



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:57 AM UTC

PDB ID : 9CI3 / pdb_00009ci3
EMDB ID : EMD-45609
Title : Structure of the LRRK2/14-3-3 complex
Authors : Martinez Fiesco, J.A.; Zhang, P.
Deposited on : 2024-07-02
Resolution : 3.96 Å(reported)

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

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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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

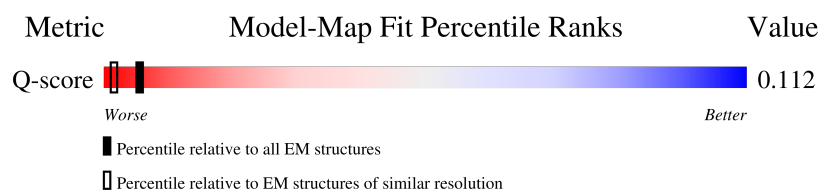
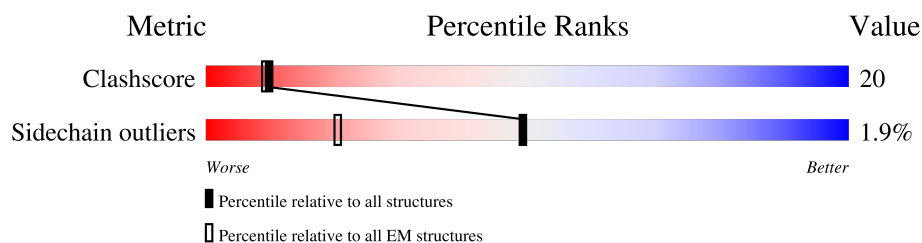
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



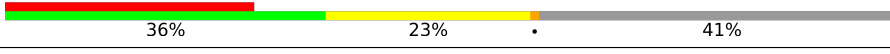
The reported resolution of this entry is 3.96 Å.

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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7646 (3.46 - 4.46)

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	B	265	
1	C	265	
2	A	2562	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15926 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 14-3-3 protein gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	237	Total	C	N	O	S	0	0
			1909	1190	325	384	10		
1	B	240	Total	C	N	O	S	0	0
			1935	1204	330	391	10		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	initiating methionine	UNP P61981
C	-16	GLY	-	expression tag	UNP P61981
C	-15	SER	-	expression tag	UNP P61981
C	-14	HIS	-	expression tag	UNP P61981
C	-13	HIS	-	expression tag	UNP P61981
C	-12	HIS	-	expression tag	UNP P61981
C	-11	HIS	-	expression tag	UNP P61981
C	-10	HIS	-	expression tag	UNP P61981
C	-9	HIS	-	expression tag	UNP P61981
C	-8	SER	-	expression tag	UNP P61981
C	-7	GLY	-	expression tag	UNP P61981
C	-6	GLU	-	expression tag	UNP P61981
C	-5	ASN	-	expression tag	UNP P61981
C	-4	LEU	-	expression tag	UNP P61981
C	-3	TYR	-	expression tag	UNP P61981
C	-2	PHE	-	expression tag	UNP P61981
C	-1	GLN	-	expression tag	UNP P61981
C	0	GLY	-	expression tag	UNP P61981
B	-17	MET	-	initiating methionine	UNP P61981
B	-16	GLY	-	expression tag	UNP P61981
B	-15	SER	-	expression tag	UNP P61981
B	-14	HIS	-	expression tag	UNP P61981
B	-13	HIS	-	expression tag	UNP P61981
B	-12	HIS	-	expression tag	UNP P61981
B	-11	HIS	-	expression tag	UNP P61981
B	-10	HIS	-	expression tag	UNP P61981

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP P61981
B	-8	SER	-	expression tag	UNP P61981
B	-7	GLY	-	expression tag	UNP P61981
B	-6	GLU	-	expression tag	UNP P61981
B	-5	ASN	-	expression tag	UNP P61981
B	-4	LEU	-	expression tag	UNP P61981
B	-3	TYR	-	expression tag	UNP P61981
B	-2	PHE	-	expression tag	UNP P61981
B	-1	GLN	-	expression tag	UNP P61981
B	0	GLY	-	expression tag	UNP P61981

- Molecule 2 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	1521	Total	C	N	O	P	S	0	0
			12054	7711	2074	2197	2	70		

There are 36 discrepancies between the modelled and reference sequences:

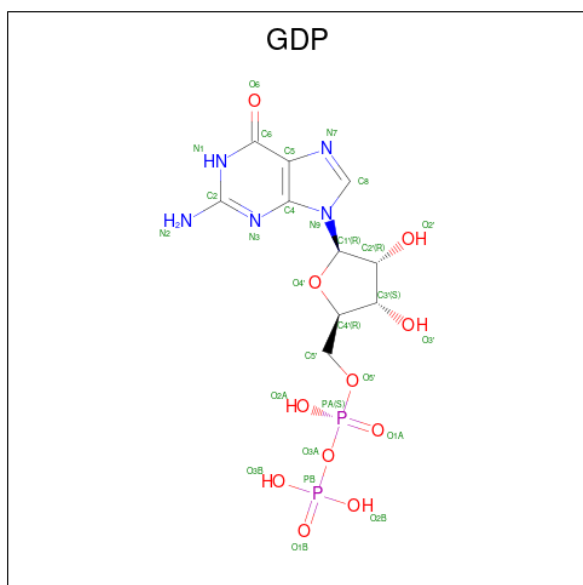
Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP Q5S007
A	-33	GLY	-	expression tag	UNP Q5S007
A	-32	SER	-	expression tag	UNP Q5S007
A	-31	ASP	-	expression tag	UNP Q5S007
A	-30	TYR	-	expression tag	UNP Q5S007
A	-29	LYS	-	expression tag	UNP Q5S007
A	-28	ASP	-	expression tag	UNP Q5S007
A	-27	HIS	-	expression tag	UNP Q5S007
A	-26	ASP	-	expression tag	UNP Q5S007
A	-25	GLY	-	expression tag	UNP Q5S007
A	-24	ASP	-	expression tag	UNP Q5S007
A	-23	TYR	-	expression tag	UNP Q5S007
A	-22	LYS	-	expression tag	UNP Q5S007
A	-21	ASP	-	expression tag	UNP Q5S007
A	-20	HIS	-	expression tag	UNP Q5S007
A	-19	ASP	-	expression tag	UNP Q5S007
A	-18	ILE	-	expression tag	UNP Q5S007
A	-17	ASP	-	expression tag	UNP Q5S007
A	-16	TYR	-	expression tag	UNP Q5S007
A	-15	LYS	-	expression tag	UNP Q5S007
A	-14	ASP	-	expression tag	UNP Q5S007
A	-13	ASP	-	expression tag	UNP Q5S007

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ASP	-	expression tag	UNP Q5S007
A	-11	ASP	-	expression tag	UNP Q5S007
A	-10	LYS	-	expression tag	UNP Q5S007
A	-9	LEU	-	expression tag	UNP Q5S007
A	-8	GLY	-	expression tag	UNP Q5S007
A	-7	LEU	-	expression tag	UNP Q5S007
A	-6	GLU	-	expression tag	UNP Q5S007
A	-5	VAL	-	expression tag	UNP Q5S007
A	-4	LEU	-	expression tag	UNP Q5S007
A	-3	PHE	-	expression tag	UNP Q5S007
A	-2	GLN	-	expression tag	UNP Q5S007
A	-1	GLY	-	expression tag	UNP Q5S007
A	0	PRO	-	expression tag	UNP Q5S007
A	50	HIS	ARG	variant	UNP Q5S007

