



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:30 AM UTC

PDB ID : 8WVW / pdb_00008wvw
EMDB ID : EMD-37874
Title : Cryo-EM structure of LGR4 in state II
Authors : Lin, C.; Chang, Z.
Deposited on : 2023-10-24
Resolution : 3.53 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

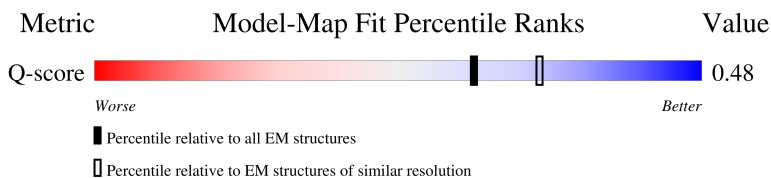
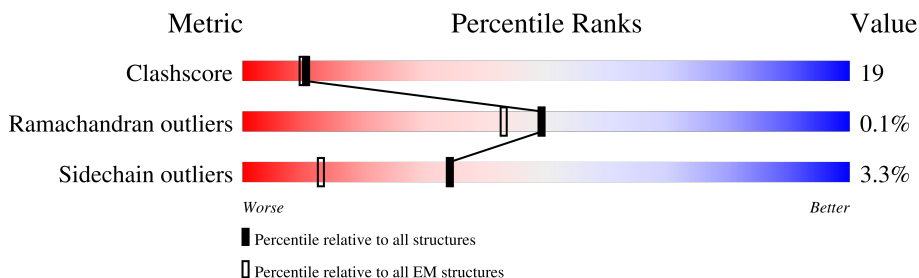
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 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	12947 (3.03 - 4.02)

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	832	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5594 atoms, of which 0 are hydrogens and 0 are deuteriums.

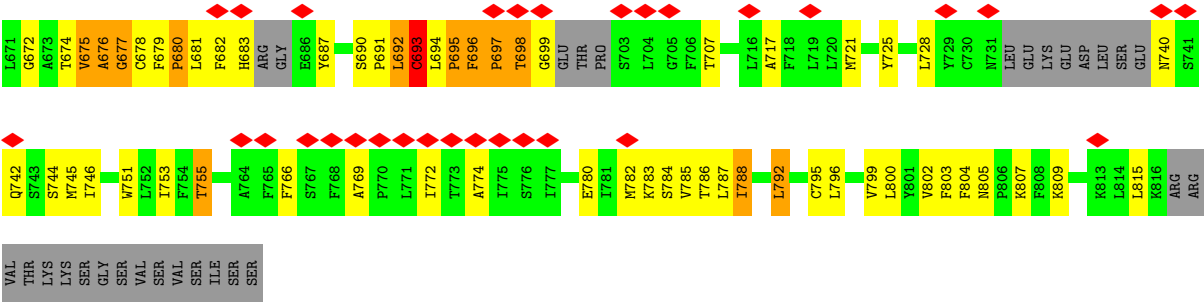
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Leucine-rich repeat-containing G-protein coupled receptor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	722	Total	C	N	O	S	0	0
			5594	3634	920	1014	26		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9BXB1
A	2	LYS	-	expression tag	UNP Q9BXB1
A	3	THR	-	expression tag	UNP Q9BXB1
A	4	ILE	-	expression tag	UNP Q9BXB1
A	5	ILE	-	expression tag	UNP Q9BXB1
A	6	ALA	-	expression tag	UNP Q9BXB1
A	7	LEU	-	expression tag	UNP Q9BXB1
A	8	SER	-	expression tag	UNP Q9BXB1
A	9	TYR	-	expression tag	UNP Q9BXB1
A	10	ILE	-	expression tag	UNP Q9BXB1
A	11	PHE	-	expression tag	UNP Q9BXB1
A	12	CYS	-	expression tag	UNP Q9BXB1
A	13	LEU	-	expression tag	UNP Q9BXB1
A	14	VAL	-	expression tag	UNP Q9BXB1
A	15	PHE	-	expression tag	UNP Q9BXB1
A	16	ALA	-	expression tag	UNP Q9BXB1
A	17	ASP	-	expression tag	UNP Q9BXB1
A	18	TYR	-	expression tag	UNP Q9BXB1
A	19	LYS	-	expression tag	UNP Q9BXB1
A	20	ASP	-	expression tag	UNP Q9BXB1
A	21	ASP	-	expression tag	UNP Q9BXB1
A	22	ASP	-	expression tag	UNP Q9BXB1
A	23	ASP	-	expression tag	UNP Q9BXB1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	162355	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.127	Depositor
Minimum map value	-2.303	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.696	Depositor
Map size (Å)	306.0, 306.0, 306.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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	1.40	120/5721 (2.1%)	1.31	72/7778 (0.9%)

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	TYR	C-N	16.21	1.47	1.33
1	A	698	THR	C-N	12.01	1.50	1.33
1	A	400	LEU	C-N	11.72	1.46	1.33
1	A	94	SER	C-N	11.53	1.50	1.33
1	A	432	GLY	C-N	10.74	1.49	1.33
1	A	457	VAL	C-N	10.18	1.46	1.33
1	A	455	ASP	C-N	9.82	1.46	1.33
1	A	253	LEU	C-N	9.73	1.47	1.33
1	A	169	PRO	C-N	9.40	1.45	1.33
1	A	434	ASN	C-N	9.25	1.47	1.33
1	A	284	LEU	C-N	-9.18	1.21	1.33
1	A	302	VAL	C-N	9.00	1.44	1.33
1	A	130	ALA	C-N	8.95	1.45	1.33
1	A	171	HIS	C-N	-8.88	1.22	1.33
1	A	328	GLY	C-N	8.82	1.45	1.33
1	A	288	GLY	C-N	8.62	1.45	1.33
1	A	81	PRO	C-N	-8.60	1.22	1.33
1	A	370	ILE	C-N	8.57	1.44	1.33
1	A	742	GLN	C-N	-8.55	1.22	1.33
1	A	257	SER	C-N	8.17	1.45	1.33
1	A	85	GLU	C-N	-8.14	1.22	1.33
1	A	283	PRO	C-N	8.10	1.45	1.33
1	A	213	ILE	C-N	-8.02	1.22	1.33
1	A	193	PRO	C-N	8.02	1.44	1.33
1	A	237	LEU	C-N	-7.95	1.21	1.33
1	A	147	ASP	C-N	-7.91	1.22	1.33
1	A	745	MET	C-N	-7.90	1.24	1.33
1	A	146	GLU	C-N	-7.84	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	GLU	C-N	7.74	1.43	1.33
1	A	299	HIS	C-N	-7.66	1.24	1.33
1	A	676	ALA	C-O	7.64	1.32	1.24
1	A	461	SER	C-N	7.57	1.45	1.33
1	A	182	LEU	C-N	7.49	1.43	1.33
1	A	95	PHE	C-N	7.44	1.43	1.33
1	A	387	GLY	C-N	7.44	1.44	1.33
1	A	273	LEU	C-N	7.40	1.43	1.33
1	A	414	PRO	C-N	7.32	1.42	1.33
1	A	230	LEU	C-N	7.29	1.43	1.33
1	A	531	PRO	C-O	-7.28	1.15	1.23
1	A	544	THR	C-N	-7.27	1.25	1.34
1	A	91	ASN	C-N	7.21	1.43	1.33
1	A	359	PRO	C-N	7.18	1.43	1.33
1	A	384	THR	C-N	-7.02	1.23	1.33
1	A	204	VAL	C-N	-6.94	1.24	1.33
1	A	422	PHE	C-N	6.93	1.43	1.33
1	A	617	GLY	C-N	-6.92	1.24	1.34
1	A	628	SER	CA-CB	-6.90	1.41	1.53
1	A	246	ALA	C-N	6.87	1.42	1.33
1	A	277	ILE	C-N	6.87	1.43	1.33
1	A	374	ARG	C-N	6.81	1.43	1.33
1	A	809	LYS	C-O	6.75	1.31	1.24
1	A	160	LEU	C-N	6.72	1.42	1.33
1	A	306	ALA	C-N	-6.71	1.23	1.33
1	A	84	GLU	C-N	-6.66	1.25	1.33
1	A	377	ILE	C-N	-6.62	1.23	1.33
1	A	746	ILE	C-N	-6.60	1.25	1.33
1	A	792	LEU	C-N	6.54	1.42	1.33
1	A	143	SER	C-N	-6.48	1.26	1.33
1	A	355	ILE	C-N	-6.45	1.24	1.33
1	A	195	PHE	C-N	-6.36	1.24	1.33
1	A	104	LEU	C-N	-6.28	1.25	1.33
1	A	329	THR	C-N	6.15	1.41	1.33
1	A	223	GLY	C-N	6.14	1.41	1.33
1	A	272	PRO	C-N	6.09	1.42	1.33
1	A	173	LEU	C-N	-6.07	1.25	1.33
1	A	405	HIS	C-N	6.05	1.41	1.33
1	A	352	TYR	C-N	6.02	1.42	1.33
1	A	606	ALA	C-N	-6.02	1.26	1.33
1	A	180	GLN	C-N	-6.01	1.25	1.33
1	A	675	VAL	C-O	-6.00	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	583	SER	CA-CB	-6.00	1.43	1.53
1	A	669	ALA	CA-CB	-5.99	1.44	1.53
1	A	661	GLN	C-N	-5.96	1.25	1.34
1	A	89	ALA	C-N	-5.91	1.25	1.33
1	A	194	ASP	C-N	-5.90	1.25	1.33
1	A	591	THR	C-N	-5.88	1.26	1.33
1	A	401	ILE	C-N	-5.87	1.25	1.33
1	A	463	SER	CA-CB	-5.87	1.44	1.52
1	A	97	HIS	C-N	5.80	1.47	1.33
1	A	451	LEU	C-N	5.77	1.41	1.33
1	A	92	ASP	C-N	5.71	1.41	1.33
1	A	780	GLU	C-N	-5.69	1.26	1.33
1	A	326	LEU	C-N	5.68	1.41	1.33
1	A	807	LYS	C-N	-5.66	1.26	1.33
1	A	172	PRO	C-N	-5.63	1.26	1.33
1	A	226	ASN	C-N	5.62	1.41	1.33
1	A	740	ASN	C-N	5.62	1.41	1.34
1	A	217	SER	C-N	5.58	1.41	1.33
1	A	367	LEU	C-N	-5.56	1.25	1.33
1	A	381	LYS	C-N	5.56	1.41	1.33
1	A	538	SER	CA-CB	-5.55	1.45	1.53
1	A	139	ASN	C-N	-5.54	1.26	1.33
1	A	248	PRO	C-N	-5.53	1.25	1.33
1	A	261	SER	CA-CB	-5.52	1.46	1.54
1	A	680	PRO	C-O	-5.48	1.16	1.24
1	A	572	SER	CA-CB	-5.47	1.45	1.53
1	A	331	ILE	C-N	-5.46	1.25	1.33
1	A	378	TYR	C-N	-5.45	1.26	1.33
1	A	281	ASP	C-N	5.42	1.39	1.33
1	A	150	GLU	C-N	-5.38	1.25	1.33
1	A	132	GLN	C-N	-5.36	1.26	1.33
1	A	264	PRO	C-O	-5.33	1.17	1.24
1	A	629	SER	CA-CB	-5.33	1.44	1.53
1	A	788	ILE	C-N	-5.31	1.25	1.33
1	A	216	LEU	C-N	-5.30	1.25	1.33
1	A	441	LEU	C-N	-5.25	1.27	1.33
1	A	632	ALA	CA-CB	-5.22	1.46	1.54
1	A	528	ALA	CA-CB	-5.17	1.47	1.54
1	A	309	VAL	C-N	-5.17	1.26	1.33
1	A	600	VAL	C-N	-5.14	1.26	1.33
1	A	105	LYS	C-N	5.12	1.43	1.34
1	A	646	SER	CA-CB	-5.11	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	GLN	C-N	-5.08	1.25	1.33
1	A	755	THR	C-N	-5.07	1.26	1.34
1	A	537	GLY	C-N	-5.06	1.26	1.33
1	A	297	ASP	C-N	-5.06	1.26	1.33
1	A	98	PRO	C-N	5.05	1.42	1.33
1	A	144	VAL	C-N	-5.04	1.26	1.33
1	A	191	SER	C-N	5.01	1.37	1.33
1	A	677	GLY	C-N	-5.00	1.27	1.34

