



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 10:46 PM EST

PDB ID : 8EM2  
EMDB ID : EMD-28232  
Title : Cryo-EM structure of the human GDH/6PGL endoplasmic bifunctional protein  
Authors : Su, C.C.  
Deposited on : 2022-09-26  
Resolution : 3.02 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
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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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

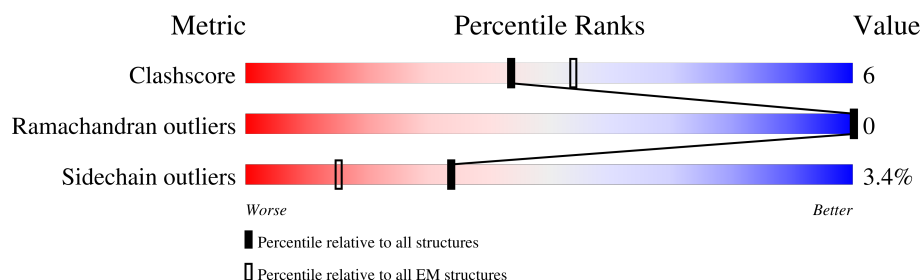
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.02 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	791	
1	B	791	

## 2 Entry composition [i](#)

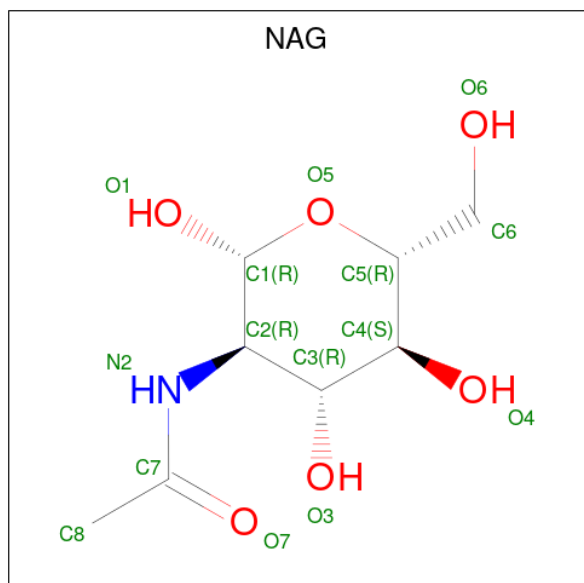
There are 2 unique types of molecules in this entry. The entry contains 8022 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GDH/6PGL endoplasmic bifunctional protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	502	Total	C	N	O	S	0	0
			4004	2555	718	719	12		
1	B	500	Total	C	N	O	S	0	0
			3990	2549	711	717	13		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	



E97	D246	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
H98	A247	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
D100	E248	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
L103	Y257	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
Q110	L111	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
L120	L120	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
H130	A131	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
A131	G132	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
L133	L133	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
A134	A134	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
G137	G137	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
F140	F140	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
S143	S143	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
E150	E150	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
D151	D151	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
I152	I152	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
A153	A153	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
I156	I156	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
N157	N157	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
S158	S158	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
S159	S159	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
C160	C160	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
G165	G165	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
A166	A166	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
D179	D179	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
T188	T188	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
D203	D203	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
G207	G207	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
A210	A210	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
V211	V211	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
I214	I214	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
R222	R222	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
L225	L225	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
D226	D226	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
N230	N230	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
R231	R231	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q525	GLN	PRO	GLU	GLN	LEU	GLN	VAL	PRO	PRO	ALA	PRO	H232
H232	H232	K357	R370	I371	L372	V380	Q381	Q390	I402	R420	K428	P434	Y447	A457	S463	F466	H467	K470	W483	T487	F488	L489	R499	F515	S516	S517	G518	R519	Q524	Q												

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196757	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 ( $e^-/\text{\AA}^2$ )	29.0	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.564	Depositor
Minimum map value	-1.189	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.29	0/4111	0.57	0/5566
1	B	0.29	0/4097	0.56	0/5550
All	All	0.29	0/8208	0.57	0/11116

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

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	4004	0	3887	49	0
1	B	3990	0	3881	52	0
2	A	14	0	13	0	0
2	B	14	0	13	1	0
All	All	8022	0	7794	99	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 6.