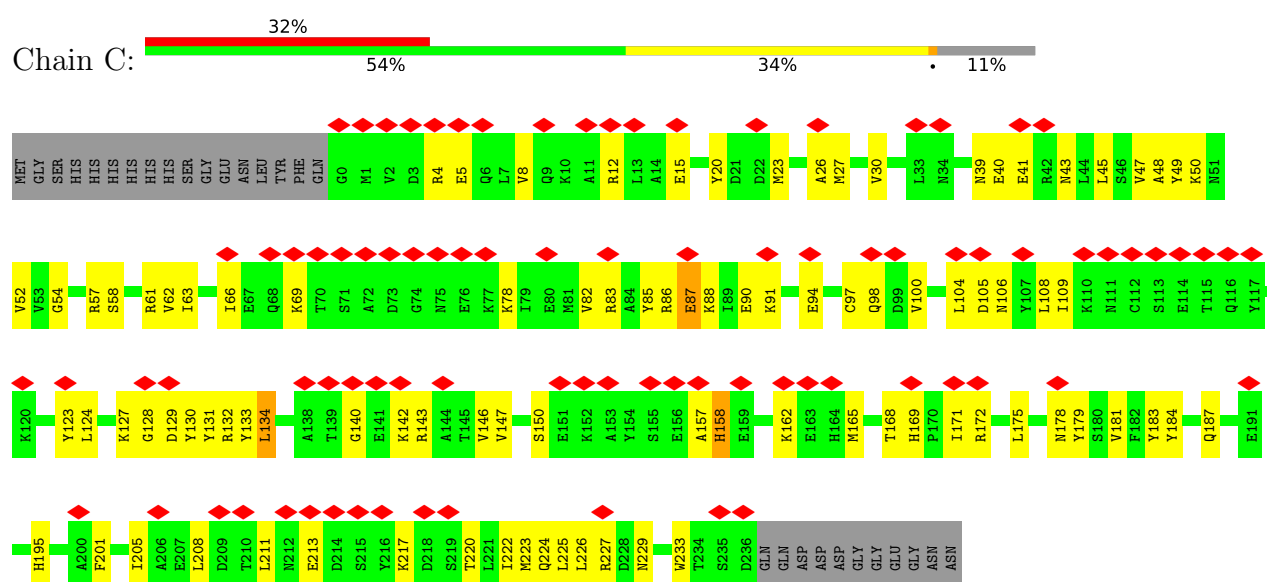
- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



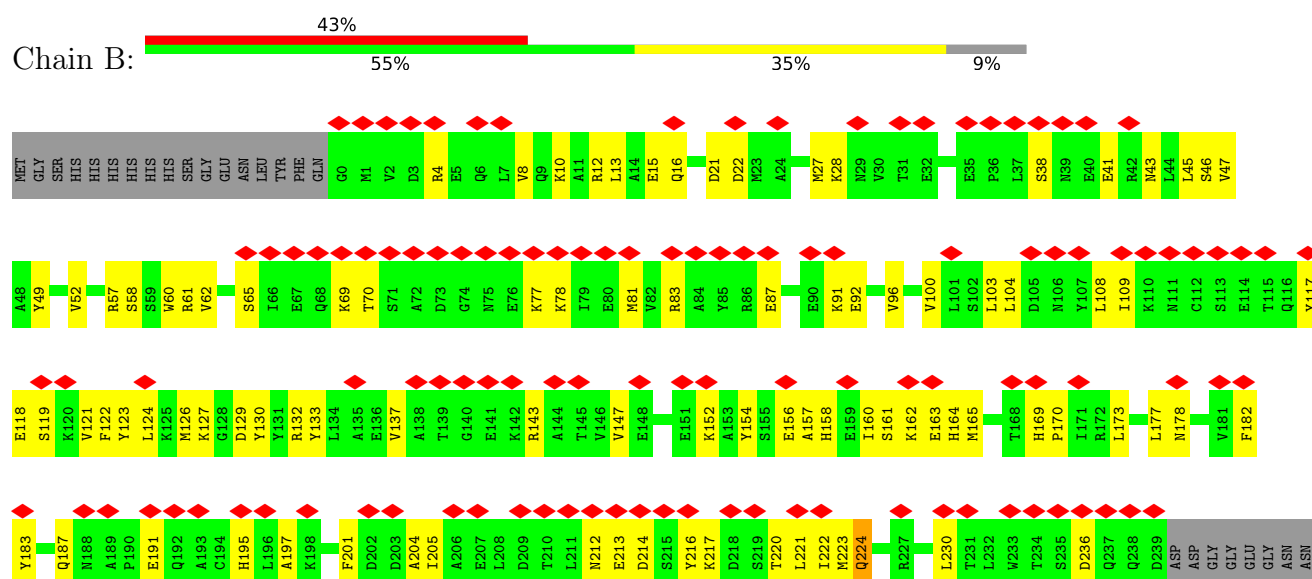
3 Residue-property plots

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: 14-3-3 protein gamma



• Molecule 1: 14-3-3 protein gamma



• Molecule 2: Leucine-rich repeat serine/threonine-protein kinase 2

T1912	D1844	L1749	D1675	I1606	S1536	GLN	W1376	F1308	L1243	M1183	N1117	F1050
S1913	D1845	V1750	H1676	M1607	E1537	ARG	P1377	K1309	W1244	K1184	K1118	P1051
L1914	P1846	H1768	R1677	A1608	R1538	K1463	I1378	H1310	S1245	F1185	I1119	S1052
R1915	R1847	L1763	I1680	I1611	K1539	K1468	R1381	I1311	R1246	S1186	G1121	Y1053
L1916		K1764	E1681	V1615	I1543	L1474	D1382	G1312	K1249	C1187	G1122	L1054
R1917		V1767	P1682	E1616	F1544	K1476	K1383	K1313	L1250	I1188	I1122	L1055
R1918		R1771	P1683	G1617	F1545	R1477	R1384	K1314	H1251	P1189	C1123	M1056
Q1919		K1772	H1684	E1618	I1548	P1480	K1385	K1315	L1252	A1190		S1058
E1920		I1775	C1686	C1618	D1549	L1482	D1387	K1316	K1258	I1192		C1059
V1922		I1776	R1686	P1619	R1550	I1481	L1388	D1317	L1257	L1194		C1059
V1923		L1777	M1687	K1620	K1551	I1482	V1389	I1319	K1259	N1194		I1060
C1925			S1688	H1621	R1552	Y1485	V1392	F1320	I1260	L1195		A1061
L1926				P1622	Q1555	V1488	F1395	L1322		P1196		N1062
L1927				K1623	L1556	N1488		Q1323	E1263	H1197		S1066
H1928				V1557	V1557	M1489	F1401	Q1324	I1264	R1198		R1067
H1929				V1558	R1558	N1490	Y1402	R1325	G1265	R1199		N1068
P1930				E1559	E1559	A1490	S1403	R1326	C1266	S1200		G1071
S1931				M1560	M1560	T1491	T1404	L1326	L1267	L1201		P1072
L1932				Q1561	Q1561	E1492	H1405	K1327	E1288	D1202		S1073
I1933				Q1562	Q1562	E1493	H1406	K1328	N1269	M1203		V1074
S1934				L1564	L1564	L1497	H1407	A1329	L1270	S1204		V1075
L1935				D1565	D1565	A1498	F1408	V1330	T1271	N1206		L1076
G1939				E1566	E1566	K1499	M1409	N1333	S1272	D1207		D1077
R1940				M1567	M1567	L1500	Y1415	R1334	L1273	R1208		P1078
P1942				P1568	P1568	R1501	L1416	M1335	Q1209	E1146		T1079
R1943				E1569	E1569	K1502	A1417	K1336	Y1210	N1147		V1080
M1944				L1569	L1569	T1503	V1418	L1337	L1211	F1148		K1081
L1945				H1574	H1574	I1504	G1424	M1338	P1212	L1149		C1082
V1946				F1575	F1575	N1506	Q1425	I1339	G1213	E1150		P1083
M1947				L1576	L1576	E1507		V1340	P1214	T1084		T1084
E1948				S1579	S1579	S1508	D1429	G1346	A1215	P1153		L1085
L1949				V1581	V1581	L1512	A1430	L1361	H1216	K1154		K1086
A1950				L1582	L1582	I1513	M1431	Q1352	W1217	V1155		Q1087
				H1583	H1583		K1432	Q1353	K1218	E1156		F1088
L1955				H1584	H1584	Q1516	P1433	L1354	S1219	S1157		S1091
R1956				F1585	F1585	L1517	W1434	M1355	L1220	F1158		Y1092
R1957				Q1586	Q1586	V1518	F1436	K1356	M1221	S1159		M1093
L1958				D1587	D1587	G1520	N1437	T1357	L1222	A1160		Q1094
L1959				P1588	P1588	Q1521	I1438	K1358	R1223	R1161		L1095
Q1960				A1589	A1589	L1522	K1439	K1359	E1224	M1162		S1096
Q1961				I1590	I1590	D1525	S1444	S1360	L1225	F1164		F1097
D1962				Q1591	Q1591	C1526	I1448	D1361	P1227	L1165		E1100
L1963				L1592	L1592	C1527	L1449	L1362	S1228	L1168		N1101
A1964				S1593	S1593	Y1527		K1293	H1229	M1169		L1102
S1965				D1594	D1594	V1528	L1454	G1363	M1230	P1170		T1103
L1966				L1595	L1595	L1530	D1455	M1364	Q1231	F1179		L1104
T1967				Y1596	Y1596	L1533	V1456	Q1365	L1232	L1171		V1105
R1968				F1597	F1597	I1534	S1457	L1297	I1234	P1172		V1106
				V1598	V1598	I1534	ASP	P1298	L1235	P1173		E1107
Q1971				E1599	E1599	L1535	GLU	L1299	D1236	S1174		K1108
H1972				W1602	W1602		LYS	D1300	L1237	M1175		T1109
R1973				L1603	L1603			E1301	D1238	I1177		L1176
T1974								S1239	E1239	L1178		E1110
A1975								K1302	H1303	L1178		L1114
L1976								L1304	N1305	K1179		E1115
H1977								F1306	Y1242	S1181		G1116
								D1307		Q1182		