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	TRP	N-CA-C	16.50	132.71	112.58
1	A	532	CYS	N-CA-CB	-10.82	93.96	110.73
1	A	531	PRO	CB-CA-C	-10.72	97.63	111.46
1	A	805	ASN	CB-CA-C	-10.26	96.32	109.65
1	A	697	PRO	O-C-N	9.12	133.18	122.23
1	A	695	PRO	CB-CA-C	-9.02	96.68	111.56
1	A	804	PHE	CA-C-O	-8.63	113.64	121.67
1	A	660	LYS	CB-CA-C	-7.99	98.33	110.88
1	A	696	PHE	CB-CA-C	-7.68	95.03	110.17
1	A	340	GLN	N-CA-C	-7.67	103.94	113.38
1	A	276	THR	CB-CA-C	-7.59	101.23	110.94
1	A	531	PRO	N-CA-C	7.45	122.76	111.14
1	A	386	GLN	O-C-N	-7.30	114.39	123.01
1	A	804	PHE	CB-CA-C	-7.28	100.86	112.07
1	A	573	SER	CA-C-N	7.28	130.04	120.28
1	A	573	SER	C-N-CA	7.28	130.04	120.28
1	A	524	PRO	N-CA-C	-7.24	97.55	112.47
1	A	122	SER	N-CA-C	-7.02	101.93	112.04
1	A	469	GLN	N-CA-C	-6.92	104.86	113.38
1	A	804	PHE	CA-CB-CG	6.88	120.68	113.80
1	A	697	PRO	N-CA-C	-6.78	104.11	113.53
1	A	362	ASN	O-C-N	-6.77	115.31	122.96
1	A	287	VAL	CA-C-N	6.70	126.70	120.34
1	A	287	VAL	C-N-CA	6.70	126.70	120.34
1	A	675	VAL	CA-C-O	-6.68	114.32	121.27
1	A	638	LEU	N-CA-C	-6.48	105.41	113.38
1	A	680	PRO	CA-N-CD	-6.32	103.15	112.00
1	A	96	ILE	O-C-N	-6.29	116.47	123.26
1	A	473	PHE	N-CA-C	-6.26	104.95	112.59
1	A	667	LEU	N-CA-C	-6.26	105.80	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ILE	CA-C-N	6.13	126.10	120.21
1	A	192	ILE	C-N-CA	6.13	126.10	120.21
1	A	680	PRO	N-CA-CB	6.12	109.68	103.25
1	A	631	SER	N-CA-C	-6.08	105.86	113.28
1	A	547	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	627	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	643	ARG	N-CA-C	-5.88	104.86	112.68
1	A	36	ASP	CA-C-N	-5.84	112.32	122.83
1	A	36	ASP	C-N-CA	-5.84	112.32	122.83
1	A	524	PRO	CB-CA-C	5.81	121.15	111.56
1	A	287	VAL	O-C-N	-5.80	116.93	123.20
1	A	680	PRO	O-C-N	-5.79	114.83	122.64
1	A	744	SER	O-C-N	-5.69	115.95	122.09
1	A	566	SER	N-CA-C	-5.68	107.00	114.04
1	A	282	ASN	O-C-N	-5.66	117.86	121.88
1	A	358	LEU	CA-C-N	5.66	126.96	120.85
1	A	358	LEU	C-N-CA	5.66	126.96	120.85
1	A	658	HIS	CA-C-O	-5.62	114.58	120.32
1	A	338	LEU	N-CA-C	-5.62	105.30	111.82
1	A	336	ASN	CB-CA-C	-5.58	104.36	111.22
1	A	121	PRO	N-CA-C	-5.49	101.16	112.47
1	A	96	ILE	CA-C-N	5.48	128.27	120.49
1	A	96	ILE	C-N-CA	5.48	128.27	120.49
1	A	538	SER	CB-CA-C	-5.45	101.01	113.33
1	A	192	ILE	O-C-N	-5.43	116.07	121.12
1	A	144	VAL	CA-C-N	5.42	125.89	120.52
1	A	144	VAL	C-N-CA	5.42	125.89	120.52
1	A	693	CYS	CA-C-O	-5.37	115.75	122.03
1	A	642	GLU	CB-CA-C	-5.32	100.39	109.65
1	A	339	CYS	CA-CB-SG	-5.29	102.24	114.40
1	A	340	GLN	CA-C-N	-5.24	113.46	122.79
1	A	340	GLN	C-N-CA	-5.24	113.46	122.79
1	A	666	ALA	N-CA-C	-5.21	106.60	113.17
1	A	668	LEU	N-CA-C	-5.21	106.70	113.16
1	A	275	ARG	CB-CA-C	-5.17	99.59	110.45
1	A	247	LEU	O-C-N	5.08	125.86	121.34
1	A	692	LEU	N-CA-C	-5.07	106.94	113.02
1	A	386	GLN	CA-C-N	5.06	130.75	121.85
1	A	386	GLN	C-N-CA	5.06	130.75	121.85
1	A	697	PRO	CA-C-N	-5.03	113.14	122.60
1	A	697	PRO	C-N-CA	-5.03	113.14	122.60
1	A	669	ALA	O-C-N	5.00	129.46	122.36

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	5594	0	5633	212	0
All	All	5594	0	5633	212	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 19.

