



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 05:35 pm GMT

PDB ID : 6ZH2
EMDB ID : EMD-11211
Title : Cryo-EM structure of DNA-PKcs (State 1)
Authors : Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2020-06-20
Resolution : 3.92 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

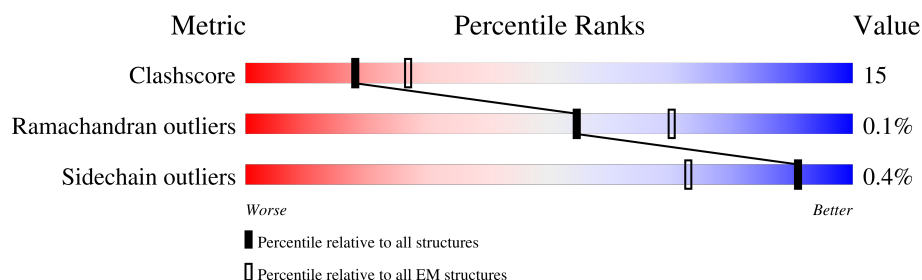
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.92 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	4156	

i

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.

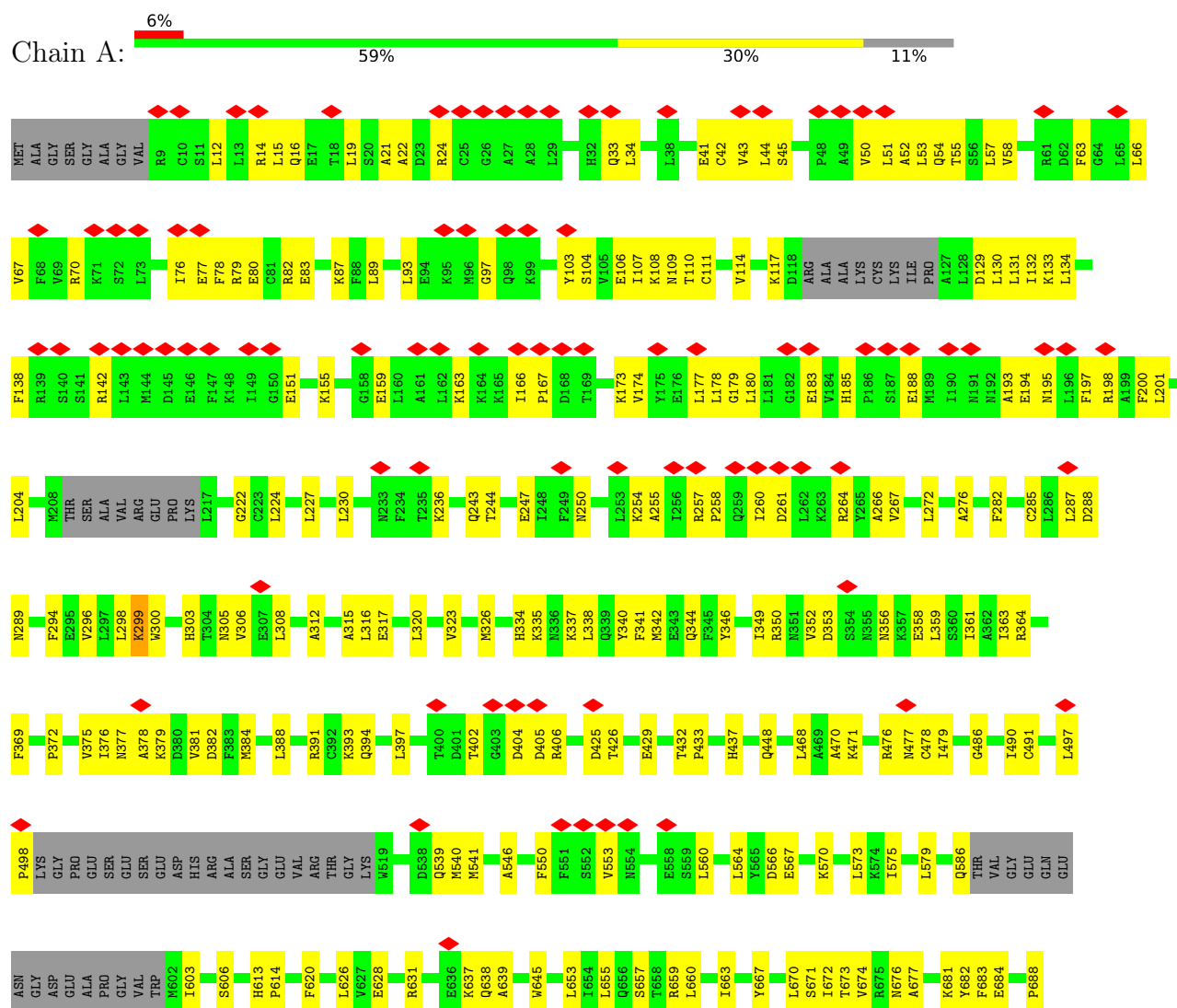
- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit,DNA-depen
dent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA
-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subuni
t,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic
subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3704	Total	C	N	O	S	0	0
			29313	18814	4959	5348	192		

