



## wwPDB EM Validation Summary Report ⓘ

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 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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 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

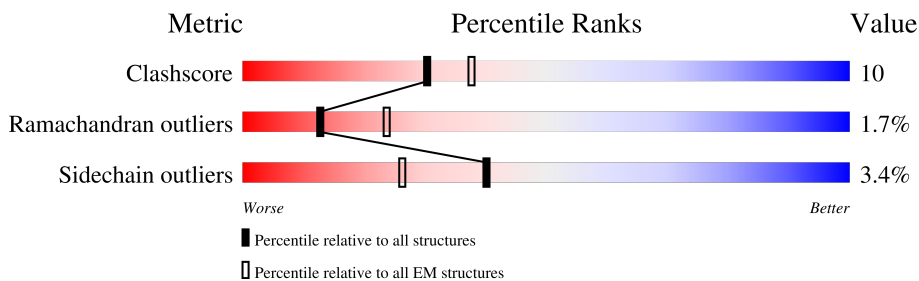
# 1 Overall quality at a glance

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  $\geq 3$ , 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	

## 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.

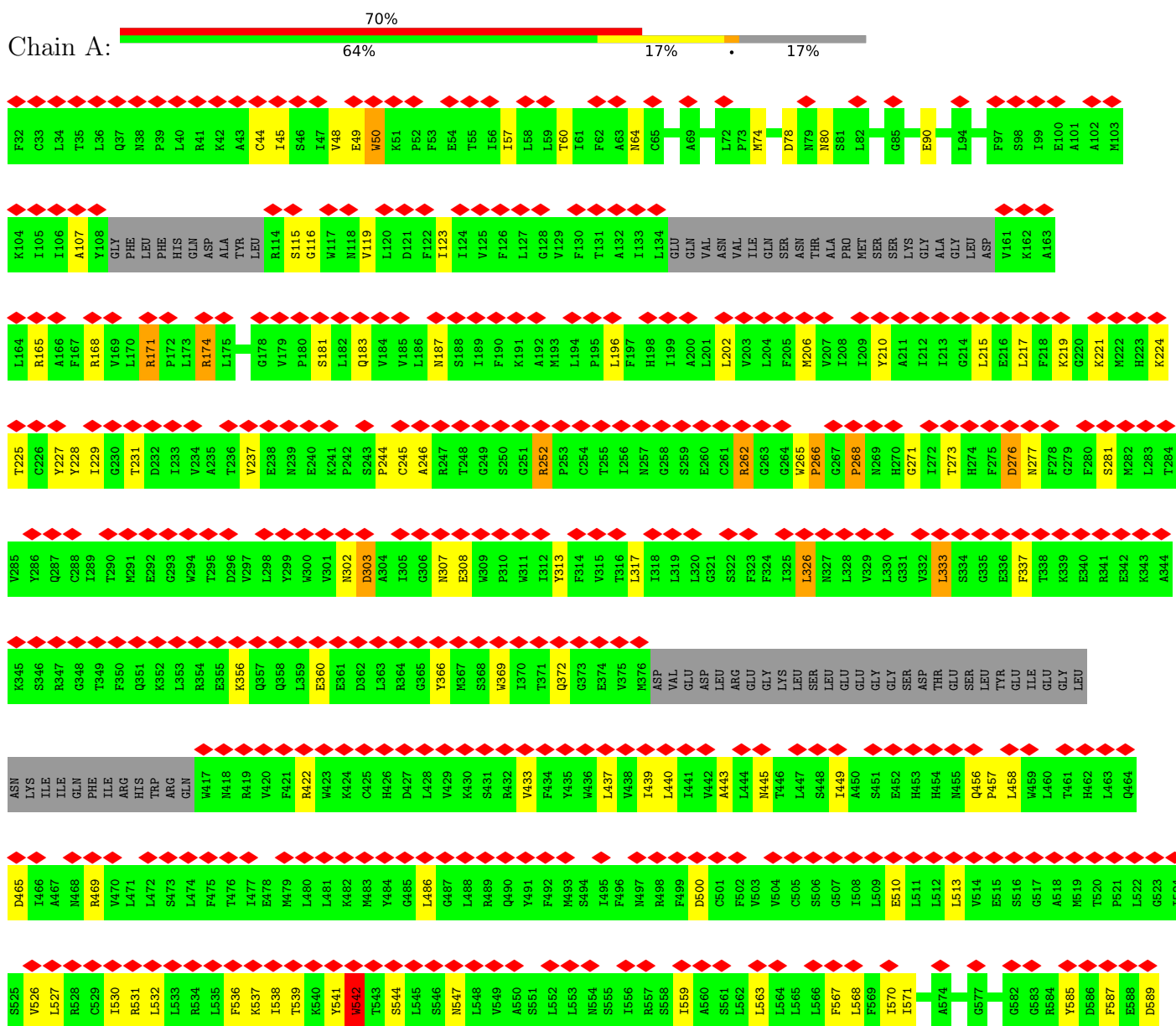
- Molecule 1 is a protein called Voltage-dependent L-type calcium channel subunit alpha-1S.

