



## wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 02:45 AM UTC

PDB ID : 7WLU / pdb\_00007wlu  
EMDB ID : EMD-32593  
Title : The Flattened Structure of mPIEZO1 in Lipid Bilayer  
Authors : Yang, X.; Lin, C.; Chen, X.; Li, S.; Li, X.; Xiao, B.  
Deposited on : 2022-01-13  
Resolution : 6.81 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:

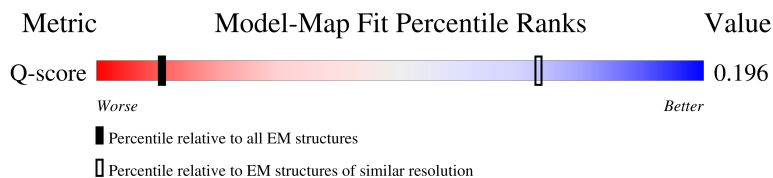
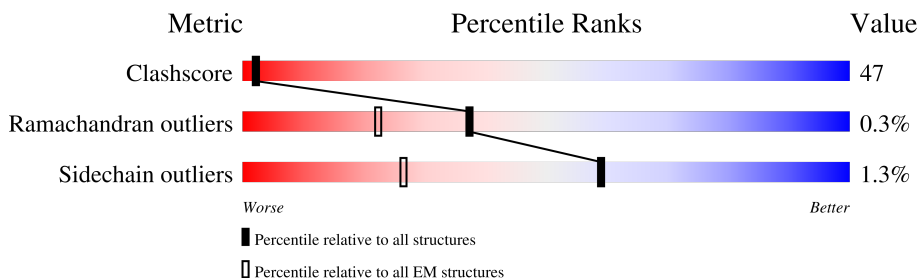
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.81 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	464 ( 6.31 - 7.30 )

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	2547	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">15%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">27%</div> <div style="text-align: center;">32%</div> <div style="text-align: center;">•</div> <div style="text-align: center;">41%</div> </div>
1	C	2547	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">15%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">27%</div> <div style="text-align: center;">32%</div> <div style="text-align: center;">•</div> <div style="text-align: center;">41%</div> </div>
1	E	2547	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">15%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">27%</div> <div style="text-align: center;">31%</div> <div style="text-align: center;">•</div> <div style="text-align: center;">41%</div> </div>

## 2 Entry composition [i](#)

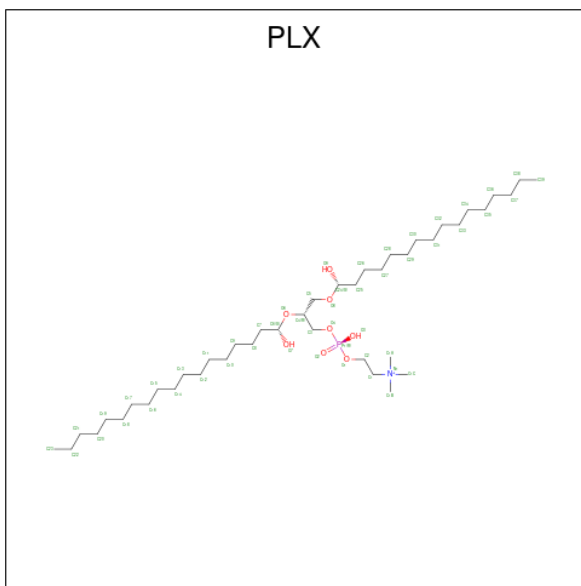
There are 2 unique types of molecules in this entry. The entry contains 34761 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1498	11535	7496	1973	2005	61	0	0
1	C	1498	11535	7496	1973	2005	61	0	0
1	E	1498	11535	7496	1973	2005	61	0	0

- Molecule 2 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOXOL (CCD ID: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	52	42	1	8	1	0
2	C	1	52	42	1	8	1	0