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,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs



I1867	I1868	K1869	K1870	Y1873	Y1874	K1875	I1876	I1877	V1879	M1880	R1883	L1884	P1885	K1886	D1887	D1888	H1889	K1891	K1892	E1893	S1894	K1895	V1899	F1900	H1901	C1904	I1905	T1906	E1907	N1909	E1910	L1911	K1913	T1914	L1915	I1916	K1917	L1918	C1919	Y1920	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938				
G1768	G1769	S1790	C1791	V1792	Q1794	L1797	V1801	F1805	D1809	P1810	S1813	R1816	R1822	L1825	L1828	H1830	C1831	S1832	L1833	D1834	A1835	E1838	F1839	S1841	T1842	I1843	A1847	L1848	L1851	K1852	S1853	R1854	F1855	T1856	K1857	L1858	N1859	E1860	T1862	S1861	F1863	D1864	T1865	Q1866	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938
Q1691	A1692	T1693	V1694	L1695	L1696	T1700	T1703	G1704	L1707	E1708	E1709	L1710	R1711	H1712	V1713	L1714	E1715	I1718	M1724	E1728	G1732	R1735	F1736	M1737	M1743	F1746	L1747	S1753	Q1754	M1762	L1766	Q1770	Q1771	H1772	E1775	F1778	Q1779	R1783	I1784	I1785	A1786	R1787	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
L1582	S1585	S1586	V1587	D1588	N1589	L1601	E1607	R1608	A1609	M1610	Q1611	K1612	H1613	Q1614	K1617	L1623	K1627	W1632	K1635	D1636	S1637	P1638	L1639	E1640	T1641	K1642	M1643	L1646	K1651	S1657	S1658	V1659	S1660	T1663	S1664	G1666	F1668	P1669	E1670	F1672	D1685	G1690	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
S1478	V1479	E1482	S1485	L1486	Y1487	Y1488	I1491	A1492	F1493	G1494	D1495	E1496	L1497	Q1498	C1499	S1502	L1503	D1504	L1505	S1512	G1513	L1514	E1516	G1523	V1529	S1530	L1531	L1532	A1541	SER	LEU	GLY	SER	GLN	SER	GLY	V1550	L1572	L1575	A1578														
D1388	Q1389	Q1390	V1391	M1392	L1395	P1396	D1397	V1398	M1401	K1404	K1407	P1410	Y1411	K1412	D1413	I1414	L1415	E1416	T1417	H1418	L1419	R1420	E1421	K1422	S1427	E1430	Y1437	G1438	P1439	Q1442	V1443	D1444	R1445	S1446	R1447	L1448	A1449	V1452	L1463	S1470	Q1471	S1472	T1473	D1474	L1475	H1477								
A1308	A1309	I1310	K1311	C1312	PHE	T1315	G1316	A1317	A1318	G1319	N1320	A1321	T1322	S1323	P1324	Q1325	E1326	E1327	E1328	K1334	V1338	V1339	R1340	I1341	M1342	L1348	T1351	S1352	P1353	W1356	K1357	L1358	L1359	D1362	H1367	L1368	M1369	R1370	V1371	L1372	V1373	E1378	F1379	A1380	S1381	I1382	I1385	I1386	G1387					
F1082	I1085	Y1086	R1087	R1090	E1091	V1100	F1101	E1102	V1105	I1106	M1107	M1108	F1109	K1099	K1000	Q1004	D1005	T1006	V1007	L1010	I1013	I1017	V1018	D1019	P1020	V1021	D1022	R1026	R1031	W1039	K1042	Y1064	A1067	H1069	N1071	A1072	F1073	K1074	R1075	L1080	A1081													
F1219	L1220	N1221	T1223	F1224	E1225	Q1231	S1233	G1234	L1235	L1236	A1237	Q1238	Y1243	L1244	R1245	G1246	P1247	F1248	S1249	L1250	Q1251	T1253	L1259	L1260	L1261	L1264	Y1267	V1281	L1282	G1283	T1294	E1285	A1286	Q1287	S1288	S1289	L1290	L1291	K1292	F1297	L1298	E1299	S1300	I1301	A1302	M1303	H1304	I1307						
