



Full wwPDB EM Validation Report ⓘ

Dec 29, 2024 – 08:42 AM EST

PDB ID : 7MP6
EMDB ID : EMD-23930
Title : Neurofibromin homodimer
Authors : Lupton, C.J.; Bayly-Jones, C.; Ellisdon, A.M.
Deposited on : 2021-05-04
Resolution : 6.25 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

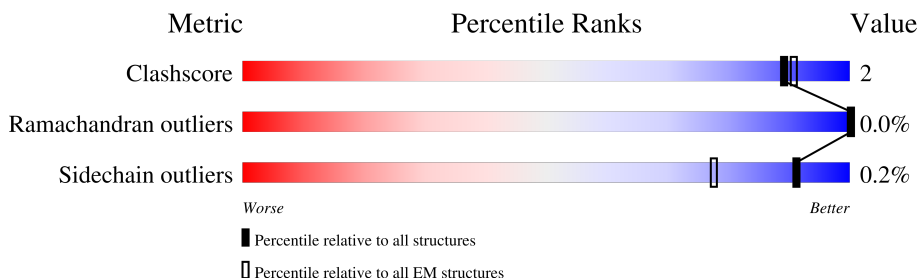
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.25 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	2826	
1	B	2826	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25464 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 Isoform I of Neurofibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1600	Total	C	N	O	S	0	0
			12704	8190	2127	2296	91		
1	B	1609	Total	C	N	O	S	0	0
			12760	8223	2136	2310	91		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P21359
A	-6	ASP	-	expression tag	UNP P21359
A	-5	TYR	-	expression tag	UNP P21359
A	-4	LYS	-	expression tag	UNP P21359
A	-3	ASP	-	expression tag	UNP P21359
A	-2	ASP	-	expression tag	UNP P21359
A	-1	ASP	-	expression tag	UNP P21359
A	0	ASP	-	expression tag	UNP P21359
A	1	LYS	-	expression tag	UNP P21359
B	-7	MET	-	initiating methionine	UNP P21359
B	-6	ASP	-	expression tag	UNP P21359
B	-5	TYR	-	expression tag	UNP P21359
B	-4	LYS	-	expression tag	UNP P21359
B	-3	ASP	-	expression tag	UNP P21359
B	-2	ASP	-	expression tag	UNP P21359
B	-1	ASP	-	expression tag	UNP P21359
B	0	ASP	-	expression tag	UNP P21359
B	1	LYS	-	expression tag	UNP P21359

- Molecule 1: Isoform I of Neurofibromin

Chain B:



GLY	ASP	THR	LYS	ASP	ASP	ASP	ALA	ALA	HIS	R5		W9		R16		K24	THR	GLY	GLN	GLN	ASN	T30		Y49		N67	MET	ARG	ILE	PHE	GLY	GLU	VAL	ALA	ASP	GLU	K77		P98	LYS	ASP	THR	MET	ARG	LEU	ASP	E106	T107	M108		Q112		L121	HIS	THR	CYS	TRP	GLU	V373
Q129		C147		R156		V166	CYS	SER	GLU	ASP	ASP	V172		K195		F199		L213		Q236	ILE	PRO	T240		R262		V266		K266	ASP	VAL	VAL	ASP	GLU	N292		R304		I334	ASN	TRP	CLU	ASP	ASN	S340		S365		ARG	GLY	SER	GLY	GLN	PRO	ASP				



LYS	TRP	GLY	Y2259
ILE	SER	PRO	
VAL	PRO	ASP	
	LYS	THR	Y2264
	GLY	SER	
	GLU	GLY	Q2281
	TYR	GLY	P2282
	LEU	TYR	
	ALA	LEU	Y2377
	ALA	ALA	R2378
	THR	ALA	
	TYR	THR	R2390
	PRO	TYR	
	THR	PRO	R2403
	VAL	THR	
	GLY	VAL	S2430
	GLN	ARG	
	THR	CYS	
	SER	SER	
	LEU	LEU	
	PRO	LYS	
	ARG	HIS	
	ALA	ARG	
	LYS	ALA	
	SER	LYS	
	LEU	SER	
	THR	LEU	
	LEU	THR	
	ASP	LEU	
	ASP	ASP	
	GLY	MET	
	GLN	MET	
	PRO	GLU	
	ASN	PRO	
	VAL	ASN	
	PRO	VAL	
	ALA	PRO	
	MET	ALA	
	THR	ASN	
	ASP	THR	
	HIS	LYS	
	LEU	LYS	
	THR	THR	
	VAL	TYR	
	SER	PRO	
	VAL	LEU	
	SER	ILE	
	THR	GLY	
	ALA	HIS	
	ASN	ARG	
	GLN	GLY	
	LEU	ARG	
	THR	LEU	
	ALA	THR	
	ASN	ASP	
	ILE	ILE	
	THR	VAL	
	ALA	GLU	
	ASN	LEU	
	ILE	THR	
	LYS	THR	
	ASN	LEU	
	SER	LEU	
	ILE	THR	
	LYS	ALA	
	ASN	THR	
	LYS	LEU	
	LYS	THR	D2591

ASN	PRO	LYS	GLY	Y2606
LEU	LYS	ARG	GLY	
SER	ARG	GLN	SER	S2626
ASN	GLU	GLU	GLY	
SER	MET	GLU	ILE	F2633
THR	THR	SER	THR	
SER	GLU	GLY	GLY	Y2669
LEU	ILE	GLY	ILE	H2670
ALA	GLU	GLY	GLY	E2671
THR	SER	THR	THR	
SER	PRO	THR	THR	
GLN	PRO	THR	THR	P2675
HIS	PRO	THR	THR	
SER	LYS	THR	THR	
PRO	LYS	THR	THR	G2689
GLY	MET	THR	THR	
ILE	ARG	THR	THR	R2692
ASP	ARG	THR	THR	F2693
LYS	VAL	THR	THR	
GLU	ALA	THR	THR	F2697
ASN	GLU	THR	THR	
VAL	LYS	THR	THR	
GLU	THR	THR	THR	
VAL	GLN	THR	THR	
THR	THR	THR	THR	
SER	THR	THR	THR	
LEU	THR	THR	THR	
GLN	THR	THR	THR	
ALA	THR	THR	THR	
SER	THR	THR	THR	
GLY	THR	THR	THR	
THR	THR	THR	THR	
ARG	THR	THR	THR	
HIS	THR	THR	THR	
LEU	THR	THR	THR	
THR	THR	THR	THR	
ASN	THR	THR	THR	
GLY	THR	THR	THR	
THR	THR	THR	THR	
ILE	THR	THR	THR	
LYS	THR	THR	THR	
LYS	THR	THR	THR	

LYS
ILE
VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	95564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.365	Depositor
Minimum map value	-0.873	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	515.808, 515.808, 515.808	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.388, 2.388, 2.388	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	0.61	0/12925	0.98	39/17476 (0.2%)
1	B	0.61	1/12983 (0.0%)	0.98	42/17558 (0.2%)
All	All	0.61	1/25908 (0.0%)	0.98	81/35034 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1897	ASN	C-N	8.97	1.54	1.34

