



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:45 AM UTC

PDB ID : 5W1R / pdb_00005w1r
EMDB ID : EMD-8751
Title : Cryo-EM structure of DNAPKcs
Authors : Sharif, H.; Li, Y.; Wu, H.
Deposited on : 2017-06-04
Resolution : 4.40 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

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>.

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

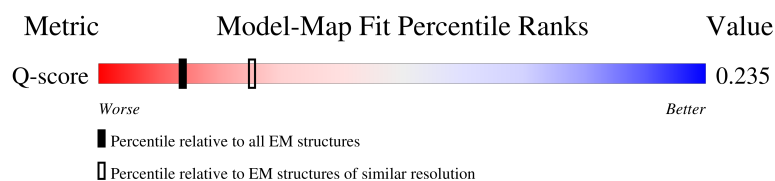
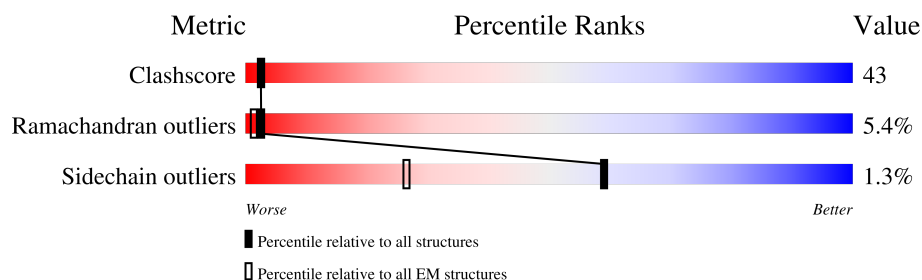
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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	4128	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25559 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3563	Total	C	N	O	S	0	0
			25559	16187	4350	4889	133		

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: DNA-dependent protein kinase catalytic subunit



L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448	A1449	V1452	S1453	L1463	L1464	H1465	L1466	I1467	P1469	L1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
R1340	I1341	M1342	E1343	F1344	M1350	T1351	T1352	P1353	E1354	K1357	L1358	K1361	D1362	L1363	C1364	N1365	T1366	H1367	L1368	M1369	R1370	V1371	L1372	V1373	T1375	L1376	G1377	E1378	P1379	A1380	G1383	F1384	N1385	I1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
T1275	V1276	A1277	G1278	L1279	Q1280	V1281	L1282	G1283	T1284	E1285	L1286	Q1287	S1288	S1289	L1290	K1291	K1292	V1293	V1294	A1295	F1296	F1297	L1298	E1299	A1302	M1303	H1304	T1307	ALA	ALA	GLU	LYS	CYS	PHE	GLY	THR	ALA	ALA	GLY	ASN	THR	S1323	E1326	G1327	E1328	R1329	Y1330	K1334	C1335	T1336	V1337	V1338	V1339			
PRO	LEU	LEU	PRO	GLY	ASN	ARG	SER	PRO	ASN	LEU	TRP	LEU	LYS	ASP	VAL	K1213	E1214	E1215	G1216	V1217	L1220	I1221	M1222	T1223	F1224	G1228	Q1231	L1236	A1237	Q1238	P1239	R1245	G1246	F1248	S1249	Q1251	A1252	T1253	L1254	L1257	D1258	L1259	L1260	C1266	I1271	E1272	E1273	R1274								
I1131	D1132	H1133	L1134	C1135	I1138	K1139	K1140	K1141	H1142	V1143	K1147	A1148	K1149	K1150	R1151	L1152	L1153	P1154	F1157	P1158	P1159	S1160	A1161	S1162	L1163	C1164	L1165	L1166	D1167	L1168	L1169	K1170	H1171	L1172	L1173	G1176	G1177	R1178	P1179	Q1180	THR	GLU	CYS	ARG	HIS	LYS	SER	ILE	GLU	LEU	PHE	THR	LYS	PHE	VAL	
L1063	L1068	L1069	P1070	A1071	A1072	F1073	K1074	R1075	A1078	S1079	L1080	A1081	F1082	N1083	N1084	I1085	Y1086	R1087	E1088	F1089	R1090	E1091	S1094	L1095	V1096	E1097	Q1098	F1099	V1100	F1101	A1102	A1103	L1104	V1105	I1106	Y1107	S1110	L1113	A1114	H1115	A1116	D1117	E1118	K1119	S1120	L1121	G1122	T1123	I1124	C1127	C1128	D1129	A1130			
K1000	F1001	E1002	S1003	Q1004	D1005	T1006	A1007	A1008	L1009	L1010	E1011	A1012	L1013	L1014	D1015	G1016	I1017	V1018	D1019	P1020	V1021	D1022	S1023	T1024	L1025	R1026	D1027	F1028	E1029	G1030	R1031	K1032	I1033	R1034	E1035	F1036	L1037	K1038	W1039	S1040	I1041	K1042	I1043	I1044	T1045	Q1048	Q1049	E1050	K1051	S1052	P1053	V1054	M1055	T1056	L1059	F1060
M937	Y938	G963	G964	Q965	I966	N967	K968	N969	L970	L971	T972	V973	T974	S975	S976	D977	E978	M979	M980	K981	Y982	Y983	D987	ARG	GLU	LYS	LYS	ARG	PHE	LEU	SER	PHE	ALA	VAL	PRO	PHE	R999	E900	P903	V904	L911	V914	T915	L919	D923	R924	Q925	I928	A929	A930	C931	E932	L933	L934		
M937	Y938	G963	G964	Q965	I966	N967	K968	N969	L970	L971	T972	V973	T974	S975	S976	D977	E978	M979	M980	K981	Y982	Y983	D987	ARG	GLU	LYS	LYS	ARG	PHE	LEU	SER	PHE	ALA	VAL	PRO	PHE	R999	E900	P903	V904	L911	V914	T915	L919	D923	R924	Q925	I928	A929	A930	C931	E932	L933	L934		
K1000	F1001	E1002	S1003	Q1004	D1005	T1006	A1007	A1008	L1009	L1010	E1011	A1012	L1013	L1014	D1015	G1016	I1017	V1018	D1019	P1020	V1021	D1022	S1023	T1024	L1025	R1026	D1027	F1028	E1029	G1030	R1031	K1032	I1033	R1034	E1035	F1036	L1037	K1038	W1039	S1040	I1041	K1042	I1043	I1044	T1045	Q1048	Q1049	E1050	K1051	S1052	P1053	V1054	M1055	T1056	L1059	F1060
L1063	L1068	L1069	P1070	A1071	A1072	F1073	K1074	R1075	A1078	S1079	L1080	A1081	F1082	N1083	N1084	I1085	Y1086	R1087	E1088	F1089	R1090	E1091	S1094	L1095	V1096	E1097	Q1098	F1099	V1100	F1101	A1102	A1103	L1104	V1105	I1106	Y1107	S1110	L1113	A1114	H1115	A1116	D1117	E1118	K1119	S1120	L1121	G1122	T1123	I1124	C1127	C1128	D1129	A1130			
I1131	D1132	H1133	L1134	C1135	I1138	K1139	K1140	K1141	H1142	V1143	K1147	A1148	K1149	K1150	R1151	L1152	L1153	P1154	F1157	P1158	P1159	S1160	A1161	S1162	L1163	C1164	L1165	L1166	D1167	L1168	L1169	K1170	H1171	L1172	L1173	G1176	G1177	R1178	P1179	Q1180	THR	GLU	CYS	ARG	HIS	LYS	SER	ILE	GLU	LEU	PHE	THR	LYS	PHE	VAL	
PRO	LEU	LEU	PRO	GLY	ASN	ARG	SER	PRO	ASN	LEU	TRP	LEU	LYS	ASP	VAL	K1213	E1214	E1215	G1216	V1217	L1220	I1221	M1222	T1223	F1224	G1228	Q1231	L1236	A1237	Q1238	P1239	R1245	G1246	F1248	S1249	Q1251	A1252	T1253	L1254	L1257	D1258	L1259	L1260	C1266	I1271	E1272	E1273	R1274								
T1275	V1276	A1277	G1278	L1279	Q1280	V1281	L1282	G1283	T1284	E1285	L1286	Q1287	S1288	S1289	L1290	K1291	K1292	V1293	V1294	A1295	F1296	F1297	L1298	E1299	A1302	M1303	H1304	T1307	ALA	ALA	GLU	LYS	CYS	PHE	GLY	THR	ALA	ALA	GLY	ASN	THR	S1323	E1326	G1327	E1328	R1329	Y1330	K1334	C1335	T1336	V1337	V1338	V1339			
R1340	I1341	M1342	E1343	F1344	M1350	T1351	T1352	P1353	E1354	K1357	L1358	K1361	D1362	L1363	C1364	N1365	T1366	H1367	L1368	M1369	R1370	V1371	L1372	V1373	T1375	L1376	G1377	E1378	P1379	A1380	G1383	F1384	N1385	I1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448	A1449	V1452	S1453	L1463	L1464	H1465	L1466	I1467	P1469	L1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448	A1449	V1452	S1453	L1463	L1464	H1465	L1466	I1467	P1469	L1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448	A1449	V1452	S1453	L1463	L1464	H1465	L1466	I1467	P1469	L1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448	A1449	V1452	S1453	L1463	L1464	H1465	L1466	I1467	P1469	L1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448	A1449	V1452	S1453	L1463	L1464	H1465	L1466	I1467	P1469	L1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448	A1449	V1452	S1453	L1463	L1464	H1465	L1466	I1467	P1469	L1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448	A1449	V1452	S1453	L1463	L1464	H1465	L1466	I1467	P1469	L1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448	A1449	V1452	S1453	L1463	L1464	H1465	L1466	I1467	P1469	L1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448	A1449	V1452	S1453	L1463	L1464	H1465	L1466	I1467	P1469	L1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448	A1449	V1452	S1453	L1463	L1464	H1465	L1466	I1467	P1469	L1386	G1387	D1388	V1391	A1392	A1393	H1394	L1395	D1397	V1398	K1404	Y1411	I1414	L1415	H1418	D1495	E1496	R1497	Q1498	C1499			
L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1447	L1448																																

