



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:02 AM UTC

PDB ID : 9B8K / pdb_00009b8k
EMDB ID : EMD-44348
Title : Cryo-EM structure of human dysferlin monomer
Authors : Huang, H.L.; Heissler, S.M.; Chinthalapudi, K.
Deposited on : 2024-03-30
Resolution : 2.96 Å(reported)

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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

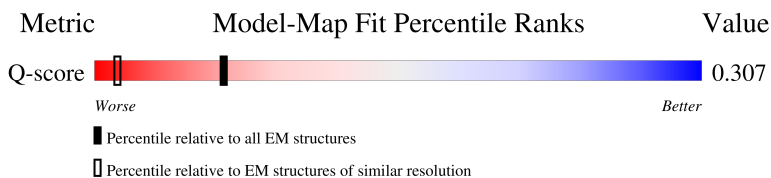
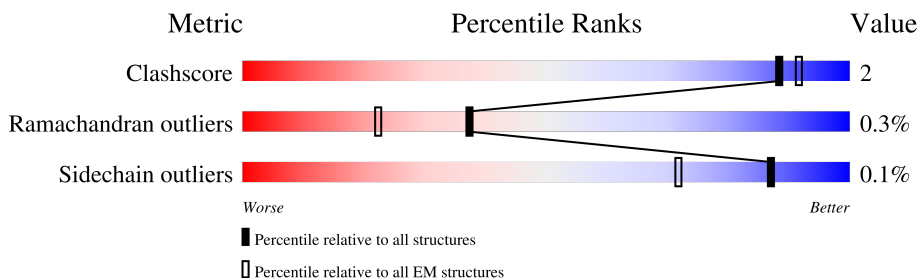
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	13155 (2.46 - 3.46)

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	2080	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14231 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 Dysferlin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1761	14231	9085	2426	2648	72	0	0



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	271263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.950	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0639	Depositor
Map size ($\text{\AA}$)	456.192, 456.192, 456.192	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.891, 0.891, 0.891	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	0/14601	1.01	212/19798 (1.1%)

There are no bond length outliers.

