



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:06 PM UTC

PDB ID : 5Y3R / pdb_00005y3r
EMDB ID : EMD-6803
Title : Cryo-EM structure of Human DNA-PK Holoenzyme
Authors : Yin, X.; Liu, M.; Tian, Y.; Wang, J.; Xu, Y.
Deposited on : 2017-07-29
Resolution : 6.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

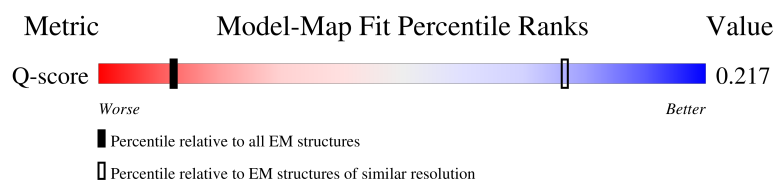
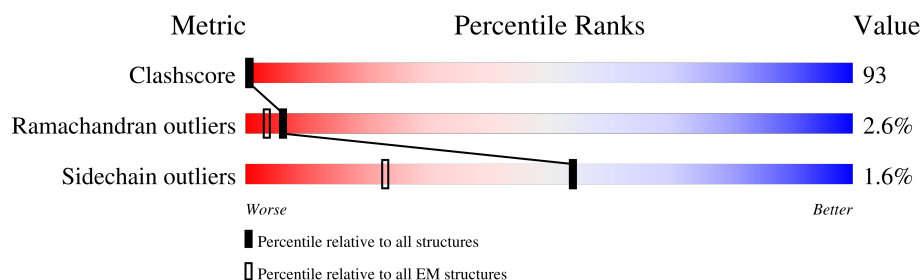
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	531 (6.10 - 7.10)

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	501	
2	B	536	
3	K	15	
4	D	34	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	36	100%
6	C	4119	11% 11% 73% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38766 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	493	Total	C	N	O	S	0	0
			3982	2550	675	739	18		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	526	Total	C	N	O	S	0	0
			4210	2696	707	784	23		

- Molecule 3 is a protein called PRKDC-Helix.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 4 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	34	Total	C	N	O	P	0	0
			700	336	123	207	34		

- Molecule 5 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	36	Total	C	N	O	P	0	0
			733	354	132	212	35		

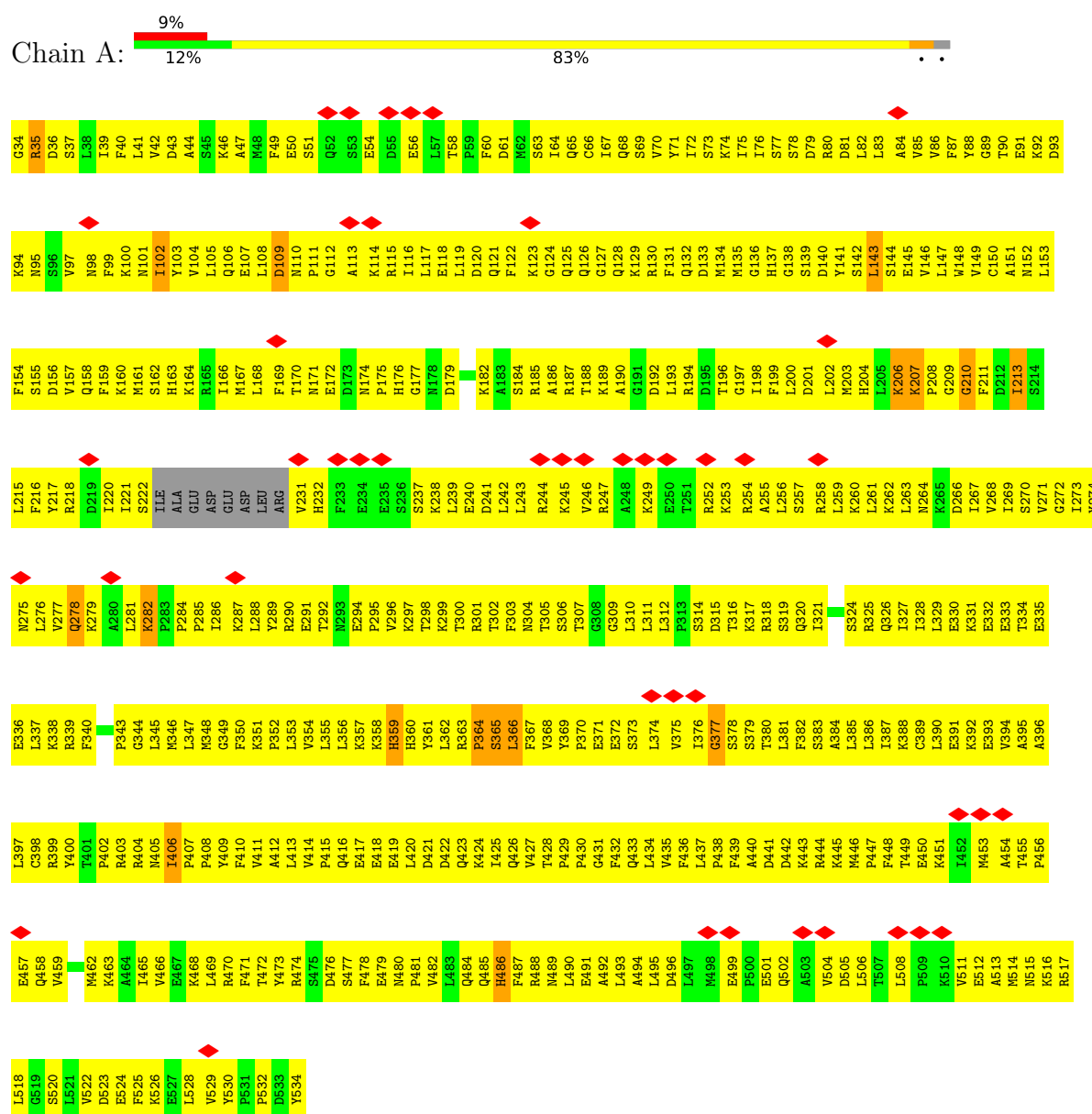
- Molecule 6 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	3636	Total	C	N	O	S	0	0
			29066	18608	4912	5356	190		

