



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:50 PM UTC

PDB ID : 6BYO / pdb_00006byo
EMDB ID : EMD-9513
Title : Residue assignment correction to the voltage gated calcium Cav1.1 rabbit alpha 1 subunit PDB entries 3JBR & 5GJV
Authors : Cardozo, T.J.; Martinez-Ortiz, W.
Deposited on : 2017-12-21
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

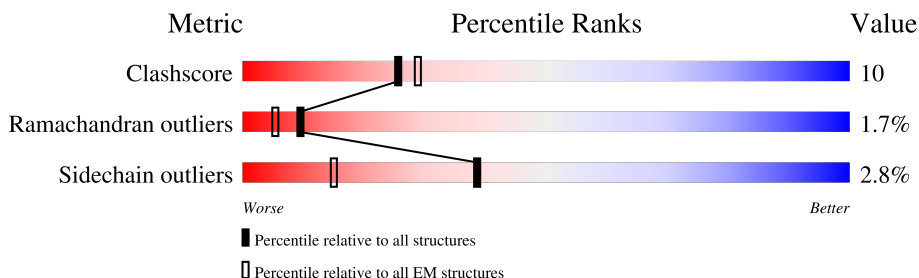
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	1357	70% 64% 17% • 17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18470 atoms, of which 9312 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.

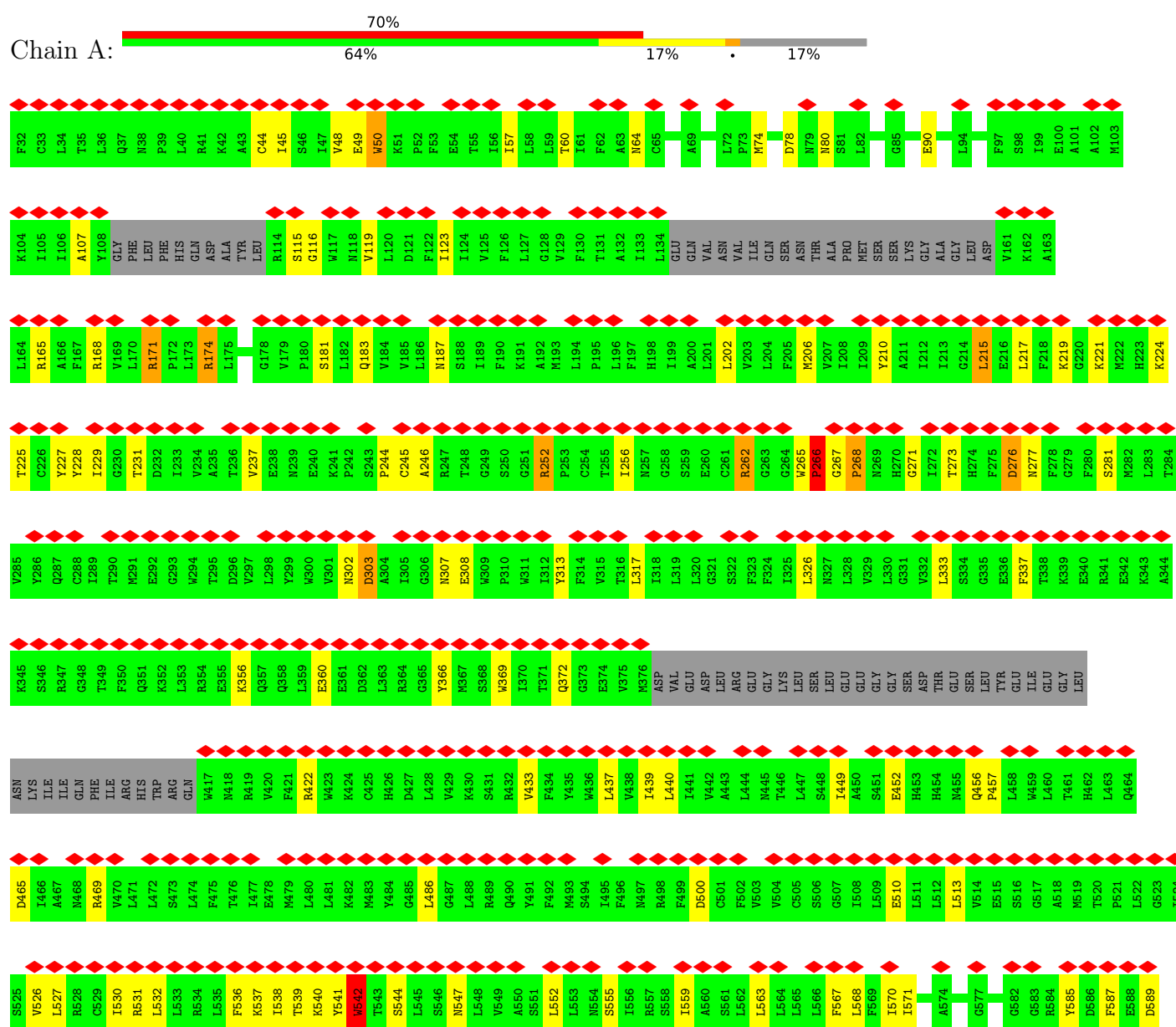
- Molecule 1 is a protein called Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1129	Total	C	H	N	O	S	0	0
			18470	6056	9312	1471	1565	66		

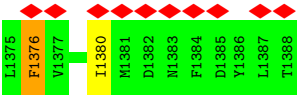
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1S







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	527833	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.294	Depositor
Minimum map value	-0.187	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.044	Depositor
Map size ($\text{\AA}$)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	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	0.62	3/9380 (0.0%)	0.91	24/12722 (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	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	ARG	C-O	24.08	1.48	1.24
1	A	540	LYS	CA-C	7.46	1.63	1.52
1	A	171	ARG	C-N	7.09	1.42	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	LYS	N-CA-C	-11.02	98.94	112.38
1	A	171	ARG	CA-C-N	-10.24	109.22	119.87
1	A	171	ARG	C-N-CA	-10.24	109.22	119.87
1	A	171	ARG	O-C-N	8.96	129.14	120.71
1	A	633	PRO	CB-CA-C	8.18	123.62	111.68
1	A	957	CYS	CB-CA-C	-8.10	95.66	109.51
1	A	1341	GLU	N-CA-C	-6.92	106.03	114.75
1	A	181	SER	CB-CA-C	6.84	124.03	110.42
1	A	281	SER	N-CA-C	-6.82	103.93	111.36
1	A	281	SER	CB-CA-C	6.66	122.18	110.85
1	A	452	GLU	N-CA-C	6.42	119.05	111.02
1	A	1174	ALA	N-CA-C	6.41	124.45	110.80
1	A	1174	ALA	CB-CA-C	-6.40	97.68	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	GLY	N-CA-C	6.39	119.67	112.00
1	A	440	LEU	CB-CA-C	5.94	121.63	110.63
1	A	976	LYS	O-C-N	5.78	130.11	122.36
1	A	1102	ILE	N-CA-C	5.74	114.58	108.95
1	A	897	ARG	CB-CA-C	5.53	120.25	110.85
1	A	266	PRO	CB-CA-C	-5.33	104.03	110.00
1	A	171	ARG	N-CA-C	5.25	120.61	113.16
1	A	897	ARG	N-CA-C	-5.23	105.66	111.36
1	A	215	LEU	N-CA-C	5.18	117.01	111.36
1	A	1044	PHE	N-CA-C	-5.14	105.59	111.14
1	A	256	ILE	N-CA-C	-5.05	107.41	111.91