L2483	H2433	Y2364	C2302	K2240	L2179	L2115	V2048	V1978
T2494	I2365	I2365	L2303	M2241	L2132	K2116	I2049	A1979
W2496	A2366	A2366	S2304	T2242	D2183	E2117	Y2050	D1980
D2497	Q2367	Q2367	E2305	T2243	L2184	N2118	N2051	R1983
N2499	Q2368	Q2368	S2306	S2244	N2185	P2119	Q2052	H1986
P2500	N2369	N2369	T2307	V2245	Q2120	E2121	Q2053	S1987
H2502	S2370	S2370	N2308	C2247	E2187	R2122	A2054	I1991
E2503	Q2376	Q2376	S2309	N2251	Y2189	G2188	D2055	Y2056
E2504	D2377	D2377	T2310	S2252	T2190	P2123	Y2057	V1992
E2505	K2378	K2378	E2311	F2253	S2191	T2124	S2058	R1993
Q2506	K2379	K2379	N2312	F2254	E2192	A2126	F2059	D1994
N2507	T2380	T2380	N2313	K2255	E2194	Q2127	G2060	L1995
E2508	E2381	E2381	V2314	Q2256	A2195	V2128	L2061	K1996
K2509	K2382	K2382	N2315	S2257	D2196	F2129	L2062	L2001
H2510	L2383	L2383	W2316	Q2258	S2197	L2132	L2067	L2002
Y2449	C2384	C2384	G2317	Q2259	R2198	L2131	G2071	P2007
N2450	G2385	G2385	C2318	Q2260	T2199	L2132	R2072	N2008
E2512	L2386	L2386	C2319	N2261	L2200	N2133	I2073	A2009
V2513	C2389	C2389	G2320	L2262	L2201	E2136	E2075	I2011
K2514	V2390	V2390	T2321	L2263	L2202	L2137	E2076	I2012
K2515	F2324	F2324	F2325	L2264	L2203	V2138	L2077	K2013
E2516	F2326	F2326	S2327	V2265	L2204	C2139	L2078	K2014
A2518	R2394	R2394	E2328	T2267	V2205	T2141	F2079	I2015
E2519	E2395	E2395	N2329	A2268	H2206	R2142	P2080	A2016
K2520	V2396	V2396	F2330	D2269	L2207	I2144	N2081	D2017
M2521	M2397	M2397	T2331	G2270	P2208	L2145	E2082	Y2018
R2522	VAL	VAL	L2332	L2271	V2209	L2146	N2084	G2019
R2523	LYS	LYS	Q2333	L2272	E2210	P2147	F2083	I2020
T2524	GLU	GLU	K2334	A2273	E2212	K2148	D2084	A2021
S2525	ASN	ASN	L2335	I2274	S2213	N2149	E2085	Q2022
V2526	LYS	LYS	T2336	F2275	W2214	V2150	L2086	Y2023
E2527	SER	SER	E2337	E2276	I2215	T2151	E2087	C2024
	LYS	LYS	T2338	D2277	V2216	E2152	I2088	C2025
	MET	MET	T2339	K2278	S2217	G2159	Q2089	R2026
	SER	SER	R2340	T2279	G2218	H2159	G2090	N2027
	TYR	TYR	S2341	V2280	T2219	H2160	K2091	GLY
	S2411	S2411	Q2342	K2281	Q2220	N2161	L2092	ILE
	G2412	G2412	L2343	L2282	G2222	S2162	P2093	LYS
	R2413	R2413	F2344	K2283	T2223	R2163	T2031	T2031
	V2414	V2414	S2345	G2284	L2224	N2164	S2032	S2032
	K2415	K2415	T2346	A2285	L2225	A2165	E2033	E2033
	T2416	T2416	A2347	A2286	V2226	S2166	G2034	G2034
	L2419	L2419	A2348	L2287	T2227	T2167	K2097	T2035
	Q2420	Q2420	F2349	L2288	N2228	W2168	Y2099	P2036
	K2421	K2421	S2350	L2290	T2229	L2169	G2100	G2037
	N2422	N2422	D2351	I2291	E2230	G2170	C2101	F2038
	T2423	T2423	S2352	N2292	D2231	C2171	A2102	R2039
	A2424	A2424	N2353	I2293	G2232	G2172	P2105	A2040
	L2425	L2425	T2354	G2294	K2233	H2173	M2106	P2041
	W2426	W2426	I2355	N2295	K2234	T2174	V2107	E2042
	I2427	I2427	T2356	V2296	R2235	R2175	E2108	V2043
	G2428	G2428	V2357	S2297	H2236	G2177	K2109	A2044
	T2429	T2429	D2360	T2298	T2237	I2111	L2110	R2045
	G2430	G2430	T2361	L2300	L2238	K2112	K2113	G2046
			A2362	M2301	E2239	Q2178	C2114	N2047
			L2363					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	2.360	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.122	Depositor
Map size (Å)	325.62, 325.62, 325.62	wwPDB
Map dimensions	402, 402, 402	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.17	0/1963	0.46	0/2648
1	C	0.17	0/1937	0.43	0/2613
2	A	0.19	0/12271	0.46	6/16603 (0.0%)
All	All	0.18	0/16171	0.46	6/21864 (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
2	A	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	938	PRO	CA-N-CD	-9.96	98.06	112.00
2	A	938	PRO	CB-CA-C	7.04	123.18	111.56
2	A	938	PRO	N-CA-CB	-6.67	96.25	103.25
2	A	2142	ARG	N-CA-C	6.30	116.77	107.88
2	A	2500	LEU	N-CA-C	5.83	122.68	109.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2142	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	B	1935	0	1898	84	0
1	C	1909	0	1878	82	0
2	A	12054	0	12234	475	0
3	A	28	0	12	0	0
All	All	15926	0	16022	626	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 626 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)
2:A:1240:LYS:HD2	2:A:1243:LEU:HD22	1.54	0.90
1:C:225:LEU:O	1:C:229:ASN:ND2	2.08	0.87
2:A:1437:ASN:HD21	2:A:1702:MET:HE3	1.37	0.86
1:C:57:ARG:NH2	2:A:935:SEP:O2P	2.11	0.84
2:A:2456:ARG:NH1	2:A:2475:TYR:OH	2.11	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	B	211/231 (91%)	209 (99%)	2 (1%)	70	76
1	C	208/231 (90%)	203 (98%)	5 (2%)	43	63
2	A	1346/2310 (58%)	1320 (98%)	26 (2%)	50	67
All	All	1765/2772 (64%)	1732 (98%)	33 (2%)	49	67