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	2669	TYR	CB-CG-CD2	-7.55	116.47	121.00
1	B	304	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	B	2669	TYR	CB-CG-CD2	-7.53	116.48	121.00
1	B	156	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	914	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	156	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	B	914	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	2129	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	2390	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	2129	ARG	NE-CZ-NH1	6.97	123.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2377	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	A	2377	TYR	CB-CG-CD2	-6.88	116.88	121.00
1	A	2390	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	2032	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	2032	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	1949	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	440	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	B	1949	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	1025	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	440	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	B	2606	VAL	CA-CB-CG2	6.64	120.87	110.90
1	A	2606	VAL	CA-CB-CG2	6.63	120.84	110.90
1	A	1025	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	1000	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	1968	TYR	CB-CG-CD1	-6.43	117.14	121.00
1	B	1000	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	930	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	930	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	A	765	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	765	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	416	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	1026	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	897	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	1026	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	897	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	1849	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	433	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	B	1849	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	897	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	5	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	433	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	B	5	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	B	897	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	B	416	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	1853	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	A	1853	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	A	2403	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	1066	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	2214	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	2214	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	1066	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	2237	ARG	NE-CZ-NH1	5.53	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2098	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	1038	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	2237	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	1038	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	2403	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	2378	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	734	ASN	CB-CA-C	5.47	121.34	110.40
1	A	734	ASN	CB-CA-C	5.45	121.30	110.40
1	A	2098	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	2063	TYR	CB-CG-CD2	-5.34	117.79	121.00
1	A	2378	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	720	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	711	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	711	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	2063	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	720	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	601	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	16	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	B	1176	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	1176	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	601	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	692	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	B	262	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	692	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	A	2669	TYR	CB-CG-CD1	5.09	124.06	121.00
1	A	16	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	B	2669	TYR	CB-CG-CD1	5.08	124.05	121.00
1	B	764	ARG	NE-CZ-NH2	5.02	122.81	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	CYS	Mainchain
1	A	1853	TYR	Sidechain
1	A	2693	PHE	Sidechain
1	A	49	TYR	Sidechain
1	B	147	CYS	Mainchain
1	B	1853	TYR	Sidechain
1	B	2693	PHE	Sidechain
1	B	49	TYR	Sidechain

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	12704	0	13032	48	0
1	B	12760	0	13087	50	0
All	All	25464	0	26119	89	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 (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1916:SER:CB	1:B:1920:LEU:HD23	1.67	1.24
1:B:1865:LEU:HA	1:B:1898:GLU:OE1	1.46	1.15
1:B:1916:SER:HB3	1:B:1920:LEU:HD23	1.14	1.09
1:A:1987:ASP:OD1	1:A:2032:ARG:NH2	1.94	0.99
1:A:1987:ASP:OD1	1:A:2032:ARG:CZ	2.18	0.92
1:A:1987:ASP:OD1	1:A:2032:ARG:NH1	2.05	0.90
1:A:2019:SER:O	1:A:2020:GLY:O	1.90	0.88
1:B:1916:SER:HB3	1:B:1920:LEU:CD2	2.01	0.87
1:A:2015:VAL:HG11	1:B:1882:ASN:O	1.76	0.86
1:B:1920:LEU:HD12	1:B:1923:LEU:HD23	1.55	0.85
1:B:1916:SER:OG	1:B:1920:LEU:HD23	1.76	0.84
1:B:1839:LEU:HD11	1:B:1920:LEU:HD11	1.61	0.83
1:B:1891:SER:HG	1:B:1931:TRP:HE1	1.26	0.81
1:B:1916:SER:CB	1:B:1920:LEU:CD2	2.58	0.80
1:B:1839:LEU:HD13	1:B:1927:TYR:OH	1.86	0.76
1:B:2087:THR:HG23	1:B:2230:VAL:HG21	1.71	0.73
1:B:1916:SER:OG	1:B:1920:LEU:CD2	2.38	0.72
1:A:2015:VAL:HB	1:B:1882:ASN:ND2	2.04	0.72
1:A:2087:THR:HG23	1:A:2230:VAL:HG21	1.71	0.72
1:B:1889:SER:HA	1:B:1892:LYS:HE2	1.76	0.68
1:A:1889:SER:HA	1:A:1892:LYS:HE2	1.76	0.68
1:A:1179:PHE:CZ	1:A:1183:LEU:HD11	2.29	0.67
1:B:1179:PHE:CZ	1:B:1183:LEU:HD11	2.29	0.66
1:B:1834:LEU:HD22	1:B:1901:LEU:HD13	1.78	0.65
1:A:1892:LYS:HB3	1:A:1930:PRO:HG2	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1839:LEU:CD1	1:B:1920:LEU:HD11	2.29	0.63
1:A:2015:VAL:HB	1:B:1882:ASN:HD22	1.61	0.63
1:A:2071:ASN:HA	1:A:2074:ASP:HB3	1.81	0.62
1:B:1165:ILE:HD11	1:B:1832:THR:HG21	1.80	0.62
1:A:1165:ILE:HD11	1:A:1832:THR:HG21	1.80	0.62
1:B:2071:ASN:HA	1:B:2074:ASP:HB3	1.81	0.62
1:A:195:LYS:HG2	1:A:199:PHE:CE2	2.35	0.61
1:B:195:LYS:HG2	1:B:199:PHE:CE2	2.35	0.61
1:A:1892:LYS:HB3	1:A:1930:PRO:CG	2.30	0.60
1:B:1834:LEU:CD2	1:B:1901:LEU:HD13	2.32	0.60
1:A:1872:LEU:HD22	1:B:2113:CYS:HB2	1.85	0.58
1:A:2113:CYS:HB2	1:B:1872:LEU:HD22	1.85	0.58
1:A:1987:ASP:CG	1:A:2032:ARG:HH22	2.09	0.56
1:B:108:MET:HG2	1:B:112:GLN:NE2	2.21	0.56
1:A:108:MET:HG2	1:A:112:GLN:NE2	2.21	0.55
1:B:2087:THR:CG2	1:B:2230:VAL:HG21	2.39	0.52
1:B:1153:LEU:HD21	1:B:1164:SER:HB3	1.92	0.52
1:A:1153:LEU:HD21	1:A:1164:SER:HB3	1.92	0.51
1:A:2018:ALA:HB2	1:A:2067:LEU:HD21	1.92	0.51
1:B:1183:LEU:HD13	1:B:1833:LEU:HD22	1.92	0.51
1:A:2018:ALA:HB2	1:A:2067:LEU:CD2	2.42	0.50
1:A:1183:LEU:HD13	1:A:1833:LEU:HD22	1.92	0.50
1:B:1891:SER:OG	1:B:1931:TRP:NE1	2.23	0.50
1:A:2087:THR:CG2	1:A:2230:VAL:HG21	2.39	0.48
1:B:1165:ILE:CD1	1:B:1832:THR:HG21	2.43	0.48
1:A:1165:ILE:CD1	1:A:1832:THR:HG21	2.43	0.48
1:A:2071:ASN:HA	1:A:2074:ASP:CB	2.44	0.47
1:B:2071:ASN:HA	1:B:2074:ASP:CB	2.44	0.47
1:A:1878:CYS:SG	1:B:2153:ALA:HB2	2.56	0.46
1:A:2153:ALA:HB2	1:B:1878:CYS:SG	2.56	0.46
1:A:1846:PRO:CG	1:B:2157:PHE:HB2	2.46	0.45
1:B:894:PHE:CE2	1:B:898:LEU:HD11	2.51	0.45
1:A:894:PHE:CE2	1:A:898:LEU:HD11	2.51	0.45
1:A:2157:PHE:HB2	1:B:1846:PRO:CG	2.46	0.45
1:A:1162:MET:HA	1:A:1165:ILE:HD12	1.99	0.45
1:B:1162:MET:HA	1:B:1165:ILE:HD12	1.99	0.45
1:B:1833:LEU:HA	1:B:1836:ILE:HG12	1.99	0.44
1:A:1833:LEU:HA	1:A:1836:ILE:HG12	1.99	0.44
1:B:213:ILE:HD13	1:B:266:VAL:HG12	2.00	0.44
1:A:213:ILE:HD13	1:A:266:VAL:HG12	1.99	0.44
1:A:1929:THR:HB	1:A:1930:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:851:CYS:HB2	1:B:891:VAL:HG21	2.00	0.43
1:B:2626:SER:HA	1:B:2633:PHE:CD1	2.53	0.43
1:A:2015:VAL:HG22	1:A:2066:MET:HB3	1.99	0.43
1:A:851:CYS:HB2	1:A:891:VAL:HG21	2.01	0.43
1:A:2626:SER:HA	1:A:2633:PHE:CD1	2.53	0.43
1:B:2079:LEU:HD23	1:B:2204:TRP:CE3	2.54	0.42
1:B:1976:TRP:CZ3	1:B:1979:LEU:HD13	2.54	0.42
1:A:2689:GLY:O	1:A:2692:ARG:HB3	2.20	0.42
1:B:2689:GLY:O	1:B:2692:ARG:HB3	2.20	0.42
1:A:2079:LEU:HD23	1:A:2204:TRP:CE3	2.54	0.42
1:A:1172:ASP:CG	1:A:1175:THR:HG23	2.40	0.42
1:B:1179:PHE:CE2	1:B:1183:LEU:HD11	2.55	0.42
1:B:1924:CYS:HA	1:B:1927:TYR:CE2	2.55	0.42
1:B:1172:ASP:CG	1:B:1175:THR:HG23	2.40	0.41
1:B:1905:PHE:CE1	1:B:1909:CYS:SG	3.13	0.41
1:A:2019:SER:C	1:A:2020:GLY:O	2.55	0.41
1:A:1179:PHE:CE2	1:A:1183:LEU:HD11	2.55	0.41
1:B:2281:GLN:CG	1:B:2282:PRO:HD3	2.51	0.41
1:A:2281:GLN:CG	1:A:2282:PRO:HD3	2.51	0.41
1:A:1180:MET:HA	1:A:1183:LEU:HD12	2.03	0.41
1:A:2113:CYS:SG	1:A:2128:LEU:HB3	2.61	0.41
1:A:537:HIS:CD2	1:A:537:HIS:H	2.39	0.41
1:A:2213:GLN:HG3	1:A:2217:PHE:CE2	2.57	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	1532/2826 (54%)	1504 (98%)	27 (2%)	1 (0%)	48	83
1	B	1545/2826 (55%)	1518 (98%)	27 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3077/5652 (54%)	3022 (98%)	54 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2020	GLY