T2355	T2356	G2276	L2277	K2000	L2200	N2135	E2070	V1994	Y1920	ASP	ARG	F1722	A1647	I1567	L1500
N2357	E2357	G2279	L2279	T2201	T2202	P2136	Q2071	E1995	F1923	VAL	GLY	F1723	L1648	L1571	F1501
D2358	D2358	T2203	P2203	P2203	T2203	V2138	H2077	R1999	E1930	LYS	CYS	M1724	A1649	L1572	L1503
M2359	M2359	G2204	G2204	G2204	G2204	P2139	D2078	R2000	E1930	ARG	VAL	Q1725	A1650	K1573	D1504
D2361	T2361	V2205	V2205	V2205	V2205	L2140	D2079	K2001	L1933	PHE	GLN	Q1726	K1651	N1574	L1505
D2362	T2362	D2208	D2208	D2208	D2208	F2142	V2080	K2002	L1933	THR	VAL	R1727	Q1654	L1575	L1506
C2363	C2363	L2216	L2216	L2216	L2216	K2143	L2081	K2003	R1937	L1857	GLY	E1728	S1658	D1576	C1507
N2364	N2364	N2217	N2217	N2217	N2217	L2144	L2081	Y2004	R1938	L1858	LEU	F1729	VAL	L1577	K1508
P2286	P2286	L2219	L2219	L2219	L2219	F2145	L2083	K2009	Y1940	G1732	SER	P1730	SER	A1578	Q1509
N2367	N2367	L2220	L2220	L2220	L2220	A2147	L2083	E2010	H1941	T1865	ASN	P1731	PHE	V1579	L1510
T2368	T2368	K2221	K2221	K2221	K2221	K2148	M2085	A2011	A1944	Q1866	THR	R1735	THR	E1581	A1511
K2369	K2369	L2222	L2222	L2222	L2222	L2149	M2086	D2086	Y1945	T1867	SER	F1736	VAL	L1580	F1519
S2370	S2370	V2223	V2223	V2223	V2223	V2150	E2092	A2011	A1945	T1868	HIS	N1737	GLY	L1582	A1520
P2371	P2371	T2151	T2151	T2151	T2151	D2018	L2088	D2018	Y1945	K1869	THR	F1736	THR	F1521	F1521
A2375	A2375	T2152	T2152	T2152	T2152	G2021	P2096	G2021	I1949	M1870	GLY	N1738	SER	S1585	L1524
D2376	D2376	E2154	E2154	E2154	E2154	P2022	L2097	P2022	S1960	K1871	PHE	N1739	ASN	D1588	C1525
F2377	F2377	V2156	V2156	V2156	V2156	S2023	T2098	S2023	V1951	M1870	PRO	V1740	THR	N1589	E1526
N2379	N2379	P2159	P2159	P2159	P2159	Y2024	L2100	Y2024	C1953	M1871	GLU	E1750	SER	T1590	ARG
N2380	N2380	K2227	K2227	K2227	K2227	M2025	V2101	M2025	C1954	Y1874	VAL	E1751	VAL	K1591	LEU
A2381	A2381	A2229	A2229	A2229	A2229	S2027	K2102	S2027	K1875	K1875	THR	L1752	THR	M1593	VAL
V2382	V2382	F2231	F2231	F2231	F2231	L2028	H2103	L2028	I1876	I1876	THR	E1760	THR	S1594	SER
F2383	F2383	R2232	R2232	R2232	R2232	L2031	M2104	L2031	L1877	L1877	TYR	L1747	TYR	A1595	LEU
F2384	F2384	H2233	H2233	H2233	H2233	A2032	H2105	A2032	D1878	D1878	I1676	L1748	LEU	V1596	LEU
L2385	L2385	N2234	N2234	N2234	N2234	L2033	H2106	L2033	M1879	M1879	S1677	A1749	ASN	N1597	ASN
E2315	E2315	L2238	L2238	L2238	L2238	D2033	H2107	D2033	Y1881	Y1881	L1678	E1750	PRO	N1598	PRO
Y2316	Y2316	L2241	L2241	L2241	L2241	S2034	H2108	S2034	S1882	S1882	A1680	E1751	ALA	G1599	ALA
A2317	A2317	C2244	C2244	C2244	C2244	S2037	H2109	S2037	L1884	L1884	D1681	E1751	VAL	M1600	VAL
A2319	A2319	L2244	L2244	L2244	L2244	E2038	H2110	E2038	P1885	P1885	D1682	E1751	LEU	A1609	LEU
A2320	A2320	D2247	D2247	D2247	D2247	S2041	H2111	S2041	K1886	K1886	K1683	E1751	SER	GLN	SER
E2321	E2321	C2248	C2248	C2248	C2248	Q2042	H2112	Q2042	H1890	H1890	T1682	E1751	THR	GLN	THR
V2322	V2322	L2249	L2249	L2249	L2249	F2043	H2113	F2043	A1891	A1891	K1684	E1751	ALA	LYS	ALA
G2324	G2324	L2250	L2250	L2250	L2250	F2045	H2114	F2045	K1892	K1892	D1685	E1751	SER	LYS	SER
L2325	L2325	L2251	L2251	L2251	L2251	S2046	H2115	S2046	F1972	F1972	D1686	E1751	GLY	GLY	GLY
L2326	L2326	L2252	L2252	L2252	L2252	T2047	H2116	T2047	N1974	N1974	L1687	E1751	SER	SER	SER
L2327	L2327	P2252	P2252	P2252	P2252	Q2048	H2117	Q2048	L1975	L1975	L1688	E1751	GLY	GLY	GLY
R2328	R2328	R2254	R2254	R2254	R2254	Q2050	H2118	Q2050	C1904	C1904	L1689	E1751	LEU	LEU	LEU
