



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 08:54 AM UTC

PDB ID : 9NWD / pdb_00009nwd
EMDB ID : EMD-46688
Title : Human E3 ligase UBR4-KCMF1-calmodulin complex (N-terminal)
Authors : Yang, Z.; Haakonsen, D.L.; Heider, M.; Witus, S.R.; Zelter, A.; Beschauner, T.; MacCoss, M.J.; Rape, M.
Deposited on : 2025-03-22
Resolution : 3.40 Å(reported)

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

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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

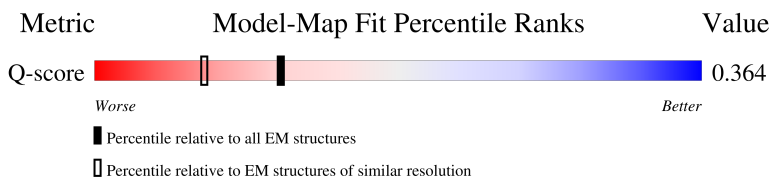
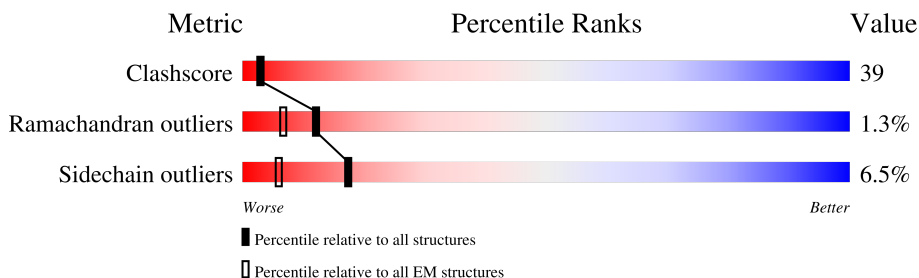
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	5183	
1	B	5183	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21667 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 E3 ubiquitin-protein ligase UBR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1396	Total	C	N	O	S	0	0
			10853	6909	1833	2049	62		
1	B	1387	Total	C	N	O	S	0	0
			10814	6883	1831	2038	62		

SER	GLY	L1554	Q1490	M1412	S1333	L1270	S1191	L1128	H1057	K986	A846	G772
SER	PRO	Q1555	L1491	A1413	L1334	G1271	K1192	S1129	H1058	E987	Q847	D773
THR	SER	L1556	L1492	A1414	E1335	T1272	K1193	V1131	I1059	K988	M848	P774
MET	HIS	H1557	Q1493	A1415	L1336	L1273	K1194	Q1132	K989	W918	R849	E778
THR	LEU	N1558	L1496	A1416	L1337	C1274	L1195	Q1133	K1060	Y991	F850	C779
LYS	SER	A1559	T1497	E1417	L1338	L1278	Q1196	S1134	Q1061	L999	V851	L780
LYS	VAL	A1560	T1497	E1417	L1339	L1278	G1197	S1134	G1062	H921	P852	L780
ALA	ASP	A1561	T1497	E1417	L1339	L1278	F1198	L1135	M1063	F922	L853	K761
VAL	GLY	D1562	V1427	V1427	E1342	P1279	F1198	L1135	A1068	Q1000	W82	V782
GLN	GLY	V1563	L1428	K1428	A1281	L1280	A1199	H1138	A1068	Y1001	L854	W783
ASP	GLY	L1564	L1428	K1428	E1345	A1281	A1200	F1139	A1068	S924	L855	W783
VAL	GLY	S1565	F1430	F1430	L1346	S1283	V1201	S1140	L1071	D925	A856	F786
ARG	ALA	S1566	F1431	F1431	L1347	L1284	A1203	S1141	L1072	A926	R857	L787
VAL	ILE	C1567	T1432	T1432	A1346	K1285	I2004	M1142	L1072	P928	L858	S788
ILE	GLY	K1568	A1433	R1433	L1349	H1286	G1205	A1143	A1075	H929	L859	S788
THR	VAL	Q1569	L1434	V1434	V1350	L1287	G1206	A1143	S1076	W1007	L860	T789
VAL	ASP	V1570	F1435	F1435	Y1351	L1288	S1207	ALA	S1077	P930	L861	K791
CYS	SER	L1571	T1438	E1439	K1353	L1289	R1208	THR	T1077	R931	F862	Q792
ALA	ASP	S1572	T1438	E1439	L1354	S1290	C1209	ASP	G1080	Q793	Y864	N793
LYS	THR	Q1573	E1439	E1439	L1354	L1291	K1210	PRO	S1081	C934	L865	A794
VAL	VAL	C1574	N1443	N1443	G1357	V1292	A1211	HIS	S1082	V935	L866	L795
HIS	GLY	V1575	M1444	M1444	L1361	L1293	T1212	LYS	V1083	L936	H867	Q796
ALA	GLY	V1576	L1445	L1445	L1361	L1294	T1213	S1151	K1084	P1015	Q868	G797
LYS	LEU	V1577	S1445	L1446	L1361	T1295	L1214	S1152	E1087	Y1019	Y869	V798
ASP	ALA	E1578	L1514	L1447	H1385	G1296	G1215	L1154	E1088	I1020	V874	V799
VAL	VAL	K1579	G1516	L1447	H1385	P1297	P1216	T1154	E1088	D943	P800	P800
SER	GLY	L1580	L1517	L1447	N1369	L1298	T1217	K1155	I1089	D944	Y875	S801
PRO	ILE	N1581	L1518	H1448	S1370	L1299	L1218	K1156	V1090	Q1022	L876	E802
ALA	SER	A1582	L1519	L1449	S1371	V1300	V1219	E1091	E1091	S1024	F877	N807
ASP	ASP	P1520	C1450	C1450	L1372	W1301	Q1220	L1159	F1094	N1025	E878	V808
LYS	VAL	M1521	L1453	L1453	L1372	S1302	N1221	P1160	F1094	M1026	Q881	E809
ALA	GLN	T1522	L1456	L1456	L1376	E1304	L1222	A1161	R1096	S1027	L885	H810
LYS	GLY	T1523	L1456	L1456	L1376	M1305	P1223	L1162	Q1097	P1028	Q812	L811
THR	ASP	F1524	V1459	V1459	C1380	N1306	S1224	Q1164	I1098	A952	P887	M813
ILE	SER	M1525	E1460	E1460	Q1382	P1307	V1226	L1165	F1101	M1030	P888	
PHE	ASP	N1528	R1463	R1463	Q1382	Q1308	Y1229	P1167	E1032	S1031	F889	L816
CYS	GLY	G1529	L1464	L1464	Y1383	Q1309	Y1229	P1167	E1032	E1032	G890	L817
ASP	ASP	D1530	L1464	L1464	L1384	V1310	Y1233	T1168	C1033	C1033	TRP	
LYS	GLY	G1531	W1467	W1467	Q1387	I1311	Y1233	Y1169	D1105	D1034	ALA	F821
LYS	ASN	F1534	L1468	L1468	L1387	T1313	P1242	S1171	L1036	I1035	GLY	G825
GLY	LEU	P1535	T1469	T1469	Q1392	L1314	N1243	F1172	H1037	D964	SER	
GLY	LEU	E1536	R1470	R1470	A1393	L1315	T1244	T1173	E965	E965	SER	
LYS	GLY	L1537	M1471	M1471	A1393	P1316	G1245	R1174	L1038	L1038	GLN	I829
LYS	GLY	M1538	M1471	M1471	R1394	L1317	S1246	A1175	L1039	L1040	ASP	L830
LYS	GLY	V1539	S1474	S1474	L1394	L1318	W1247	Y1176	R1040	W1041	ASP	S831
LYS	GLY	V1540	S1474	S1474	M1397	L1319	W1247	L1177	A968	A969	ASN	F833
ALA	LEU	M1541	K1477	K1477	E1398	E1320	F1251	L1178	SER	SER	V834	
LEU	THR	A1542	D1478	D1478	E1399	T1323	A1252	L1178	F1116	L973	Q835	
VAL	GLN	T1543	D1479	D1479	F1400	E1324	T1255	L1045	S1117	L974	ARG	
LYS	LYS	L1544	D1480	D1480	F1401	E1325	T1255	L1046	A975	A975	ARG	
ARG	ARG	A1545	Q1481	Q1481	S1402	V1326	T1256	I1047	A976	A976	A903	
THR	THR	S1546	Q1481	Q1481	D1403	V1326	T1256	S1048	A976	A976	T904	
THR	PHE	A1547	V1484	V1484	D1403	E1327	P1257	I1121	L980	L980	T905	
VAL	MET	G1548	I1485	I1485	G1405	E1328	P1257	S1049	P906	P906	P906	
GLY	ASN	Q1549	Q1486	Q1486	E1406	I1329	Y1261	V1051	T982	T982	Y908	
GLY	GLY	G1550	E1487	E1487	L1407	S1330	Y1261	L1124	V983	V983	H909	
GLY	GLY	A1551	N1488	N1488	L1407	S1331	A1268	W1053	R984	R984	G910	
ARG	THR	H1553	M1489	M1489	M1411	N1332	H1269	P1190	A1127	A1127	D845	