All (212) 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:676:ALA:O	1:A:680:PRO:HD3	1.50	1.10
1:A:637:MET:HE2	1:A:717:ALA:HB1	1.52	0.89
1:A:442:VAL:HG13	1:A:463:SER:OG	1.74	0.86
1:A:677:GLY:O	1:A:680:PRO:HD2	1.76	0.85
1:A:67:ASN:OD1	1:A:91:ASN:ND2	2.12	0.81
1:A:523:THR:O	1:A:524:PRO:C	2.23	0.80
1:A:769:ALA:HB2	1:A:782:MET:HE1	1.63	0.80
1:A:109:VAL:HG22	1:A:133:SER:HB3	1.63	0.79
1:A:570:LEU:HD23	1:A:574:LYS:HE2	1.65	0.78
1:A:252:GLU:HA	1:A:276:THR:HG23	1.66	0.78
1:A:672:GLY:O	1:A:675:VAL:HG22	1.85	0.77
1:A:772:ILE:HG23	1:A:774:ALA:H	1.50	0.76
1:A:570:LEU:HD23	1:A:574:LYS:CE	2.17	0.75
1:A:189:ILE:HD11	1:A:211:ASN:HD21	1.53	0.74
1:A:85:GLU:OE1	1:A:109:VAL:HB	1.89	0.72
1:A:179:LEU:HD21	1:A:182:LEU:HB2	1.72	0.72
1:A:84:GLU:HA	1:A:107:LEU:HA	1.72	0.71
1:A:695:PRO:HG2	1:A:696:PHE:HD1	1.54	0.71
1:A:695:PRO:HG2	1:A:696:PHE:CD1	2.26	0.71
1:A:89:ALA:HB1	1:A:113:GLN:HG2	1.72	0.70
1:A:194:ASP:HA	1:A:220:CYS:HA	1.74	0.70
1:A:207:HIS:HA	1:A:231:ASP:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PRO:O	1:A:125:ILE:HG12	1.94	0.68
1:A:406:SER:HA	1:A:429:PRO:HB3	1.76	0.68
1:A:345:LEU:HD21	1:A:348:LEU:HD13	1.77	0.67
1:A:676:ALA:O	1:A:679:PHE:HB3	1.95	0.67
1:A:51:VAL:HG21	1:A:76:ALA:HB1	1.76	0.67
1:A:358:LEU:HD11	1:A:377:ILE:HD13	1.77	0.66
1:A:128:LEU:HD12	1:A:131:LEU:HD21	1.77	0.66
1:A:637:MET:HB2	1:A:721:MET:HE2	1.76	0.66
1:A:680:PRO:HB2	1:A:687:TYR:CZ	2.31	0.66
1:A:697:PRO:CD	1:A:698:THR:H	2.08	0.66
1:A:755:THR:HG21	1:A:796:LEU:HD21	1.77	0.65
1:A:679:PHE:O	1:A:680:PRO:C	2.38	0.65
1:A:146:GLU:OE1	1:A:171:HIS:ND1	2.30	0.64
1:A:204:VAL:HG13	1:A:228:GLU:HG3	1.79	0.64
1:A:618:CYS:O	1:A:693:CYS:SG	2.56	0.64
1:A:536:LEU:HD13	1:A:598:ASP:CG	2.23	0.64
1:A:721:MET:HG2	1:A:753:ILE:HD12	1.78	0.63
1:A:251:LYS:HD3	1:A:275:ARG:HH21	1.64	0.63
1:A:312:PHE:CD2	1:A:335:PRO:HG2	2.33	0.63
1:A:680:PRO:HG2	1:A:687:TYR:OH	1.97	0.63
1:A:416:THR:HG23	1:A:437:ASN:HB2	1.80	0.63
1:A:692:LEU:HD13	1:A:787:LEU:HD13	1.79	0.63
1:A:796:LEU:HA	1:A:799:VAL:HB	1.81	0.62
1:A:523:THR:O	1:A:525:SER:N	2.33	0.61
1:A:583:SER:OG	1:A:632:ALA:HB2	2.01	0.60
1:A:640:THR:HG23	1:A:725:TYR:HD1	1.65	0.60
1:A:520:ILE:H	1:A:520:ILE:HD12	1.66	0.60
1:A:664:VAL:HG12	1:A:664:VAL:O	2.02	0.60
1:A:224:LEU:HD13	1:A:227:LEU:HD12	1.83	0.60
1:A:122:SER:OG	1:A:145:PRO:HG2	2.01	0.60
1:A:238:GLY:HA2	1:A:259:SER:O	2.02	0.59
1:A:558:LEU:O	1:A:562:THR:HG23	2.03	0.58
1:A:679:PHE:O	1:A:681:LEU:N	2.36	0.58
1:A:275:ARG:HG3	1:A:275:ARG:O	2.02	0.58
1:A:566:SER:O	1:A:567:CYS:C	2.45	0.58
1:A:355:ILE:HB	1:A:375:ASN:HD22	1.69	0.57
1:A:523:THR:HG22	1:A:524:PRO:N	2.19	0.56
1:A:442:VAL:HG13	1:A:463:SER:HG	1.68	0.56
1:A:141:ILE:HB	1:A:163:ASN:ND2	2.21	0.56
1:A:640:THR:HG23	1:A:725:TYR:CD1	2.41	0.56
1:A:637:MET:O	1:A:637:MET:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ARG:NH1	1:A:598:ASP:OD2	2.39	0.55
1:A:425:LEU:HB2	1:A:444:ASN:HD22	1.71	0.55
1:A:338:LEU:HD12	1:A:339:CYS:H	1.70	0.55
1:A:355:ILE:HB	1:A:375:ASN:ND2	2.22	0.55
1:A:310:GLN:HB2	1:A:330:LYS:HE2	1.88	0.55
1:A:677:GLY:O	1:A:680:PRO:CD	2.51	0.55
1:A:637:MET:HE2	1:A:717:ALA:CB	2.29	0.55
1:A:250:LEU:HD22	1:A:274:LEU:HD12	1.88	0.54
1:A:682:PHE:O	1:A:683:HIS:HB2	2.07	0.54
1:A:117:LEU:HB2	1:A:139:ASN:ND2	2.22	0.54
1:A:637:MET:CA	1:A:721:MET:HE2	2.37	0.54
1:A:637:MET:CB	1:A:721:MET:HE2	2.37	0.54
1:A:312:PHE:CD2	1:A:335:PRO:CG	2.91	0.54
1:A:677:GLY:O	1:A:678:CYS:C	2.47	0.53
1:A:570:LEU:HD23	1:A:574:LYS:HE3	1.91	0.53
1:A:674:THR:O	1:A:675:VAL:C	2.50	0.53
1:A:766:PHE:CE2	1:A:785:VAL:HG11	2.44	0.53
1:A:579:LEU:HD22	1:A:670:PHE:HE2	1.72	0.53
1:A:237:LEU:HB2	1:A:258:ASN:HD21	1.74	0.53
1:A:262:VAL:O	1:A:262:VAL:HG23	2.09	0.52
1:A:274:LEU:HD21	1:A:277:ILE:HG12	1.90	0.52
1:A:683:HIS:C	1:A:683:HIS:CD2	2.87	0.52
1:A:471:CYS:SG	1:A:526:THR:HG21	2.48	0.52
1:A:815:LEU:HD23	1:A:815:LEU:O	2.09	0.52
1:A:107:LEU:HD21	1:A:128:LEU:CD1	2.40	0.52
1:A:55:LEU:HD12	1:A:80:PHE:CZ	2.45	0.52
1:A:699:GLY:HA2	1:A:707:THR:HG21	1.92	0.51
1:A:681:LEU:HD23	1:A:687:TYR:CE2	2.45	0.51
1:A:190:SER:O	1:A:213:ILE:HA	2.11	0.51
1:A:189:ILE:HD11	1:A:211:ASN:ND2	2.22	0.51
1:A:642:GLU:CD	1:A:642:GLU:O	2.54	0.51
1:A:680:PRO:CG	1:A:687:TYR:OH	2.59	0.51
1:A:694:LEU:HB3	1:A:695:PRO:HD2	1.93	0.51
1:A:74:GLU:HB3	1:A:97:HIS:NE2	2.26	0.51
1:A:374:ARG:HD2	1:A:398:ARG:HB3	1.92	0.51
1:A:536:LEU:HD13	1:A:598:ASP:CB	2.42	0.50
1:A:101:LEU:CD2	1:A:128:LEU:HD21	2.41	0.50
1:A:117:LEU:HB2	1:A:139:ASN:HD21	1.76	0.50
1:A:640:THR:CG2	1:A:725:TYR:HD1	2.25	0.50
1:A:254:GLY:HA2	1:A:278:HIS:HB2	1.92	0.50
1:A:555:PHE:HE2	1:A:803:PHE:CE2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:THR:CG2	1:A:796:LEU:HD21	2.41	0.50
1:A:212:LYS:O	1:A:212:LYS:HD3	2.12	0.50
1:A:338:LEU:HD12	1:A:339:CYS:N	2.25	0.50
1:A:349:ASP:HA	1:A:371:SER:OG	2.12	0.50
1:A:697:PRO:CD	1:A:698:THR:N	2.75	0.50
1:A:214:ARG:HD3	1:A:236:ASN:O	2.12	0.50
1:A:529:PHE:CE1	1:A:783:LYS:HG3	2.47	0.50
1:A:783:LYS:HA	1:A:786:THR:HG22	1.92	0.49
1:A:203:LEU:HD11	1:A:206:LEU:HD13	1.94	0.49
1:A:35:CYS:SG	1:A:36:ASP:N	2.85	0.49
1:A:110:LEU:HB3	1:A:134:LEU:HD12	1.95	0.49
1:A:336:ASN:C	1:A:337:ASN:CG	2.80	0.49
1:A:576:PHE:O	1:A:580:ILE:HG13	2.12	0.49
1:A:107:LEU:HD21	1:A:128:LEU:HD12	1.94	0.49
1:A:792:LEU:O	1:A:795:CYS:HB3	2.13	0.49
1:A:31:ALA:O	1:A:32:PRO:C	2.55	0.48
1:A:531:PRO:HD2	1:A:691:PRO:HG3	1.96	0.48
1:A:66:MET:HE3	1:A:66:MET:HA	1.95	0.48
1:A:103:GLY:O	1:A:105:LYS:NZ	2.47	0.48
1:A:728:LEU:HD12	1:A:728:LEU:O	2.14	0.48
1:A:186:LEU:HD12	1:A:210:ASN:HB2	1.96	0.47
1:A:55:LEU:HD12	1:A:80:PHE:HZ	1.78	0.47
1:A:101:LEU:HG	1:A:128:LEU:HD21	1.96	0.47
1:A:110:LEU:HG	1:A:112:LEU:HD11	1.96	0.47
1:A:631:SER:O	1:A:635:LEU:HD12	2.15	0.47
1:A:681:LEU:HD23	1:A:687:TYR:HE2	1.78	0.47
1:A:421:SER:HB2	1:A:442:VAL:O	2.15	0.47
1:A:464:VAL:HB	1:A:465:PRO:HD2	1.96	0.47
1:A:404:ILE:HG13	1:A:425:LEU:HD21	1.96	0.46
1:A:442:VAL:CG1	1:A:463:SER:OG	2.56	0.46
1:A:679:PHE:C	1:A:681:LEU:N	2.71	0.46
1:A:179:LEU:HD23	1:A:200:LEU:HD13	1.98	0.46
1:A:190:SER:C	1:A:213:ILE:HA	2.40	0.46
1:A:352:TYR:CE1	1:A:374:ARG:HG3	2.51	0.46
1:A:352:TYR:HE1	1:A:374:ARG:HG3	1.80	0.46
1:A:769:ALA:CB	1:A:782:MET:HE1	2.40	0.46
1:A:310:GLN:O	1:A:331:ILE:HA	2.16	0.46
1:A:121:PRO:O	1:A:125:ILE:HG23	2.15	0.46
1:A:590:TYR:CD1	1:A:625:ALA:HB2	2.50	0.46
1:A:113:GLN:HE22	1:A:135:ARG:HD3	1.80	0.46
1:A:329:THR:HG22	1:A:331:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:PHE:HB3	1:A:707:THR:HG23	1.98	0.46
1:A:751:TRP:HB3	1:A:800:LEU:HD21	1.98	0.45
1:A:784:SER:O	1:A:788:ILE:HG22	2.15	0.45
1:A:97:HIS:CD2	1:A:99:LYS:H	2.34	0.45
1:A:171:HIS:HB3	1:A:172:PRO:HD3	1.99	0.45
1:A:252:GLU:HA	1:A:276:THR:CG2	2.43	0.45
1:A:536:LEU:HD13	1:A:598:ASP:HB2	1.99	0.45
1:A:547:PHE:CZ	1:A:551:VAL:HG21	2.52	0.45
1:A:637:MET:HB2	1:A:721:MET:CE	2.43	0.45
1:A:530:LYS:HE3	1:A:613:GLU:OE2	2.17	0.44
1:A:72:LEU:CD2	1:A:93:LEU:HD11	2.47	0.44
1:A:697:PRO:HD2	1:A:698:THR:H	1.80	0.44
1:A:108:LYS:O	1:A:132:GLN:N	2.45	0.44
1:A:682:PHE:O	1:A:683:HIS:CB	2.64	0.44
1:A:697:PRO:CG	1:A:698:THR:H	2.31	0.44
1:A:240:PHE:CE2	1:A:267:ALA:HB1	2.53	0.44
1:A:251:LYS:HA	1:A:274:LEU:HA	1.99	0.44
1:A:637:MET:HA	1:A:721:MET:HE2	2.00	0.44
1:A:692:LEU:HD11	1:A:787:LEU:HD22	1.99	0.44
1:A:468:TYR:HE2	1:A:613:GLU:OE2	2.01	0.44
1:A:334:ILE:CG1	1:A:355:ILE:HD13	2.48	0.44
1:A:347:THR:HA	1:A:369:GLU:HB3	2.00	0.44
1:A:111:THR:HA	1:A:135:ARG:HB2	2.00	0.43
1:A:247:LEU:HD13	1:A:250:LEU:HD12	2.00	0.43
1:A:401:ILE:HD12	1:A:423:ASN:ND2	2.33	0.43
1:A:641:VAL:HG12	1:A:641:VAL:O	2.17	0.43
1:A:125:ILE:HA	1:A:128:LEU:HD23	1.99	0.43
1:A:167:GLU:CA	1:A:189:ILE:HG22	2.48	0.43
1:A:186:LEU:HD11	1:A:210:ASN:HD22	1.84	0.43
1:A:425:LEU:HB2	1:A:444:ASN:ND2	2.34	0.43
1:A:518:ILE:HD12	1:A:519:ILE:H	1.84	0.42
1:A:530:LYS:HD3	1:A:530:LYS:HA	1.93	0.42
1:A:697:PRO:CG	1:A:698:THR:N	2.81	0.42
1:A:203:LEU:HD13	1:A:224:LEU:HD22	2.01	0.42
1:A:250:LEU:CD2	1:A:253:LEU:HB2	2.50	0.42
1:A:262:VAL:O	1:A:264:PRO:HD3	2.19	0.42
1:A:536:LEU:CD1	1:A:598:ASP:HB2	2.50	0.42
1:A:128:LEU:HB3	1:A:131:LEU:HD23	2.02	0.42
1:A:188:LYS:HB2	1:A:188:LYS:HE3	1.91	0.42
1:A:587:MET:HB2	1:A:628:SER:HB3	2.02	0.42
1:A:189:ILE:CD1	1:A:211:ASN:HD21	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:PHE:O	1:A:696:PHE:CD2	2.72	0.42
1:A:462:LEU:HD22	1:A:473:PHE:CE2	2.55	0.41
1:A:258:ASN:HD22	1:A:260:ILE:HD11	1.85	0.41
1:A:678:CYS:SG	1:A:682:PHE:CE2	3.13	0.41
1:A:333:SER:O	1:A:333:SER:OG	2.35	0.41
1:A:721:MET:CG	1:A:753:ILE:HD12	2.47	0.41
1:A:590:TYR:CE1	1:A:625:ALA:HB2	2.56	0.41
1:A:83:LEU:HD12	1:A:83:LEU:HA	1.90	0.41
1:A:348:LEU:HB2	1:A:367:LEU:HD11	2.03	0.41
1:A:531:PRO:CD	1:A:691:PRO:HG3	2.51	0.41
1:A:93:LEU:HB2	1:A:115:ASN:ND2	2.35	0.41
1:A:121:PRO:HB2	1:A:125:ILE:HG23	2.03	0.41
1:A:87:GLN:NE2	1:A:89:ALA:HB3	2.36	0.41
1:A:110:LEU:HB2	1:A:131:LEU:HD11	2.02	0.41
1:A:83:LEU:O	1:A:107:LEU:HA	2.21	0.41
1:A:251:LYS:HG2	1:A:275:ARG:NE	2.36	0.41
1:A:336:ASN:C	1:A:337:ASN:OD1	2.64	0.41
1:A:463:SER:OG	1:A:463:SER:O	2.35	0.41
1:A:465:PRO:HD2	1:A:469:GLN:HE21	1.86	0.41
1:A:167:GLU:HA	1:A:189:ILE:HG22	2.03	0.41
1:A:557:LEU:HD23	1:A:557:LEU:HA	1.86	0.41
1:A:696:PHE:CD2	1:A:696:PHE:C	2.99	0.40
1:A:377:ILE:HB	1:A:399:ASN:HD22	1.87	0.40
1:A:579:LEU:HD22	1:A:670:PHE:CE2	2.54	0.40
1:A:336:ASN:O	1:A:337:ASN:CG	2.64	0.40
1:A:122:SER:HB3	1:A:148:SER:OG	2.22	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	708/832 (85%)	644 (91%)	63 (9%)	1 (0%)	48 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	523	THR