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1344	TYR	Peptide
1	A	228	TYR	Peptide
1	A	229	ILE	Peptide
1	A	237	VAL	Peptide
1	A	266	PRO	Peptide
1	A	268	PRO	Peptide
1	A	456	GLN	Peptide
1	A	628	GLY	Peptide
1	A	629	GLY	Peptide

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	9158	9312	9304	187	0
All	All	9158	9312	9304	187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (187) 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:1296:ASP:OD2	1:A:1302:ARG:NH2	1.72	1.23
1:A:224:LYS:O	1:A:266:PRO:HG3	1.44	1.17
1:A:984:GLU:OE1	1:A:986:ARG:NH1	1.81	1.11
1:A:1203:ASP:OD2	1:A:1229:ARG:HD2	1.56	1.03
1:A:959:ASP:OD2	1:A:988:ARG:NH1	1.96	0.98
1:A:956:SER:HB3	1:A:1022:ARG:HH11	1.28	0.95
1:A:820:ASP:HB2	1:A:821:PRO:HA	1.52	0.91
1:A:955:PHE:CE1	1:A:992:HIS:CD2	2.61	0.89
1:A:231:THR:O	1:A:262:ARG:NH2	2.06	0.88
1:A:356:LYS:NZ	1:A:360:GLU:OE2	2.06	0.88
1:A:956:SER:HB3	1:A:1022:ARG:NH1	1.90	0.86
1:A:245:CYS:SG	1:A:246:ALA:N	2.48	0.86
1:A:538:ILE:O	1:A:541:TYR:HD1	1.59	0.86
1:A:500:ASP:OD1	1:A:537:LYS:NZ	2.09	0.85
1:A:955:PHE:CE1	1:A:992:HIS:NE2	2.43	0.85
1:A:215:LEU:O	1:A:219:LYS:HG3	1.77	0.84
1:A:820:ASP:HB2	1:A:821:PRO:CA	2.09	0.81
1:A:955:PHE:CZ	1:A:992:HIS:CD2	2.68	0.81
1:A:439:ILE:HG12	1:A:541:TYR:OH	1.80	0.81
1:A:966:GLU:OE2	1:A:969:ARG:NH1	2.14	0.80
1:A:903:ARG:HB2	1:A:904:PRO:HD3	1.61	0.80
1:A:942:PHE:CD2	1:A:1048:TYR:HD1	1.99	0.79
1:A:90:GLU:OE1	1:A:168:ARG:NH2	2.16	0.79
1:A:942:PHE:HD2	1:A:1048:TYR:HD1	1.28	0.79
1:A:821:PRO:HG3	1:A:1286:MET:HG2	1.66	0.76
1:A:820:ASP:H	1:A:821:PRO:HA	1.50	0.75
1:A:587:PHE:HE2	1:A:625:MET:HE3	1.51	0.75
1:A:224:LYS:O	1:A:266:PRO:CG	2.32	0.75
1:A:1046:ILE:O	1:A:1049:ILE:HG22	1.87	0.75
1:A:544:SER:OG	1:A:547:ASN:HB3	1.87	0.74
1:A:908:ILE:HD11	1:A:1276:MET:HG2	1.68	0.74
1:A:841:SER:O	1:A:845:VAL:HG23	1.89	0.72
1:A:171:ARG:O	1:A:174:ARG:HB2	1.89	0.72
1:A:268:PRO:HB2	1:A:273:THR:HB	1.71	0.71
1:A:632:TYR:HB3	1:A:633:PRO:HD3	1.70	0.71
1:A:587:PHE:CE2	1:A:625:MET:HE3	2.24	0.71
1:A:591:GLU:OE2	1:A:593:ARG:NH1	2.24	0.70
1:A:820:ASP:CB	1:A:821:PRO:CA	2.68	0.70
1:A:591:GLU:OE2	1:A:593:ARG:NH2	2.25	0.70
1:A:820:ASP:HB2	1:A:821:PRO:C	2.18	0.69
1:A:955:PHE:CZ	1:A:992:HIS:HD2	2.10	0.69
1:A:836:ASP:CG	1:A:900:ARG:HH12	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:TRP:CZ3	1:A:1020:LEU:HD22	2.29	0.68
1:A:976:LYS:NZ	1:A:984:GLU:OE2	2.19	0.67
1:A:538:ILE:O	1:A:541:TYR:CD1	2.45	0.67
1:A:942:PHE:HD2	1:A:1048:TYR:CD1	2.11	0.66
1:A:372:GLN:NE2	1:A:486:LEU:O	2.29	0.66
1:A:836:ASP:OD2	1:A:900:ARG:NH1	2.29	0.65
1:A:206:MET:HE2	1:A:317:LEU:HD12	1.78	0.65
1:A:333:LEU:HD11	1:A:1064:VAL:HG11	1.77	0.64
1:A:302:ASN:OD1	1:A:307:ASN:HB3	1.98	0.64
1:A:836:ASP:OD2	1:A:900:ARG:NH2	2.30	0.64
1:A:568:LEU:O	1:A:568:LEU:HD23	1.98	0.63
1:A:276:ASP:O	1:A:277:ASN:HB3	1.99	0.62
1:A:957:CYS:SG	1:A:958:ASN:N	2.72	0.62
1:A:115:SER:O	1:A:119:VAL:HG13	2.00	0.62
1:A:942:PHE:CD2	1:A:1048:TYR:CD1	2.87	0.62
1:A:820:ASP:N	1:A:821:PRO:HA	2.11	0.61
1:A:541:TYR:O	1:A:542:TRP:HB2	2.00	0.61
1:A:823:ARG:NH2	1:A:1341:GLU:OE2	2.33	0.60
1:A:439:ILE:CG1	1:A:541:TYR:OH	2.50	0.59
1:A:819:GLU:HG2	1:A:897:ARG:HH21	1.67	0.59
1:A:1016:TRP:HZ3	1:A:1020:LEU:HD22	1.67	0.59
1:A:1099:ARG:O	1:A:1100:CYS:SG	2.60	0.59
1:A:822:ILE:HG21	1:A:1291:LYS:H	1.68	0.59
1:A:836:ASP:CG	1:A:900:ARG:NH1	2.62	0.58
1:A:1016:TRP:CD1	1:A:1017:PRO:HD3	2.38	0.58
1:A:846:GLU:HG3	1:A:847:ILE:N	2.19	0.58
1:A:591:GLU:OE2	1:A:593:ARG:CZ	2.52	0.58
1:A:965:GLU:CD	1:A:990:TRP:HE1	2.11	0.57
1:A:369:TRP:O	1:A:369:TRP:HD1	1.87	0.57
1:A:45:ILE:HG12	1:A:107:ALA:HA	1.86	0.57
1:A:542:TRP:N	1:A:542:TRP:HE3	2.02	0.57
1:A:183:GLN:O	1:A:187:ASN:OD1	2.22	0.57
1:A:1203:ASP:CG	1:A:1229:ARG:HD2	2.29	0.57
1:A:820:ASP:CB	1:A:821:PRO:HA	2.19	0.56
1:A:911:ALA:O	1:A:915:LYS:HE2	2.05	0.56
1:A:1016:TRP:O	1:A:1020:LEU:N	2.28	0.56
1:A:74:MET:HB3	1:A:78:ASP:HB3	1.87	0.56
1:A:1339:ASP:O	1:A:1341:GLU:N	2.34	0.56
1:A:265:TRP:HZ2	1:A:271:GLY:HA2	1.70	0.55
1:A:844:THR:O	1:A:847:ILE:HG13	2.06	0.55
1:A:225:THR:HG23	1:A:266:PRO:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASN:O	1:A:308:GLU:HG2	2.07	0.55
1:A:1016:TRP:CG	1:A:1017:PRO:HD3	2.43	0.54
1:A:1173:LYS:O	1:A:1175:ARG:N	2.40	0.54
1:A:820:ASP:OD2	1:A:829:ASN:ND2	2.41	0.54
1:A:510:GLU:OE2	1:A:531:ARG:CG	2.57	0.53
1:A:843:PHE:O	1:A:846:GLU:HG2	2.07	0.53