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

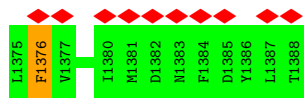
### 3 Residue-property plots

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



T590	E591	V592	R593	R594	S595	N596	F597	D598	N599	F600	Q602	A603	L604	I605	S606	V607	F608	Q609	V610	L611	T612	G613	E614	D615	S618	Y621	N622	M625	A626	Y627	G628	G629	P630	S631	Y632	P633	G634	V635	L636	V637	C638	F641	I642	L644	F645	V646	C647	G648	N649	Y650	I651	L652	L653								
M654	V655	F656	L657	A658	I659	A660	V661	D662	M663	L664	A665	E666	A667	E668	S669	LEU	THR	SER	ALA	GLN	LYS	ALA	LYS	ALA	E614	GLU	ARG	GLY	LYS	ARG	GLU	LYS	LEU	ARG	GLU	GLY	LYS	SER	VAL	LEU	ALA	GLN	LEU	LYS	LYS	ALA	VAL	GLN	PRO	LYS	GLY	GLY	GLY								
ILE	PRO	THR	THR	ALA	LYS	LEU	LYS	VAL	ASP	GLU	PHE	GLU	ASN	VAL	LYS	ASP	PRO	TYR	PRO	ALA	LYS	ALA	PHE	GLY	ASP	GLY	ARG	GLU	PRO	GLY	ILE	VAL	ARG	PRO	PRO	GLU	ALA	GLY	SER	LEU	LEU	VAL	PRO	PRO	LYS	GLY	GLY	ILE													
PRO	GLU	ALA	SER	SER	PHE	PHE	ILE	PHE	SER	PRO	THR	ASN	LYS	V788	R789	V790	L791	C792	H793	R794	I795	V796	N797	GLY	ALA	LEU	HIS	LYS	GLY	SER	PHE	CYS	R860	N861	Y862	F863	N864	I865	L866	D867	A814	A815	L816	A817	A818	E819	D820	P821	I822	R823	A824	E825	S826	E827	N829	O830	I831	L832	G833		
Y834	F835	D836	I837	A838	F839	T840	S841	H842	F843	T844	V845	E846	I847	V848	L849	M851	T852	T853	Y854	GLY	PHE	LEU	ALA	LEU	HIS	LYS	GLY	SER	PHE	CYS	R860	N861	Y862	F863	N864	I865	L866	D867	A814	A815	L816	A817	A818	E819	D820	P821	I822	R823	A824	E825	S826	E827	N829	O830	I831	L832	G833				
R894	T895	L896	R897	H898	L899	R900	V901	L902	R903	P904	L905	R906	A907	I908	N909	R910	A911	R912	G913	V914	L914	R915	H916	V917	V918	Q919	C920	V921	F922	V923	A924	R925	R926	T927	N928	G929	N930	I931	V932	L933	V934	T935	T936	L937	L938	Q939	F940	H941	F942	A943	A944	I945	G946	V947	THR	ILE	SER	V892	V893		
F954	F955	S956	C957	N958	D959	L960	S961	K962	M963	T964	E965	E966	E967	C968	R969	G970	Y971	Y972	Y973	V974	Y975	K976	D977	G978	D979	T981	Q982	N983	E984	L985	A924	R986	P987	R988	Q989	Q990	I991	H992	N993	D994	F995	H996	F997	D998	N999	V1000	L1001	S1002	A1003	M1004	M1005	S1006	L1007	F1008	T1009	V1010	S1011	T1012	F1013		
E1014	G1015	W1016	Q1017	Q1018	L1019	L1020	Y1021	R1022	A1023	I1024	D1025	S1026	N1027	E1028	E1029	D1030	M1031	C1032	P1033	V1034	Y1035	M1036	M1037	R1038	V1039	E1040	M1041	A1042	I1043	F1044	F1045	I1046	I1047	Y1048	I1049	I1050	L1051	I1052	A1053	F1054	F1055	M1056	M1057	M1058	I1059	V1060	V1061	G1062	F1063	V1064	I1065	V1066	T1067	F1068	Q1069	E1070	Q1071	G1072	E1073		
T1074	E1075	Y1076	K1077	M1078	C1079	E1080	L1081	D1082	K1083	M1084	Q1085	R1086	Q1087	C1088	V1089	Q1090	Y1091	A1092	L1093	K1094	A1095	R1096	P1097	L1098	R1099	C1100	Y1101	I1102	P1103	K1104	N1105	P1106	Y1107	Q1108	Y1109	Q1110	V1111	W1112	Y1113	V1114	V1115	T1116	S1117	S1118	Y1119	F1120	E1121	Y1122	L1123	M1124	F1125	A1126	L1127	I1128	M1129	L1130	T1131	L1132	I1133		
C1134	L1135	G1136	M1137	Q1138	H1139	Y1140	H1141	Q1142	S1143	E1144	E1145	M1146	N1147	H1148	S1150	D1151	L1152	L1153	M1154	V1155	A1156	F1157	T1158	I1159	I1160	F1161	T1162	L1163	E1164	M1165	I1166	L1167	K1168	L1169	L1170	A1171	F1172	K1173	A1174	R1175	G1176	Y1177	F1178	F1179	D1180	P1181	W1182	M1183	V1184	F1185	D1186	F1187	L1188	I1189	V1190	I1191	G1192	S1193			
I1194	I1195	I1196	L1197	L1198	S1200	E1201	I1202	D1203	T1204	F1205	LEU	ALA	SER	SER	GLY	LEU	TYR	CYS	GLY	GLY	CYS	GLY	ASN	VAL	ASP	PRO	ASP	GLU	SER	ALA	R1229	I1230	S1231	S1232	A1233	F1234	F1235	R1236	L1237	F1238	R1239	V1240	M241	M242	L1243	I1244	K1245	R1242	L1243	I1244	K1245	L1246	L1247	S1248	R1249	A1250	E1251	G1252	V1253	R1254	
T1255	L1256	L1257	W1258	T1259	F1260	I1261	K1262	S1263	A1264	Q1265	A1266	L1267	P1268	Y1269	V1270	A1271	L1272	L1273	I1274	V1275	M1276	L1277	F1278	F1279	I1280	Y1281	A1282	V1283	I1284	G1285	M1286	Q1287	M1288	F1289	G1290	K1291	I1292	A1293	L1294	V1295	D1296	G1297	T1298	L1299	I1300	N1301	R1302	N1303	N1304	N1305	F1306	Q1307	T1308	F1309	C1368	A1369	F1370	Q1311	A1312	V1313	L1314
L1315	L1316	F1317	R1318	C1319	A1320	T1321	G1322	E1323	A1324	W1325	Q1326	E1327	I1328	L1329	A1331	C1332	S1333	Y1334	G1335	K1336	L1337	C1338	D1339	P1340	E1341	S1342	D1343	Y1344	A1345	P1346	G1347	E1348	E1349	Y1350	T1351	C1352	G1353	M1355	F1356	A1357	Y1358	Y1359	Y1360	F1361	I1362	S1363	F1364	Y1365	M1366	L1367	C1368	A1369	F1370	L1371	I1372	V1373	M1374				