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	628/730 (86%)	607 (97%)	21 (3%)	33 58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	CYS
1	A	122	SER
1	A	260	ILE
1	A	276	THR
1	A	337	ASN
1	A	338	LEU
1	A	339	CYS
1	A	340	GLN
1	A	463	SER
1	A	517	GLN
1	A	518	ILE
1	A	522	CYS
1	A	523	THR
1	A	525	SER
1	A	526	THR
1	A	532	CYS
1	A	583	SER
1	A	643	ARG
1	A	690	SER
1	A	693	CYS

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Mol	Chain	Res	Type
1	A	802	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	180	GLN
1	A	199	ASN
1	A	210	ASN
1	A	258	ASN
1	A	375	ASN
1	A	386	GLN
1	A	438	GLN
1	A	458	ASN
1	A	469	GLN
1	A	658	HIS
1	A	683	HIS
1	A	797	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

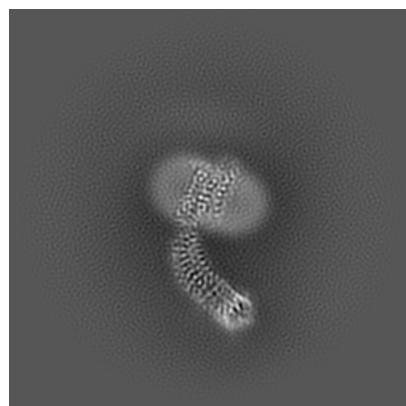
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37874. These allow visual inspection of the internal detail of the map and identification of artifacts.

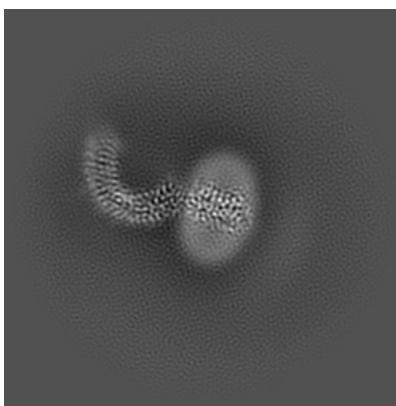
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