All (99) 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:214:ILE:HG21	1:B:275:VAL:HG12	1.75	0.68
1:B:231:ARG:HD3	1:B:351:GLY:H	1.61	0.66
1:B:32:GLY:HA3	1:B:143:SER:HB2	1.80	0.63
1:A:237:VAL:HG22	1:A:371:ILE:HG22	1.83	0.59
1:B:68:THR:O	1:B:110:GLN:NE2	2.36	0.58
1:A:218:ARG:NH1	1:A:275:VAL:O	2.36	0.58
1:B:272:LEU:HD12	1:B:356:LEU:HD21	1.85	0.58
1:A:74:GLN:HG3	1:A:108:TYR:HB3	1.85	0.58
1:A:218:ARG:NH2	1:A:277:MET:O	2.36	0.57
1:A:68:THR:O	1:A:110:GLN:NE2	2.37	0.57
1:A:162:PRO:HD3	1:A:168:LEU:HD13	1.86	0.57
1:A:134:ARG:HH21	1:A:136:ALA:HA	1.69	0.56
1:B:31:LEU:HD21	1:B:140:PHE:HD2	1.70	0.56
1:A:499:ARG:NH2	1:A:510:LEU:O	2.39	0.55
1:A:179:ASP:N	1:A:179:ASP:OD1	2.39	0.55
1:A:231:ARG:HG3	1:A:351:GLY:H	1.72	0.55
1:B:210:ALA:HB3	1:B:402:ILE:HG22	1.89	0.54
1:B:257:TYR:O	1:B:261:ARG:NE	2.41	0.54
1:B:203:ASP:OD1	1:B:203:ASP:N	2.41	0.53
1:A:32:GLY:HA3	1:A:143:SER:HB2	1.91	0.53
1:B:248:GLU:OE1	1:B:319:GLN:NE2	2.43	0.52
1:B:463:SER:O	1:B:467:HIS:ND1	2.42	0.52
1:A:305:ARG:O	1:A:305:ARG:NH1	2.43	0.52
1:A:60:PHE:HB3	1:A:62:PHE:HE1	1.75	0.52
1:B:252:SER:OG	1:B:323:GLU:OE1	2.28	0.51
1:B:499:ARG:NH2	1:B:524:GLN:O	2.43	0.51
1:B:68:THR:H	1:B:110:GLN:HE22	1.58	0.51
1:B:264:LEU:HG	1:B:268:LEU:HD12	1.92	0.51
1:A:151:ASP:OD1	1:A:151:ASP:N	2.40	0.50
1:B:92:PRO:HA	1:B:95:CYS:HB3	1.93	0.50
1:B:179:ASP:N	1:B:179:ASP:OD1	2.45	0.50
1:B:309:VAL:HG22	1:B:339:ALA:HB3	1.93	0.49
1:B:156:ILE:HA	1:B:160:CYS:HB2	1.95	0.49
1:B:81:LEU:HD13	1:B:103:LEU:HD23	1.95	0.49
1:B:157:ASN:HD21	2:B:801:NAG:HN2	1.61	0.49
1:B:260:ILE:HA	1:B:264:LEU:HB2	1.95	0.49
1:B:246:ASP:OD1	1:B:246:ASP:N	2.43	0.48
1:A:70:PRO:HD3	1:A:110:GLN:HE21	1.77	0.48
1:B:211:VAL:HG23	1:B:402:ILE:HG21	1.93	0.48
1:A:31:LEU:HD21	1:A:156:ILE:HD11	1.95	0.48
1:A:288:ALA:HA	1:A:291:ARG:HG2	1.96	0.48
1:A:272:LEU:HD22	1:A:356:LEU:HD11	1.96	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ALA:HA	1:A:81:LEU:HD12	1.94	0.48
1:A:509:ARG:NH1	1:B:390:GLN:O	2.47	0.48
1:A:162:PRO:HB2	1:A:166:ALA:HB3	1.95	0.48
1:A:321:ARG:NH2	1:A:326:LYS:O	2.47	0.47
1:A:216:PRO:O	1:A:220:GLN:NE2	2.47	0.47
1:B:270:GLU:O	1:B:274:LEU:HG	2.14	0.47
1:B:263:VAL:HG13	1:B:264:LEU:HD12	1.97	0.47
1:B:483:TRP:O	1:B:487:THR:OG1	2.29	0.47
1:A:228:LEU:HB3	1:A:373:PHE:HE2	1.80	0.47
1:B:264:LEU:O	1:B:269:THR:OG1	2.33	0.47
1:B:282:ASN:OD1	1:B:285:SER:N	2.48	0.47
1:A:264:LEU:HA	1:A:268:LEU:HB2	1.97	0.46
1:B:151:ASP:OD1	1:B:151:ASP:N	2.46	0.46
1:B:344:ILE:HD11	1:B:349:TRP:HB2	1.98	0.46
1:B:517:SER:OG	1:B:518:GLY:N	2.45	0.46
1:A:54:ALA:O	1:A:56:ARG:NH1	2.48	0.46
1:A:264:LEU:O	1:A:269:THR:OG1	2.28	0.46
1:B:370:ARG:HH21	1:B:372:LEU:HD22	1.79	0.46
1:B:84:LEU:HB2	1:B:99:LYS:HE2	1.97	0.46
1:A:288:ALA:O	1:A:292:HIS:ND1	2.38	0.46
1:A:226:ASP:HA	1:A:229:TRP:HD1	1.81	0.45
1:B:294:LEU:HA	1:B:297:PHE:HD2	1.81	0.45
1:A:324:LEU:HB2	1:A:326:LYS:HE2	1.99	0.45
1:B:288:ALA:O	1:B:292:HIS:ND1	2.45	0.45
1:A:239:ILE:HG22	1:A:268:LEU:HD22	1.99	0.45
1:A:242:LYS:O	1:A:365:ARG:HA	2.16	0.45
1:B:268:LEU:HA	1:B:271:VAL:HG12	1.98	0.45
1:B:230:ASN:HB3	1:B:232:HIS:H	1.82	0.45
1:A:414:VAL:HG21	1:A:421:PRO:HG3	1.99	0.44
1:B:137:GLY:HA2	1:B:166:ALA:HB1	1.99	0.44
1:A:417:ASN:OD1	1:A:417:ASN:N	2.50	0.44
1:B:111:LEU:HD11	1:B:120:LEU:HD12	1.98	0.44
1:B:339:ALA:HB2	1:B:357:MET:HG2	2.00	0.44
1:B:153:ALA:HA	1:B:156:ILE:HD12	2.00	0.44
1:A:259:VAL:HG12	1:A:335:PRO:HB2	2.01	0.43
1:A:406:ASP:HB3	1:A:436:LEU:HD21	2.00	0.43
1:A:138:ARG:HB3	1:A:140:PHE:HE1	1.84	0.43
1:A:514:GLU:OE1	1:A:523:SER:OG	2.27	0.43
1:B:303:LEU:HD23	1:B:489:LEU:HD22	1.99	0.43
1:A:471:ASN:N	1:A:471:ASN:OD1	2.51	0.42
1:B:26:VAL:HG21	1:B:466:PHE:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TRP:O	1:A:487:THR:OG1	2.23	0.42
1:B:225:LEU:HD12	1:B:225:LEU:HA	1.93	0.42
1:B:515:PHE:HA	1:B:519:ARG:O	2.20	0.42
1:A:242:LYS:NZ	1:B:380:VAL:O	2.45	0.42
1:B:37:LEU:HA	1:B:40:LYS:HB3	2.02	0.41
1:B:470:LYS:HD2	1:B:470:LYS:HA	1.89	0.41
1:A:370:ARG:HG3	1:A:399:VAL:HG22	2.01	0.41
1:A:344:ILE:HB	1:A:349:TRP:HB2	2.00	0.41
1:A:415:SER:HB2	1:A:418:LEU:HD12	2.02	0.41
1:B:150:GLU:O	1:B:153:ALA:HB3	2.20	0.41
1:A:407:LEU:HD23	1:A:407:LEU:HA	1.94	0.41
1:A:517:SER:OG	1:A:518:GLY:N	2.53	0.41
1:A:231:ARG:HD3	1:A:350:GLU:HB3	2.03	0.41
1:A:29:ILE:HG23	1:A:63:HIS:HB2	2.03	0.40
1:B:207:GLY:HA3	1:B:457:ALA:HB1	2.03	0.40
1:A:340:VAL:HG21	1:A:486:TRP:HH2	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	498/791 (63%)	478 (96%)	20 (4%)	0	100	100
1	B	496/791 (63%)	474 (96%)	22 (4%)	0	100	100
All	All	994/1582 (63%)	952 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	417/667 (62%)	402 (96%)	15 (4%)	30	62
1	B	418/667 (63%)	405 (97%)	13 (3%)	35	67
All	All	835/1334 (63%)	807 (97%)	28 (3%)	34	65

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	CYS
1	A	94	HIS
1	A	106	SER
1	A	116	ASP
1	A	122	LYS
1	A	134	ARG
1	A	205	TYR
1	A	220	GLN
1	A	222	ARG
1	A	230	ASN
1	A	264	LEU
1	A	279	LEU
1	A	317	SER
1	A	337	PHE
1	A	471	ASN
1	B	30	LEU
1	B	39	LYS
1	B	58	HIS
1	B	90	MET
1	B	94	HIS
1	B	95	CYS
1	B	97	GLU
1	B	134	ARG
1	B	222	ARG
1	B	337	PHE
1	B	381	GLN
1	B	428	LYS

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Mol	Chain	Res	Type
1	B	447	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	220	GLN
1	A	314	GLN
1	B	107	GLN
1	B	110	GLN
1	B	127	GLN
1	B	221	ASN
1	B	381	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](#)