## 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 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

The worst 5 of 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

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	TYR	Peptide
1	A	229	ILE	Peptide
1	A	237	VAL	Peptide
1	A	266	PRO	Peptide

*Continued on next page...*



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Mol	Chain	Res	Type	Group
1	A	268	PRO	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.

The worst 5 of 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
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

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%)	<b>9</b>   45

5 of 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

### 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

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1199	LEU
1	A	1249	ARG
1	A	1306	PHE
1	A	800	TRP
1	A	794	ARG

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.

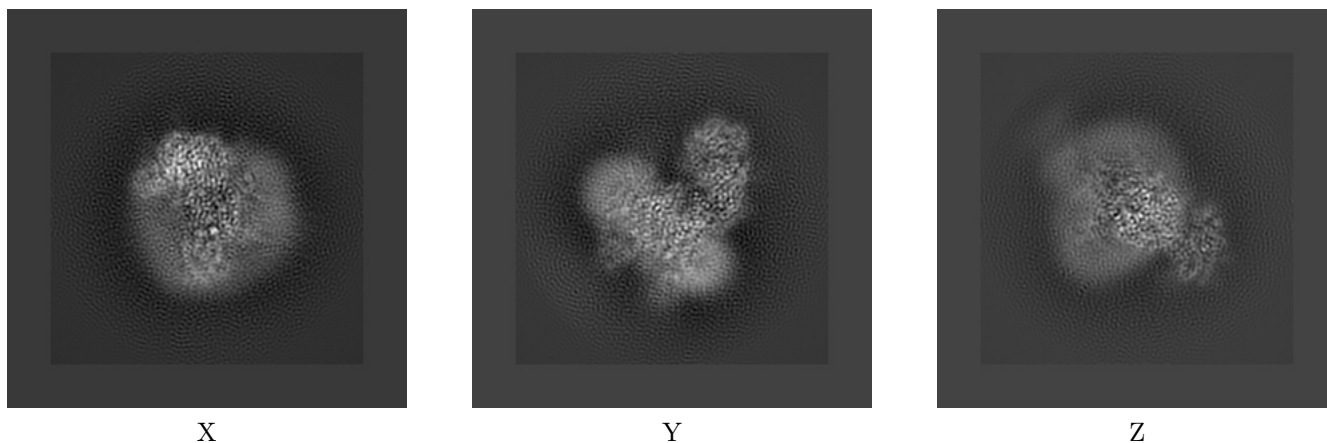
## 6 Map visualisation [i](#)

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](#)