A1308	A1309	I1310	K1311	C1312	PHE	T1315	G1316	A1317	A1318	G1319	N1320	A1321	T1322	S1323	P1324	Q1325	E1326	E1327	E1328	K1334	V1338	V1339	R1340	I1341	M1342	L1348	T1351	S1352	P1353	W1356	K1357	L1358	L1359	D1362	H1367	L1368	M1369	R1370	V1371	L1372	V1373	E1378	F1379	A1380	S1381	I1382	I1385	I1386	G1387					
D1388	Q1389	Q1390	V1391	M1392	L1395	P1396	D1397	V1398	M1401	K1404	K1407	P1410	Y1411	K1412	D1413	I1414	L1415	E1416	T1417	H1418	L1419	R1420	E1421	K1422	S1427	E1430	Y1437	G1438	P1439	Q1442	V1443	D1444	R1445	S1446	R1447	L1448	A1449	V1452	L1463	S1470	Q1471	S1472	T1473	D1474	L1475	H1477								
S1478	V1479	E1482	S1485	L1486	Y1487	Y1488	I1491	A1492	F1493	G1494	D1495	E1496	L1497	Q1498	C1499	S1502	L1503	D1504	L1505	S1512	G1513	L1514	E1516	G1523	V1529	S1530	L1531	L1532	A1541	SER	LEU	GLY	SER	GLN	SER	GLY	V1550	L1572	L1575	A1578														
L1582	S1585	S1586	V1587	D1588	N1589	L1601	E1607	R1608	A1609	M1610	Q1611	K1612	H1613	Q1614	K1617	L1623	K1627	W1632	K1635	D1636	S1637	P1638	L1639	E1640	T1641	K1642	M1643	L1646	K1651	S1657	S1658	V1659	S1660	T1663	S1664	G1666	F1668	P1669	E1670	F1672	D1685	G1690	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
Q1691	A1692	T1693	V1694	L1695	L1696	T1700	T1703	G1704	L1707	E1708	E1709	L1710	R1711	H1712	V1713	L1714	E1715	I1718	M1724	E1728	G1732	R1735	F1736	M1737	M1743	F1746	L1747	S1753	Q1754	M1762	L1766	Q1770	Q1771	H1772	E1775	F1778	Q1779	R1783	I1784	I1785	A1786	R1787	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
L1582	S1585	S1586	V1587	D1588	N1589	L1601	E1607	R1608	A1609	M1610	Q1611	K1612	H1613	Q1614	K1617	L1623	K1627	W1632	K1635	D1636	S1637	P1638	L1639	E1640	T1641	K1642	M1643	L1646	K1651	S1657	S1658	V1659	S1660	T1663	S1664	G1666	F1668	P1669	E1670	F1672	D1685	G1690	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
Q1691	A1692	T1693	V1694	L1695	L1696	T1700	T1703	G1704	L1707	E1708	E1709	L1710	R1711	H1712	V1713	L1714	E1715	I1718	M1724	E1728	G1732	R1735	F1736	M1737	M1743	F1746	L1747	S1753	Q1754	M1762	L1766	Q1770	Q1771	H1772	E1775	F1778	Q1779	R1783	I1784	I1785	A1786	R1787	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
L1582	S1585	S1586	V1587	D1588	N1589	L1601	E1607	R1608	A1609	M1610	Q1611	K1612	H1613	Q1614	K1617	L1623	K1627	W1632	K1635	D1636	S1637	P1638	L1639	E1640	T1641	K1642	M1643	L1646	K1651	S1657	S1658	V1659	S1660	T1663	S1664	G1666	F1668	P1669	E1670	F1672	D1685	G1690	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
Q1691	A1692	T1693	V1694	L1695	L1696	T1700	T1703	G1704	L1707	E1708	E1709	L1710	R1711	H1712	V1713	L1714	E1715	I1718	M1724	E1728	G1732	R1735	F1736	M1737	M1743	F1746	L1747	S1753	Q1754	M1762	L1766	Q1770	Q1771	H1772	E1775	F1778	Q1779	R1783	I1784	I1785	A1786	R1787	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
