



wwPDB EM Validation Summary Report ⓘ

Jun 3, 2025 – 12:42 PM EDT

PDB ID : 9D9Z / pdb_00009d9z
EMDB ID : EMD-46686
Title : Structure of human UBR4-KCMF1-CaM E3 ligase complex (Silencing Factor of the Integrated stress response, SiFI)
Authors : Yang, Z.; Rape, M.
Deposited on : 2024-08-21
Resolution : 3.40 Å(reported)

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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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

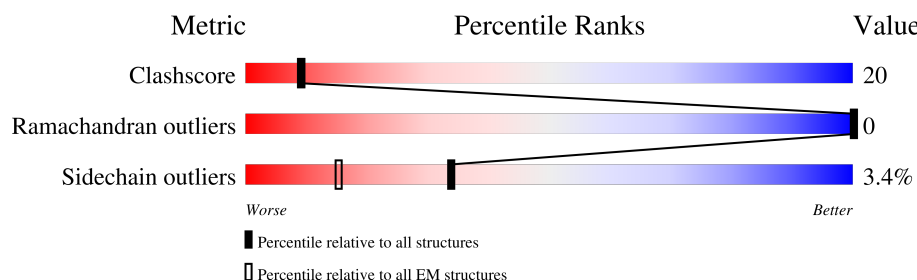
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	5205	<div> <div>50%</div> <div>45%</div> <div>29%</div> <div>25%</div> </div>
1	B	5205	<div> <div>50%</div> <div>46%</div> <div>28%</div> <div>24%</div> </div>
2	C	149	<div> <div>83%</div> <div>51%</div> <div>43%</div> <div>• •</div> </div>
2	D	149	<div> <div>85%</div> <div>47%</div> <div>46%</div> <div>• •</div> </div>
3	E	381	<div> <div>34%</div> <div>30%</div> <div>17%</div> <div>52%</div> </div>
3	F	381	<div> <div>35%</div> <div>29%</div> <div>18%</div> <div>52%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	A	5202	-	-	X	-
4	ZN	B	5202	-	-	X	-
5	CA	D	202	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 66746 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 UBR4 (endogenously FLAG-tagged at the N-terminus),E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3917	Total	C	N	O	S	0	0
			30658	19475	5230	5749	204		
1	B	3946	Total	C	N	O	S	0	0
			30933	19647	5279	5802	205		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	144	Total	C	N	O	S	0	0
			1134	696	182	247	9		
2	D	143	Total	C	N	O	S	0	0
			1127	692	181	245	9		

- Molecule 3 is a protein called E3 ubiquitin-protein ligase KCMF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	182	Total	C	N	O	S	0	0
			1435	881	250	288	16		
3	F	182	Total	C	N	O	S	0	0
			1435	881	250	288	16		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	6	Total	Zn	0
			6	6	
4	B	6	Total	Zn	0
			6	6	
4	E	4	Total	Zn	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
4	F	4	Total	Zn	0
			4	4	

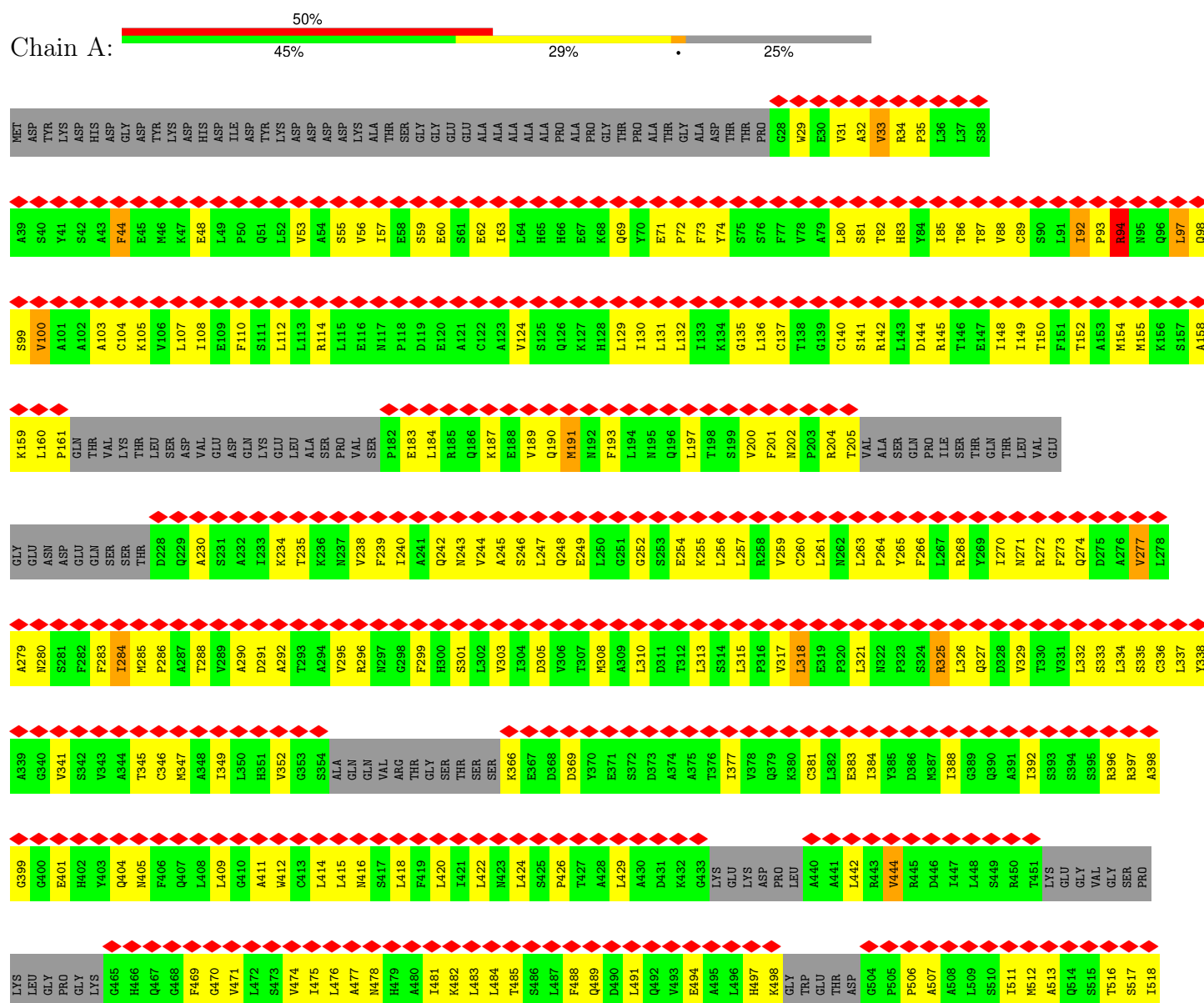
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	C	2	Total	Ca	0
			2	2	
5	D	2	Total	Ca	0
			2	2	

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: UBR4 (endogenously FLAG-tagged at the N-terminus),E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4