WORLDWIDE
PDB
PROTEIN DATA BANK

D1126	H1057	L973	ASN	M813	V729	LEU	GLU	THR	ASP	PRO	ASP	V352	N280	GLU	A158	I63
A1126	L1058	D981	SER	L816	T730	ALA	GLU	ASP	GLU	PRO	G353	G352	N281	GLY	K159	H66
A1127	I1059	D981	ARG	I817	Q733	ALA	ASP	GLU	LEU	ALA	S354	ALA	F282	ASN	P161	
K1129	Q1061	R985	ARG	F821	A738	L646	SER	IS11	GLN	A441	GLN	GLN	M285	ASP	THR	E70
K1130	G1062	R986	THR	R827	P739	F647	ASP	IS18	ASP	R443	VAL	VAL	M286	GLN	THR	Y71
V1131	M1063	T992	THR	R827	F740	L648	ASP	Q519	ASP	R444	ARG	ARG	F286	SER	LYS	P72
Q1132	K1064	A993	THR	L830	W745	G649	ASP	R520	ASP	R445	THR	THR	F287	GLY	THR	F73
V1133	E1065	E995	THR	S831	P746	L650	GLU	IS21	GLU	D446	SER	SER	T288	THR	LEU	Y74
S1134	H1067	A996	THR	L832	L747	L654	PRO	Q522	THR	I447	SER	SER				
L1135	A1068		THR	F833	H750	L655	ILE	R523	THR	L448	SER	SER	D281	THR	THR	T82
			THR	Q835			LEU	L524	THR				A294	ASP	ASP	H83
			THR	L836	L754	L659	GLY	IS25	GLU	T451	SER	SER	V295	VAL	GLU	Y84
			THR	L840	S755		GLN	D526	GLU	R296	GLU	GLU	A230	ASP	ASP	I85
			THR	L844	R759	L663	THR	V527	GLY	R297	THR	THR	N297	GLN	GLN	T86
			THR	M844	L760	L667	GLU	V528	VAL	E371	VAL	VAL	K234	LYS	LYS	V88
			THR	M848	L761	L669	GLU	P529	GLY	I377	GLY	GLY	K236	GLU	GLU	C89
			THR	M849	L762		GLU	L530	SER	V378	SER	SER	N237	LEU	LEU	S90
			THR	M850	L763		GLU	M531	PRO	Q379	LYS	LYS	S301	ALA	ALA	L91
			THR	V851	Q765	R671	SER	L535	GLY	K381	GLY	GLY	K380	SER	SER	I92
			THR	V852	H766	L674	LYS	L537	GLY	L382	GLY	GLY	V303	PRO	PRO	P93
			THR	L853	K767	S677	GLU	L538	GLY				T312	VAL	VAL	Q96
			THR	L855	A768	L678	LYS	S539	GLY				L313	SER	SER	L97
			THR	L856		L683	LYS	L539	GLY				S314	THR	THR	Q98
			THR	L857	D773	L686	LYS	L540	GLY				P316	THR	THR	C104
			THR	L858	E778	L689	LYS	L541	GLY				V317	THR	THR	L112
			THR	L859	C779	L694	LYS	L542	GLY				L318	THR	THR	L113
			THR	L860	L780	L698	LYS	L543	GLY				E319	THR	THR	L114
			THR	L861	K781	L699	LYS	L544	GLY				P320	THR	THR	R114
			THR	L862	L782	L703	LYS	L545	GLY				L321	THR	THR	L115
			THR	L863	W783	L704	LYS	L546	GLY				N322	THR	THR	E120
			THR	L864		L705	LYS	L547	GLY				P323	THR	THR	A121
			THR	L865	F786	L706	LYS	L548	GLY				S324	THR	THR	C122
			THR	L866	L787	L707	LYS	L549	GLY				R325	THR	THR	L194
			THR	L867		L708	LYS	L550	GLY				L326	THR	THR	A123
			THR	L868		L709	LYS	L551	GLY				Q327	THR	THR	V124
			THR	L869		L710	LYS	L552	GLY				D328	THR	THR	L129
			THR	L870		L711	LYS	L553	GLY				V331	THR	THR	I130
			THR	L871		L712	LYS	L554	GLY				L332	THR	THR	L131
			THR	L872		L713	LYS	L555	GLY				S333	THR	THR	L132
			THR	L873		L714	LYS	L556	GLY				L334	THR	THR	I133
			THR	L874		L715	LYS	L557	GLY				S335	THR	THR	L136
			THR	L875		L716	LYS	L558	GLY				F419	THR	THR	L137
			THR	L876		L717	LYS	L559	GLY				L420	THR	THR	P203
			THR	L877		L718	LYS	L560	GLY				L421	THR	THR	R204
			THR	L878		L719	LYS	L561	GLY				L422	THR	THR	T205
			THR	L879		L720	LYS	L562	GLY				L423	THR	THR	R142
			THR	L880		L721	LYS	L563	GLY				L424	THR	THR	L143
			THR	L881		L722	LYS	L564	GLY				L425	THR	THR	D144
			THR	L882		L723	LYS	L565	GLY				L426	THR	THR	E147
			THR	L883		L724	LYS	L566	GLY				L427	THR	THR	F151
			THR	L884		L725	LYS	L567	GLY				L428	THR	THR	M164
			THR	L885		L726	LYS	L568	GLY				L429	THR	THR	K156
			THR	L886		L727	LYS	L569	GLY				L430	THR	THR	S157
			THR	L887		L728	LYS	L570	GLY				L431	THR	THR	
			THR	L888		L729	LYS	L571	GLY				L432	THR	THR	
			THR	L889		L730	LYS	L572	GLY				L433	THR	THR	
			THR	L890		L731	LYS	L573	GLY				L434	THR	THR	
			THR	L891		L732	LYS	L574	GLY				L435	THR	THR	
			THR	L892		L733	LYS	L575	GLY				L436	THR	THR	
			THR	L893		L734	LYS	L576	GLY				L437	THR	THR	
			THR	L894		L735	LYS	L577	GLY				L438	THR	THR	
			THR	L895		L736	LYS	L578	GLY				L439	THR	THR	
			THR	L896		L737	LYS	L579	GLY				L440	THR	THR	
			THR	L897		L738	LYS	L580	GLY				L441	THR	THR	
			THR	L898		L739	LYS	L581	GLY				L442	THR	THR	
			THR	L899		L740	LYS	L582	GLY				L443	THR	THR	
			THR	L900		L741	LYS	L583	GLY				L444	THR	THR	
			THR	L901		L742	LYS	L584	GLY				L445	THR	THR	
			THR	L902		L743	LYS	L585	GLY				L446	THR	THR	
			THR	L903		L744	LYS	L586	GLY				L447	THR	THR	
			THR	L904		L745	LYS	L587	GLY				L448	THR	THR	
			THR	L905		L746	LYS	L588	GLY				L449	THR	THR	
			THR	L906		L747	LYS	L589	GLY				L450	THR	THR	
			THR	L907		L748	LYS	L590	GLY				L451	THR	THR	
			THR	L908		L749	LYS	L591	GLY				L452	THR	THR	
			THR	L909		L750	LYS	L592	GLY				L453	THR	THR	
			THR	L910		L751	LYS	L593	GLY				L454	THR	THR	
			THR	L911		L752	LYS	L594	GLY				L455	THR	THR	
			THR	L912		L753	LYS	L595	GLY				L456	THR	THR	
			THR	L913		L754	LYS	L596	GLY				L457	THR	THR	
			THR	L914		L755	LYS	L597	GLY				L458	THR	THR	
			THR	L915		L756	LYS	L598	GLY				L459	THR	THR	
			THR	L916		L757	LYS	L599	GLY				L460	THR	THR	
			THR	L917		L758	LYS	L600	GLY				L461	THR	THR	
			THR	L918		L759	LYS	L601	GLY				L462	THR	THR	
			THR	L919		L760	LYS	L602	GLY				L463	THR	THR	
			THR	L920		L761	LYS	L603	GLY				L464	THR	THR	
			THR	L921		L762	LYS	L604	GLY				L465	THR	THR	
			THR	L922		L763	LYS	L605	GLY				L466	THR	THR	
			THR	L923		L764	LYS	L606	GLY				L467	THR	THR	
			THR	L924		L765	LYS	L607	GLY				L468	THR	THR	
			THR	L925		L766	LYS	L608	GLY				L469	THR	THR	
			THR	L926		L767	LYS	L609	GLY				L470	THR	THR	
			THR	L927		L768	LYS	L610	GLY				L471	THR	THR	
			THR	L928		L769	LYS	L611	GLY				L472	THR	THR	
			THR	L929		L770	LYS	L612	GLY				L473	THR	THR	
			THR	L930		L771	LYS	L613	GLY				L474	THR	THR	
			THR	L931		L772	LYS	L614	GLY				L475	THR	THR	
			THR	L932		L773	LYS	L615	GLY				L476	THR	THR	
			THR	L933		L774	LYS	L616	GLY				L477	THR	THR	
			THR	L934		L775	LYS	L617	GLY				L478	THR	THR	
			THR	L935		L776	LYS	L618	GLY				L479	THR	THR	
			THR	L936		L777	LYS	L619	GLY				L480	THR	THR	
			THR	L937		L778	LYS	L620	GLY				L481	THR	THR	
			THR	L938		L779	LYS	L621	GLY				L482	THR	THR	
			THR	L939		L780	LYS	L622	GLY				L483	THR	THR	
			THR	L940		L781	LYS	L623	GLY				L484	THR	THR	
			THR	L941		L782	LYS	L624	GLY				L485	THR	THR	
			THR	L942		L783	LYS	L625	GLY				L486	THR	THR	
			THR	L943		L784	LYS	L626	GLY				L487	THR	THR	
			THR	L944		L785	LYS	L627	GLY				L488	THR	THR	
			THR	L945		L786	LYS	L628	GLY				L489	THR	THR	
			THR	L946		L787	LYS	L629	GLY				L490	THR	THR	
			THR	L947		L788	LYS	L630	GLY				L491	THR	THR	
			THR	L948		L789	LYS	L631	GLY				L492	THR	THR	
			THR	L949		L790	LYS	L632	GLY				L493	THR	THR	
			THR	L950		L791	LYS	L633	GLY							