*Continued on next page...*

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	E	1	52	42	1	8	1	0

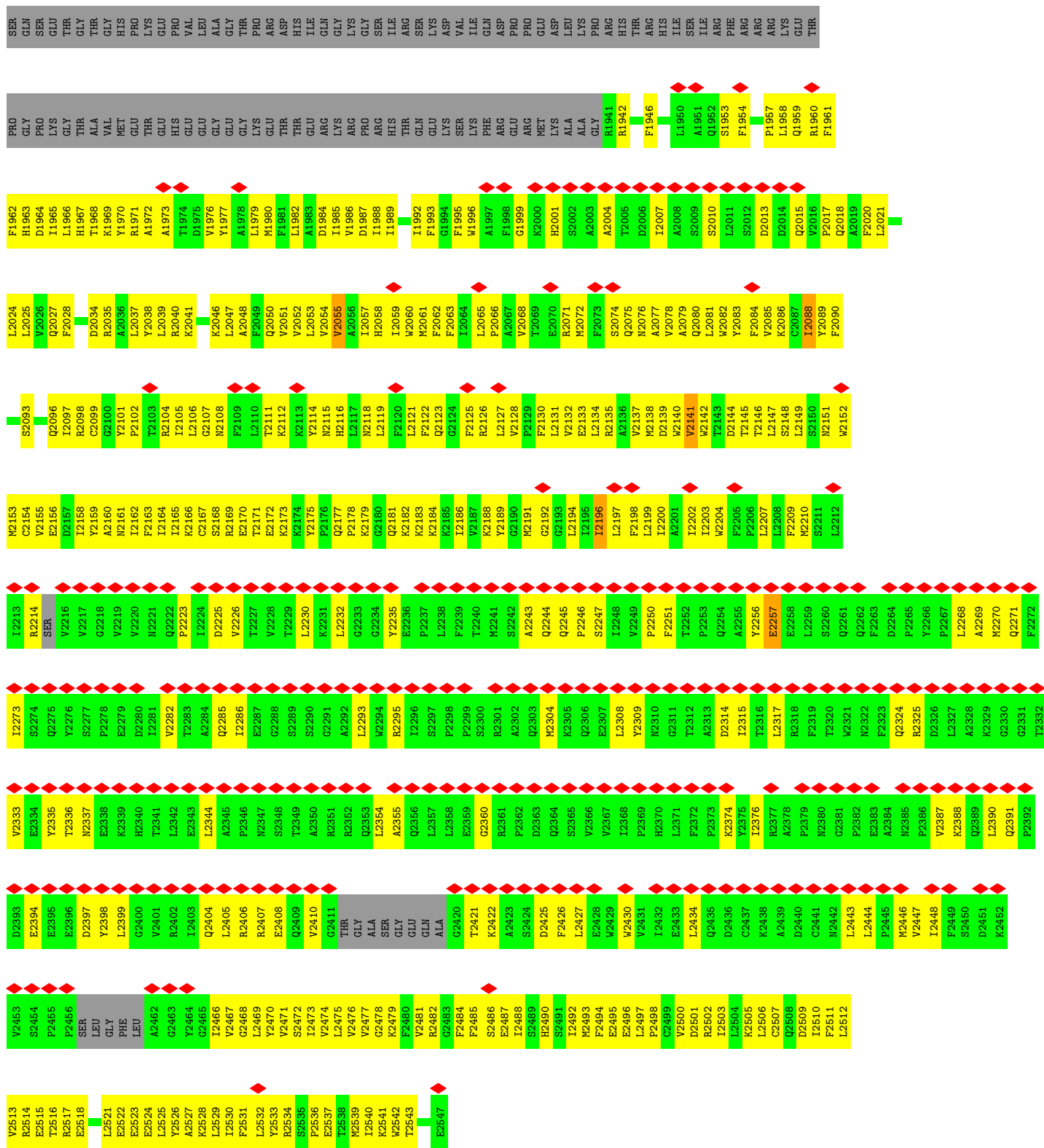


L815	V827	M828	N829	W836	A837	F838	P841	R844	F845	K870	I871	V872	N873	N874	HIS	GLU	GLN	TRP	SER	SER	ASN	ASN	THR	THR	THR	GLU	PRO	PHE	PRO	PRO	ASN	THR	ASN	ASN	LEU	GLN	PRO	LEU	GLU	ILE	ASN	GLN	SER	LEU	LEU	TYR	ARG	GLY	PRO	VAL	ASP	PRO	PRO	ALA	ALA	TRP	F912	H951																																																																																																																			
GLN	GLN	ALA	L1016	PRO	L1017	LEU	L1018	PRO	ALA	L1020	ALA	L1021	GLN	L1022	VAL	L1082	CYS	R1024	ALA	ALA	R1025	ASP	S985	T966	R967	Q968	R1031	R969	L970	D973	L974	S976	C977	L978	R979	Y980	F981	L982	N983	F984	F985	L1045	F986	Y987	K988	F989	L991	E992	F995	L996	M997	A998	Y999	N1000	V1001	Q1020	C1059	G1003	Q1004	Y1062	R1005	M1006	M1007	F1008	R1065	M1009	V1010	L1011	L1012	H1013																																																																																																							
G1014	C1015	W1016	L1017	V1018	A1019	I1020	L1021	L1022	R1023	VAL	R1024	ALA	R1025	E1027	A1028	I1029	A1030	Q968	R1031	L1032	W1033	W1034	N1035	L1036	C1037	L1038	F1039	L1040	T1041	L1042	F1043	L1044	L1045	L1046	Q1047	L1048	L1049	L1050	L1052	L1053	G1054	M1054	P1055	P1056	A1057	L1058	Q1120	R1121	M1122	A1123	GLY	ILE	ASN	THR	W1064	ASP	R1065	HIS	V1066	W1067	L1068	L1069	L1070	M1071	M1072	N1073																																																																																																											
S1074	A1075	I1077	K1078	W1079	L1080	Y1081	L1082	P1083	F1086	A1087	A1088	P1089	M1090	S1091	T1092	M1093	L1094	I1095	S1096	D1097	F1098	L1099	L1100	L1101	L1102	S1105	Q1106	Q1107	W1108	Q1109	V1110	F1111	S1112	A1113	E1114	R1115	T1116	E1117	E1118	W1119	Q1120	R1121	M1122	A1123	GLY	ILE	ASN	THR	W1176	Y1177	S1178	R1179	G1181	L1182	G1183	Y1184	L1185	L1186	A1187	C1188	F1189	Y1190	L1191	L1192	L1193	G1194	G1195	L1196	G1135																																																																																																								
E1136	P1137	M1138	P1139	I1140	P1141	M1142	F1143	I1144	H1145	L1146	R1147	S1148	Y1149	L1150	D1151	M1152	L1153	K1154	V1155	A1156	V1157	F1158	R1159	Y1160	L1161	F1162	W1163	L1164	V1165	L1166	V1167	V1168	V1169	F1170	V1171	A1172	T1175	R1176	I1177	S1178	F1180	G1181	L1182	G1183	Y1184	L1185	L1186	A1187	C1188	F1189	Y1190	L1191	L1192	L1193	G1194	G1195	L1196	T1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	W1210	D1211	C1212	L1213	L1214	L1215	Y1216	M1217	V1218	T1219	I1220	I1221	I1222	S1223	K1224	M1225	M1226	L1227	L1228	L1229	L1230	S1231	C1232	V1233	E1236	Q1237	M1238	Q1239	S1240	N1241	F1242	C1243	W1244	V1245	I1246	Q1247	L1248	F1249	S1250	L1251	V1252	V1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	D1282	S1284	I1285	C1286	F1287	F1288	F1289	L1290	L1291	L1292	L1293	R1294	R1295	I1296	F1297	F1302	L1303	H1304	V1305	S1306	A1307	D1308	L1309	K1310	A1311	T1312	A1313	L1314	Q1315	A1316	S1317	R1318	G1319	F1320	A1321
T1197	L1198	L1199	Q1200	K1201	D1202	T1203	R1204	A1205	L1206	L1207	V1208	L1209	W1210	D1211	C1212	L1213	L1214	L1215	Y1216	M1217	V1218	T1219	I1220	I1221	I1222	S1223	K1224	M1225	M1226	L1227	L1228	L1229	L1230	S1231	C1232	V1233	E1236	Q1237	M1238	Q1239	S1240	N1241	F1242	C1243	W1244	V1245	I1246	Q1247	L1248	F1249	S1250	L1251	V1252	V1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	D1282	S1284	I1285	C1286	F1287	F1288	F1289	L1290	L1291	L1292	L1293	R1294	R1295	I1296	F1297	F1302	L1303	H1304	V1305	S1306	A1307	D1308	L1309	K1310	A1311	T1312	A1313	L1314	Q1315	A1316	S1317	R1318	G1319	F1320	A1321																																																										