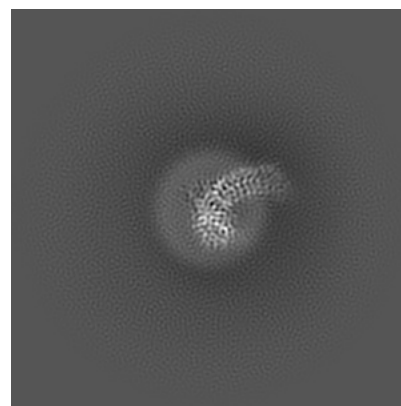
6.1.1 Primary map



X

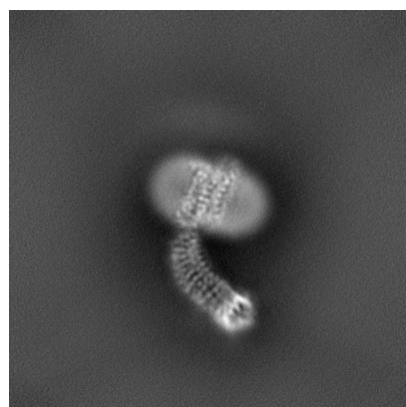


Y

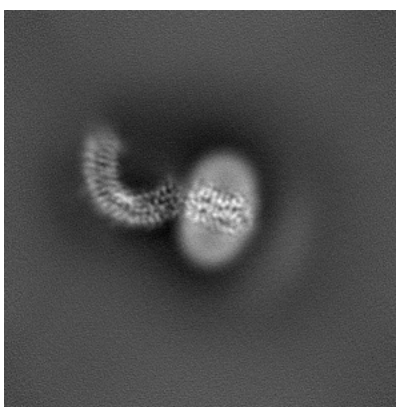


Z

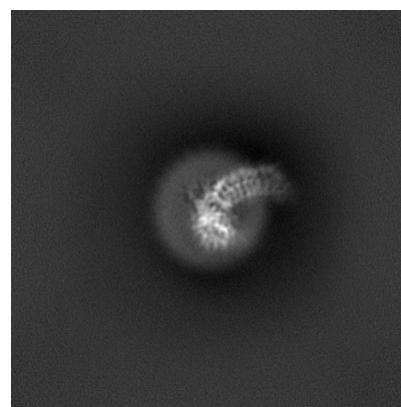
6.1.2 Raw map



X



Y

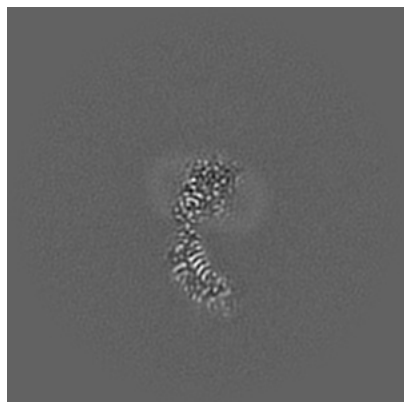


Z

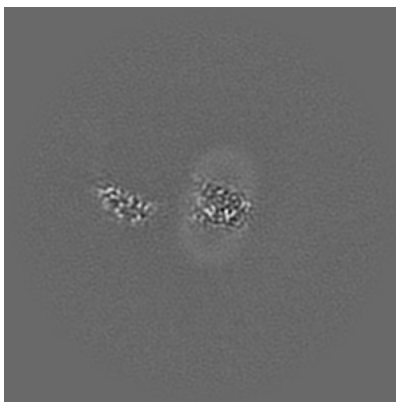
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

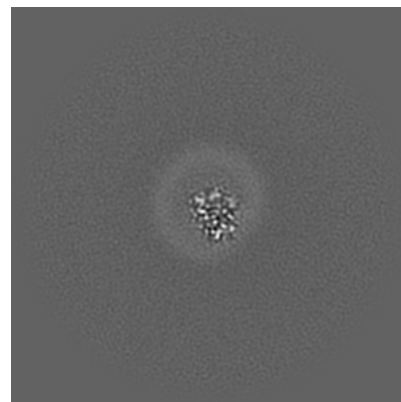
6.2.1 Primary map



X Index: 180

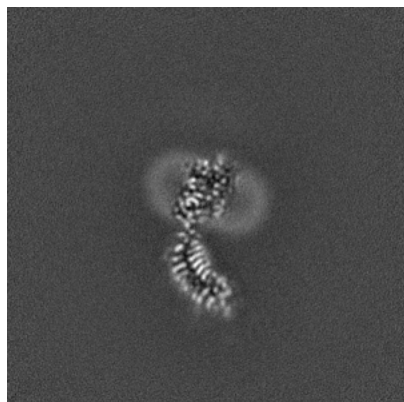


Y Index: 180

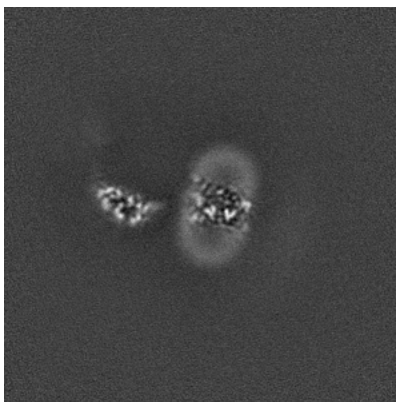


Z Index: 180

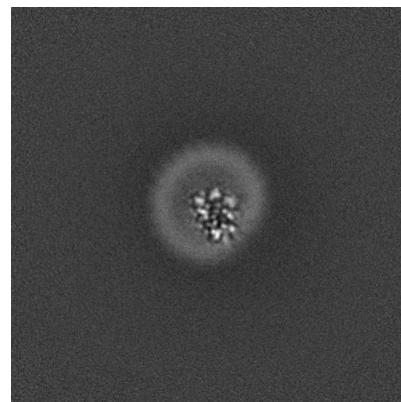
6.2.2 Raw map



X Index: 180



Y Index: 180

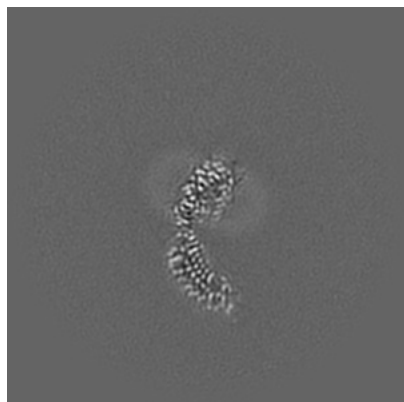


Z Index: 180

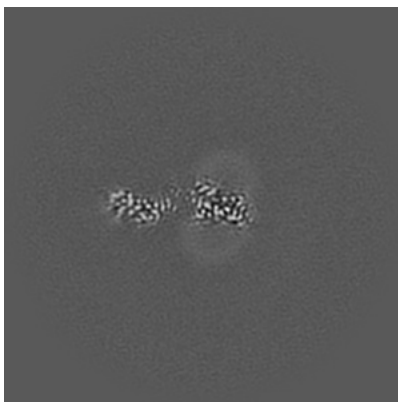
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

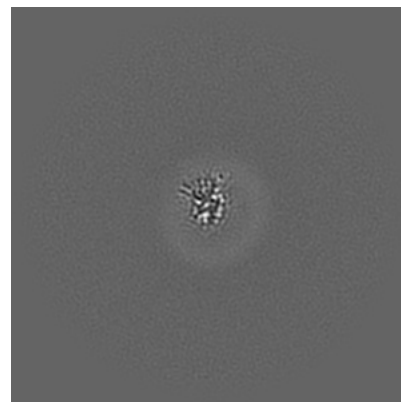
6.3.1 Primary map



X Index: 183

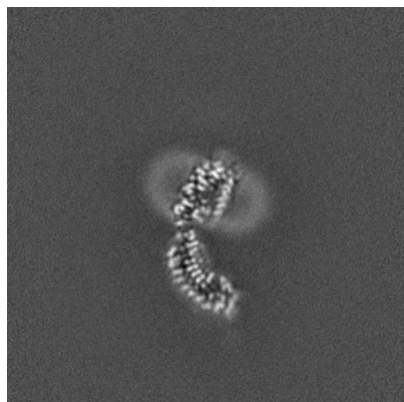


Y Index: 171

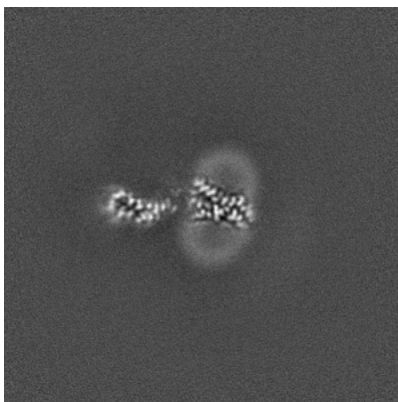


Z Index: 207

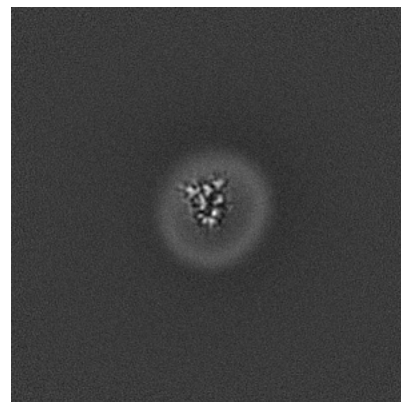
6.3.2 Raw map



X Index: 184



Y Index: 172

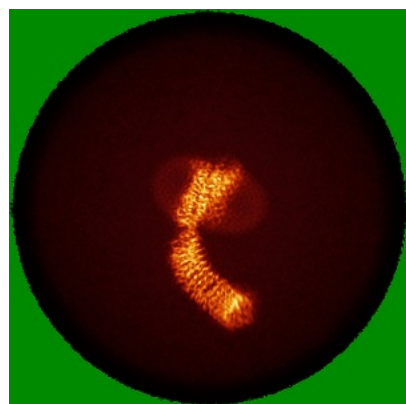


Z Index: 204

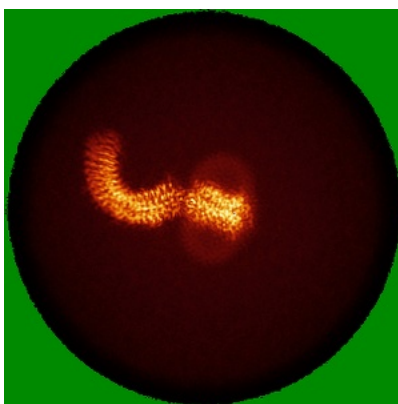
The images above show the largest variance slices of the map in three orthogonal directions.