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2397	MET
2	A	2436	LEU
2	A	2500	LEU
2	A	1192	ILE
2	A	1175	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	1854	GLN
2	A	2420	GLN
2	A	2506	ASN
2	A	1986	HIS
2	A	1068	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SEP	A	910	2	8,9,10	1.60	1 (12%)	7,12,14	1.30	1 (14%)
2	SEP	A	935	2	8,9,10	1.57	1 (12%)	7,12,14	1.52	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	A	910	2	-	1/6/8/10	-
2	SEP	A	935	2	-	5/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	935	SEP	P-O1P	3.47	1.61	1.50
2	A	910	SEP	P-O1P	3.47	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	935	SEP	OG-CB-CA	3.57	111.62	108.14
2	A	910	SEP	OG-CB-CA	2.88	110.94	108.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	935	SEP	N-CA-CB-OG
2	A	935	SEP	C-CA-CB-OG
2	A	935	SEP	CB-OG-P-O1P
2	A	935	SEP	CB-OG-P-O2P
2	A	935	SEP	CB-OG-P-O3P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	910	SEP	3	0
2	A	935	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GDP	A	2601	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	A	2601	-	-	2/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	GDP	C5-C4	3.12	1.47	1.38
3	A	2601	GDP	C6-N1	-2.36	1.34	1.38
3	A	2601	GDP	C5-N7	-2.18	1.34	1.39

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	GDP	C5-C4-N3	-6.28	118.40	128.39
3	A	2601	GDP	C2-N3-C4	5.12	121.12	112.30
3	A	2601	GDP	N9-C4-N3	4.57	135.09	125.95
3	A	2601	GDP	C6-C5-N7	3.21	136.14	130.29
3	A	2601	GDP	C4-C5-N7	-2.65	106.47	110.67

There are no chirality outliers.

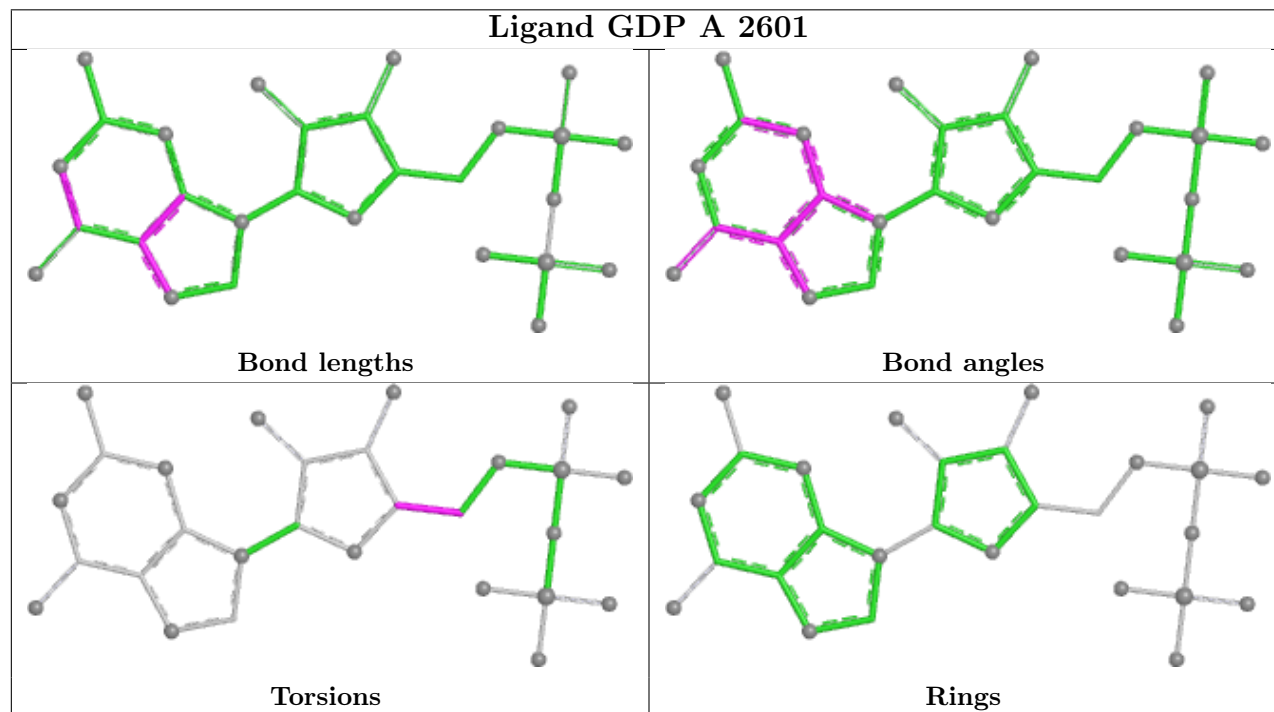
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2601	GDP	O4'-C4'-C5'-O5'
3	A	2601	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

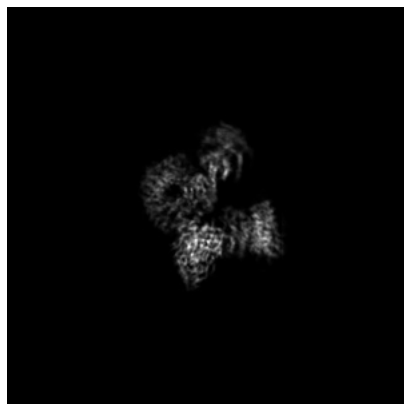
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45609. These allow visual inspection of the internal detail of the map and identification of artifacts.

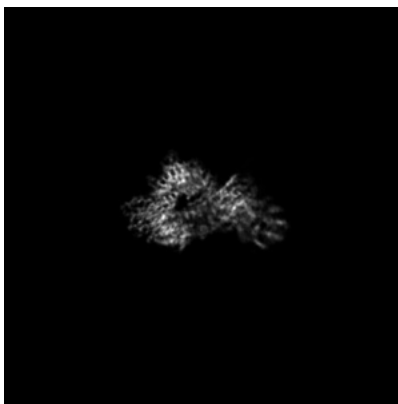
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