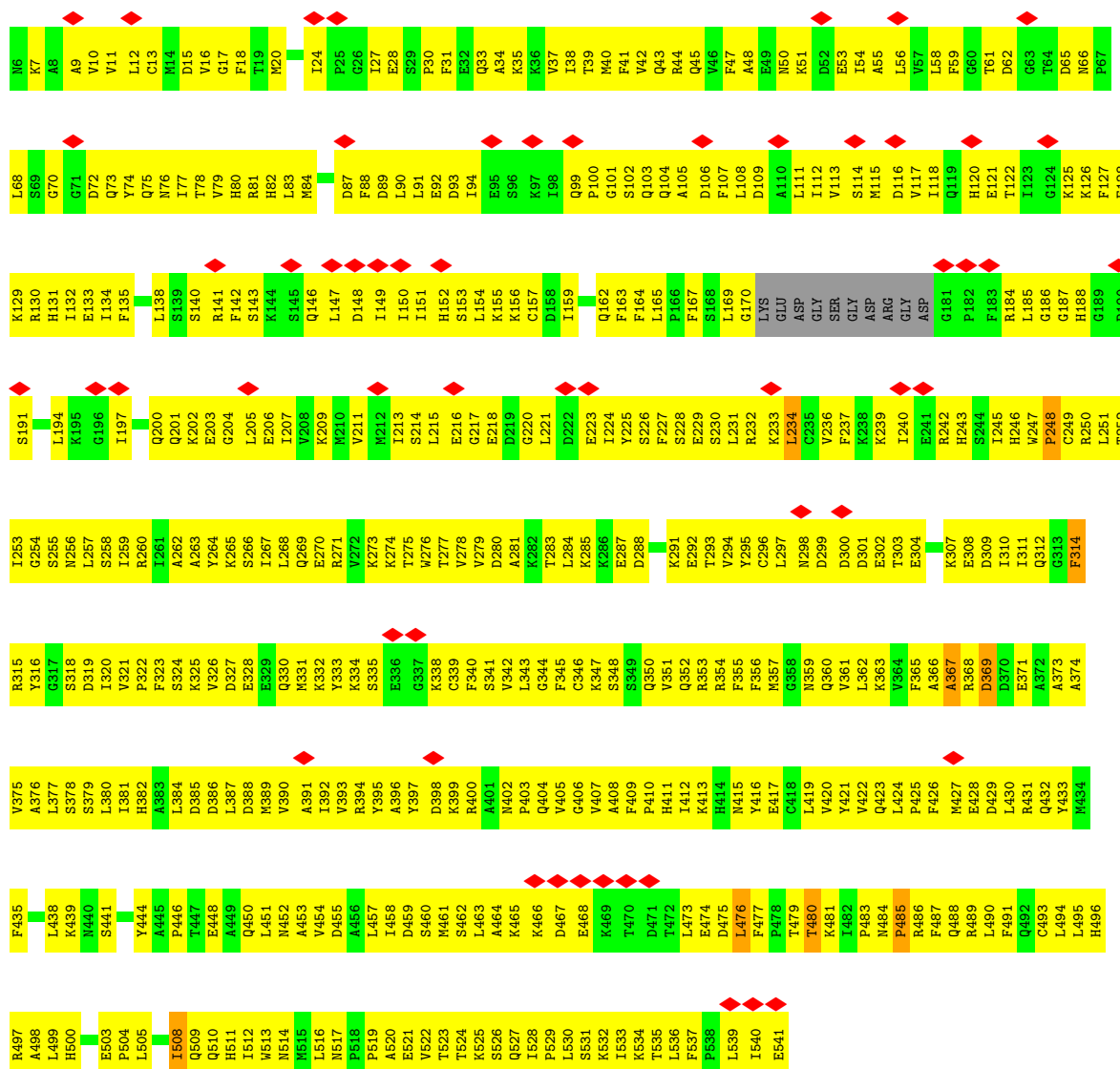
3 Residue-property plots

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.

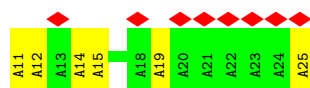
- Molecule 1: X-ray repair cross-complementing protein 6



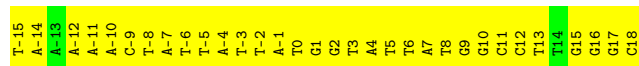
- Molecule 2: X-ray repair cross-complementing protein 5



• Molecule 3: PRKDC-Helix



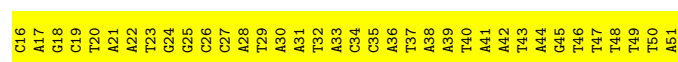
• Molecule 4: DNA (34-MER)



• Molecule 5: DNA (36-MER)

Chain E:

100%



• Molecule 6: DNA-dependent protein kinase catalytic subunit

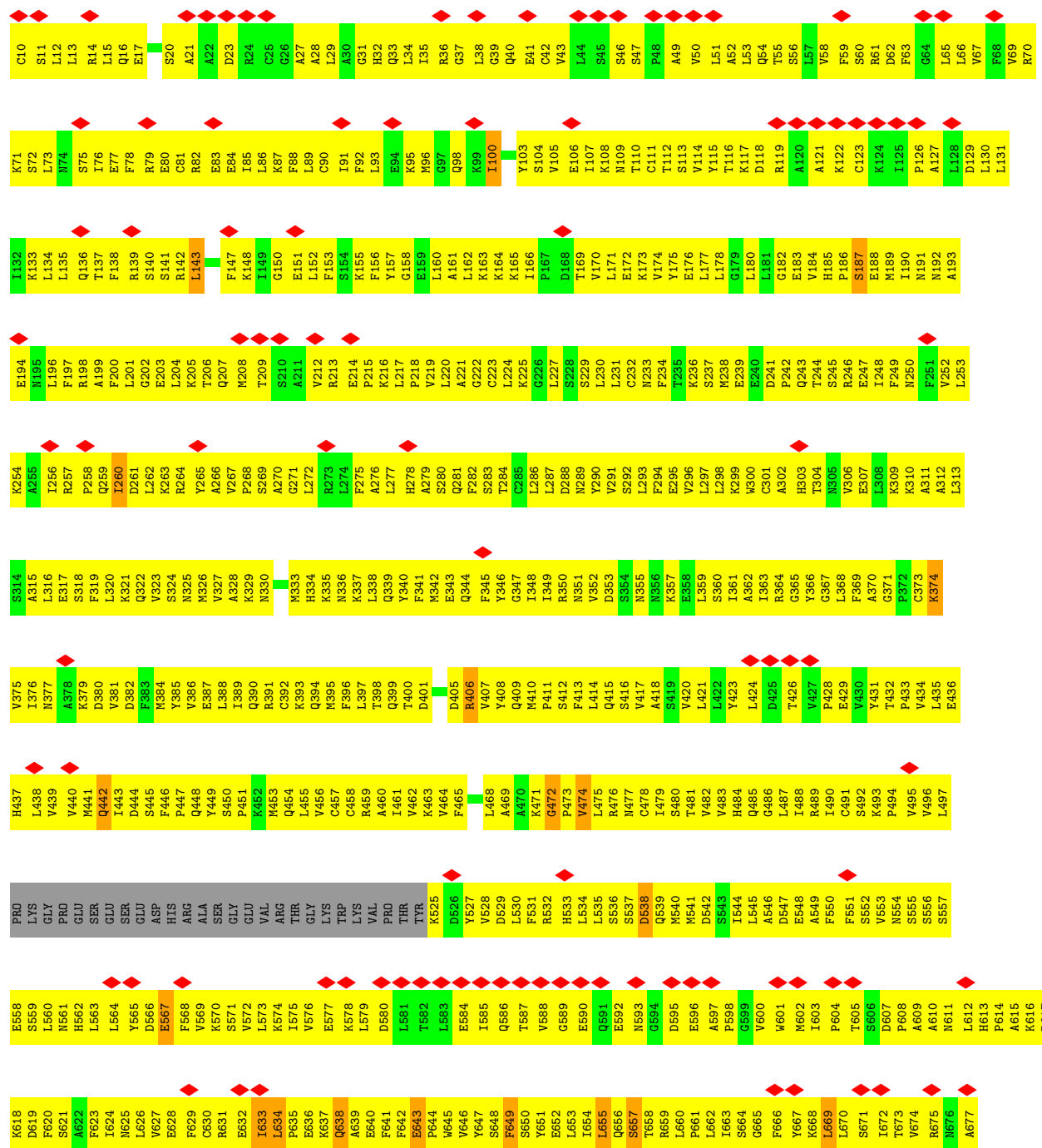
Chain C:

