



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 08:40 PM UTC

PDB ID : 7XJY / pdb_00007xjy
EMDB ID : EMD-33237
Title : Cryo-EM structure of Oryza sativa plastid glycyl-tRNA synthetase (apo form)
Authors : Yu, Z.; Wu, Z.; Li, Y.; Lu, G.; Lin, J.
Deposited on : 2022-04-19
Resolution : 3.60 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

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.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

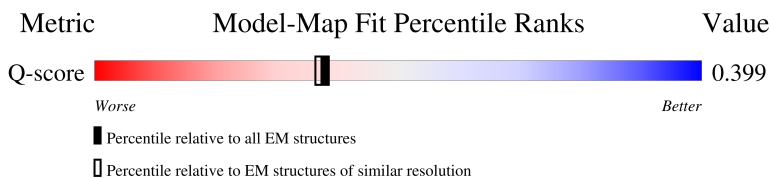
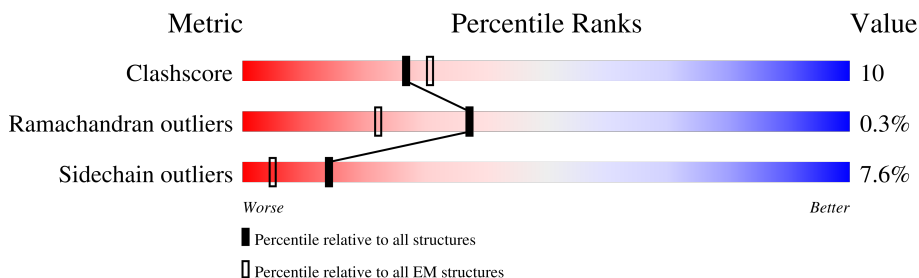
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	1045	16% 51% 20% • 27%
1	B	1045	15% 52% 19% • 27%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12070 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 Glycine-tRNA ligase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	763	Total	C	N	O	S	0	0
			6034	3856	1029	1125	24		
1	B	763	Total	C	N	O	S	0	0
			6036	3857	1032	1123	24		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	HIS	-	expression tag	UNP Q0DFB6
A	-17	HIS	-	expression tag	UNP Q0DFB6
A	-16	HIS	-	expression tag	UNP Q0DFB6
A	-15	HIS	-	expression tag	UNP Q0DFB6
A	-14	HIS	-	expression tag	UNP Q0DFB6
A	-13	HIS	-	expression tag	UNP Q0DFB6
A	-12	HIS	-	expression tag	UNP Q0DFB6
A	-11	HIS	-	expression tag	UNP Q0DFB6
A	-10	GLY	-	expression tag	UNP Q0DFB6
A	-9	SER	-	expression tag	UNP Q0DFB6
A	-8	SER	-	expression tag	UNP Q0DFB6
A	-7	LEU	-	expression tag	UNP Q0DFB6
A	-6	GLU	-	expression tag	UNP Q0DFB6
A	-5	VAL	-	expression tag	UNP Q0DFB6
A	-4	LEU	-	expression tag	UNP Q0DFB6
A	-3	PHE	-	expression tag	UNP Q0DFB6
A	-2	GLN	-	expression tag	UNP Q0DFB6
A	-1	GLY	-	expression tag	UNP Q0DFB6
A	0	PRO	-	expression tag	UNP Q0DFB6
A	439	PRO	LEU	conflict	UNP Q0DFB6
A	925	THR	ALA	conflict	UNP Q0DFB6
A	998	LYS	ARG	conflict	UNP Q0DFB6
B	-18	HIS	-	expression tag	UNP Q0DFB6
B	-17	HIS	-	expression tag	UNP Q0DFB6
B	-16	HIS	-	expression tag	UNP Q0DFB6
B	-15	HIS	-	expression tag	UNP Q0DFB6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q0DFB6
B	-13	HIS	-	expression tag	UNP Q0DFB6
B	-12	HIS	-	expression tag	UNP Q0DFB6
B	-11	HIS	-	expression tag	UNP Q0DFB6
B	-10	GLY	-	expression tag	UNP Q0DFB6
B	-9	SER	-	expression tag	UNP Q0DFB6
B	-8	SER	-	expression tag	UNP Q0DFB6
B	-7	LEU	-	expression tag	UNP Q0DFB6
B	-6	GLU	-	expression tag	UNP Q0DFB6
B	-5	VAL	-	expression tag	UNP Q0DFB6
B	-4	LEU	-	expression tag	UNP Q0DFB6
B	-3	PHE	-	expression tag	UNP Q0DFB6
B	-2	GLN	-	expression tag	UNP Q0DFB6
B	-1	GLY	-	expression tag	UNP Q0DFB6
B	0	PRO	-	expression tag	UNP Q0DFB6
B	439	PRO	LEU	conflict	UNP Q0DFB6
B	925	THR	ALA	conflict	UNP Q0DFB6
B	998	LYS	ARG	conflict	UNP Q0DFB6



GLN	PRO	LEU	GLU	ASP	PHE	PHE	THR	THR	ASN	VAL	PHE	VAL	MET	ALA	GLU	GLU	ASP	GLU	GLU	LYS	VAL	GLY	LEU	VAL	ASP	ARG	ASN	ASN	ASN	ARG	LEU	LEU	ALA	ALA	LEU	LEU	PRO	PRO	GLY	PHE																			
TTR	SER	ARG	PRO	THR	ARG	ILE	ILE	ARG	GLY	LYS	GLU	ILE	GLY	SER	ALA	LEU	GLU	VAL	GLU	LYS	VAL	ASP	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ALA																				
E861	V862	V863	Q864	F865	V866	T867	R868	R869	R870	E871	Q872	L873	L874	VAL	ASP	GLU	GLY	ILE	VAL	ARG	SER	VAL	LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ALA																				
V901	G902	L903	F904	G905	A906	G907	C908	Q909	P910	S911	S912	T913	N914	D915	P916	F917	G918	L919	A920	R921	I922	S923	Y924	G925	L926	V927	Q928	I929	L930	V931	E932	N933	K934	K935	N936	F937	D938	L939	T940	K941	A942	L943	T944	L945	V946	A947	E948	E949	Q950	P951	I952	T953	I954	D955	S956	G957	V958	I959	S960

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18283	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.991	Depositor
Minimum map value	-2.897	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.133	Depositor
Recommended contour level	0.7	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/6159	0.64	6/8351 (0.1%)
1	B	0.42	1/6161 (0.0%)	0.61	4/8353 (0.0%)
All	All	0.41	1/12320 (0.0%)	0.63	10/16704 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	TYR	C-O	-8.39	1.14	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	807	GLY	N-CA-C	6.88	120.10	111.85
1	B	807	GLY	N-CA-C	6.03	118.57	111.63
1	B	807	GLY	CA-C-O	-5.86	117.36	122.16
1	A	807	GLY	CA-C-O	-5.54	117.20	122.13
1	A	673	ASP	N-CA-C	-5.51	106.76	112.93
1	B	125	LEU	N-CA-C	-5.46	105.43	111.71
1	A	554	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	821	ARG	N-CA-C	-5.40	104.79	111.33
1	A	824	TYR	CB-CA-C	-5.20	102.72	110.88
1	A	672	MET	CB-CA-C	-5.19	100.70	110.67

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	6034	0	6038	124	0
1	B	6036	0	6045	117	0
All	All	12070	0	12083	239	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 10.