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	1438/2520 (57%)	1436 (100%)	2 (0%)	92	95
1	B	1444/2520 (57%)	1441 (100%)	3 (0%)	92	94
All	All	2882/5040 (57%)	2877 (100%)	5 (0%)	91	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TRP
1	A	16	ARG
1	B	9	TRP
1	B	16	ARG
1	B	1984	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	112	GLN

5.3.3 RNA ⓘ

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.

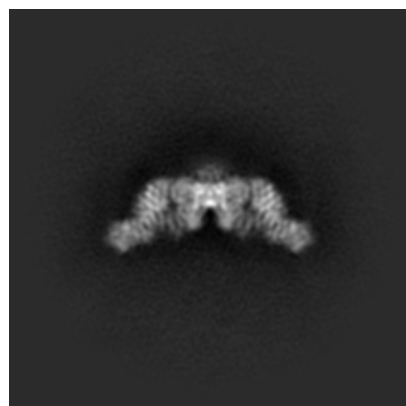
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23930. These allow visual inspection of the internal detail of the map and identification of artifacts.

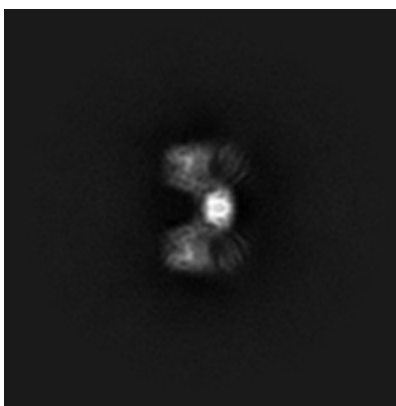
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

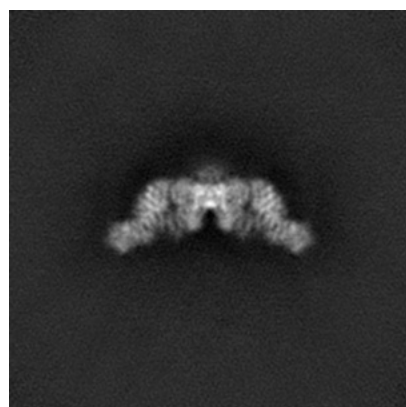


Y

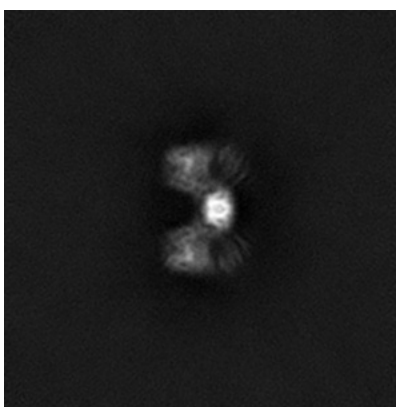


Z

6.1.2 Raw map



X



Y



Z

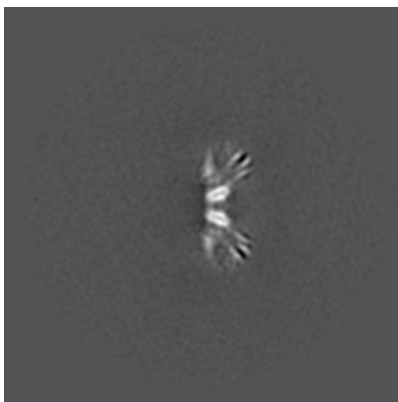
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