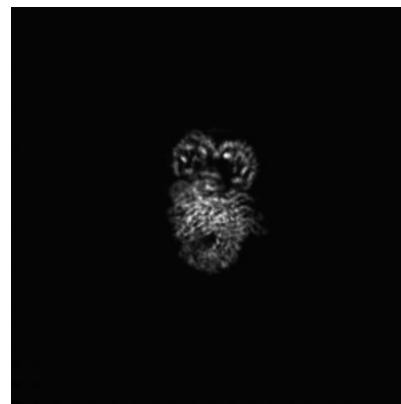
6.1.1 Primary map



X

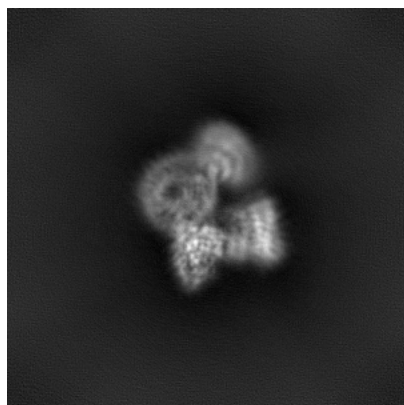


Y

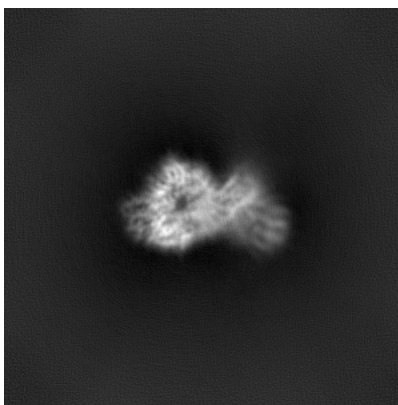


Z

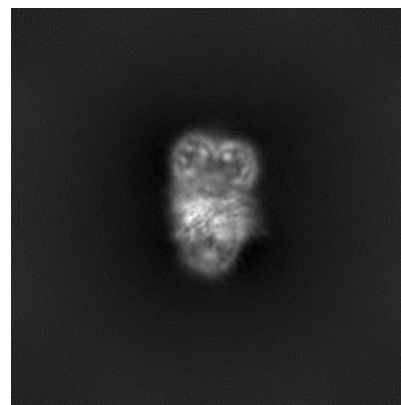
6.1.2 Raw map



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: 201

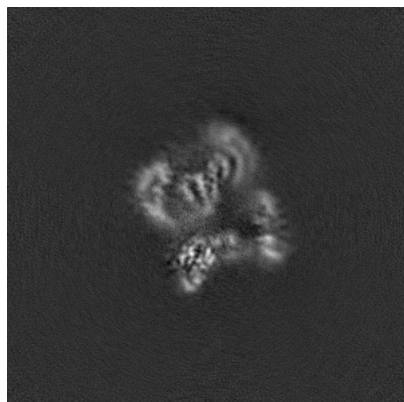


Y Index: 201

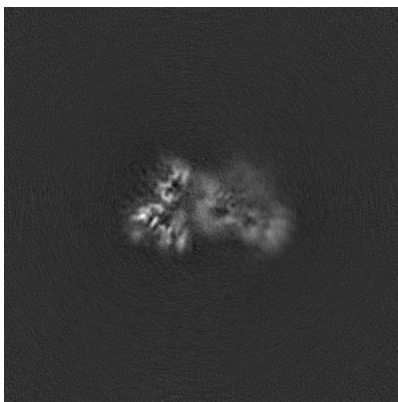


Z Index: 201

6.2.2 Raw map



X Index: 201



Y Index: 201



Z Index: 201

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

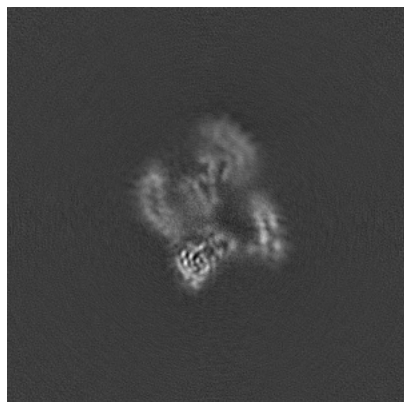


Y Index: 189

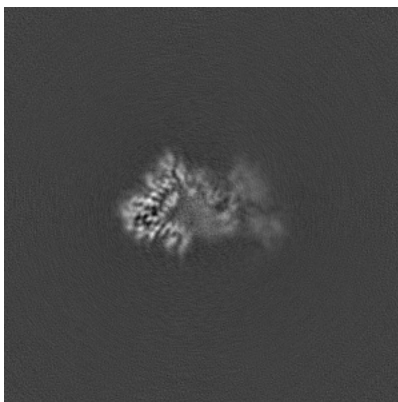


Z Index: 167

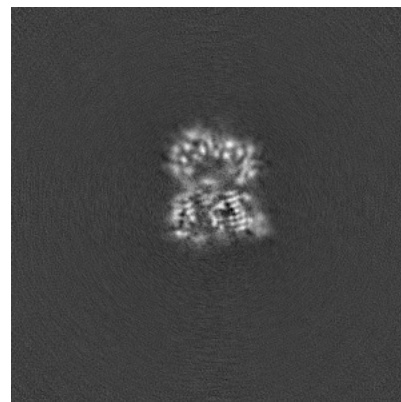
6.3.2 Raw map



X Index: 193



Y Index: 189

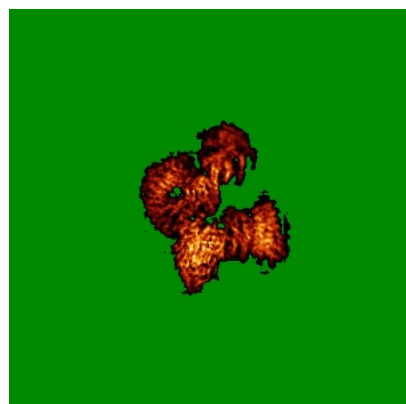


Z Index: 166

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

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

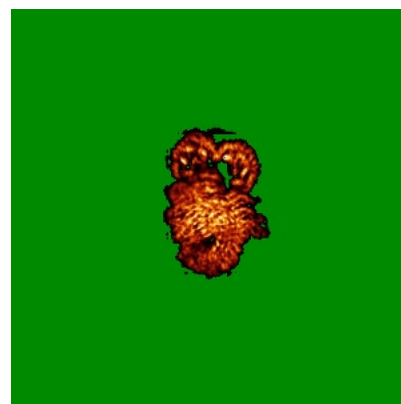
6.4.1 Primary map



X

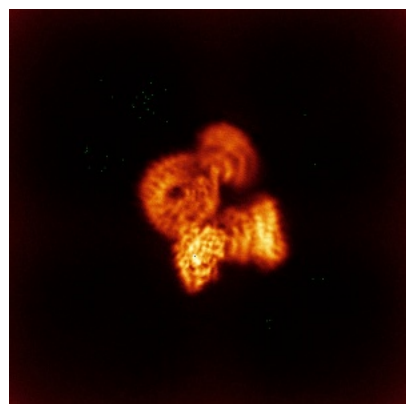


Y

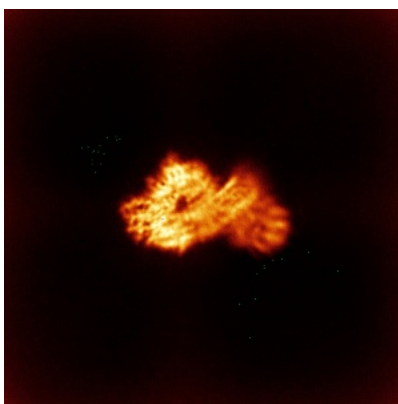


Z

6.4.2 Raw map



X



Y

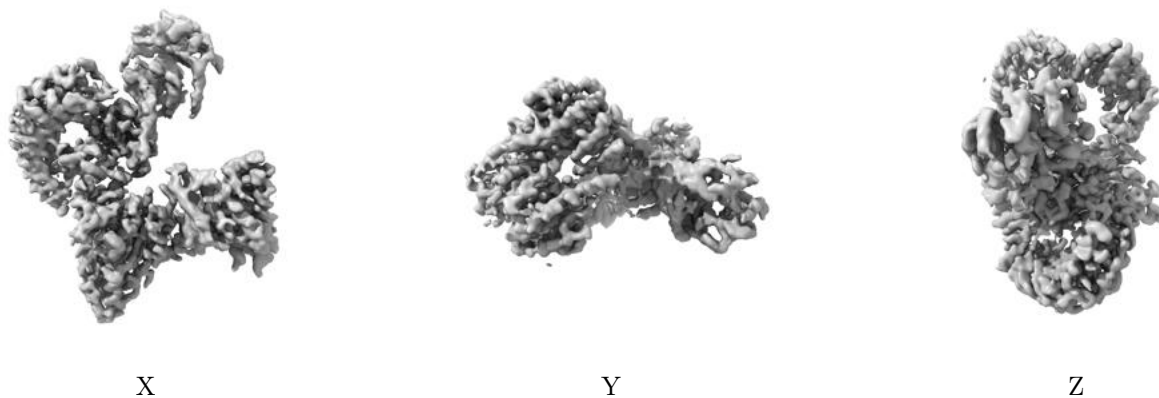


Z

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

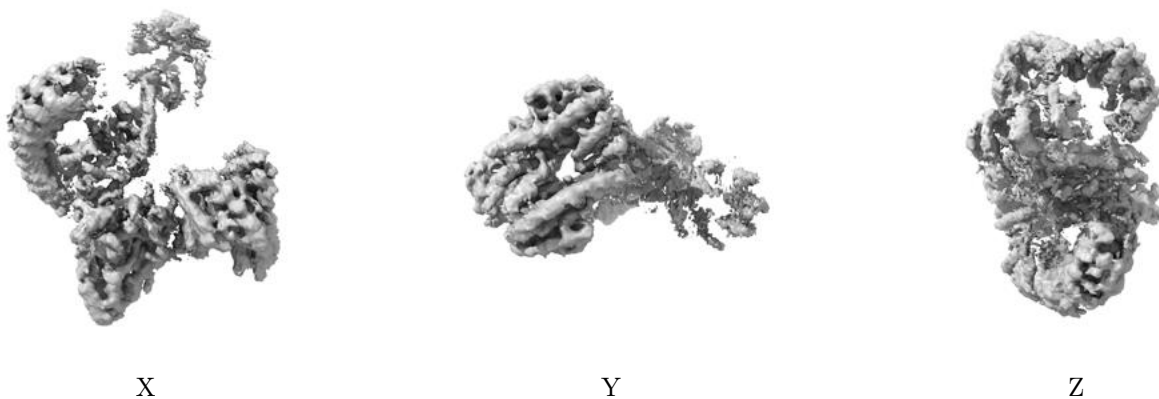
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.122. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