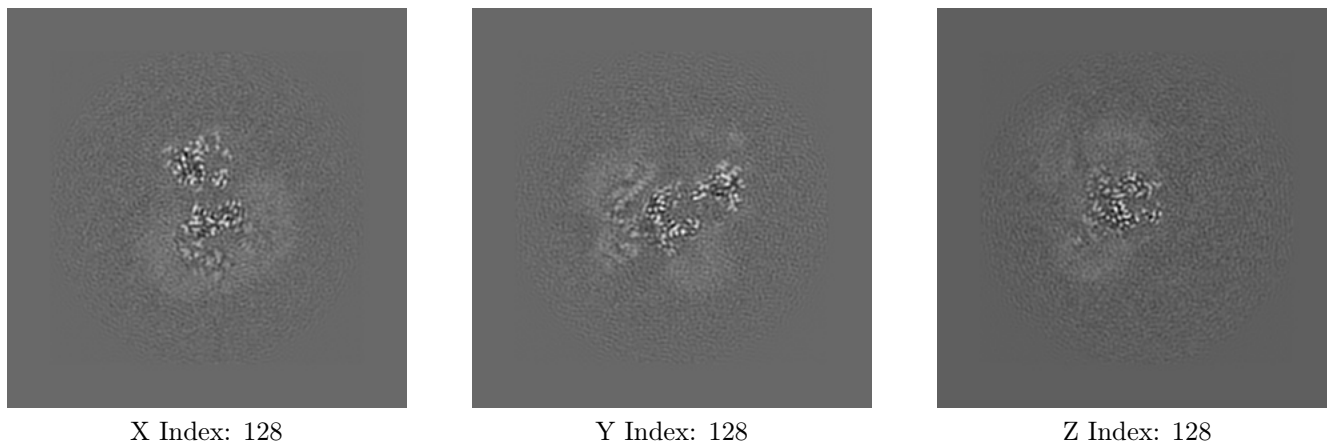
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

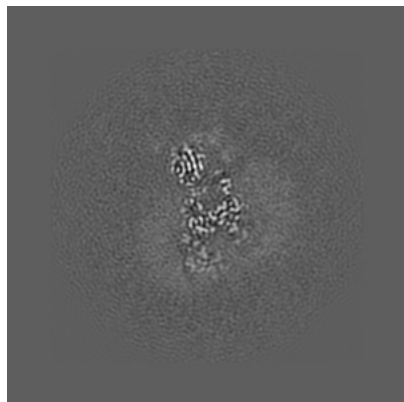
#### 6.2.1 Primary map



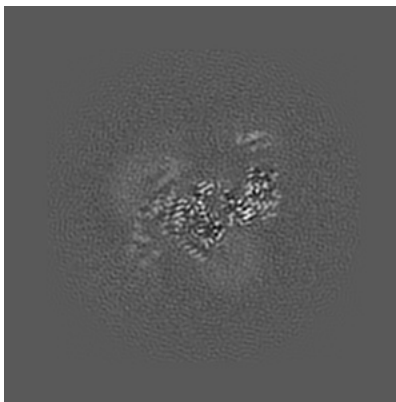
The images above show central slices of the map in three orthogonal directions.

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

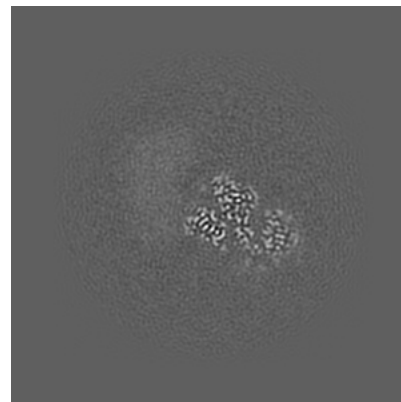
### 6.3.1 Primary map



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.

