



Full wwPDB EM Validation Report (i)

Nov 27, 2022 – 03:25 AM EST

PDB ID : 6BYO
EMDB ID : EMD-9513
Title : Residue assignment correction to the voltage gated calcium Cav1.1 rabbit al-pha 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 (i) 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 \(i\)](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbit : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

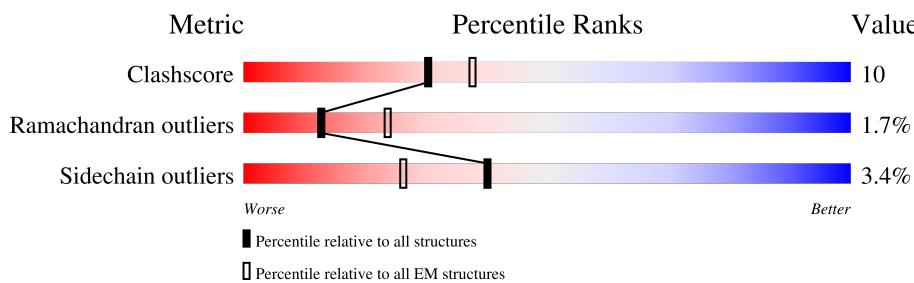
1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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				
			70%	64%	17%	.	17%
1	A	1357					

2 Entry composition [\(i\)](#)

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.

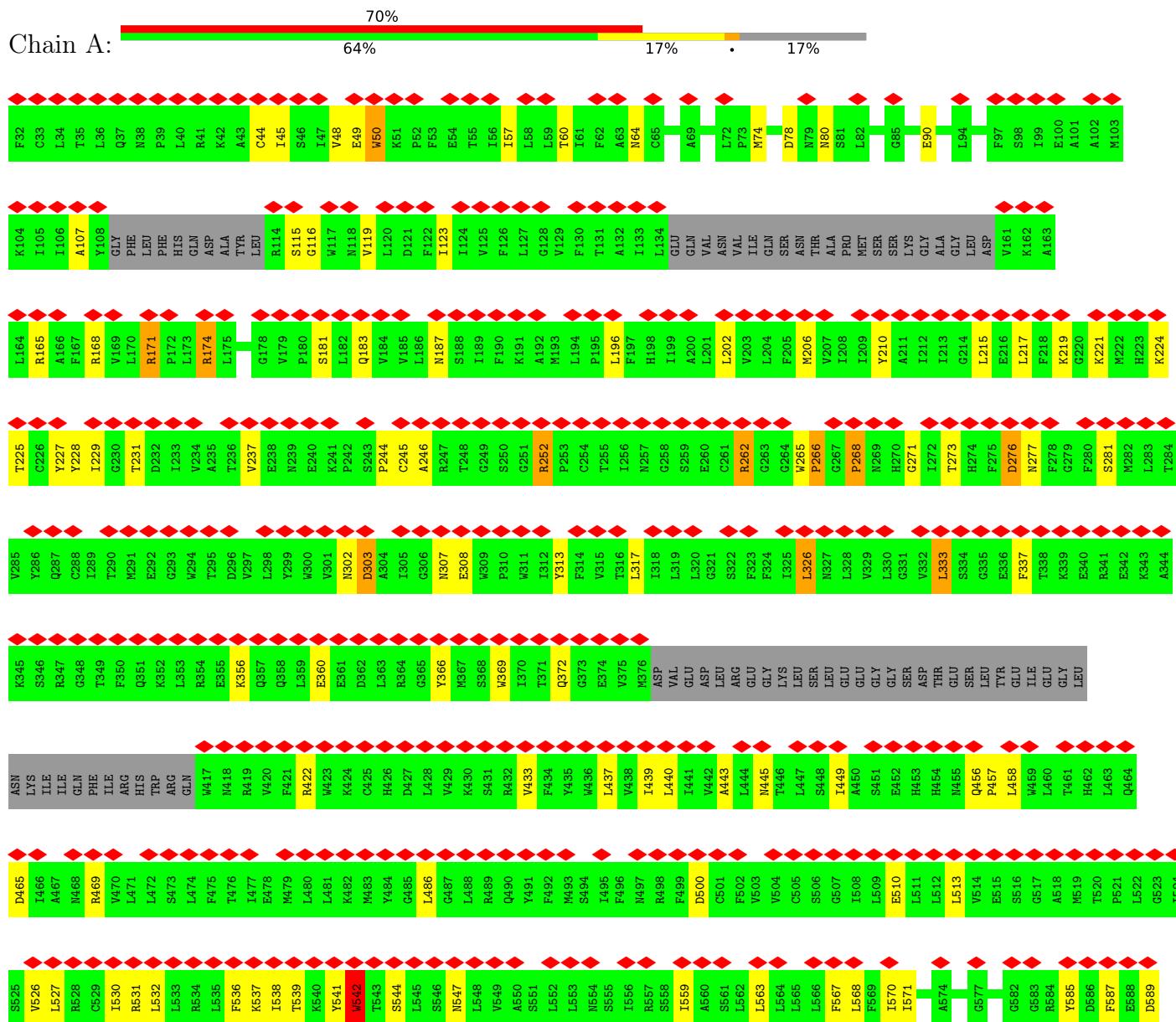
- Molecule 1 is a protein called Voltage-dependent L-type calcium channel subunit alpha-1S.