TYR	ASP	PRO	LYS	GLU	MET	MET	THR	ARG	ASP	ASP	ASP	CYS	LEU	LEU	PRO	PRO	VAL	GLU	E1277	A1278	G1279	I1280	W1281	D1282	S1284	I1285	C1286	F1287	F1288	F1289	L1290	L1291	L1292	L1293	R1294	R1295	I1296	F1297	F1302	L1303	H1304	V1305	S1306	A1307	D1308	L1309	K1310	A1311	T1312	A1313	L1314	Q1315	A1316	S1317	R1318	G1319	F1320	A1321																																																																																																																			
L1322	Y1323	M1324	A1325	L1328	K1329	S1330	I1331	M1332	F1333	H1334	R1335	Q1336	I1337	E1338	E1339	K1340	S1341	L1342	A1343	Q1344	L1345	K1346	R1347	Q1348	M1349	K1350	R1351	I1352	R1353	A1354	K1355	L1356	E1357	K1358	R1359	Q1361	S1362	Q1363	A1364	SER	ARG	GLY	GLN	LEU	GLM	GLM	SER	LYS	ASP	ASP	PRO	ALA	ALA	ALA	GLN	GLN	ASP	Q1337	F1438	Q1439	M1440	A1441	Y1442																																																																																																														
PRO	ASP	SER	PRO	GLY	SER	SER	PRO	PRO	PRO	ARG	GLN	TRP	TRP	TRP	TRP	TRP	D1401	D1402	A1403	A1404	T1405	V1406	F1407	H1408	S1409	G1410	D1411	Y1412	F1413	L1414	F1415	E1416	S1417	D1418	GLU	GLU	GLU	GLU	GLU	ALA	ALA	LEU	PRO	GLU	ASP	MET	ALA	G1490	M1494	M1495	Q1496	R1497	T1501	M1502	Q1503	F1504	L1505	W1506	V1507	L1508	G1509																																																																																																																
Q1443	V1446	T1447	T1451	W1452	L1453	R1454	Q1455	R1456	R1457	A1458	R1459	A1460	R1461	Q1462	Q1463	R1464	A1465	E1466	Q1467	L1468	ALA	SER	GLY	GLY	ASP	ASN	ASN	PRO	L1540	L1541	T1542	THR	GLY	E1544	L1545	L1546	G1549	E1549	F1550	V1551	R1552	R1553	G1554	V1555	L1556	D1557	Q1558	L1559	TYR	VAL	GLY	GLU	GLN	ASP	GLU	ALA	THR	SER	THR	ALA	LEU	LEU	LEU	GLY	GLY																																																																																																												
Q1510	A1511	T1512	V1513	D1514	G1515	L1516	R1517	W1518	W1519	L1520	R1521	A1522	F1523	T1524	K1525	L1526	H1527	R1528	T1529	M1530	S1531	L1532	V1533	L1534	C1535	A1536	E1537	R1538	Y1539	L1540	L1541	T1542	THR	GLY	E1544	L1545	L1546	G1549	E1549	F1550	V1551	R1552	R1553	G1554	V1555	L1556	D1557	Q1558	L1559	TYR	VAL	GLY	GLU	GLN	ASP	GLU	ALA	THR	SER	THR	ALA	LEU	LEU	GLY	GLY																																																																																																												
PRO	VAL	GLU	THR	ARG	ASP	GLY	PRO	ALA	ARG	ARG	ALA	SER	SER	GLY	LEU	GLY	ALA	GLU	PRO	LEU	SER	SER	MET	THR	ASP	ASP	THR	SER	SER	PRO	LEU	SER	THR	GLY	TYR	ASN	THR	THR	ARG	SER	GLY	SER	GLU	GLU	ILE	VAL	THR	THR	ASP	ALA	GLY	GLY	ASP	LEU	GLN	ALA	GLY	THR	SER	THR	ALA	LEU	LEU	HIS	GLY																																																																																																												
SER	GLN	GLU	LEU	LEU	ALA	ASN	ALA	ARG	THR	ARG	MET	ARG	ARG	THR	THR	THR	THR	ASP	ASP	ASP	THR	SER	SER	THR	PRO	LEU	LEU	LEU	LEU	THR	THR	GLY	TYR	ASN	THR	THR	ARG	SER	GLY	SER	GLU	GLU	ILE	VAL	THR	THR	ASP	ALA	GLY	GLY	ASP	LEU	GLN	ALA	GLY	THR	SER	THR	ALA	LEU	LEU	HIS	GLY																																																																																																														
R1657	E1658	L1659	E1660	E1661	A1662	E1663	R1664	F1665	E1666	A1667	Q1668	Q1669	G1670	R1671	T1672	R1677	A1678	G1679	Y1680	Q1681	C1682	V1683	H1686	S1687	E1688	L1689	L1690	C1691	Y1692	F1693	I1694	L1695	I1696	L1697	N1698	H1699	M1700																																																																																																																																								