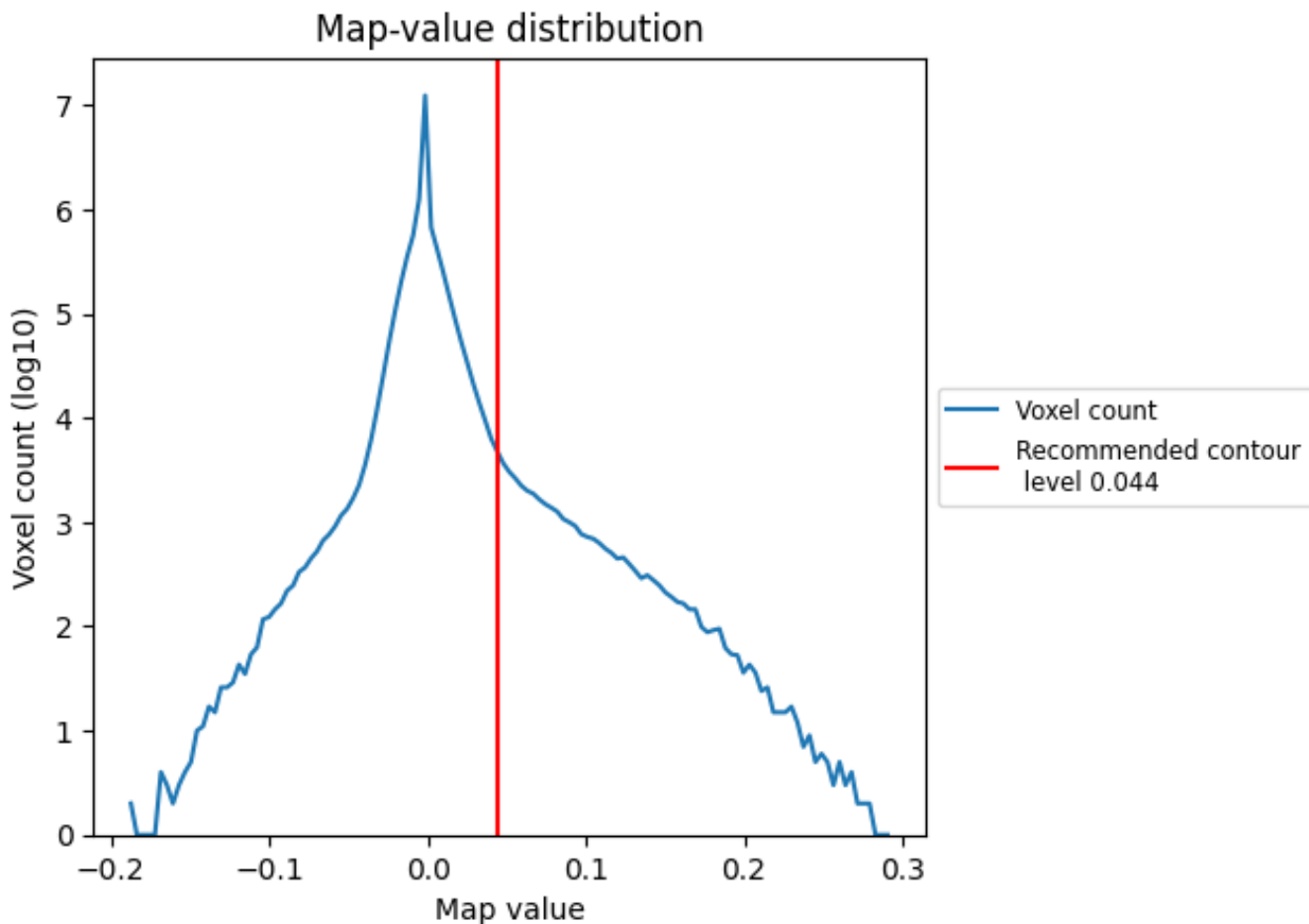
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

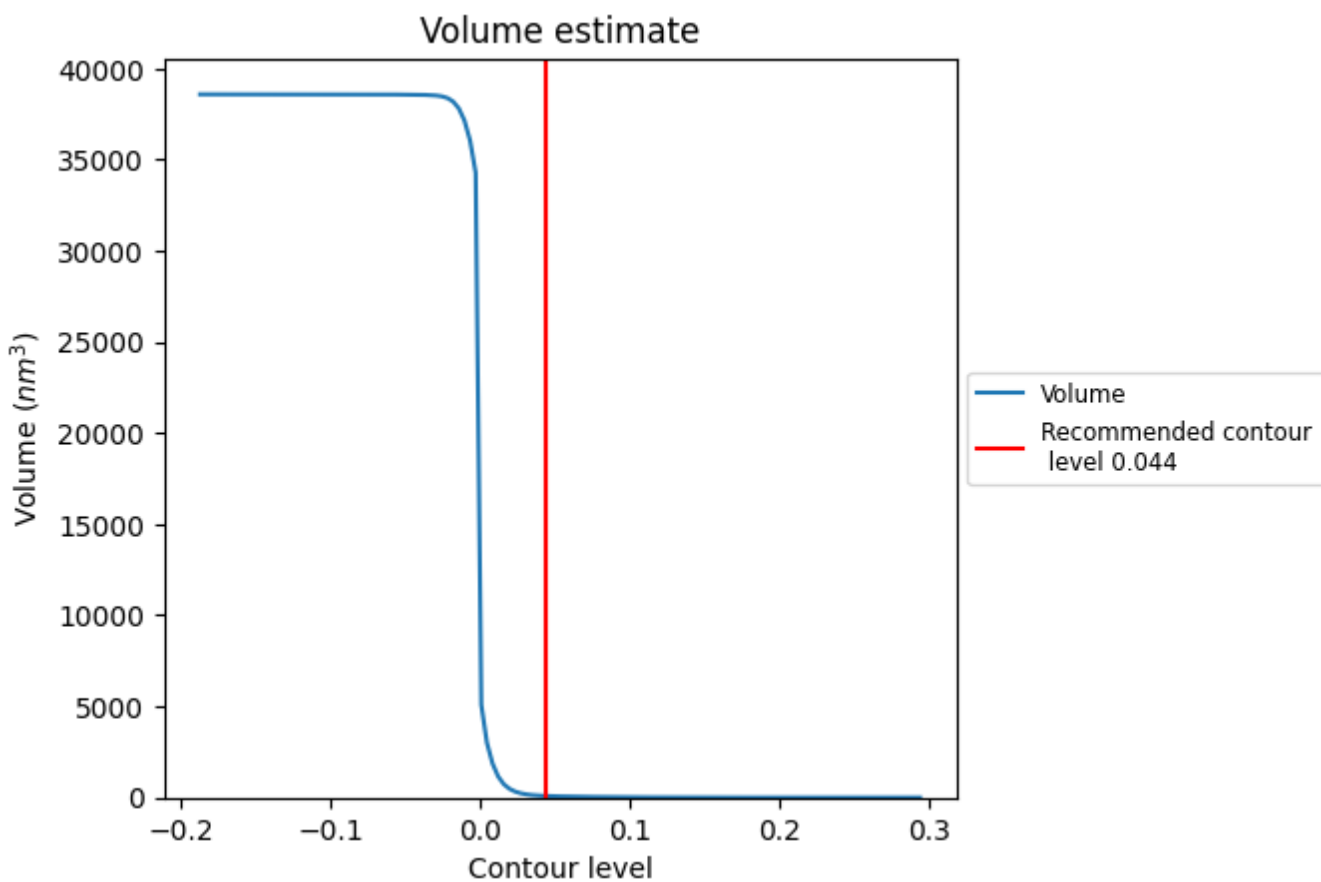
This section contains the results of statistical analysis of the map.