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

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



	T1255	L1315	C1134	T1074	V834	N654	T590
	L1256	L1316	L1135	E1075	V835	V655	E591
	L1257	F1517	G1136	V1076	D835	THR	V592
	M1258	R1318	M1137	K1077	P017	A1A	R593
	T1259	C1319	Q1138	N1078	Q1018	L1A	R594
	F1260	A1320	S1200	H1139	L1019	LYS	D595
	E1201	T1321	I1202	E1140	L1079	PHE	V596
	I1261	K1262	D1203	H1141	L1080	PHE	F597
	S1263	E1523	P1264	Q1142	L1081	SER	V651
	F1204	F1205	Q1265	S1143	D1082	ASP	V652
	W1325	A1266	E1144	E1144	K1083	PRO	D598
	LEU	ALA	ALA	ALA	K1084	GLU	N653
	LEU	SER.	E1145	E1145	N1084	GLU	N654
	LEU	TYR	S1150	S1150	Q1085	ASP	V655
	V1270	A1271	L1267	D1150	V1089	ASP	V656
	V1330	A1331	E1328	H1148	E1086	ASP	V657
	E1332	S1268	P1268	C1148	K1087	ASP	V658
	GLY	GLY	GLY	GLY	E1087	ASP	V659
	Y1269	V1274	Q1265	Q1149	E1028	ASP	V660
	V1270	A1266	E1326	V1154	I1024	ASP	V660
	V1332	C1326	Q1265	V1155	D1025	ASP	V660
	E1331	A1332	E1328	V1156	S1026	ASP	V660
	L1272	I1328	P1268	V1157	M1027	ASP	V660
	LEU	LEU	LEU	LEU	E966	ASP	V660
	Y1273	V1333	F1278	L1153	A1082	ASP	V660
	L1279	Y1334	F1279	L1154	K1083	ASP	V660
	V1330	D1339	Q1274	V1155	V1034	ASP	V660
	E1332	K1336	M1276	V1156	K1094	ASP	V660
	L1337	A1344	C1338	V1157	E1035	ASP	V660
	F1278	F1279	Q1285	F1158	P1036	ASP	V660
	V1280	D1339	G1285	M1158	V1037	ASP	V660
	Y1281	P1340	S1231	V1159	V1038	ASP	V660
	E1344	A1282	S1231	V1160	V1039	ASP	V660
	L1277	A1344	E1344	V1161	C1100	ASP	V660
	F1278	A1344	F1278	V1162	A1041	ASP	V660
	V1280	D1339	F1279	L1163	A1096	ASP	V660
	Y1281	P1340	Q1285	E1164	P1097	ASP	V660
	E1344	A1282	E1344	P1164	P1097	ASP	V660
	L1337	F1278	V1280	P1165	V1038	ASP	V660
	F1278	D1339	F1279	V1165	V1039	ASP	V660
	V1280	P1340	Q1285	V1166	V1039	ASP	V660
	Y1281	E1344	A1345	V1167	V1040	ASP	V660
	E1344	A1282	F1278	V1168	V1040	ASP	V660
	L1337	F1278	V1280	V1168	V1040	ASP	V660
	F1278	D1339	F1279	V1169	V1040	ASP	V660
	V1280	P1340	Q1285	V1169	V1040	ASP	V660
	Y1281	E1344	A1345	V1170	V1040	ASP	V660
	E1344	A1282	F1278	V1170	V1040	ASP	V660
	L1337	F1278	V1280	V1170	V1040	ASP	V660
	F1278	D1339	F1279	V1171	V1040	ASP	V660
	V1280	P1340	Q1285	V1171	V1040	ASP	V660
	Y1281	E1344	A1345	V1172	V1040	ASP	V660
	E1344	A1282	F1278	V1172	V1040	ASP	V660
	L1337	F1278	V1280	V1172	V1040	ASP	V660
	F1278	D1339	F1279	V1173	V1040	ASP	V660
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	E1344	A1282	F1278	V1174	V1040	ASP	V660
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	L1337	F1278	V1280	V1176	V1040	ASP	V660
	F1278	D1339	F1279	V1177	V1040	ASP	V660
	V1280	P1340	Q1285	V1177	V1040	ASP	V660
	Y1281	E1344	A1345	V1178	V1040	ASP	V660
	E1344	A1282	F1278	V1178	V1040	ASP	V660
	L1337	F1278	V1280	V1178	V1040	ASP	V660
	F1278	D1339	F1279	V1179	V1040	ASP	V660
	V1280	P1340	Q1285	V1179	V1040	ASP	V660
	Y1281	E1344	A1345	V1179	V1040	ASP	V660
	E1344	A1282	F1278	V1179	V1040	ASP	V660
	L1337	F1278	V1280	V1179	V1040	ASP	V660
	F1278	D1339	F1279	V1180	V1040	ASP	V660
	V1280	P1340	Q1285	V1180	V1040	ASP	V660
	Y1281	E1344	A1345	V1180	V1040	ASP	V660
	E1344	A1282	F1278	V1180	V1040	ASP	V660
	L1337	F1278	V1280	V1180	V1040	ASP	V660
	F1278	D1339	F1279	V1181	V1040	ASP	V660
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	E1344	A1282	F1278	V1181	V1040	ASP	V660
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	Y1281	E1344	A1345	V1182	V1040	ASP	V660
	E1344	A1282	F1278	V1182	V1040	ASP	V660
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	E1344	A1282	F1278	V1183	V1040	ASP	V660
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	E1344	A1282	F1278	V1185	V1040	ASP	V660
	L1337	F1278	V1280	V1185	V1040	ASP	V660
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	E1344	A1282	F1278	V1186	V1040	ASP	V660
	L1337	F1278	V1280	V1186	V1040	ASP	V660
	F1278	D1339	F1279	V1187	V1040	ASP	V660
	V1280	P1340	Q1285	V1187	V1040	ASP	V660
	Y1281	E1344	A1345	V1187	V1040	ASP	V660
	E1344	A1282	F1278	V1187	V1040	ASP	V660
	L1337	F1278	V1280	V1187	V1040	ASP	V660
	F1278	D1339	F1279	V1188	V1040	ASP	V660
	V1280	P1340	Q1285	V1188	V1040	ASP	V660
	Y1281	E1344	A1345	V1188	V1040	ASP	V660
	E1344	A1282	F1278	V1188	V1040	ASP	V660
	L1337	F1278	V1280	V1188	V1040	ASP	V660
	F1278	D1339	F1279	V1189	V1040	ASP	V660
	V1280	P1340	Q1285	V1189	V1040	ASP	V660
	Y1281	E1344	A1345	V1189	V1040	ASP	V660
	E1344	A1282	F1278	V1189	V1040	ASP	V660
	L1337	F1278	V1280	V1189	V1040	ASP	V660
	F1278	D1339	F1279	V1190	V1040	ASP	V660
	V1280	P1340	Q1285	V1190	V1040	ASP	V660
	Y1281	E1344	A1345	V1190	V1040	ASP	V660
	E1344	A1282	F1278	V1190	V1040	ASP	V660
	L1337	F1278	V1280	V1190	V1040	ASP	V660
	F1278	D1339	F1279	V1191	V1040	ASP	V660
	V1280	P1340	Q1285	V1191	V1040	ASP	V660
	Y1281	E1344	A1345	V1191	V1040	ASP	V660
	E1344	A1282	F1278	V1191	V1040	ASP	V660
	L1337	F1278	V1280	V1191	V1040	ASP	V660
	F1278	D1339	F1279	V1192	V1040	ASP	V660
	V1280	P1340	Q1285	V1192	V1040	ASP	V660
	Y1281	E1344	A1345	V1192	V1040	ASP	V660
	E1344	A1282	F1278	V1192	V1040	ASP	V660
	L1337	F1278	V1280	V1192	V1040	ASP	V660
	F1278	D1339	F1279	V1193	V1040	ASP	V660
	V1280	P1340	Q1285	V1193	V1040	ASP	V660
	Y1281	E1344	A1345	V1193	V1040	ASP	V660
	E1344	A1282	F1278	V1193	V1040	ASP	V660
	L1337	F1278	V1280	V1193	V1040	ASP	V660
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	E1344	A1282	F1278	V1194	V1040	ASP	V660
	L1337	F1278	V1280	V1194	V1040	ASP	V660
	F1278	D1339	F1279	V1195	V1040	ASP	V660
	V1280	P1340	Q1285	V1195	V1040	ASP	V660
	Y1281	E1344	A1345	V1195	V1040	ASP	V660
	E1344	A1282	F1278	V1195	V1040	ASP	V660
	L1337	F1278	V1280	V1195	V1040	ASP	V660
	F1278	D1339	F1279	V1196	V1040	ASP	V660
	V1280	P1340	Q1285	V1196	V1040	ASP	V660
	Y1281	E1344	A1345	V1196	V1040	ASP	V660
	E1344	A1282	F1278	V1196	V1040	ASP	V660
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	E1344	A1282	F1278	V1197	V1040	ASP	V660
	L1337	F1278	V1280	V1197	V1040	ASP	V660
	F1278	D1339	F1279	V1198	V1040	ASP	V660
	V1280	P1340	Q1285	V1198	V1040	ASP	V660
	Y1281	E1344	A1345	V1198	V1040	ASP	V660
	E1344	A1282	F1278	V1198	V1040	ASP	V660
	L1337	F1278	V1280	V1198	V1040	ASP	V660
	F1278	D1339	F1279	V1199	V1040	ASP	V660
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	Y1281	E1344	A1345	V1199	V1040	ASP	V660
	E1344	A1282	F1278	V1199	V1040	ASP	V660
	L1337	F1278	V1280	V1199	V1040	ASP	V660
	F1278	D1339	F1279	V1200	V1040	ASP	V660
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	Y1281	E1344	A1345	V1200	V1040	ASP	V660
	E1344	A1282	F1278	V1200	V1040	ASP	V660
	L1337	F1278	V1280	V1200	V1040	ASP	V660
	F1278	D1339	F1279	V1201	V1040	ASP	V660