1:A:303:ASP:OD2	1:A:1302:ARG:NH1	2.41	0.53
1:A:1299:GLN:HG2	1:A:1327:GLU:HB3	1.91	0.52
1:A:1333:SER:OG	1:A:1334:TYR:N	2.42	0.52
1:A:632:TYR:HB3	1:A:633:PRO:CD	2.38	0.52
1:A:366:TYR:O	1:A:369:TRP:HB3	2.09	0.52
1:A:542:TRP:N	1:A:542:TRP:CE3	2.77	0.51
1:A:589:ASP:OD2	1:A:593:ARG:NH2	2.43	0.51
1:A:836:ASP:OD1	1:A:900:ARG:NH1	2.42	0.51
1:A:819:GLU:CG	1:A:897:ARG:HH21	2.22	0.51
1:A:820:ASP:CB	1:A:821:PRO:C	2.83	0.51
1:A:1042:ALA:O	1:A:1046:ILE:HG13	2.11	0.51
1:A:225:THR:HA	1:A:266:PRO:HB3	1.92	0.51
1:A:276:ASP:O	1:A:277:ASN:CB	2.57	0.51
1:A:1016:TRP:N	1:A:1017:PRO:CD	2.73	0.51
1:A:1015:GLY:HA3	1:A:1326:GLN:OE1	2.10	0.50
1:A:1082:ASP:HB3	1:A:1085:GLN:HG2	1.92	0.50
1:A:842:VAL:O	1:A:845:VAL:HB	2.11	0.50
1:A:964:THR:OG1	1:A:965:GLU:N	2.44	0.50
1:A:536:PHE:O	1:A:539:THR:OG1	2.27	0.49
1:A:1263:SER:O	1:A:1265:GLN:N	2.41	0.49
1:A:1312:ALA:O	1:A:1316:LEU:HD13	2.13	0.49
1:A:567:PHE:O	1:A:571:ILE:HG12	2.13	0.49
1:A:965:GLU:HA	1:A:990:TRP:CZ2	2.48	0.49
1:A:1293:ALA:HB2	1:A:1339:ASP:H	1.77	0.49
1:A:49:GLU:O	1:A:50:TRP:O	2.31	0.48
1:A:816:LEU:HD21	1:A:901:VAL:HG12	1.95	0.48
1:A:1106:PRO:HA	1:A:1109:TYR:HB3	1.95	0.48
1:A:1318:ARG:HH21	1:A:1328:ILE:HD11	1.77	0.48
1:A:836:ASP:OD2	1:A:900:ARG:CZ	2.60	0.48
1:A:942:PHE:HA	1:A:945:ILE:HG22	1.95	0.48
1:A:1131:ASN:O	1:A:1135:LEU:HD13	2.14	0.48
1:A:44:CYS:O	1:A:48:VAL:HG23	2.14	0.48
1:A:165:ARG:O	1:A:168:ARG:HG2	2.14	0.48
1:A:433:VAL:O	1:A:437:LEU:N	2.44	0.48
1:A:965:GLU:OE1	1:A:990:TRP:NE1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:TYR:CZ	1:A:1351:THR:HG23	2.48	0.48
1:A:1047:ILE:O	1:A:1051:LEU:HG	2.14	0.48
1:A:206:MET:CE	1:A:317:LEU:HD12	2.43	0.47
1:A:638:CYS:O	1:A:642:ILE:HG12	2.14	0.47
1:A:1082:ASP:OD1	1:A:1083:LYS:N	2.46	0.47
1:A:513:LEU:HD23	1:A:527:LEU:HD11	1.97	0.47
1:A:227:TYR:HD2	1:A:262:ARG:HG2	1.80	0.47
1:A:1201:GLU:O	1:A:1204:THR:OG1	2.32	0.47
1:A:993:ASN:O	1:A:995:PHE:N	2.40	0.47
1:A:1319:CYS:SG	1:A:1328:ILE:HD12	2.55	0.47
1:A:202:LEU:HD23	1:A:202:LEU:O	2.14	0.47
1:A:217:LEU:HD11	1:A:1237:LEU:HD11	1.96	0.46
1:A:244:PRO:O	1:A:252:ARG:HD3	2.16	0.46
1:A:465:ASP:O	1:A:469:ARG:HG3	2.16	0.46
1:A:542:TRP:HE3	1:A:542:TRP:H	1.61	0.46
1:A:843:PHE:O	1:A:846:GLU:CG	2.63	0.46
1:A:1060:PHE:HZ	1:A:1376:PHE:CE1	2.35	0.46
1:A:225:THR:HG21	1:A:227:TYR:CZ	2.52	0.45
1:A:813:SER:HA	1:A:816:LEU:HB3	1.98	0.45
1:A:820:ASP:N	1:A:821:PRO:CA	2.79	0.45
1:A:539:THR:C	1:A:541:TYR:N	2.68	0.45
1:A:1244:ILE:HG23	1:A:1247:LEU:HD21	1.99	0.45
1:A:959:ASP:HB3	1:A:972:TYR:CE2	2.52	0.45
1:A:1045:PHE:O	1:A:1049:ILE:HB	2.16	0.45
1:A:823:ARG:HH21	1:A:823:ARG:CG	2.30	0.45
1:A:953:LYS:NZ	1:A:1029:GLU:OE2	2.49	0.45
1:A:979:ASP:OD1	1:A:979:ASP:N	2.48	0.45
1:A:252:ARG:HD2	1:A:1302:ARG:HH11	1.82	0.44
1:A:823:ARG:HH21	1:A:823:ARG:HG2	1.82	0.44
1:A:956:SER:CB	1:A:1022:ARG:HH11	2.13	0.44
1:A:552:LEU:O	1:A:555:SER:OG	2.28	0.43
1:A:1104:LYS:HG3	1:A:1105:ASN:H	1.83	0.43
1:A:1096:ARG:HB3	1:A:1097:PRO:HD2	2.00	0.43
1:A:1331:ALA:O	1:A:1336:LYS:HG3	2.18	0.43
1:A:210:TYR:O	1:A:313:TYR:OH	2.37	0.43
1:A:217:LEU:HD23	1:A:217:LEU:HA	1.86	0.43
1:A:1307:GLN:NE2	1:A:1339:ASP:OD2	2.51	0.43
1:A:1334:TYR:O	1:A:1334:TYR:CG	2.72	0.43
1:A:1049:ILE:CG2	1:A:1050:ILE:N	2.81	0.43
1:A:369:TRP:C	1:A:369:TRP:CD1	2.95	0.43
1:A:959:ASP:CG	1:A:988:ARG:HH11	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:GLU:HA	1:A:990:TRP:HZ2	1.83	0.42
1:A:559:ILE:HG22	1:A:563:LEU:HB2	2.01	0.42
1:A:819:GLU:HG2	1:A:897:ARG:NH2	2.34	0.42
1:A:116:GLY:HA2	1:A:119:VAL:CG1	2.50	0.42
1:A:326:LEU:HD23	1:A:326:LEU:O	2.19	0.42
1:A:49:GLU:C	1:A:50:TRP:O	2.63	0.41
1:A:632:TYR:CB	1:A:633:PRO:CD	2.98	0.41
1:A:594:ARG:HA	1:A:594:ARG:HD2	1.93	0.41
1:A:526:VAL:O	1:A:530:ILE:HG13	2.20	0.41
1:A:337:PHE:HZ	1:A:660:ALA:HB1	1.84	0.41
1:A:449:ILE:HG12	1:A:532:LEU:HD23	2.03	0.41
1:A:570:ILE:HD13	1:A:570:ILE:HG21	1.82	0.41
1:A:966:GLU:CD	1:A:969:ARG:NH1	2.78	0.41
1:A:116:GLY:HA2	1:A:119:VAL:HG13	2.03	0.41
1:A:585:TYR:HA	1:A:587:PHE:CE1	2.55	0.41
1:A:57:ILE:HA	1:A:60:THR:HG22	2.03	0.40
1:A:90:GLU:CD	1:A:168:ARG:NH2	2.79	0.40
1:A:599:ASN:CG	1:A:601:PRO:HD2	2.47	0.40
1:A:903:ARG:HB2	1:A:904:PRO:CD	2.42	0.40
1:A:955:PHE:CD1	1:A:992:HIS:NE2	2.86	0.40
1:A:1195:ILE:HD12	1:A:1195:ILE:HA	1.96	0.40
1:A:844:THR:HG21	1:A:875:LEU:HB2	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	1113/1357 (82%)	978 (88%)	116 (10%)	19 (2%)	7	35