All (239) 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:A:616:VAL:HG22	1:A:744:PHE:CE1	1.85	1.10
1:B:670:TYR:HA	1:B:740:ILE:HD11	1.65	0.79
1:B:803:LEU:HB2	1:B:819:LEU:HD21	1.68	0.76
1:A:30:LEU:O	1:A:198:GLN:NE2	2.20	0.73
1:B:833:ASN:O	1:B:835:LYS:NZ	2.21	0.73
1:B:372:ILE:HA	1:B:375:LYS:HD2	1.71	0.72
1:A:616:VAL:CG2	1:A:744:PHE:CE1	2.68	0.71
1:B:521:ASN:HD21	1:B:535:LYS:HE3	1.55	0.71
1:A:75:GLU:OE2	1:A:308:ARG:NH2	2.22	0.71
1:B:347:GLU:HB3	1:B:502:PHE:HB3	1.72	0.70
1:A:833:ASN:O	1:A:835:LYS:NZ	2.23	0.70
1:A:111:LYS:HB2	1:A:183:SER:HB3	1.73	0.70
1:A:608:LEU:HD21	1:A:667:LYS:HG2	1.75	0.69
1:A:386:TYR:HD1	1:A:554:ASP:HA	1.59	0.68
1:B:616:VAL:HG22	1:B:744:PHE:CE1	2.29	0.67
1:A:174:SER:HB3	1:A:179:LEU:HD21	1.75	0.67
1:B:771:GLU:HB3	1:B:783:PRO:HB3	1.77	0.67
1:A:372:ILE:HA	1:A:375:LYS:HD2	1.77	0.66
1:A:771:GLU:HB3	1:A:783:PRO:HB3	1.78	0.66
1:B:75:GLU:OE2	1:B:308:ARG:NH2	2.29	0.65
1:A:756:ALA:HB1	1:A:761:LEU:HB2	1.78	0.65
1:B:174:SER:HB3	1:B:179:LEU:HD21	1.78	0.65
1:B:585:GLN:HA	1:B:588:ILE:HD12	1.78	0.64
1:A:803:LEU:HD12	1:A:819:LEU:HG	1.79	0.64
1:A:544:HIS:O	1:A:547:GLU:HB2	1.98	0.63
1:B:135:HIS:ND1	1:B:161:ASP:OD2	2.30	0.63
1:B:544:HIS:O	1:B:547:GLU:HB2	1.98	0.62
1:A:50:VAL:H	1:B:33:GLN:HE22	1.48	0.62
1:A:347:GLU:HB3	1:A:502:PHE:HB3	1.80	0.61
1:A:585:GLN:HA	1:A:588:ILE:HD12	1.81	0.61
1:A:829:ILE:O	1:A:833:ASN:ND2	2.28	0.60
1:A:117:SER:HB2	1:A:168:PHE:HZ	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LYS:HB2	1:B:183:SER:HB3	1.83	0.59
1:A:135:HIS:ND1	1:A:161:ASP:OD2	2.36	0.59
1:A:611:ASP:HB3	1:A:747:LEU:HD21	1.84	0.59
1:A:350:THR:OG1	1:A:351:GLU:O	2.21	0.58
1:B:386:TYR:HB3	1:B:553:ILE:O	2.02	0.58
1:A:771:GLU:CD	1:A:784:LYS:H	2.12	0.58
1:B:541:LEU:O	1:B:545:THR:N	2.35	0.58
1:A:107:GLN:HE21	1:A:109:ILE:HD11	1.67	0.58
1:B:491:ASN:OD1	1:B:491:ASN:N	2.33	0.58
1:A:782:PHE:O	1:A:784:LYS:NZ	2.36	0.58
1:A:561:ARG:NH1	1:A:565:ASP:OD1	2.37	0.58
1:A:71:VAL:O	1:A:111:LYS:NZ	2.37	0.57
1:B:71:VAL:O	1:B:111:LYS:NZ	2.36	0.57
1:A:616:VAL:CG2	1:A:744:PHE:CZ	2.88	0.57
1:B:107:GLN:HE21	1:B:109:ILE:HD11	1.70	0.57
1:A:674:THR:HB	1:A:758:ARG:NH2	2.20	0.57
1:B:829:ILE:O	1:B:833:ASN:ND2	2.28	0.56
1:B:756:ALA:HB1	1:B:761:LEU:HB2	1.86	0.56
1:A:602:ASP:OD1	1:A:660:ARG:NH2	2.39	0.56
1:B:561:ARG:NH1	1:B:565:ASP:OD1	2.39	0.56
1:A:756:ALA:HA	1:A:759:ASP:HB2	1.88	0.56
1:B:151:ALA:HA	1:B:173:GLN:O	2.06	0.56
1:B:602:ASP:N	1:B:602:ASP:OD1	2.39	0.55
1:A:231:GLU:O	1:A:278:ARG:NH2	2.39	0.55
1:B:771:GLU:CD	1:B:784:LYS:H	2.14	0.55
1:A:753:ARG:HG3	1:A:766:ALA:HB1	1.87	0.55
1:B:753:ARG:HG3	1:B:766:ALA:HB1	1.88	0.55
1:A:602:ASP:OD1	1:A:602:ASP:N	2.40	0.54
1:A:756:ALA:O	1:A:760:GLY:N	2.40	0.54
1:A:57:GLU:OE1	1:A:57:GLU:N	2.38	0.54
1:A:575:GLY:O	1:A:629:LYS:NZ	2.35	0.54
1:A:562:ILE:O	1:A:566:SER:OG	2.26	0.54
1:B:388:THR:HG21	1:B:592:GLU:OE1	2.07	0.54
1:A:164:GLU:OE1	1:A:192:ARG:NH1	2.41	0.54
1:B:147:PRO:HB2	1:B:290:PHE:HE1	1.73	0.54
1:B:796:ARG:NH1	1:B:822:ILE:HA	2.23	0.54
1:B:42:TYR:O	1:B:45:SER:OG	2.26	0.53
1:A:705:GLU:HA	1:A:729:ALA:HB1	1.90	0.53
1:A:246:GLU:HG3	1:A:296:LEU:HD11	1.90	0.53
1:A:251:SER:O	1:A:254:SER:OG	2.27	0.53
1:A:815:ASP:H	1:A:816:PRO:HD2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ALA:HB3	1:A:541:LEU:HG	1.90	0.53
1:A:770:PHE:O	1:A:773:THR:OG1	2.24	0.53
1:A:491:ASN:OD1	1:A:491:ASN:N	2.35	0.53
1:B:670:TYR:CA	1:B:740:ILE:HD11	2.38	0.53
1:B:231:GLU:O	1:B:278:ARG:NH2	2.41	0.52
1:A:238:ILE:HG23	1:A:271:ALA:HB1	1.91	0.52
1:B:238:ILE:HG23	1:B:271:ALA:HB1	1.91	0.52
1:B:350:THR:OG1	1:B:351:GLU:O	2.27	0.52
1:A:796:ARG:HH12	1:A:822:ILE:HA	1.75	0.52
1:B:725:ILE:HG12	1:B:787:PRO:HB3	1.92	0.52
1:A:725:ILE:HG12	1:A:787:PRO:HB3	1.92	0.52
1:B:575:GLY:O	1:B:629:LYS:NZ	2.40	0.51
1:B:611:ASP:HB3	1:B:747:LEU:HD21	1.93	0.51
1:A:602:ASP:CG	1:A:660:ARG:HH21	2.18	0.51
1:B:356:HIS:O	1:B:360:GLU:HG2	2.11	0.51
1:B:260:PRO:O	1:B:264:HIS:ND1	2.42	0.51
1:A:151:ALA:HA	1:A:173:GLN:O	2.11	0.51
1:B:735:ASP:HB3	1:B:752:ALA:HB2	1.93	0.51
1:B:768:ALA:HB2	1:B:787:PRO:HB2	1.92	0.51
1:B:347:GLU:OE1	1:B:542:TYR:OH	2.22	0.50
1:A:347:GLU:OE1	1:A:542:TYR:OH	2.20	0.50
1:A:138:ARG:HG3	1:A:140:VAL:HG23	1.94	0.50
1:A:502:PHE:HZ	1:A:536:VAL:HB	1.76	0.50
1:A:42:TYR:O	1:A:45:SER:OG	2.27	0.50
1:A:161:ASP:N	1:A:161:ASP:OD1	2.44	0.50
1:A:768:ALA:HB2	1:A:787:PRO:HB2	1.94	0.50
1:B:222:GLU:OE2	1:B:226:SER:OG	2.27	0.50
1:B:523:SER:OG	1:B:524:CYS:N	2.44	0.50
1:A:351:GLU:OE1	1:A:497:PRO:HD2	2.11	0.50
1:B:796:ARG:HH12	1:B:822:ILE:HA	1.77	0.49
1:A:521:ASN:HD21	1:A:535:LYS:HE3	1.77	0.49
1:B:194:LEU:HD12	1:B:198:GLN:HE21	1.77	0.49
1:B:75:GLU:CD	1:B:308:ARG:HH21	2.17	0.49
1:A:674:THR:HB	1:A:758:ARG:CZ	2.43	0.49
1:B:538:ALA:HB3	1:B:541:LEU:HG	1.93	0.49
1:A:818:GLY:O	1:A:822:ILE:HB	2.12	0.49
1:B:351:GLU:OE1	1:B:497:PRO:HD2	2.13	0.49
1:A:260:PRO:O	1:A:264:HIS:ND1	2.45	0.49
1:A:352:GLU:N	1:A:352:GLU:OE1	2.46	0.48
1:A:252:LEU:HD13	1:A:260:PRO:HB2	1.94	0.48
1:B:489:ASN:O	1:B:490:SER:OG	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLU:HG3	1:B:296:LEU:HD11	1.93	0.48
1:B:531:LEU:HD22	1:B:534:PHE:HD1	1.77	0.48
1:B:252:LEU:HD13	1:B:260:PRO:HB2	1.96	0.47
1:B:388:THR:HG22	1:B:391:ARG:HG2	1.95	0.47
1:B:465:ALA:O	1:B:469:LEU:HG	2.14	0.47