2 ligands 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
2	NAG	A	801	1	14,14,15	0.28	0	17,19,21	0.52	0
2	NAG	B	801	-	14,14,15	0.66	0	17,19,21	0.87	1 (5%)

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
2	NAG	A	801	1	-	3/6/23/26	0/1/1/1
2	NAG	B	801	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	NAG	C1-O5-C5	3.33	116.64	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAG	C8-C7-N2-C2
2	A	801	NAG	O7-C7-N2-C2
2	A	801	NAG	O5-C5-C6-O6
2	B	801	NAG	C4-C5-C6-O6
2	B	801	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

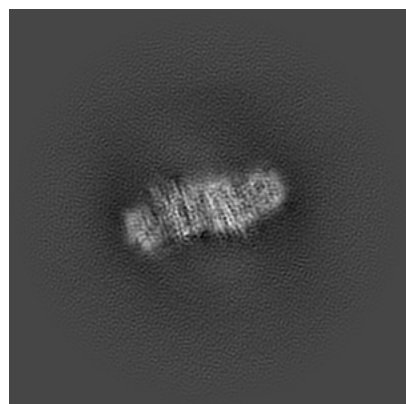
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28232. These allow visual inspection of the internal detail of the map and identification of artifacts.

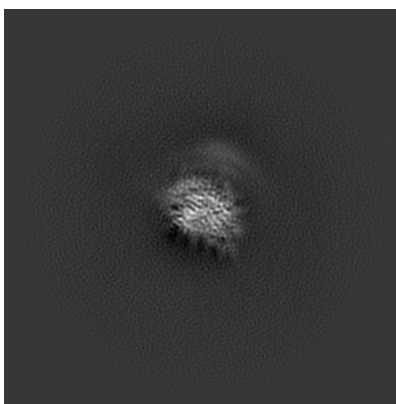
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

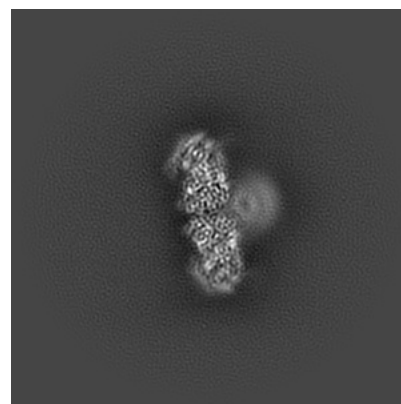
#### 6.1.1 Primary map



X

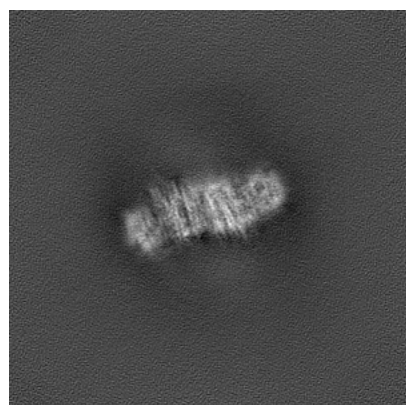


Y

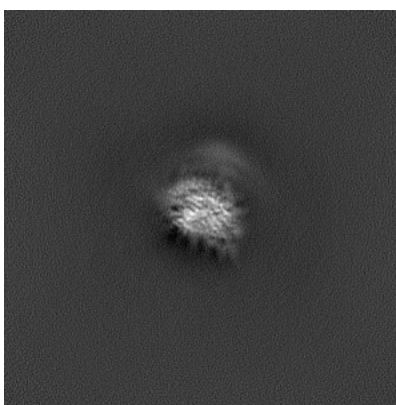


Z

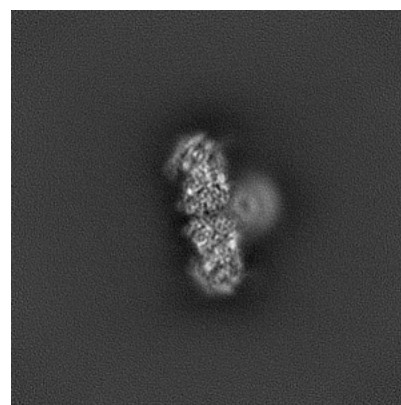
#### 6.1.2 Raw map



X



Y

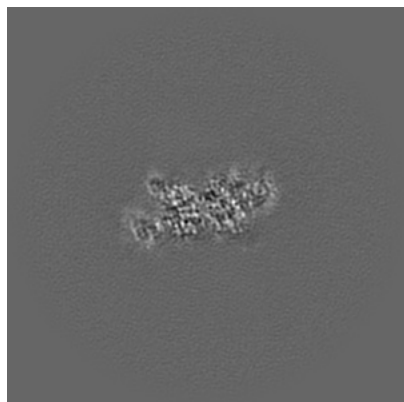


Z

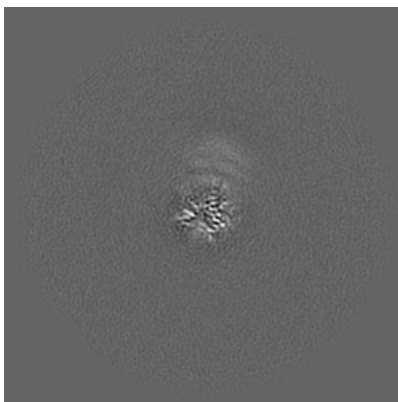
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