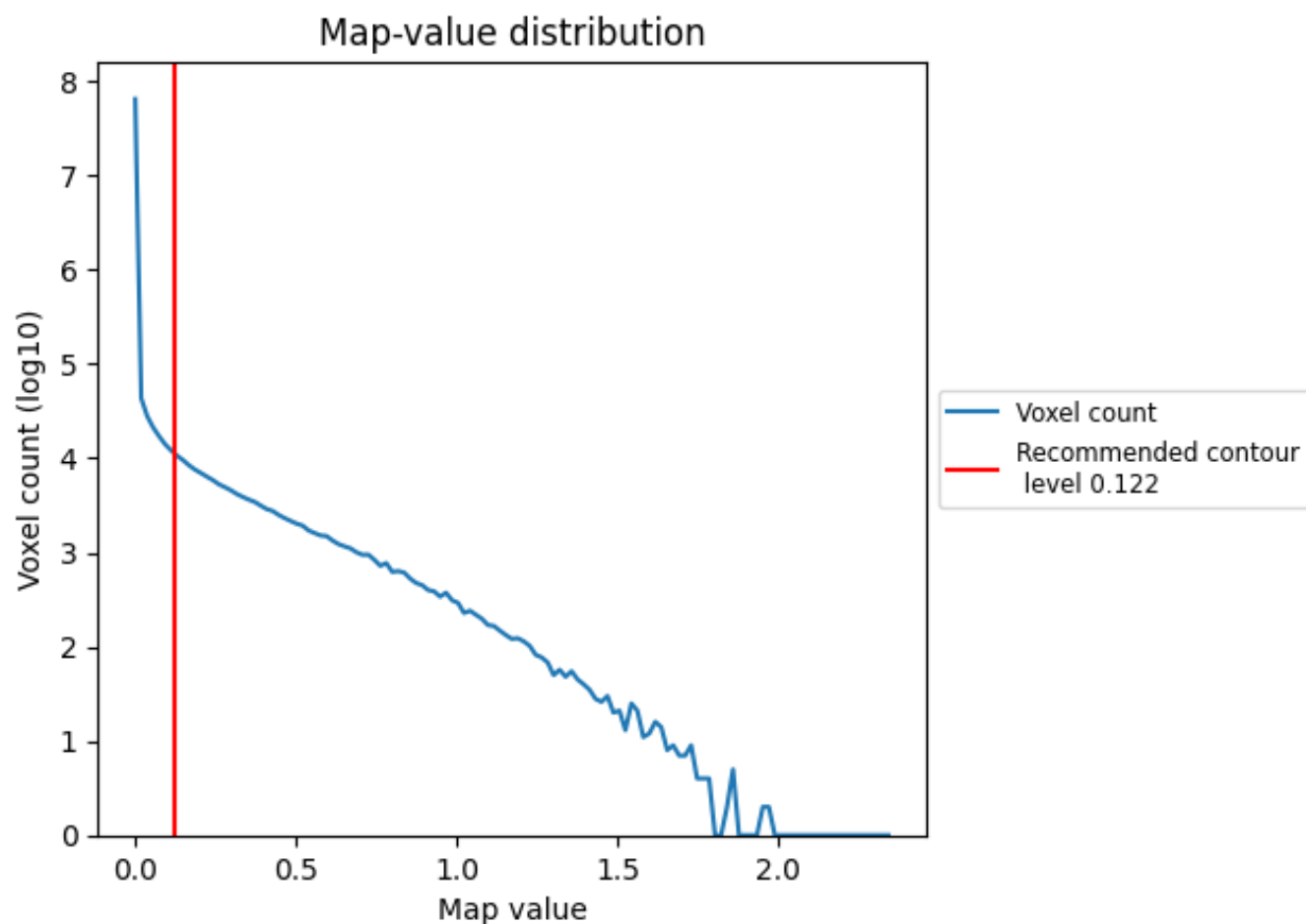
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

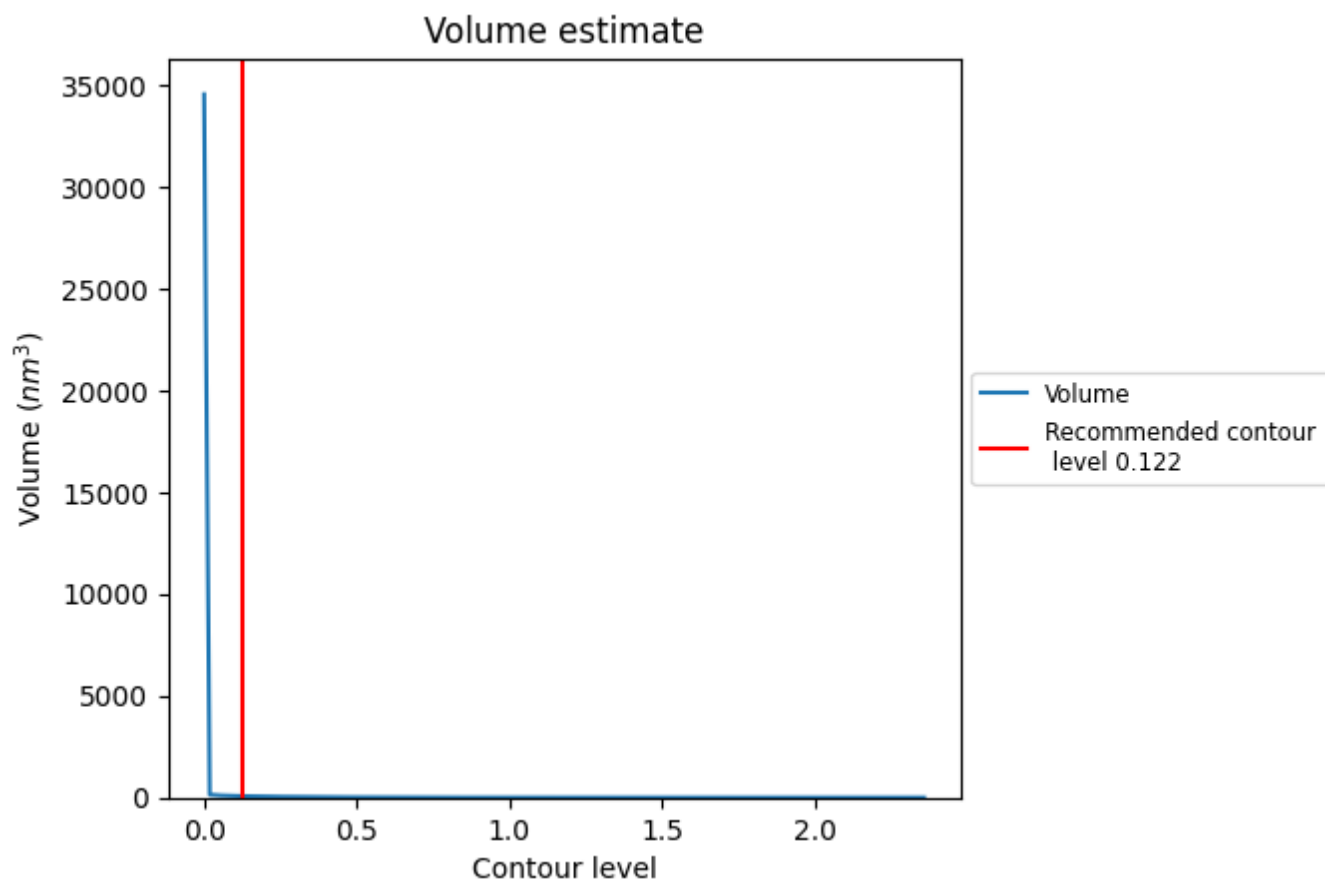
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