1:B:770:PHE:O	1:B:773:THR:OG1	2.32	0.47
1:A:465:ALA:O	1:A:469:LEU:HG	2.14	0.47
1:A:735:ASP:HB3	1:A:752:ALA:HB2	1.96	0.47
1:A:761:LEU:HD23	1:A:765:ILE:HG21	1.96	0.47
1:B:161:ASP:OD1	1:B:161:ASP:N	2.45	0.47
1:A:283:VAL:HG13	1:A:284:THR:HG23	1.97	0.47
1:B:371:GLN:HB3	1:B:375:LYS:HE3	1.97	0.47
1:B:811:SER:HB2	1:B:816:PRO:HG3	1.96	0.47
1:B:796:ARG:O	1:B:800:LEU:HG	2.15	0.46
1:A:809:GLN:HB2	1:A:810:PRO:HD3	1.97	0.46
1:B:251:SER:O	1:B:254:SER:OG	2.31	0.46
1:A:702:LYS:O	1:A:705:GLU:HG2	2.15	0.46
1:B:138:ARG:HG3	1:B:140:VAL:HG23	1.97	0.46
1:A:531:LEU:HD13	1:A:534:PHE:CD1	2.50	0.46
1:A:796:ARG:O	1:A:800:LEU:HG	2.16	0.46
1:A:523:SER:OG	1:A:524:CYS:N	2.48	0.46
1:A:556:GLN:O	1:A:557:GLU:C	2.57	0.46
1:B:705:GLU:HA	1:B:729:ALA:HB1	1.98	0.46
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.81	0.46
1:A:611:ASP:HB3	1:A:747:LEU:CD2	2.46	0.46
1:A:798:ASP:OD1	1:A:850:GLN:NE2	2.49	0.45
1:B:352:GLU:OE1	1:B:352:GLU:N	2.49	0.45
1:B:65:PRO:HB3	1:B:262:TYR:HD2	1.82	0.45
1:A:815:ASP:N	1:A:816:PRO:HD2	2.32	0.45
1:A:365:LEU:HB2	1:A:480:ILE:HD11	1.97	0.45
1:B:386:TYR:HD1	1:B:554:ASP:HA	1.81	0.45
1:A:473:LEU:HD23	1:A:473:LEU:HA	1.75	0.45
1:B:37:GLN:O	1:B:37:GLN:NE2	2.49	0.45
1:A:51:MET:HG3	1:A:79:VAL:HG22	1.99	0.45
1:A:783:PRO:HD2	1:A:829:ILE:HG12	1.97	0.45
1:B:702:LYS:O	1:B:705:GLU:HG2	2.16	0.45
1:B:117:SER:HB2	1:B:168:PHE:HZ	1.82	0.45
1:B:383:VAL:HG22	1:B:396:VAL:HG22	1.99	0.45
1:A:383:VAL:HG22	1:A:396:VAL:HG22	1.99	0.45
1:A:391:ARG:NH2	1:A:500:TRP:HH2	2.15	0.45
1:A:733:MET:C	1:A:735:ASP:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PHE:CE1	1:A:166:THR:HG21	2.53	0.44
1:A:531:LEU:HD22	1:A:534:PHE:HD1	1.82	0.44
1:A:796:ARG:NH1	1:A:822:ILE:HA	2.32	0.44
1:B:256:TRP:O	1:B:257:LEU:HD23	2.17	0.44
1:A:610:LYS:O	1:A:614:ILE:HG13	2.17	0.44
1:B:473:LEU:HD23	1:B:473:LEU:HA	1.80	0.44
1:B:371:GLN:HB3	1:B:375:LYS:NZ	2.33	0.44
1:B:798:ASP:OD1	1:B:850:GLN:NE2	2.51	0.44
1:A:371:GLN:HB3	1:A:375:LYS:HE3	1.99	0.44
1:B:97:PRO:HA	1:B:202:HIS:CD2	2.53	0.44
1:B:288:ARG:O	1:B:292:ARG:HG3	2.18	0.44
1:B:868:ARG:NH1	1:B:872:GLN:HB2	2.33	0.44
1:A:288:ARG:O	1:A:292:ARG:HG3	2.18	0.43
1:A:222:GLU:OE2	1:A:226:SER:OG	2.32	0.43
1:A:541:LEU:O	1:A:545:THR:N	2.45	0.43
1:B:616:VAL:CG2	1:B:744:PHE:CE1	3.01	0.43
1:B:765:ILE:O	1:B:769:LEU:HG	2.18	0.43
1:A:775:PRO:O	1:A:796:ARG:NH2	2.51	0.43
1:B:556:GLN:O	1:B:559:LYS:N	2.51	0.43
1:B:209:THR:O	1:B:210:LYS:C	2.61	0.43
1:B:756:ALA:O	1:B:760:GLY:N	2.51	0.43
1:B:809:GLN:O	1:B:810:PRO:C	2.61	0.43
1:A:65:PRO:HB3	1:A:262:TYR:HD2	1.83	0.43
1:A:543:LEU:O	1:A:547:GLU:HG3	2.17	0.43
1:A:101:GLN:OE1	1:A:229:TYR:HE2	2.02	0.43
1:A:815:ASP:O	1:A:816:PRO:C	2.61	0.43
1:B:818:GLY:O	1:B:819:LEU:HB2	2.19	0.43
1:B:240:LYS:HB3	1:B:240:LYS:HE3	1.81	0.43
1:A:703:ARG:HD3	1:A:851:PRO:HD3	2.01	0.43
1:B:676:LYS:HB2	1:B:681:PHE:CE2	2.53	0.43
1:B:354:PRO:O	1:B:358:VAL:HG23	2.19	0.42
1:A:670:TYR:O	1:A:674:THR:HG23	2.19	0.42
1:A:721:MET:O	1:A:725:ILE:HG13	2.19	0.42
1:A:728:ALA:HB2	1:A:765:ILE:HG23	2.00	0.42
1:B:783:PRO:HD2	1:B:829:ILE:HG12	2.00	0.42
1:A:51:MET:HE2	1:A:51:MET:HB3	1.79	0.42
1:A:559:LYS:HE3	1:A:584:VAL:HG11	2.01	0.42
1:B:160:MET:HE1	1:B:196:SER:OG	2.20	0.42
1:B:623:TYR:O	1:B:625:PRO:HD3	2.20	0.42
1:A:147:PRO:O	1:A:150:GLY:N	2.52	0.42
1:B:498:ILE:O	1:B:499:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:VAL:HG13	1:B:284:THR:HG23	2.01	0.42
1:B:615:THR:CG2	1:B:746:SER:OG	2.68	0.42
1:B:526:LEU:HD23	1:B:526:LEU:HA	1.89	0.42
1:B:819:LEU:HD23	1:B:819:LEU:HA	1.84	0.42
1:A:193:ILE:O	1:A:197:LEU:HG	2.19	0.41
1:A:154:LEU:HD12	1:A:486:MET:HB3	2.02	0.41
1:A:580:PRO:O	1:A:584:VAL:HG23	2.20	0.41
1:B:91:SER:HB2	1:B:230:LEU:HD21	2.03	0.41
1:A:371:GLN:HB3	1:A:375:LYS:NZ	2.35	0.41
1:A:617:MET:HE2	1:A:617:MET:HB3	1.84	0.41
1:B:235:VAL:O	1:B:239:GLN:HG3	2.20	0.41
1:B:101:GLN:OE1	1:B:229:TYR:HE2	2.03	0.41
1:B:556:GLN:O	1:B:557:GLU:C	2.64	0.41
1:A:762:SER:HB3	1:A:765:ILE:HG13	2.01	0.41
1:B:172:GLN:NE2	1:B:486:MET:HB2	2.36	0.41
1:B:559:LYS:HE3	1:B:584:VAL:HG11	2.03	0.41
1:A:354:PRO:O	1:A:358:VAL:HG23	2.20	0.41
1:B:147:PRO:O	1:B:150:GLY:N	2.53	0.41
1:B:193:ILE:O	1:B:197:LEU:HG	2.21	0.41
1:A:615:THR:HG23	1:A:746:SER:OG	2.21	0.41
1:A:798:ASP:HA	1:A:846:VAL:HG11	2.03	0.41
1:A:825:GLY:O	1:A:826:LEU:C	2.63	0.41
1:B:191:GLU:OE2	1:B:214:TYR:OH	2.33	0.41
1:B:628:SER:HB2	1:B:635:LEU:HD21	2.03	0.41
1:B:769:LEU:O	1:B:772:ILE:HG22	2.21	0.41
1:B:774:LEU:HD13	1:B:781:VAL:HG23	2.02	0.41
1:A:64:ASN:OD1	1:A:66:LEU:N	2.34	0.41
1:A:531:LEU:HD13	1:A:534:PHE:CE1	2.56	0.41
1:B:747:LEU:HB3	1:B:751:MET:HG2	2.03	0.41
1:A:50:VAL:H	1:B:33:GLN:NE2	2.16	0.40
1:B:712:ALA:HB2	1:B:790:VAL:HG11	2.03	0.40
1:A:235:VAL:O	1:A:239:GLN:HG3	2.21	0.40
1:A:256:TRP:O	1:A:257:LEU:HD23	2.21	0.40
1:B:64:ASN:OD1	1:B:66:LEU:N	2.34	0.40
1:B:543:LEU:O	1:B:547:GLU:HG3	2.21	0.40
1:B:721:MET:O	1:B:725:ILE:HG13	2.22	0.40
1:B:256:TRP:CE3	1:B:303:LEU:HD11	2.56	0.40
1:A:769:LEU:O	1:A:772:ILE:HG22	2.22	0.40
1:B:121:PHE:CE1	1:B:166:THR:HG21	2.56	0.40
1:B:803:LEU:HD12	1:B:819:LEU:HG	2.02	0.40
1:A:160:MET:HE1	1:A:196:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:O	1:A:182:VAL:HG13	2.22	0.40
1:A:498:ILE:O	1:A:499:ARG:HD3	2.21	0.40