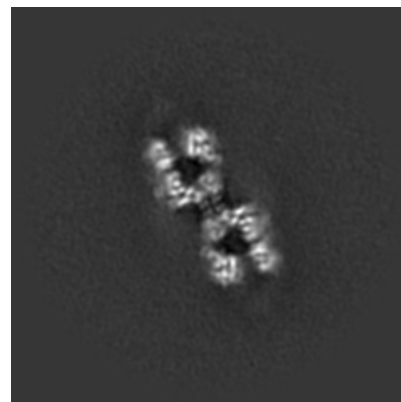
6.2.1 Primary map



X Index: 108

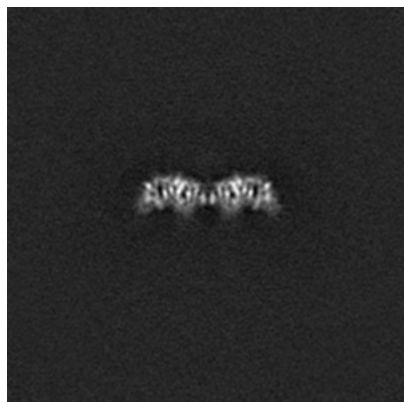


Y Index: 108

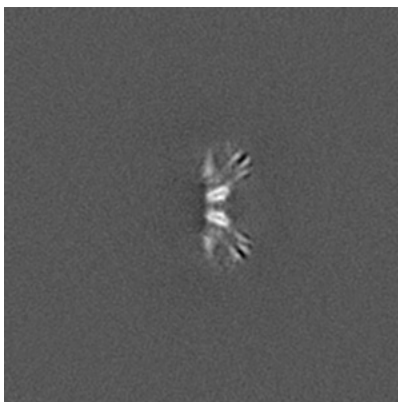


Z Index: 108

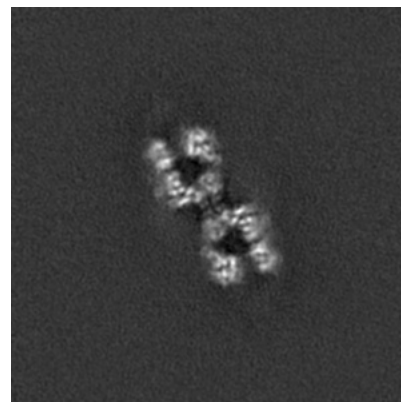
6.2.2 Raw map



X Index: 108



Y Index: 108



Z Index: 108

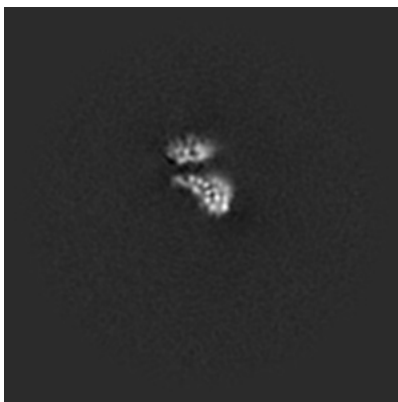
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 105



Y Index: 76



Z Index: 112

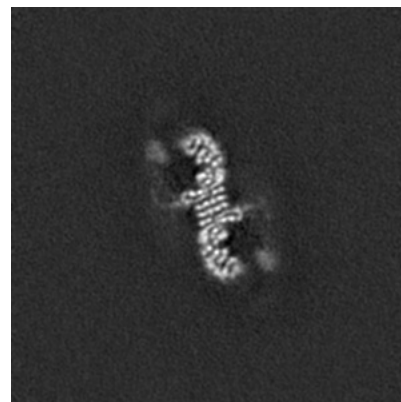
6.3.2 Raw map



X Index: 105



Y Index: 76

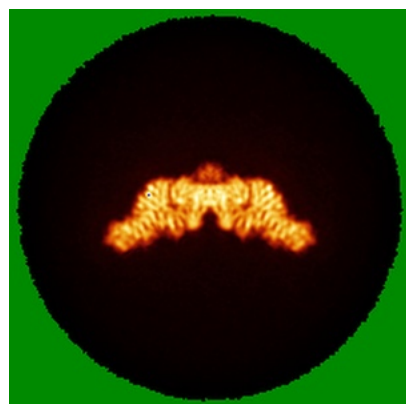


Z Index: 112

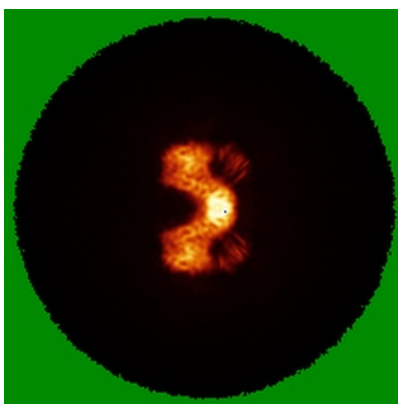
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X



Y

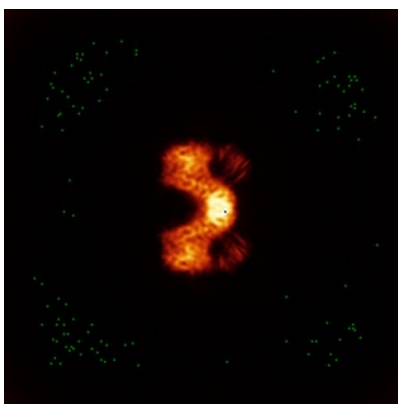


Z

6.4.2 Raw map



X



Y

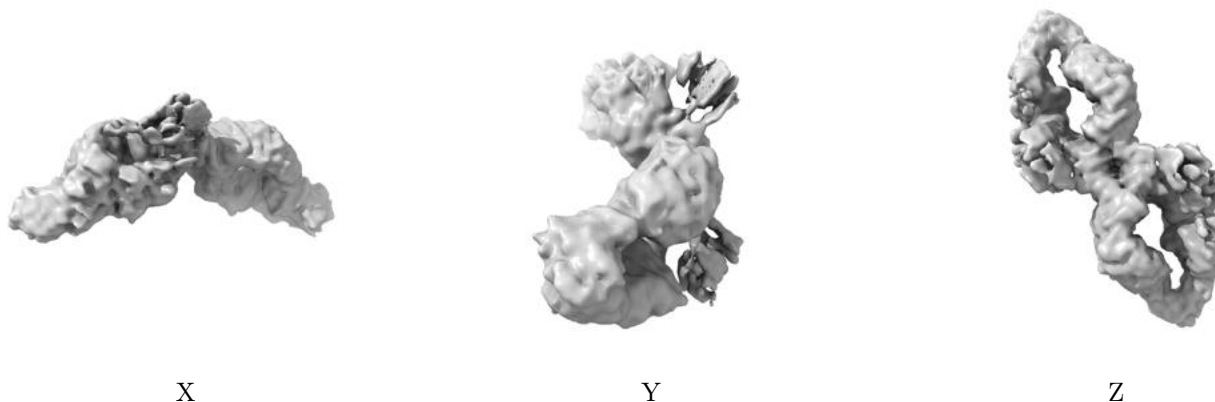


Z

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.