### 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](#)

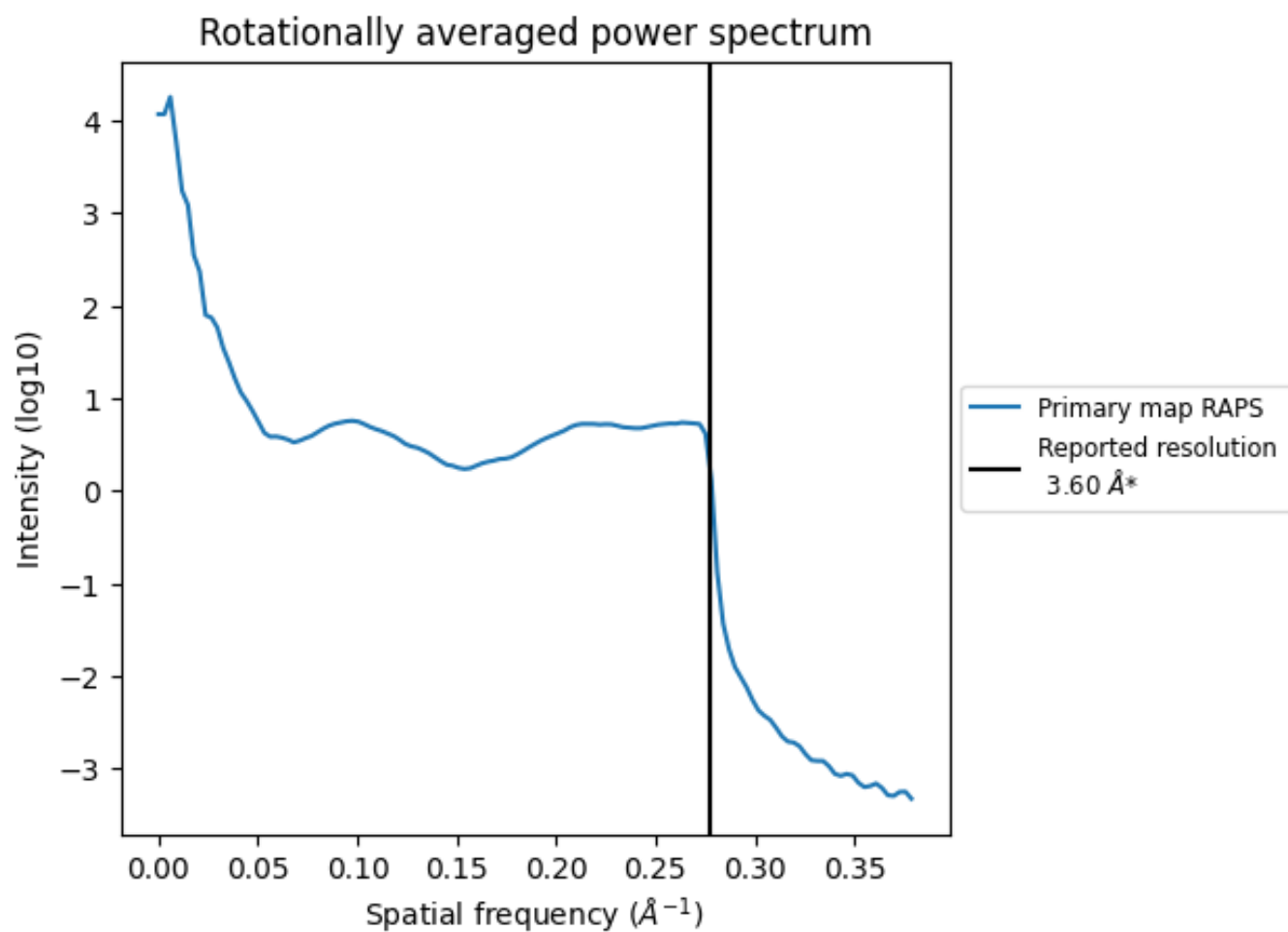


The volume at the recommended contour level is 87 nm<sup>3</sup>; this corresponds to an approximate mass of 79 kDa.