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	757/1045 (72%)	723 (96%)	32 (4%)	2 (0%)	36	65
1	B	757/1045 (72%)	723 (96%)	31 (4%)	3 (0%)	30	61
All	All	1514/2090 (72%)	1446 (96%)	63 (4%)	5 (0%)	37	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	815	ASP
1	A	816	PRO
1	B	557	GLU
1	B	819	LEU
1	B	810	PRO

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	659/898 (73%)	604 (92%)	55 (8%)	10	35
1	B	659/898 (73%)	614 (93%)	45 (7%)	14	42
All	All	1318/1796 (73%)	1218 (92%)	100 (8%)	14	39

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	33	GLN
1	A	36	ILE
1	A	41	ASP
1	A	53	CYS
1	A	79	VAL
1	A	118	GLN
1	A	125	LEU
1	A	126	SER
1	A	132	VAL
1	A	161	ASP
1	A	183	SER
1	A	185	GLU
1	A	191	GLU
1	A	196	SER
1	A	200	VAL
1	A	209	THR
1	A	212	ILE
1	A	221	ASN
1	A	236	ASP
1	A	259	ILE
1	A	275	LEU
1	A	277	SER
1	A	290	PHE
1	A	307	THR
1	A	315	LEU
1	A	350	THR
1	A	388	THR
1	A	470	THR
1	A	491	ASN
1	A	529	SER
1	A	552	LEU
1	A	553	ILE
1	A	554	ASP
1	A	566	SER

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Mol	Chain	Res	Type
1	A	586	GLU
1	A	598	ILE
1	A	602	ASP
1	A	640	THR
1	A	650	VAL
1	A	665	ASP
1	A	667	LYS
1	A	671	LYS
1	A	675	GLN
1	A	676	LYS
1	A	707	THR
1	A	740	ILE
1	A	741	VAL
1	A	750	ILE
1	A	809	GLN
1	A	811	SER
1	A	813	THR
1	A	819	LEU
1	A	822	ILE
1	A	827	VAL
1	B	30	LEU
1	B	41	ASP
1	B	53	CYS
1	B	54	SER
1	B	79	VAL
1	B	118	GLN
1	B	125	LEU
1	B	126	SER
1	B	132	VAL
1	B	161	ASP
1	B	183	SER
1	B	185	GLU
1	B	191	GLU
1	B	196	SER
1	B	200	VAL
1	B	209	THR
1	B	212	ILE
1	B	221	ASN
1	B	259	ILE
1	B	275	LEU
1	B	277	SER
1	B	307	THR

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Mol	Chain	Res	Type
1	B	350	THR
1	B	351	GLU
1	B	388	THR
1	B	491	ASN
1	B	500	TRP
1	B	529	SER
1	B	552	LEU
1	B	554	ASP
1	B	555	MET
1	B	598	ILE
1	B	602	ASP
1	B	626	VAL
1	B	640	THR
1	B	650	VAL
1	B	676	LYS
1	B	707	THR
1	B	741	VAL
1	B	750	ILE
1	B	809	GLN
1	B	810	PRO
1	B	811	SER
1	B	813	THR
1	B	821	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	234	ASN
1	A	237	ASN
1	A	643	ASN
1	B	33	GLN
1	B	198	GLN
1	B	234	ASN
1	B	400	ASN
1	B	521	ASN
1	B	564	HIS
1	B	643	ASN
1	B	809	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.

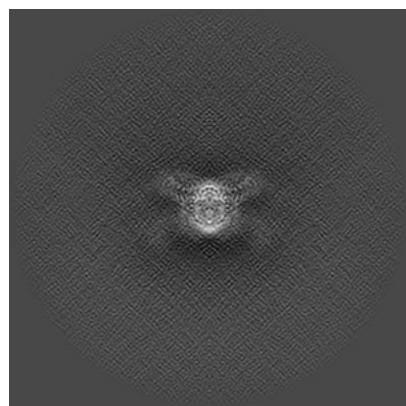
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33237. These allow visual inspection of the internal detail of the map and identification of artifacts.

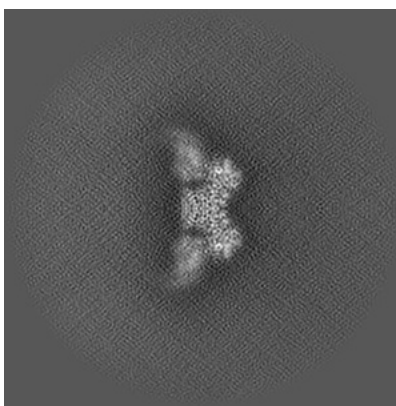
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

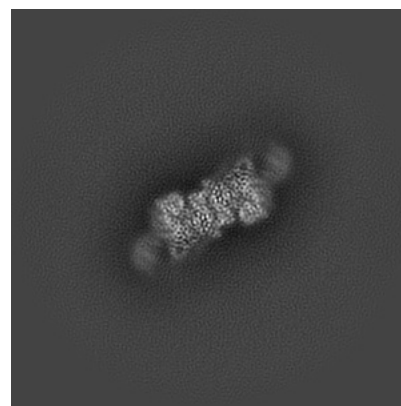
6.1.1 Primary map



X

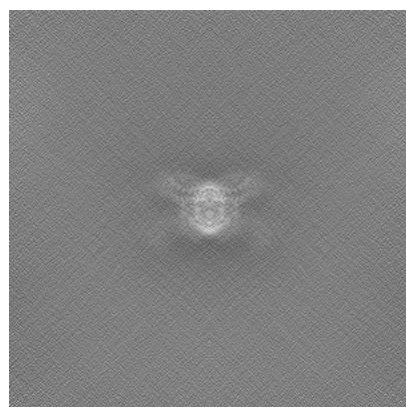


Y

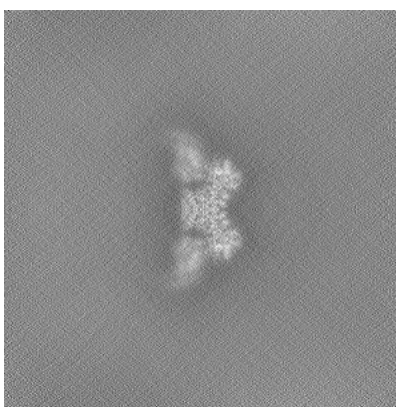


Z

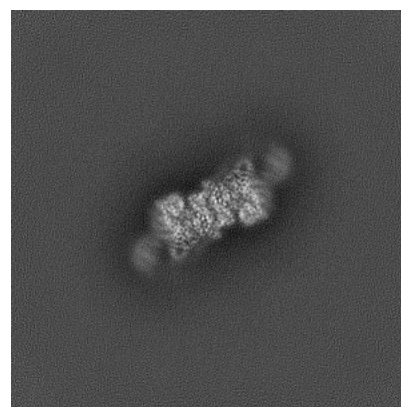
6.1.2 Raw map



X



Y



Z

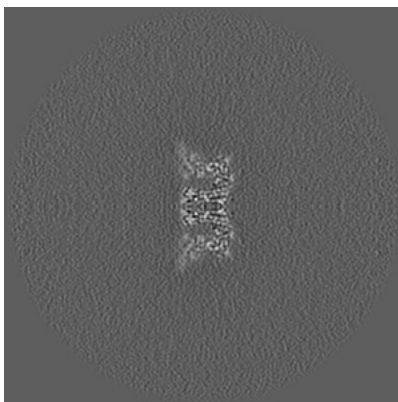
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