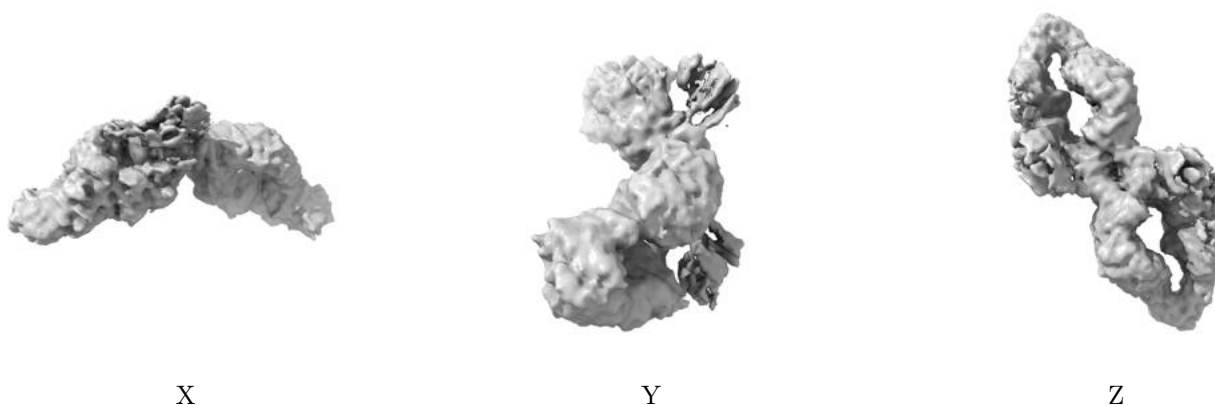
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

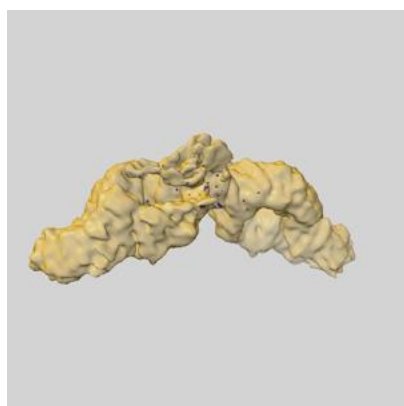
6.6 Mask visualisation [i](#)

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

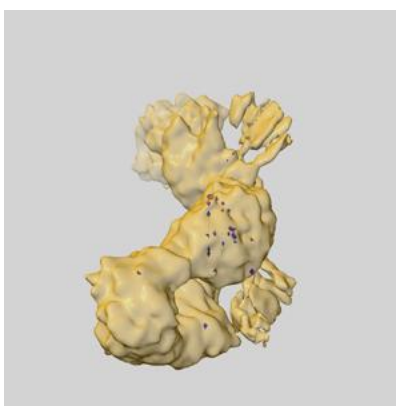
A mask typically either:

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

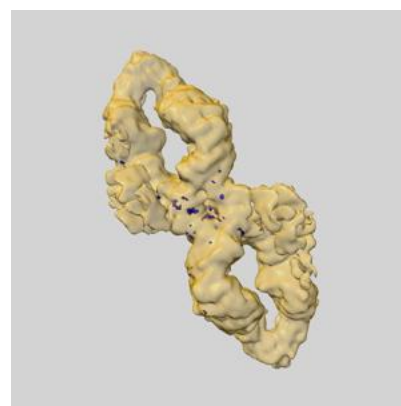
6.6.1 emd_23930_msk_1.map [i](#)