11%

11%

73%

12%



L1406	K1407	M1408	S1409	P1410	Y1411	K1412	D1413	L1414	L1415	E1416	W1356	G1355	L1417	L1418	L1358	L1359	K1360	K1361	D1362	L1363	L1424	A1425	A1426	Q1427	S1428	I1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	Q1442	V1443	D1444	R1445	S1446	R1447	L1448	S1453	K1456	Q1457	L1458	H1459	R1460	A1461	G1462	L1463	L1464	H1465	F1466	L1467	L1468	
T1346	T1347	L1348	L1349	N1350	T1351	K1352	P1353	E1354	G1355	W1356	K1357	L1358	L1359	K1360	K1361	D1362	L1363	L1364	H1365	T1366	H1367	L1368	M1369	R1370	V1371	L1372	V1373	Q1374	T1375	L1376	C1377	E1378	P1379	A1380	S1381	I1382	G1383	F1384	N1385	I1386	G1387	D1388	V1389	K1390	V1391	M1392	A1393	H1394	L1395	P1396	D1397	V1398	C1399	M1400	N1401	L1402	M1403	K1404	A1405		
T1284	E1285	A1286	Q1287	S1288	L1291	K1292	A1295	F1296	F1297	L1298	E1299	S1300	T1301	A1302	M1303	H1304	D1305	I1306	T1307	A1308	ALA	GLU	CYS	PHE	GLY	THR	GLY	ALA	GLY	ASN	ARG	THR	S1323	P1324	Q1325	E1326	G1327	E1328	R1329	Y1330	N1331	Y1332	S1333	K1334	C1335	T1336	V1337	V1338	R1340	M1342	E1343	F1344	T1345								
L1220	I1221	T1222	F1224	G1227	G1228	C1229	G1230	Q1231	P1232	S1233	G1234	I1235	L1236	A1237	Q1238	P1239	T1240	L1241	L1242	Y1243	F1248	S1249	L1250	Q1251	A1252	T1253	L1254	C1255	W1256	L1257	D1258	L1259	L1260	L1261	A1262	A1263	E1265	C1266	Y1267	T1268	F1270	I1271	G1272	A1273	R1274	T1275	G1276	G1277	L1278	Q1280	V1281	G1283									
V1100	F1101	E1102	A1103	L1104	V1105	I1106	Y1107	M1108	E1109	S1110	L1111	A1112	L1113	A1114	H1115	A1116	F1117	E1118	K1119	G1120	L1121	G1122	T1123	I1124	Q1125	Q1126	C1127	C1128	A1130	I1131	D1132	A1133	C1135	R1136	I1137	I1138	E1139	K1140	K1141	H1142	V1143	S1144	L1145	N1146	K1147	A1148	K1149	K1150	R1151	R1152	L1153	P1154	L1155	G1156	F1157	P1158	P1159				
S1040	I1041	Q1042	Q1043	L1044	T1045	P1046	Q1047	Q1048	Q1049	E1050	K1051	S1052	P1053	V1054	M1055	L1056	K1057	S1058	L1059	F1060	K1061	R1062	L1063	Y1064	S1065	L1066	A1067	L1068	H1069	P1070	N1071	A1072	F1073	K1074	R1075	L1076	G1077	A1078	S1079	L1080	A1081	F1082	N1083	N1084	I1085	Y1086	R1087	E1088	F1089	R1090	E1091	E1092	E1093	S1094	L1095	V1096	E1097	K1098	F1099		
T980	R981	Q982	L983	Y984	E985	P986	L987	V988	M989	Q990	L991	T992	H993	W994	F995	T996	N997	N998	K999	K1000	F1001	E1002	S1003	Q1004	D1005	T1006	V1007	A1008	L1009	L1010	E1011	P949	E950	E951	G952	G953	G954	E955	P956	P957	F958	R959	E990	K902	P903	V904	L968	P967	L969	R970	R971	R972	R973	D977	Q978	V979					
M858	L859	G860	S861	L862	G863	G864	Q865	L866	N867	K868	M869	L870	L871	T872	W873	T874	S875	S876	D877	E878	M880	K881	S882	Y883	V884	A885	W886	D887	R888	E889	G892	K890	R891	L892	S893	F894	A895	V896	P897	F898	R899	E900	K902	P903	V904	L968	P967	L969	R970	R971	R972	R973	D908	V909	R910	R911	P912	R913	V914	T915	L917
G798	Y799	L800	K801	S802	A803	A804	L805	S806	D807	E808	T809	LYS	ASN	ASN	TRP	GLU	VAL	SER	ALA	LEU	SER	ARG	ALA	ALA	GLN	LYS	PHE	ASN	LYS	VAL	VAL	VAL	ASN	LEU	SER	ASN	GLU	ALA	I846	S847	L848	E849	R906	R907	R908	I851	R852	L793	R853	V855	R856	Q857									
H738	N739	I740	I741	E742	L743	L744	V745	VAL	A747	Y748	V749	P750	SER	LEU	L752	L753	Q754	A755	A756	K757	L758	L759	L760	S761	Y762	T763	P764	L765	A766	E767	V768	G769	L770	N771	A772	L773	A774	E775	W776	S777	Y779	I780	D781	R782	H783	M785	Q786	P787	Y788	Y789	K790	L791	I792	L793	P794	C795	L796	D797			
K678	K679	I680	K681	Y682	PHE	GLU	GLY	VAL	SER	PRO	LYS	SER	LEU	LYS	HIS	SER	PRO	GLU	ASP	PRO	GLU	K700	Y701	S702	C703	A704	A705	L706	F707	W708	K709	F710	G711	K712	E713	V714	A715	E716	K717	M718	K719	Q720	Y721	K722	D723	E724	L725	L726	A727	S728	C729	L730	T731	F732	L733	L734	S735	L736	P737		