4 Experimental information (i)

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 (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	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	0.59	1/9380 (0.0%)	0.75	21/12722 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	ARG	C-O	13.19	1.48	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1174	ALA	CB-CA-C	-8.28	97.68	110.10
1	A	957	CYS	CB-CA-C	-7.37	95.66	110.40
1	A	181	SER	CB-CA-C	7.33	124.03	110.10
1	A	333	LEU	CA-CB-CG	7.24	131.94	115.30
1	A	949	LEU	CA-CB-CG	7.08	131.59	115.30
1	A	281	SER	CB-CA-C	6.36	122.18	110.10
1	A	954	PHE	CB-CG-CD1	6.32	125.23	120.80
1	A	326	LEU	CA-CB-CG	6.04	129.18	115.30
1	A	440	LEU	CB-CA-C	6.01	121.63	110.20
1	A	458	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	644	LEU	CB-CG-CD2	-5.72	101.28	111.00
1	A	954	PHE	CB-CG-CD2	-5.70	116.81	120.80
1	A	443	ALA	CB-CA-C	5.63	118.54	110.10
1	A	997	PHE	CB-CG-CD1	5.58	124.70	120.80
1	A	1316	LEU	CB-CG-CD2	-5.51	101.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	1188	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	597	PHE	CB-CG-CD1	5.30	124.51	120.80
1	A	1337	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	333	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	A	653	LEU	CA-CB-CG	5.03	126.87	115.30