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1398	CYS	CA-C-N	8.59	125.85	119.66
1	A	1398	CYS	C-N-CA	8.59	125.85	119.66
1	A	1799	PRO	CA-C-N	8.16	128.11	120.03
1	A	1799	PRO	C-N-CA	8.16	128.11	120.03
1	A	1624	GLU	CA-C-N	8.16	128.18	119.78
1	A	1624	GLU	C-N-CA	8.16	128.18	119.78
1	A	1744	GLY	CA-C-N	7.97	127.99	119.78
1	A	1744	GLY	C-N-CA	7.97	127.99	119.78
1	A	1878	LEU	CA-C-N	7.95	127.67	119.56
1	A	1878	LEU	C-N-CA	7.95	127.67	119.56
1	A	1952	HIS	CA-C-N	7.88	127.59	119.56
1	A	1952	HIS	C-N-CA	7.88	127.59	119.56
1	A	1969	TRP	CA-C-N	7.83	127.78	120.03
1	A	1969	TRP	C-N-CA	7.83	127.78	120.03
1	A	1399	PRO	CA-C-N	7.81	127.96	120.31
1	A	1399	PRO	C-N-CA	7.81	127.96	120.31
1	A	1796	ARG	CA-C-N	7.79	127.74	120.03
1	A	1796	ARG	C-N-CA	7.79	127.74	120.03
1	A	1281	LYS	CA-C-N	7.64	127.60	120.03
1	A	1281	LYS	C-N-CA	7.64	127.60	120.03
1	A	391	LEU	CA-C-N	7.60	127.56	120.03
1	A	391	LEU	C-N-CA	7.60	127.56	120.03
1	A	487	ALA	CA-C-N	7.57	127.20	119.56
1	A	487	ALA	C-N-CA	7.57	127.20	119.56
1	A	1552	TYR	CA-C-N	7.50	127.43	119.85
1	A	1552	TYR	C-N-CA	7.50	127.43	119.85
1	A	439	ASN	CA-C-N	7.50	127.42	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	ASN	C-N-CA	7.50	127.42	119.85
1	A	575	LEU	CA-C-N	7.43	127.43	119.78
1	A	575	LEU	C-N-CA	7.43	127.43	119.78
1	A	1688	GLY	CA-C-N	7.41	127.12	119.56
1	A	1688	GLY	C-N-CA	7.41	127.12	119.56
1	A	1594	ASP	CA-C-N	7.41	127.12	119.56
1	A	1594	ASP	C-N-CA	7.41	127.12	119.56
1	A	345	GLY	CA-C-N	7.41	127.04	119.56
1	A	345	GLY	C-N-CA	7.41	127.04	119.56
1	A	356	ASP	CA-C-N	7.37	127.00	119.56
1	A	356	ASP	C-N-CA	7.37	127.00	119.56
1	A	1768	ARG	CA-C-N	7.30	127.22	119.85
1	A	1768	ARG	C-N-CA	7.30	127.22	119.85
1	A	1377	ASN	CA-C-N	7.29	126.99	119.56
1	A	1377	ASN	C-N-CA	7.29	126.99	119.56
1	A	1772	SER	CA-C-N	7.28	126.91	119.56
1	A	1772	SER	C-N-CA	7.28	126.91	119.56
1	A	1591	GLN	CA-C-N	7.27	127.19	119.85
1	A	1591	GLN	C-N-CA	7.27	127.19	119.85
1	A	1311	PRO	CA-C-N	7.25	127.17	119.85
1	A	1311	PRO	C-N-CA	7.25	127.17	119.85
1	A	1761	VAL	CA-C-N	7.23	127.19	120.03
1	A	1761	VAL	C-N-CA	7.23	127.19	120.03
1	A	1019	PRO	CA-C-N	7.16	126.86	119.56
1	A	1019	PRO	C-N-CA	7.16	126.86	119.56
1	A	1174	ASP	CA-C-N	7.13	127.05	119.85
1	A	1174	ASP	C-N-CA	7.13	127.05	119.85
1	A	1028	VAL	CA-C-N	7.11	126.74	119.56
1	A	1028	VAL	C-N-CA	7.11	126.74	119.56
1	A	1246	GLN	CA-C-N	7.10	127.06	120.03
1	A	1246	GLN	C-N-CA	7.10	127.06	120.03
1	A	785	GLU	CA-C-N	7.06	126.69	119.56
1	A	785	GLU	C-N-CA	7.06	126.69	119.56
1	A	232	LEU	CA-C-N	7.06	126.98	119.85
1	A	232	LEU	C-N-CA	7.06	126.98	119.85
1	A	1619	ILE	CA-C-N	7.04	127.04	119.78
1	A	1619	ILE	C-N-CA	7.04	127.04	119.78
1	A	238	LYS	CA-C-N	6.99	126.75	119.76
1	A	238	LYS	C-N-CA	6.99	126.75	119.76
1	A	913	LEU	CA-C-N	6.98	126.95	119.76
1	A	913	LEU	C-N-CA	6.98	126.95	119.76
1	A	1798	GLY	CA-C-N	6.97	127.56	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1798	GLY	C-N-CA	6.97	127.56	120.38
1	A	1775	GLN	CA-C-N	6.96	127.54	119.47
1	A	1775	GLN	C-N-CA	6.96	127.54	119.47
1	A	259	SER	CA-C-N	6.95	126.86	119.85
1	A	259	SER	C-N-CA	6.95	126.86	119.85
1	A	528	SER	CA-C-N	6.94	126.93	119.78
1	A	528	SER	C-N-CA	6.94	126.93	119.78
1	A	1740	ASN	CA-C-N	6.92	126.55	119.56
1	A	1740	ASN	C-N-CA	6.92	126.55	119.56
1	A	1804	THR	CA-C-N	6.91	126.90	119.78
1	A	1804	THR	C-N-CA	6.91	126.90	119.78
1	A	1600	ASP	CA-C-N	6.91	126.83	119.85
1	A	1600	ASP	C-N-CA	6.91	126.83	119.85
1	A	790	LEU	CA-C-N	6.91	127.31	119.92
1	A	790	LEU	C-N-CA	6.91	127.31	119.92
1	A	629	LEU	CA-C-N	6.90	126.53	119.56
1	A	629	LEU	C-N-CA	6.90	126.53	119.56
1	A	1287	ILE	CA-C-N	6.90	126.87	119.76
1	A	1287	ILE	C-N-CA	6.90	126.87	119.76
1	A	1557	ASP	CA-C-N	6.90	127.05	119.87
1	A	1557	ASP	C-N-CA	6.90	127.05	119.87
1	A	1934	LYS	CA-C-N	6.89	127.30	119.93
1	A	1934	LYS	C-N-CA	6.89	127.30	119.93
1	A	933	CYS	CA-C-N	6.82	126.80	119.78
1	A	933	CYS	C-N-CA	6.82	126.80	119.78
1	A	656	LYS	CA-C-N	6.81	126.78	119.76
1	A	656	LYS	C-N-CA	6.81	126.78	119.76
1	A	1790	PHE	CA-C-N	6.79	126.75	119.76
1	A	1790	PHE	C-N-CA	6.79	126.75	119.76
1	A	325	ASP	CA-C-N	6.79	126.42	119.56
1	A	325	ASP	C-N-CA	6.79	126.42	119.56
1	A	1252	MET	CA-C-N	6.76	126.73	119.76
1	A	1252	MET	C-N-CA	6.76	126.73	119.76
1	A	1265	GLN	CA-C-N	6.74	126.70	119.76
1	A	1265	GLN	C-N-CA	6.74	126.70	119.76
1	A	1554	LEU	CA-C-N	6.70	126.62	119.85
1	A	1554	LEU	C-N-CA	6.70	126.62	119.85
1	A	1680	LEU	CA-C-N	6.69	126.87	120.31
1	A	1680	LEU	C-N-CA	6.69	126.87	120.31
1	A	1221	PRO	CA-C-N	6.67	126.65	119.78
1	A	1221	PRO	C-N-CA	6.67	126.65	119.78
1	A	1196	ASN	CA-C-N	6.64	126.56	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1196	ASN	C-N-CA	6.64	126.56	119.85
1	A	501	LYS	CA-C-N	6.64	126.89	119.32
1	A	501	LYS	C-N-CA	6.64	126.89	119.32
1	A	1018	ILE	CA-C-N	6.62	127.19	120.38
1	A	1018	ILE	C-N-CA	6.62	127.19	120.38
1	A	537	ASP	CA-C-N	6.60	126.73	119.87
1	A	537	ASP	C-N-CA	6.60	126.73	119.87
1	A	809	VAL	CA-C-N	6.58	126.54	119.76
1	A	809	VAL	C-N-CA	6.58	126.54	119.76
1	A	1310	PRO	CA-C-N	6.57	127.15	120.38
1	A	1310	PRO	C-N-CA	6.57	127.15	120.38
1	A	1099	GLU	CA-C-N	6.56	126.47	119.85
1	A	1099	GLU	C-N-CA	6.56	126.47	119.85
1	A	1694	ASP	N-CA-C	-6.56	98.76	108.79
1	A	1105	GLY	CA-C-N	6.55	128.03	119.84
1	A	1105	GLY	C-N-CA	6.55	128.03	119.84
1	A	1414	ARG	CA-C-N	6.54	126.46	119.85
1	A	1414	ARG	C-N-CA	6.54	126.46	119.85
1	A	1560	ILE	CA-C-N	6.52	126.48	119.76
1	A	1560	ILE	C-N-CA	6.52	126.48	119.76
1	A	1321	VAL	CA-C-N	6.50	126.53	119.90
1	A	1321	VAL	C-N-CA	6.50	126.53	119.90
1	A	838	TYR	CA-C-N	6.49	126.44	119.76
1	A	838	TYR	C-N-CA	6.49	126.44	119.76
1	A	1139	ARG	CA-C-N	6.48	126.40	119.85
1	A	1139	ARG	C-N-CA	6.48	126.40	119.85
1	A	919	ARG	CA-C-N	6.44	126.40	119.76
1	A	919	ARG	C-N-CA	6.44	126.40	119.76
1	A	730	THR	CA-C-N	6.43	126.12	119.56
1	A	730	THR	C-N-CA	6.43	126.12	119.56
1	A	988	CYS	CA-C-N	6.43	126.35	119.85
1	A	988	CYS	C-N-CA	6.43	126.35	119.85
1	A	417	ASP	CA-C-N	6.43	126.95	120.14
1	A	417	ASP	C-N-CA	6.43	126.95	120.14
1	A	1391	LEU	CA-C-N	6.41	126.33	119.85
1	A	1391	LEU	C-N-CA	6.41	126.33	119.85
1	A	350	ALA	CA-C-N	6.40	127.55	120.45
1	A	350	ALA	C-N-CA	6.40	127.55	120.45
1	A	1902	ILE	CA-C-N	6.35	126.30	119.76
1	A	1902	ILE	C-N-CA	6.35	126.30	119.76
1	A	1326	LYS	CA-C-N	6.34	126.29	119.76
1	A	1326	LYS	C-N-CA	6.34	126.29	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	SER	CA-C-N	6.33	126.02	119.56
1	A	273	SER	C-N-CA	6.33	126.02	119.56
1	A	1431	ASP	CA-C-N	6.33	126.02	119.56
1	A	1431	ASP	C-N-CA	6.33	126.02	119.56
1	A	722	GLN	CA-C-N	6.33	126.24	119.85
1	A	722	GLN	C-N-CA	6.33	126.24	119.85
1	A	1574	GLY	CA-C-N	6.30	127.72	119.84
1	A	1574	GLY	C-N-CA	6.30	127.72	119.84
1	A	448	LEU	CA-C-N	6.28	126.80	120.14
1	A	448	LEU	C-N-CA	6.28	126.80	120.14
1	A	1563	PRO	CA-C-N	6.28	126.31	119.90
1	A	1563	PRO	C-N-CA	6.28	126.31	119.90
1	A	1309	TYR	CA-C-N	6.25	126.82	120.38
1	A	1309	TYR	C-N-CA	6.25	126.82	120.38
1	A	280	GLU	CA-C-N	6.24	126.16	119.85
1	A	280	GLU	C-N-CA	6.24	126.16	119.85
1	A	370	ARG	CA-C-N	6.24	126.15	119.85
1	A	370	ARG	C-N-CA	6.24	126.15	119.85
1	A	1695	GLN	CA-C-O	6.22	127.03	119.38
1	A	981	LEU	CA-C-N	6.20	126.22	119.90
1	A	981	LEU	C-N-CA	6.20	126.22	119.90
1	A	1307	LEU	CA-C-N	6.19	126.14	119.76
1	A	1307	LEU	C-N-CA	6.19	126.14	119.76
1	A	901	TYR	CA-C-N	6.17	126.11	119.76
1	A	901	TYR	C-N-CA	6.17	126.11	119.76
1	A	1213	GLU	CA-C-N	6.09	126.54	119.47
1	A	1213	GLU	C-N-CA	6.09	126.54	119.47
1	A	311	GLU	CA-C-N	6.09	126.45	119.93
1	A	311	GLU	C-N-CA	6.09	126.45	119.93
1	A	843	VAL	CA-C-N	6.08	126.25	119.32
1	A	843	VAL	C-N-CA	6.08	126.25	119.32
1	A	1023	LYS	CA-C-N	6.07	126.39	119.83
1	A	1023	LYS	C-N-CA	6.07	126.39	119.83
1	A	1258	PHE	CA-C-N	6.05	125.96	119.85
1	A	1258	PHE	C-N-CA	6.05	125.96	119.85
1	A	535	PHE	CA-C-N	5.97	125.99	119.90
1	A	535	PHE	C-N-CA	5.97	125.99	119.90
1	A	1354	SER	CA-C-N	5.91	125.82	119.85
1	A	1354	SER	C-N-CA	5.91	125.82	119.85
1	A	1873	PHE	CA-C-N	5.88	127.19	119.84
1	A	1873	PHE	C-N-CA	5.88	127.19	119.84
1	A	216	LYS	CA-C-N	5.87	126.17	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	LYS	C-N-CA	5.87	126.17	119.83
1	A	1713	ALA	CA-C-N	5.87	126.17	119.83
1	A	1713	ALA	C-N-CA	5.87	126.17	119.83
1	A	1932	MET	CA-C-N	5.86	125.82	119.78
1	A	1932	MET	C-N-CA	5.86	125.82	119.78
1	A	515	LEU	CA-C-N	5.81	126.11	119.83
1	A	515	LEU	C-N-CA	5.81	126.11	119.83
1	A	960	LEU	CA-C-N	5.78	126.17	119.47
1	A	960	LEU	C-N-CA	5.78	126.17	119.47
1	A	848	MET	CA-C-N	5.72	125.57	119.28
1	A	848	MET	C-N-CA	5.72	125.57	119.28
1	A	1697	ARG	CA-C-N	5.57	125.40	119.28
1	A	1697	ARG	C-N-CA	5.57	125.40	119.28
1	A	1220	GLN	CA-C-N	5.42	125.96	120.38
1	A	1220	GLN	C-N-CA	5.42	125.96	120.38
1	A	1562	MET	CA-C-N	5.40	125.94	120.38
1	A	1562	MET	C-N-CA	5.40	125.94	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14231	0	13968	54	0
All	All	14231	0	13968	54	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 2.