I1299	N1239	Q1179	Q1119	I1059	L999	E939	Q879	H819	R759	K699	ALA	GLY	I1299	N1239	Q1179	Q1119	I1059	L999	E939	Q879	H819	R759	K699	ASP	Q519
V1300	E1240	N1180	S1120	K1060	Q1000	A940	V880	N820	L760	G700	R540	SER	V1300	E1240	N1180	S1120	K1060	Q1000	A940	V880	N820	L760	G700	SER	R520
W1301	F1241	F1181	I1121	Q1061	Y1001	S941	Q881	F821	R641	S701	R641	GLN	W1301	F1241	F1181	I1121	Q1061	Y1001	S941	Q881	F821	R641	S701	GLN	Q522
S1302	P1242	N1182	Y1122	G1062	Y1002	E942	H882	T822	L762	S702	D643	ASP	S1302	P1242	N1182	Y1122	G1062	Y1002	E942	H882	T822	L762	S702	ASP	Q523
D1303	N1243	E1183	T1123	M1063	F1003	D943	N883	E823	I763	D703	P644	ASP	D1303	N1243	E1183	T1123	M1063	F1003	D943	N883	E823	I763	D703	ASP	R523
E1304	I1244	E1184	L1124	K1064	L1004	D944	L884	T824	W764	E704	L524	ASP	E1304	I1244	E1184	L1124	K1064	L1004	D944	L884	T824	W764	E704	ASP	L524
M1305	G1245	THR	D1125	A1065	I1005	L945	L885	Q825	Q765	E705	D526	SER	M1305	G1245	THR	D1125	A1065	I1005	L945	L885	Q825	Q765	E705	SER	I525
N1306	S1246	THR	A1126	E1066	L1006	N946	S886	R826	H766	F706	D526	GLY	N1306	S1246	THR	A1126	E1066	L1006	N946	S886	R826	H766	F706	GLY	D526
P1307	W1247	GLU	A1127	H1067	W1007	R947	P887	R827	K767	A707	S527	PRO	P1307	W1247	GLU	A1127	H1067	W1007	R947	P887	R827	K767	A707	PRO	S527
P1308	R1248	LVS	I1128	A1068	R1008	L948	P888	A828	A768	A708	V528	LEU	P1308	R1248	LVS	I1128	A1068	R1008	L948	P888	A828	A768	A708	LEU	V528
Q1309	M1249	P1190	S1129	S1069	I1009	D949	PHE	R829	S769	A709	G649	GLN	Q1309	M1249	P1190	S1129	S1069	I1009	D949	PHE	R829	S769	A709	GLN	P529
V1310	A1250	K1191	S1130	S1070	L1010	S950	TRP	L830	A770	L710	L530	GLN	V1310	A1250	K1191	S1130	S1070	L1010	S950	TRP	L830	A770	L710	GLN	P530
I1311	F1251	K1192	V1131	L1071	G1011	V951	ALA	S831	Q771	Y711	M531	PHE	I1311	F1251	K1192	V1131	L1071	G1011	V951	ALA	S831	Q771	Y711	PHE	M531
R1312	A1252	E1193	Q1132	E1073	I1012	A952	SER	L832	G772	H712	N532	GLY	R1312	A1252	E1193	Q1132	E1073	I1012	A952	SER	L832	G772	H712	GLY	N532
T1313	N1253	K1194	V1133	E1073	L1013	C953	GLY	F833	D773	F713	L533	GLY	T1313	N1253	K1194	V1133	E1073	L1013	C953	GLY	F833	D773	F713	GLY	L533
L1314	D1254	L1195	S1134	A1075	P1014	D954	SER	V834	P774	N714	L534	TLE	L1314	D1254	L1195	S1134	A1075	P1014	D954	SER	V834	P774	N714	TLE	L534
L1315	T1255	Q1196	L1135	L1075	P1015	V955	ASP	Q835	D775	H715	L535	SER	L1315	T1255	Q1196	L1135	L1075	P1015	V955	ASP	Q835	D775	H715	SER	L535
P1316	I1256	G1197	D1136	S1076	S1016	L956	SER	T836	V776	S716	T536	PRO	P1316	I1256	G1197	D1136	S1076	S1016	L956	SER	T836	V776	S716	PRO	T536
F1198	P1257	F1198	E1137	T1077	K1017	F957	SER	R837	F777	L717	L537	SER	F1198	P1257	F1198	E1137	T1077	K1017	F957	SER	R837	F777	L717	SER	L537
L1317	S1258	A1199	H1138	T1078	T1018	S958	ARG	Q838	E778	V718	L538	GLY	L1317	S1258	A1199	H1138	T1078	T1018	S958	ARG	Q838	E778	V718	GLY	L538
L1318	E1259	A1200	F1139	K1079	Y1019	K959	ARG	E839	C779	T719	S539	LVS	L1318	E1259	A1200	F1139	K1079	Y1019	K959	ARG	E839	C779	T719	LVS	S539
L1319	S1260	V1201	S1140	C1080	I1020	L960	A903	L840	L780	S720	T540	ALA	L1319	S1260	V1201	S1140	C1080	I1020	L960	A903	L840	L780	S720	ALA	T540
S1321	Y1261	L1202	K1141	S1081	N1021	V961	T904	S841	K781	S720	S541	PRO	S1321	Y1261	L1202	K1141	S1081	N1021	V961	T904	S841	K781	S720	PRO	S541
S1322	I1262	A1203	M1142	V1082	Q1022	K962	T905	V842	W782	L722	Y542	PRO	S1322	I1262	A1203	M1142	V1082	Q1022	K962	T905	V842	W782	L722	PRO	Y542
T1323	S1263	I1204	A1143	V1083	L1023	Y963	P906	N843	W783	Q723	R543	PRO	T1323	S1263	I1204	A1143	V1083	L1023	Y963	P906	N843	W783	Q723	PRO	R543
E1324	A1264	G1205	ALA	K1084	S1024	D964	L907	N844	D784	S724	K544	PRO	E1324	A1264	G1205	ALA	K1084	S1024	D964	L907	N844	D784	S724	PRO	K544
S1325	V1265	S1206	GLY	Y1085	M1025	E965	Y908	D845	R785	P725	A545	PRO	S1325	V1265	S1206	GLY	Y1085	M1025	E965	Y908	D845	R785	P725	PRO	A545
V1326	Q1266	S1207	THR	D1086	N1026	L966	H909	A846	F786	N726	C546	PRO	V1326	Q1266	S1207	THR	D1086	N1026	L966	H909	A846	F786	N726	PRO	C546
A1327	A1267	R1208	PRO	V1087	S1027	Y967	G310	Q847	L787	L727	V547	PRO	A1327	A1267	R1208	PRO	V1087	S1027	Y967	G310	Q847	L787	L727	PRO	V547
E1328	A1268	C1209	HIS	E1088	P1028	A968	F911	N848	S788	Q728	L548	LEU	E1328	A1268	C1209	HIS	E1088	P1028	A968	F911	N848	S788	Q728	LEU	L548
L1329	H1269	K1210	S1151	I1089	E1029	A969	K912	R849	T789	N729	Q549	GLY	L1329	H1269	K1210	S1151	I1089	E1029	A969	K912	R849	T789	N729	GLY	Q549
S1330	L1270	A1211	S1152	V1090	M1030	L970	E913	F850	W790	M730	R549	GLY	S1330	L1270	A1211	S1152	V1090	M1030	L970	E913	F850	W790	M730	GLY	Q549
S1331	G1271	M1212	E1153	E1091	S1031	T971	V914	H851	K791	L731	R671	SER	S1331	G1271	M1212	E1153	E1091	S1031	T971	V914	H851	K791	L731	SER	R671
M1332	T1272	T1213	I1154	E1092	E1032	A972	E915	P852	Q792	L732	N672	PRO	M1332	T1272	T1213	I1154	E1092	E1032	A972	E915	P852	Q792	L732	PRO	N672
S1333	L1273	L1214	T1155	Y1093	C1033	L974	E916	L853	N793	Q733	V673	ARG	S1333	L1273	L1214	T1155	Y1093	C1033	L974	E916	L853	N793	Q733	ARG	V673
L1334	C1274	G1215	K1156	F1094	D1034	L974	N917	T854	A794	Q734	L674	LVS	L1334	C1274	G1215	K1156	F1094	D1034	L974	N917	T854	A794	Q734	LVS	G554
E1335	S1275	P1216	N1157	A1095	I1035	A975	W918	L855	L795	L735	S675	SER	E1335	S1275	P1216	N1157	A1095	I1035	A975	W918	L855	L795	L735	SER	S675
R1336	Q1276	T1217	L1158	R1096	L1036	A976	S919	A856	Q796	G736	V676	PRO	R1336	Q1276	T1217	L1158	R1096	L1036	A976	S919	A856	Q796	G736	PRO	S675
I1337	S1277	L1218	L1159	Q1097	H1037	G977	K920	R857	G797	V737	S677	LVS	I1337	S1277	L1218	L1159	Q1097	H1037	G977	K920	R857	G797	V737	LVS	S677
L1338	L1278	V1219	P1160	I1098	T1038	S978	H921	L858	W798	A738	L678	GLN	L1338	L1278	V1219	P1160	I1098	T1038	S978	H921	L858	W798	A738	GLN	L678
G1339	P1279	Q1220	A1161	S1099	L1039	Q979	F922	L859	W799	F739	S679	ALA	G1339	P1279	Q1220	A1161	S1099	L1039	Q979	F922	L859	W799	F739	ALA	S679
P1340	L1280	N1221	T1162	S1100	R1040	L980	S923	L860	P800	F740	E680	PRO	P1340	L1280	N1221	T1162	S1100	R1040	L980	S923	L860	P800	F740	PRO	E680
A1341	A1281	L1222	L1163	F1101	W1041	D981	S924	L861	S801	S741	H681	GLY	A1341	A1281	L1222	L1163	F1101	W1041	D981	S924	L861	S801	S741	GLY	E681
E1342	A1282	P1223	L1163	C1102	S1042	T982	D925	R862	E802	E742	H682	LVS	E1342	A1282	P1223	L1163	C1102	S1042	T982	D925	R862	E802	E742	LVS	THR
S1343	S1283	S1224	L1165	S1103	S1043	V983	A926	D863	T803	G743	N683	GLY	S1343	S1283	S1224	L1165	S1103	S1043	V983	A926	D863	T803	G743	GLY	ASP
D1344	L1284	S1225	I1166	T1104	R1044	R984	V927	Y864	E804	P744	A684	ASN	D1344	L1284	S1225	I1166	T1104	R1044	R984	V927	Y864	E804	P744	ASN	SER
E1345	R1285	V1226	D1167	D1105	L1045	R985	P928	L865	D805	W745	T685	THR	E1345	R1285	V1226	D1167	D1105	L1045	R985	P928	L865	D805	W745	THR	THR
F1346	H1286	Q1227	T1168	C1106	R1046	K986	R1046	L866	P746	P746	L686	TYR	F1346	H1286	Q1227	T1168	C1106	R1046	K986	R1046	L866	P746	P746	TYR	TYR
L1347	T1287	T1228	Y1169	T1107	I1047	E987	P930	R867	N807	L747	A687	GLY	L1347	T1287	T1228	Y1169	T1107	I1047	E987	P930	R867	N807	L747	GLY	TYR
A1348	L1288	V1229	A1170	T1108	S1048	N988	R931	Q868	W808	V748	S688	GLY	A1348	L1288	V1229	A1170	T1108	S1048	N988	R931	Q868	W808	V748	GLY	ASP
R1349	L1289	C1230	S1171	L1109	S1049	K989	S1049	Y869	E809	I749	T689	LVS	R1349	L1289	C1230	S1171	L1109	S1049	K989	S1049	Y869	E809	I749	LVS	THR
V1350	S1290	E1231	F1172	L1110	Y1050	N990	Y933	S870	H810	H750	D694	THR	V1350	S1290	E1231	F1172	L1110	Y1050	N990	Y933	S870	H810	H750	THR	THR
Y1351	L1291	S1232	T1173	Q1111	V1051	V991	C934	R871	L811	F751	K691	SER	Y1351	L1291	S1232	T1173	Q1111	V1051	V991	C934	R871	L811	F751	SER	SER
E1352	V1292	W1233	R1174	L1112	N1052	T992	V935	A872	Q812	Q752	E692	THR	E1352	V1292	W1233	R1174	L1112	N1052	T992	V935	A872	Q812	Q752	THR	SER
K1353	R1293	N1234	A1175	H1113	W1053	A993	L936	P873	N813	S753	V693	ASP	K1353	R1293	N1234	A1175	H1113	W1053	A993	L936	P873	N813	S753	ASP	PHE
L1354	L1294	N1235	Y1176	E1114	I1054	A994	S937	V874	L814	L754	D694	PHE	L1354	L1294	N1235	Y1176	E1114	I1054	A994	S937	V874	L814	L754	PHE	THR