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	180	0
All	All	9158	9312	9304	180	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 (180) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:955:PHE:CZ	1:A:992:HIS:HD2	2.10	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:820:ASP:HB2	1:A:821:PRO:C	2.18	0.65
1:A:333:LEU:HD11	1:A:1064:VAL:HG11	1.77	0.64
1:A:836:ASP:CG	1:A:900:ARG:HH12	2.00	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: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: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:206:MET:HE2	1:A:317:LEU:HD12	1.87	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
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:836:ASP:CG	1:A:900:ARG:NH1	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:965:GLU:CD	1:A:990:TRP:HE1	2.11	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:1203:ASP:CG	1:A:1229:ARG:HD2	2.29	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:539:THR:C	1:A:541:TYR:N	2.68	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:1201:GLU:O	1:A:1204:THR:OG1	2.32	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: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:820:ASP:CB	1:A:821:PRO:C	2.83	0.44
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:587:PHE:HE2	1:A:625:MET:HE2	1.83	0.44
1:A:956:SER:CB	1:A:1022:ARG:HH11	2.13	0.44
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:587:PHE:HE2	1:A:625:MET:CE	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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%)	9 45

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

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Mol	Chain	Res	Type
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 [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1002/1196 (84%)	968 (97%)	34 (3%)	37 69

All (34) 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
1	A	445	ASN
1	A	542	TRP
1	A	597	PHE
1	A	794	ARG
1	A	800	TRP

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Mol	Chain	Res	Type
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	955	PHE
1	A	986	ARG
1	A	988	ARG
1	A	997	PHE
1	A	1120	PHE
1	A	1121	GLU
1	A	1122	TYR
1	A	1131	ASN
1	A	1199	LEU
1	A	1249	ARG
1	A	1276	MET
1	A	1302	ARG
1	A	1306	PHE
1	A	1376	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	455	ASN
1	A	579	GLN
1	A	992	HIS
1	A	1148	HIS

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides 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.

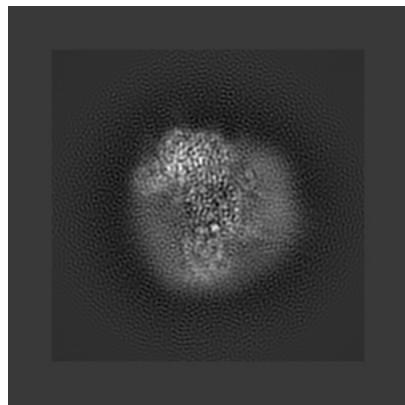
6 Map visualisation (i)

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.

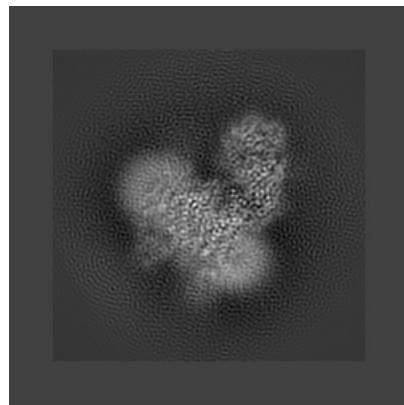
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

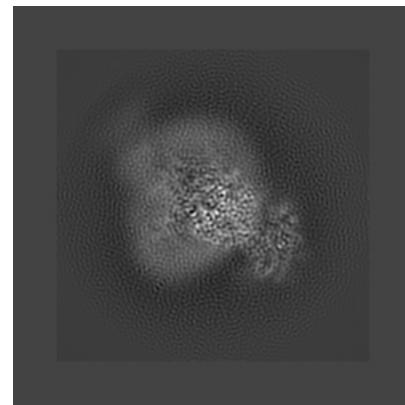
6.1.1 Primary map



X



Y

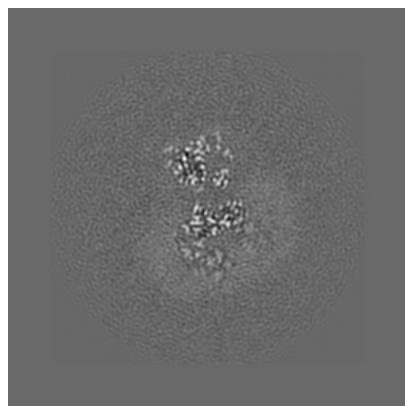


Z

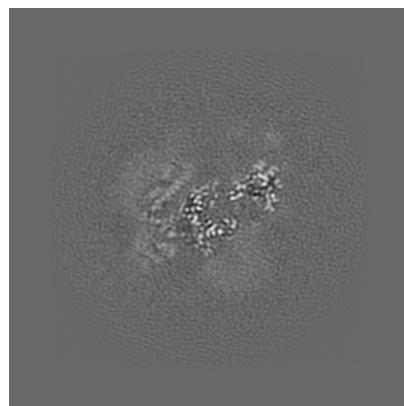
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

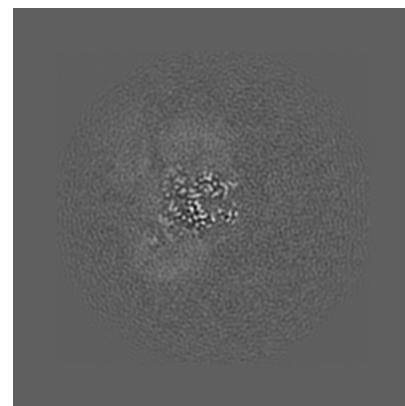
6.2.1 Primary map



X Index: 128



Y Index: 128

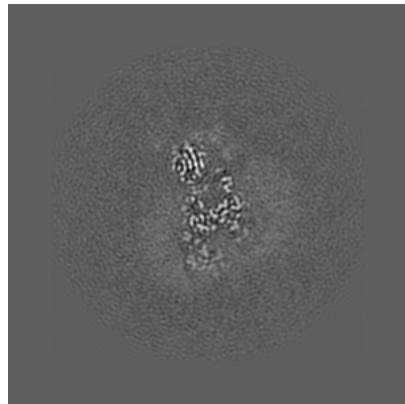


Z Index: 128

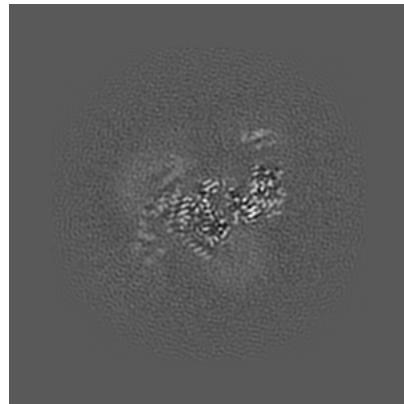
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