SER	PHE	TYR	ALA	CYS	TYR	ALA	THR	HIS
	TRP	TYR	ASP	ASN	THR	MET	GLN	GLN
	ALA	PHE	THR	GLY	PHE	ALA	VAL	LEU
	VAL	THR	GLY	LEU	THR	MET	LEU	LYS
	ASP	VAL	GLY	LEU	ARG	GLN	GLY	LEU
	LEU	LEU	GLY	PRO	VAL	LYS	THR	ILE
	ALA	ALA	GLY	VAL	VAL	ALA	ASP	LEU
	GLY	ILE	ARG	TRP	ALA	LEU	ASP	LEU
	LEU	THR	GLU	GLY	GLY	LEU	SER	GLN
	LEU	ILE	GLU	PRO	GLU	GLY	ILE	LYS
SER	MET	LEU	ASN	HIS	GLU	THR	PRO	GLY
	PHE	PRO	ILE	VAL	MET	LEU	ASN	ILE
	LYS	PRO	HIS	PRO	GLU	GLY	LEU	THR
	LYS	GLU	HIS	GLU	ASN	MET	HIS	GLN
	ASP	GLN	ILE	SER	LYS	THR	LYS	ASN
	PRO	TRP	PRO	ALA	PRO	THR	LEU	ALA
	THR	ARG	TYR	PHE	ARG	GLU	LEU	LEU
	SER	ALA	ILE	ALA	LYS	ASN	GLN	ASP
	ASN	THR	HIS	GLN	GLN	LYS	VAL	TYR
	LEU	THR	ARG	CYS	THR	GLY	SER	MET
PRO	GLY	VAL	THR	GLY	THR	LEU	LEU	LYS
	GLY	ILE	LEU	ALA	ARG	VAL	ASP	LYS
	TRP	LEU	THR	HIS	THR	THR	GLY	HIS
	ASN	ARG	VAL	ASN	VAL	LYS	ILE	PRO
	SER	LEU	ASN	TYR	HIS	ALA	ALA	THR
	SER	LEU	THR	LEU	PHE	LEU	LEU	LYS
	LEU	VAL	THR	GLN	ASN	LEU	ALA	ASN
	GLU	THR	ARG	GLU	ILE	LYS	GLU	LEU
	GLY	THR	ILE	GLY	THR	LEU	GLU	ASP
	LEU	THR	THR	THR	THR	VAL	GLN	TYR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126259	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.801	Depositor
Minimum map value	-0.495	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.068	Depositor
Map size ($\text{\AA}$)	432.64, 432.64, 432.64	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.832, 0.832, 0.832	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	0.89	21/11051 (0.2%)	1.14	66/15000 (0.4%)
1	B	0.99	22/11008 (0.2%)	1.26	65/14932 (0.4%)
All	All	0.95	43/22059 (0.2%)	1.20	131/29932 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	12
All	All	0	16

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	878	GLU	CA-C	-8.95	1.41	1.52
1	A	789	THR	CA-C	-8.80	1.41	1.52
1	A	855	LEU	CA-C	-8.66	1.40	1.52
1	A	858	LEU	CA-C	-8.53	1.41	1.52
1	A	782	VAL	CA-C	-8.30	1.42	1.52

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	855	LEU	N-CA-C	-13.01	96.76	112.89
1	B	1451	GLY	N-CA-C	-12.54	98.98	114.16
1	A	789	THR	N-CA-C	-12.48	97.67	111.28
1	B	1083	VAL	N-CA-C	-12.02	96.91	110.62
1	A	860	LEU	N-CA-C	-11.29	98.99	111.07

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1008	ARG	Sidechain
1	A	1174	ARG	Sidechain
1	A	1394	ARG	Sidechain
1	A	849	ARG	Sidechain
1	B	272	ARG	Sidechain

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	10853	0	10929	945	0
1	B	10814	0	10915	803	0
All	All	21667	0	21844	1708	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 39.

The worst 5 of 1708 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LEU:HD11	1:B:332:LEU:CD2	1.51	1.36
1:B:89:CYS:SG	1:B:239:PHE:HD2	1.54	1.30
1:A:1399:GLU:O	1:A:1403:ASP:OD1	1.56	1.20
1:B:89:CYS:SG	1:B:239:PHE:CD2	2.32	1.20
1:A:73:PHE:CD1	1:A:159:LYS:HA	1.80	1.17

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	1372/5183 (26%)	1288 (94%)	63 (5%)	21 (2%)	8	30
1	B	1359/5183 (26%)	1262 (93%)	82 (6%)	15 (1%)	11	38
All	All	2731/10366 (26%)	2550 (93%)	145 (5%)	36 (1%)	12	33

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	889	PHE
1	A	906	PRO
1	A	907	LEU
1	A	909	HIS
1	A	1031	SER

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	1218/4521 (27%)	1151 (94%)	67 (6%)	19	46
1	B	1217/4521 (27%)	1126 (92%)	91 (8%)	12	38
All	All	2435/9042 (27%)	2277 (94%)	158 (6%)	17	42

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	943	ASP
1	B	1338	LEU
1	B	1033	CYS
1	B	1131	VAL
1	B	1486	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	979	GLN
1	B	1528	ASN
1	B	1057	HIS
1	B	1249	ASN
1	B	1589	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 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.

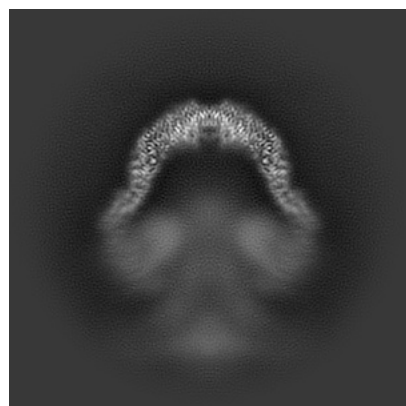
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46688. These allow visual inspection of the internal detail of the map and identification of artifacts.