P2085	I2025	N1960	C1900	Q1840	E1722	LYS	S1601	V1539	S1479	L1419	Y1359
F2086	Y2026	P1961	V1901	A1841	D1723	L1663	S1602	V1540	D1480	S1420	N1360
Y2087	D2027	C1962	L1902	L1842	G1724	C1664	Y1602	M1541	Q1481	A1421	I1361
T2088	L2028	S1963	S1903	S1843	S1725	T1665	L1603	A1542	L1482	K1422	L1362
T2089	C2029	S1904	S1904	E1844	C1726	F1666	A1604	T1543	D1483	F1423	A1363
N2090	V2030	D1965	F1905	H1845	L1727	T1667	V1606	L1544	V1484	C1424	N1364
V2091	D2031	Y1966	H1906	H1846	A1728	I1668	T1607	A1545	I1485	N1425	H1365
L2092	A2032	L1967	G1907	T1847	L1729	T1669	N1608	S1546	Q1486	R1426	A1366
L2093	L2033	A1968	R1908	V1848	VAL	GLN	A1609	A1547	E1487	V1427	A1367
I2094	S2034	C1970	VAL	E1849	LYS	GLY	L1610	G1548	N1488	L1428	P1368
N2095	P2035	G1971	GLU	K1850	THR	PHE	SER	Q1549	R1489	K1429	N1369
H2096	T2036	L1972	GLY	A1851	PRO	MET	ASN	G1550	Q1490	F1430	S1370
E2097	F2037	K1973	CYS	I1852	SER	ASN	GLN	A1551	L1491	F1431	G1371
D2098	Y2038	H1976	ARG	E1853	GLY	Q1676	ASN	G1552	L1492	T1432	L1372
L2099	F2039	V1977	E1797	M1854	GLY	H1677	GLY	H1553	Q1493	K1433	D1373
K2100	L2040	S1978	S1915	T1855	MET	Y1678	GLN	L1554	L1494	L1434	E1374
D2101	L2041	L1978	H1916	D1856	SER	Y1679	GLY	Q1555	L1495	F1435	S1375
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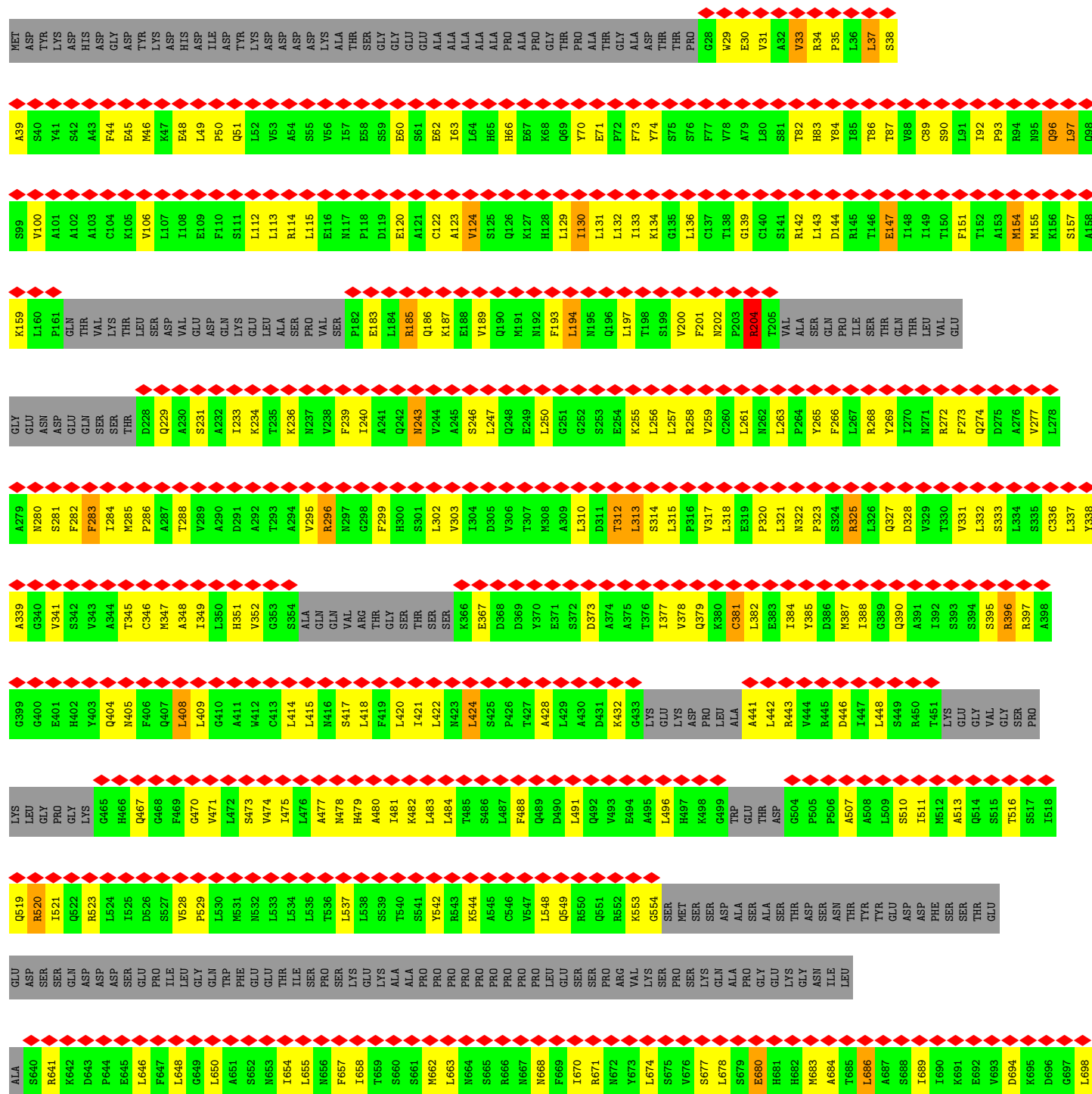




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- Molecule 1: UBR4 (endogenously FLAG-tagged at the N-terminus),E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4



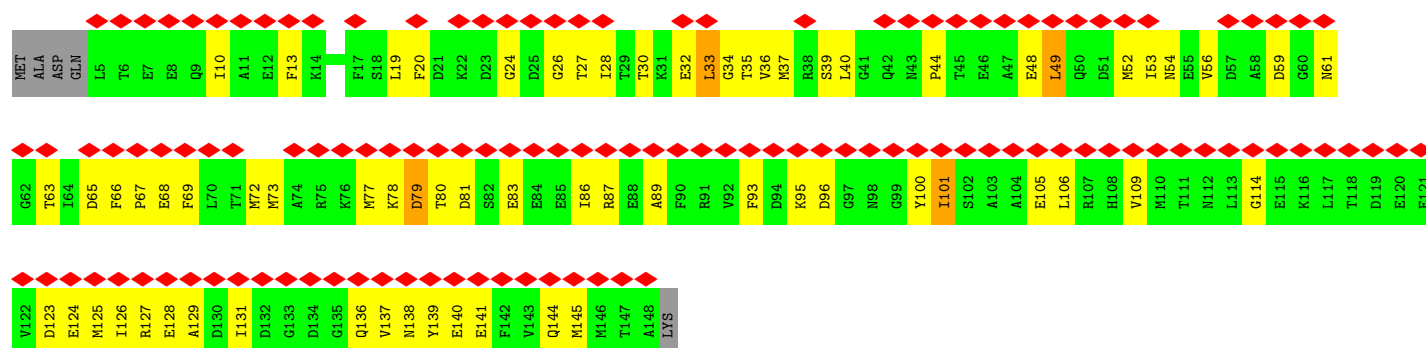
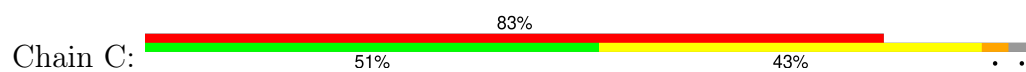
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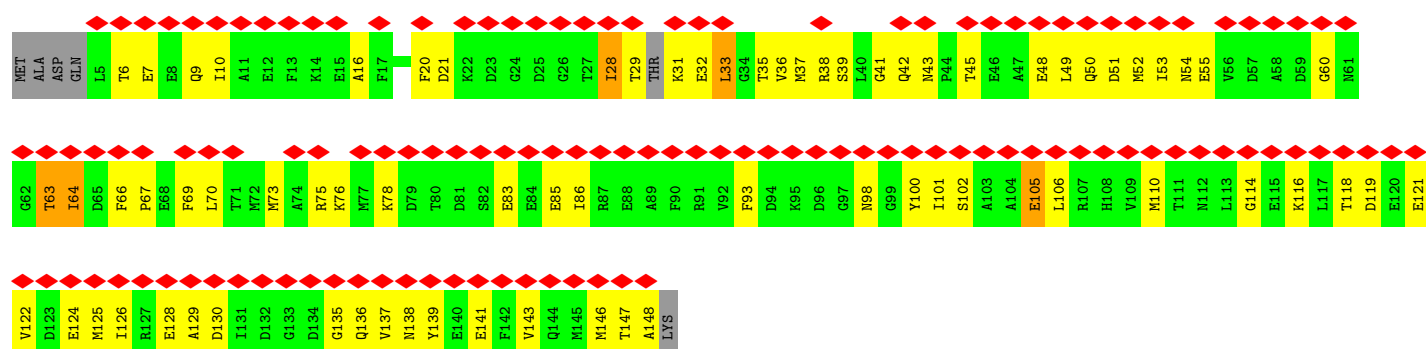
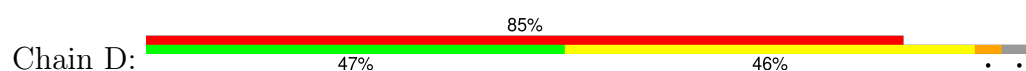


T4230	D4231	L4232	Q4233	Q4234	L4238	K4239	L4244	F4248	R4256	H4257	F4258	K4259	L4260	S4260	R4261	G4264	L4267	L4271	C4272	L4273	R4274	L4275	K4275	L4276	V4277	V4278	Q4279	R4280	T4284	D4285	E4286	T4287	Q4288	D4289	M4290	D4297	E4303	K4307	F4309	H4310	A4311	V4312	C4313	L4314	E4315	T4316	R4319	T4328	S4229							
GLU	ALA	LEU	THR	T4044	P4047	C4048	C4049	N4050	E4051	I4052	H4053	W4059	F4060	K4061	R4062	W4071	L4075	P4076	L4077	R4078	G4079	I4080	D4081	G4082	N4083	G4084	K4085	A4086	P4087	S4088	K4089	S4090	E4091	L4092	R4093	H4094	L4095	L4096	L4097	T4098	E4099	K4100	Y4101	V4102	W4103	R4104	W4105	K4106	Q4107	F4108	L4109	S4110	R4111	R4112	G4113	
K4114	R4115	T4116	S4117	L4118	L4119	D4120	L4123	G4124	H4125	W4126	N4127	F4128	L4129	R4130	Q4131	V4132	F4134	T4135	C4146	I4155	R4158	K4159	L4165	Q4169	L4170	L4173	L4186	Y4187	I4191	H4195	W4196	V4205	L4206	P4207	L4212	K4215	L4216	L4221	A4222	L4223	E4224	L4228	S4229													
F4250	L3251	V3256	L3259	I3270	M3273	F3274	H3275	Q3285	R3286	T3287	F3288	N3289	W3290	S3291	K3292	F3293	A3294	I3295	D3298	L3301	Y3302	F3303	L3304	L3305	Q3306	V3307	L3310	F3309	L3310	V3311	D3312	V3315	V3318	Y3324	L3319	L3320	L3327	L3323	D3324	C3325	S3326	L3327	C3328	G3329	S3330	K3331	V3332	L3333	A3334	E3335	L3336	A3337				
ALA	SER	SER	GLY	SER	SER	SER	SER	ALA	PRO	VAL	ALA	ALA	SER	SER	GLY	GLN	ALA	THR	THR	GLN	SER	LYS	SER	THR	LYS	LYS	LYS	GLU	GLU	LYS	GLU	LYS	GLU	GLY	GLU	THR	SER	G3385	S3386	Q3387	E3388	C3392	L3395	V3396	N3397	A3398	D3404									
K3405	E3406	T3407	L3408	I3409	Q3410	F3411	L3412	L3416	L3417	E3418	S3419	N3420	V3424	R3425	N3438	S3439	S3440	Q3443	L3447	L3450	S3453	L3454	W3455	P3456	E3457	L3458	P3459	A3460	Y3461	A3465	V3469	D3470	S3490	V3494	E3495	I3496	L3497	H3507	P3508	N3511	I3512	Y3513	H3514	T3515	L3516											
L3519	V3520	E3521	Y3525	Y3526	L3527	C3532	L3533	V3534	V3540	C3543	L3547	S3548	S3549	I3550	K3551	V3552	Y3556	Q3561	I3566	I3571	G3579	D3580	L3581	K3582	R3583	V3587	R3588	T3589	I3590	N3595	Q3600	A3601	E3604	L3605	K3606	N3607	K3608	P3609	T3621	P3622	G3623	E3626	V3627													
K3628	I3629	D3630	L3631	P3632	L3633	L3640	M3641	L3642	E3643	F3644	A3645	D3646	F3647	Y3648	E3649	N3650	V3651	Q3652	A3653	S3654	T3655	E3656	T3657	L3658	Q3659	C3660	P3661	R3662	C3663	S3664	A3665	S3666	V3667	P3668	A3669	N3670	P3671	V3672	C3674	Q3675	N3676	C3677	G3678	E3679	N3680	V3681	Y3682	Q3683	C3684	H3685	K3686	C3687	R3688	N3691	Y3692	D3693
E3694	K3695	L3699	C3703	G3704	F3705	C3706	R3710	F3711	D3712	F3713	Y3714	L3715	Y3716	A3717	K3718	V3723	E3727	N3728	E3729	E3730	D3731	R3732	K3733	K3734	A3735	I3739	L3742	A3746	D3747	R3748	V3749	Y3750	H3756	R3757	P3758	Q3759	L3760	E3761	N3762	L3763	L3764	C3765	K3766	V3767	A3770	E3773	K3774	P3775								
Q3776	D3777	D3778	S3779	G3780	T3781	A3782	G3783	G3784	L3785	S3786	T3787	S3788	S3789	A3790	S3791	V3792	N3793	R3794	Y3795	L3796	L3797	Q3798	L3799	Y3803	C3807	E3813	K3820	S3824	R3825	L3829	R3836	K3841	SER	SER	ARG	THR	SER	V3847	Q3848	P3849	T3850	F3851	T3852	A3853	S3854	Q3855	T4856	ARG	ALA	LEU	SER					
VAL	LEU	GLY	CYS	H3866	T3867	S3868	C3872	Y3873	G3874	V3879	T3880	E3881	H3882	C3883	I3884	L3887	R3888	A3889	N3893	P3894	A3895	L3896	R3897	H3898	I3899	L3900	V3901	S3902	G3903	G3904	L3905	L3909	F3910	N3913	A3918	A3919	A3920	M3921	R3922	V3925	R3926	Q3927	L3928	M3929	L3932	N3936	A3939									
T3940	T3948	G3949	K3950	V3951	K3956	D3963	L3968	Y3970	K3971	H3972	L3973	I3974	S3975	C3985	W3986	E3987	L3988	L3994	S3995	L3996	F3997	L3998	W4001	N4002	L4003	K4004	T4005	P4006	V4007	N4011	L4012	C4016	L4019	L4020	Q4021	L4024	K4025	P4026	P4027	S4031	K4035	D4036	VAL	PRO	VAL											