L1582	S1585	S1586	V1587	D1588	N1589	L1601	E1607	R1608	A1609	M1610	Q1611	K1612	H1613	Q1614	K1617	L1623	K1627	W1632	K1635	D1636	S1637	P1638	L1639	E1640	T1641	K1642	M1643	L1646	K1651	S1657	S1658	V1659	S1660	T1663	S1664	G1666	F1668	P1669	E1670	F1672	D1685	G1690	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
Q1691	A1692	T1693	V1694	L1695	L1696	T1700	T1703	G1704	L1707	E1708	E1709	L1710	R1711	H1712	V1713	L1714	E1715	I1718	M1724	E1728	G1732	R1735	F1736	M1737	M1743	F1746	L1747	S1753	Q1754	M1762	L1766	Q1770	Q1771	H1772	E1775	F1778	Q1779	R1783	I1784	I1785	A1786	R1787	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
L1582	S1585	S1586	V1587	D1588	N1589	L1601	E1607	R1608	A1609	M1610	Q1611	K1612	H1613	Q1614	K1617	L1623	K1627	W1632	K1635	D1636	S1637	P1638	L1639	E1640	T1641	K1642	M1643	L1646	K1651	S1657	S1658	V1659	S1660	T1663	S1664	G1666	F1668	P1669	E1670	F1672	D1685	G1690	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
Q1691	A1692	T1693	V1694	L1695	L1696	T1700	T1703	G1704	L1707	E1708	E1709	L1710	R1711	H1712	V1713	L1714	E1715	I1718	M1724	E1728	G1732	R1735	F1736	M1737	M1743	F1746	L1747	S1753	Q1754	M1762	L1766	Q1770	Q1771	H1772	E1775	F1778	Q1779	R1783	I1784	I1785	A1786	R1787	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
L1582	S1585	S1586	V1587	D1588	N1589	L1601	E1607	R1608	A1609	M1610	Q1611	K1612	H1613	Q1614	K1617	L1623	K1627	W1632	K1635	D1636	S1637	P1638	L1639	E1640	T1641	K1642	M1643	L1646	K1651	S1657	S1658	V1659	S1660	T1663	S1664	G1666	F1668	P1669	E1670	F1672	D1685	G1690	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
Q1691	A1692	T1693	V1694	L1695	L1696	T1700	T1703	G1704	L1707	E1708	E1709	L1710	R1711	H1712	V1713	L1714	E1715	I1718	M1724	E1728	G1732	R1735	F1736	M1737	M1743	F1746	L1747	S1753	Q1754	M1762	L1766	Q1770	Q1771	H1772	E1775	F1778	Q1779	R1783	I1784	I1785	A1786	R1787	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
L1582	S1585	S1586	V1587	D1588	N1589	L1601	E1607	R1608	A1609	M1610	Q1611	K1612	H1613	Q1614	K1617	L1623	K1627	W1632	K1635	D1636	S1637	P1638	L1639	E1640	T1641	K1642	M1643	L1646	K1651	S1657	S1658	V1659	S1660	T1663	S1664	G1666	F1668	P1669	E1670	F1672	D1685	G1690	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
Q1691	A1692	T1693	V1694	L1695	L1696	T1700	T1703	G1704	L1707	E1708	E1709	L1710	R1711	H1712	V1713	L1714	E1715	I1718	M1724	E1728	G1732	R1735	F1736	M1737	M1743	F1746	L1747	S1753	Q1754	M1762	L1766	Q1770	Q1771	H1772	E1775	F1778	Q1779	R1783	I1784	I1785	A1786	R1787	A1928	G1929	E1930	Q1932	L1933	L1934	E1935	R1936	R1937	R1938		
L1582	S1585	S1586	V1587	D1588	N1589	L1601	E1607	R1608	A1609																																													