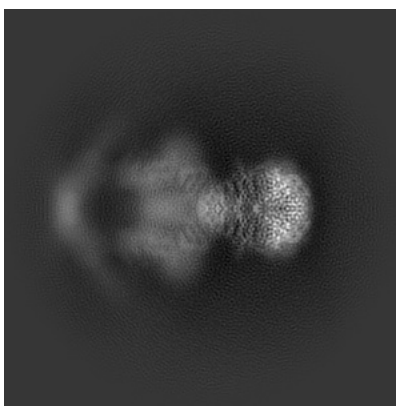
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

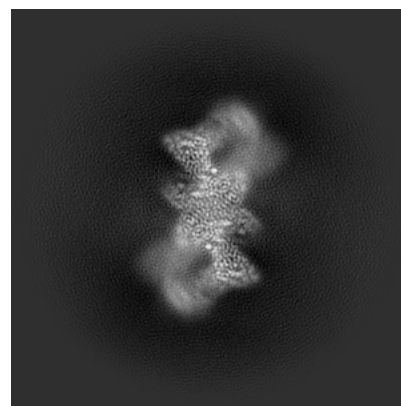
6.1.1 Primary map



X

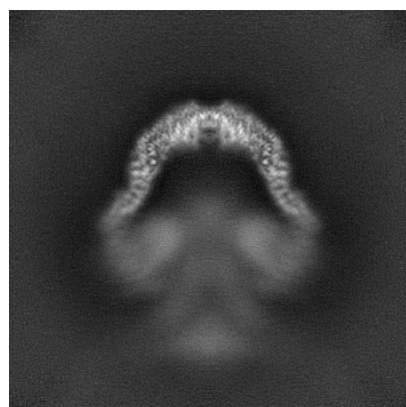


Y

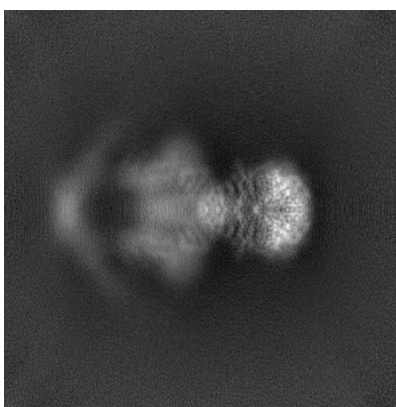


Z

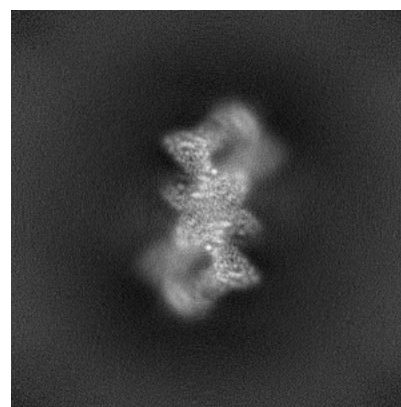
6.1.2 Raw map



X



Y

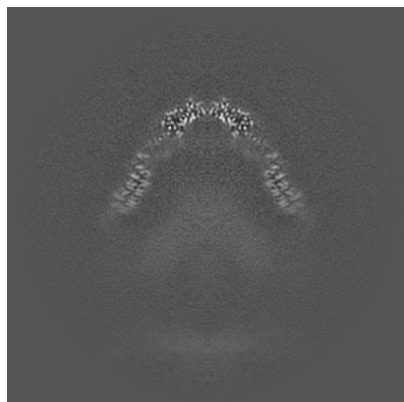


Z

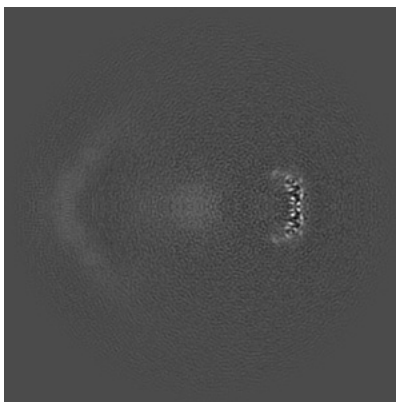
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

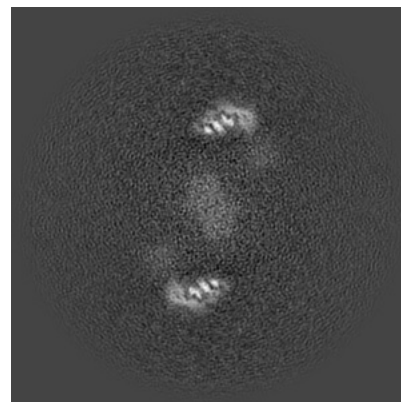
6.2.1 Primary map



X Index: 260

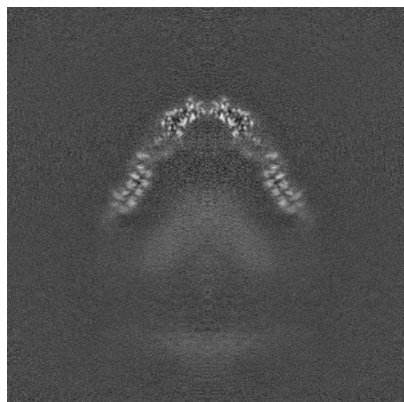


Y Index: 260

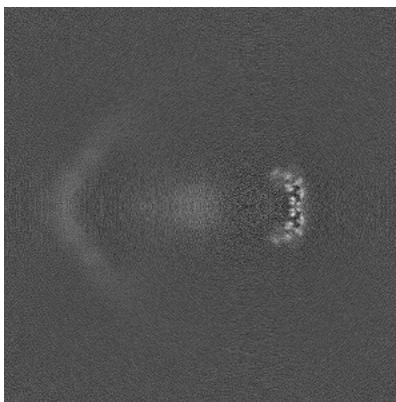


Z Index: 260

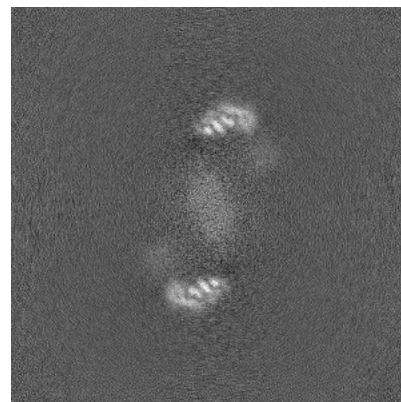
6.2.2 Raw map



X Index: 260



Y Index: 260

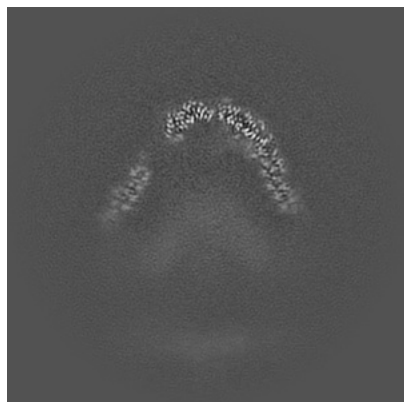


Z Index: 260

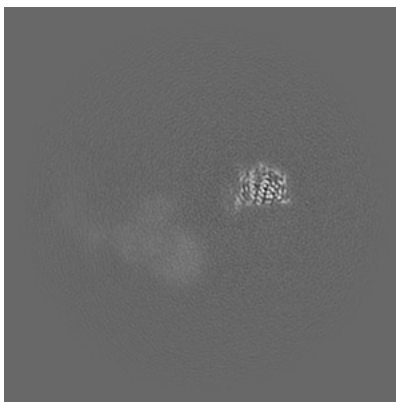
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