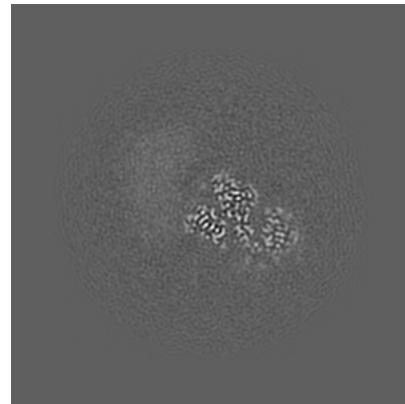
6.3.1 Primary map



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 surface views [\(i\)](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.044. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

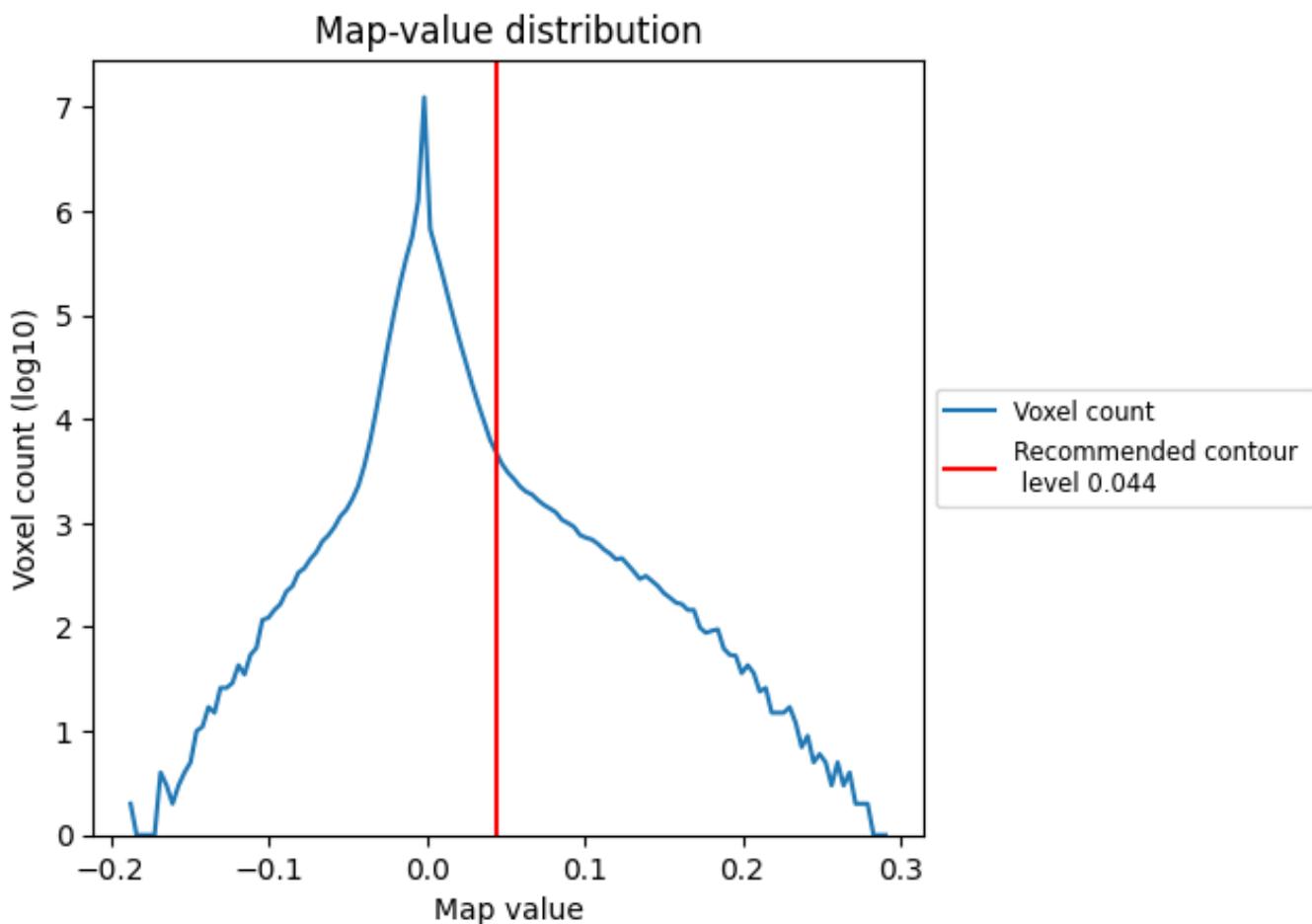
6.5 Mask visualisation

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

7 Map analysis (i)