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

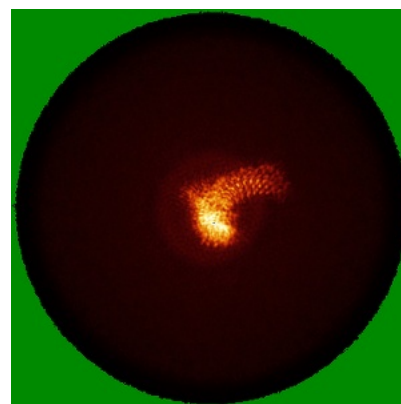
6.4.1 Primary map



X

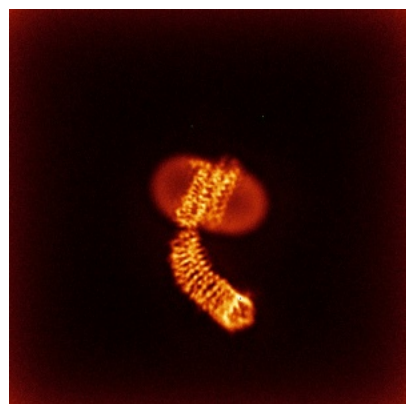


Y

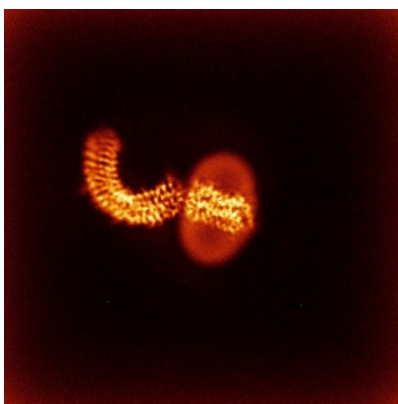


Z

6.4.2 Raw map



X



Y

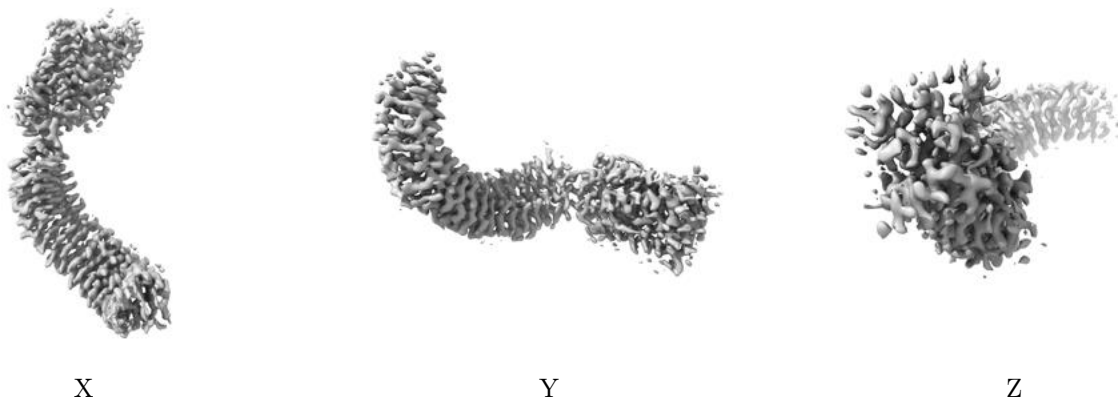


Z

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.

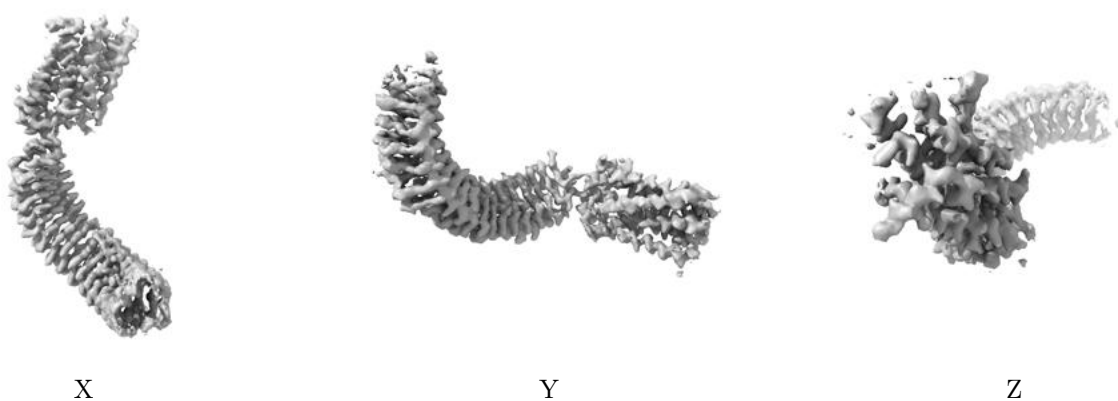
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.696. 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.

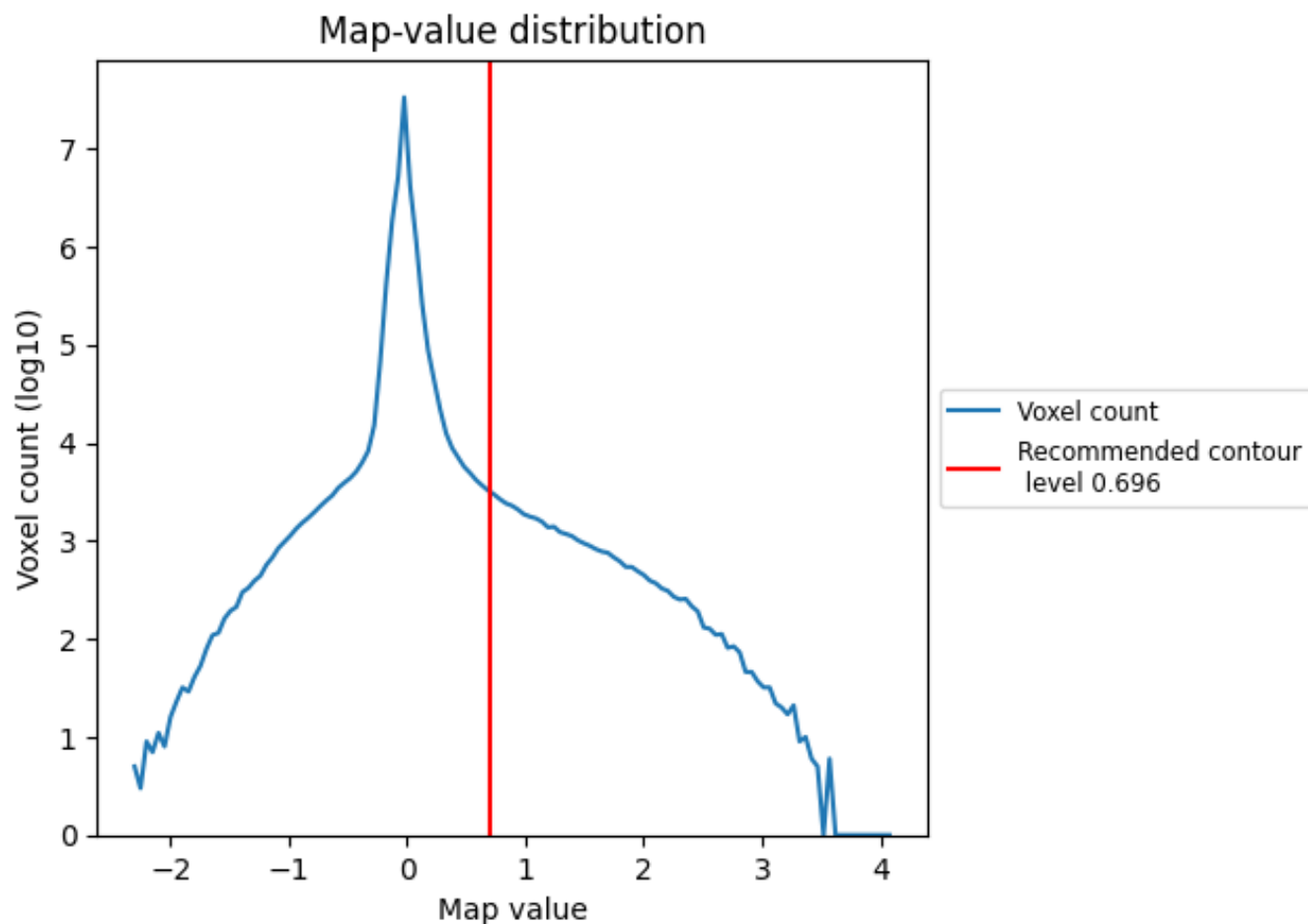
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