All (54) 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:1677:ARG:HH22	1:A:1695:GLN:HE22	1.15	0.93
1:A:1677:ARG:NH2	1:A:1695:GLN:HE22	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1693:ARG:O	1:A:1694:ASP:OD1	2.05	0.74
1:A:1677:ARG:HH22	1:A:1695:GLN:NE2	1.92	0.66
1:A:1695:GLN:HG2	1:A:1696:LEU:HG	1.80	0.63
1:A:304:ASP:OD1	1:A:304:ASP:C	2.43	0.62
1:A:1695:GLN:HG3	1:A:1794:LEU:HD13	1.84	0.59
1:A:370:ARG:N	1:A:371:PRO:CD	2.66	0.59
1:A:1121:ASP:OD2	1:A:1123:LYS:NZ	2.37	0.57
1:A:1695:GLN:HG3	1:A:1794:LEU:CD1	2.36	0.56
1:A:1695:GLN:HB3	1:A:1797:PRO:HG3	1.88	0.56
1:A:1181:PHE:O	1:A:1182:LEU:C	2.49	0.55
1:A:371:PRO:O	1:A:372:THR:C	2.48	0.54
1:A:1818:TRP:NE1	1:A:1988:THR:OG1	2.37	0.54
1:A:2000:ARG:N	1:A:2001:PRO:HD2	2.23	0.54
1:A:1354:SER:N	1:A:1355:PRO:CD	2.72	0.53
1:A:683:ASP:OD2	1:A:826:LYS:NZ	2.41	0.52
1:A:1955:TRP:O	1:A:1955:TRP:CG	2.63	0.52
1:A:413:LYS:NZ	1:A:625:ASP:OD1	2.43	0.51
1:A:765:LEU:N	1:A:766:PRO:HD2	2.25	0.51
1:A:1348:GLN:O	1:A:1350:ALA:N	2.45	0.49
1:A:1695:GLN:HE21	1:A:1794:LEU:HD13	1.78	0.49
1:A:452:PHE:HB3	1:A:453:PRO:HD3	1.95	0.48
1:A:2000:ARG:N	1:A:2001:PRO:CD	2.75	0.48
1:A:1818:TRP:NE1	1:A:1988:THR:HG1	2.10	0.47
1:A:1695:GLN:HE21	1:A:1794:LEU:CD1	2.27	0.47
1:A:1695:GLN:NE2	1:A:1794:LEU:CD1	2.78	0.46
1:A:1354:SER:N	1:A:1355:PRO:HD3	2.31	0.46
1:A:1695:GLN:CG	1:A:1794:LEU:HD13	2.45	0.46
1:A:1594:ASP:HB2	1:A:1595:PRO:CD	2.46	0.46
1:A:1510:GLU:OE1	1:A:1510:GLU:N	2.48	0.46
1:A:1129:SER:OG	1:A:1130:VAL:N	2.48	0.45
1:A:726:ASP:OD1	1:A:727:ILE:N	2.48	0.45
1:A:1779:GLU:HG2	1:A:1781:GLY:H	1.81	0.44
1:A:1434:SER:OG	1:A:1435:ALA:N	2.51	0.44
1:A:370:ARG:HB2	1:A:371:PRO:HD3	2.00	0.44
1:A:899:LEU:HG	1:A:901:TYR:H	1.82	0.43
1:A:396:ASP:OD1	1:A:397:ALA:N	2.51	0.43
1:A:1594:ASP:C	1:A:1594:ASP:OD1	2.62	0.43
1:A:1594:ASP:HB2	1:A:1595:PRO:HD2	2.01	0.43
1:A:1344:MET:O	1:A:1345:LYS:HB2	2.19	0.43
1:A:755:ALA:O	1:A:756:LEU:HB3	2.19	0.42
1:A:1206:TYR:HD2	1:A:1207:GLU:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:ASP:OD1	1:A:974:ASP:C	2.62	0.41
1:A:1818:TRP:CD1	1:A:1988:THR:HG1	2.38	0.41
1:A:1817:ILE:O	1:A:1868:ASN:N	2.54	0.41
1:A:325:ASP:OD1	1:A:325:ASP:C	2.63	0.41
1:A:1695:GLN:HG3	1:A:1794:LEU:HB3	2.02	0.41
1:A:2000:ARG:HB3	1:A:2001:PRO:HD3	2.03	0.41
1:A:311:GLU:HA	1:A:312:PRO:HD3	1.94	0.40
1:A:1816:ILE:HA	1:A:1869:TRP:O	2.22	0.40
1:A:1485:ILE:O	1:A:1485:ILE:HG22	2.20	0.40
1:A:1695:GLN:HG3	1:A:1794:LEU:CB	2.50	0.40
1:A:1935:PRO:HB3	1:A:1967:GLY:HA3	2.03	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	1757/2080 (84%)	1710 (97%)	42 (2%)	5 (0%)	36 59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1349	LEU
1	A	1975	GLU
1	A	1182	LEU
1	A	347	GLY
1	A	1638	PRO

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	1553/1833 (85%)	1551 (100%)	2 (0%)	88 95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1206	TYR
1	A	1877	TYR

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	218	GLN
1	A	380	HIS
1	A	711	GLN
1	A	746	HIS
1	A	771	GLN
1	A	851	GLN
1	A	1511	ASN
1	A	1568	HIS
1	A	1695	GLN
1	A	1775	GLN
1	A	1946	GLN
1	A	2004	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

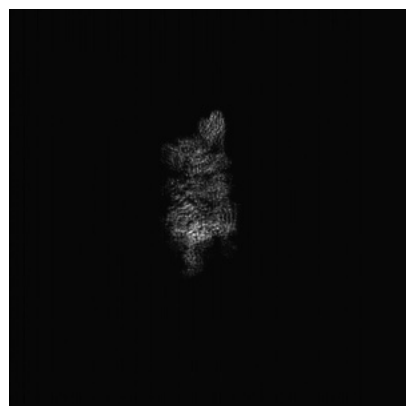
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44348. These allow visual inspection of the internal detail of the map and identification of artifacts.