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	TRP
1	A	977	ASP
1	A	1174	ALA
1	A	80	ASN
1	A	819	GLU
1	A	1344	TYR
1	A	1354	THR
1	A	994	ASP
1	A	1138	GLN
1	A	1333	SER
1	A	1355	ASN
1	A	820	ASP
1	A	903	ARG
1	A	1323	GLU
1	A	542	TRP
1	A	1294	LEU
1	A	457	PRO
1	A	252	ARG
1	A	630	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	1002/1196 (84%)	974 (97%)	28 (3%)	38 60

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

Mol	Chain	Res	Type
1	A	64	ASN
1	A	123	ILE
1	A	174	ARG
1	A	221	LYS
1	A	262	ARG
1	A	276	ASP
1	A	303	ASP
1	A	422	ARG

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Mol	Chain	Res	Type
1	A	542	TRP
1	A	794	ARG
1	A	800	TRP
1	A	823	ARG
1	A	846	GLU
1	A	866	LEU
1	A	880	LEU
1	A	892	VAL
1	A	930	ASN
1	A	954	PHE
1	A	986	ARG
1	A	997	PHE
1	A	1120	PHE
1	A	1121	GLU
1	A	1122	TYR
1	A	1199	LEU
1	A	1249	ARG
1	A	1276	MET
1	A	1376	PHE
1	A	1380	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	287	GLN
1	A	455	ASN
1	A	462	HIS
1	A	579	GLN
1	A	602	GLN
1	A	992	HIS
1	A	1058	ASN
1	A	1138	GLN
1	A	1148	HIS

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.

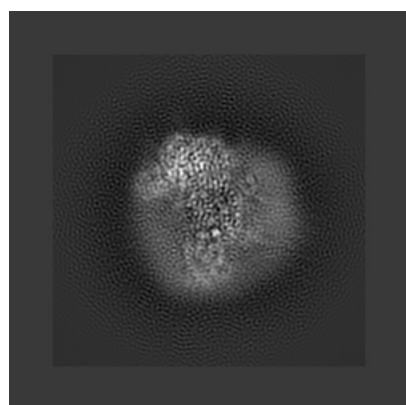
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9513. These allow visual inspection of the internal detail of the map and identification of artifacts.