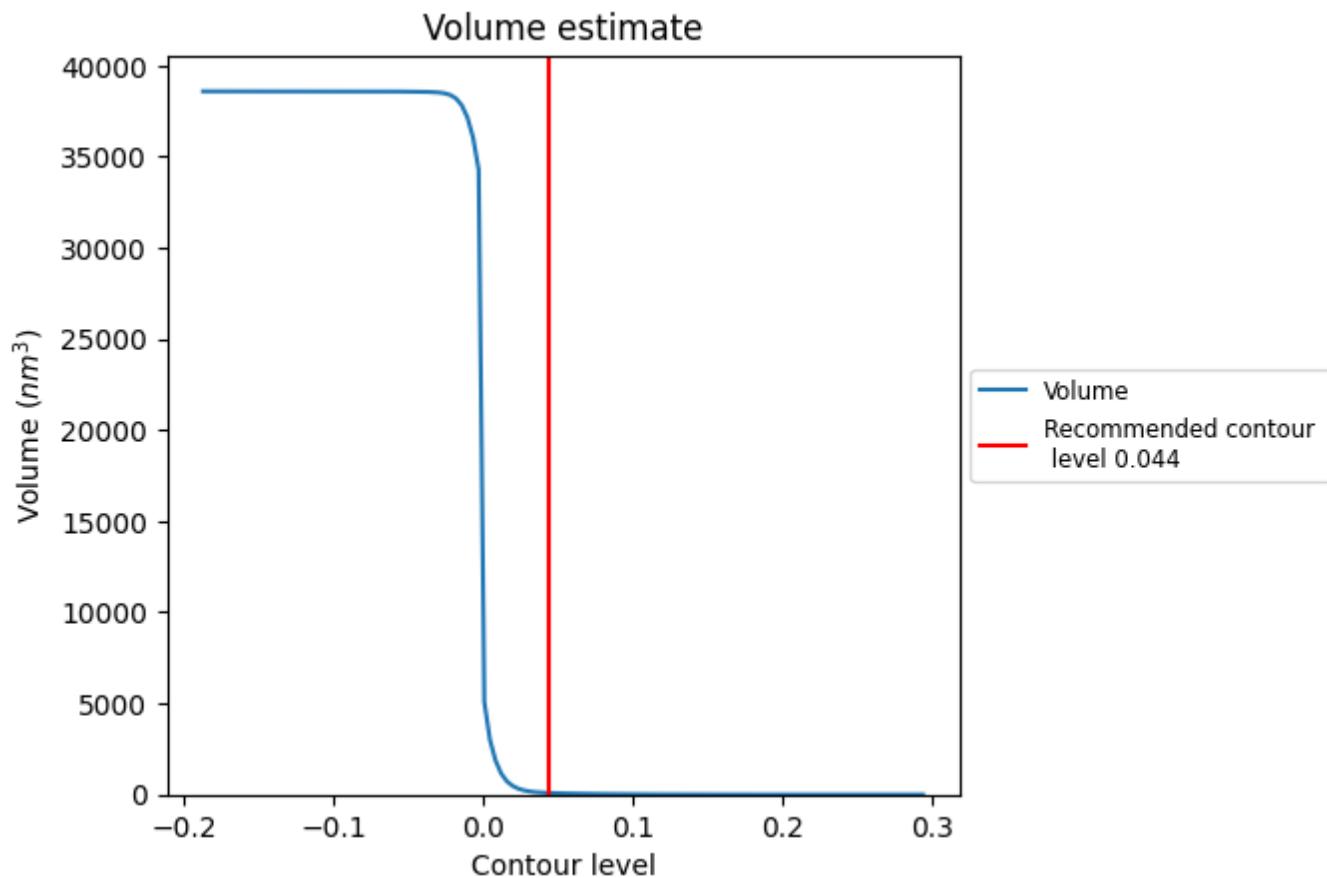
This section contains the results of statistical analysis of the map.

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.

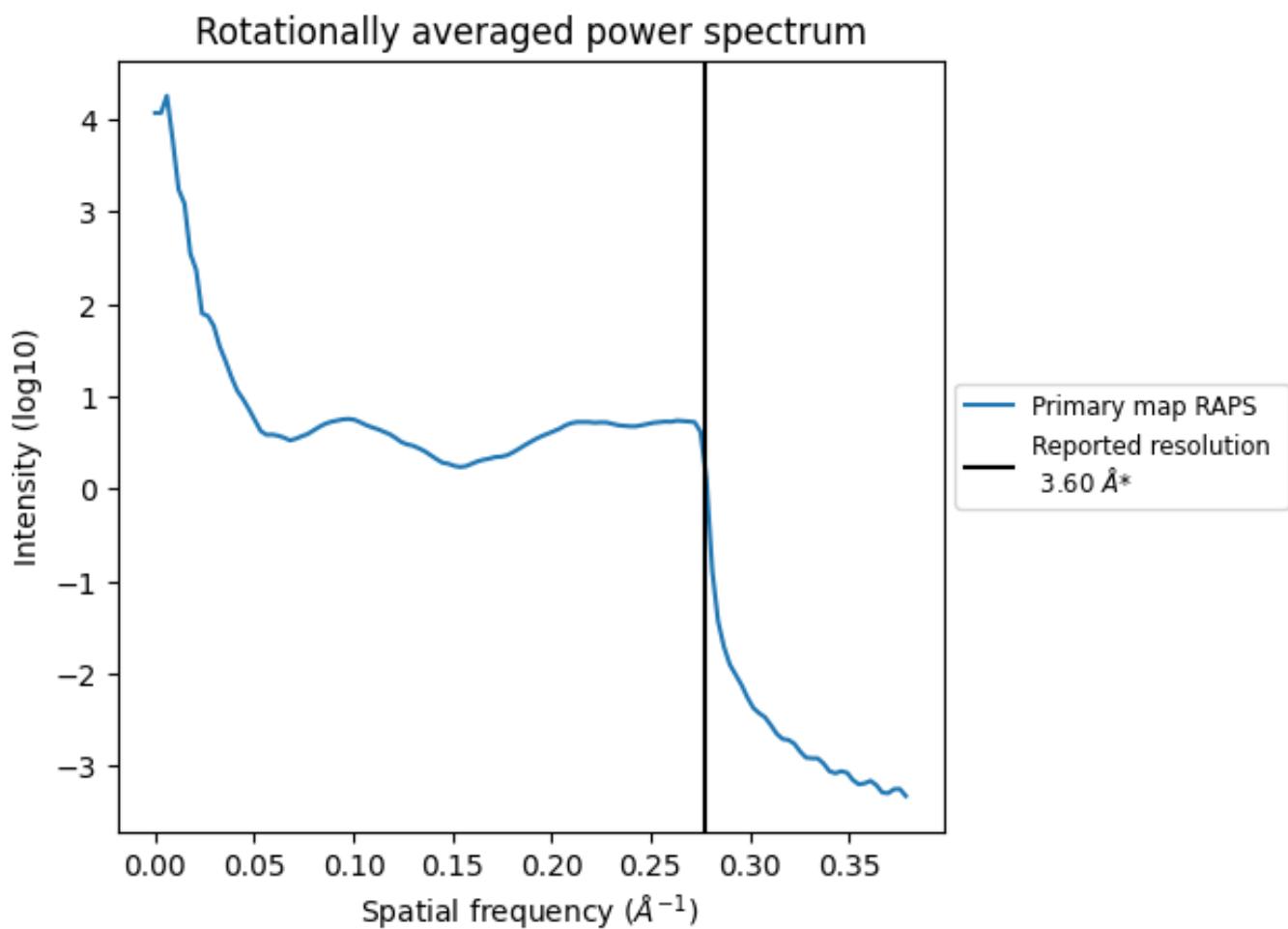
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 87 nm^3 ; 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 [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