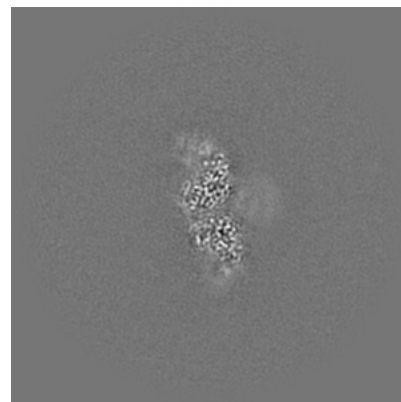
### 6.2.1 Primary map



X Index: 150

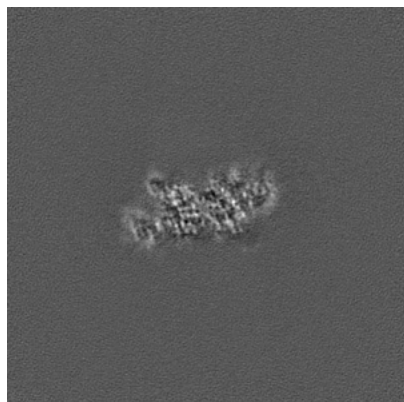


Y Index: 150

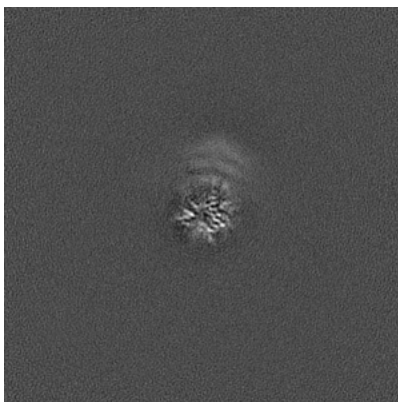


Z Index: 150

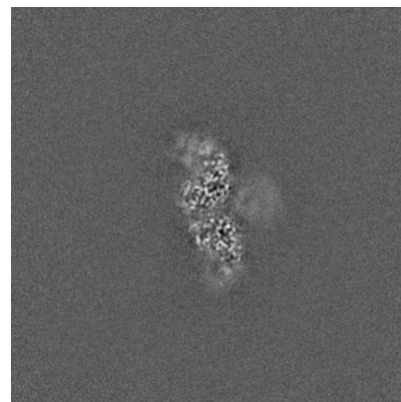
### 6.2.2 Raw map



X Index: 150



Y Index: 150



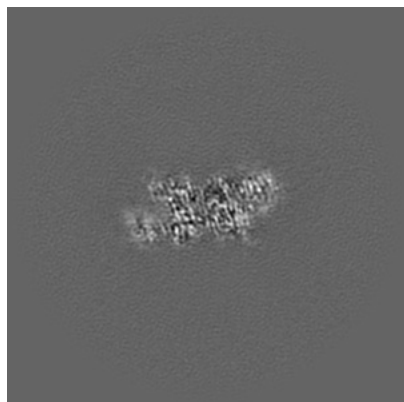
Z Index: 150

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

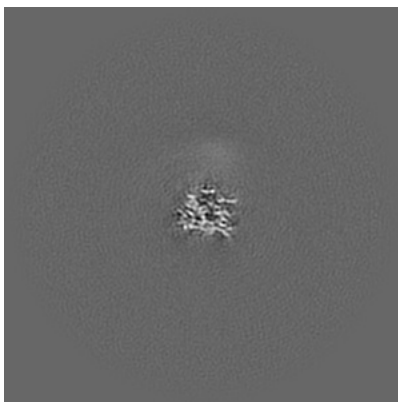


## 6.3 Largest variance slices [i](#)

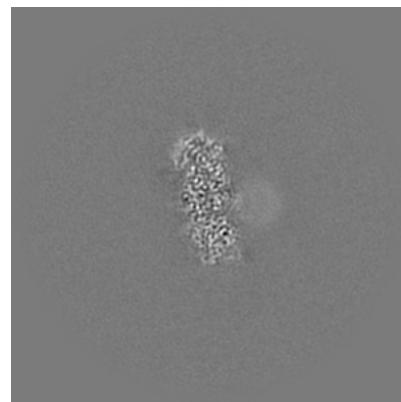
### 6.3.1 Primary map



X Index: 146



Y Index: 164

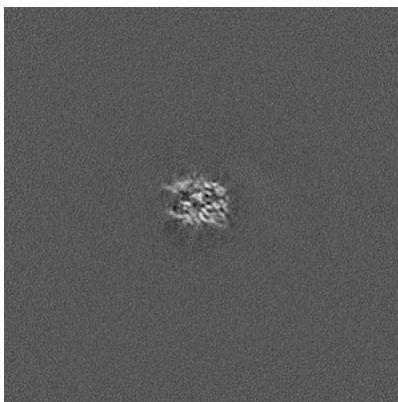


Z Index: 159

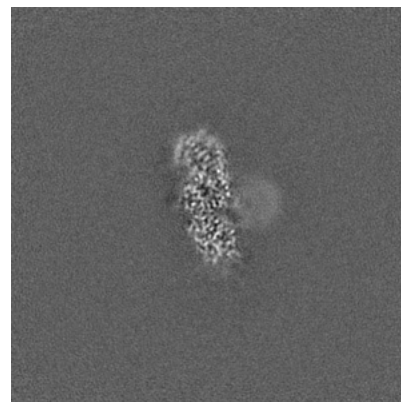
### 6.3.2 Raw map



X Index: 146



Y Index: 125

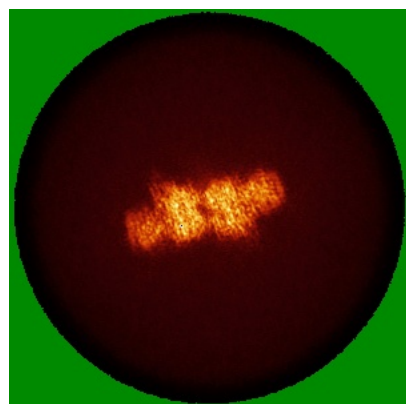


Z Index: 156

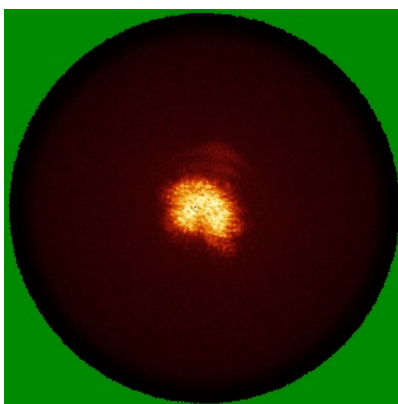
The images above show the largest variance slices of the map in three orthogonal directions.

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

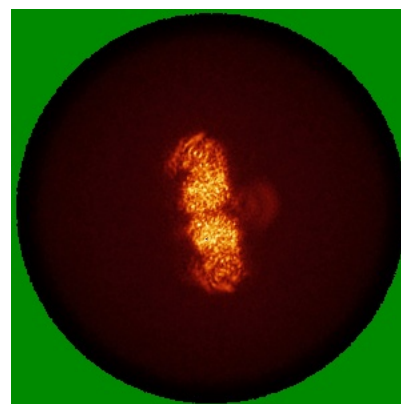
### 6.4.1 Primary map



X

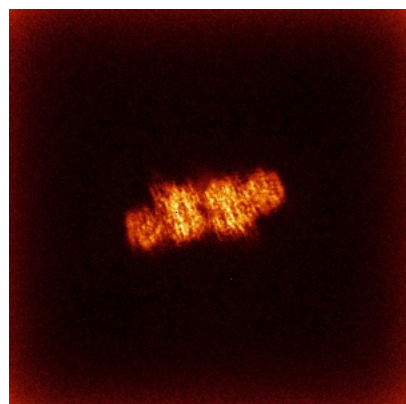


Y

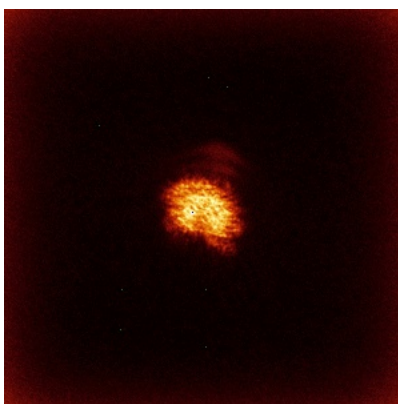


Z

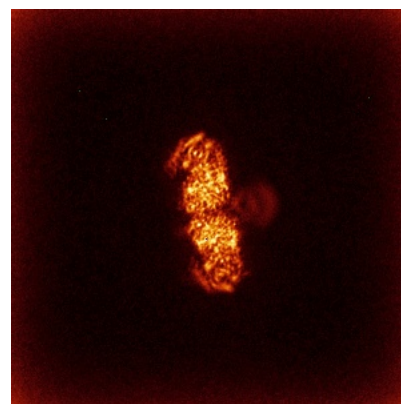
### 6.4.2 Raw map



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.