X



Y

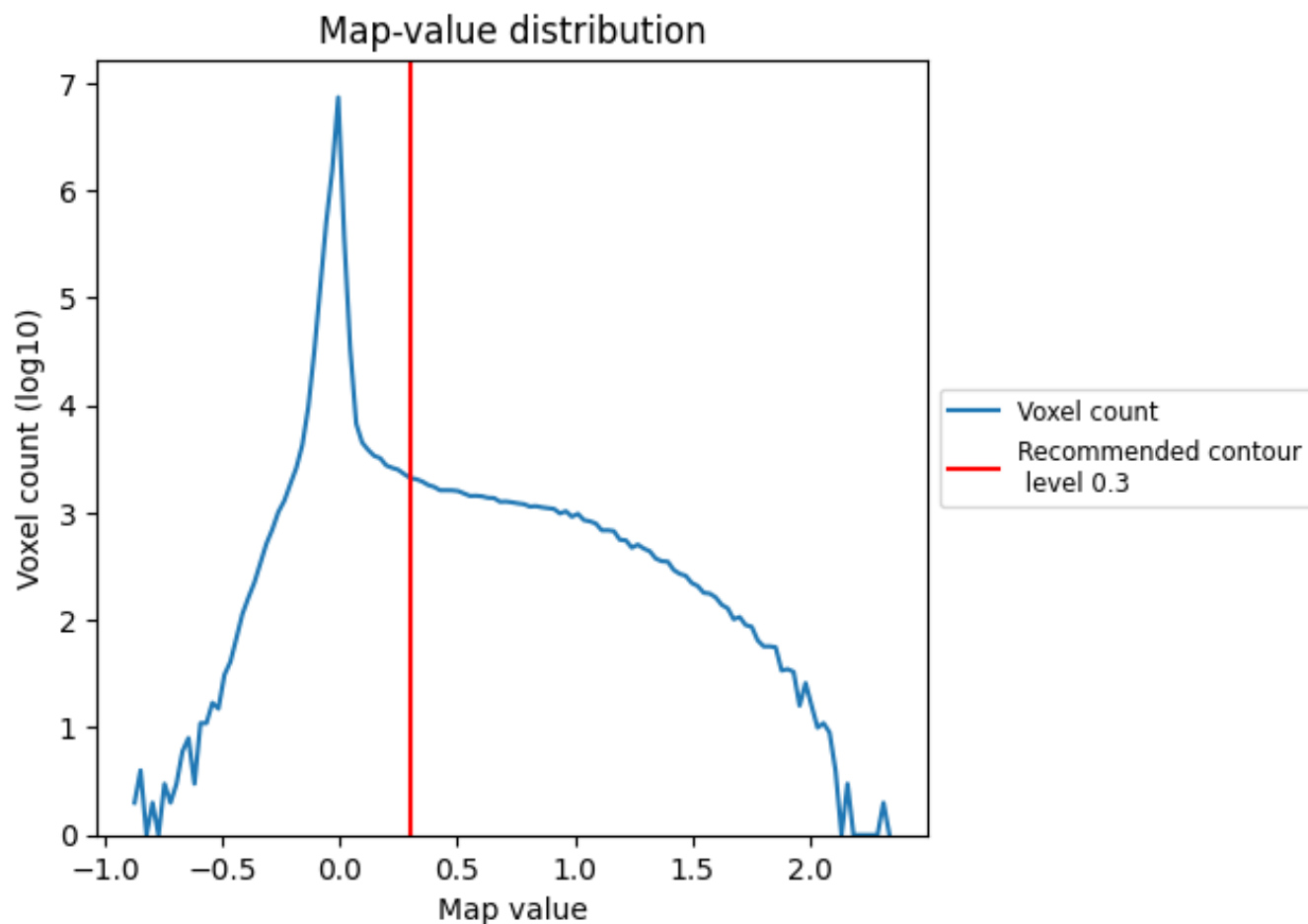


Z

7 Map analysis [i](#)

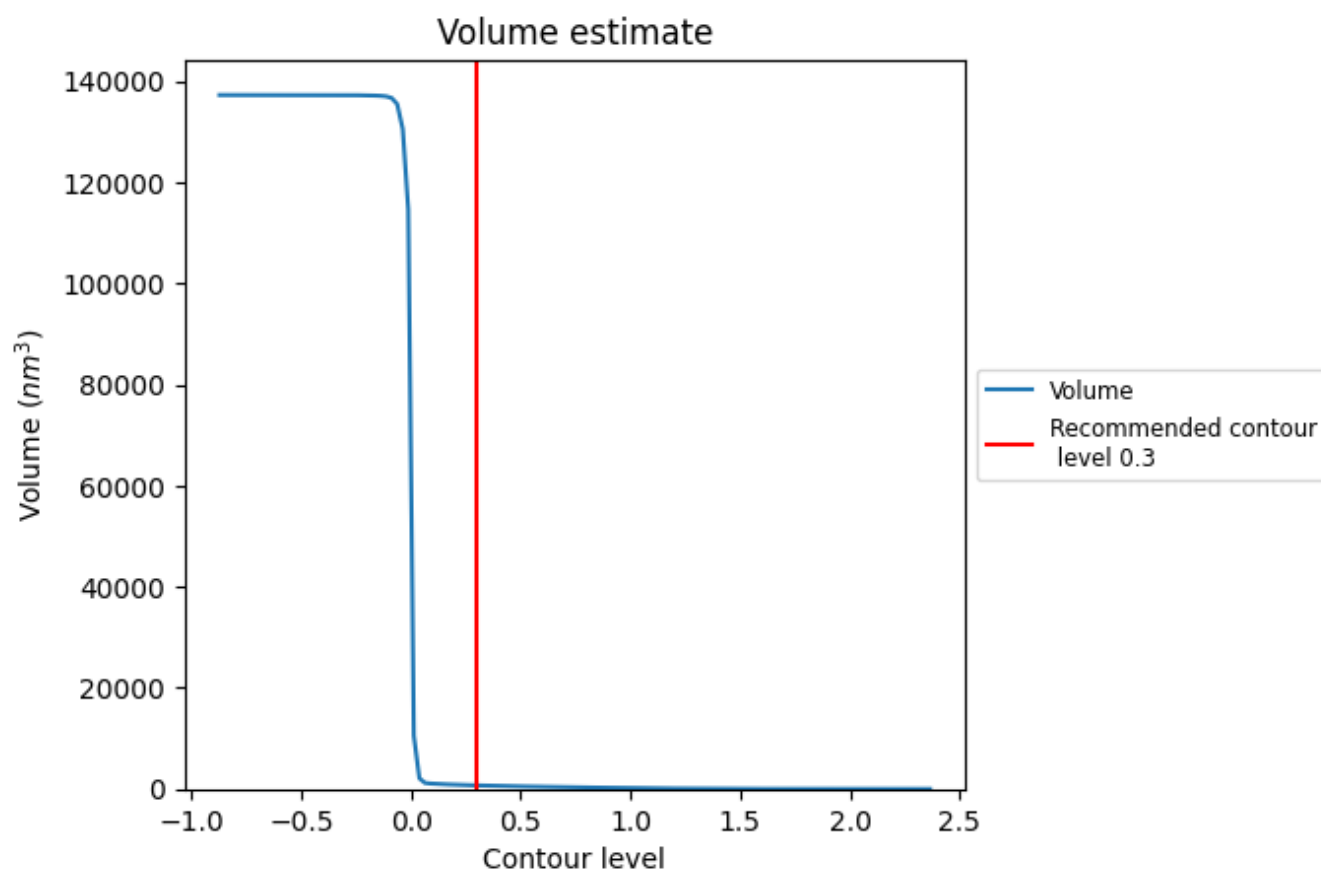
This section contains the results of statistical analysis of the map.

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.

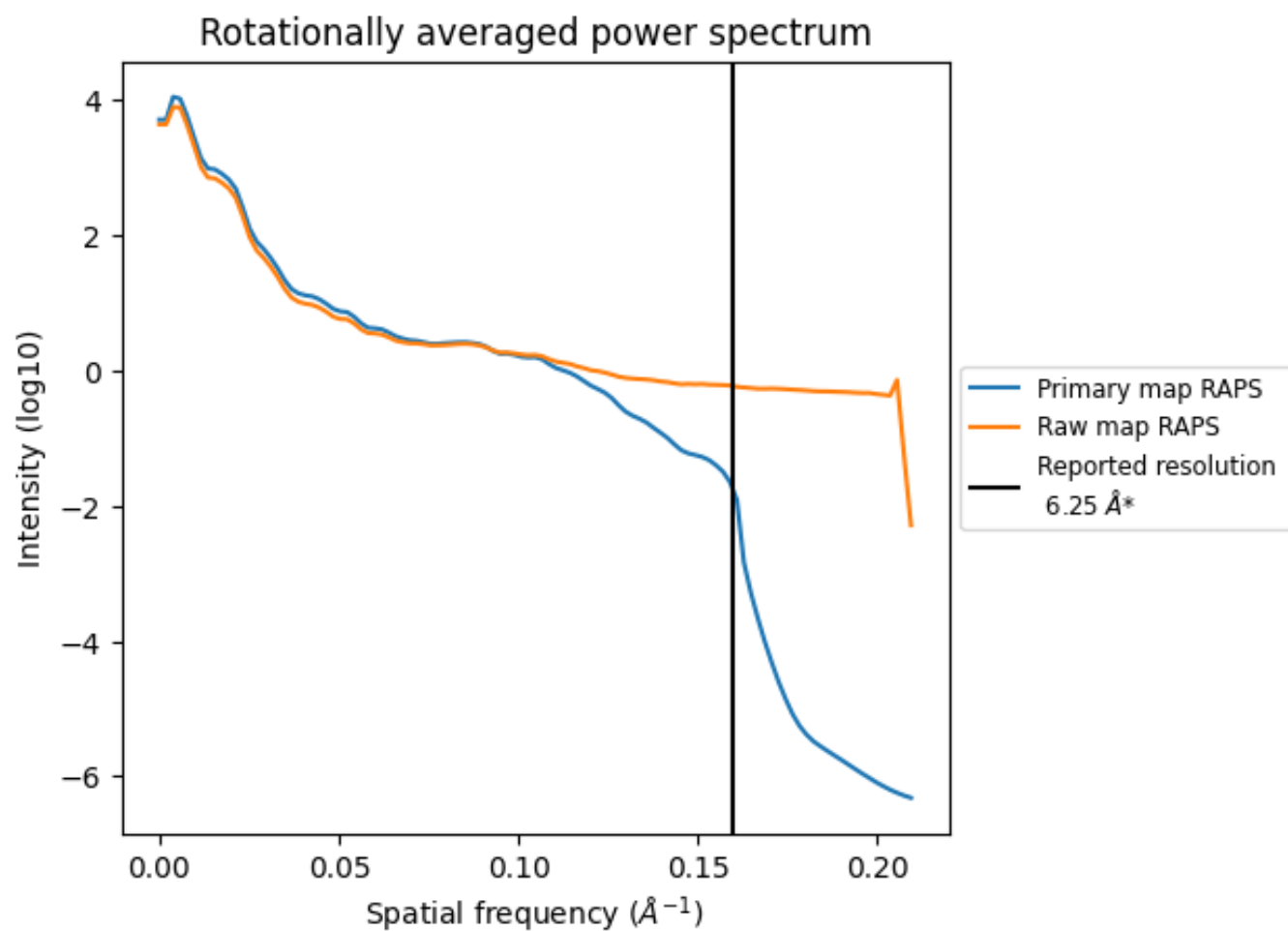
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 706 nm^3 ; this corresponds to an approximate mass of 638 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 ⓘ