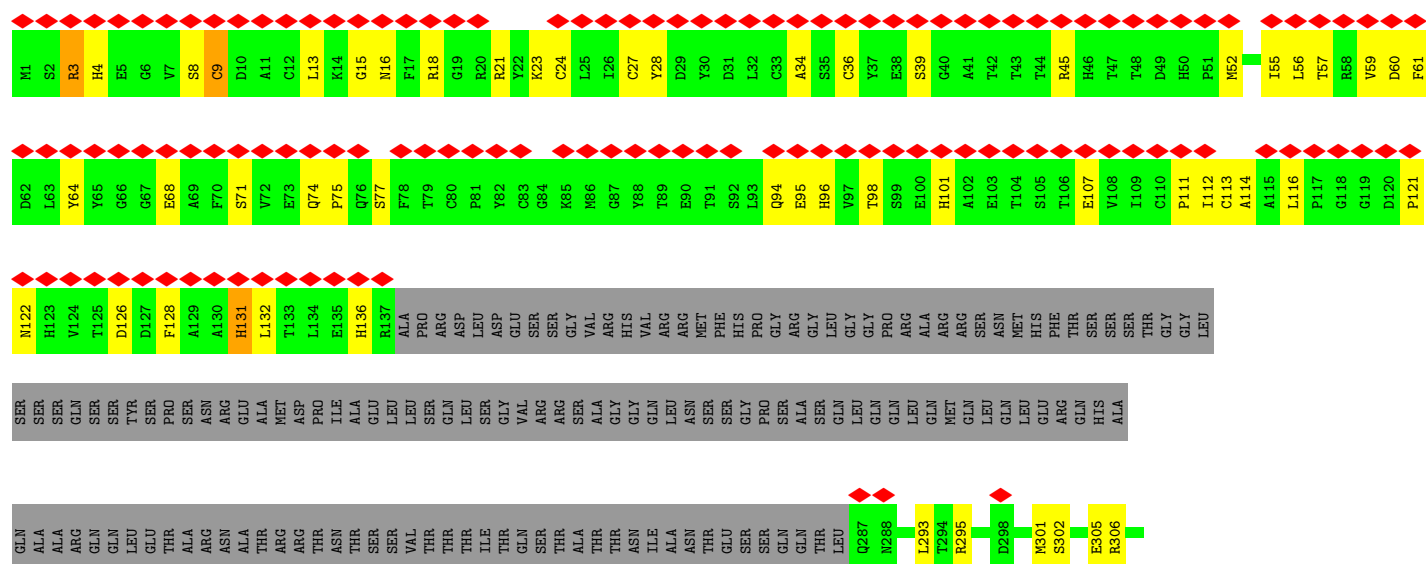
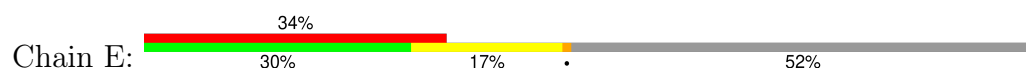
- Molecule 2: Calmodulin-1



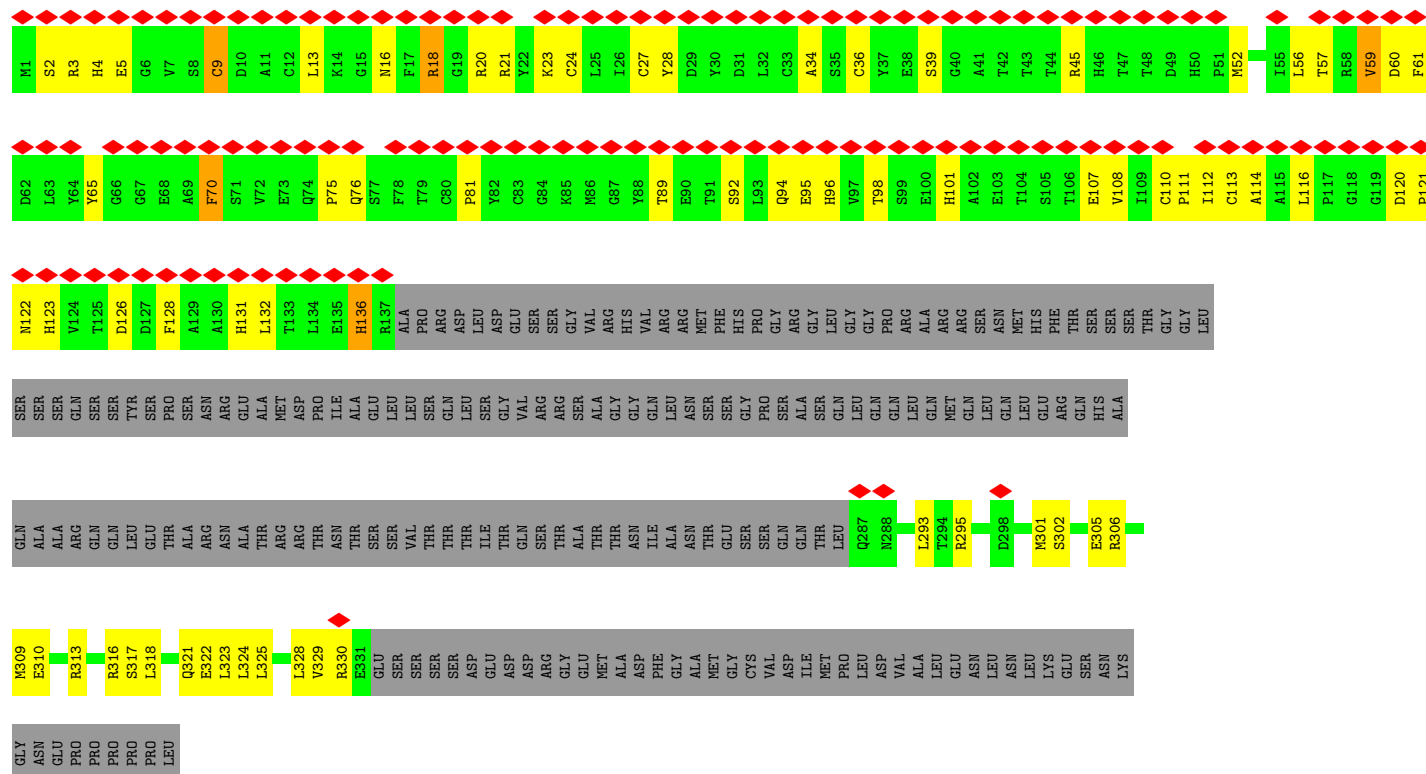
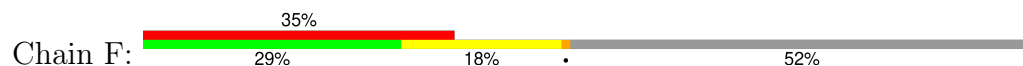
• Molecule 2: Calmodulin-1



• Molecule 3: E3 ubiquitin-protein ligase KCMF1



- Molecule 3: E3 ubiquitin-protein ligase KCMF1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126380	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.255	Depositor
Minimum map value	-0.578	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.13	Depositor
Map size (\AA)	440.16, 440.16, 440.16	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.048, 1.048, 1.048	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: CA, ZN

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	0.88	39/31195 (0.1%)	1.04	1/42247 (0.0%)
1	B	0.91	36/31477 (0.1%)	1.10	2/42619 (0.0%)
2	C	0.97	0/1146	1.24	0/1539
2	D	0.98	0/1138	1.25	0/1526
3	E	1.01	12/1463 (0.8%)	0.99	0/1978
3	F	1.00	13/1463 (0.9%)	1.01	0/1978
All	All	0.91	100/67882 (0.1%)	1.08	3/91887 (0.0%)

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	19
1	B	0	25
2	D	0	1
3	E	0	1
3	F	0	2
All	All	0	48

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1682	HIS	C-N	-10.20	1.20	1.33
1	B	1993	HIS	C-N	8.77	1.43	1.34
1	A	2290	ASP	C-N	-8.62	1.22	1.33
1	B	1865	SER	C-N	8.21	1.44	1.33
1	A	1894	LEU	C-N	-8.11	1.21	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1282	ALA	N-CA-C	-6.39	104.32	111.28
1	B	1131	VAL	N-CA-CB	5.70	117.22	110.55
1	B	529	PRO	N-CA-C	-5.06	102.05	112.47

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1008	ARG	Sidechain
1	A	325	ARG	Sidechain
1	A	849	ARG	Sidechain
1	A	94	ARG	Sidechain
1	A	985	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	30658	0	31020	1288	0
1	B	30933	0	31316	1262	0
2	C	1134	0	1063	68	0
2	D	1127	0	1055	61	0
3	E	1435	0	1344	44	0
3	F	1435	0	1344	52	0
4	A	6	0	0	2	0
4	B	6	0	0	3	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	2	0
All	All	66746	0	67142	2687	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 20.