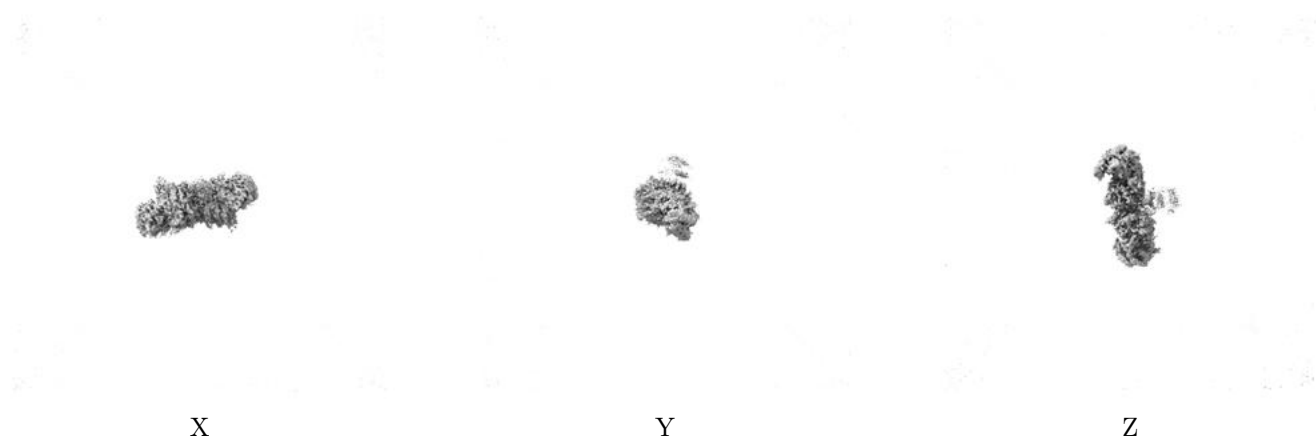
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.17. 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.

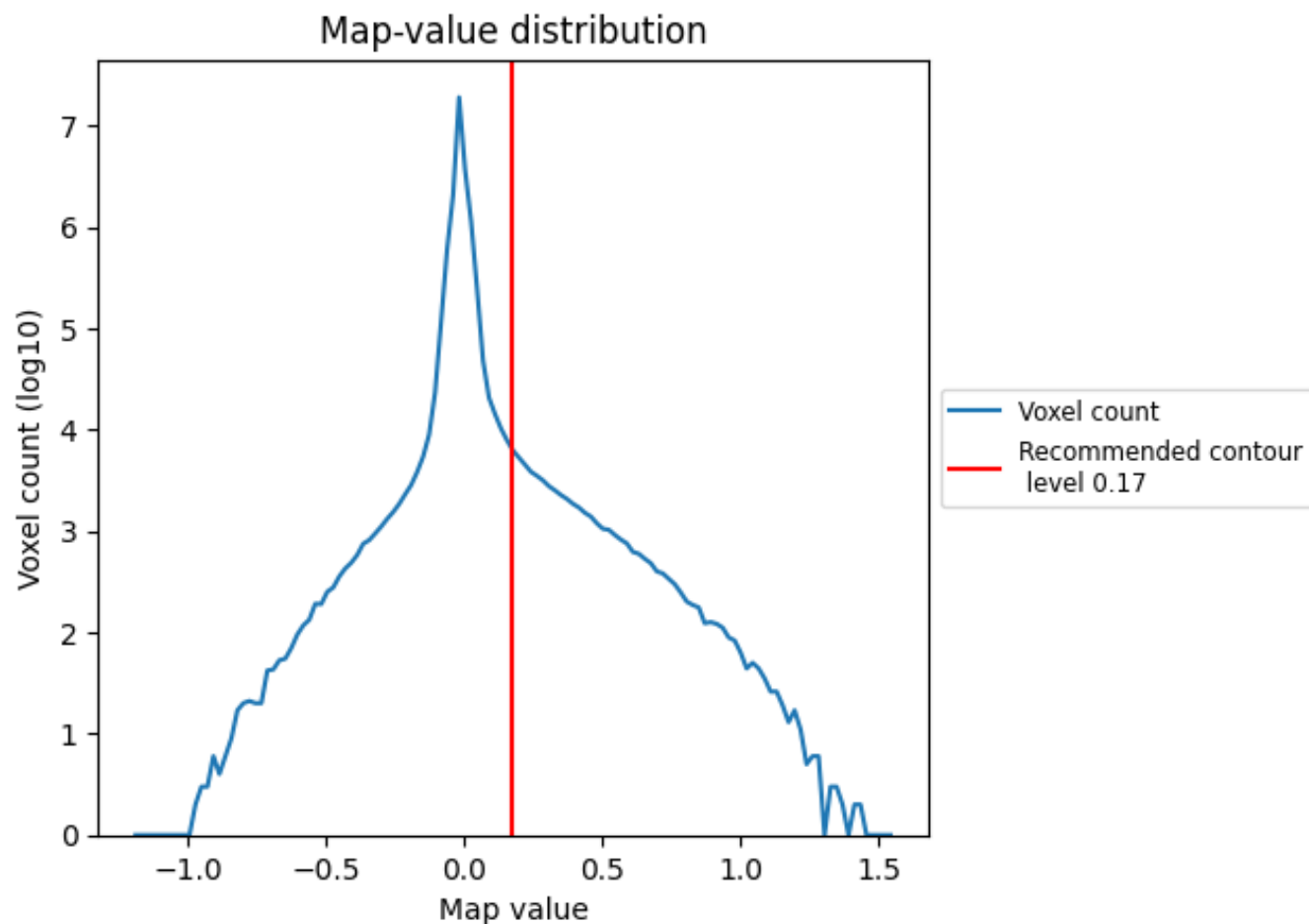
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