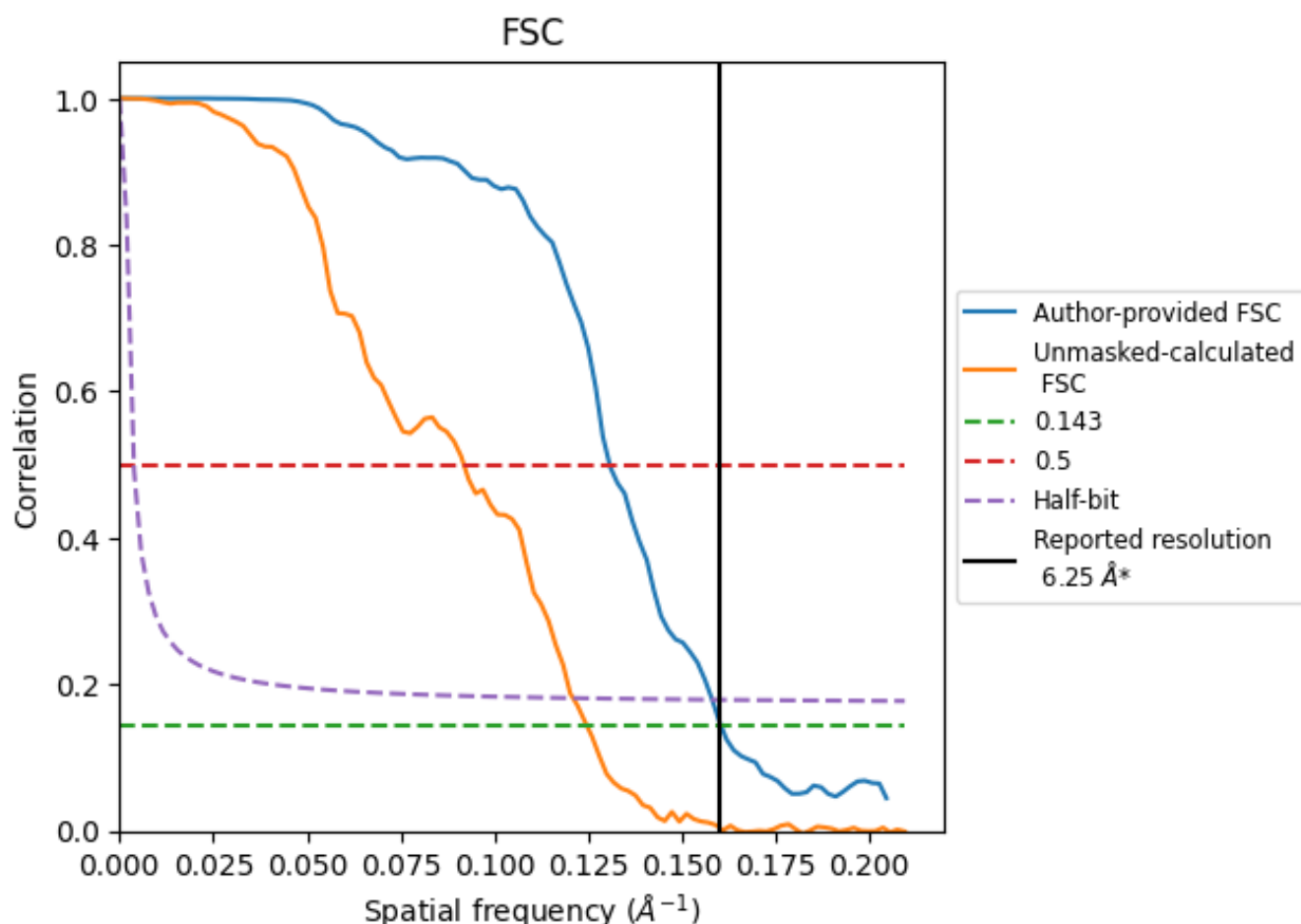


*Reported resolution corresponds to spatial frequency of 0.160 \AA^{-1}

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 0.160 \AA^{-1}

8.2 Resolution estimates [i](#)

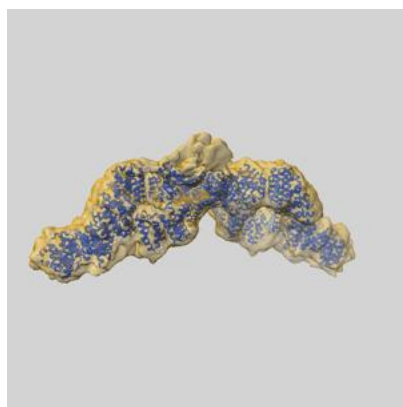
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.25	-	-
Author-provided FSC curve	6.23	7.65	6.33
Unmasked-calculated*	8.03	10.89	8.26

*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 8.03 differs from the reported value 6.25 by more than 10 %

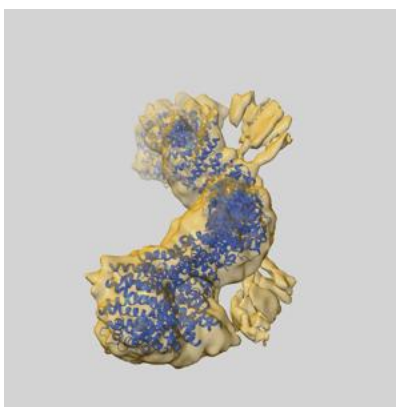
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23930 and PDB model 7MP6. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

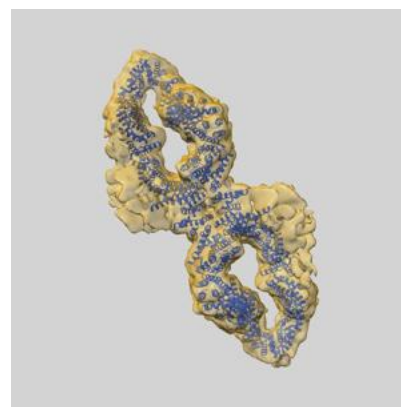
9.1 Map-model overlay [i](#)