T2201	T2202	T2203	G2204	V2205	P2206	K2207	D2208	L22149	V2150	L2211	N2089	R2090	C2093	M2094	A2095	P2096	F2097	T2098	A2099	L2100	V2101	K2102	H2103	N2104	L2165	S2166	P2167	L2168	L2169	Q2170	L2171	A2172	A2173	S2174	E2175	N2176	N2177	G2178	G2179	E2180	G2181	I2182	H2183	Y2184	M2185	V2186	V2187	E2188	I2189	V2190	A2191	T2192	H2193	G2194	S2195	L2196	T2197	G2198	K2259	F2260
L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260								
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	
L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L22									





S4084	K4085	D4086	H4087	N4088	I4089	R4090	A4091	Q4092	E4093	P4094	E4095	S4096	G4097	L4098	S4099	E4100	E4101	T4102	Q4103	V4104	K4105	C4106	L4107	M4108	D4109	Q4110	A4111	T4112	D4113	P4114	M4115	I4116	L4117	G4118	R4119	T4120	W4121	E4122	G4123	W4124	E4125	P4126	R4127	M4128															
G4024	G4025	S4026	W4027	I4028	Q4029	E4030	I4031	N4032	V4033	A4034	E4035	K4036	N4037	W4038	Y4039	R4040	Q4041	Q4042	K4043	I4044	C4045	Y4046	A4047	K4048	R4049	K4050	L4051	A4052	G4053	A4054	N4055	P4056	A4057	V4058	I4059	T4060	C4061	D4062	E4063	L4064	L4065	L4066	G4067	H4068	E4069	K4070	A4071	P4072	A4073	F4074	R4075	D4076	Y4077	V4078	A4079	V4080	A4081	R4082	G4083
L3963	T3964	R3965	Q3966	F3967	I3968	N3969	L3970	M3971	L3972	P3973	M3974	K3975	E3976	T3977	G3978	L3979	M3980	Y3981	S3982	I3983	M3984	V3985	H3986	A3987	L3988	R3989	A3990	F3991	R3992	S3993	D3994	L3997	L3998	T3999	N4000	T4001	M4002	D4003	V4004	F4005	V4006	K4007	E4008	P4009	S4010	F4011	D4012	W4013	K4014	N4015	F4016	E4017	Q4018	K4019	M4020	L4021	K4022	K4023	
R3901	S3902	H3903	F3904	A3905	S3906	S3907	H3908	A3909	L3910	I3911	C3912	I3913	S3914	H3915	W3916	I3917	L3918	G3919	I3920	G3921	D3922	R3923	H3924	L3925	N3926	N3927	F3928	M3929	V3930	A3931	M3932	E3933	T3934	G3935	G3936	V3937	I3938	G3939	I3940	D3941	F3942	G3943	H3944	G3947	S3948	A3949	T3950	Q3951	F3952	V3955	P3956	E3957	L3958	M3959	F3960	F3961	R3962		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53451	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	4700	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.139	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	390.0, 390.0, 390.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3, 1.3, 1.3	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	0.50	0/4060	0.86	7/5468 (0.1%)
2	B	0.41	0/4297	0.76	3/5798 (0.1%)
3	K	0.25	0/74	0.38	0/102
4	D	0.63	0/784	0.65	0/1209
5	E	0.59	0/822	0.66	0/1266
6	C	0.55	0/29665	0.87	26/40094 (0.1%)
All	All	0.54	0/39702	0.85	36/53937 (0.1%)

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	12
2	B	0	8
6	C	0	89
All	All	0	109

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	472	GLY	CA-C-N	11.24	133.89	119.84
6	C	472	GLY	C-N-CA	11.24	133.89	119.84
6	C	2372	PRO	N-CA-C	9.93	122.82	110.70
1	A	207	LYS	N-CA-C	-8.26	98.18	110.24
6	C	2372	PRO	CA-C-N	-7.65	110.28	119.84

There are no chirality outliers.

5 of 109 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ILE	Peptide
1	A	109	ASP	Peptide
1	A	206	LYS	Peptide
1	A	268	VAL	Peptide
1	A	35	ARG	Peptide

5.2 Too-close contacts

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	3982	0	4064	925	0
2	B	4210	0	4250	729	0
3	K	75	0	74	5	0
4	D	700	0	388	182	0
5	E	733	0	410	214	0
6	C	29066	0	29396	5491	0
All	All	38766	0	38582	7198	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 93.

The worst 5 of 7198 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)
6:C:3809:THR:HA	6:C:3930:VAL:O	1.25	1.32
6:C:3740:ILE:HB	6:C:3748:HIS:O	1.38	1.22
1:A:378:SER:O	1:A:382:PHE:HB3	1.39	1.21
6:C:700:LYS:N	6:C:703:CYS:HG	1.35	1.21
2:B:264:TYR:HB2	2:B:363:LYS:O	1.43	1.19

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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
6	C	1015/4119 (25%)	792 (78%)	197 (19%)	26 (3%)	4 25

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	C	3486	GLU
6	C	3690	PHE
6	C	4028	ILE
6	C	4005	PHE
6	C	3131	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	230/455 (50%)	228 (99%)	2 (1%)	70 79
6	C	2552/3667 (70%)	2510 (98%)	42 (2%)	55 70
All	All	2782/4122 (68%)	2738 (98%)	44 (2%)	54 70

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	C	3019	ILE
6	C	3534	ILE
6	C	3045	ILE
6	C	3120	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	C	3706	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
6	C	3112	GLN
6	C	3808	ASN
6	C	3177	ASN
6	C	3660	ASN
6	C	3951	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-6803. These allow visual inspection of the internal detail of the map and identification of artifacts.