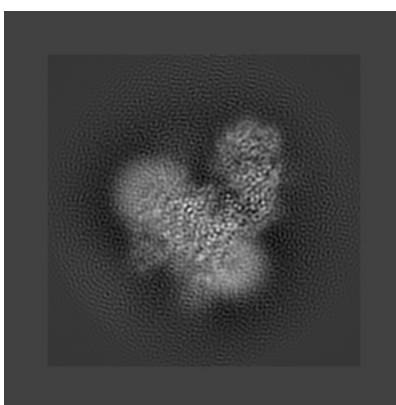
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

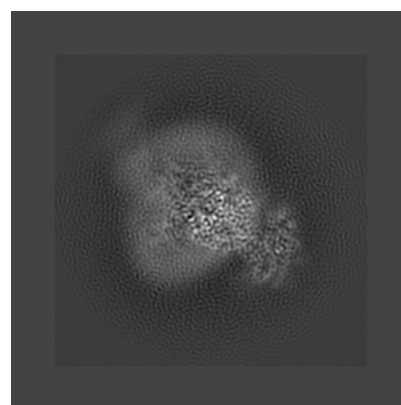
6.1.1 Primary map



X



Y

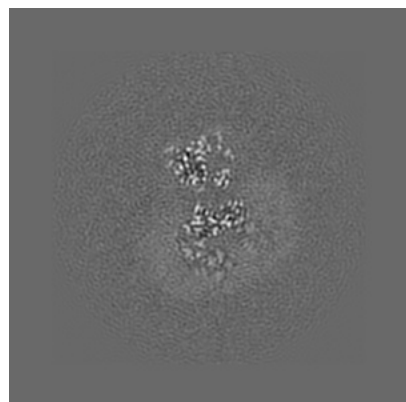


Z

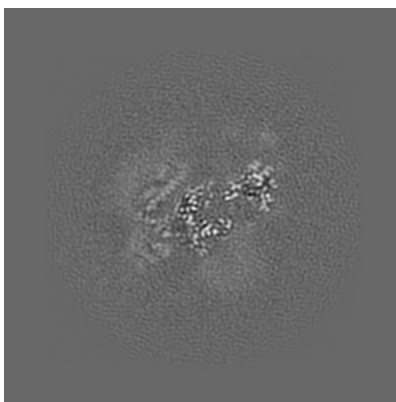
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

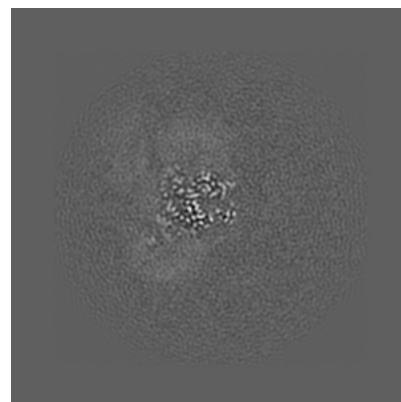
6.2.1 Primary map



X Index: 128



Y Index: 128

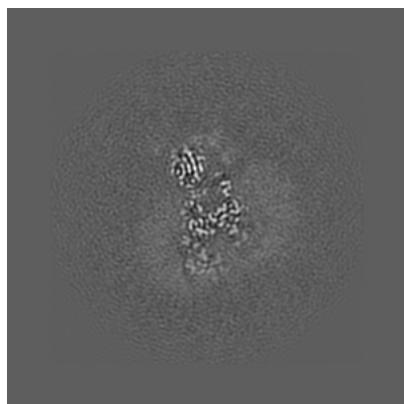


Z Index: 128

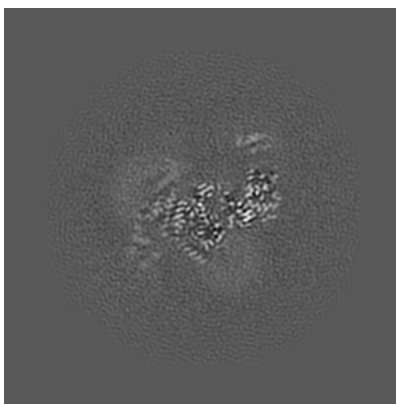
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

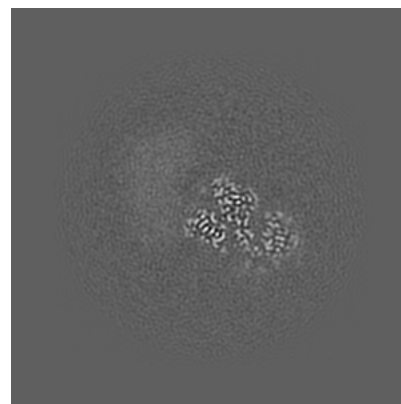
6.3.1 Primary map



X Index: 123



Y Index: 123

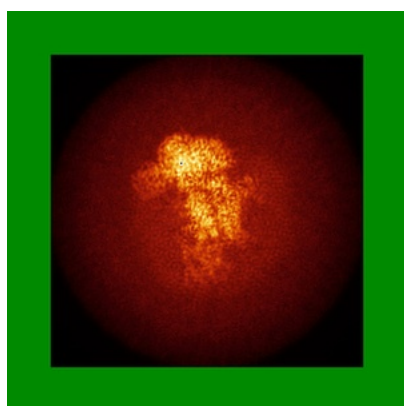


Z Index: 159

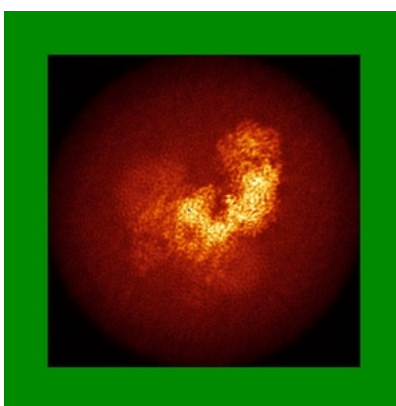
The images above show the largest variance slices of the map in three orthogonal directions.

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

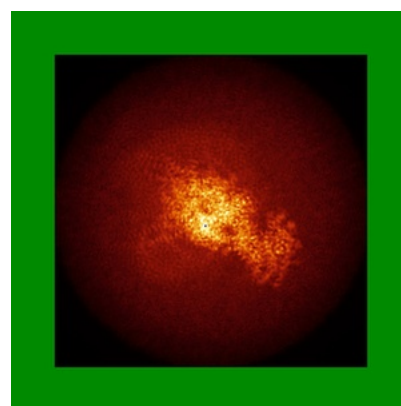
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