W4127	K4020	Q3704	P3690	T3545	K3449	R3358	L3262	I3182
W4128	L4021	Y3705	K3621	S3546	K3450	I3359	D3270	I3183
X5009	K4022	D3706	A3622	T3547	G3548	L3360	V3274	R3186
X6017	G4025	G3707	G3626	H3549	K3455	L3362	V3277	L3190
X6020	S4026	R3708	G3626	K3550	N3459	G3363	C3281	S3191
	W4027	K3710	R3629	K3551	R3462	G3364		K3192
	I4028	P3711	E3552	K3552	K3463	S3365		
	Q4029	L3712	E3553	E3553	F3465	S3366		
	E4030	P3713	R3557	R3557	L3468	S3367		
	I4031	H3716	K3561	K3561	L3472	E3368		
	N4032	I3719	K3562	K3562	E3473	E3371		
	V4033	D3723	G3638	L3562	R3474	R3380		
	A4034	E3724	H3643	G3564	Y3475	L3385		
	E4035	R3733	R3653	Q3565		S3386		
	K4036	R3737	K3654	I3568		V3389		
	K4050	R3737	K3655	F3571		L3298		
	A4054	E3747	L3656	L3575		V3300		
	W4055	D3757	S3657	L3578		L3301		
	P4056	R3763	D3658	K3579		K3302		
	I4059	I3774	P3659	P3580		T3303		
	L4064	D3776	L3666	P3581		L3306		
	L4065	D3778	L3667	L3582		L3309		
	F4074	S3779	K3669	L3583		E3309		
	R4075	A3780	K3670	V3588		W3310		
	D4076	C3781	K3671	S3589		S3314		
	Y4077	S3782	K3672	V3592		N3319		
	G4083	L3786	S3673	R3593		I3320		
	S4084	K3675	S3674	A3594		L3321		
	K4085	P3676	K3675	E3595		F3323		
	D4086	V3794	P3677	L3596		S3228		
	H4087	R3799	G3677	A3597		R3329		
	N4088	L3802	N3678	K3598		I3326		
	I4089	E3807	L3680	T3599		K3240		
	R4090	N3808	K3681	P3600		K3241		
	A4091	T3809	C3683	V3601		K3242		
	Q4092	T3819	P3684	N3602		I3243		
	E4100	T3819	P3685	K3603		L3254		
	Q4103	E3838	N3686	K3604		A3255		
	L4107	Y3839	K3687	N3605		K3256		
	Q4110	K3845	F3694	I3606		K3257		
	D4113	K3849	L3695	E3607		L3258		
	P4114	H3850	R3696	K3608		L3259		
	N4115	D3851	N3697	M3609				
	I4116	Y3855	E3610	P3532				
	F4005		E3611	T3535				
			R3612	T3536				
			M3613	F3542				
			A3616	D3544				
			D3619					
			G3703					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38575	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.95	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.199	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	280.36002, 280.36002, 280.36002	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.652, 0.652, 0.652	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	0.27	0/29777	0.44	0/40278