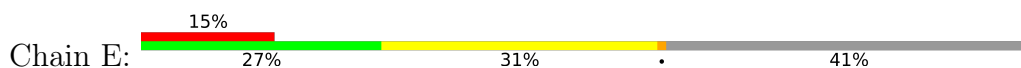






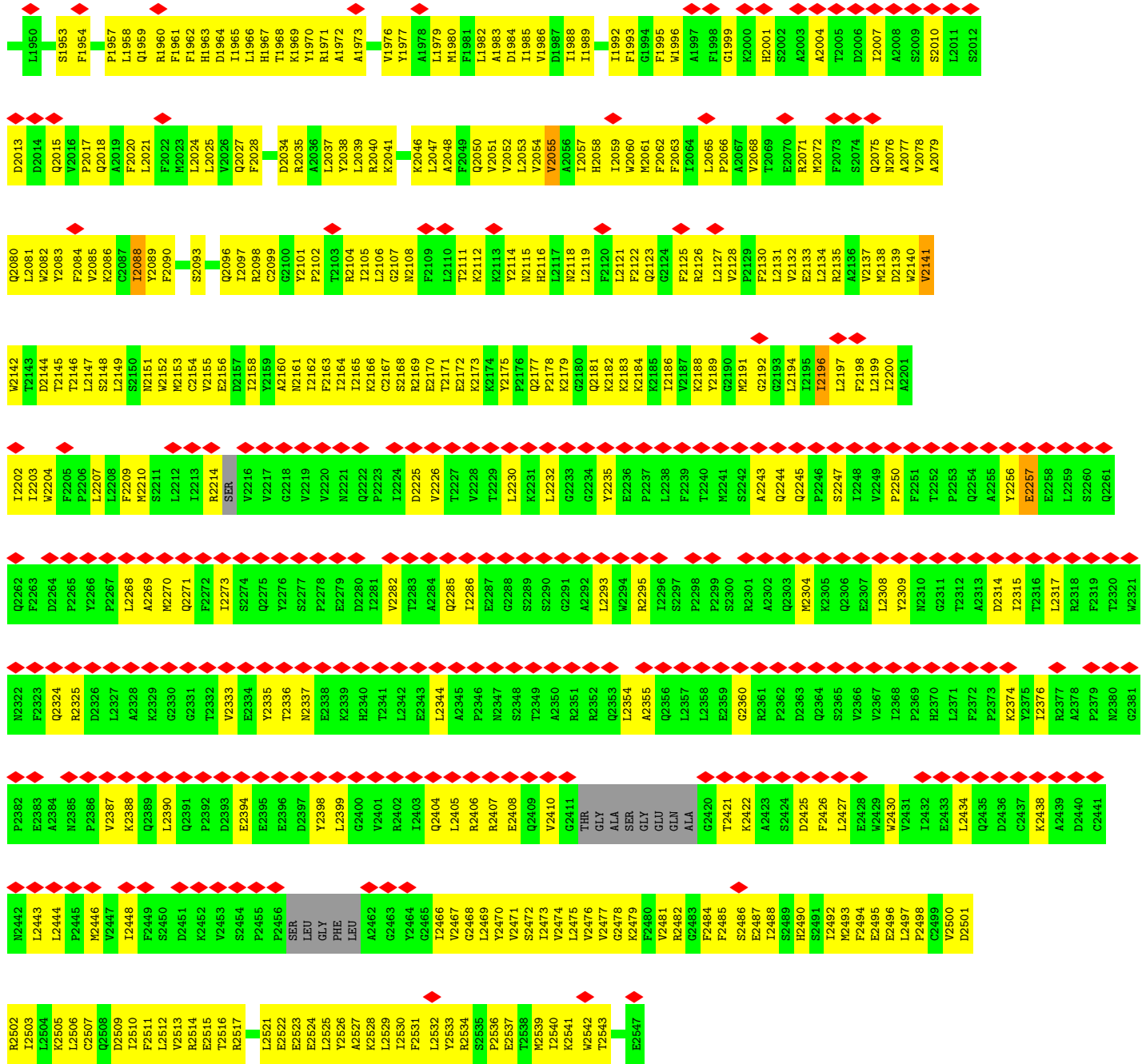


• Molecule 1: Piezo-type mechanosensitive ion channel component 1









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.137	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size ( $\text{\AA}$ )	395.28003, 395.28003, 395.28003	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.196, 2.196, 2.196	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLX

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	0.43	0/11796	0.78	3/16031 (0.0%)
1	C	0.43	0/11796	0.78	3/16031 (0.0%)
1	E	0.43	0/11796	0.78	3/16031 (0.0%)
All	All	0.43	0/35388	0.78	9/48093 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1410	GLY	N-CA-C	7.31	119.91	111.36
1	E	1410	GLY	N-CA-C	7.30	119.91	111.36
1	C	1410	GLY	N-CA-C	7.29	119.89	111.36
1	C	1738	GLU	N-CA-CB	5.56	118.39	110.16
1	A	1738	GLU	N-CA-CB	5.54	118.36	110.16

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11535	0	10972	1070	0
1	C	11535	0	10972	1080	0
1	E	11535	0	10972	1063	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	52	0	88	3	0
2	C	52	0	88	3	0
2	E	52	0	88	2	0
All	All	34761	0	33180	3163	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 47.

The worst 5 of 3163 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:1700:MET:SD	1:A:2080:GLN:HB3	1.29	1.69
1:E:1700:MET:SD	1:E:2080:GLN:HB3	1.29	1.68
1:C:1700:MET:SD	1:C:2080:GLN:HB3	1.29	1.66
1:E:1700:MET:SD	1:E:2080:GLN:CB	2.22	1.28
1:A:1700:MET:SD	1:A:2080:GLN:CB	2.22	1.27

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	1468/2547 (58%)	1376 (94%)	88 (6%)	4 (0%)	36	72
1	C	1468/2547 (58%)	1376 (94%)	88 (6%)	4 (0%)	36	72
1	E	1468/2547 (58%)	1376 (94%)	88 (6%)	4 (0%)	36	72
All	All	4404/7641 (58%)	4128 (94%)	264 (6%)	12 (0%)	37	72

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	625	TYR
1	C	625	TYR
1	E	625	TYR
1	A	605	VAL
1	C	605	VAL

### 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	1117/2246 (50%)	1103 (99%)	14 (1%)	61 74
1	C	1117/2246 (50%)	1103 (99%)	14 (1%)	61 74
1	E	1117/2246 (50%)	1103 (99%)	14 (1%)	61 74
All	All	3351/6738 (50%)	3309 (99%)	42 (1%)	59 74

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1005	ARG
1	E	1713	LEU
1	E	1018	VAL
1	E	1403	HIS
1	E	2088	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2118	ASN
1	E	1138	ASN
1	E	1109	GLN
1	E	1300	HIS
1	A	2118	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLX	C	2601	-	51,51,51	1.18	4 (7%)	53,59,59	0.87	1 (1%)
2	PLX	A	2601	-	51,51,51	1.18	4 (7%)	53,59,59	0.87	1 (1%)
2	PLX	E	2601	-	51,51,51	1.18	4 (7%)	53,59,59	0.87	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLX	C	2601	-	-	12/55/55/55	-
2	PLX	A	2601	-	-	12/55/55/55	-
2	PLX	E	2601	-	-	12/55/55/55	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2601	PLX	O6-C4	-2.76	1.41	1.44
2	E	2601	PLX	O6-C4	-2.76	1.41	1.44
2	A	2601	PLX	O6-C4	-2.73	1.41	1.44
2	C	2601	PLX	C7-C6	2.53	1.56	1.50
2	E	2601	PLX	C7-C6	2.52	1.56	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2601	PLX	C26-C25-C24	-2.40	107.79	113.38
2	A	2601	PLX	C26-C25-C24	-2.40	107.80	113.38
2	C	2601	PLX	C26-C25-C24	-2.39	107.81	113.38