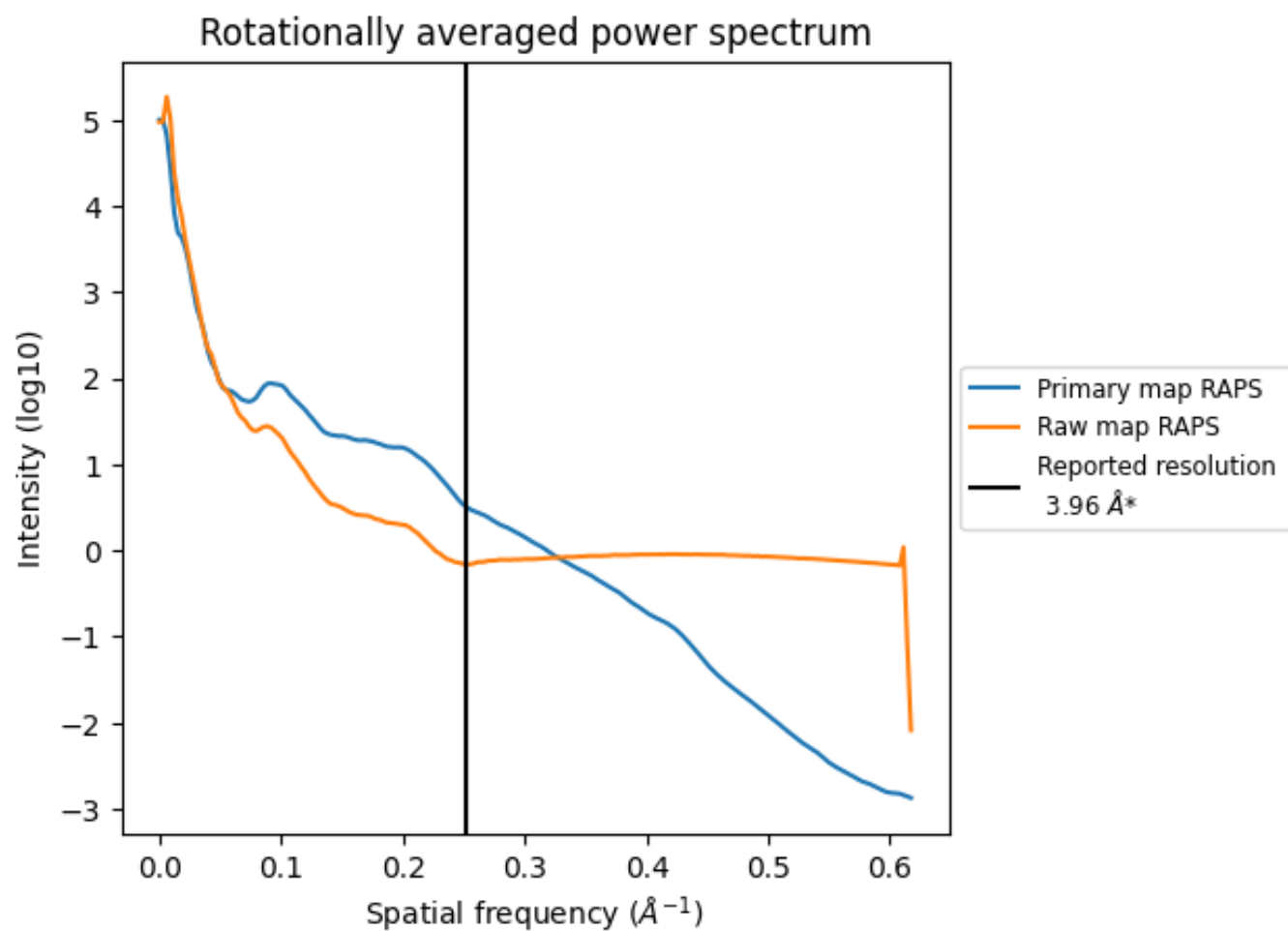
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm³; this corresponds to an approximate mass of 64 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 ⓘ

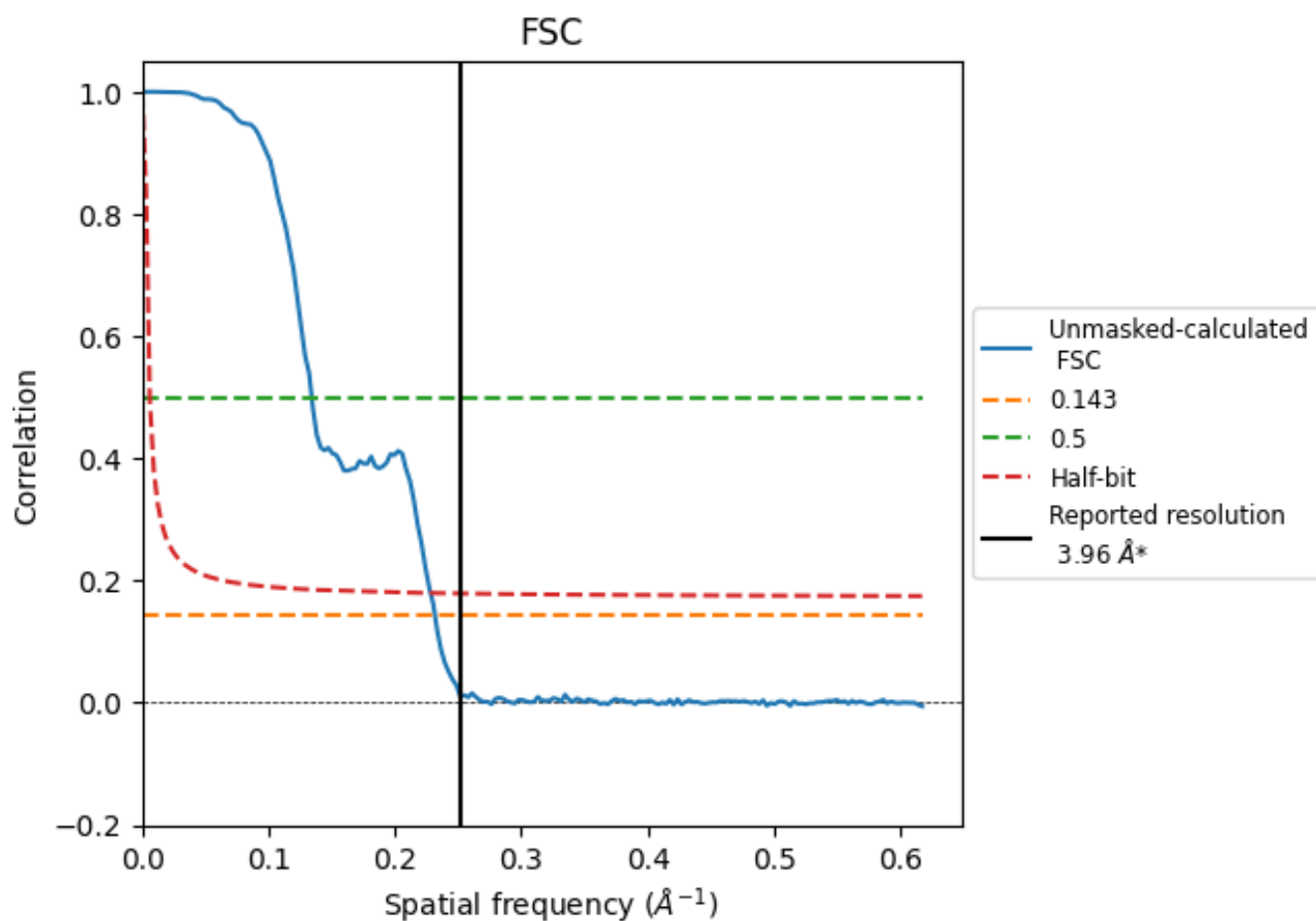


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

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 0.253 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.32	7.45	4.38