Y2329	Y2329	L2255	L2255	L2255	L2255	S2051	H2119	S2051	F1976	F1976	L1690	E1751	LEU	LEU	LEU
V2330	V2330	L2256	L2256	L2256	L2256	S2055	H2120	S2055	E1979	E1979	Q1691	E1751	LEU	LEU	LEU
K2334	K2334	E2258	E2258	E2258	E2258	S2056	H2121	S2056	N1980	N1980	T1694	E1751	LEU	LEU	LEU
N2335	N2335	K2259	K2259	K2259	K2259	Q2057	H2122	Q2057	L1981	L1981	T1695	E1751	LEU	LEU	LEU
L2336	L2336	F2260	F2260	F2260	F2260	D2058	H2123	D2058	I1982	I1982	L1696	E1751	LEU	LEU	LEU
E2343	E2343	G2262	G2262	G2262	G2262	P2059	H2124	P2059	D1983	D1983	L1697	E1751	LEU	LEU	LEU
L2344	L2344	P2265	P2265	P2265	P2265	R2060	H2125	R2060	L1984	L1984	L1698	E1751	LEU	LEU	LEU
V2345	V2345	N2266	N2266	N2266	N2266	P2061	H2126	P2061	K1985	K1985	L1699	E1751	LEU	LEU	LEU
Q2348	Q2348	K2267	K2267	K2267	K2267	A2062	H2127	A2062	R1986	R1986	L1700	E1751	LEU	LEU	LEU
L2349	L2349	S2271	S2271	S2271	S2271	T2063	H2128	T2063	T1912	T1912	L1701	E1751	LEU	LEU	LEU
K2350	K2350	V2272	V2272	V2272	V2272	F2066	H2129	F2066	T1913	T1913	L1702	E1751	LEU	LEU	LEU
Q2351	Q2351	L2276	L2276	L2276	L2276	R2067	H2130	R2067	T1914	T1914	L1703	E1751	LEU	LEU	LEU
H2352	H2352	N2354	N2354	N2354	N2354	K2068	H2131	K2068	L1915	L1915	L1704	E1751	LEU	LEU	LEU
Q2353	Q2353					R2069	H2132	R2069	L1916	L1916	L1705	E1751	LEU	LEU	LEU
N2354	N2354						H2133		F1990	F1990	L1706	E1751	LEU	LEU	LEU
							G2134		P1991	P1991	L1707	E1751	LEU	LEU	LEU
									Y1992	Y1992	L1708	E1751	LEU	LEU	LEU
									E1993	E1993	L1709	E1751	LEU	LEU	LEU
											L1710	E1751	LEU	LEU	LEU
											L1711	E1751	LEU	LEU	LEU
											L1712	E1751	LEU	LEU	LEU
											L1713	E1751	LEU	LEU	LEU
											L1714	E1751	LEU	LEU	LEU
											L1715	E1751	LEU	LEU	LEU
											L1716	E1751	LEU	LEU	LEU
											L1717	E1751	LEU	LEU	LEU
											L1718	E1751	LEU	LEU	LEU
											L1719	E1751	LEU	LEU	LEU
											L1720	E1751	LEU	LEU	LEU
											L1721	E1751	LEU	LEU	LEU
											L1722	E1751	LEU	LEU	LEU
											L1723	E1751	LEU	LEU	LEU
											L1724	E1751	LEU	LEU	LEU
											L1725	E1751	LEU	LEU	LEU
											L1726	E1751	LEU	LEU	LEU
											L1727	E1751	LEU	LEU	LEU
											L1728	E1751	LEU	LEU	LEU
											L1729	E1751	LEU	LEU	LEU
											L1730	E1751	LEU	LEU	LEU
											L1731	E1751	LEU	LEU	LEU
											L1732	E1751	LEU	LEU	LEU
											L1733	E1751	LEU	LEU	LEU
											L1734	E1751	LEU	LEU	LEU
											L1735	E1751	LEU	LEU	LEU
											L1736	E1751	LEU	LEU	LEU
											L1737	E1751	LEU	LEU	LEU
											L1738	E1751	LEU	LEU	LEU
											L1739	E1751	LEU	LEU	LEU
											L1740	E1751	LEU	LEU	LEU
											L1741	E1751	LEU	LEU	LEU
											L1742	E1751	LEU	LEU	LEU
											L1743	E1751	LEU	LEU	LEU
											L1744	E1751	LEU	LEU	LEU
											L1745	E1751	LEU	LEU	LEU
											L1746	E1751	LEU	LEU	LEU
											L1747	E1751	LEU	LEU	LEU
											L1748	E1751	LEU	LEU	LEU
											L1749	E1751	LEU	LEU	LEU
											L1750	E1751	LEU	LEU	LEU
											L1751	E1751	LEU	LEU	LEU
											L1752	E1751	LEU	LEU	LEU
											L1753	E1751	LEU	LEU	LEU
											L1754	E1751	LEU	LEU	LEU
											L1755	E1751	LEU	LEU	LEU
											L1756	E1751	LEU	LEU	LEU
											L1757	E1751	LEU	LEU	LEU
											L1758	E1751	LEU	LEU	LEU
											L1759	E1751	LEU	LEU	LEU
											L1760	E1751	LEU	LEU	LEU
											L1761	E1751	LEU	LEU	LEU
											L1762	E1751	LEU	LEU	LEU
	</														