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

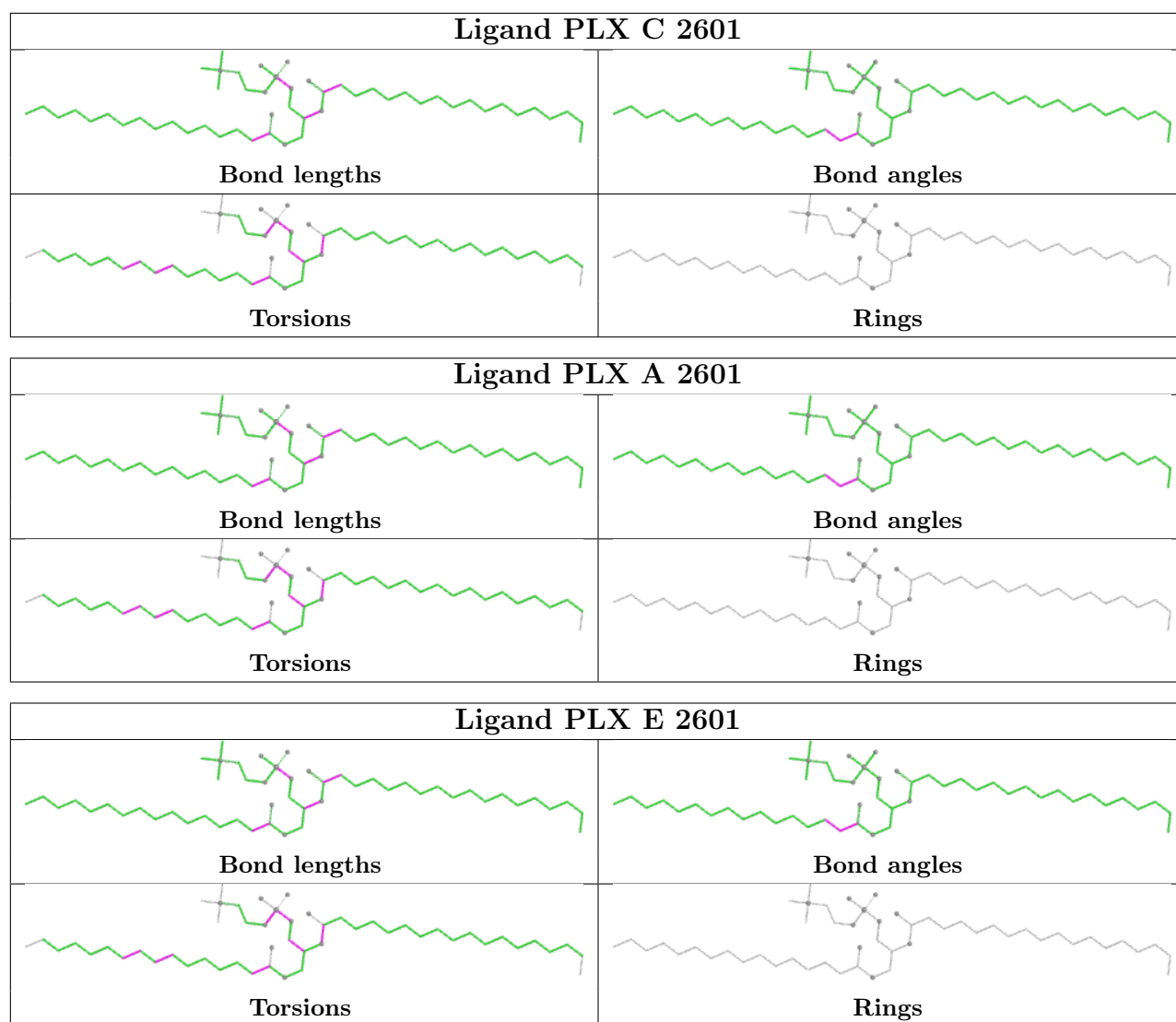
Mol	Chain	Res	Type	Atoms
2	A	2601	PLX	O7-C6-O6-C4
2	A	2601	PLX	C3-O4-P1-O1
2	A	2601	PLX	C3-O4-P1-O3
2	A	2601	PLX	C2-O1-P1-O2
2	C	2601	PLX	O7-C6-O6-C4

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2601	PLX	3	0
2	A	2601	PLX	3	0
2	E	2601	PLX	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

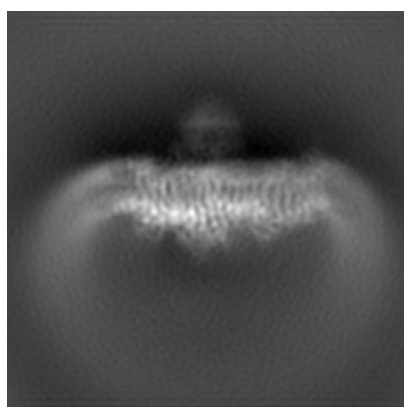
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32593. These allow visual inspection of the internal detail of the map and identification of artifacts.

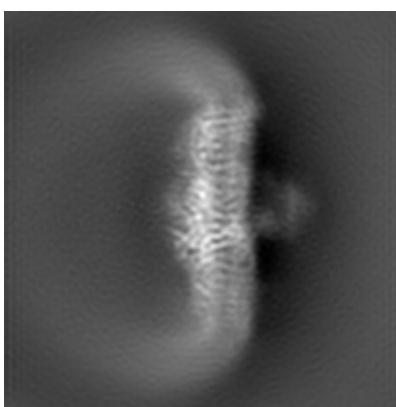
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

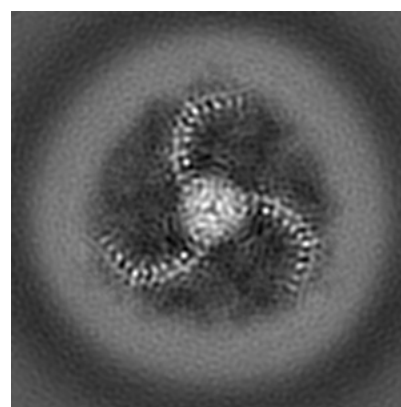
#### 6.1.1 Primary map



X



Y

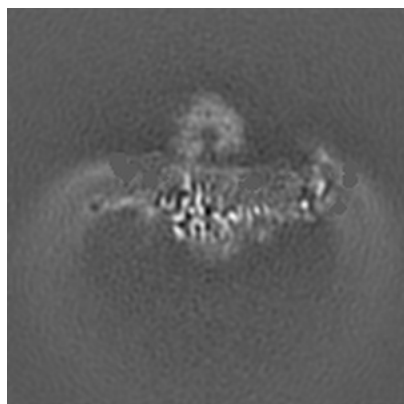


Z

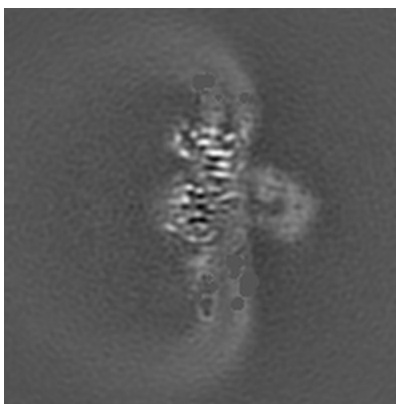
The images above show the map projected in three orthogonal directions.

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

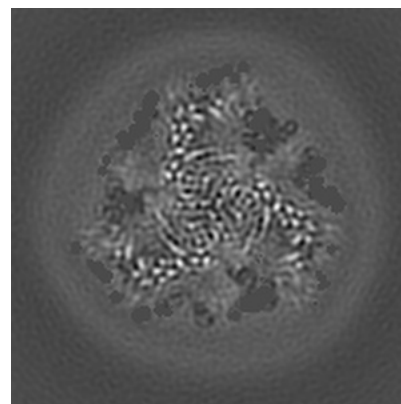
#### 6.2.1 Primary map



X Index: 90



Y Index: 90

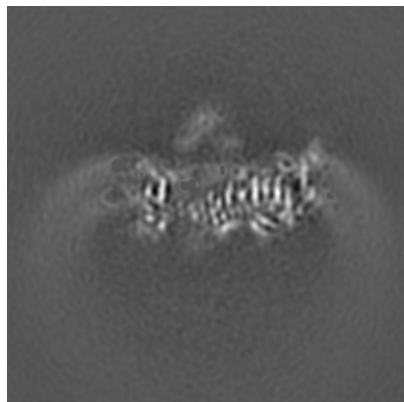


Z Index: 90

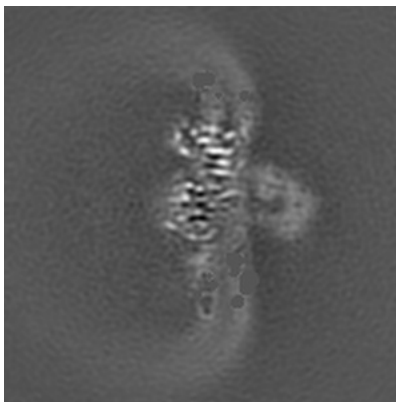
The images above show central slices of the map in three orthogonal directions.