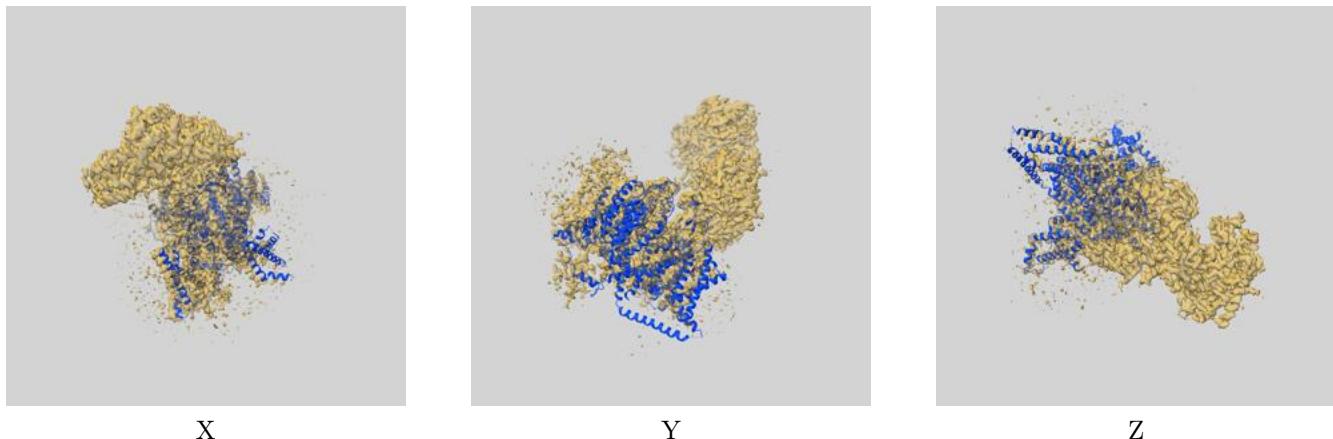
8 Fourier-Shell correlation

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

9 Map-model fit (i)

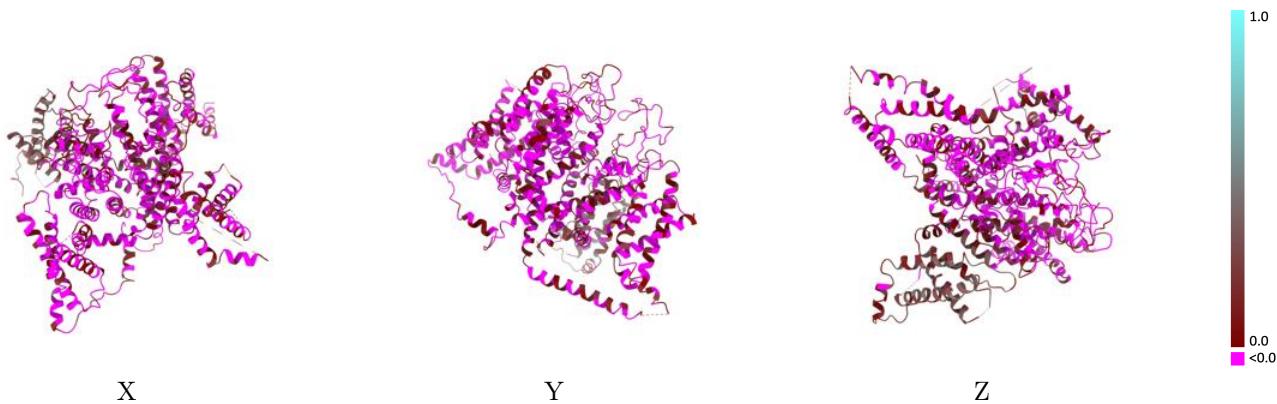
This section contains information regarding the fit between EMDB map EMD-9513 and PDB model 6BYO. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay (i)