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	289798	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.016	Depositor
Map size ($\text{\AA}$)	241.6, 241.6, 241.6	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.51, 1.51, 1.51	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	8/25994 (0.0%)	0.74	69/35463 (0.2%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3568	ILE	CA-C	6.95	1.61	1.52
1	A	3580	ASN	N-CA	6.42	1.55	1.45
1	A	1342	MET	SD-CE	6.37	1.95	1.79
1	A	3576	ASP	C-O	5.67	1.30	1.24
1	A	643	GLU	C-N	5.64	1.41	1.34

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	PHE	N-CA-C	10.57	122.80	111.28
1	A	3316	LEU	N-CA-C	-9.85	100.62	111.36
1	A	3580	ASN	N-CA-C	9.80	125.09	110.10
1	A	3348	LEU	N-CA-C	9.36	121.25	111.14
1	A	654	ILE	N-CA-C	9.00	119.81	110.72

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	25559	0	23509	2101	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	25559	0	23509	2101	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 43.

The worst 5 of 2101 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:2546:TYR:CD1	1:A:2554:PHE:CE1	1.81	1.66
1:A:995:PHE:CZ	1:A:1003:SER:N	1.69	1.57
1:A:660:LEU:HD11	1:A:733:LEU:CD2	1.34	1.54
1:A:488:ILE:HG23	1:A:616:LYS:CE	1.36	1.53
1:A:708:VAL:HG22	1:A:712:LYS:CE	1.33	1.52

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	3511/4128 (85%)	2776 (79%)	547 (16%)	188 (5%)	1 15

5 of 188 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	THR
1	A	565	TYR
1	A	623	PHE
1	A	624	ILE
1	A	638	GLN

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	2460/3671 (67%)	2429 (99%)	31 (1%)	61 72

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1959	LEU
1	A	3568	ILE
1	A	2312	TYR
1	A	3953	LEU
1	A	3416	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1466	ASN
1	A	2527	HIS
1	A	3927	ASN
1	A	1941	HIS
1	A	3278	GLN

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.

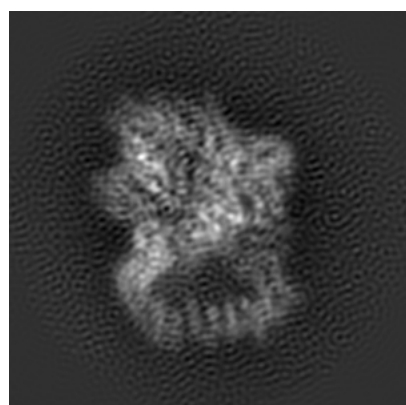
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8751. These allow visual inspection of the internal detail of the map and identification of artifacts.

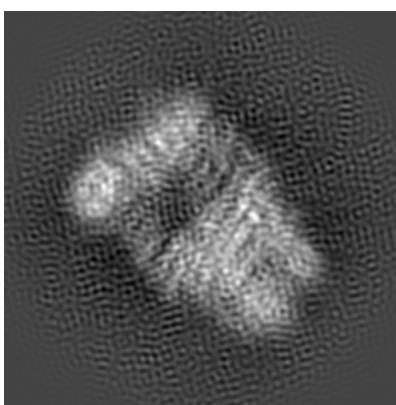
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

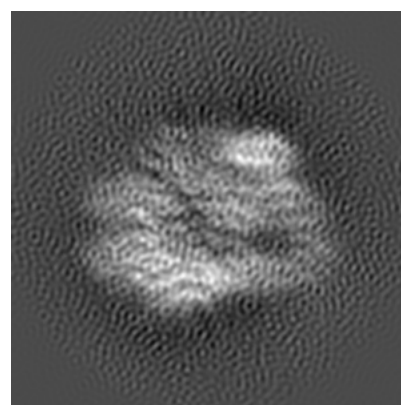
6.1.1 Primary map



X



Y

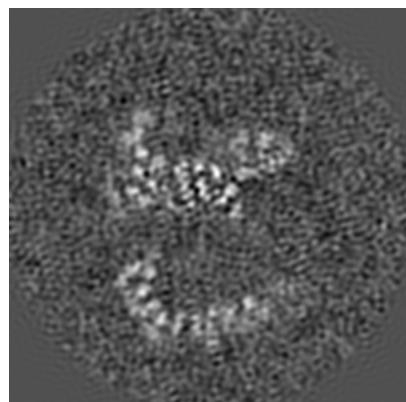


Z

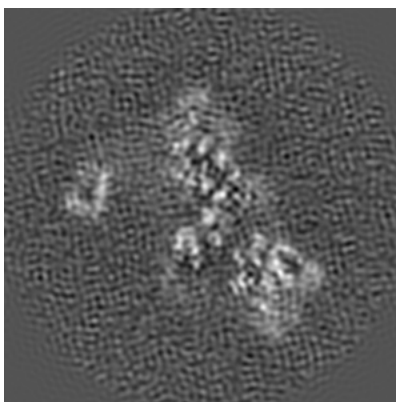
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