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

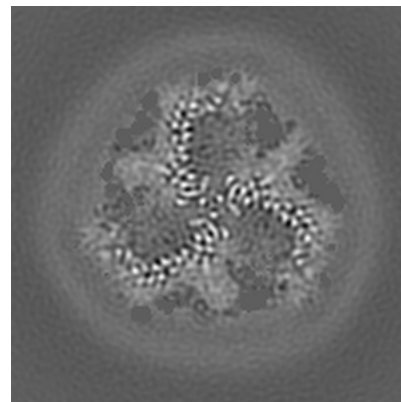
### 6.3.1 Primary map



X Index: 78



Y Index: 90

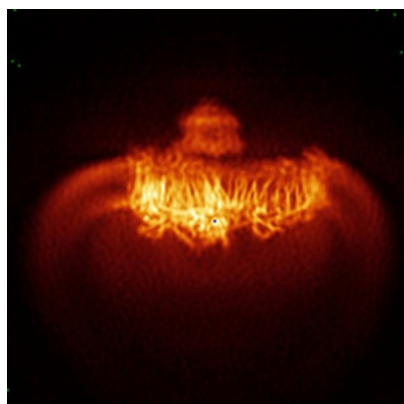


Z Index: 92

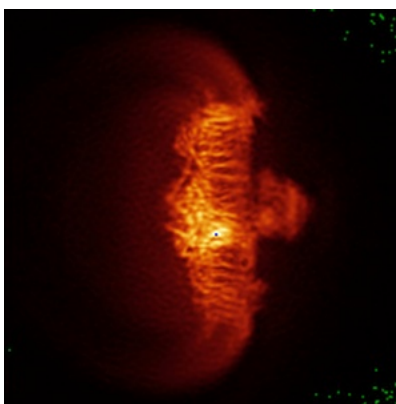
The images above show the largest variance slices of the map in three orthogonal directions.

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

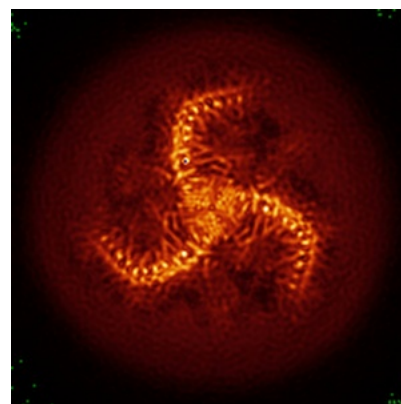
### 6.4.1 Primary map



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 [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

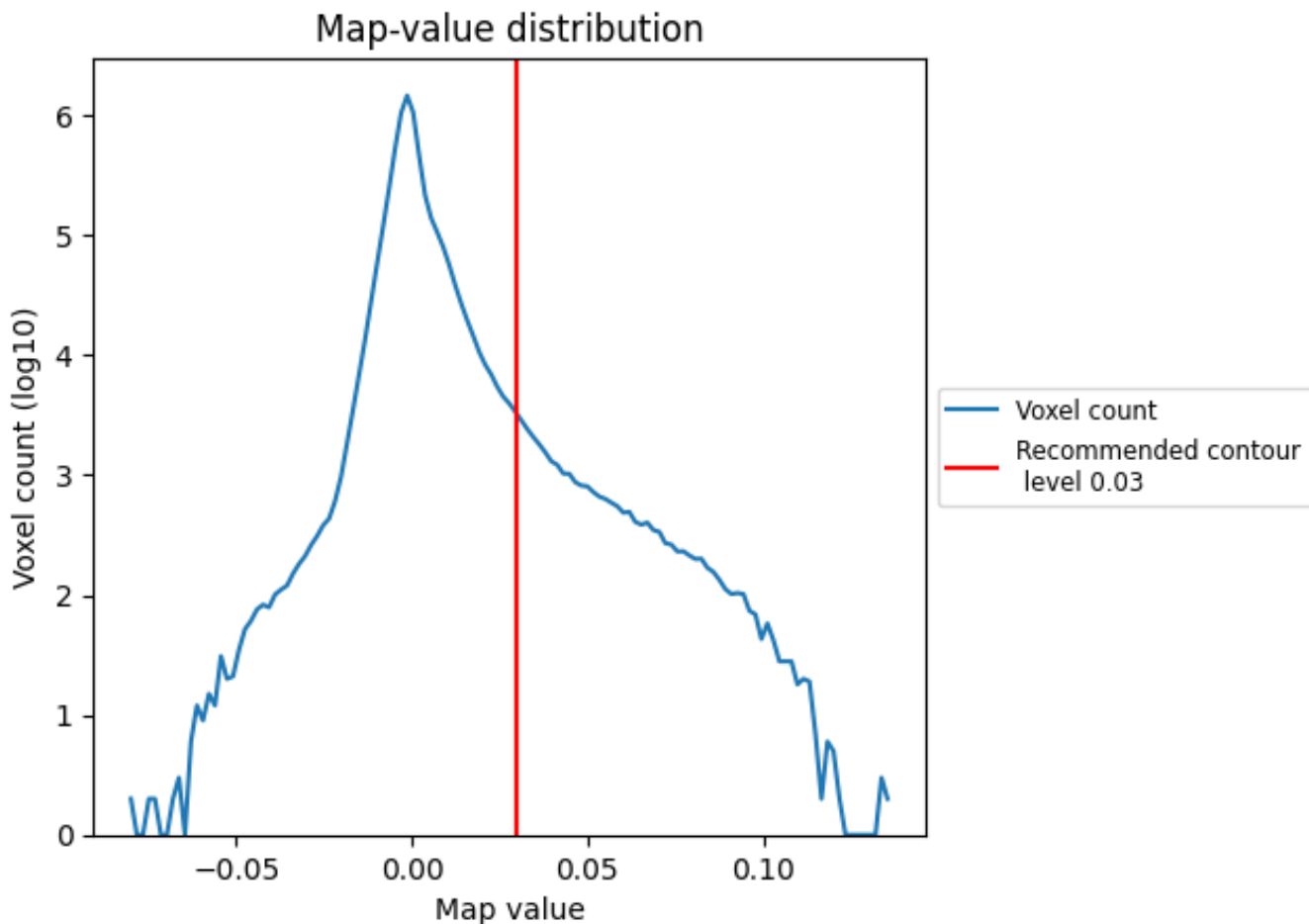
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