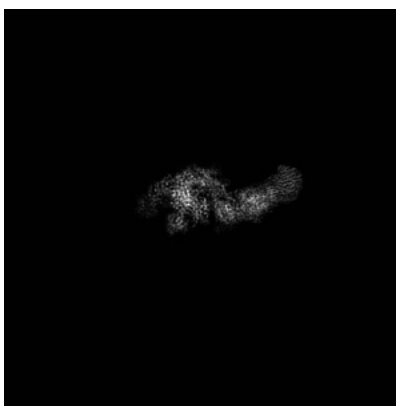
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

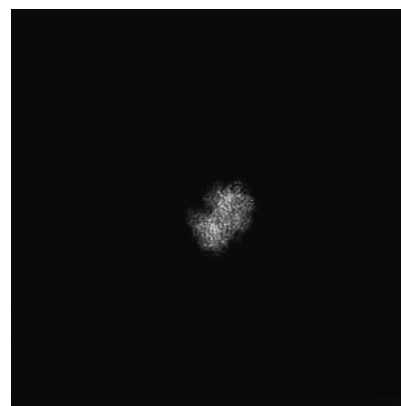
6.1.1 Primary map



X

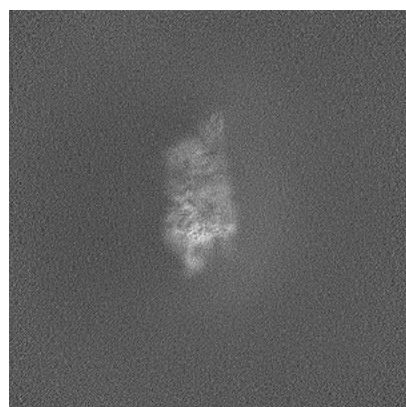


Y

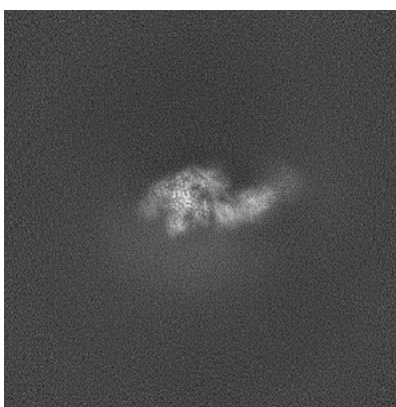


Z

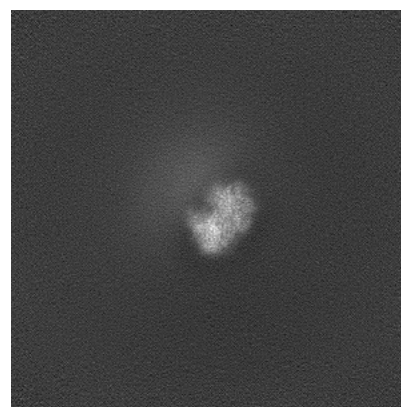
6.1.2 Raw map



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: 256

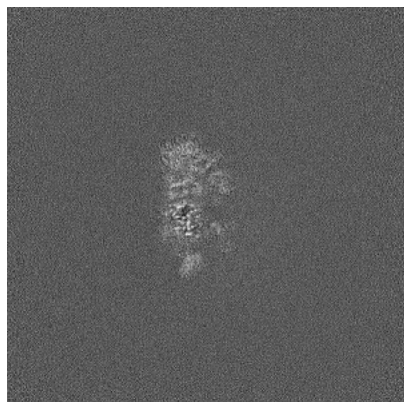


Y Index: 256

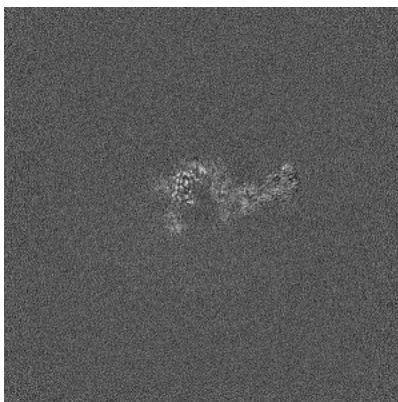


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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: 267