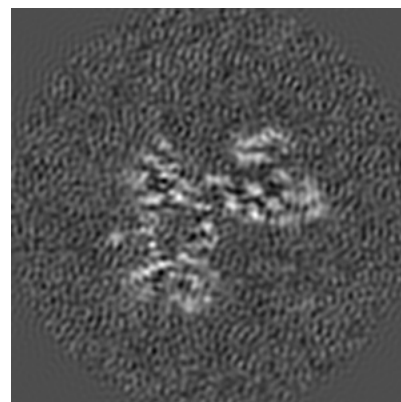
6.2.1 Primary map



X Index: 80



Y Index: 80

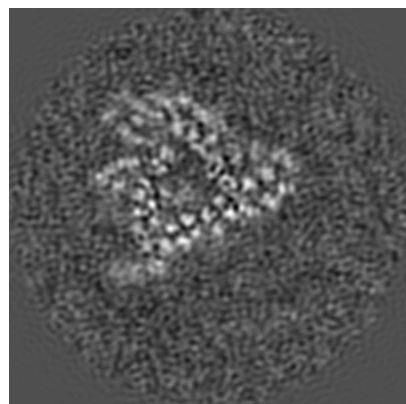


Z Index: 80

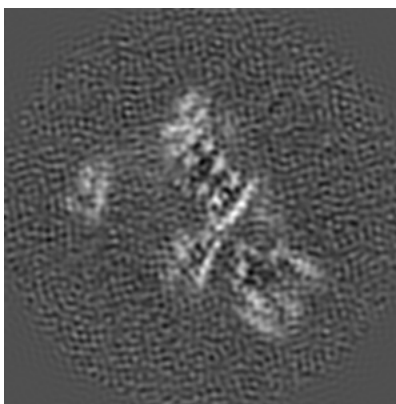
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

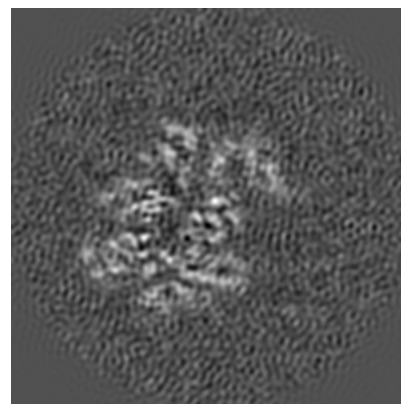
6.3.1 Primary map



X Index: 61



Y Index: 82

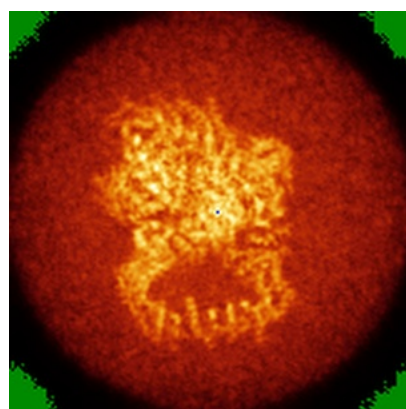


Z Index: 95

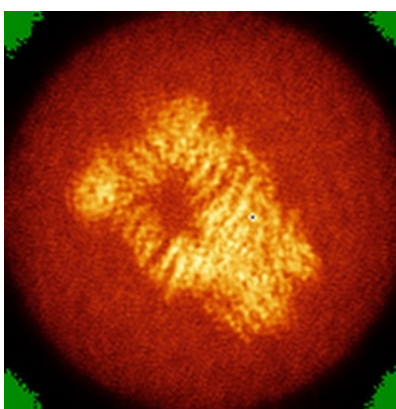
The images above show the largest variance slices of the map in three orthogonal directions.

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

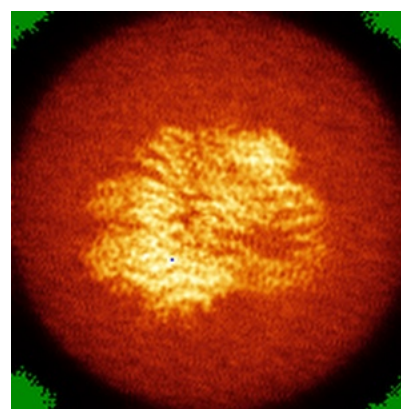
6.4.1 Primary map



X



Y

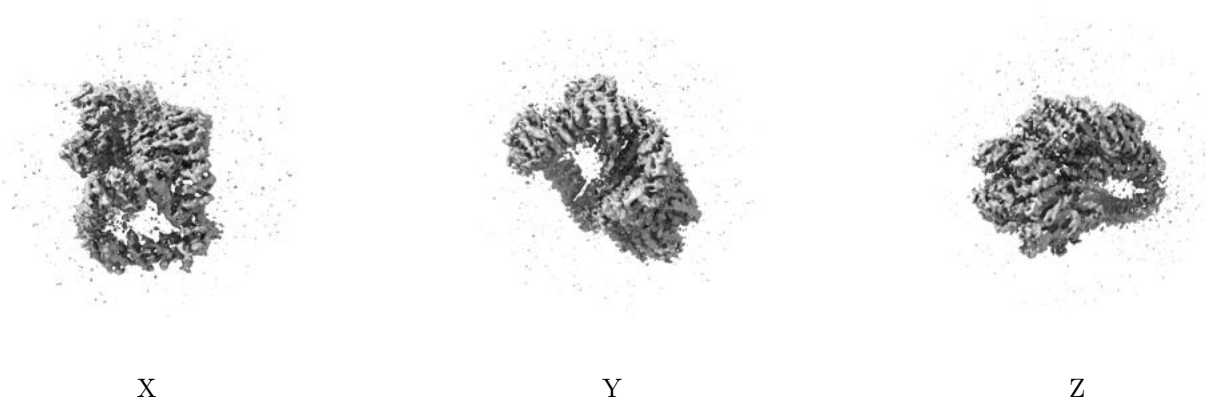


Z

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 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