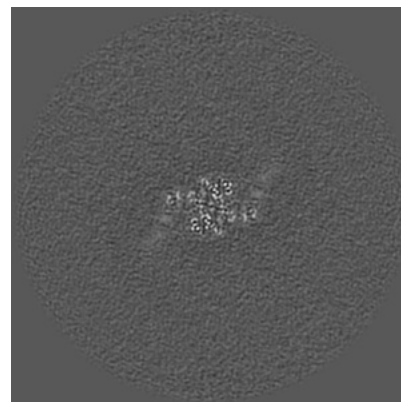
6.2.1 Primary map



X Index: 192

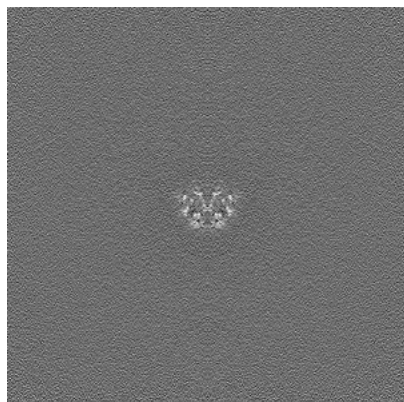


Y Index: 192

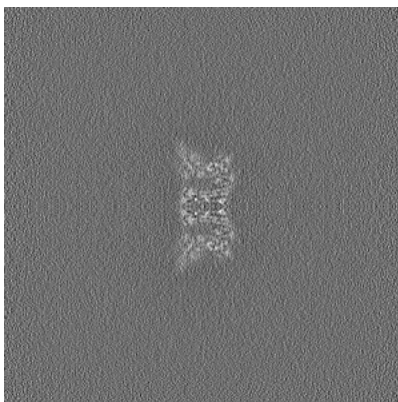


Z Index: 192

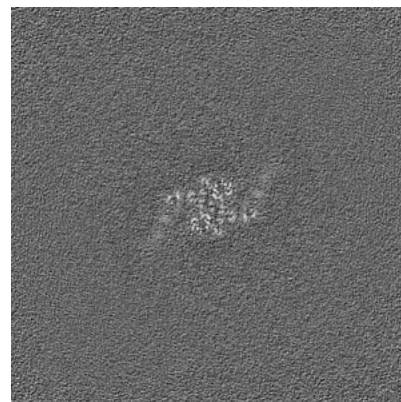
6.2.2 Raw map



X Index: 192



Y Index: 192

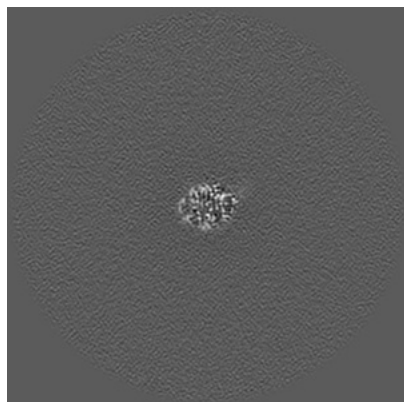


Z Index: 192

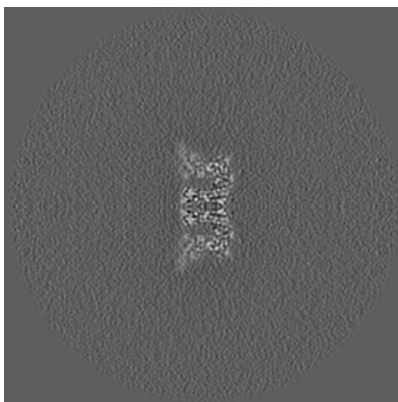
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

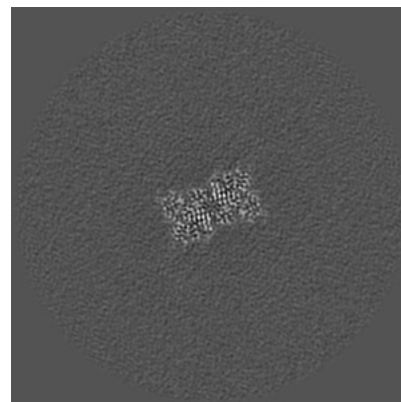
6.3.1 Primary map



X Index: 199

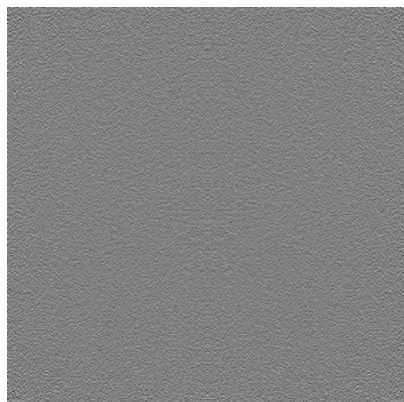


Y Index: 192

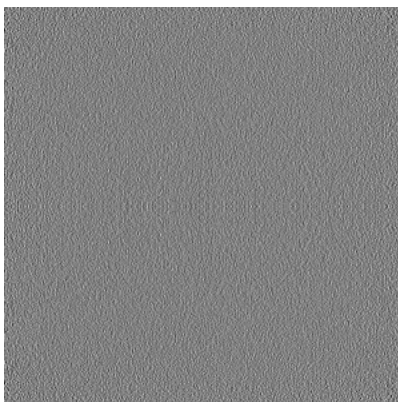


Z Index: 202

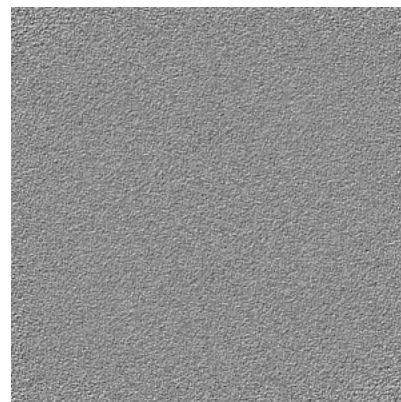
6.3.2 Raw map



X Index: 0



Y Index: 0

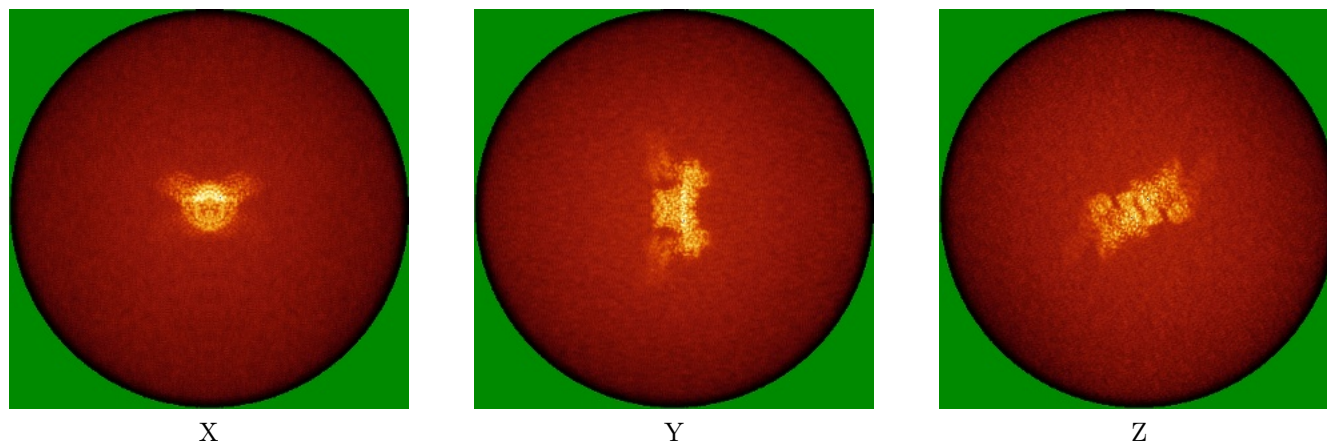


Z Index: 0

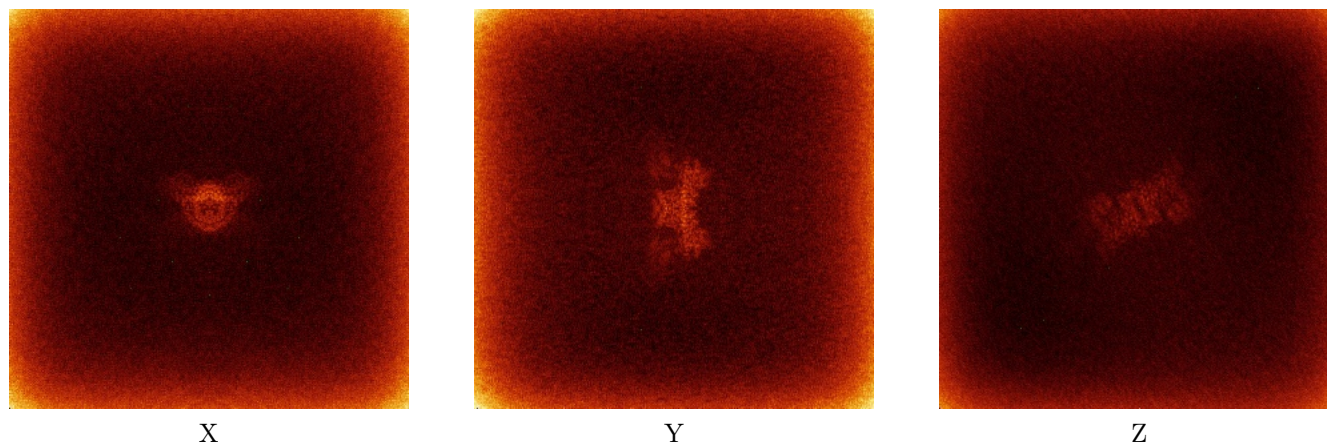
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