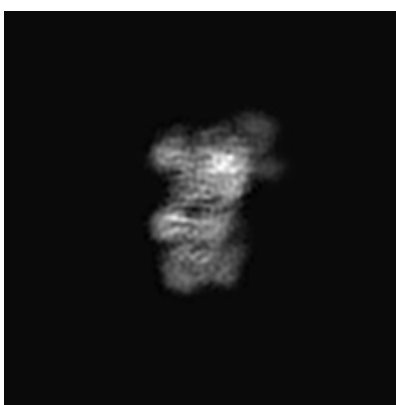
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

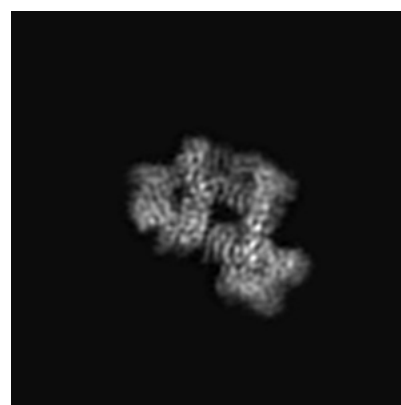
6.1.1 Primary map



X



Y

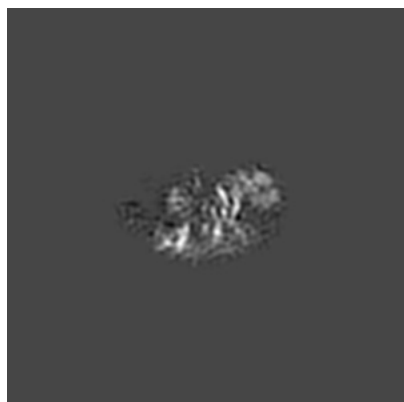


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

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: 181



Y Index: 136

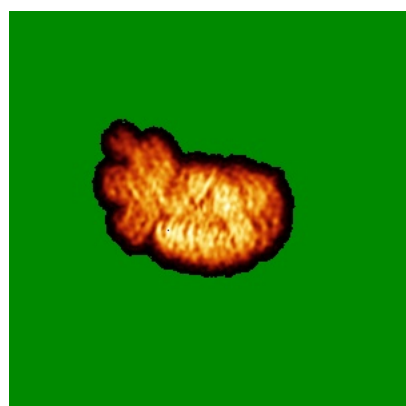


Z Index: 159

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

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

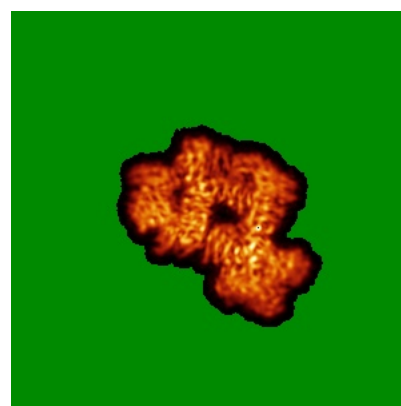
6.4.1 Primary map



X



Y

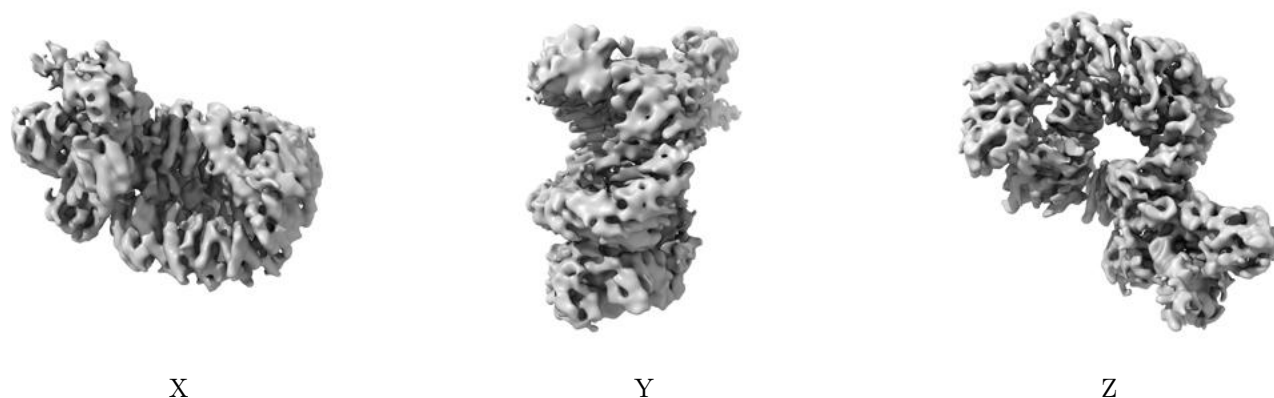


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

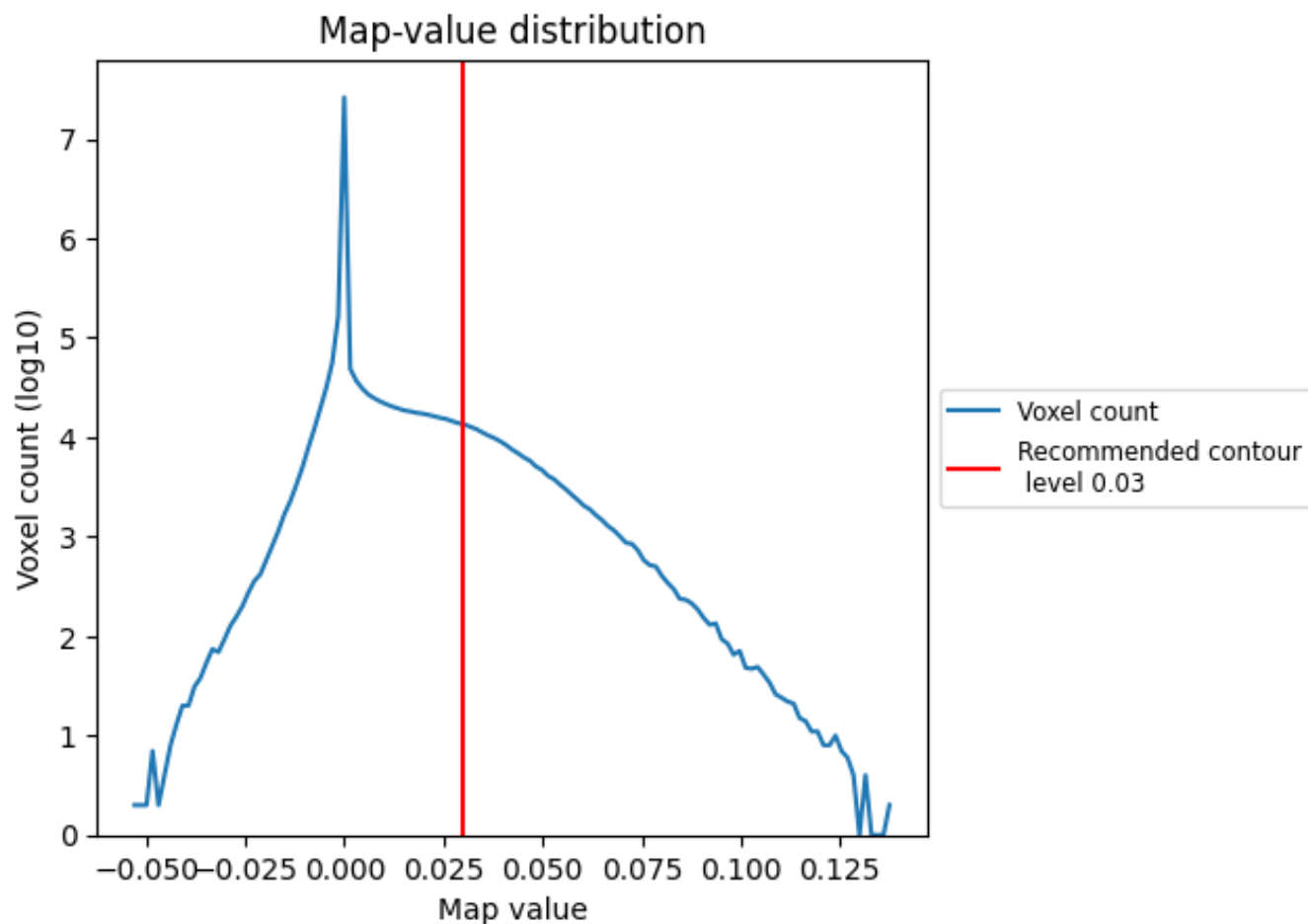
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