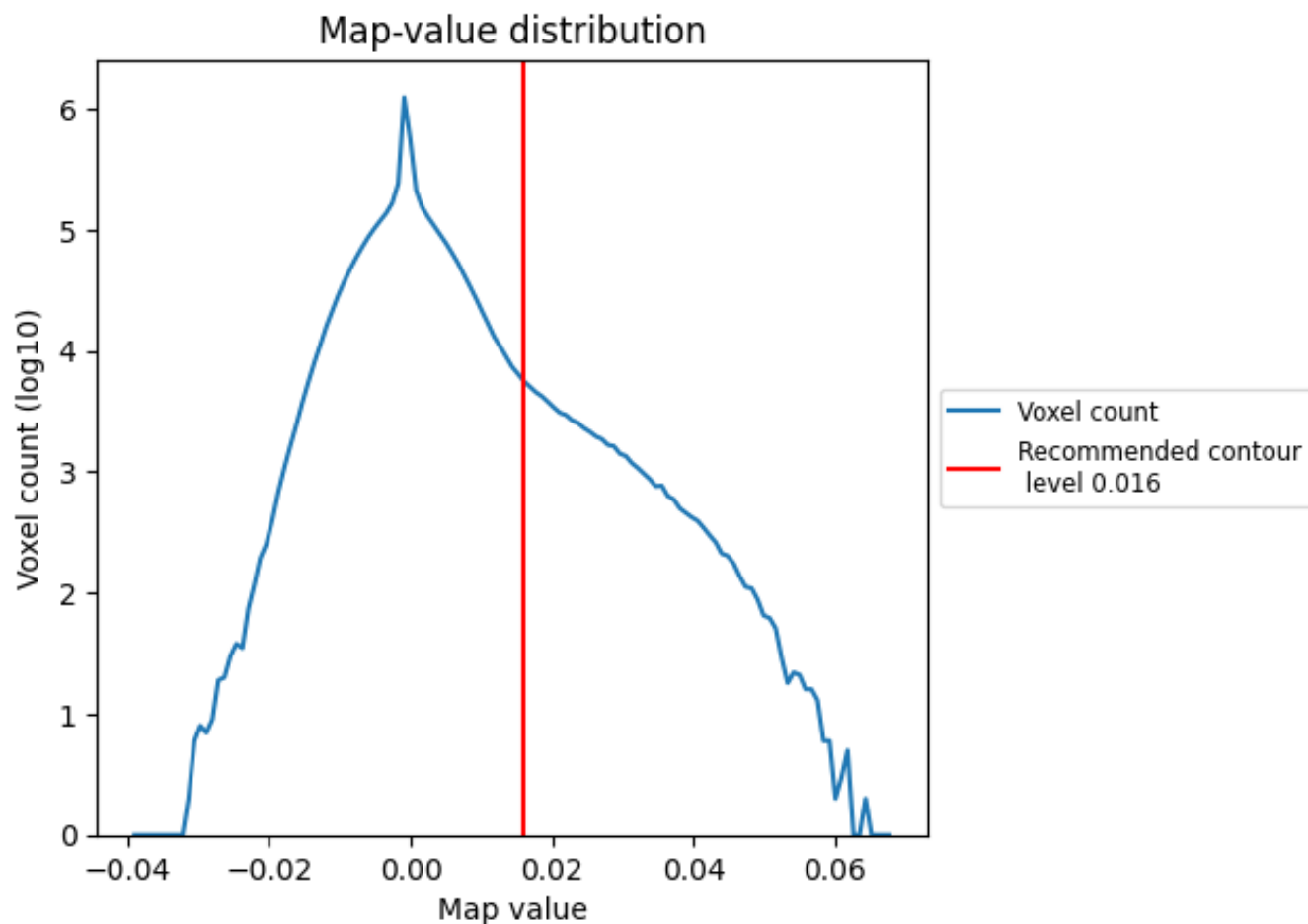
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

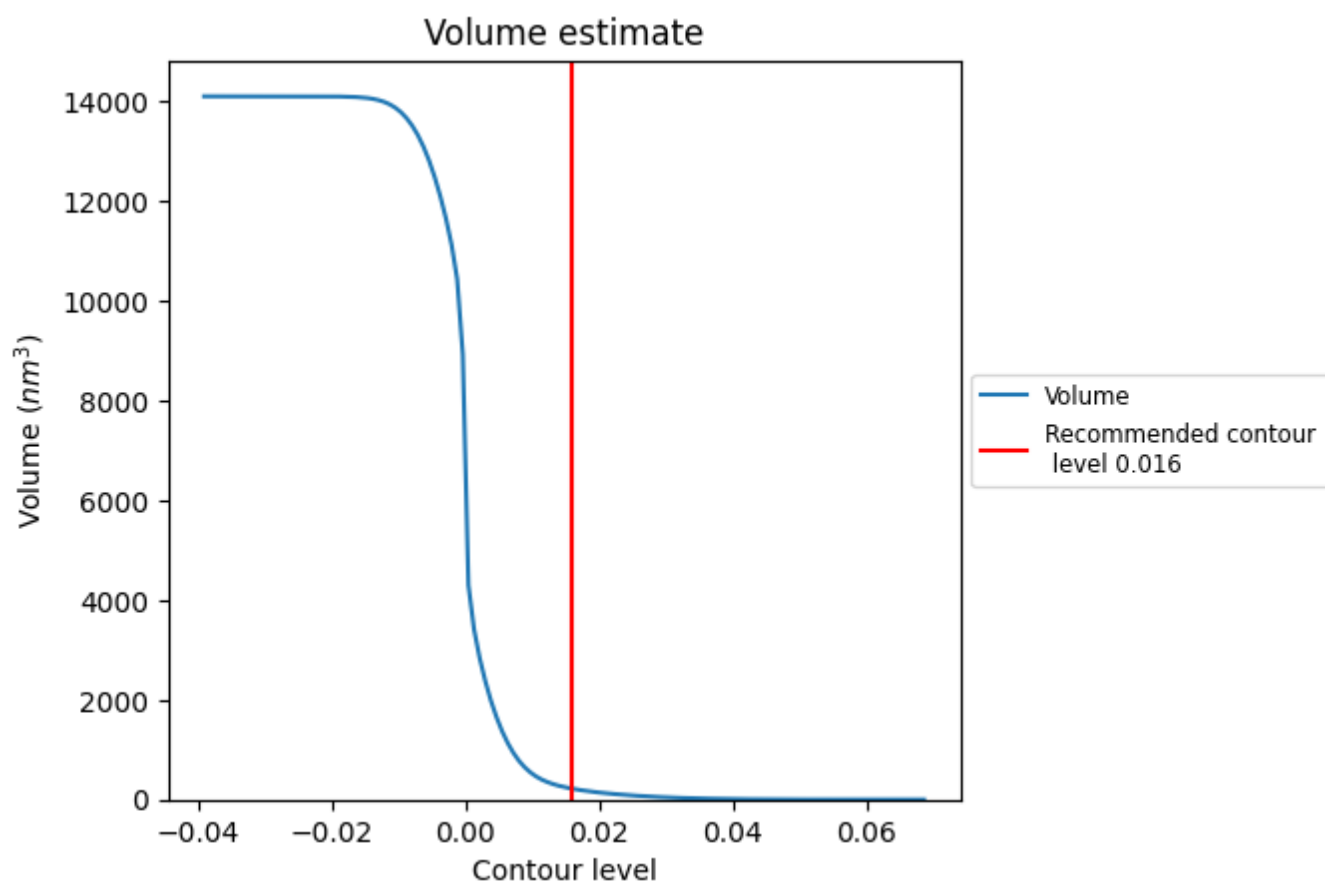
This section contains the results of statistical analysis of the map.

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.