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

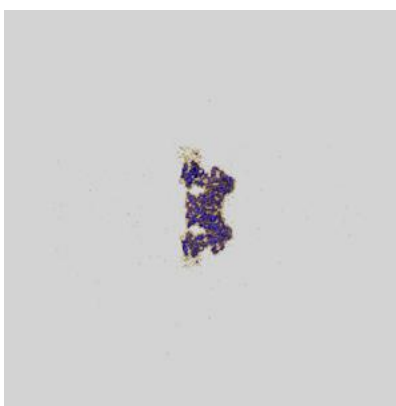
A mask typically either:

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

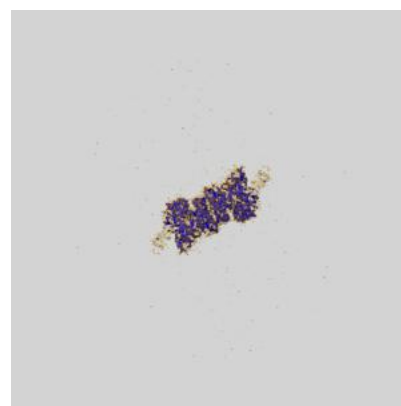
6.6.1 emd_33237_msk_1.map [i](#)



X



Y

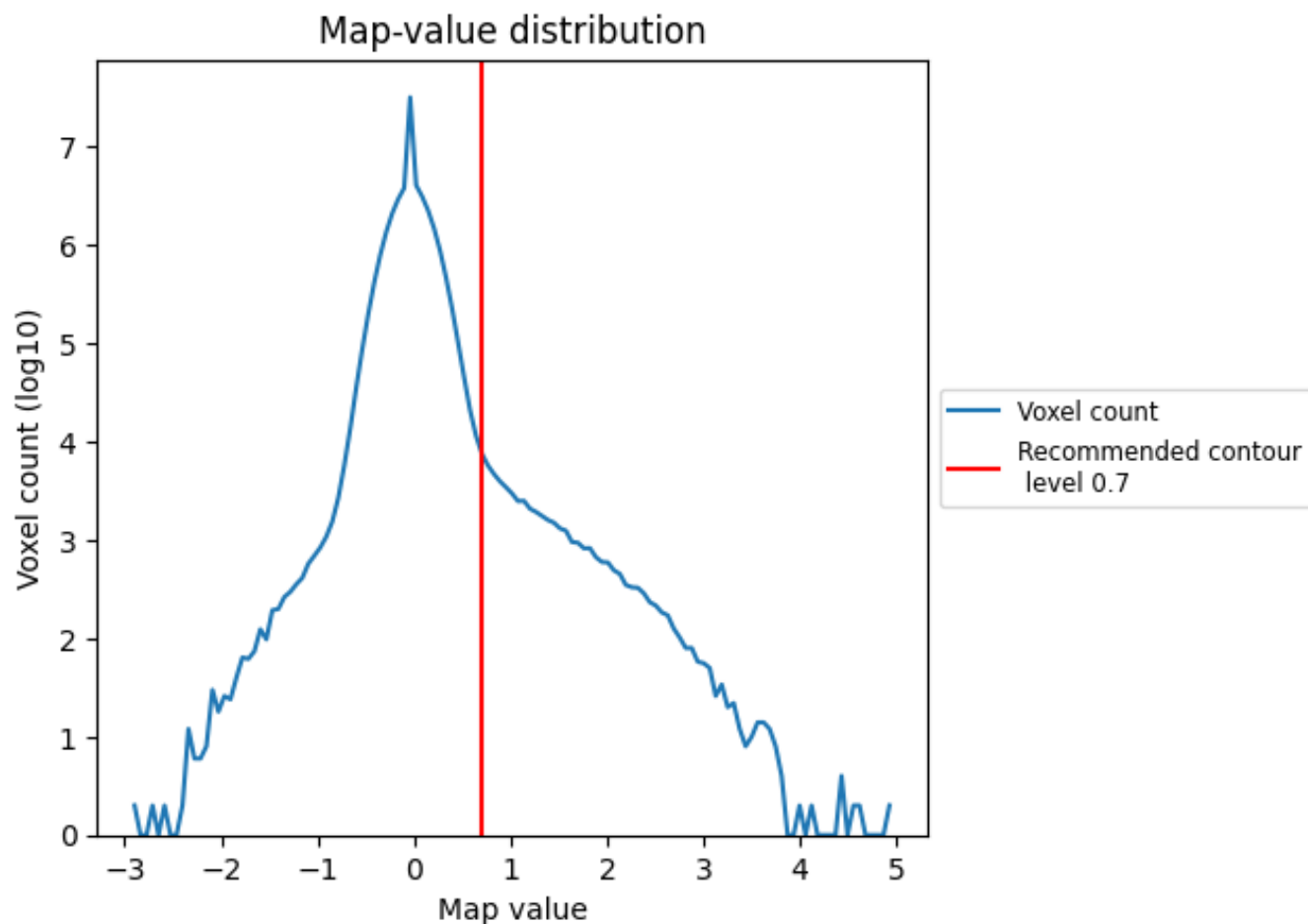


Z

7 Map analysis [i](#)

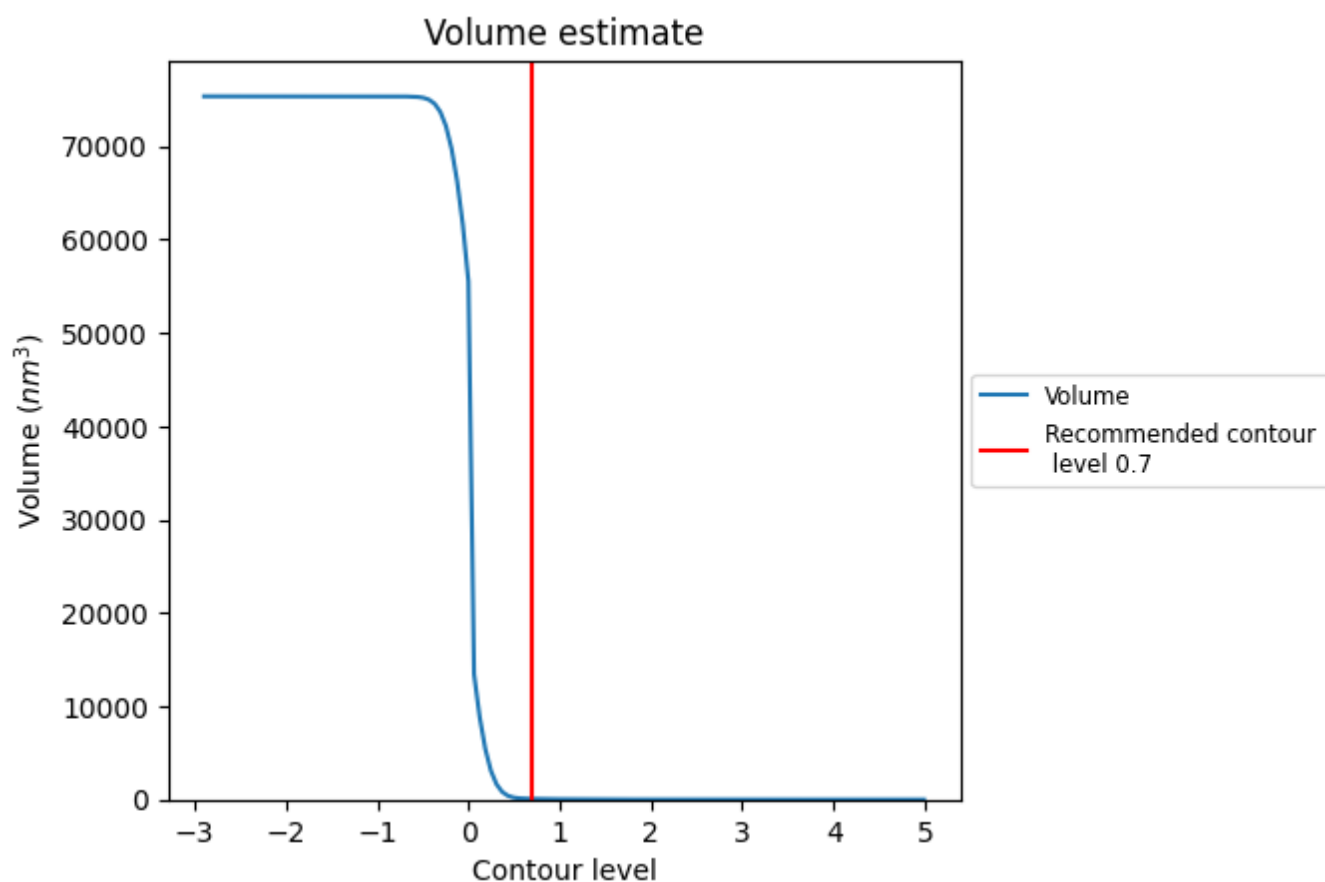
This section contains the results of statistical analysis of the map.