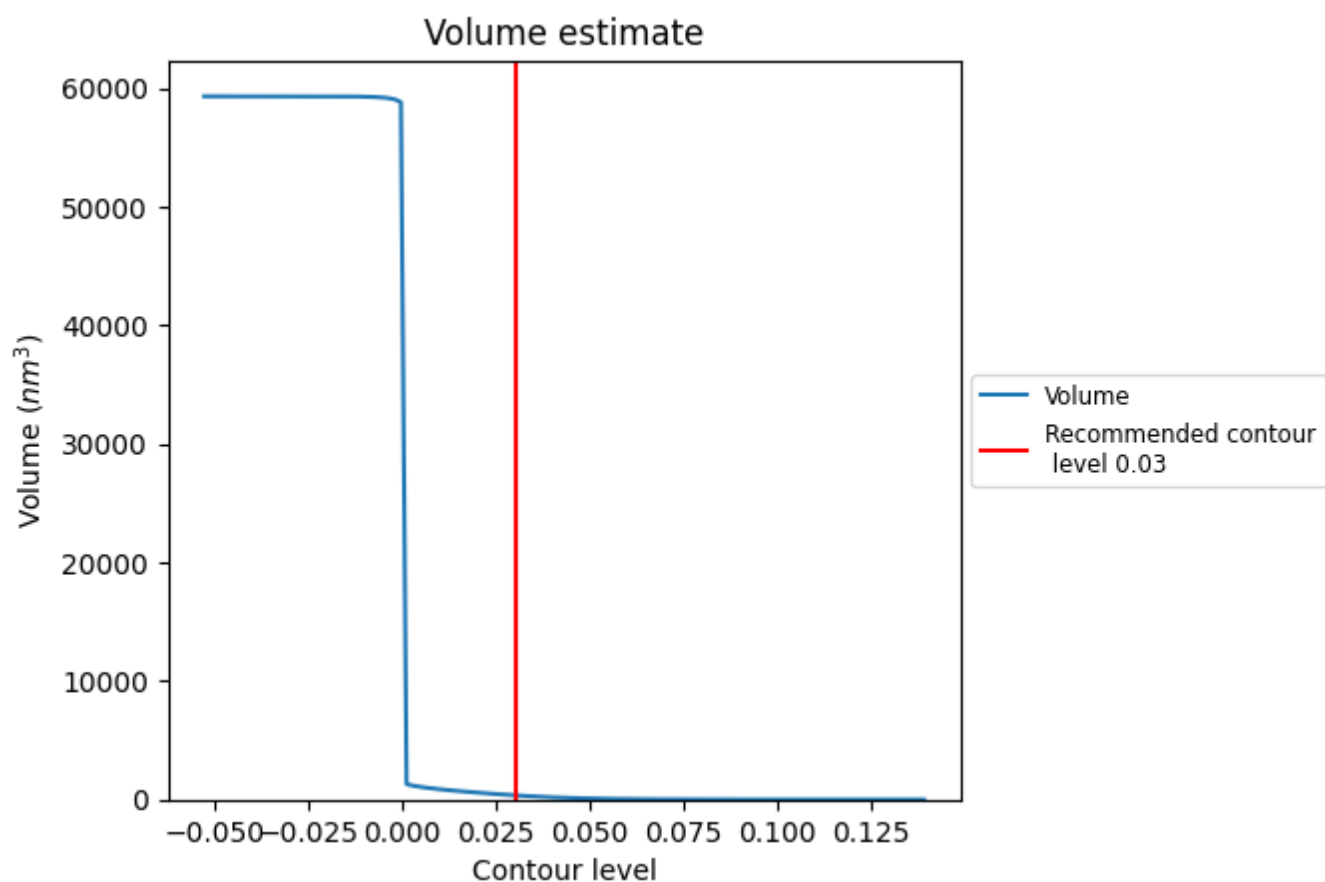
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

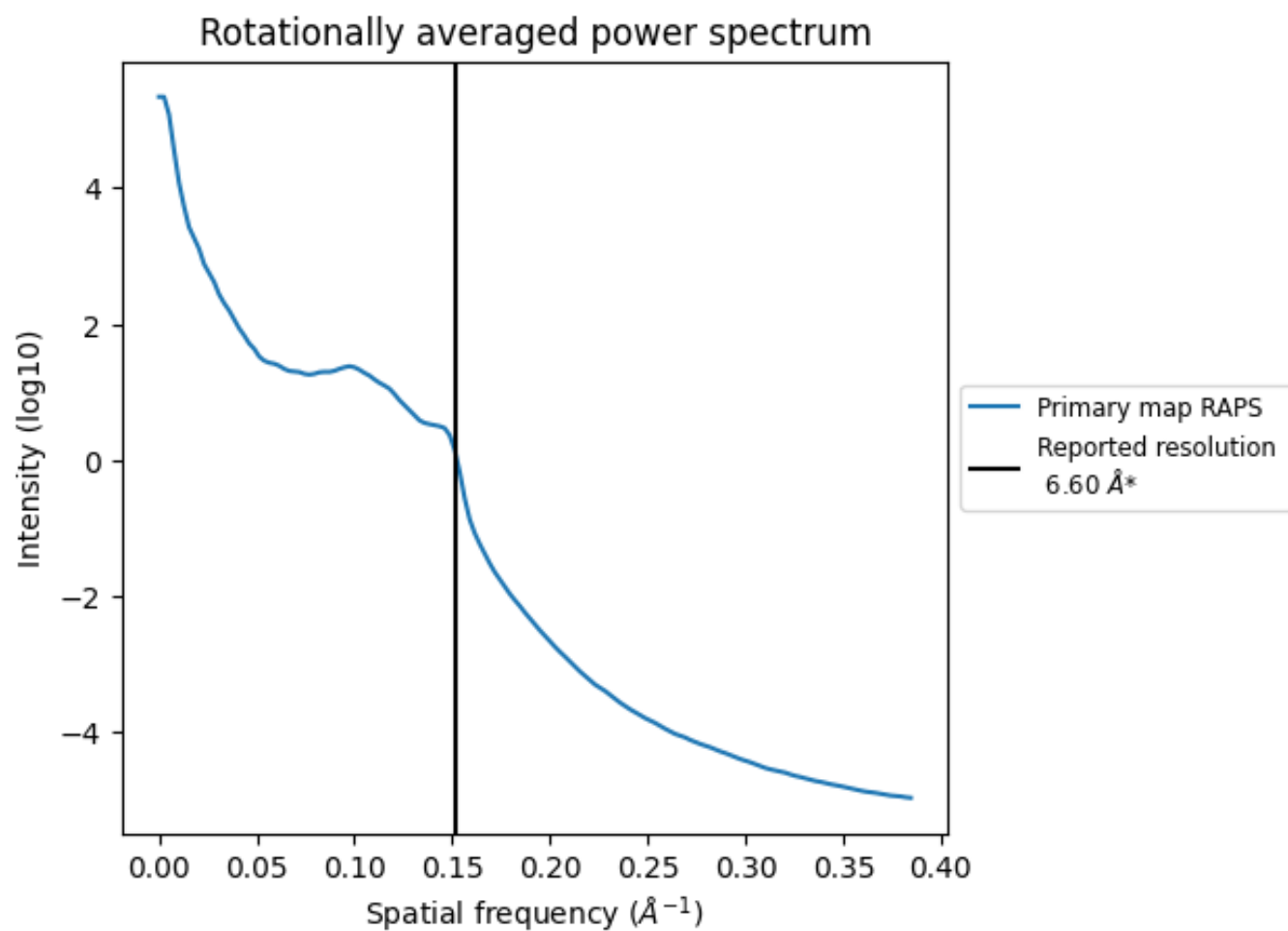
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; this corresponds to an approximate mass of 322 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 ⓘ