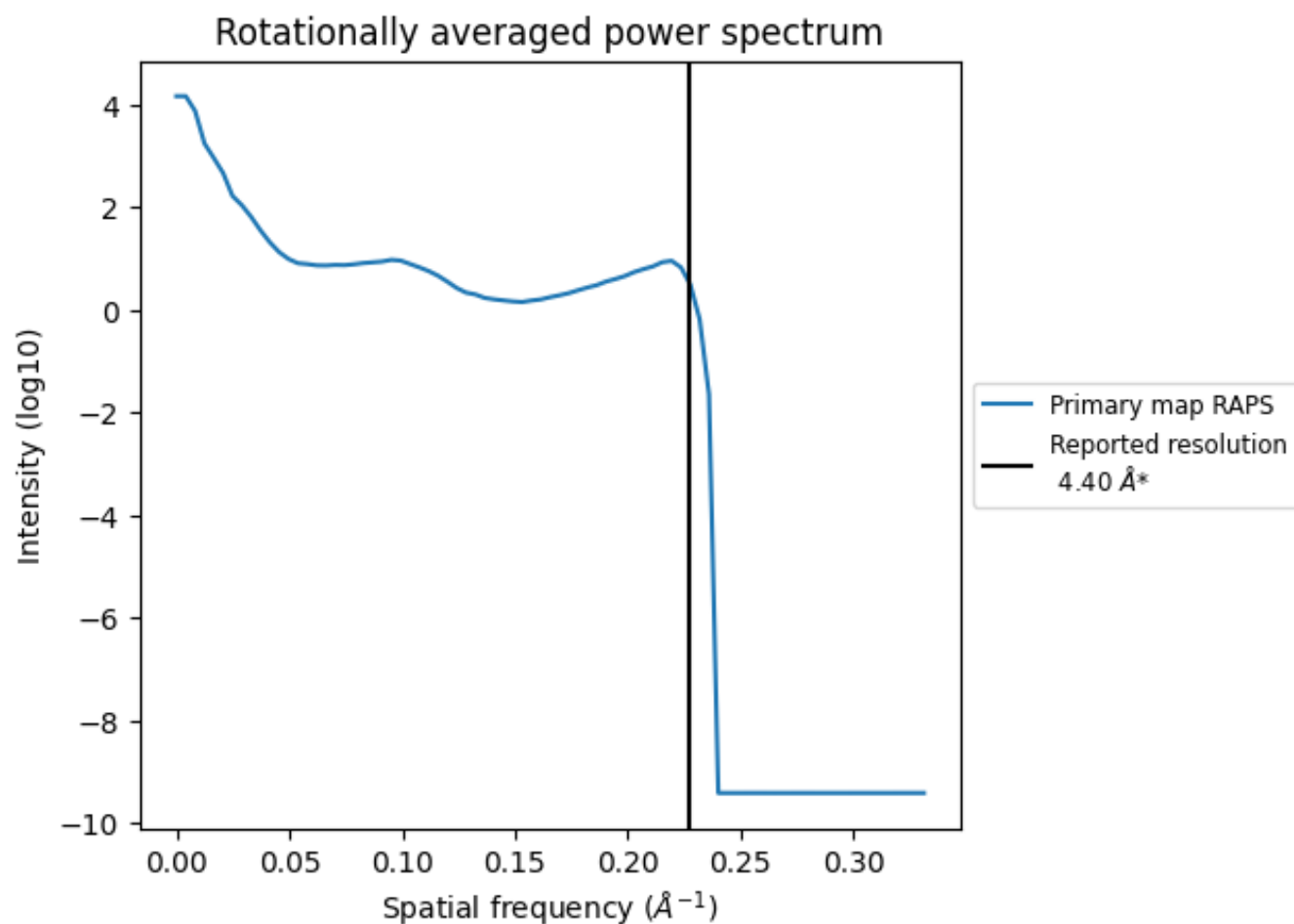
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm³; this corresponds to an approximate mass of 197 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 0.227 $\text{\AA}^{-1}$

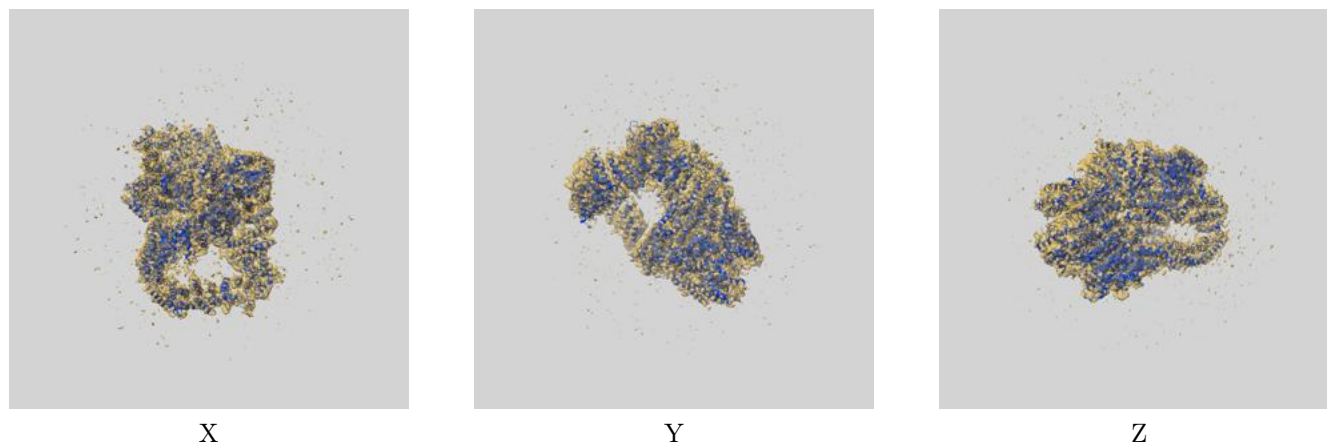
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