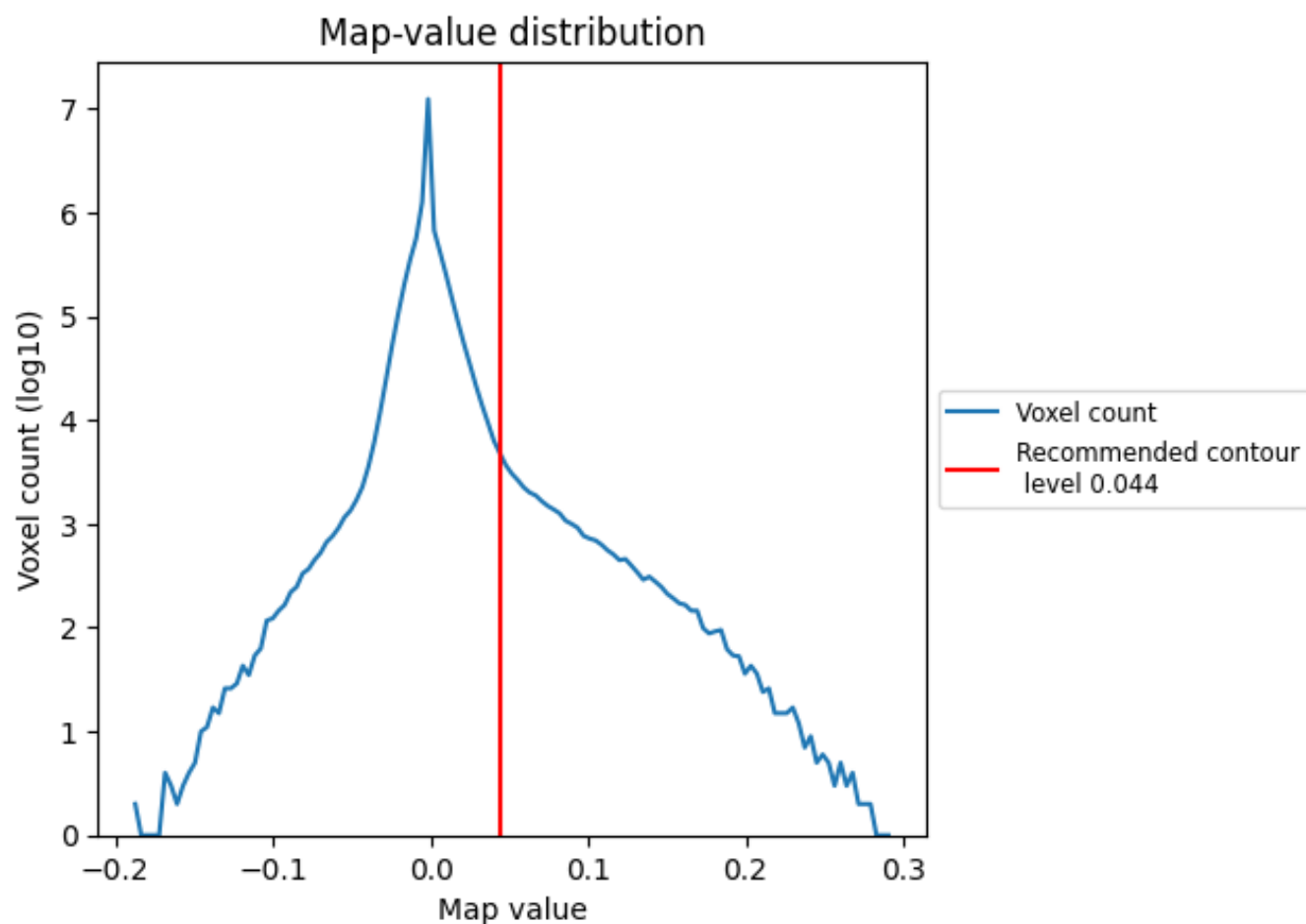
6.6 Mask visualisation

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

7 Map analysis [i](#)

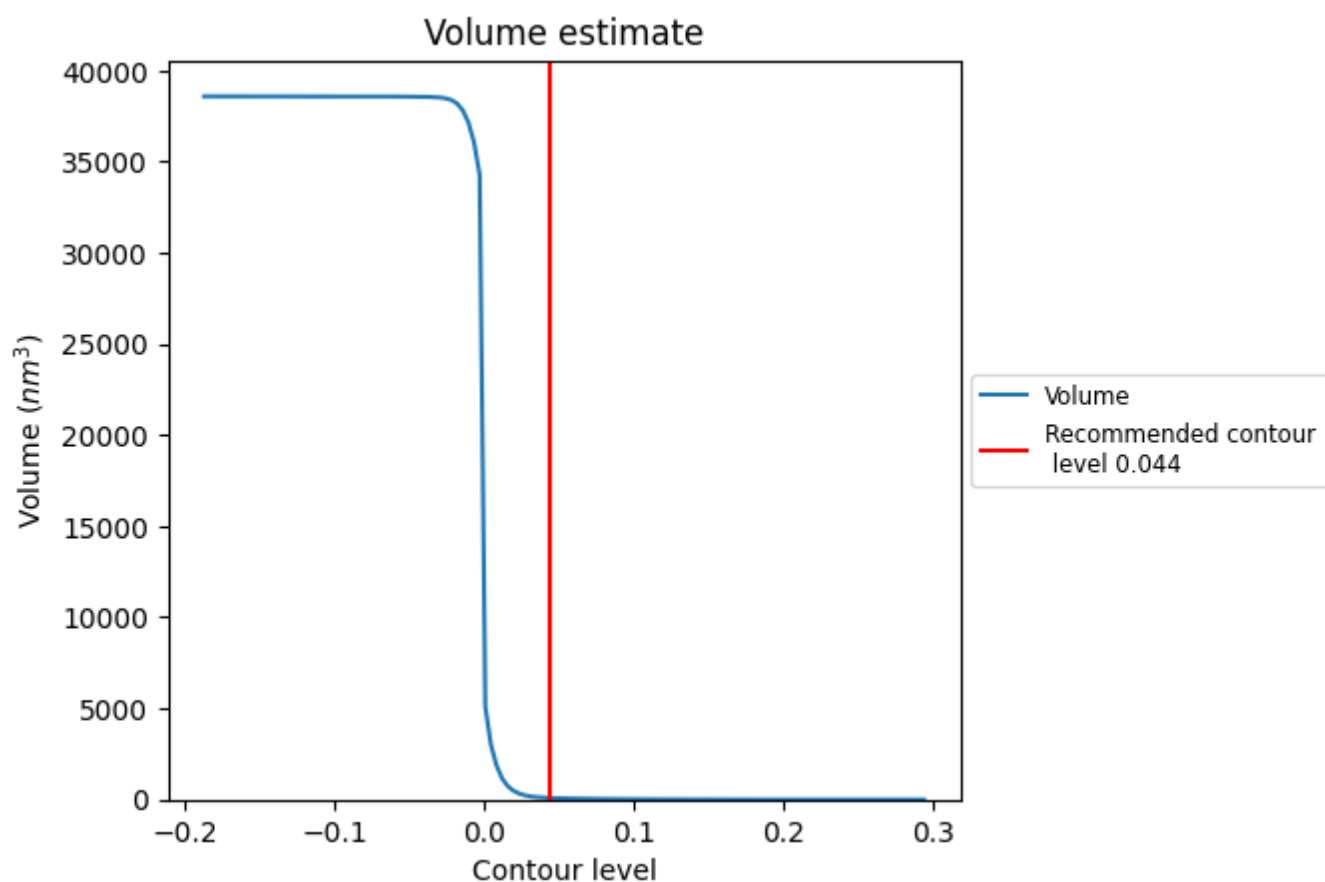
This section contains the results of statistical analysis of the map.