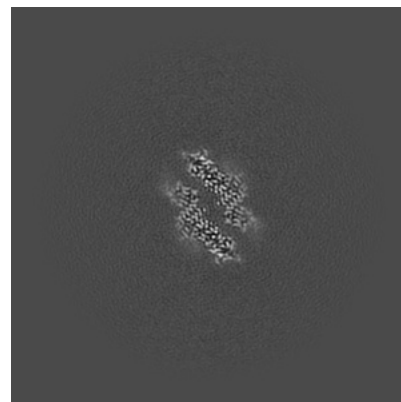
6.3.1 Primary map



X Index: 254

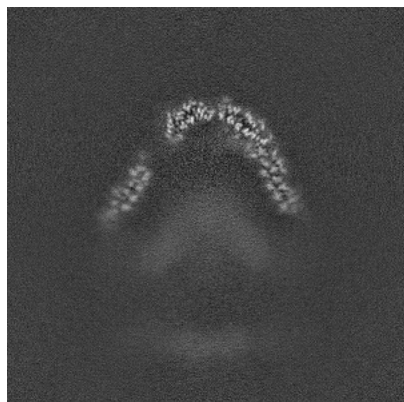


Y Index: 187

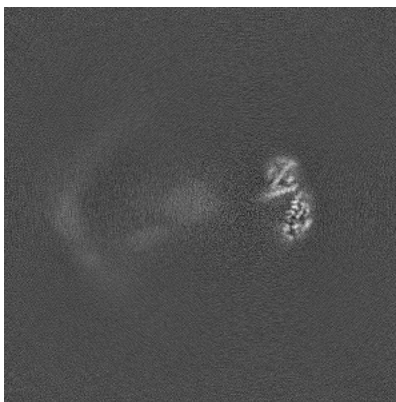


Z Index: 370

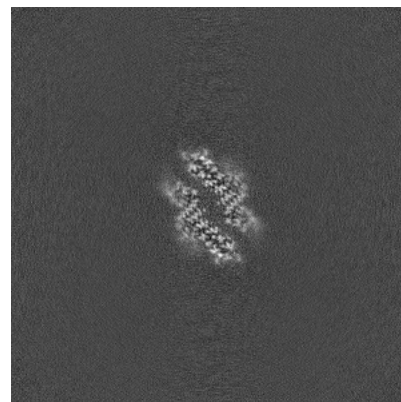
6.3.2 Raw map



X Index: 254



Y Index: 242

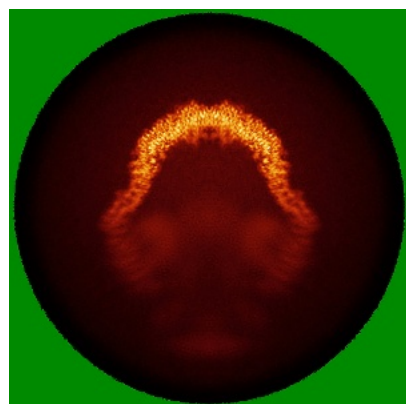


Z Index: 370

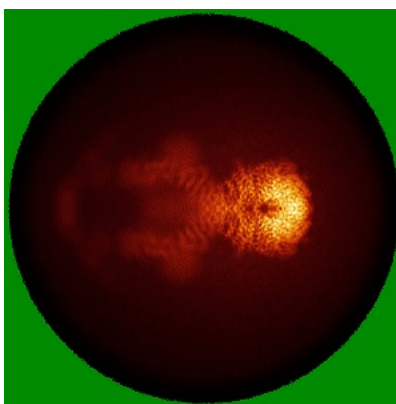
The images above show the largest variance slices of the map in three orthogonal directions.

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

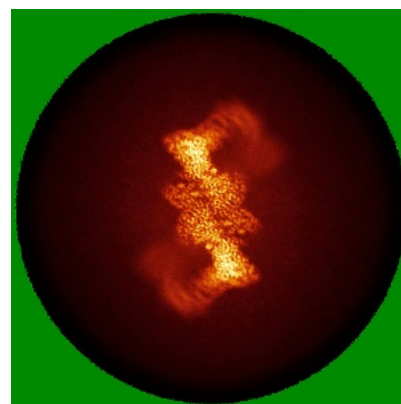
6.4.1 Primary map



X

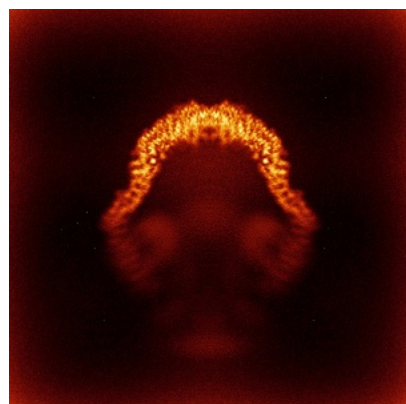


Y

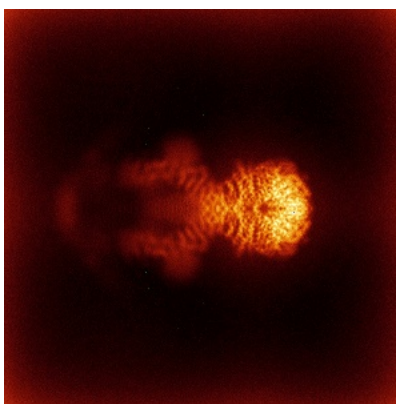


Z

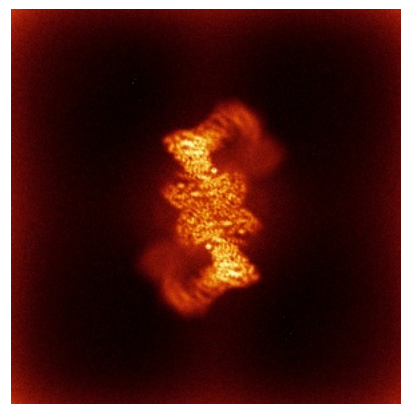
6.4.2 Raw map



X



Y

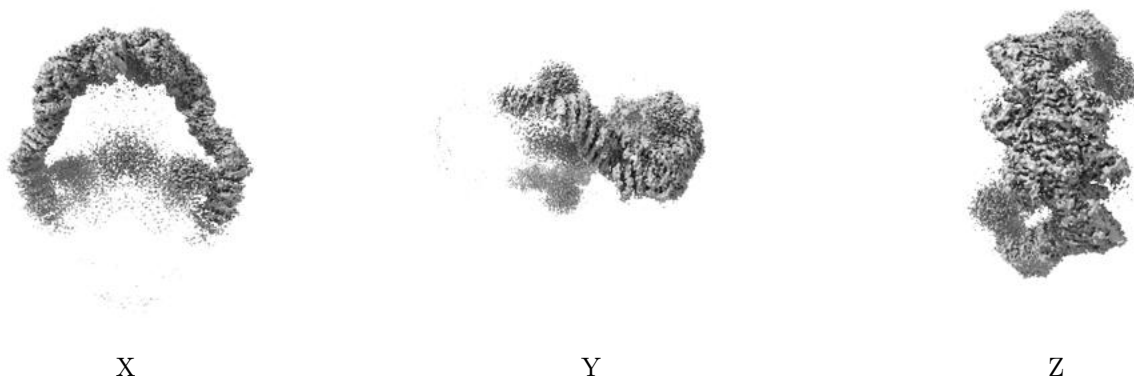


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

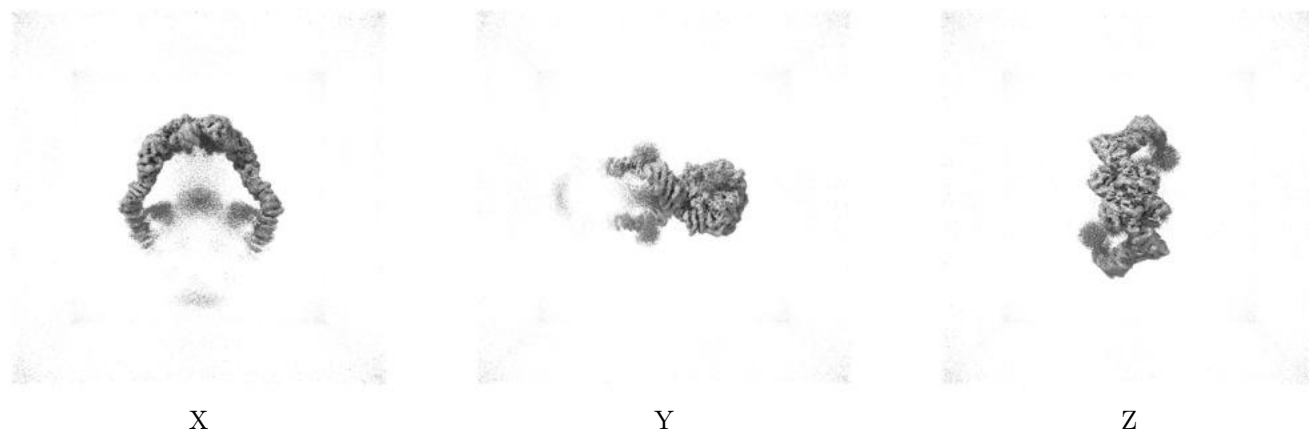
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.068. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