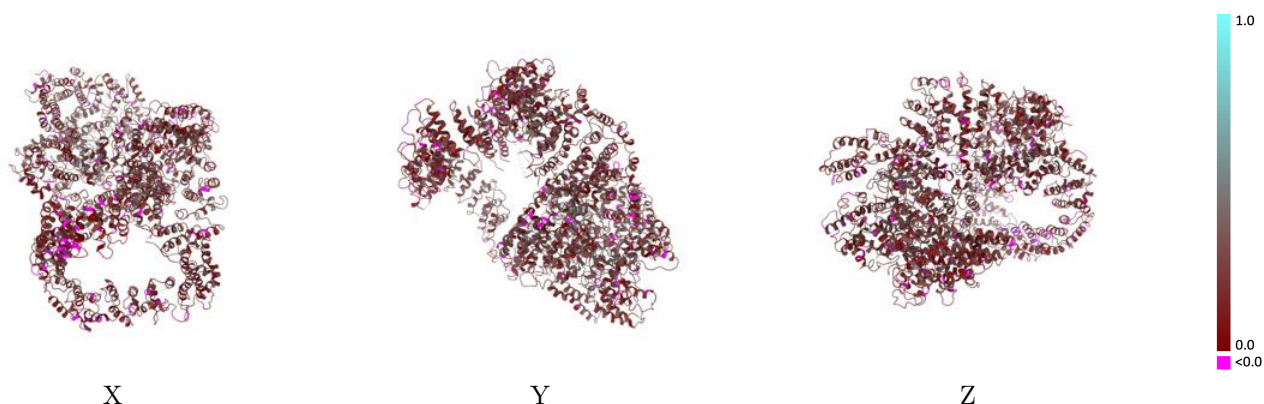
This section contains information regarding the fit between EMDB map EMD-8751 and PDB model 5W1R. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



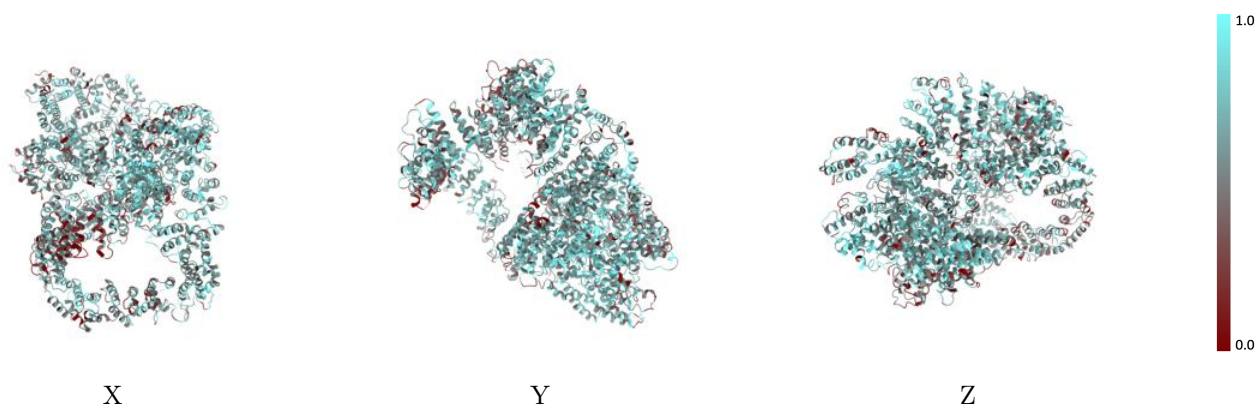
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



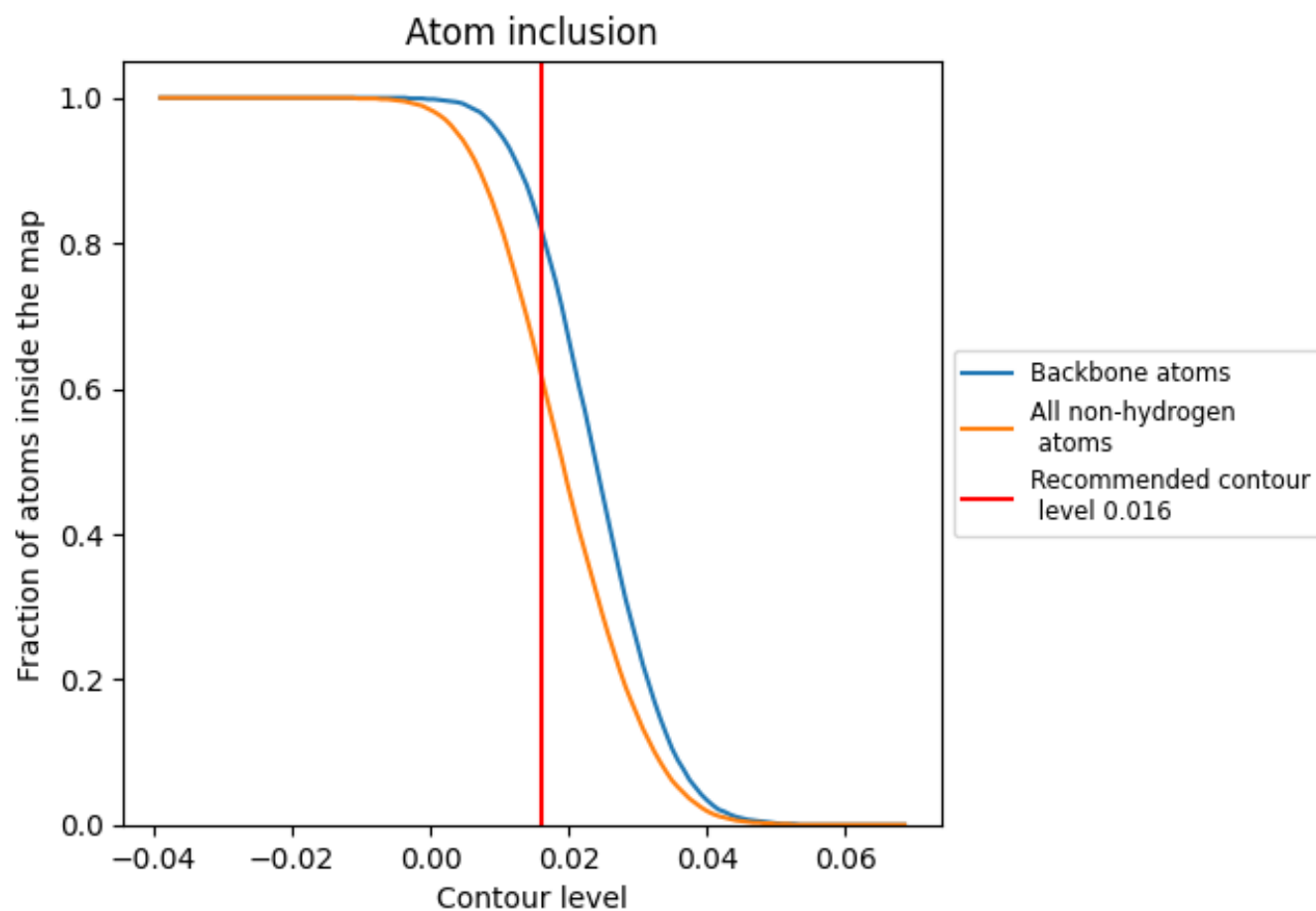
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 62% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6210	0.2350
A	0.6210	0.2350