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

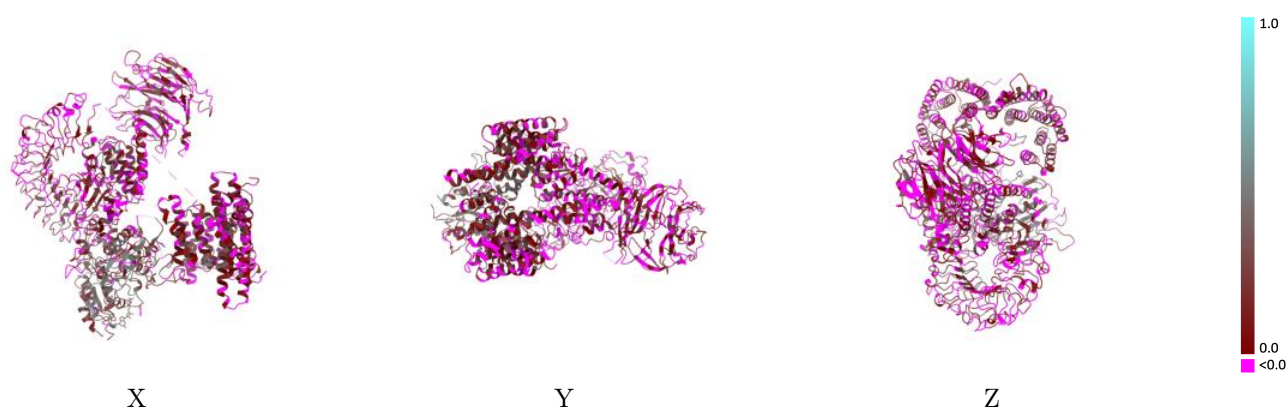
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45609 and PDB model 9CI3. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

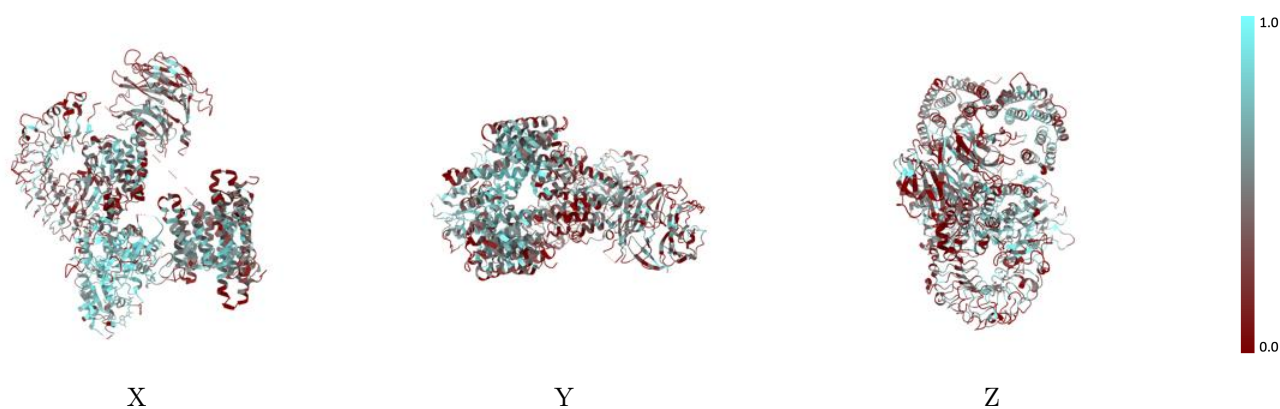
This section was not generated.

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



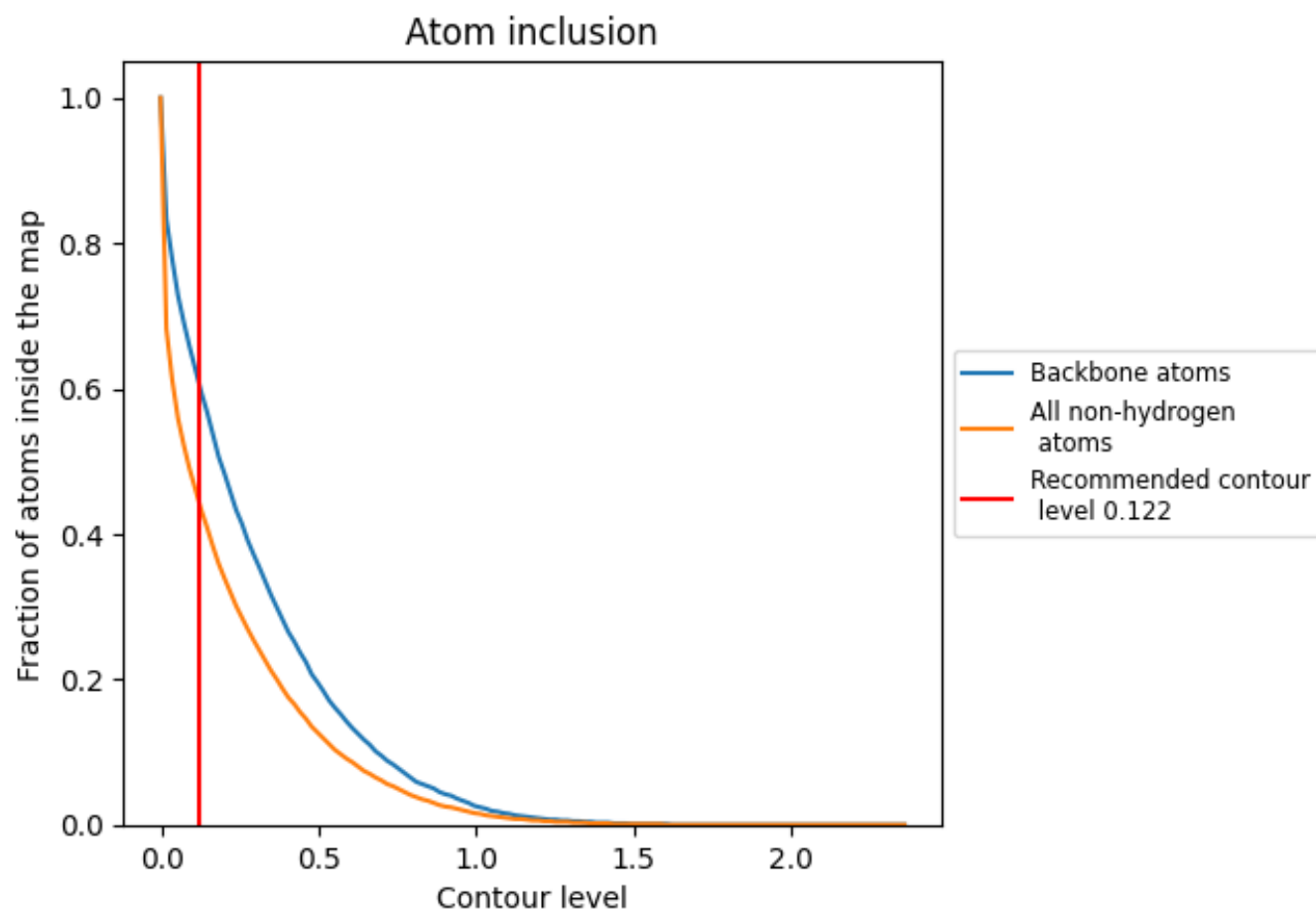
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.122).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 44% 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 (0.122) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4410	<div></div> 0.1120
A	<div></div> 0.4380	<div></div> 0.1170
B	<div></div> 0.3980	<div></div> 0.0800
C	<div></div> 0.5030	<div></div> 0.1170