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.

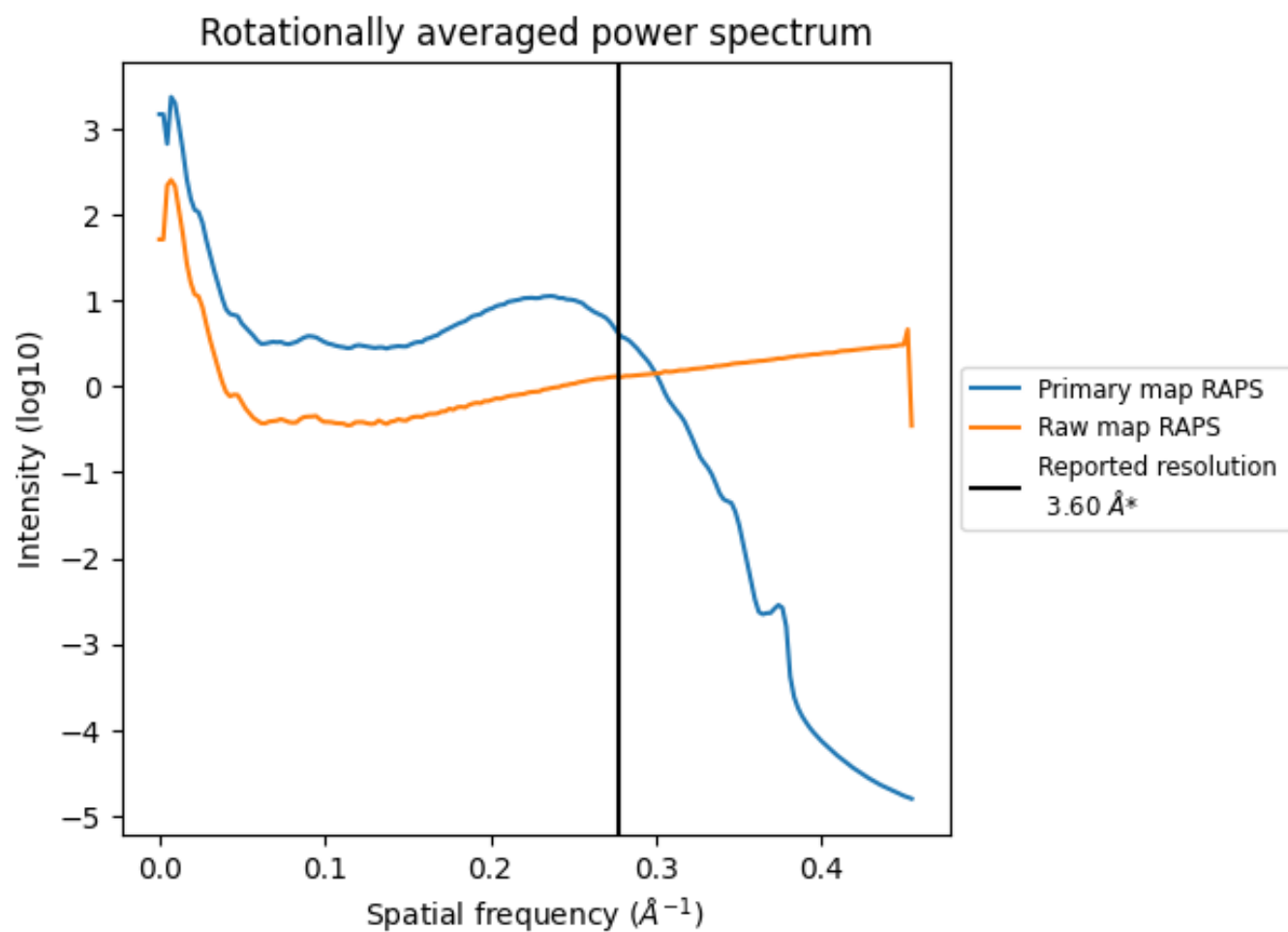
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm^3 ; this corresponds to an approximate mass of 66 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 ⓘ