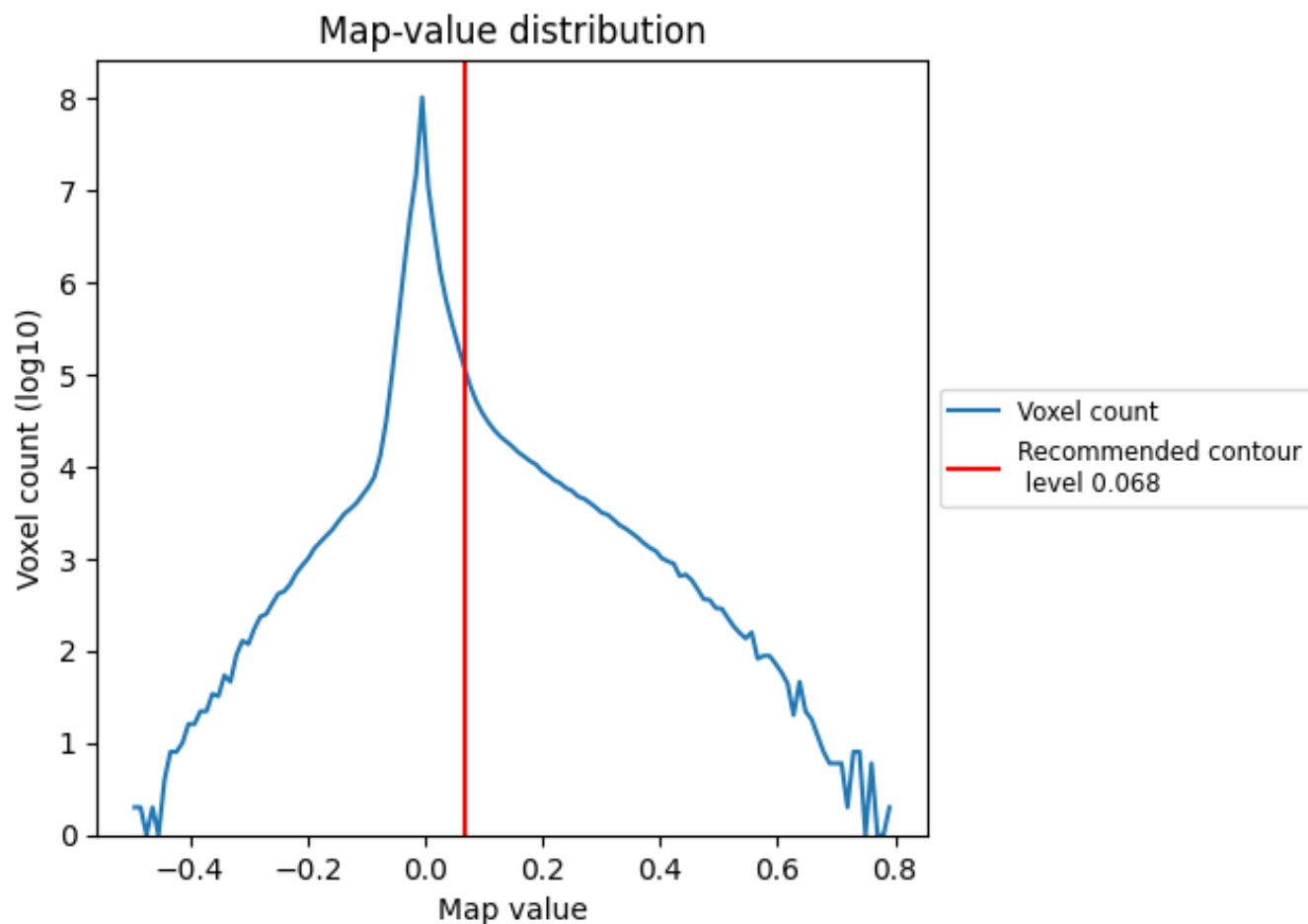
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

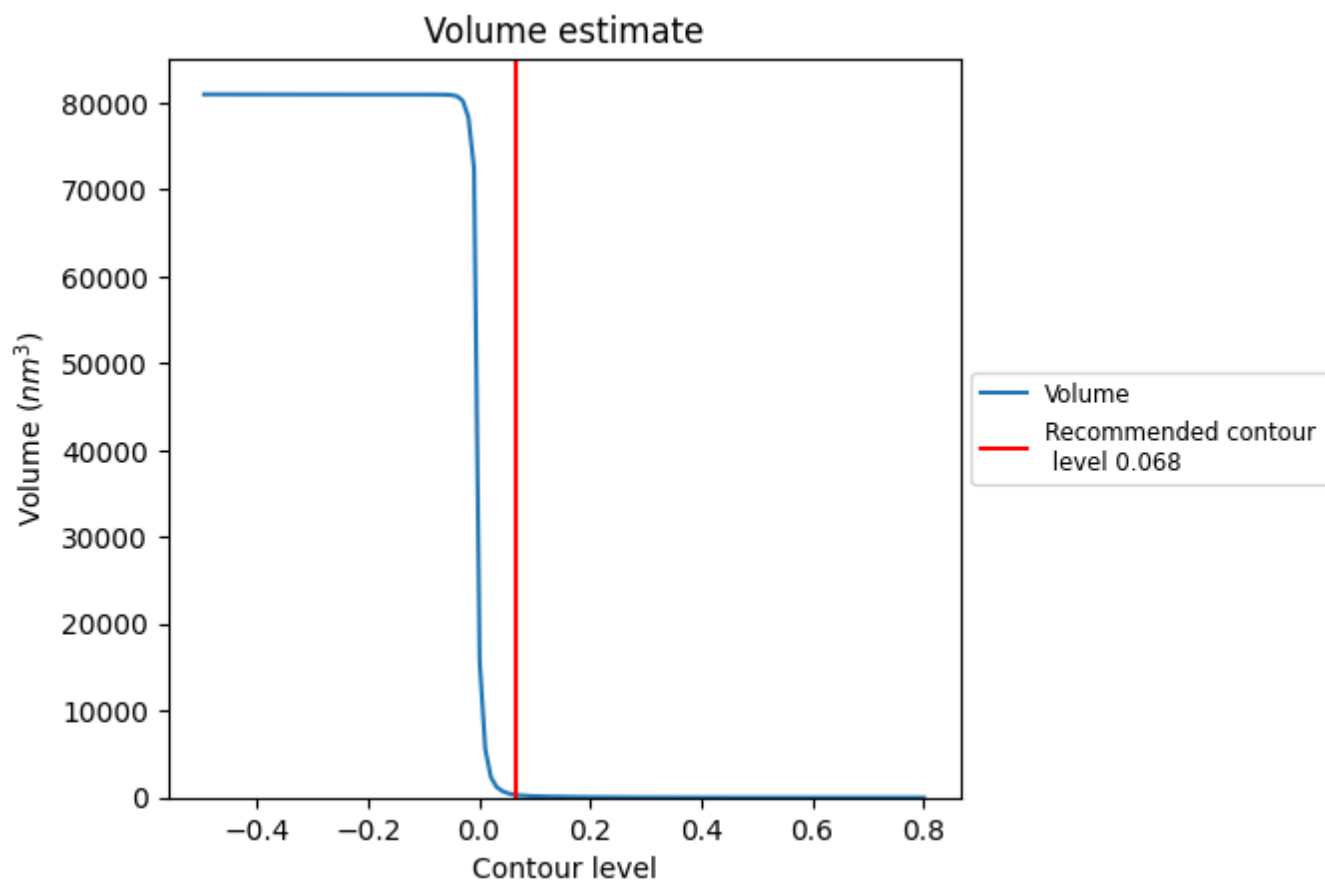
This section contains the results of statistical analysis of the map.

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.