The worst 5 of 2687 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:3270:ILE:CD1	1:B:3632:PRO:HG2	1.66	1.25
1:A:3270:ILE:CD1	1:A:3632:PRO:HG2	1.66	1.23
1:B:3087:ALA:CB	1:B:3181:ILE:HG21	1.73	1.19
1:A:73:PHE:CD1	1:A:159:LYS:HA	1.80	1.15
2:D:98:ASN:HB2	5:D:202:CA:CA	1.06	1.15

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	3853/5205 (74%)	3738 (97%)	115 (3%)	0	100	100
1	B	3884/5205 (75%)	3762 (97%)	122 (3%)	0	100	100
2	C	142/149 (95%)	136 (96%)	6 (4%)	0	100	100
2	D	139/149 (93%)	132 (95%)	7 (5%)	0	100	100
3	E	178/381 (47%)	175 (98%)	3 (2%)	0	100	100
3	F	178/381 (47%)	170 (96%)	8 (4%)	0	100	100
All	All	8374/11470 (73%)	8113 (97%)	261 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	3438/4542 (76%)	3329 (97%)	109 (3%)	34	59
1	B	3474/4542 (76%)	3347 (96%)	127 (4%)	29	54
2	C	123/127 (97%)	118 (96%)	5 (4%)	26	51
2	D	122/127 (96%)	115 (94%)	7 (6%)	17	43
3	E	162/330 (49%)	161 (99%)	1 (1%)	84	90
3	F	162/330 (49%)	159 (98%)	3 (2%)	52	71
All	All	7481/9998 (75%)	7229 (97%)	252 (3%)	34	57

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	LEU
1	B	4228	LEU
1	B	703	ASP
1	B	3968	LEU
2	C	33	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3397	ASN
1	B	3639	ASN
1	B	4766	ASN
1	A	3536	ASN
1	A	3491	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

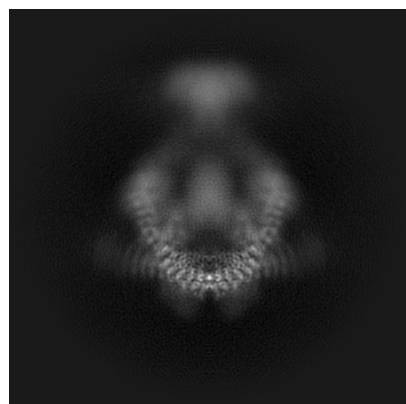
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46686. These allow visual inspection of the internal detail of the map and identification of artifacts.

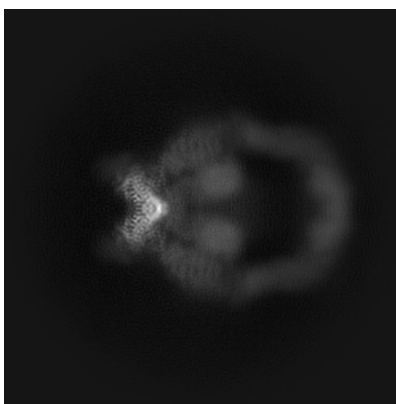
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

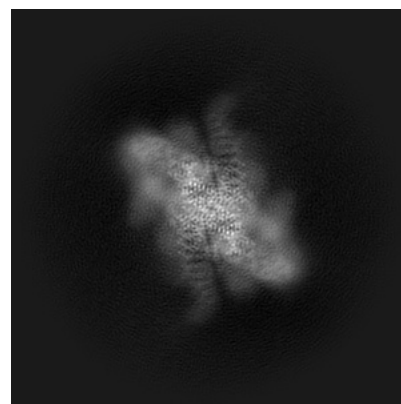
6.1.1 Primary map



X

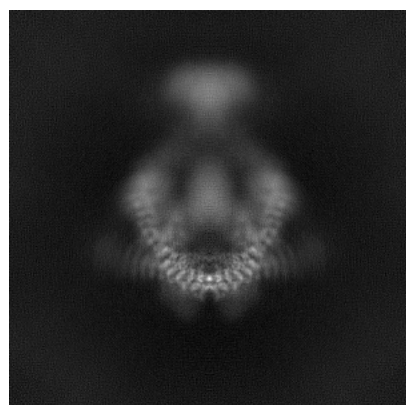


Y

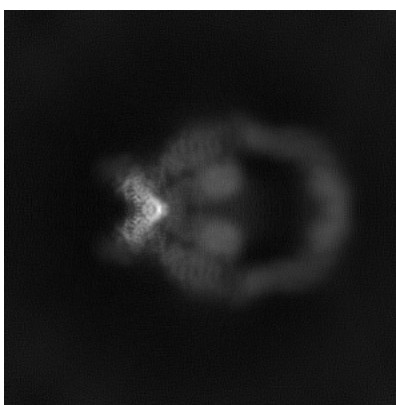


Z

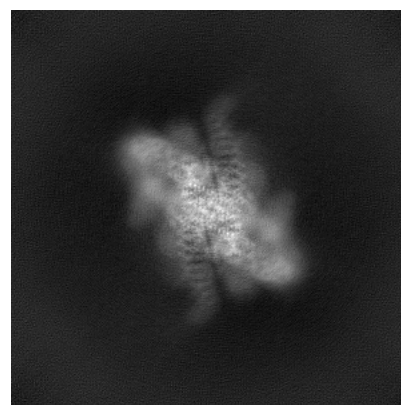
6.1.2 Raw map



X



Y

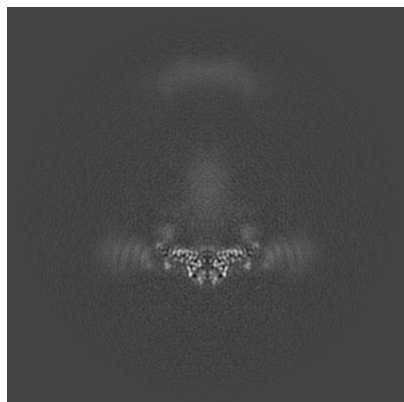


Z

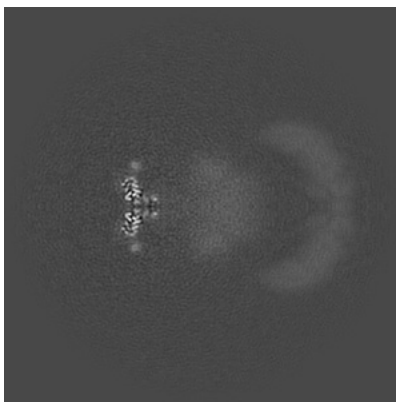
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

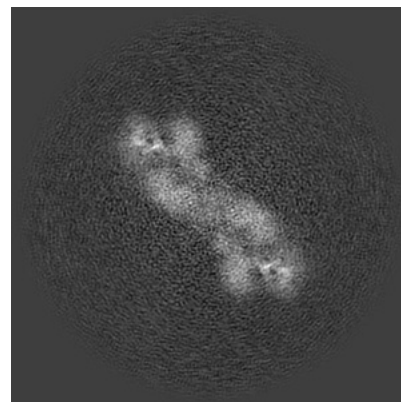
6.2.1 Primary map



X Index: 210



Y Index: 210

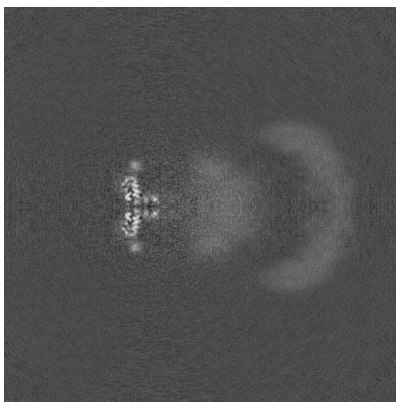


Z Index: 210

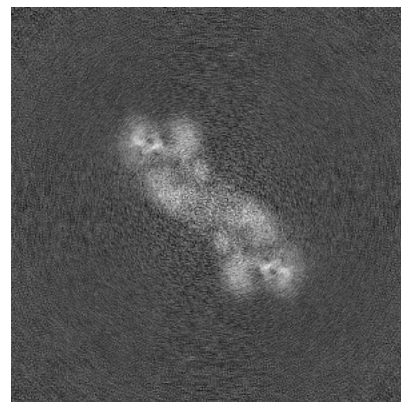
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

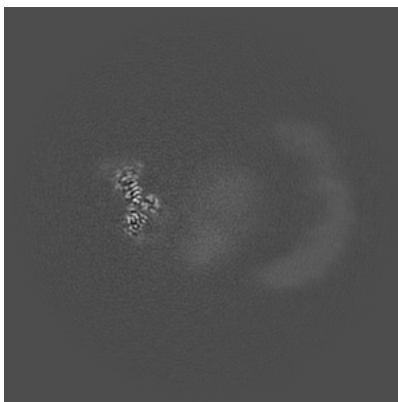
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

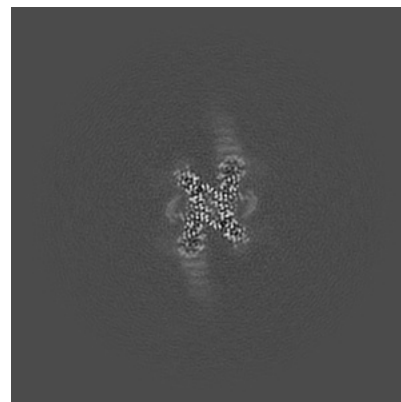
6.3.1 Primary map



X Index: 193

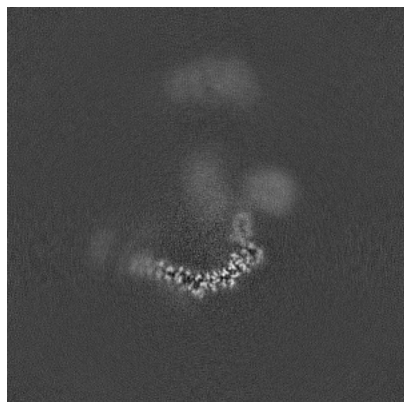


Y Index: 221

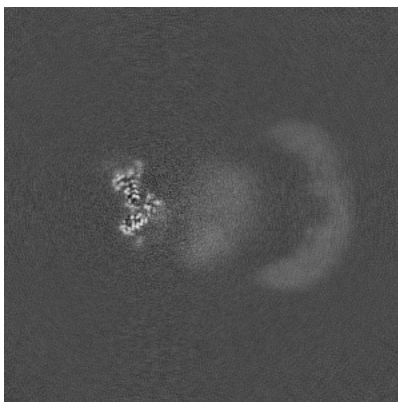


Z Index: 140

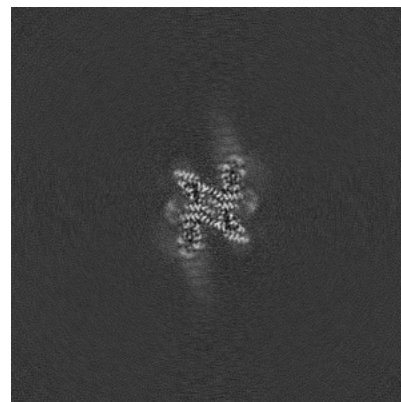
6.3.2 Raw map



X Index: 188



Y Index: 218

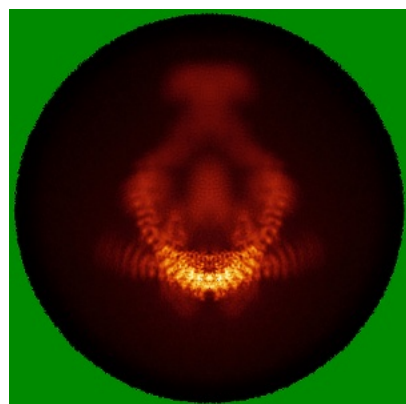


Z Index: 138

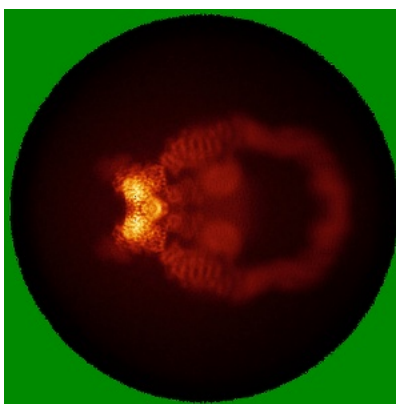
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