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.

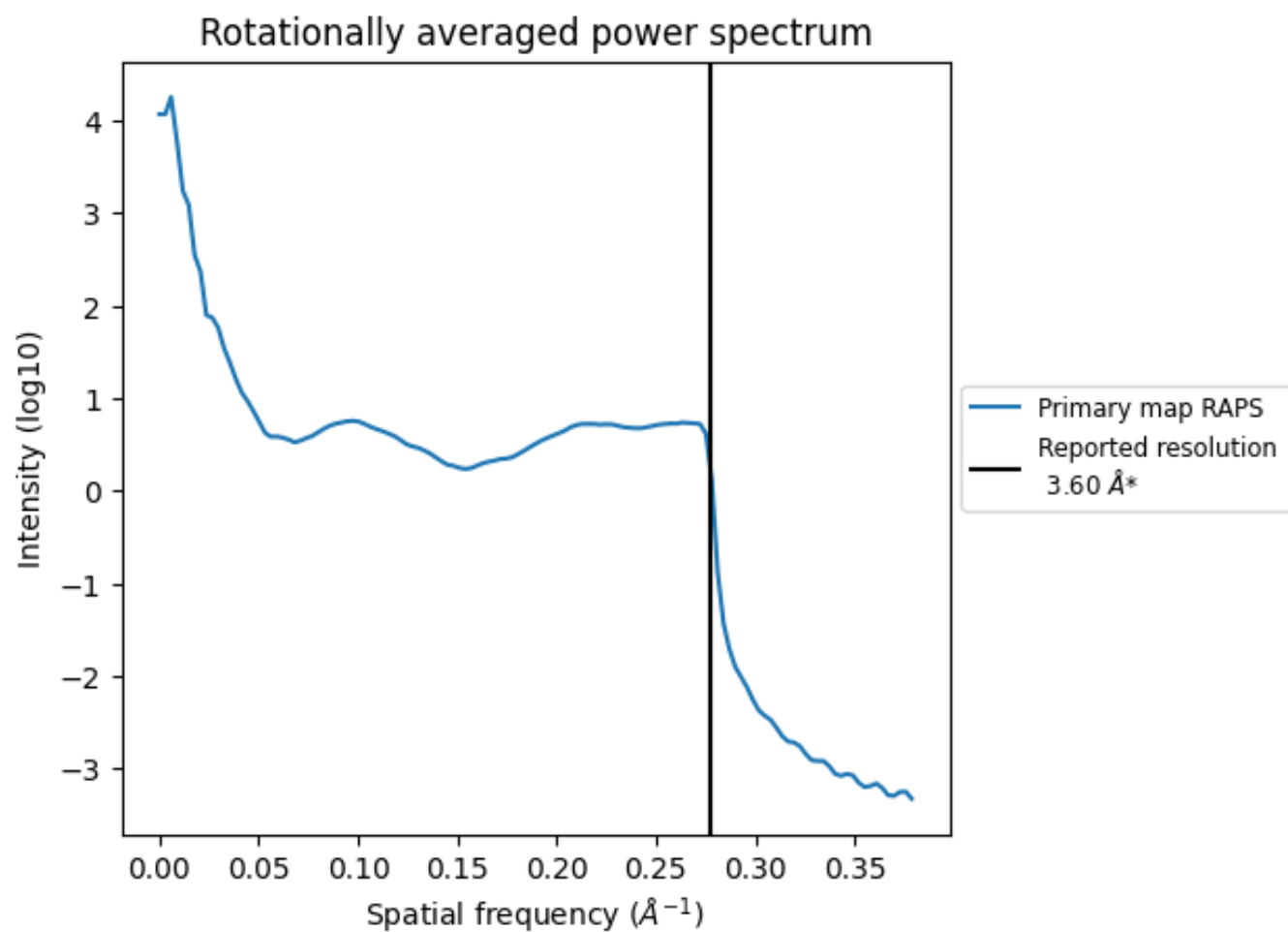
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm³; this corresponds to an approximate mass of 79 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

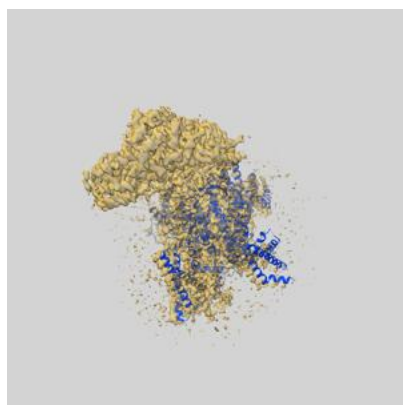
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

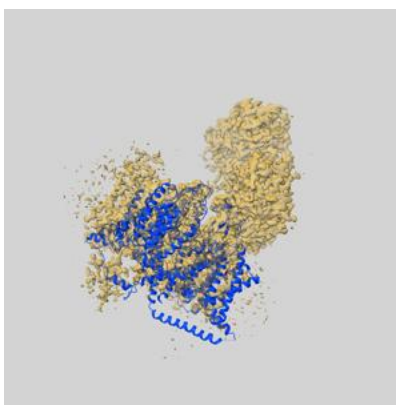
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9513 and PDB model 6BYO. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

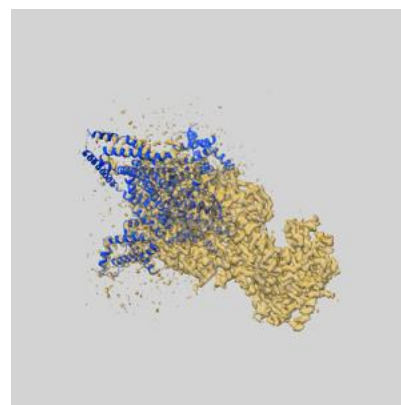
9.1 Map-model overlay [i](#)