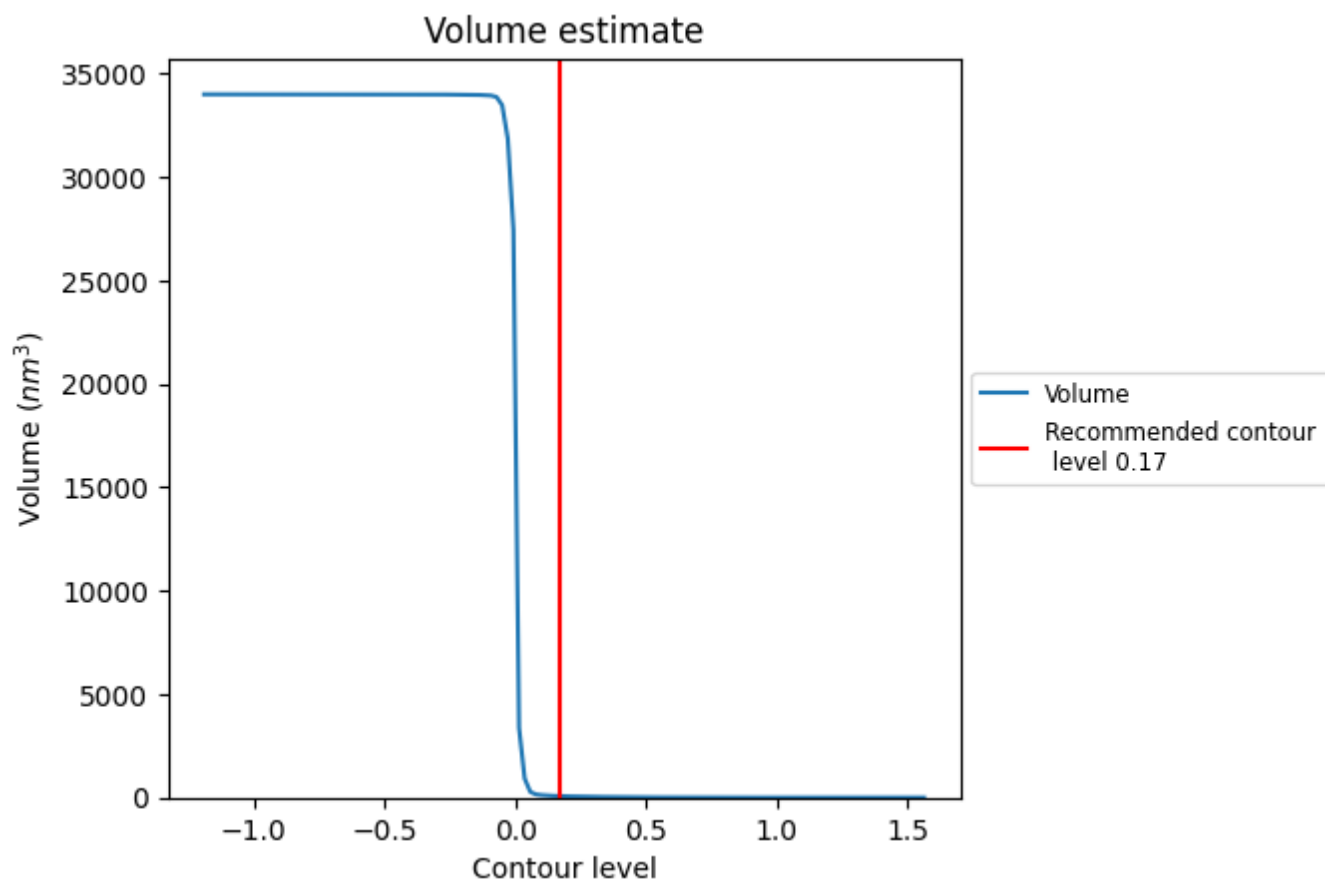
This section contains the results of statistical analysis of the map.

### 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.

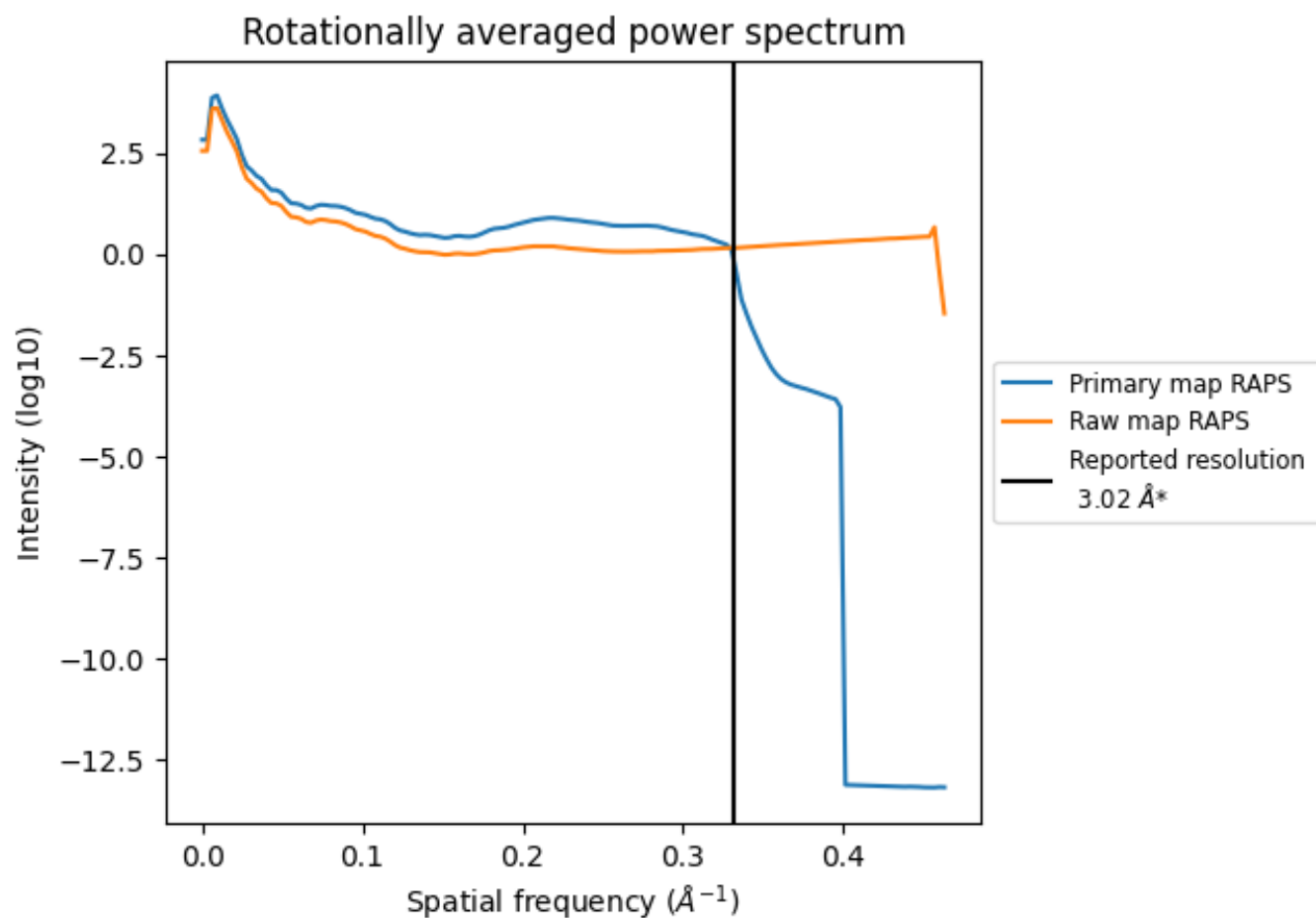
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm<sup>3</sup>; this corresponds to an approximate mass of 64 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 ⓘ