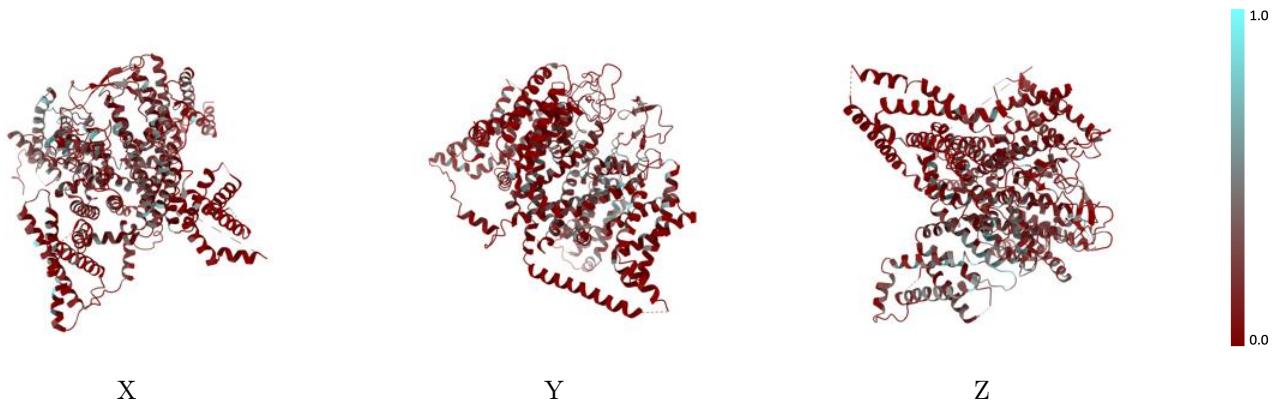
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



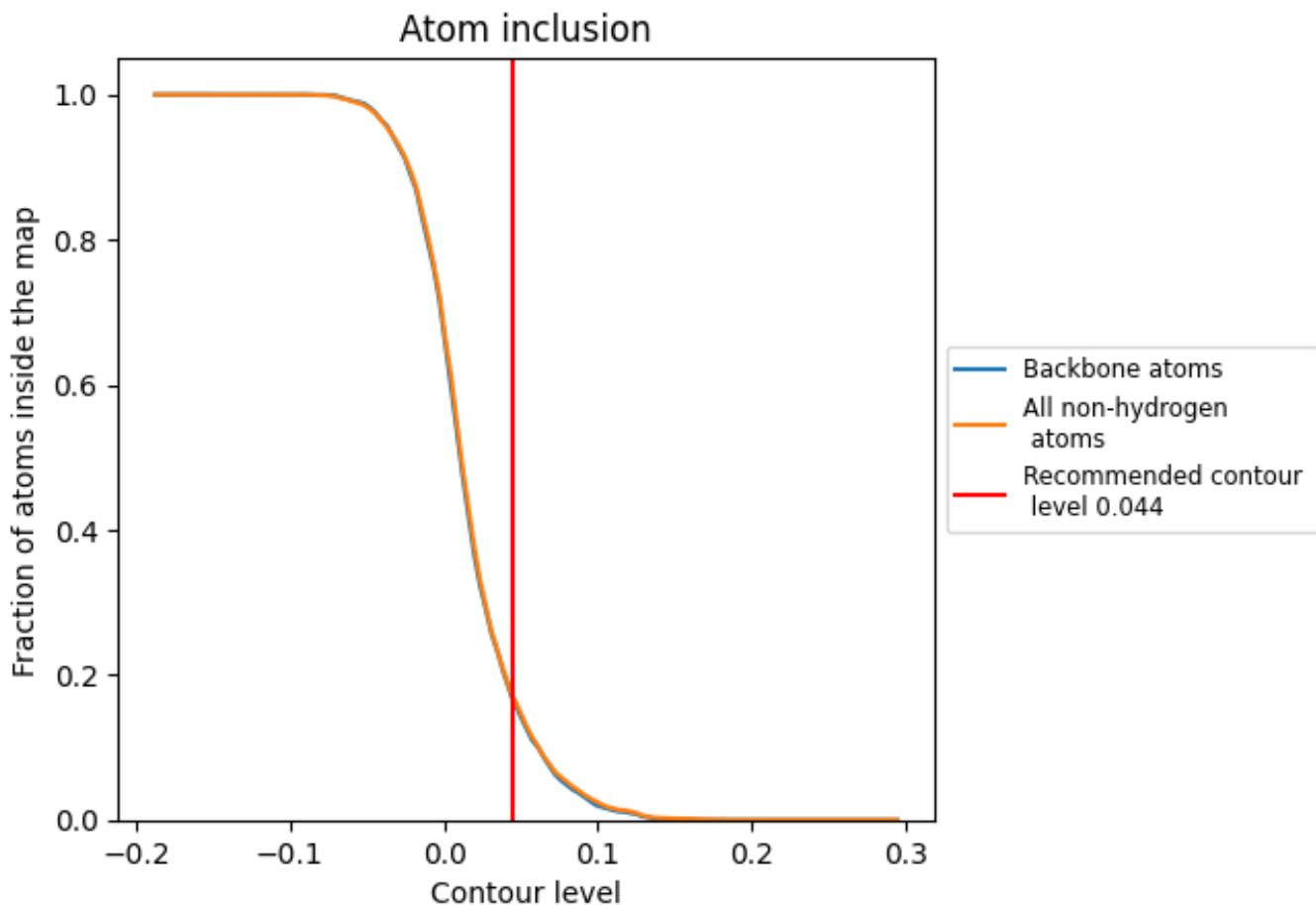
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	0.1729	-0.0110
A	0.1700	-0.0110