X



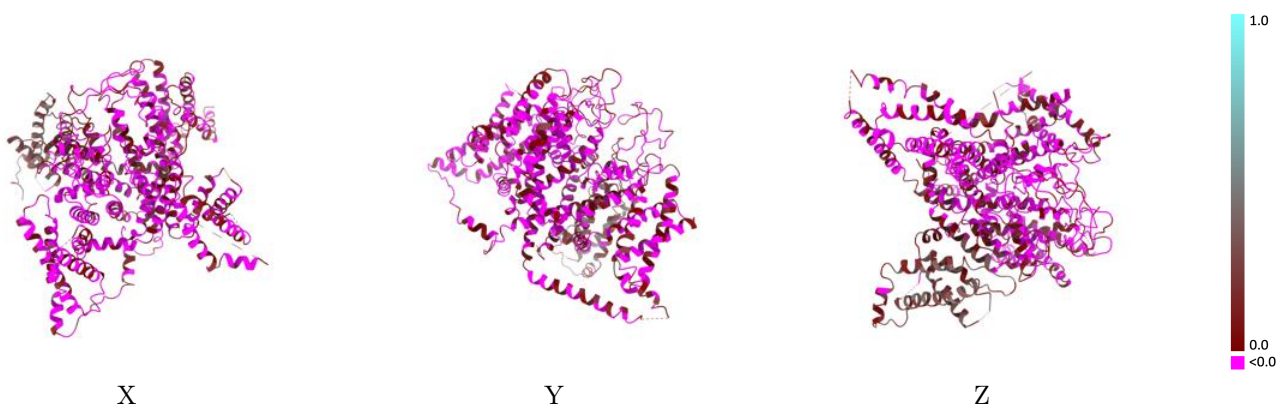
Y



Z

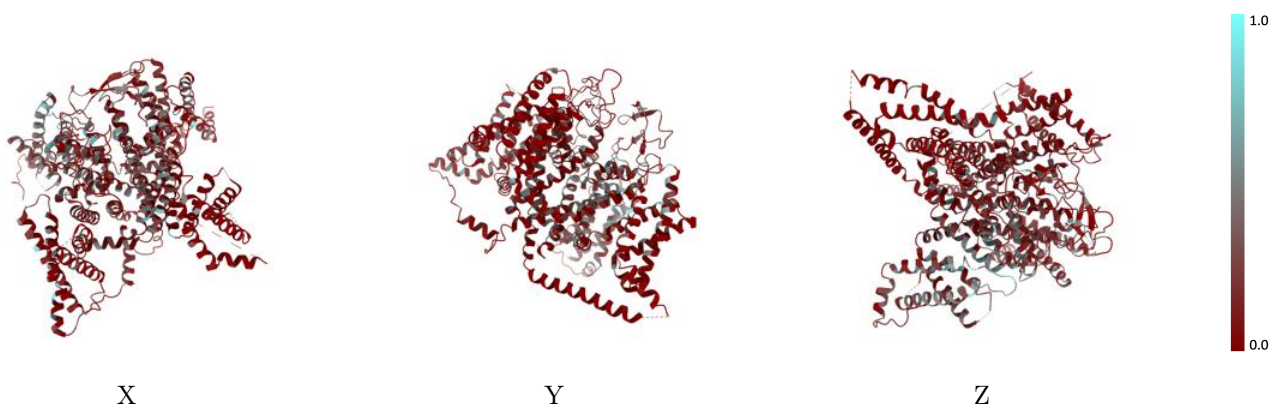
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



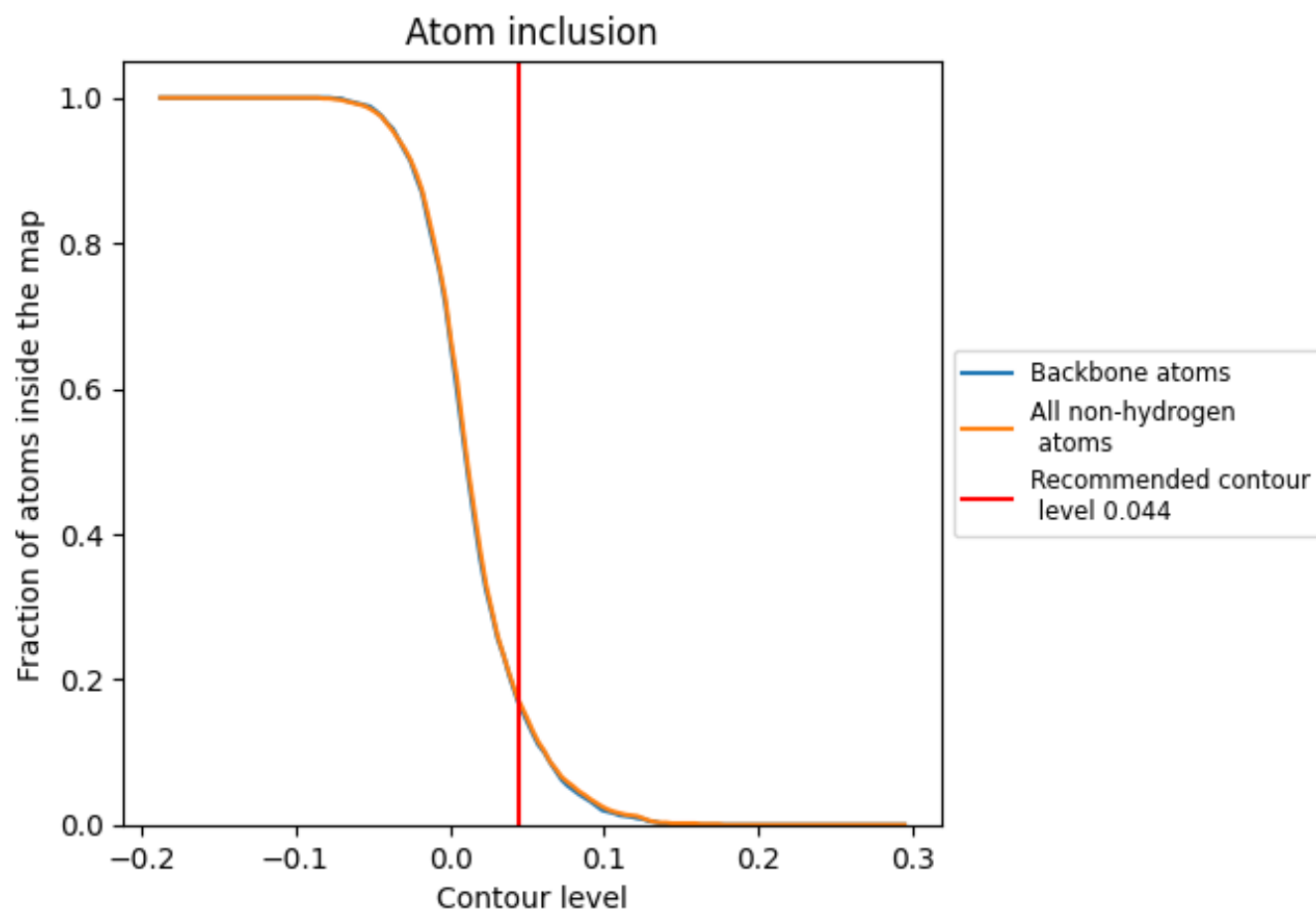
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.044).

9.4 Atom inclusion [i](#)



At the recommended contour level, 17% of all backbone atoms, 17% 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 (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1730	-0.0110
A	0.1700	-0.0110