There are no bond length outliers.

There are no bond angle outliers.

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	29313	0	29356	863	0
All	All	29313	0	29356	863	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 15.

The worst 5 of 863 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:3472:ILE:HA	1:A:3479:THR:HG21	1.22	1.15
1:A:3472:ILE:HG23	1:A:3479:THR:HB	1.38	1.02
1:A:3472:ILE:HA	1:A:3479:THR:CG2	1.93	0.98
1:A:2085:MET:N	1:A:2184:TYR:HH	1.76	0.84
1:A:3475:TYR:HB3	1:A:3478:GLU:OE2	1.77	0.84

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	3640/4156 (88%)	3354 (92%)	284 (8%)	2 (0%)	51 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3480	LEU
1	A	2787	HIS

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	3203/3671 (87%)	3190 (100%)	13 (0%)	91 94

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2283	ASN
1	A	2356	MET
1	A	3696	ARG
1	A	3478	GLU
1	A	3638	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	1611	GLN
1	A	3139	GLN
1	A	4092	GLN
1	A	356	ASN
1	A	334	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	5009:UNK	N	93.18

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	5016:UNK	C	6001:UNK	N	48.96

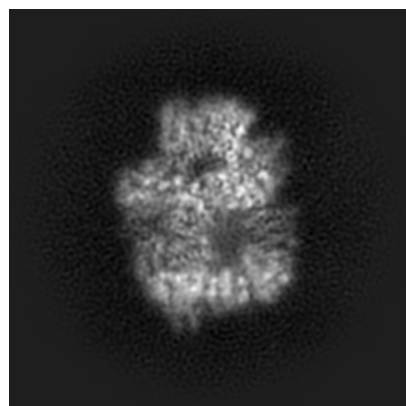
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11211. These allow visual inspection of the internal detail of the map and identification of artifacts.

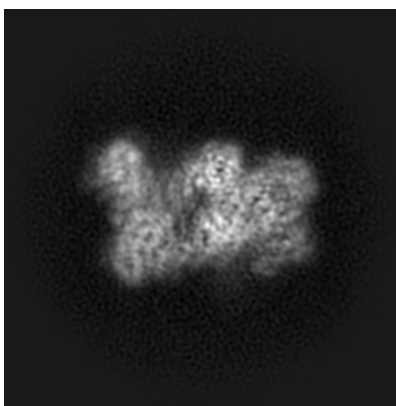
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