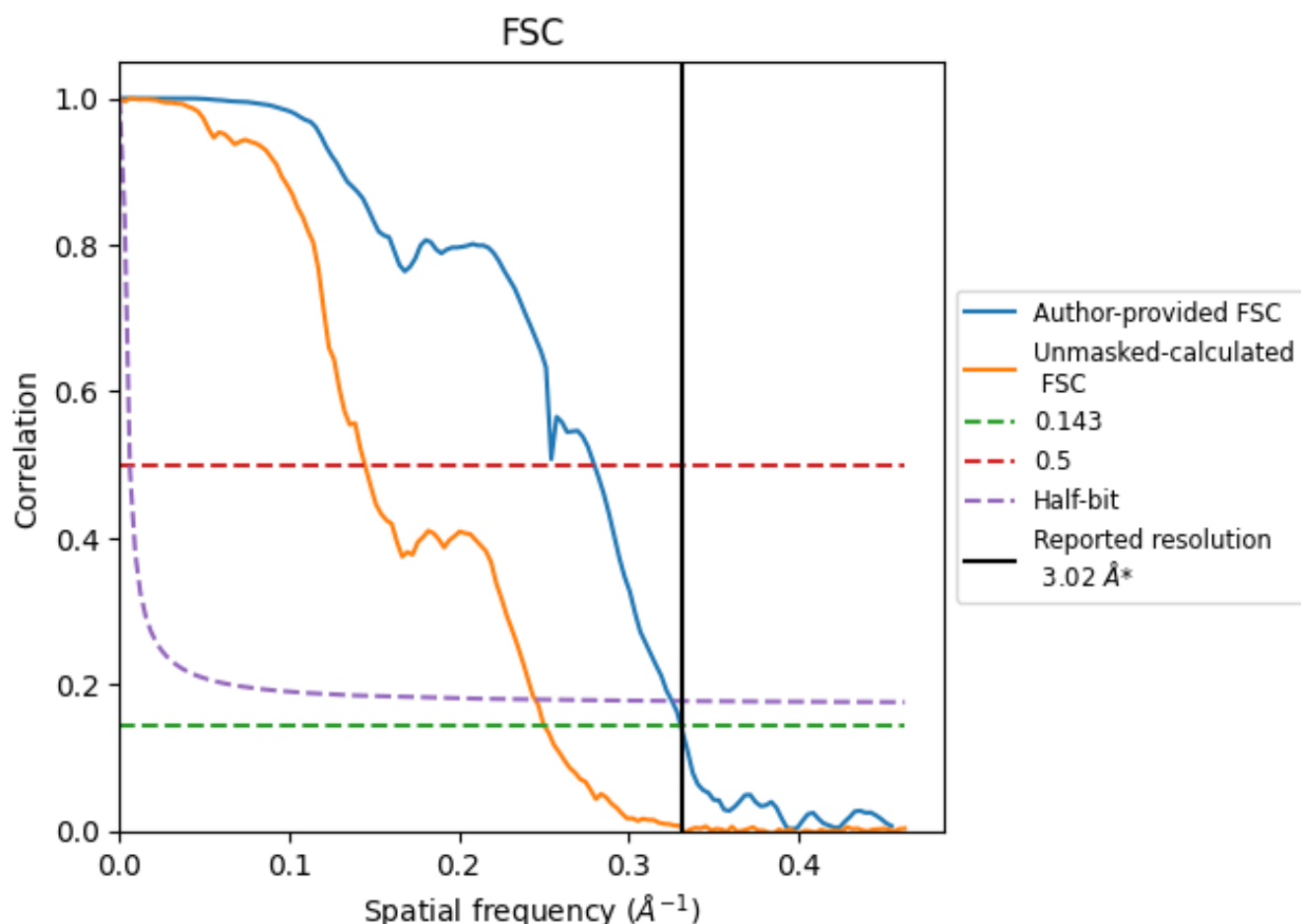


\*Reported resolution corresponds to spatial frequency of 0.331 Å<sup>-1</sup>

## 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 0.331  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.57	3.07
Unmasked-calculated*	3.99	6.92	4.08

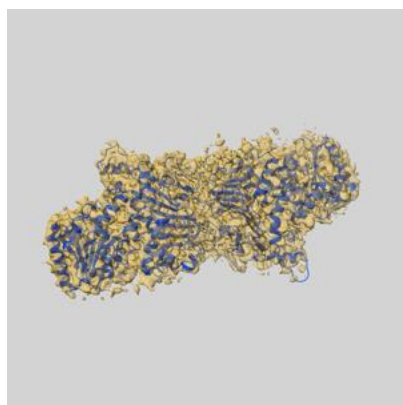
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.02 by more than 10 %



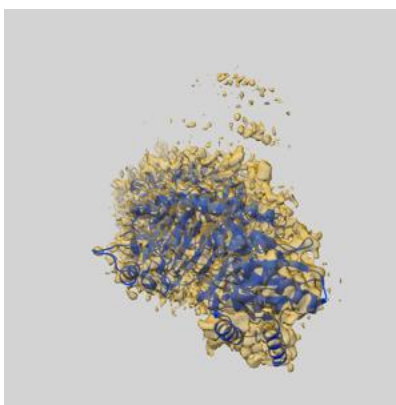
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28232 and PDB model 8EM2. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

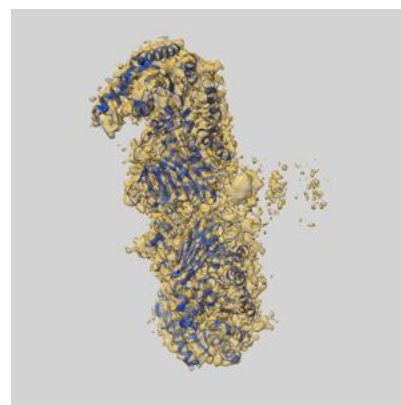
### 9.1 Map-model overlay [i](#)