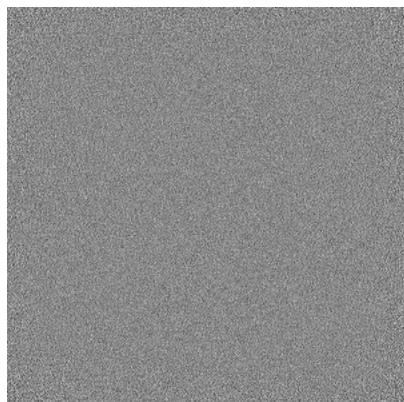


Y Index: 234

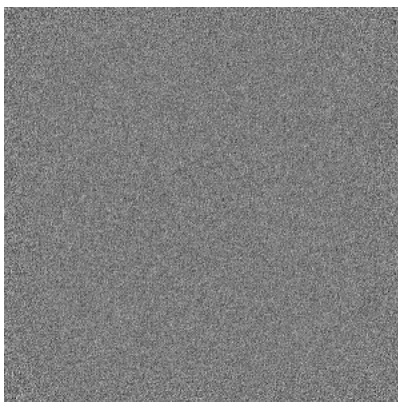


Z Index: 236

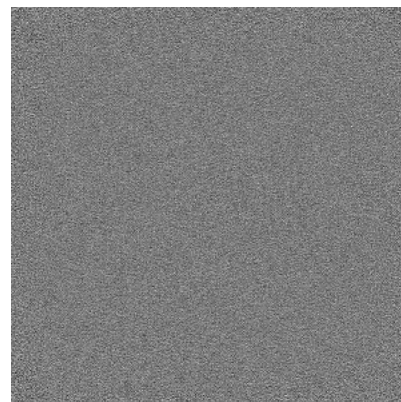
6.3.2 Raw map



X Index: 0



Y Index: 0

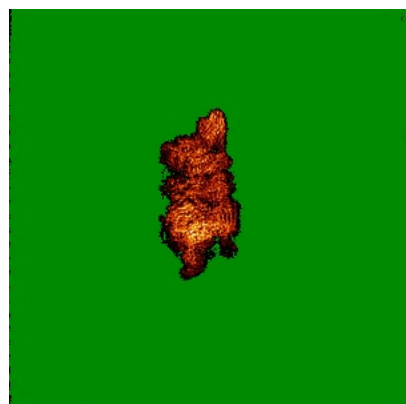


Z Index: 0

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

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

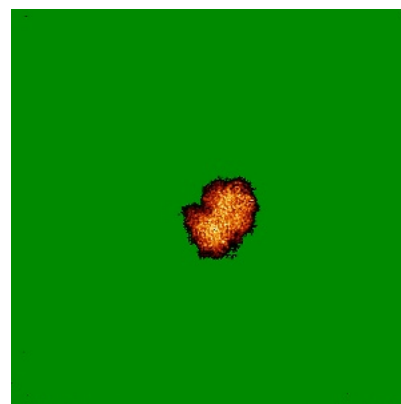
6.4.1 Primary map



X

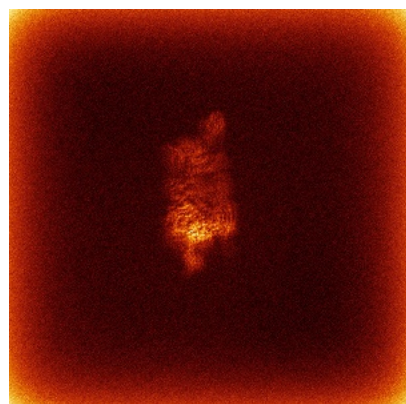


Y

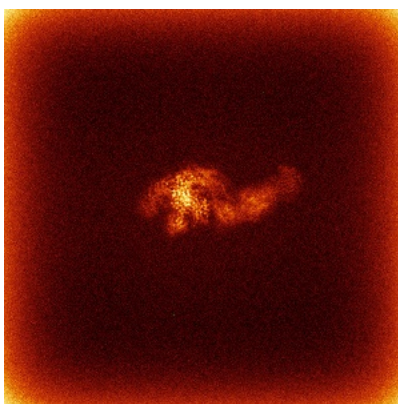


Z

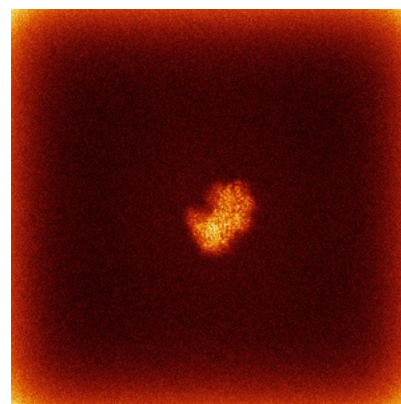
6.4.2 Raw map



X



Y

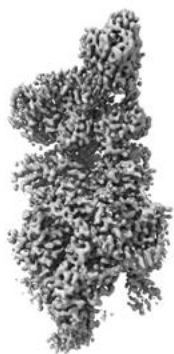


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

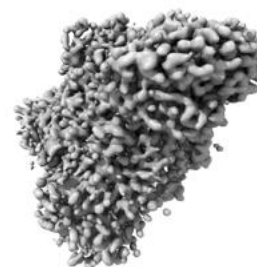
6.5.1 Primary map



X



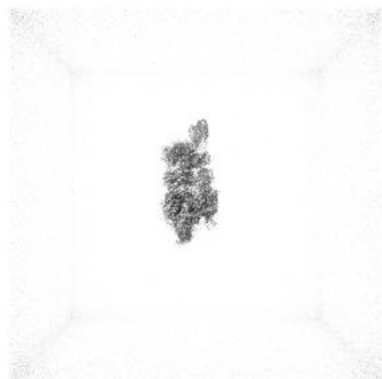
Y



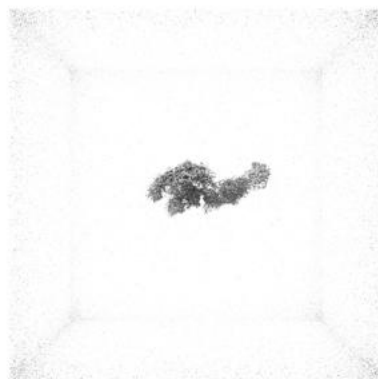
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0639. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

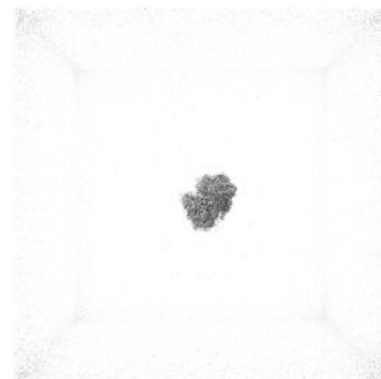
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

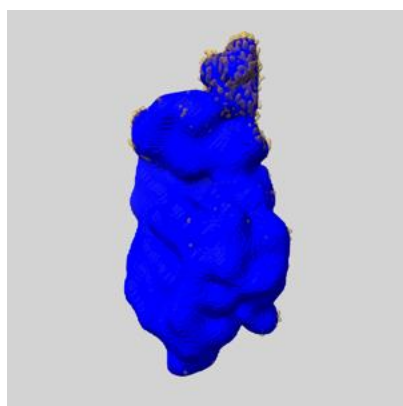
6.6 Mask visualisation [i](#)

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

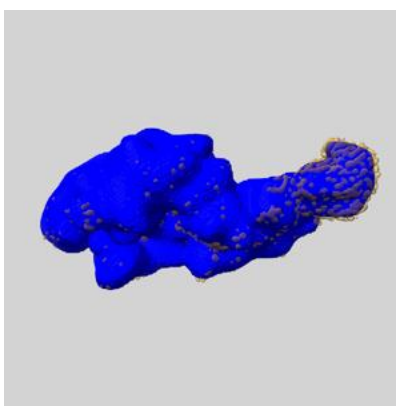
A mask typically either:

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

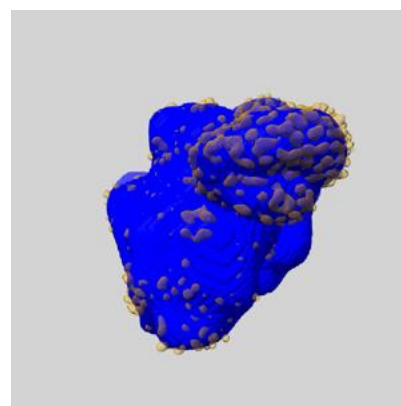
6.6.1 emd_44348_msk_1.map [i](#)