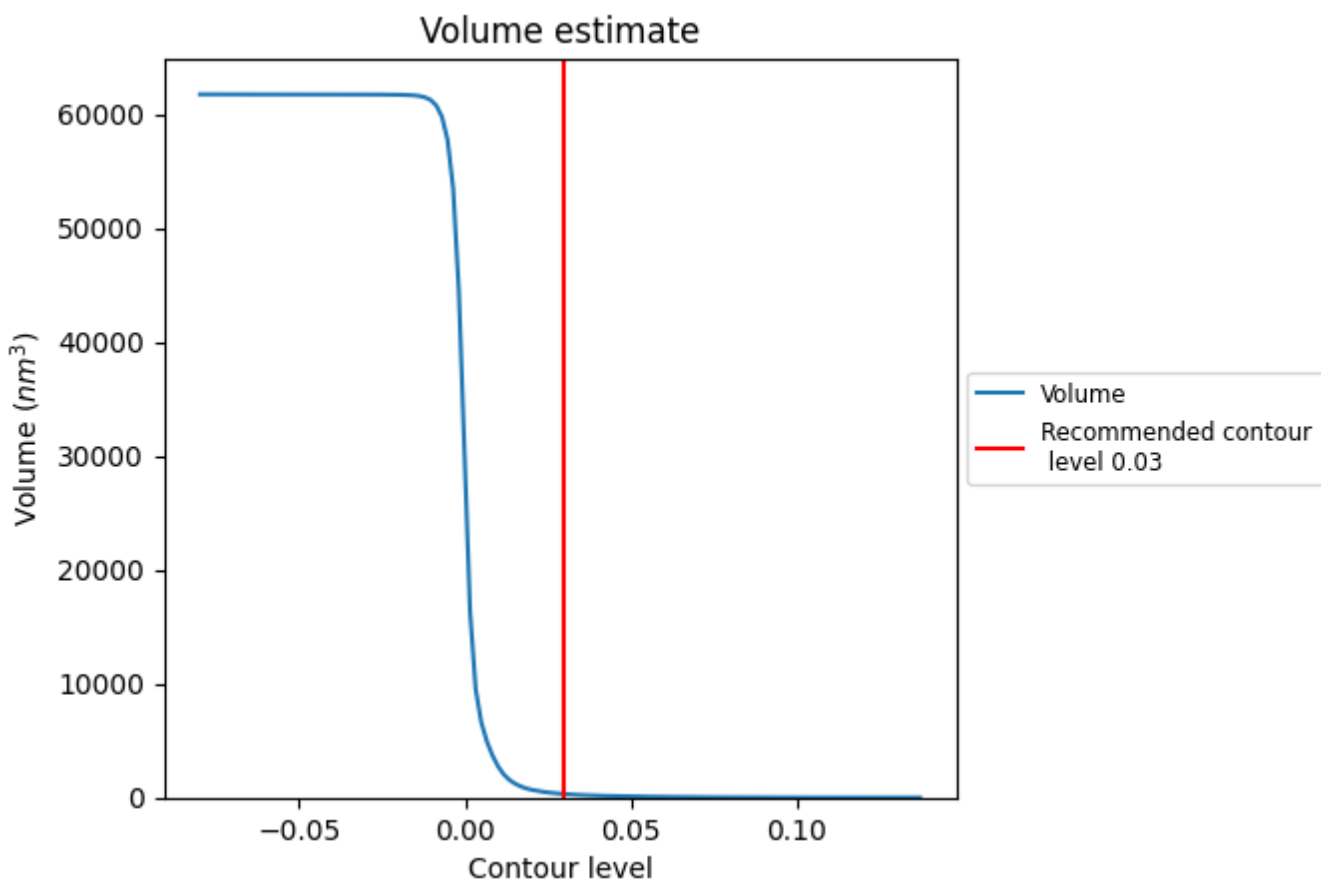
This section contains the results of statistical analysis of the map.

### 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.

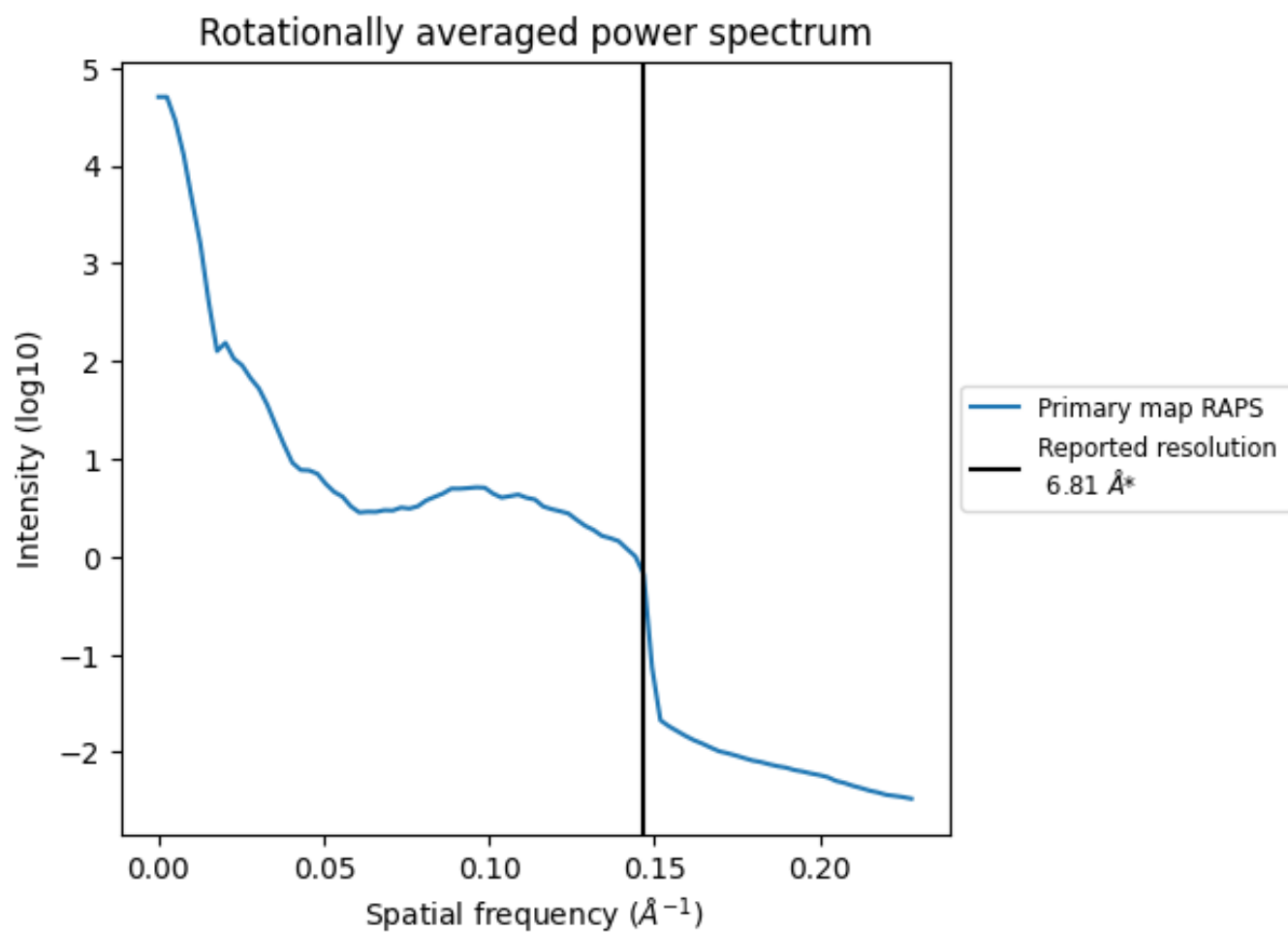
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 309 nm<sup>3</sup>; this corresponds to an approximate mass of 279 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 0.147 Å<sup>-1</sup>