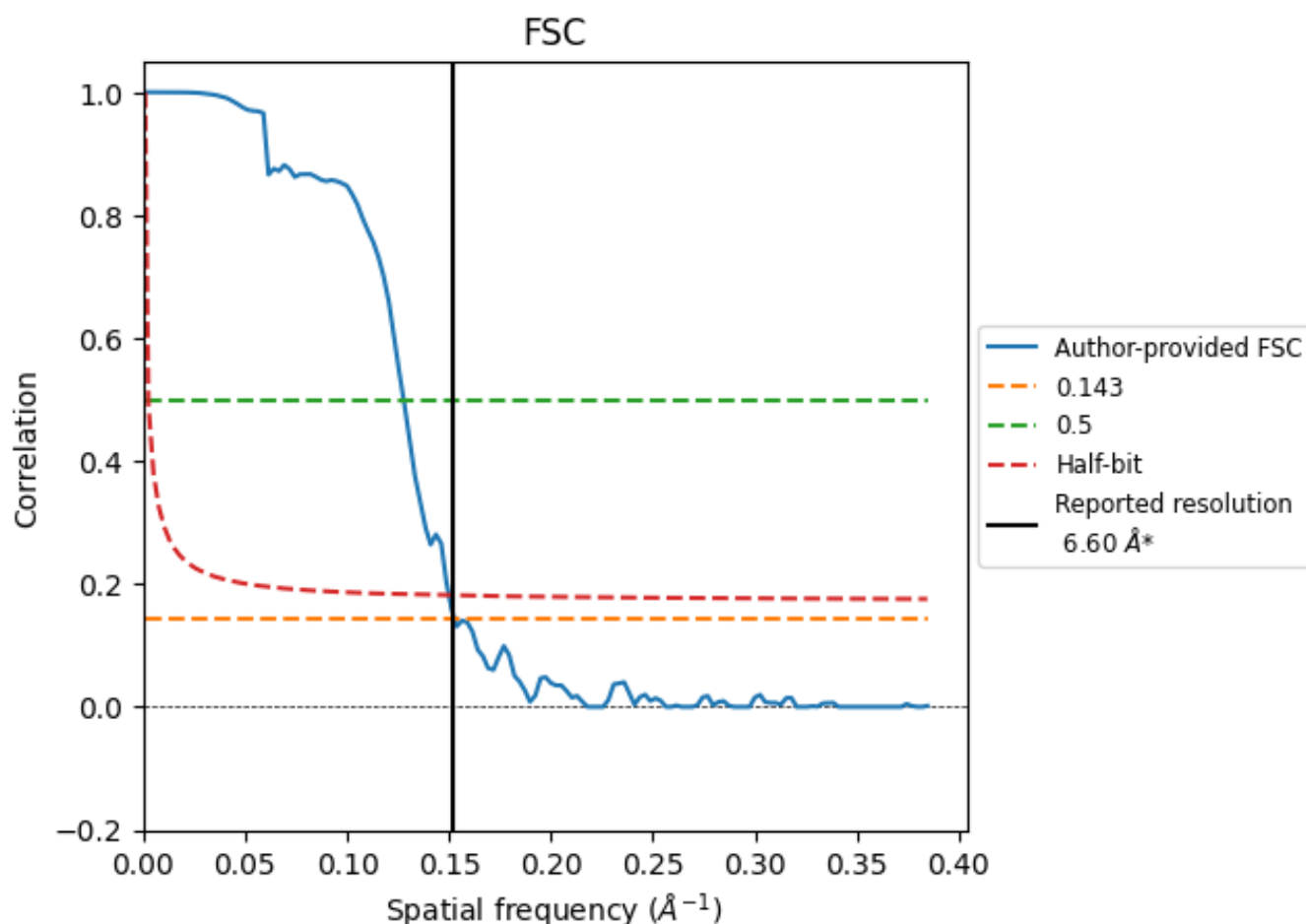


*Reported resolution corresponds to spatial frequency of 0.152 Å⁻¹

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 0.152 Å⁻¹

8.2 Resolution estimates [i](#)

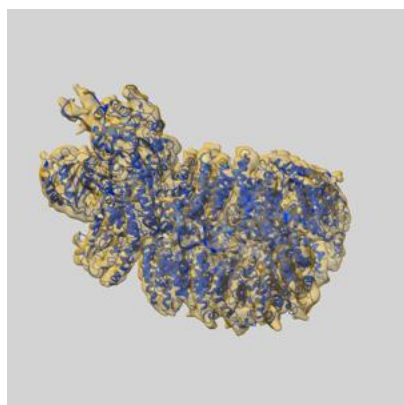
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	6.55	7.82	6.67
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

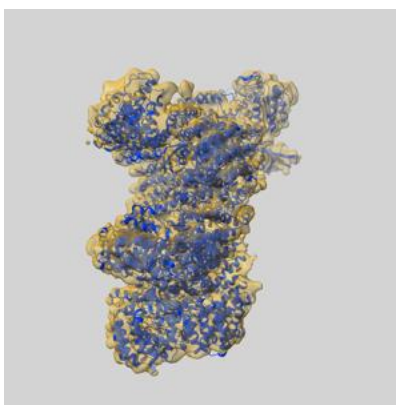
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6803 and PDB model 5Y3R. Per-residue inclusion information can be found in section [3](#) on page [5](#).