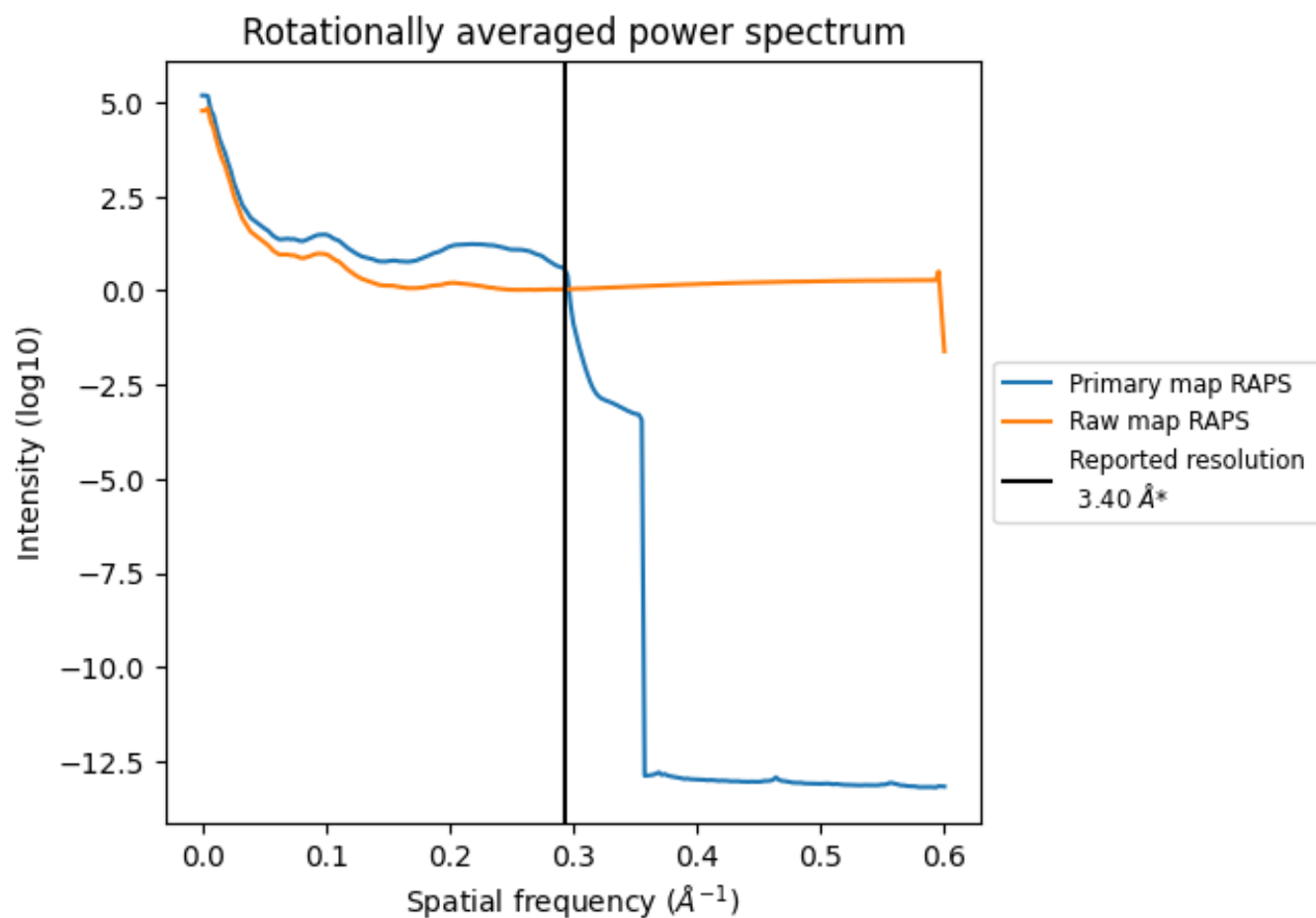
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300 nm³; this corresponds to an approximate mass of 271 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 ⓘ

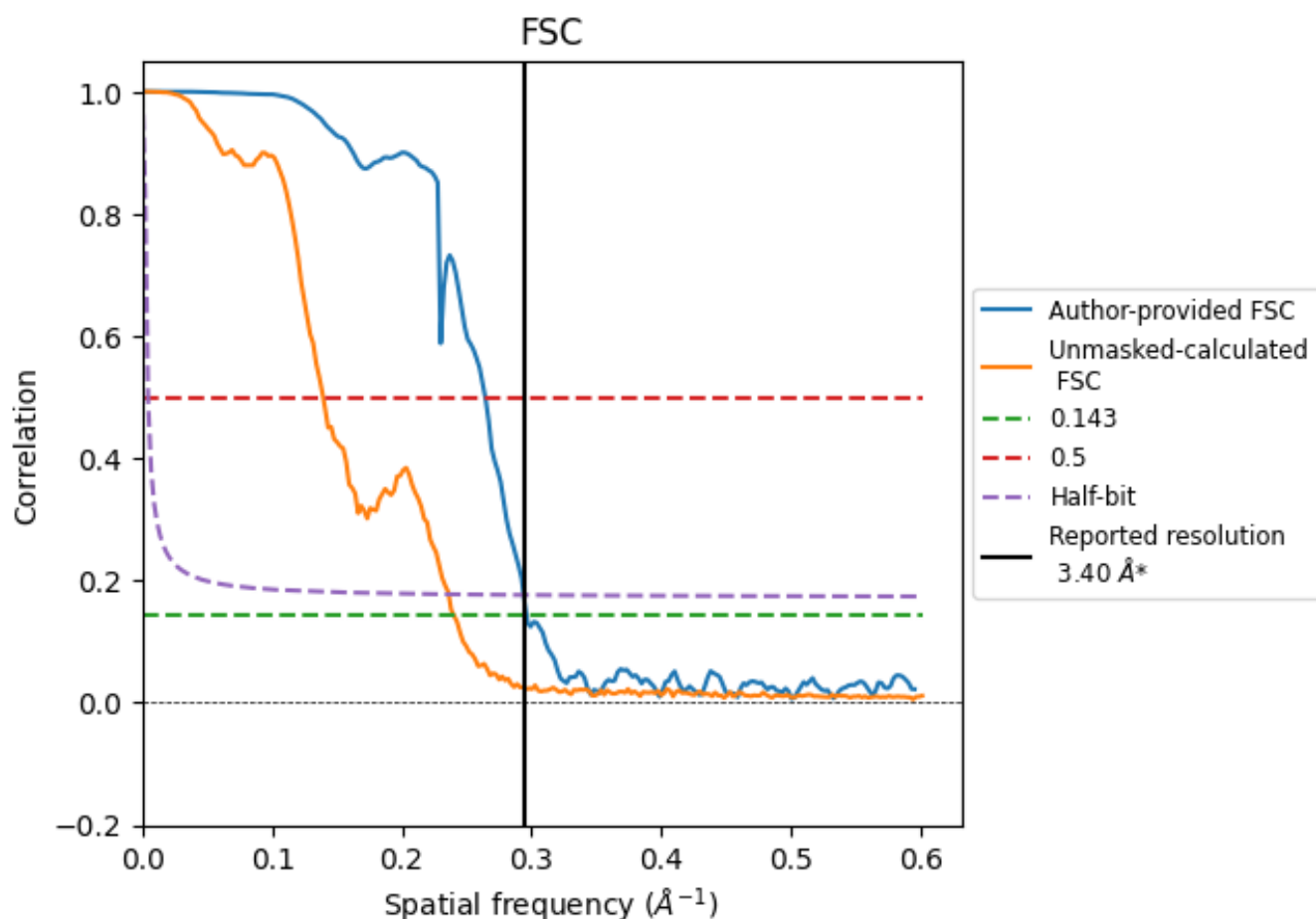


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

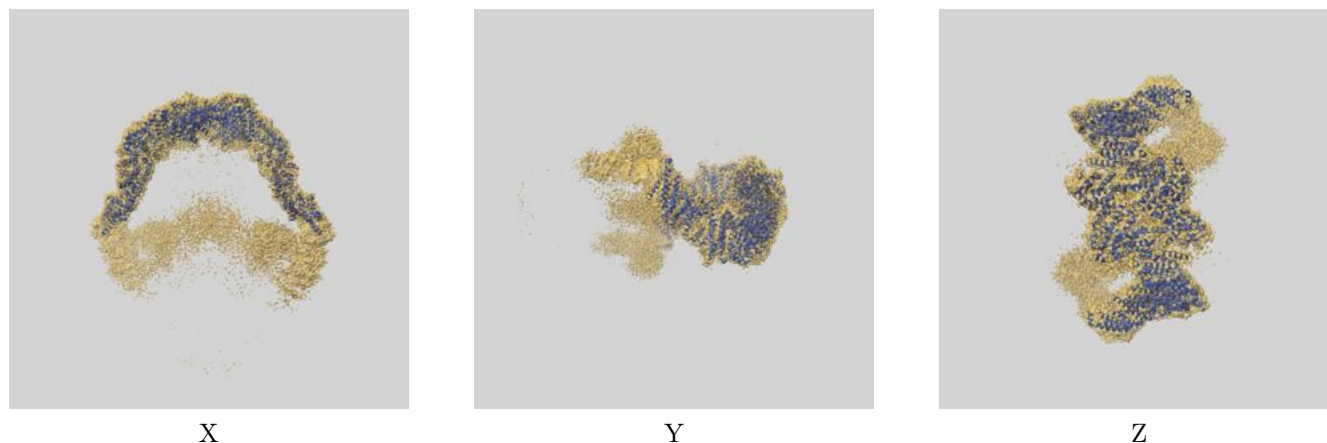
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	3.78	3.40
Unmasked-calculated*	4.16	7.17	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