X



Y

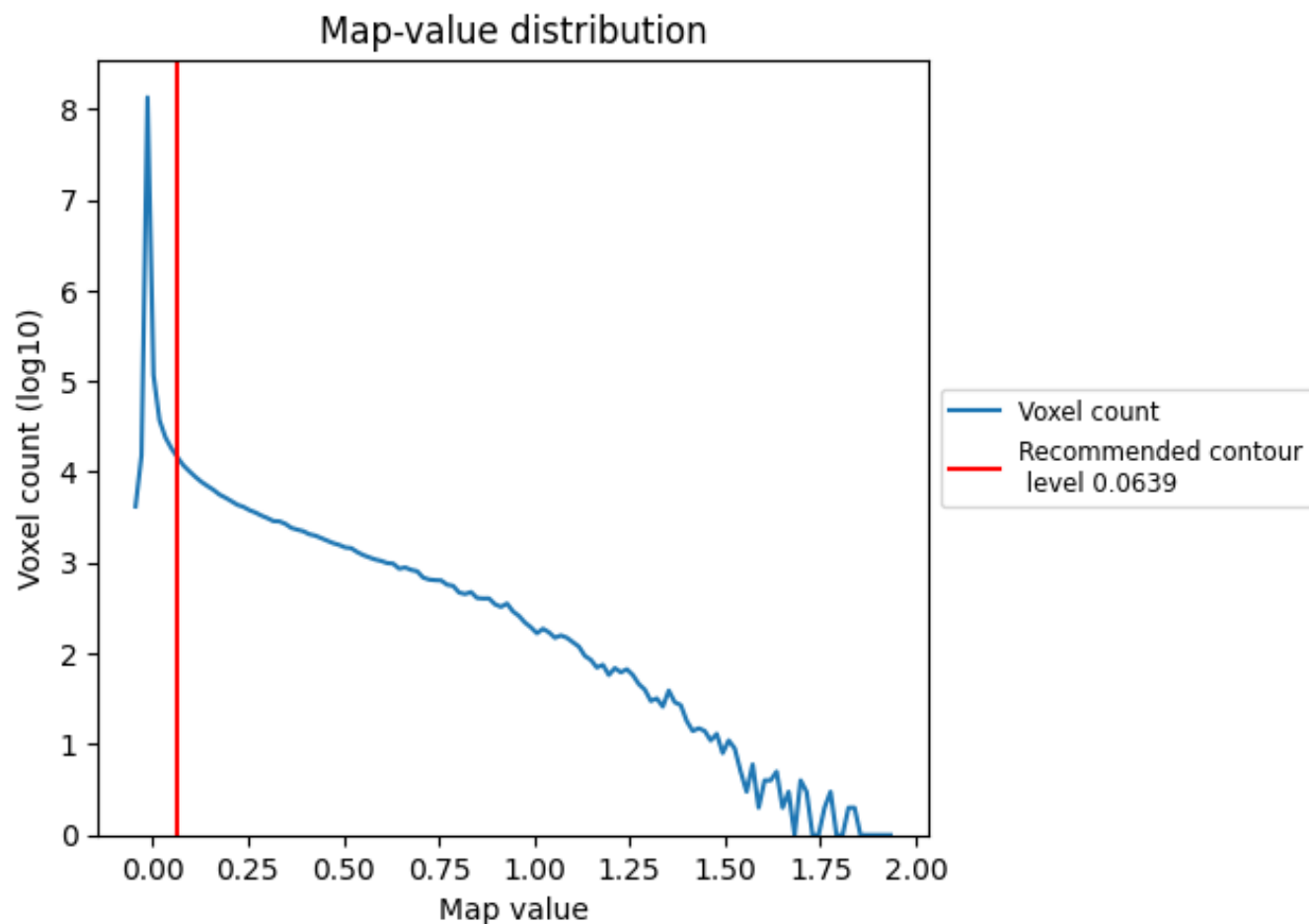


Z

7 Map analysis [i](#)

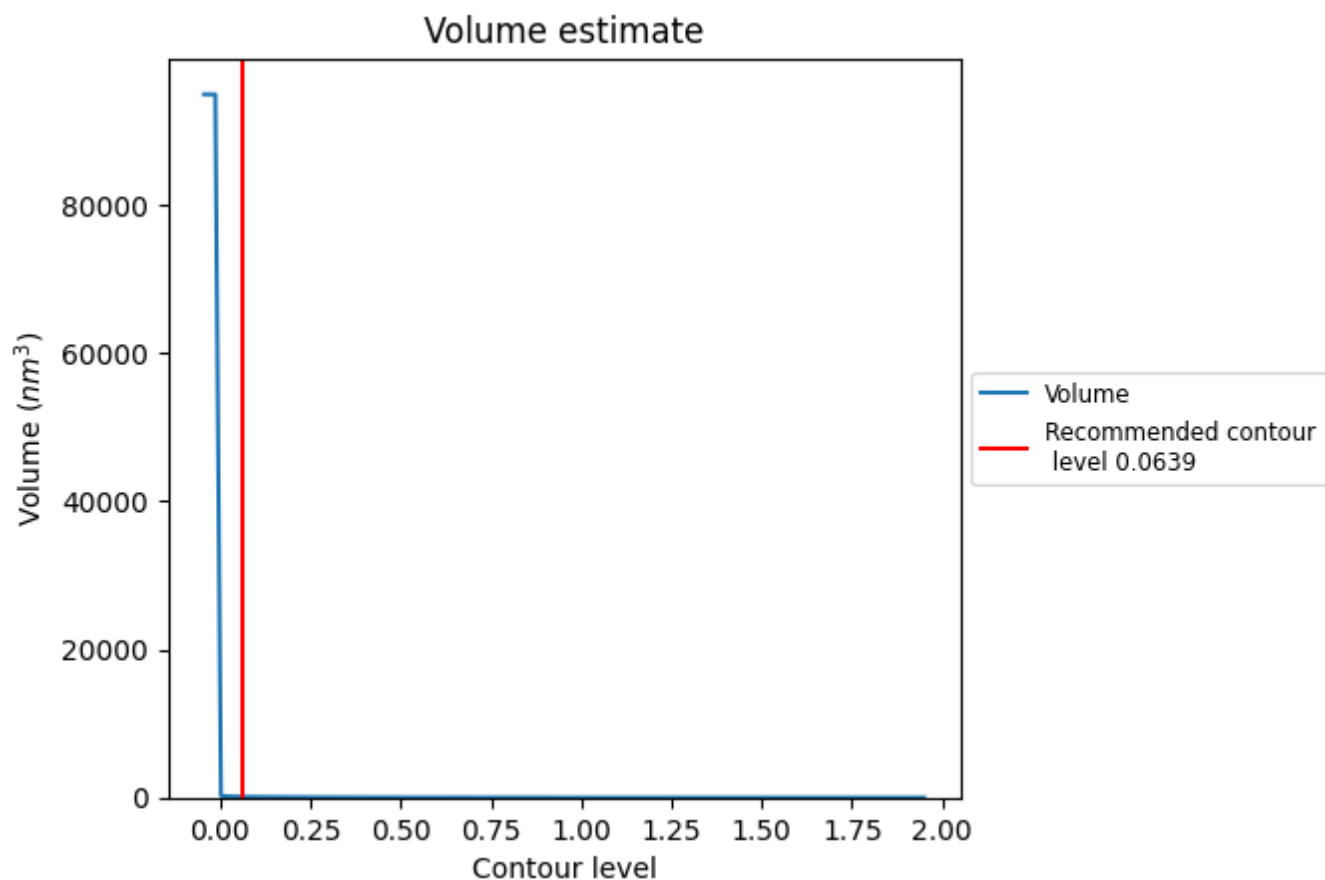
This section contains the results of statistical analysis of the map.

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.

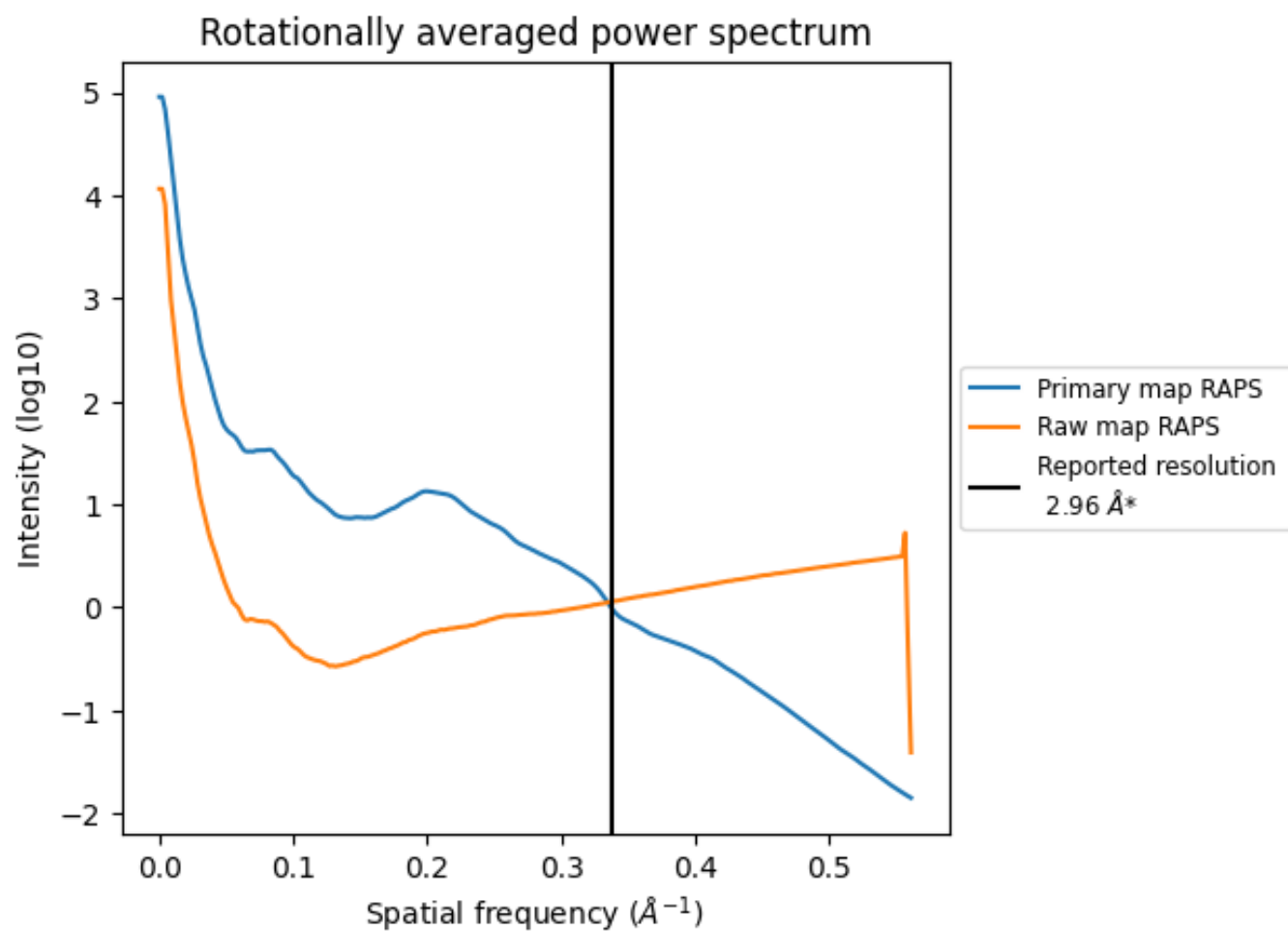
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm^3 ; this corresponds to an approximate mass of 100 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