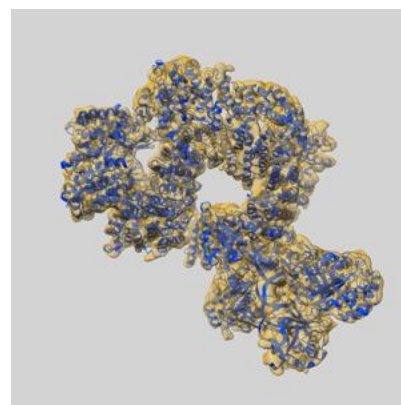
9.1 Map-model overlay [i](#)



X



Y



Z

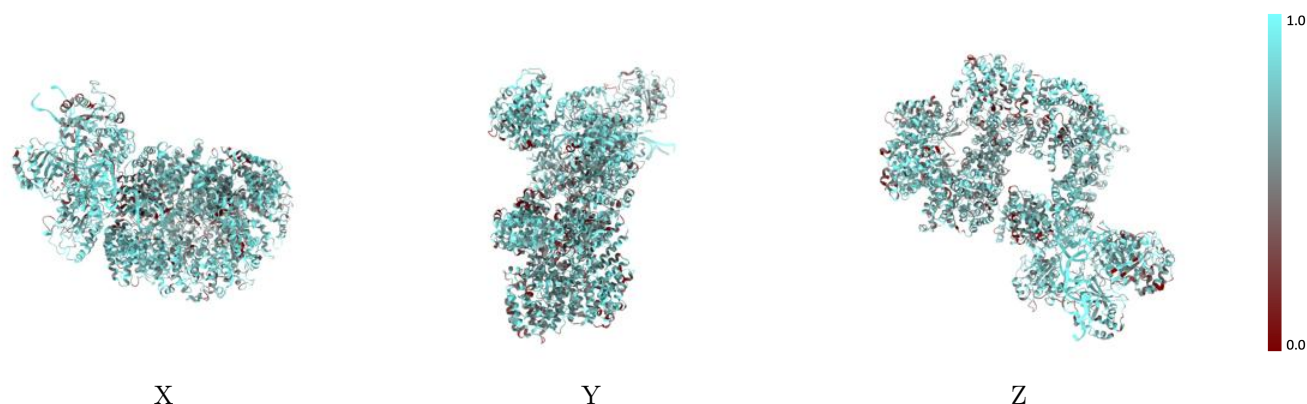
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



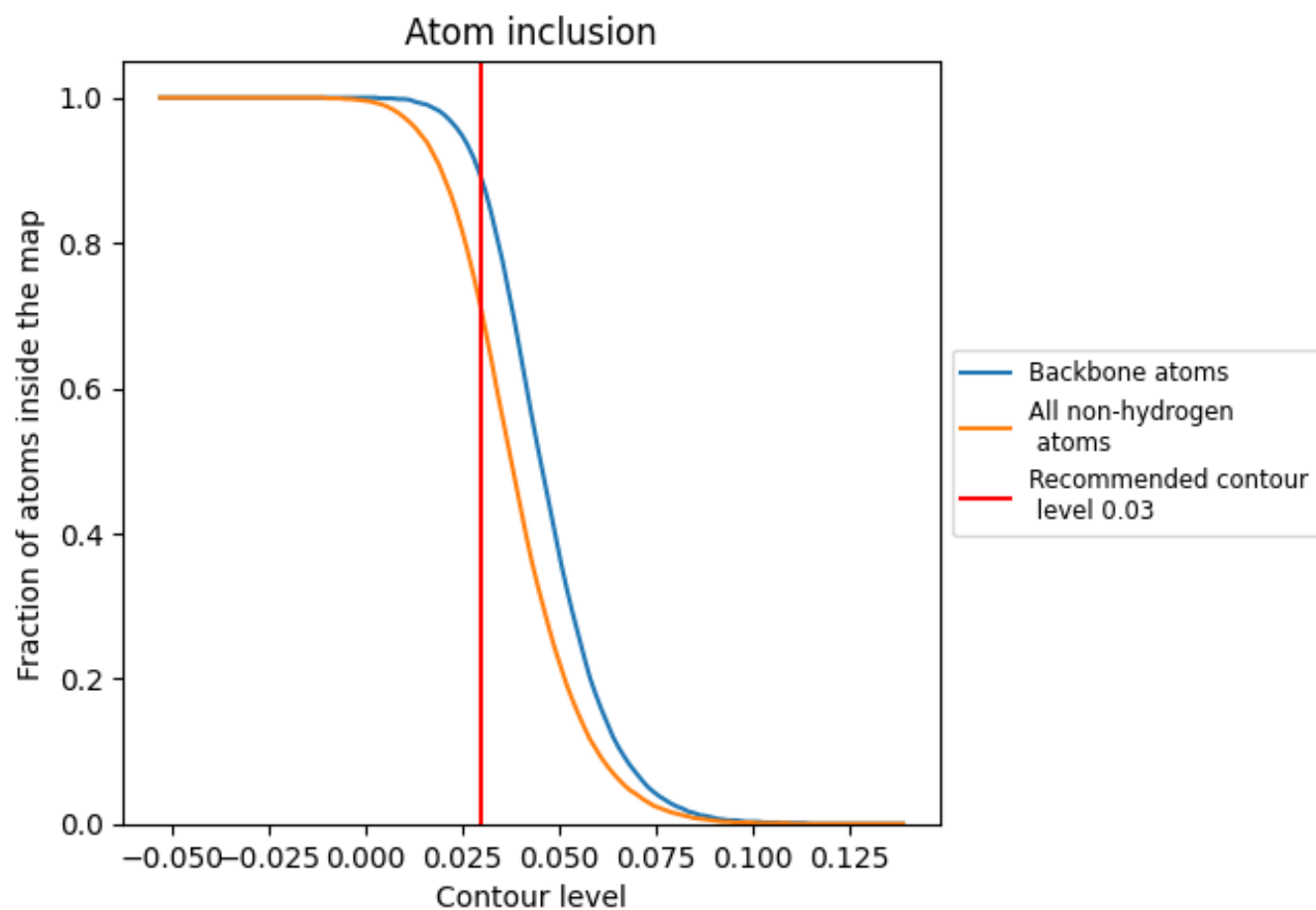
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7080	0.2170
A	0.7480	0.2360
B	0.7070	0.2250
C	0.6940	0.2110
D	0.9200	0.2680
E	0.8910	0.2590
K	0.4400	0.2940

1.0

0.0

<0.0