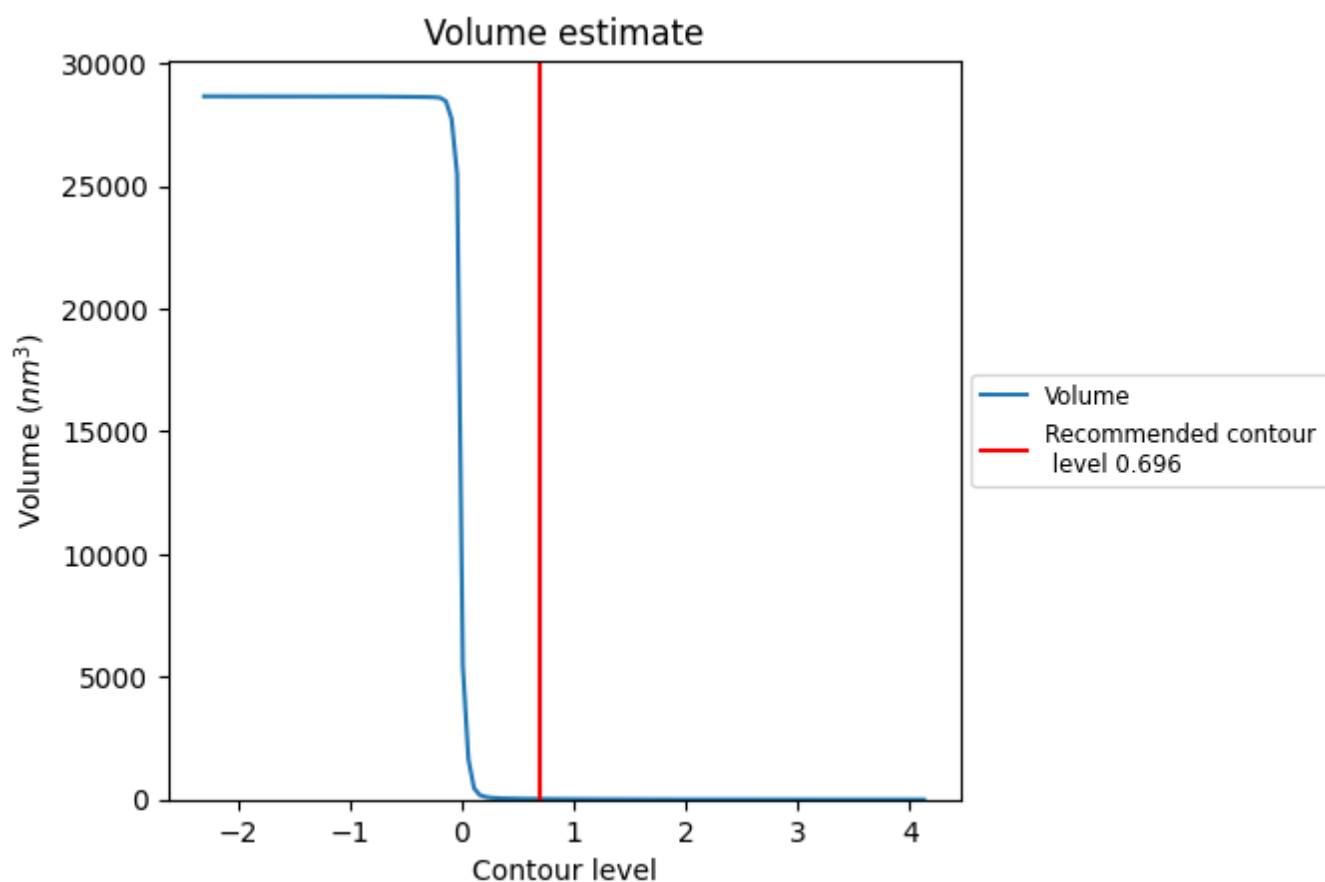
This section contains the results of statistical analysis of the map.

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.

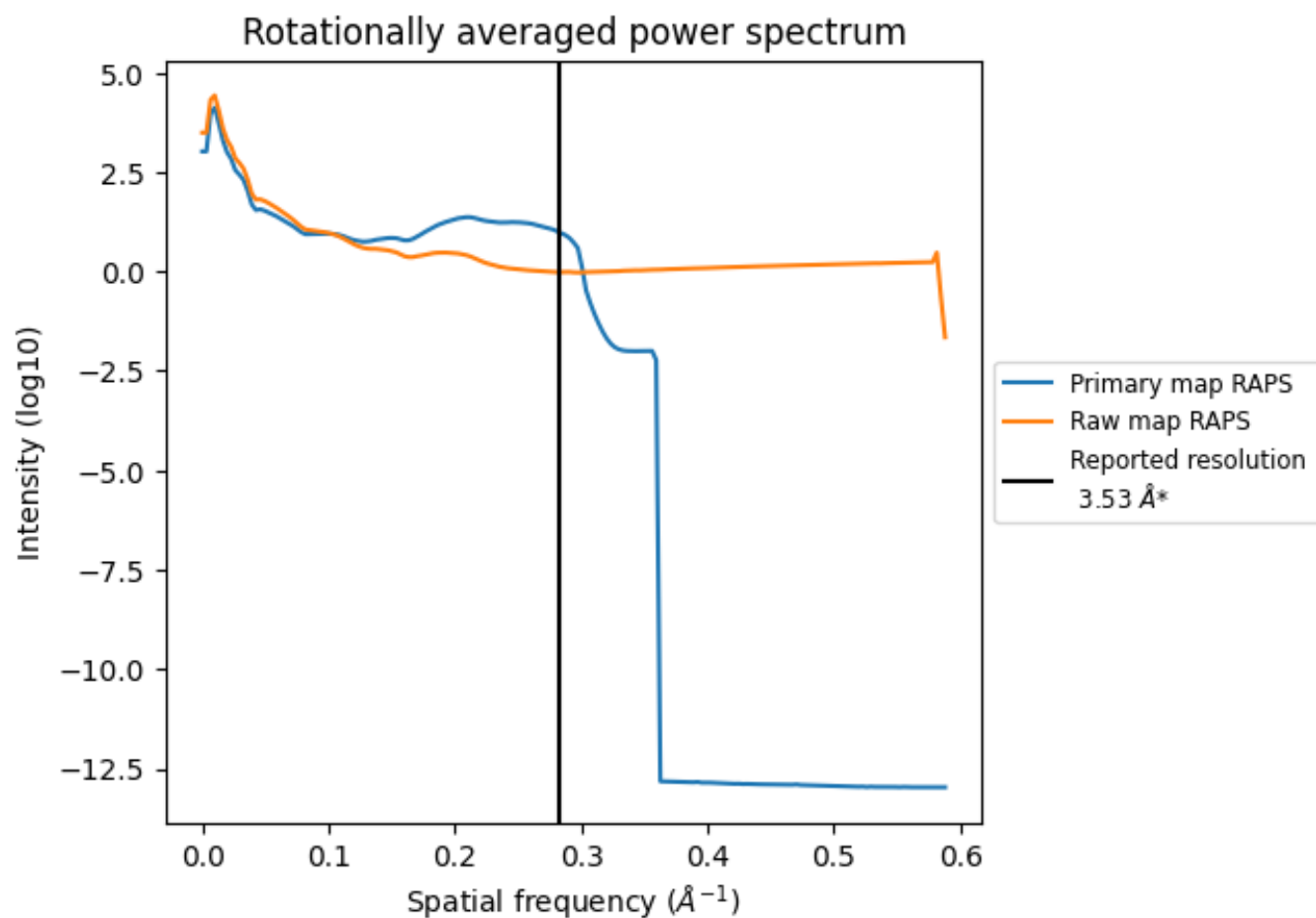
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 25 nm³; this corresponds to an approximate mass of 22 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 ⓘ

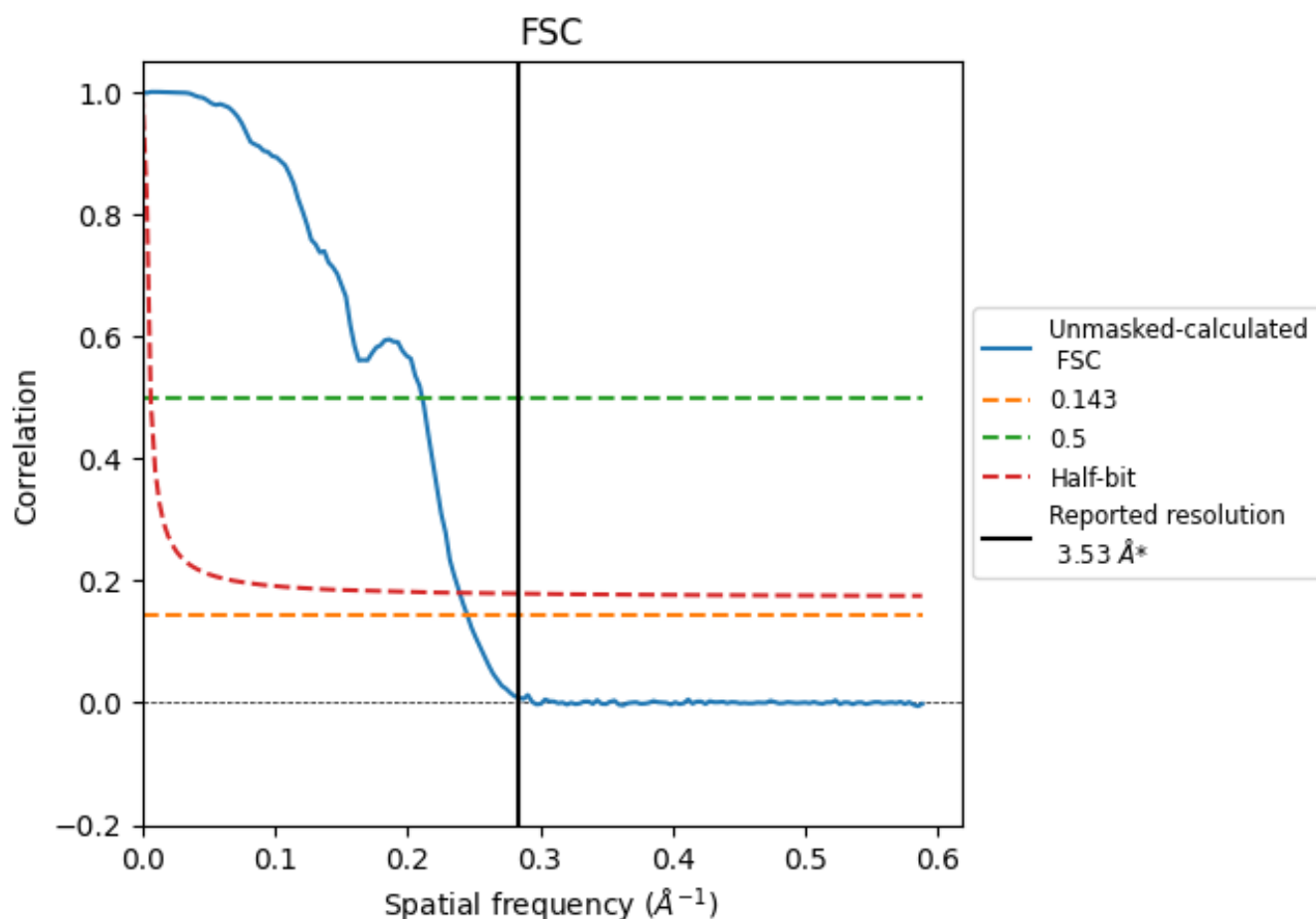


*Reported resolution corresponds to spatial frequency of 0.283 Å⁻¹

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 0.283 \AA^{-1}

8.2 Resolution estimates [i](#)

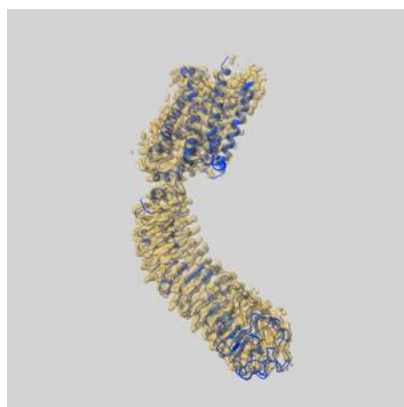
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	4.74	4.18