X



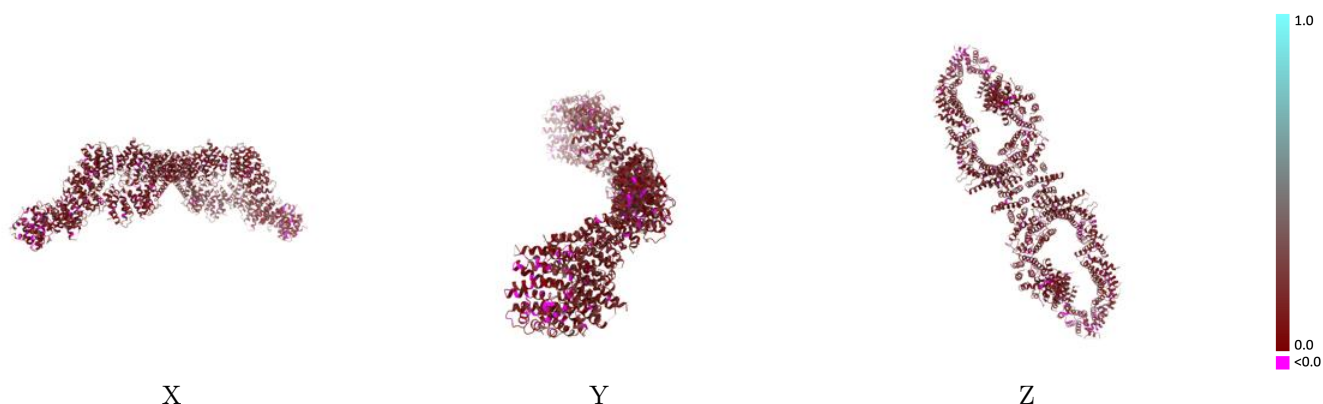
Y



Z

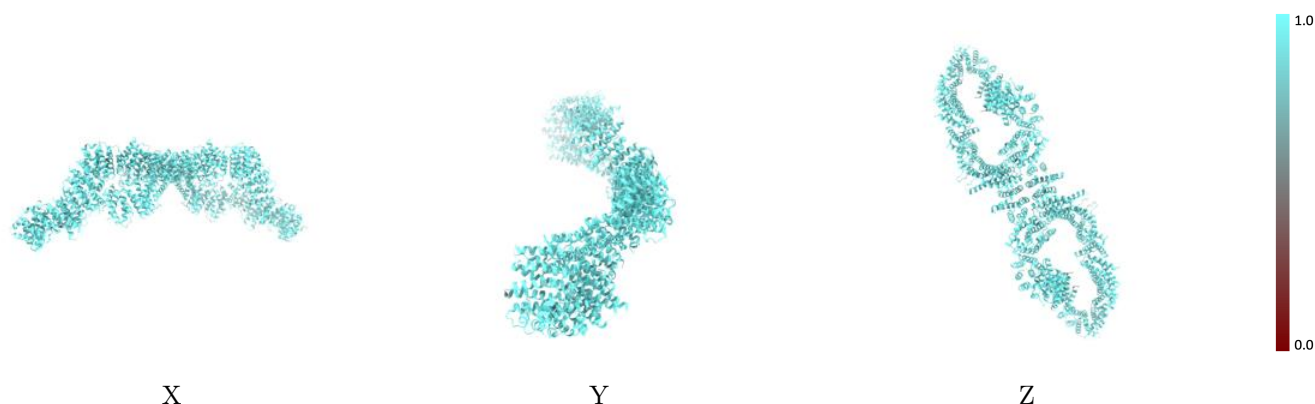
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



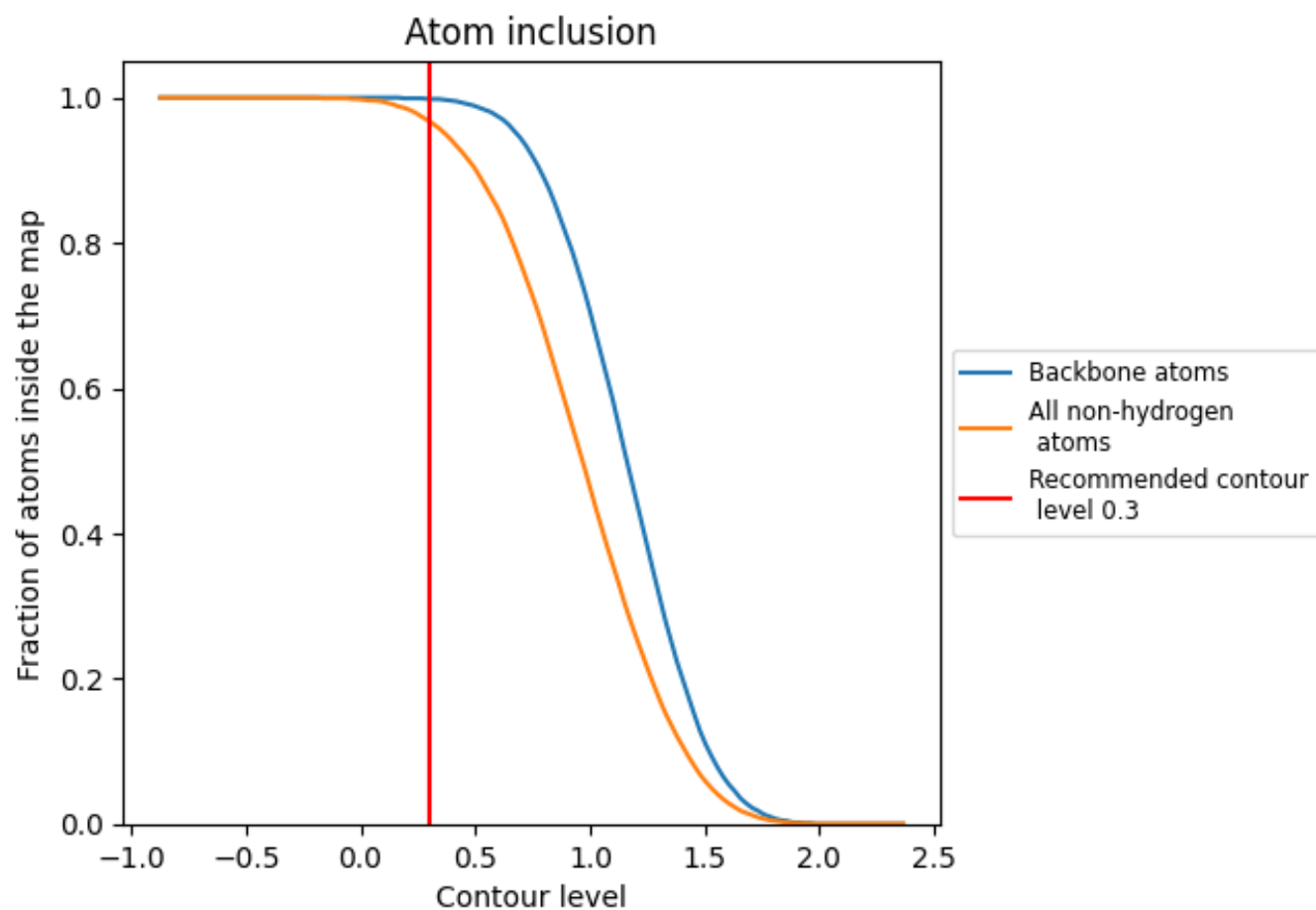
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9670	<div></div> 0.1400
A	<div></div> 0.9690	<div></div> 0.1400
B	<div></div> 0.9660	<div></div> 0.1390