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  $0.278 \text{\AA}^{-1}$

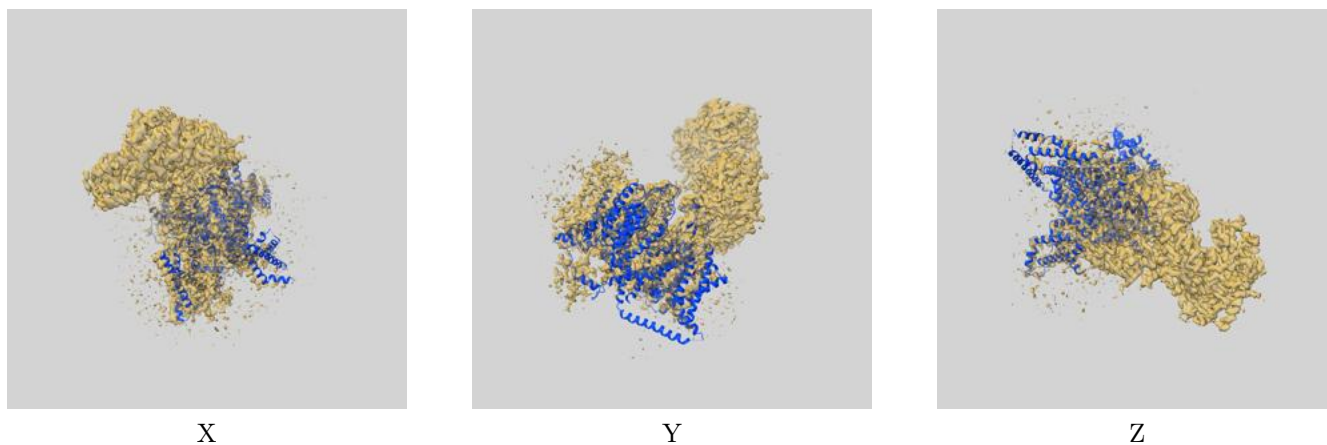
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

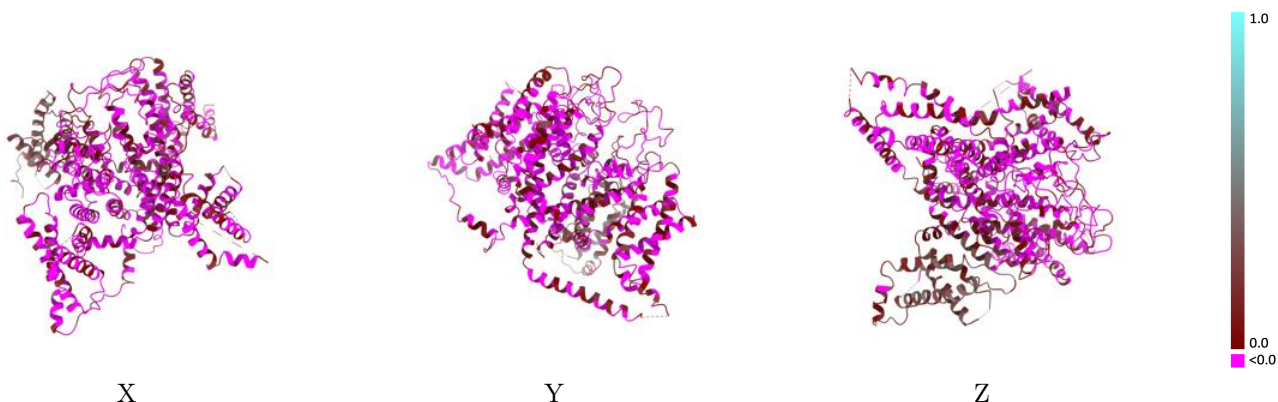
This section contains information regarding the fit between EMDB map EMD-9513 and PDB model 6BYO. Per-residue inclusion information can be found in section [3](#) on page [4](#).