X



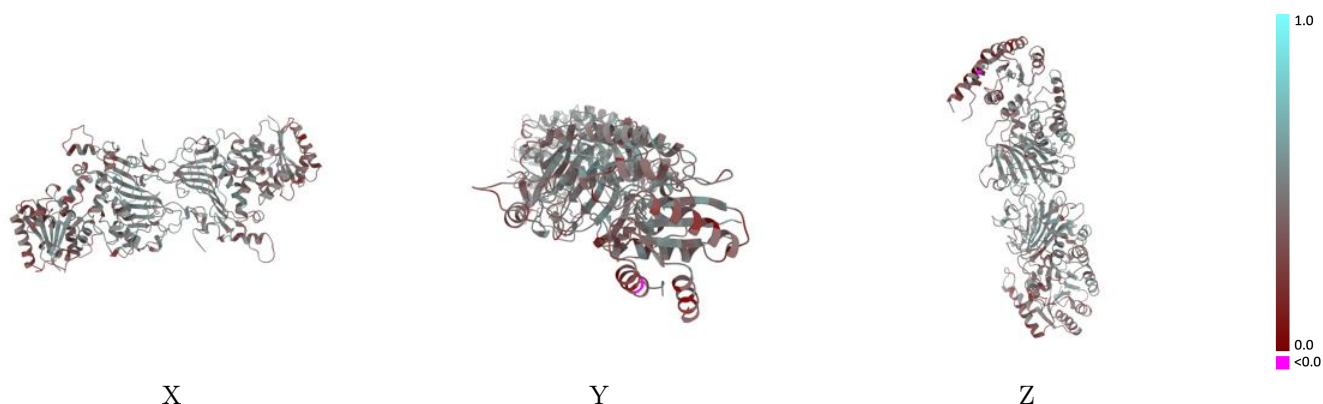
Y



Z

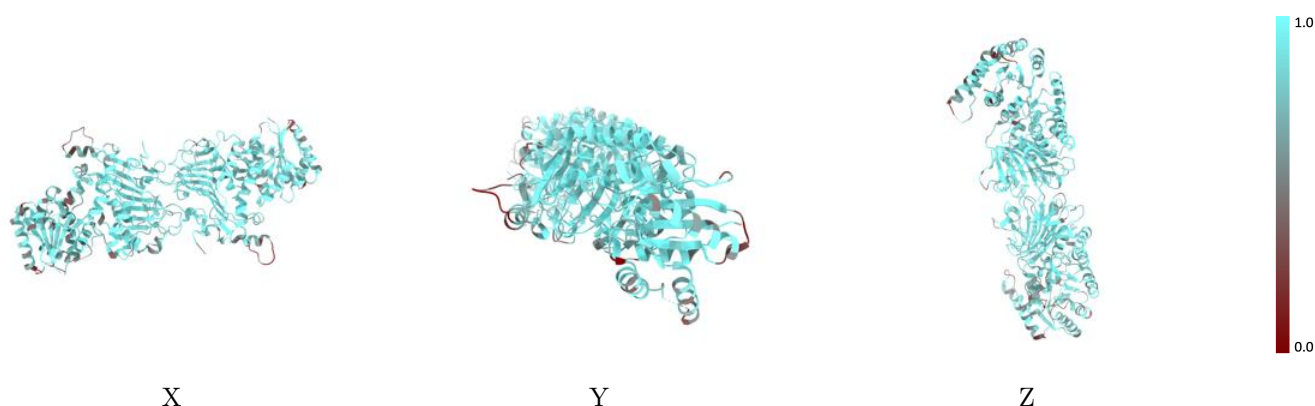
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



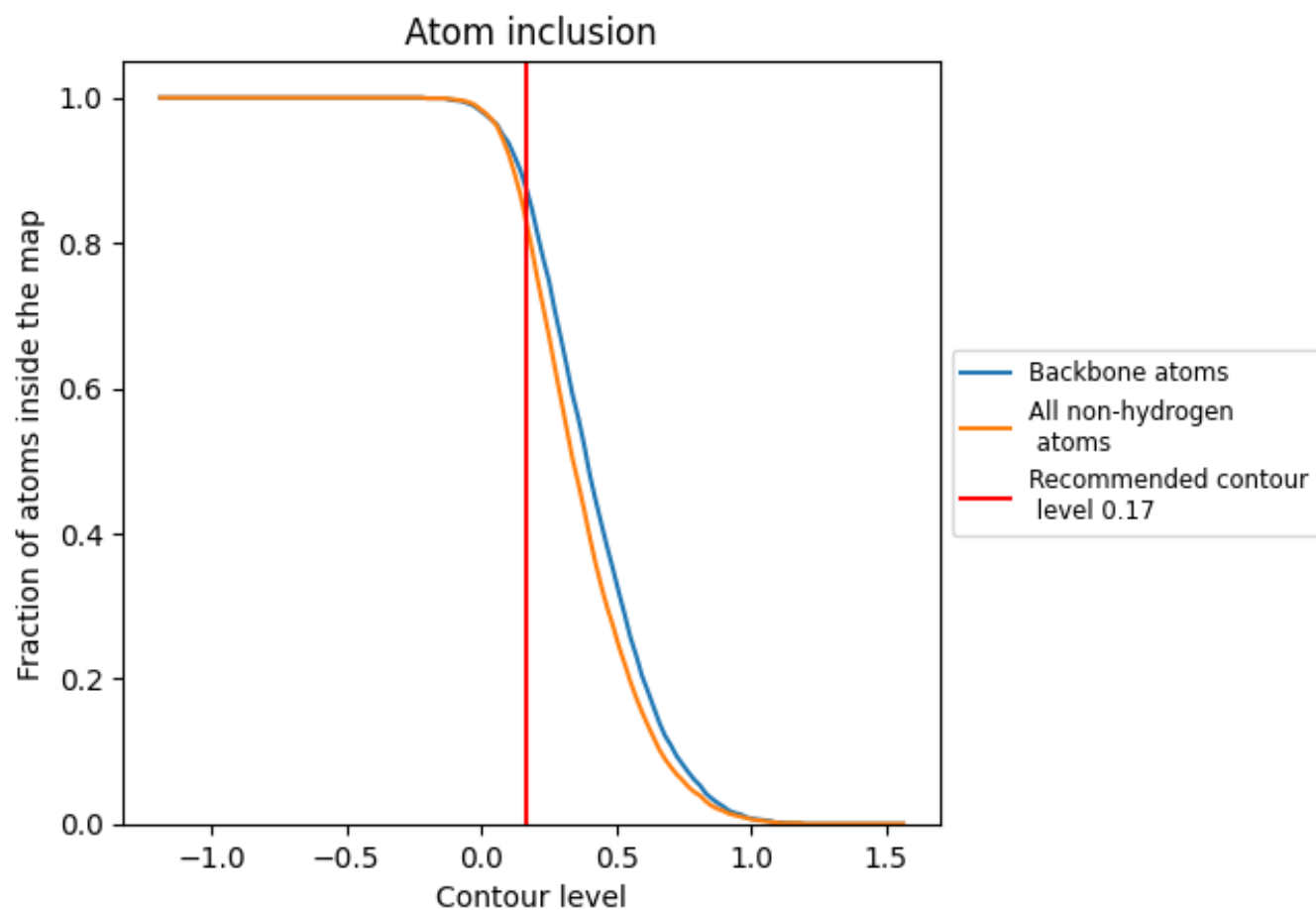
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.17).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8250	<div></div> 0.4410
A	<div></div> 0.8320	<div></div> 0.4390
B	<div></div> 0.8180	<div></div> 0.4430