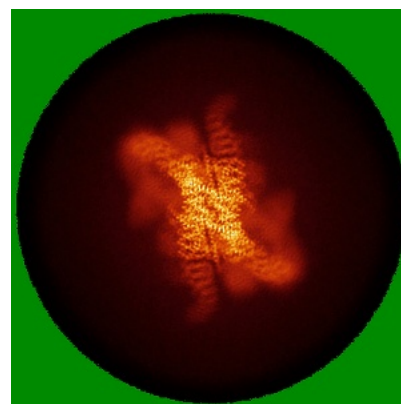
6.4.1 Primary map



X

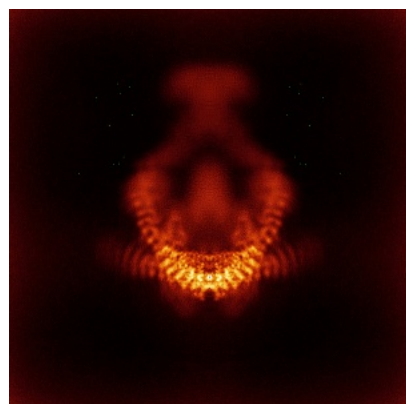


Y

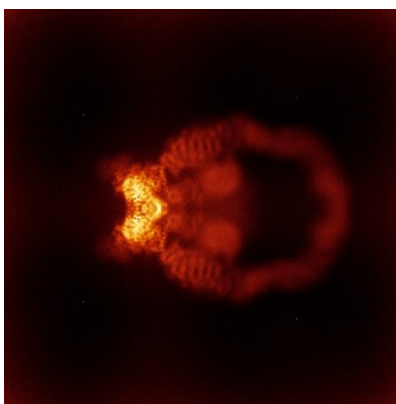


Z

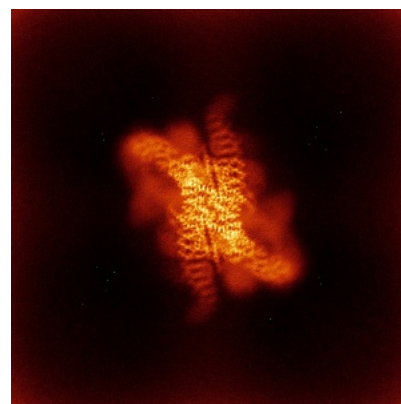
6.4.2 Raw map



X



Y

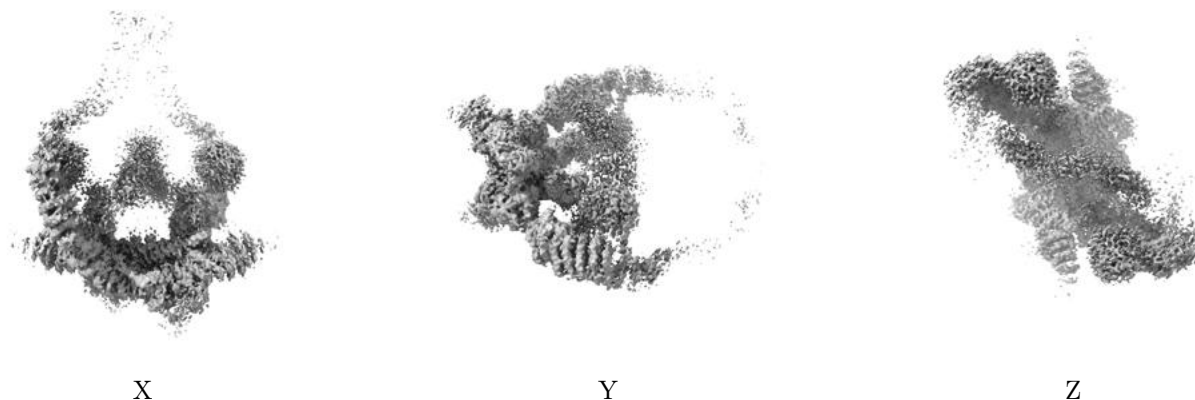


Z

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.

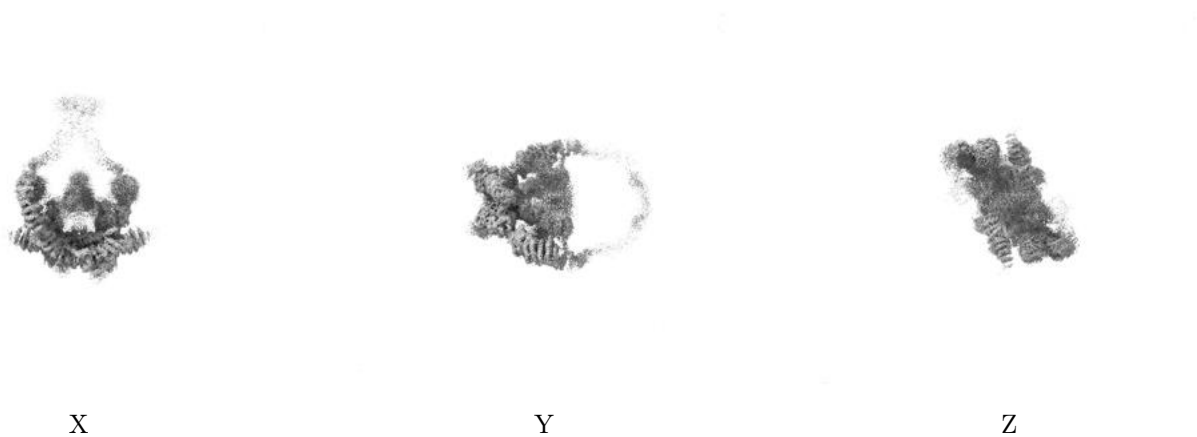
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

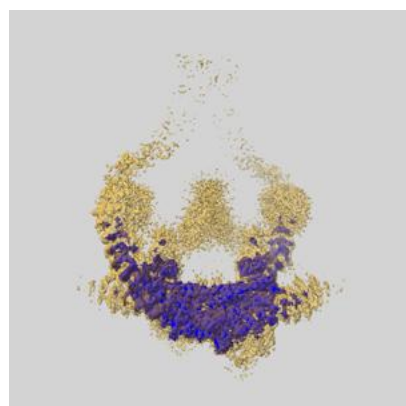
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

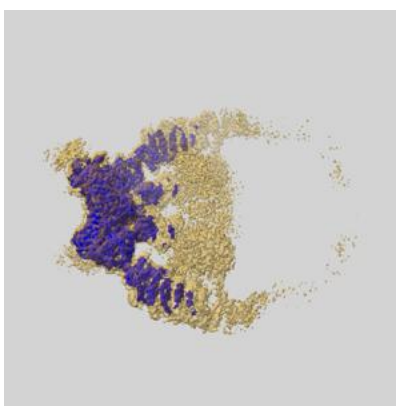
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

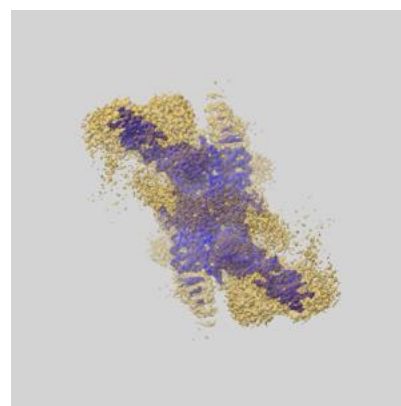
6.6.1 emd_46686_msk_1.map [i](#)