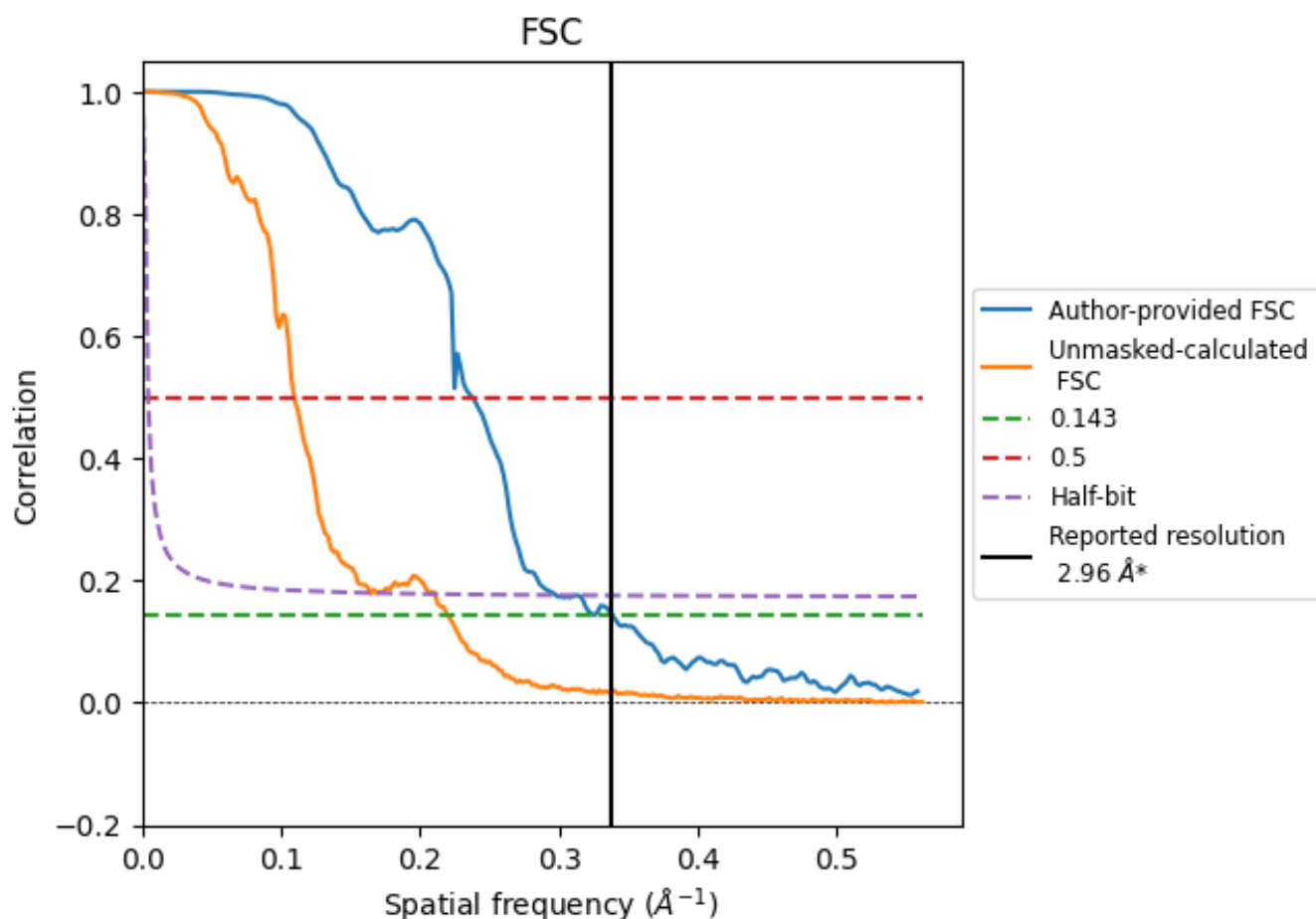


*Reported resolution corresponds to spatial frequency of 0.338 $\text{\AA}^{-1}$

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 $0.338 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

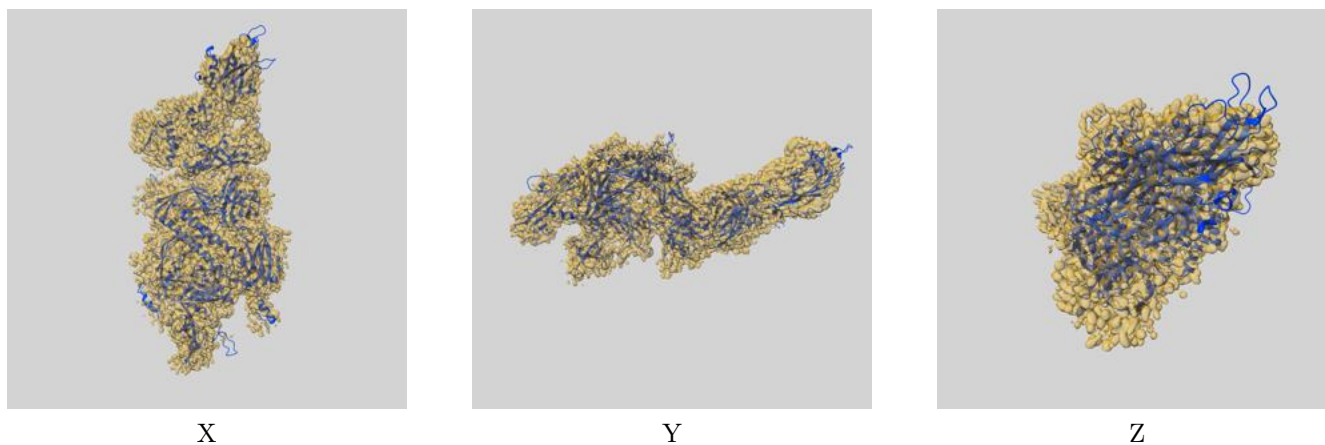
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	4.21	3.36
Unmasked-calculated*	4.55	9.15	6.09