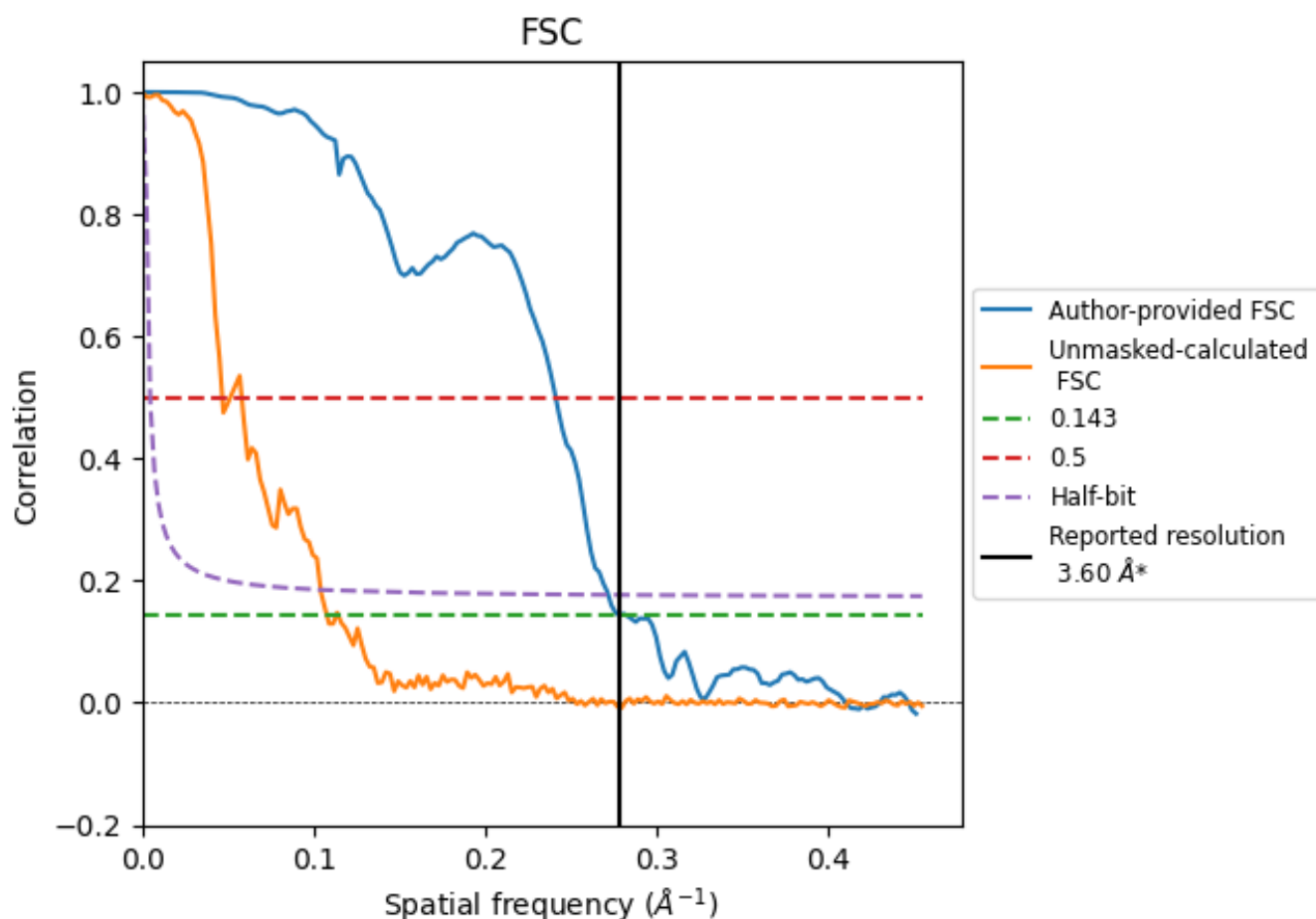


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

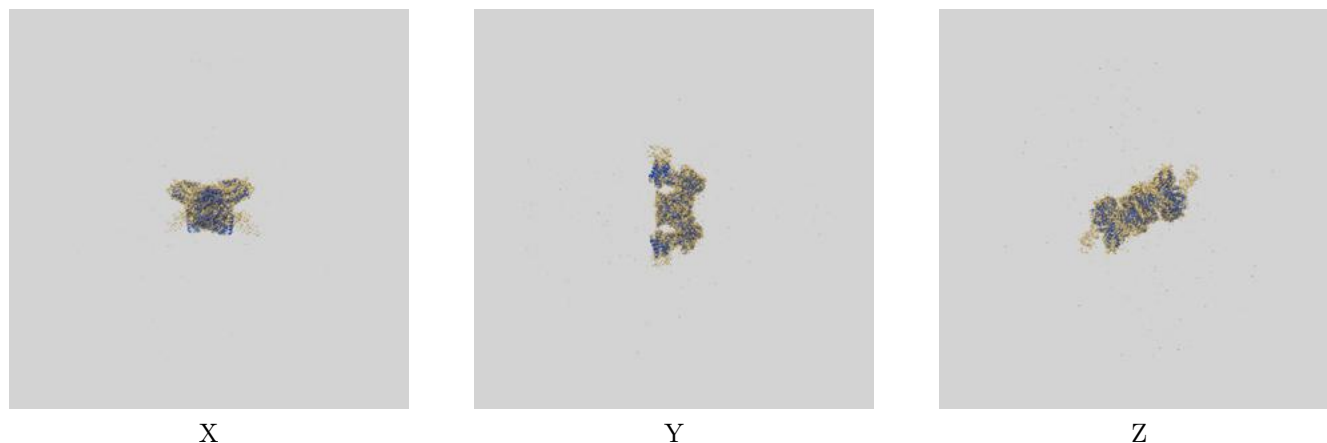
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.15	3.68
Unmasked-calculated*	9.29	21.41	9.62

*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 9.29 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

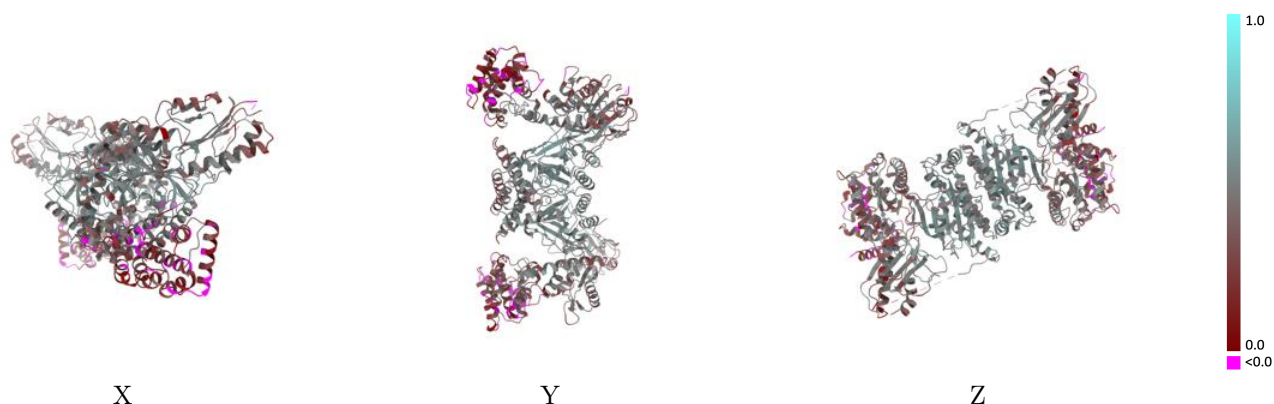
This section contains information regarding the fit between EMDB map EMD-33237 and PDB model 7XJY. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



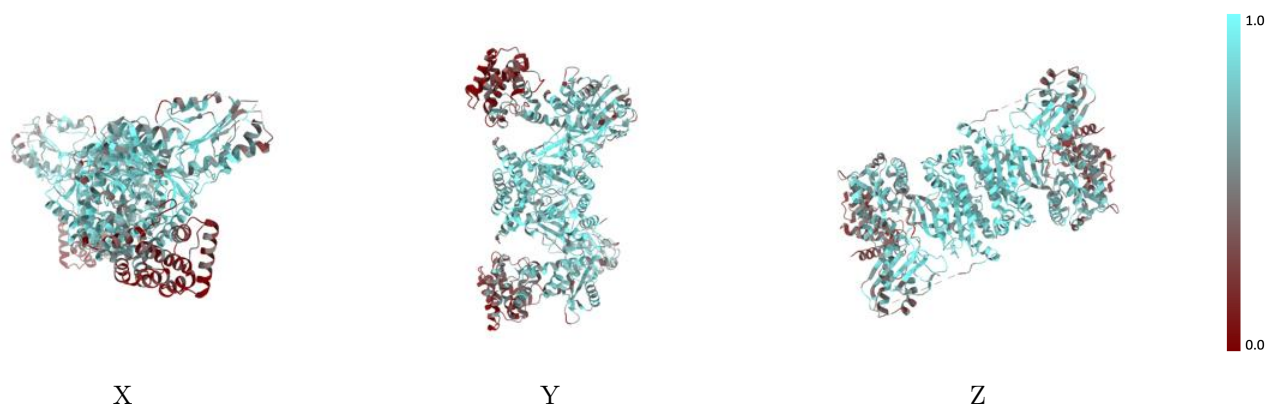
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



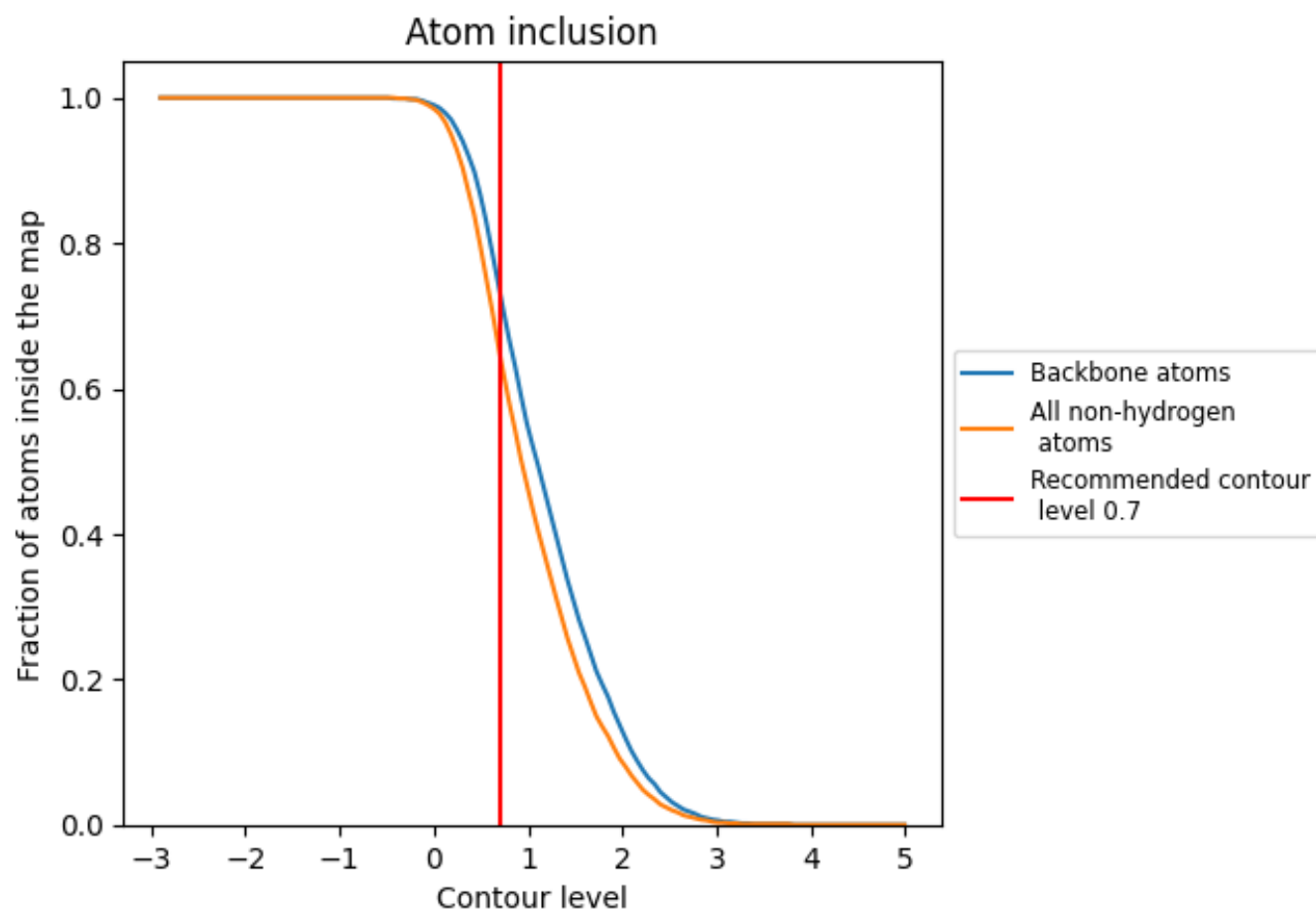
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 65% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6470	0.3990
A	0.6460	0.3990
B	0.6480	0.3990