X



Y

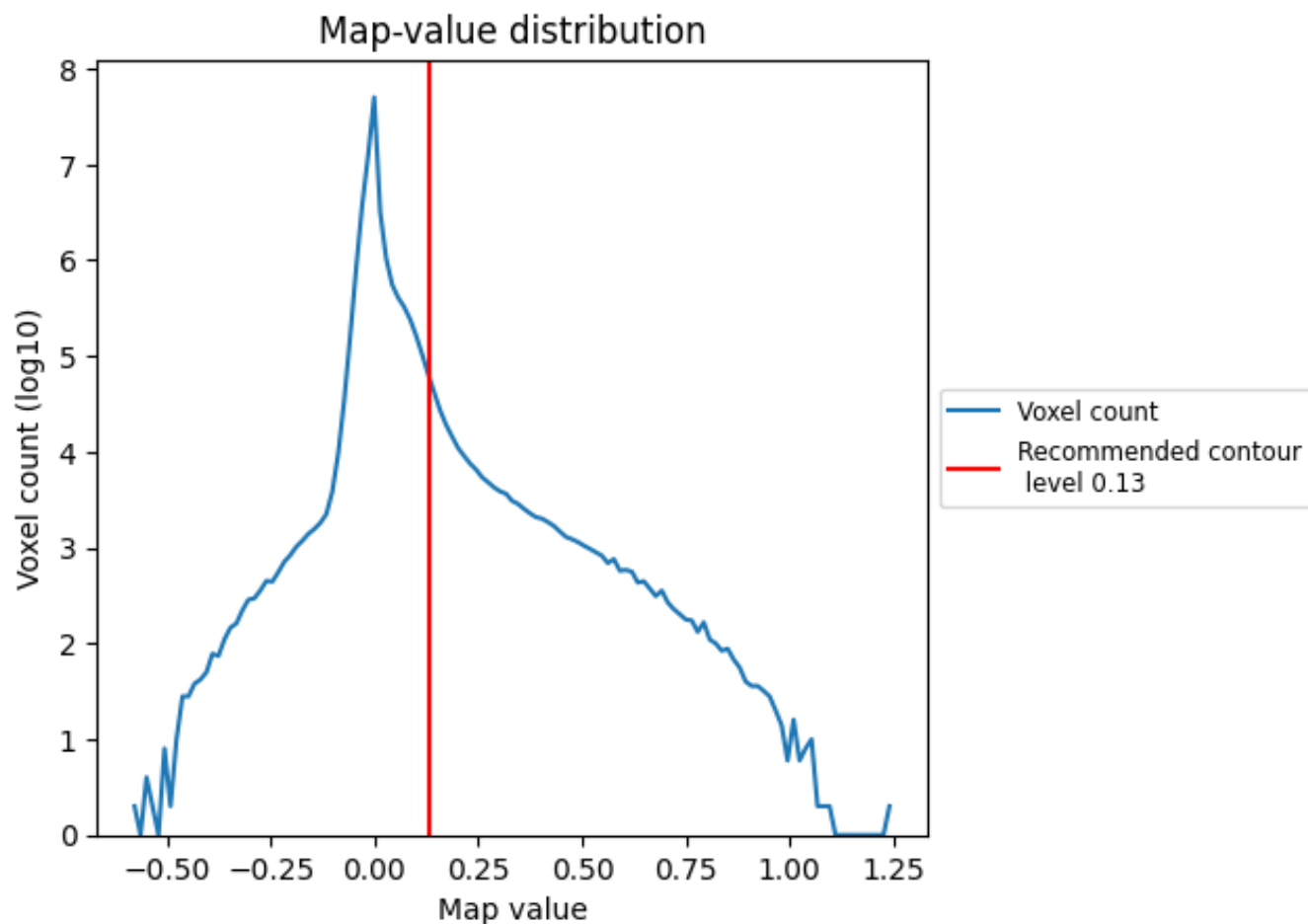


Z

7 Map analysis [i](#)

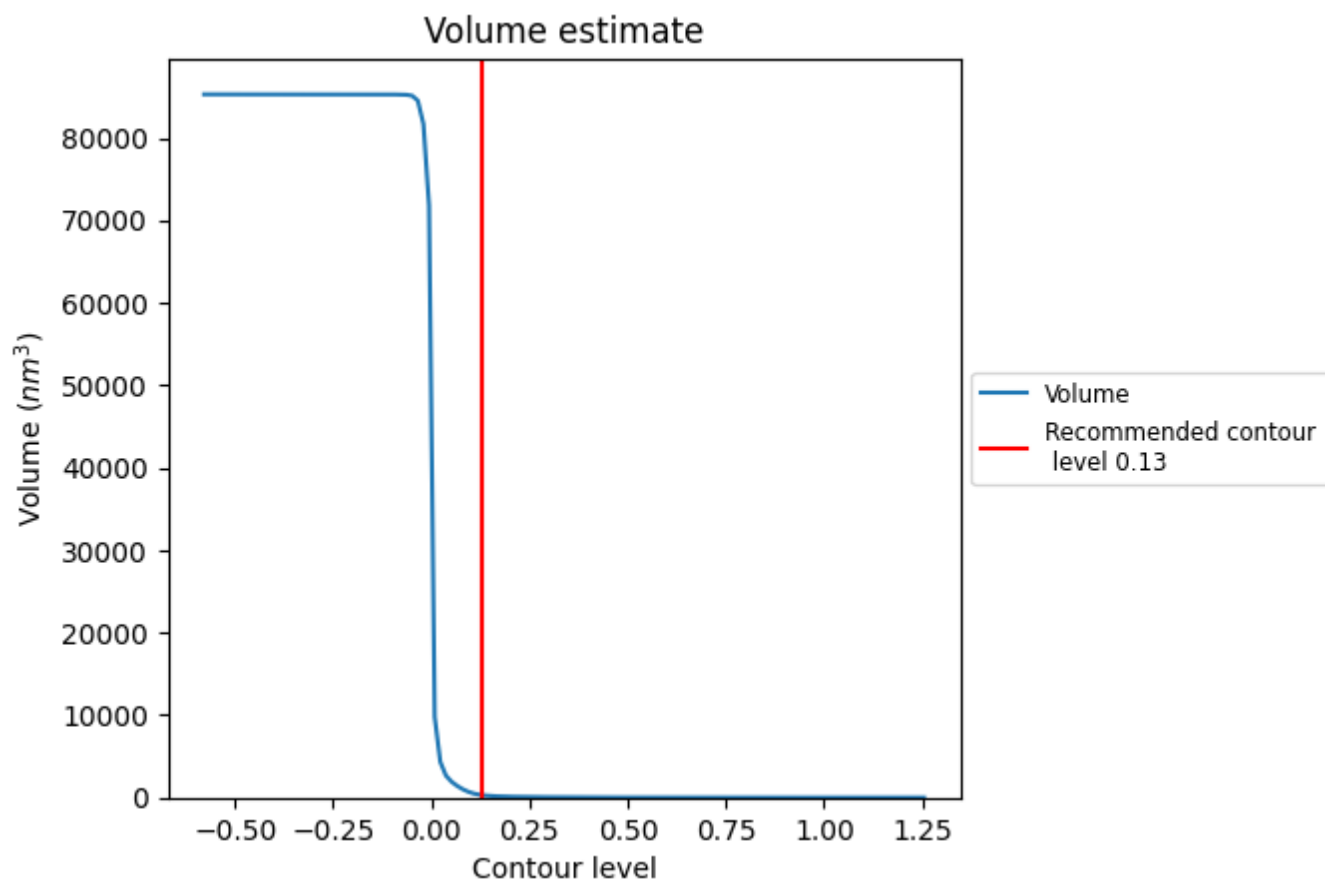
This section contains the results of statistical analysis of the map.

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.

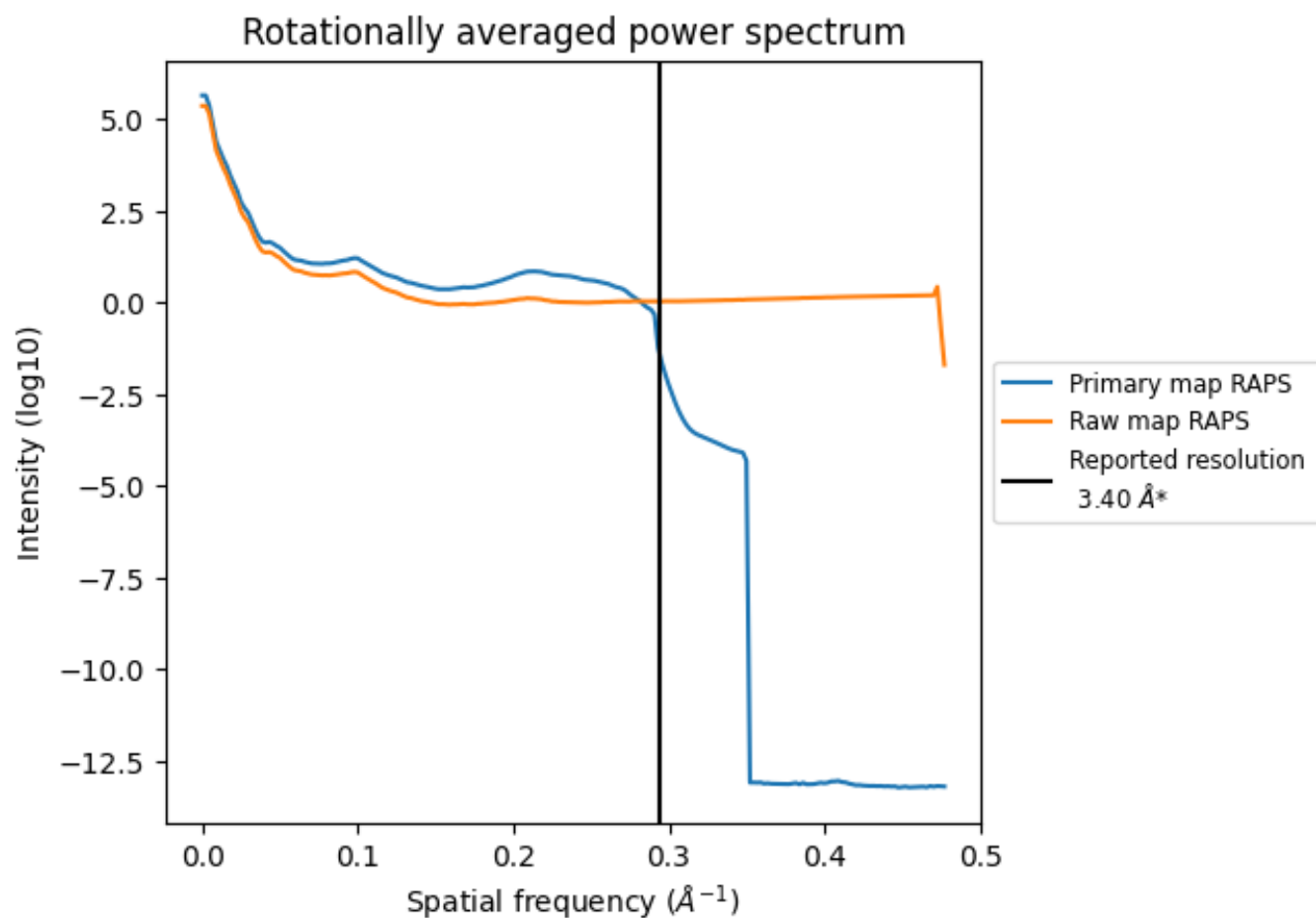
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296 nm³; this corresponds to an approximate mass of 268 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 ⓘ