*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 4.08 differs from the reported value 3.53 by more than 10 %

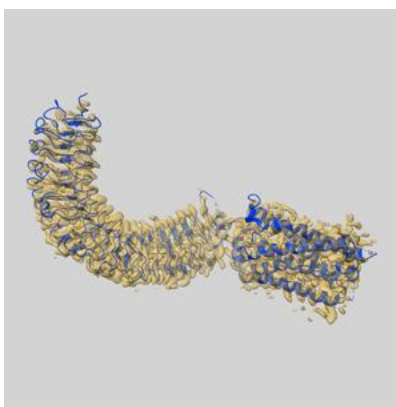
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37874 and PDB model 8WVW. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

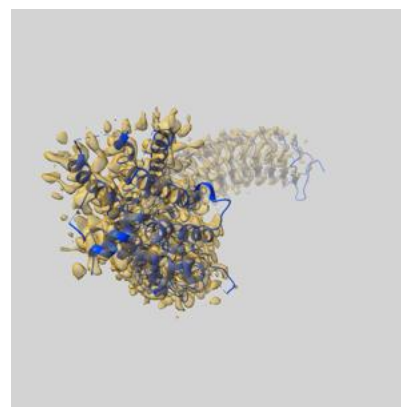
9.1 Map-model overlay [i](#)



X



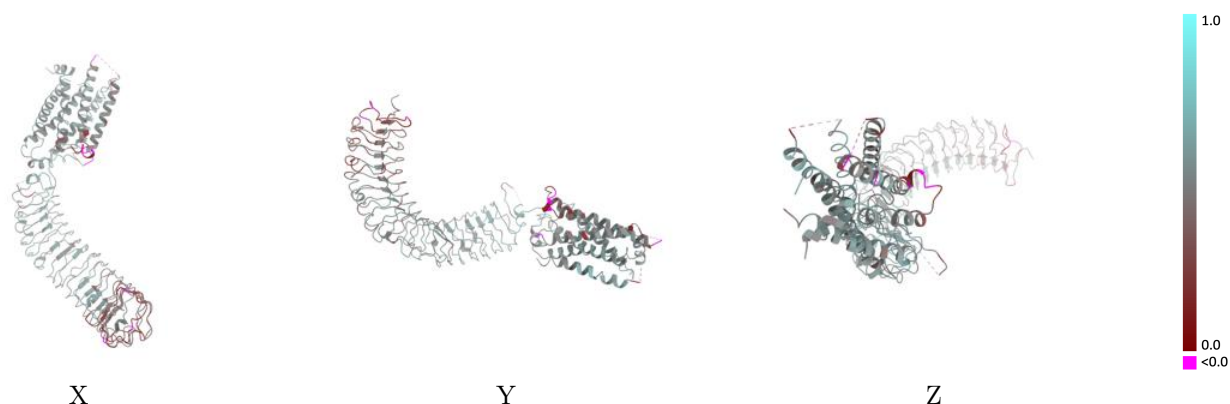
Y



Z

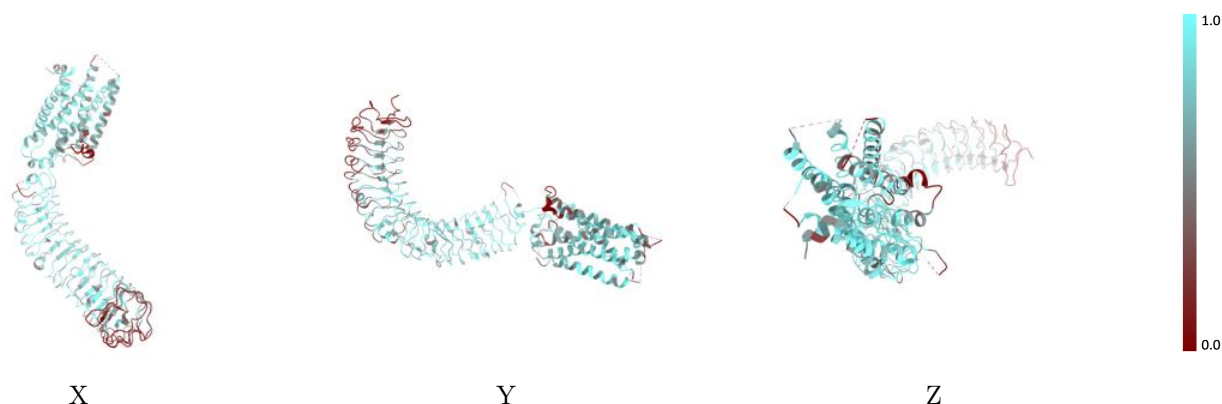
The images above show the 3D surface view of the map at the recommended contour level 0.696 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



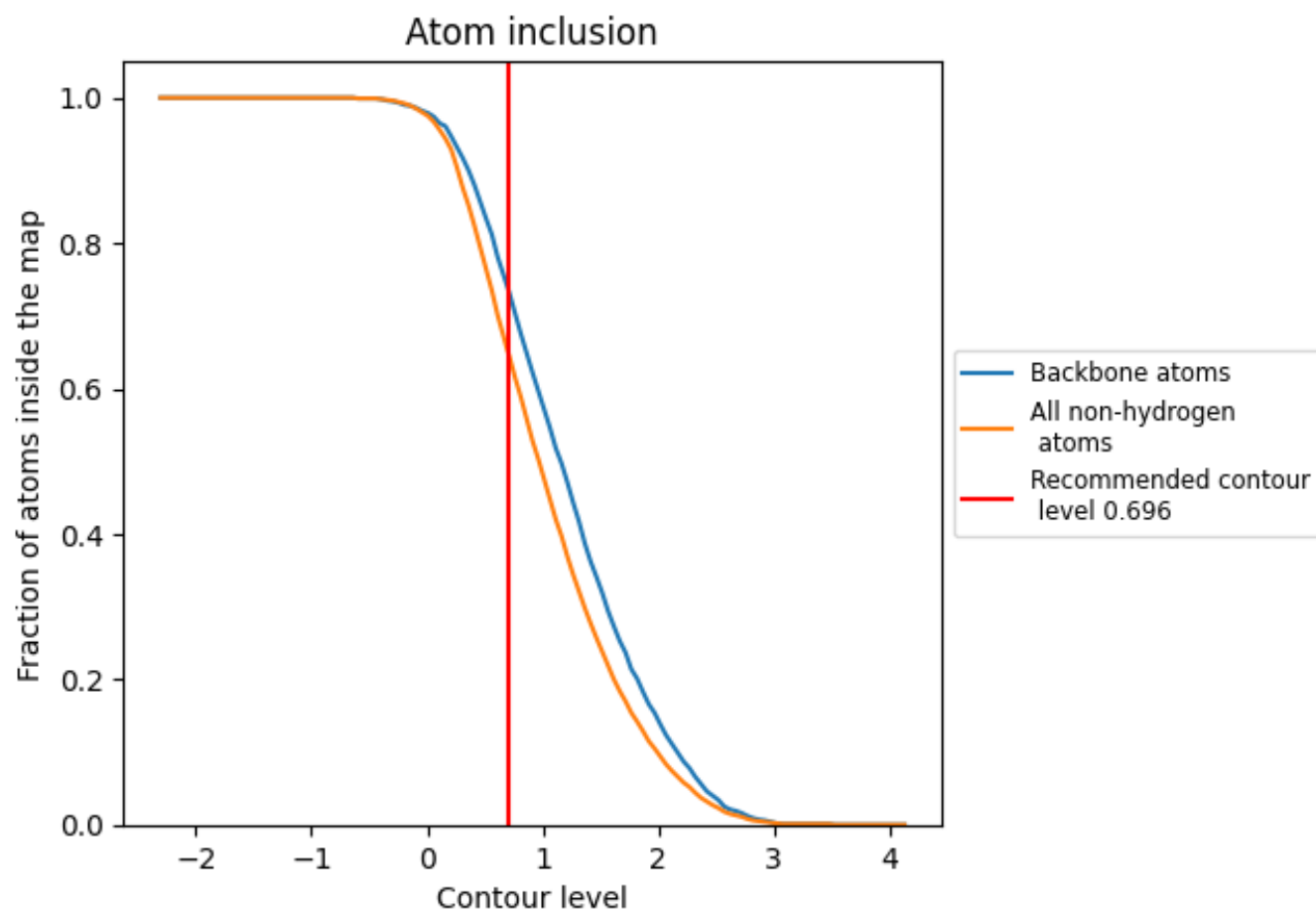
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.696).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% 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 (0.696) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6520	<div></div> 0.4800
A	<div></div> 0.6520	<div></div> 0.4800