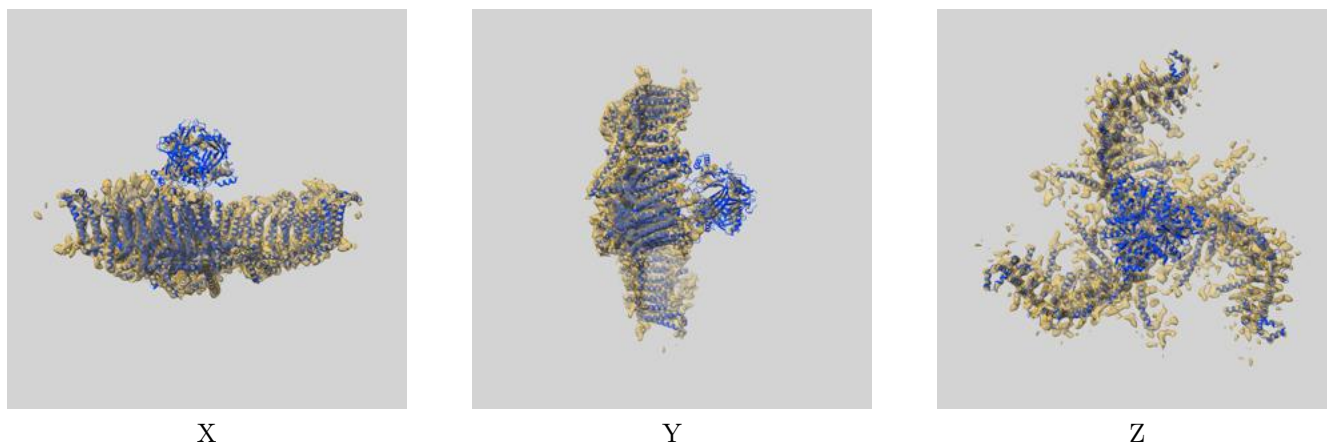
## 8 Fourier-Shell correlation

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-32593 and PDB model 7WLU. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.03 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](#)



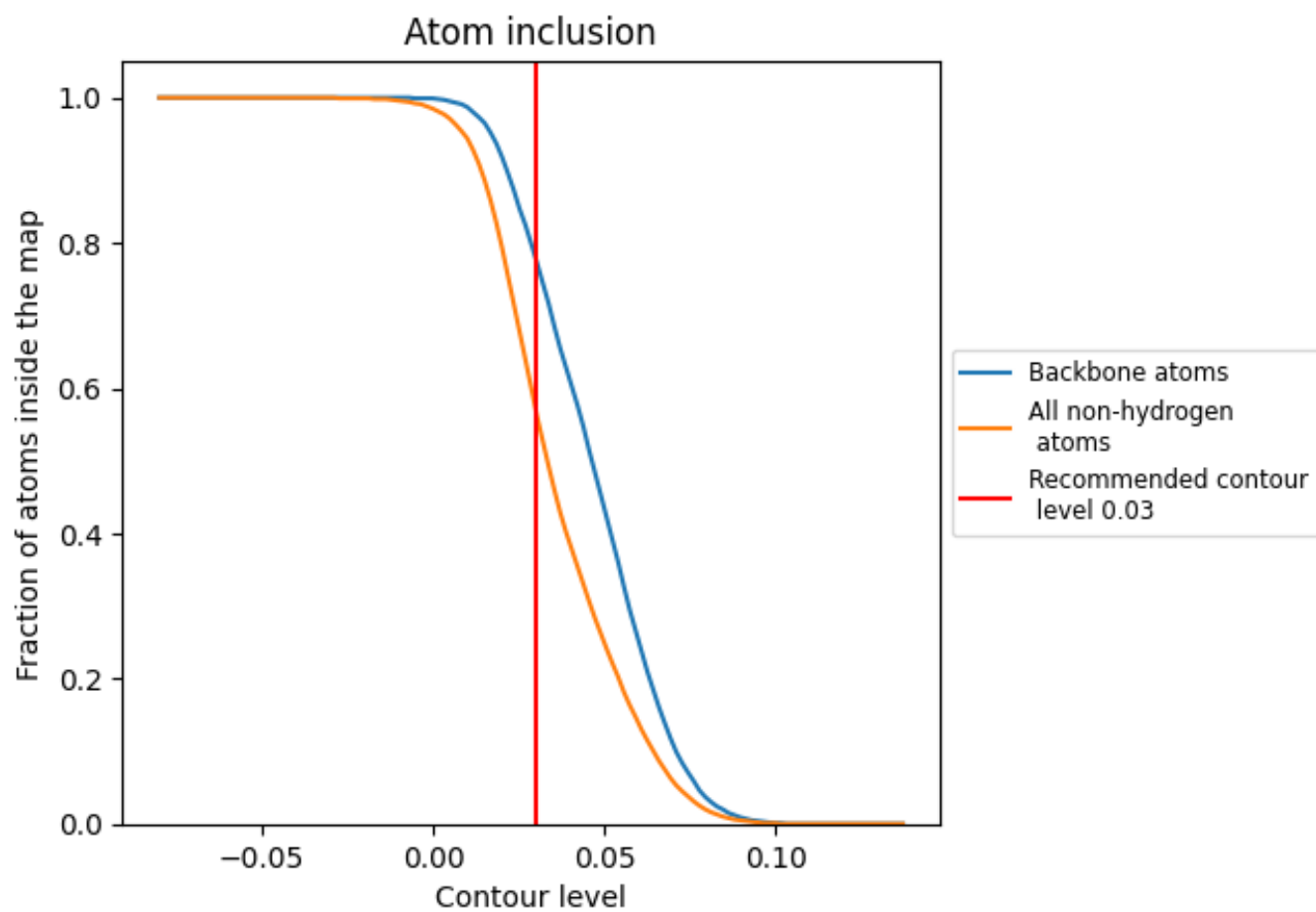
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).









## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 57% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5690	 0.1960
A	 0.5690	 0.1960
C	 0.5720	 0.1980
E	 0.5680	 0.1940