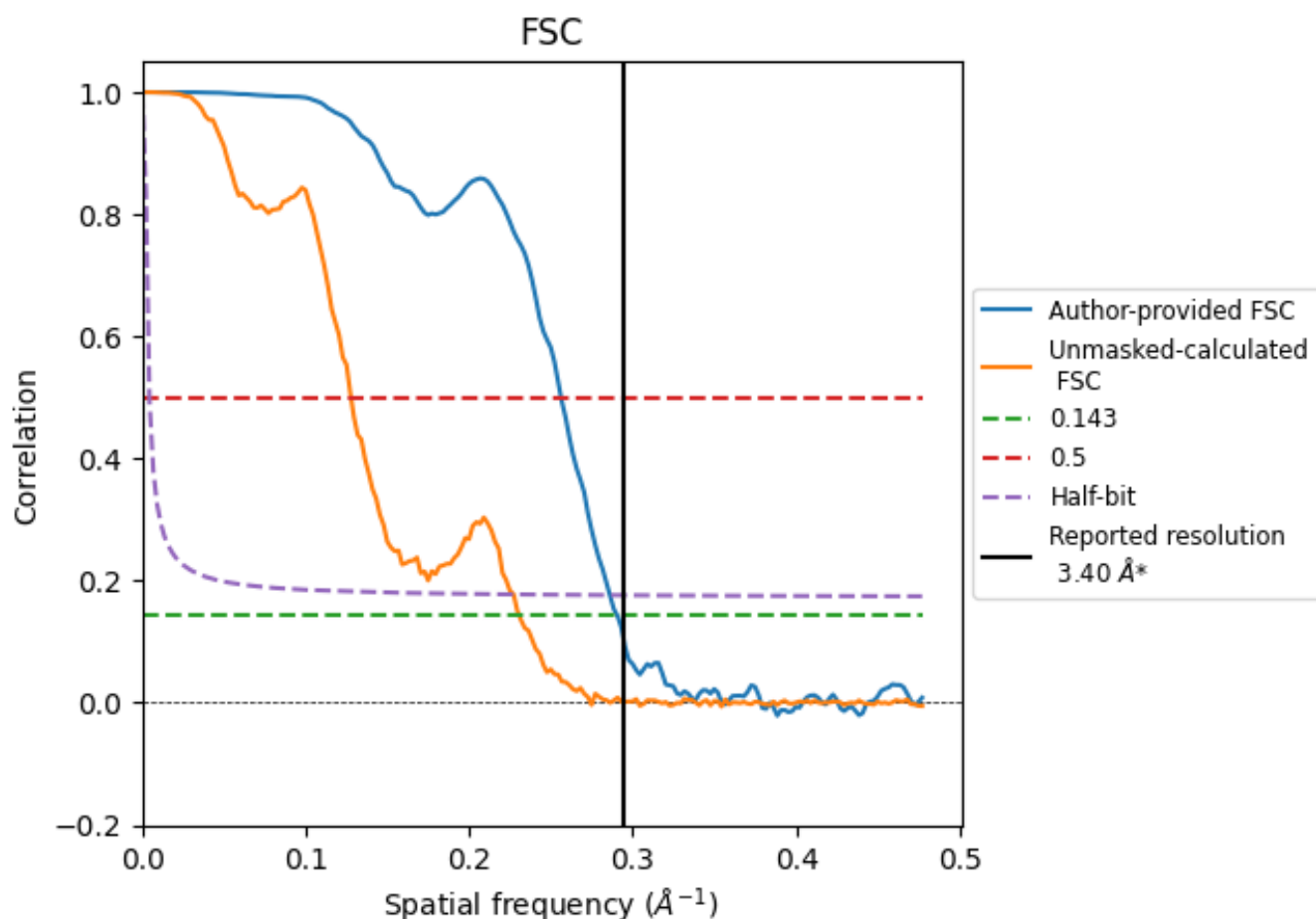


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

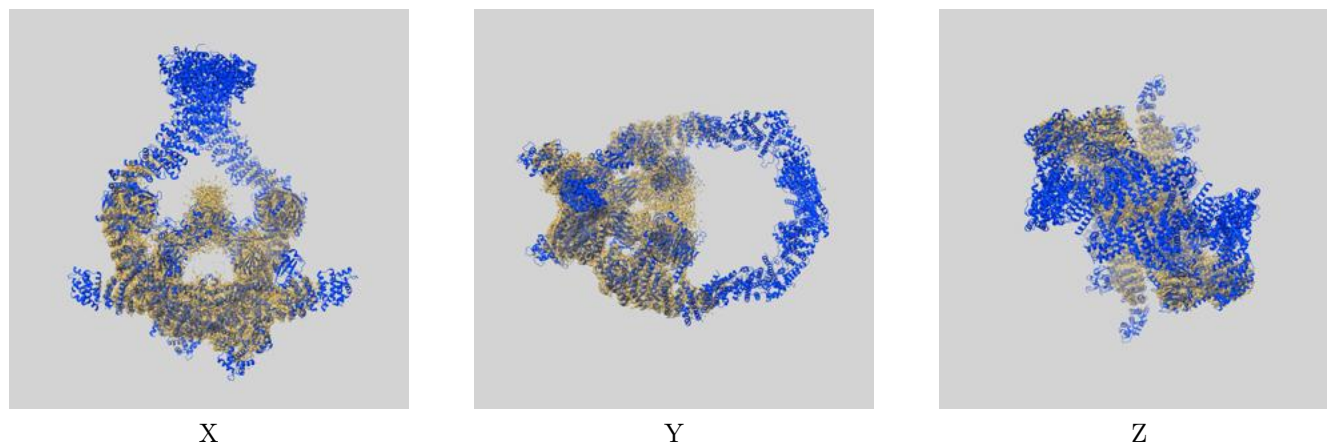
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.44	3.90	3.50
Unmasked-calculated*	4.34	7.83	4.40

*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 4.34 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

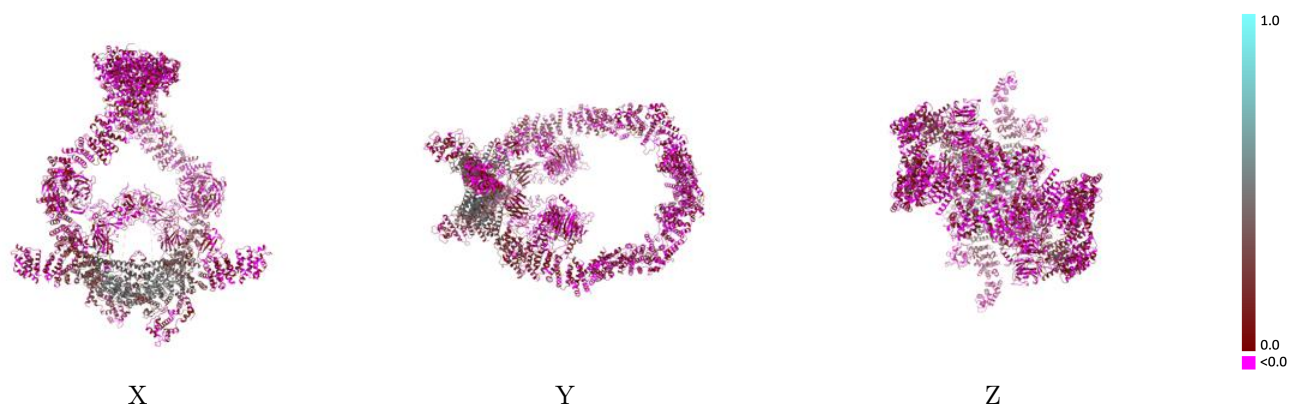
This section contains information regarding the fit between EMDB map EMD-46686 and PDB model 9D9Z. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



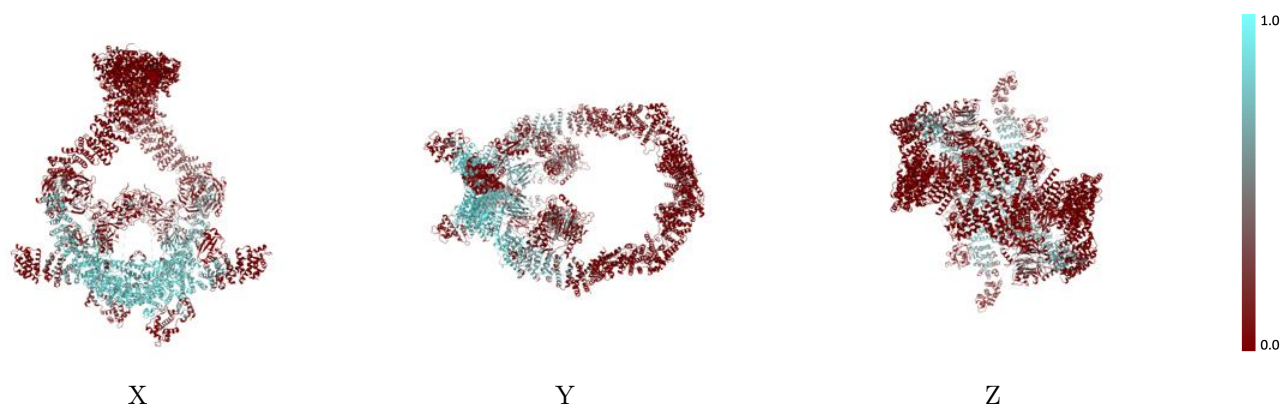
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



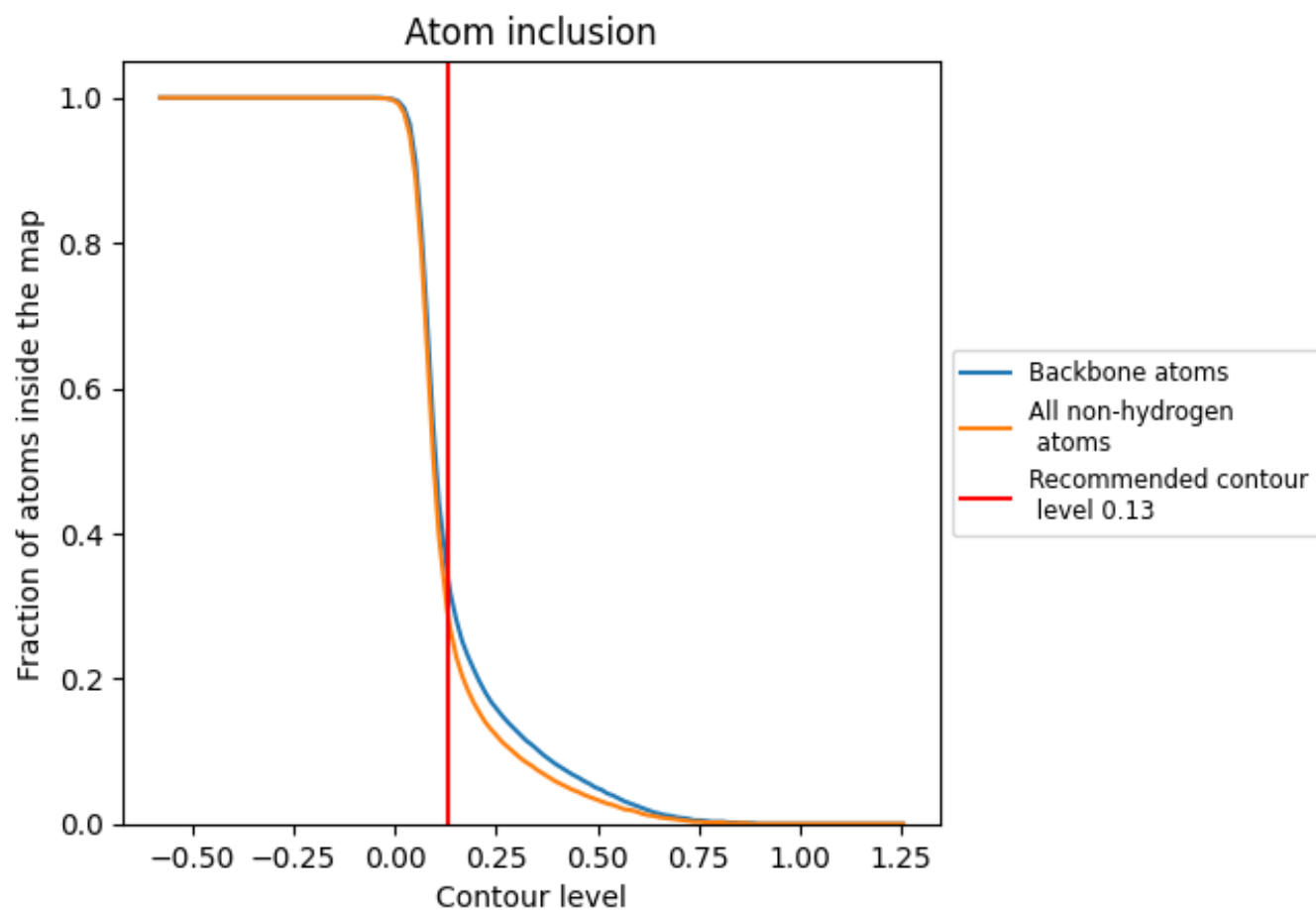
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 29% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.2930	<div><div></div></div> 0.1100
A	<div><div></div></div> 0.3000	<div><div></div></div> 0.1120
B	<div><div></div></div> 0.2990	<div><div></div></div> 0.1130
C	<div><div></div></div> 0.1500	<div><div></div></div> 0.0740
D	<div><div></div></div> 0.1350	<div><div></div></div> 0.0820
E	<div><div></div></div> 0.2720	<div><div></div></div> 0.0850
F	<div><div></div></div> 0.2740	<div><div></div></div> 0.0890

1.0

0.0

<0.0