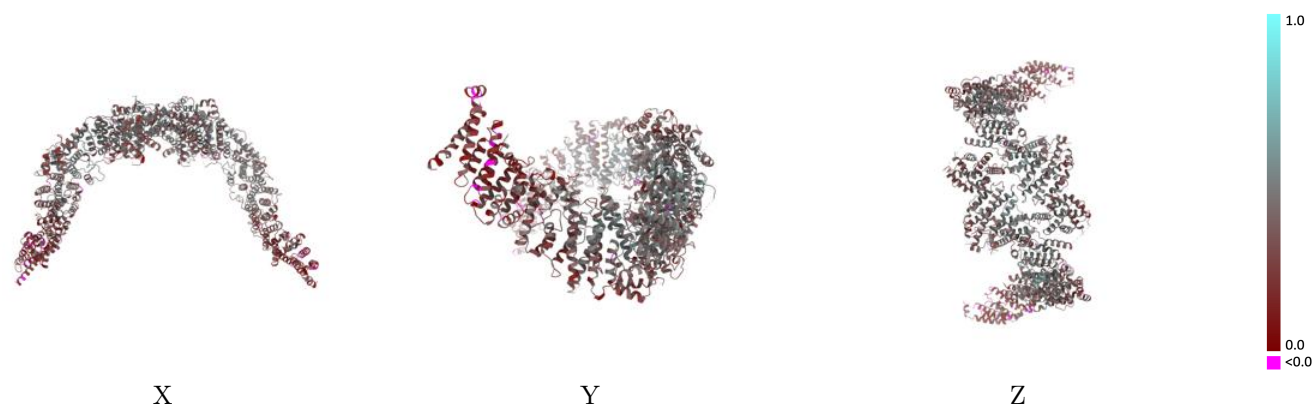
This section contains information regarding the fit between EMDB map EMD-46688 and PDB model 9NWD. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



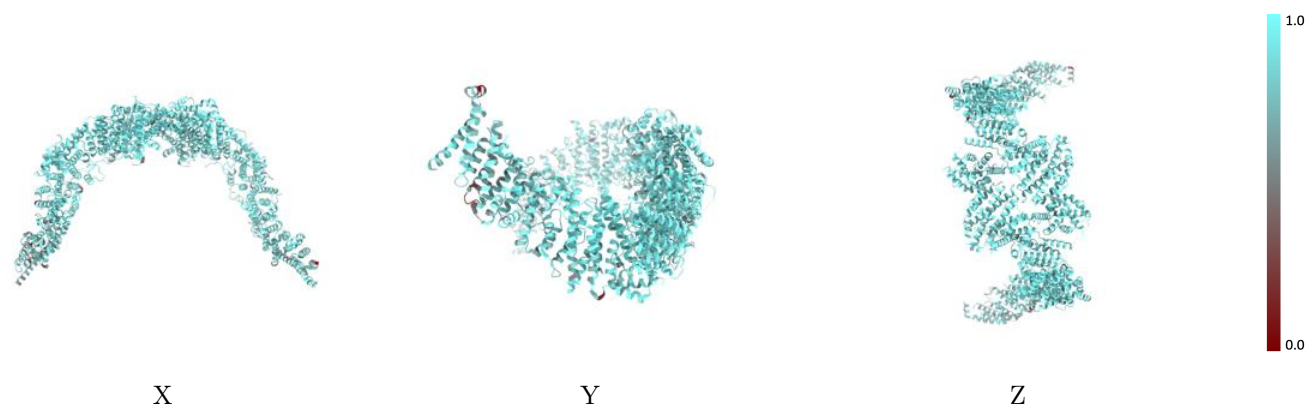
The images above show the 3D surface view of the map at the recommended contour level 0.068 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



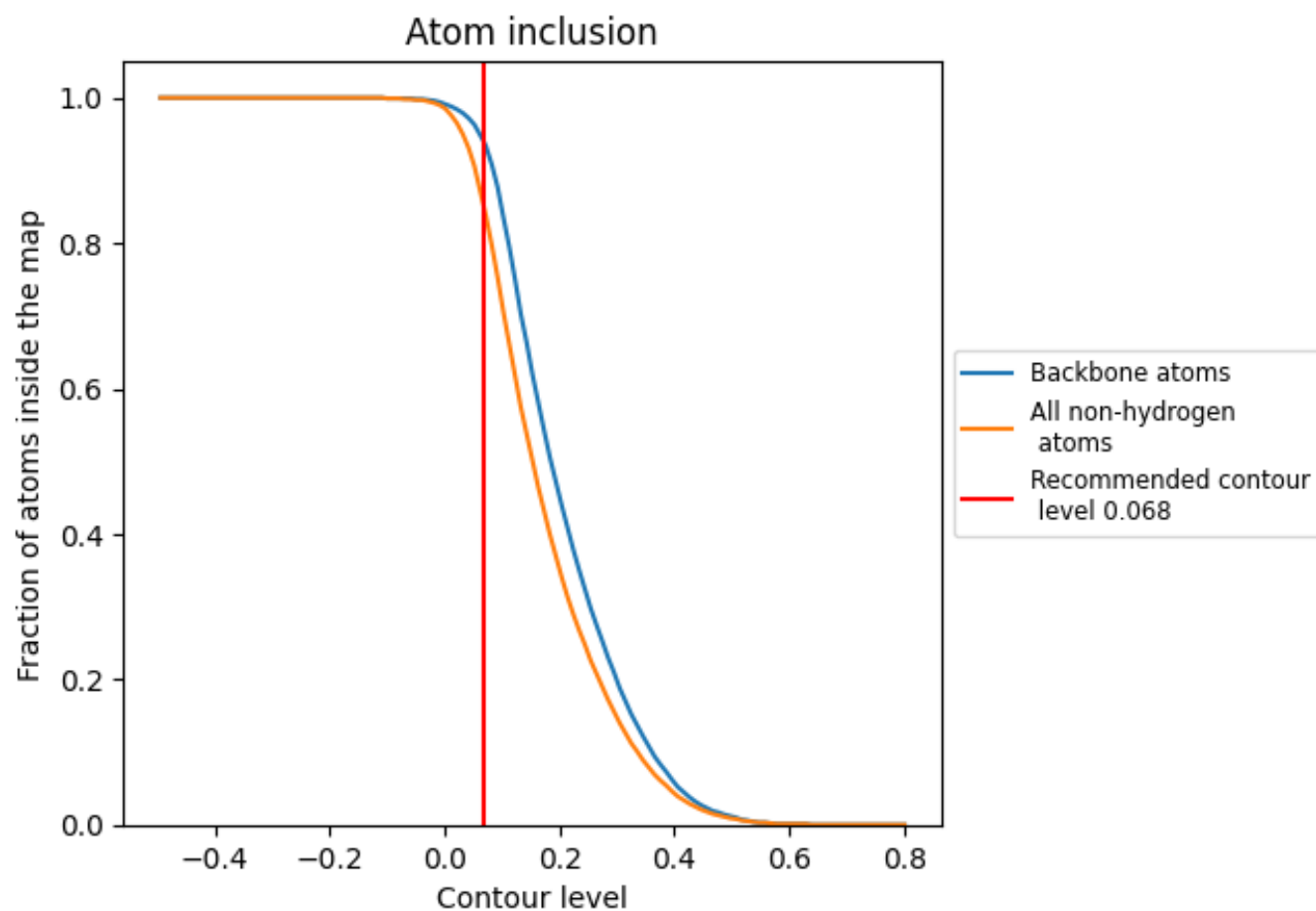
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.068).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.3640
A	0.8470	0.3600
B	0.8550	0.3680