*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 4.55 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

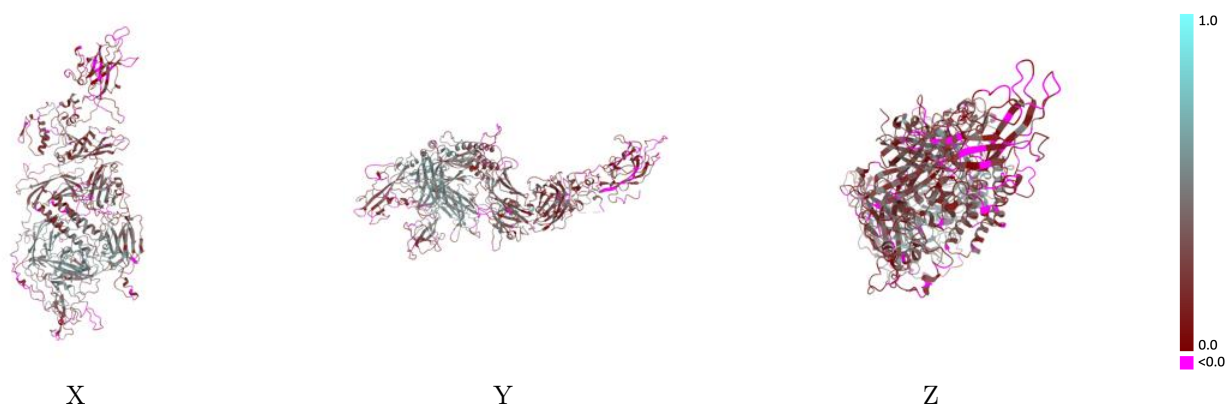
This section contains information regarding the fit between EMDB map EMD-44348 and PDB model 9B8K. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



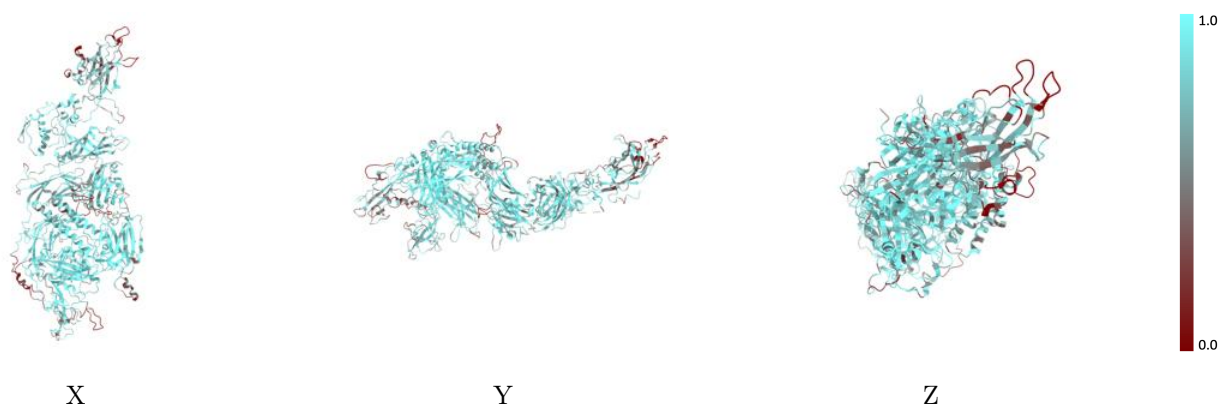
The images above show the 3D surface view of the map at the recommended contour level 0.0639 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



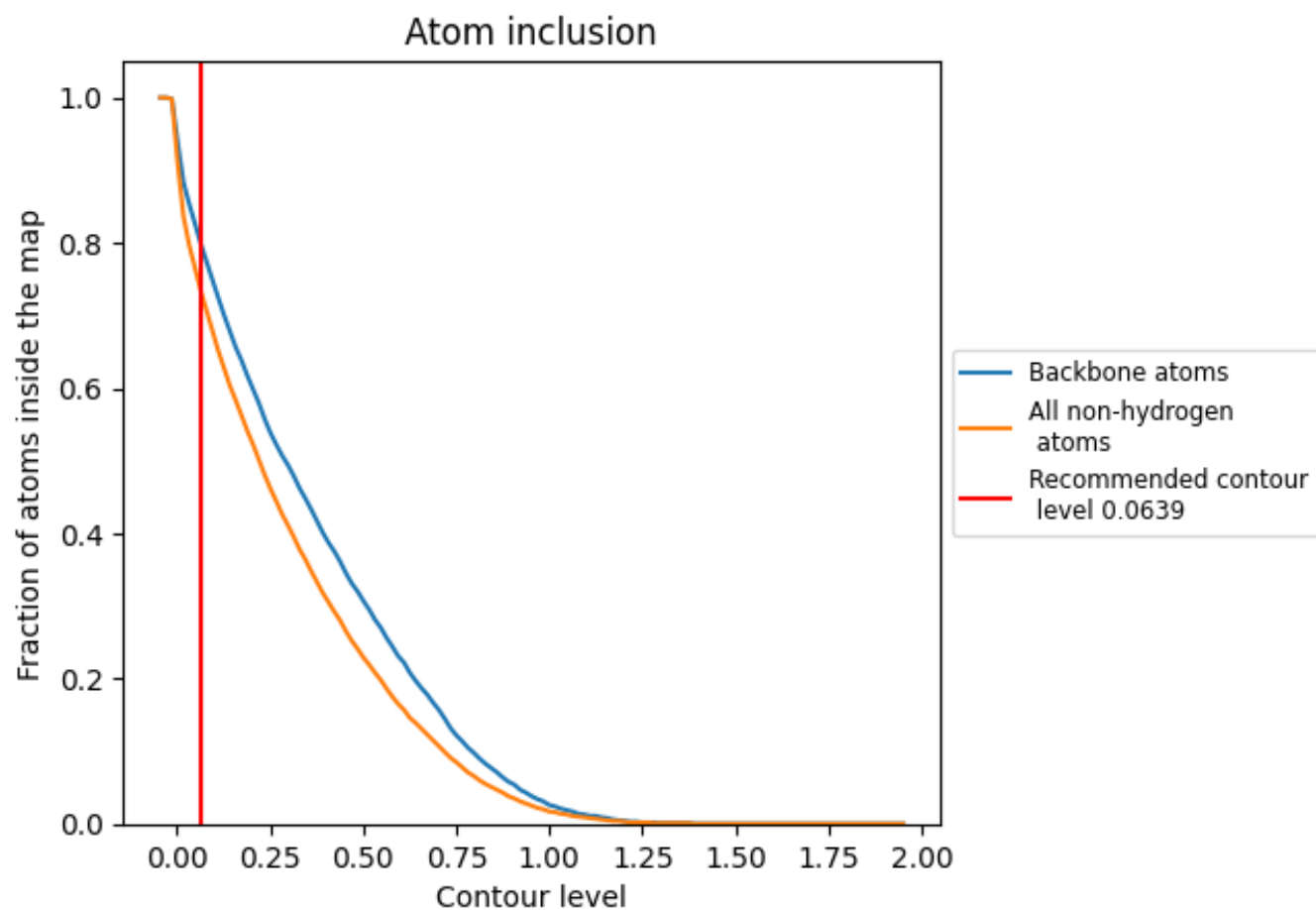
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0639).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 73% 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 (0.0639) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7340	0.3070
A	0.7340	0.3070