### 9.1 Map-model overlay [i](#)



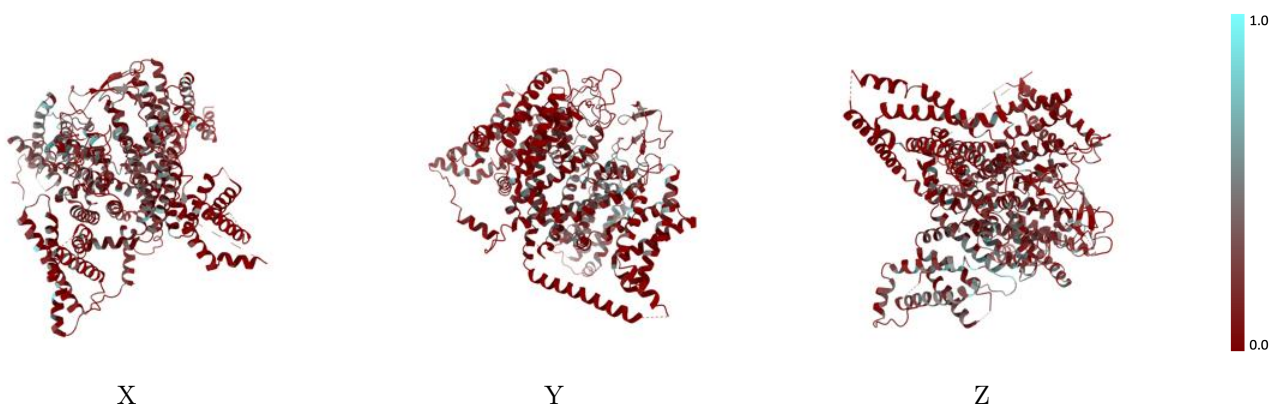
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



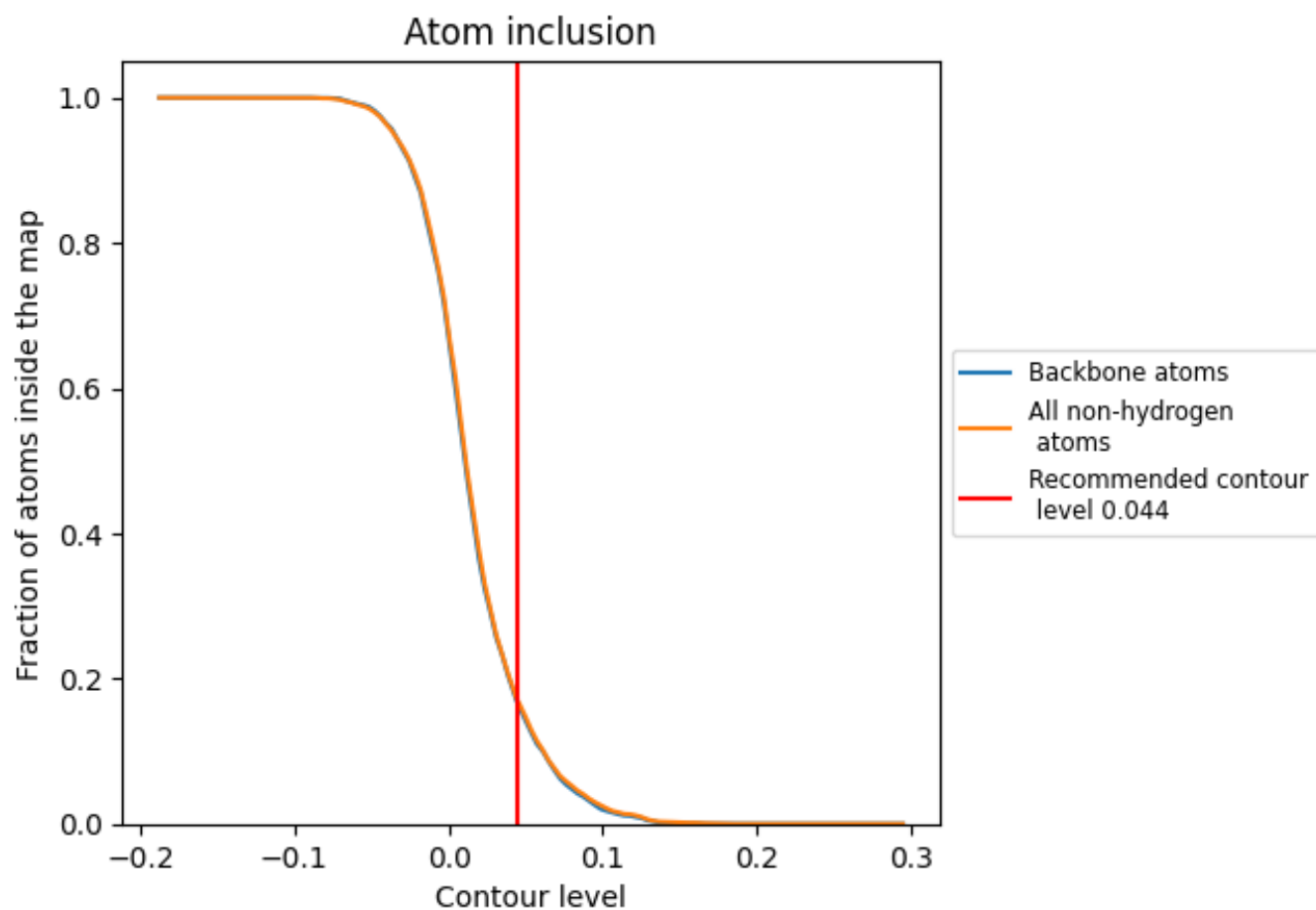
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