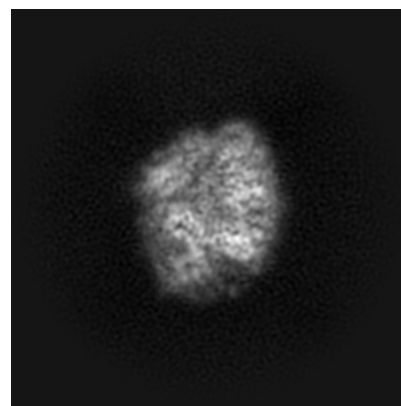
6.1.1 Primary map



X

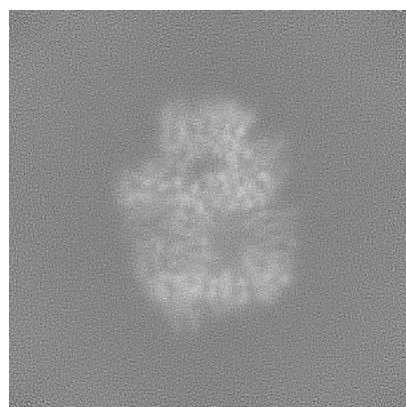


Y

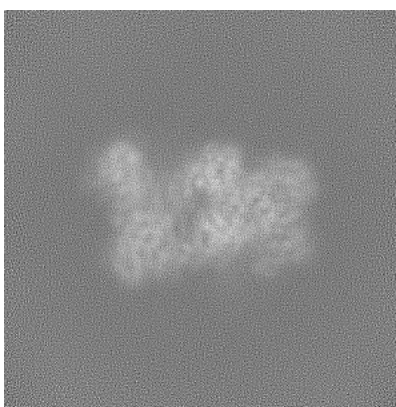


Z

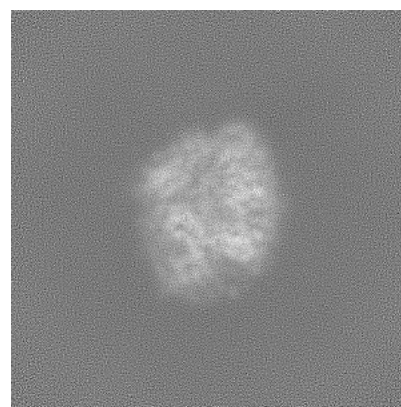
6.1.2 Raw map



X



Y

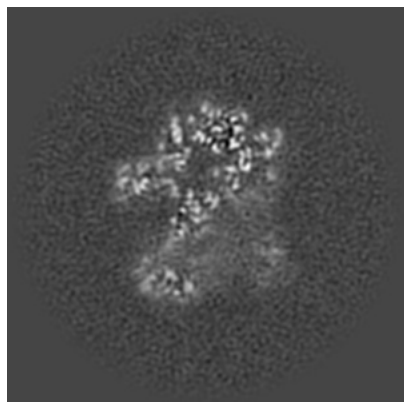


Z

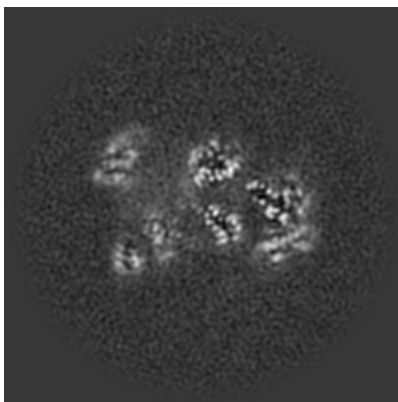
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

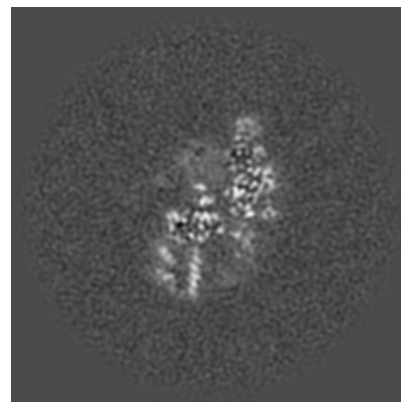
6.2.1 Primary map



X Index: 215

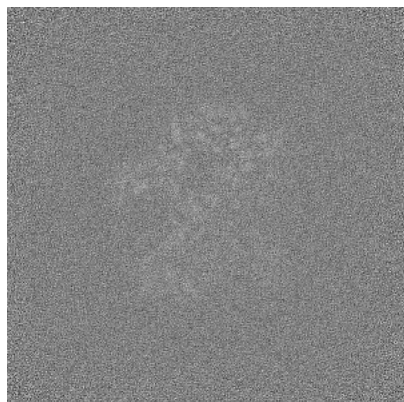


Y Index: 215

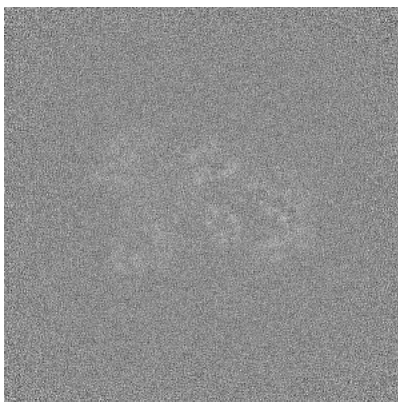


Z Index: 215

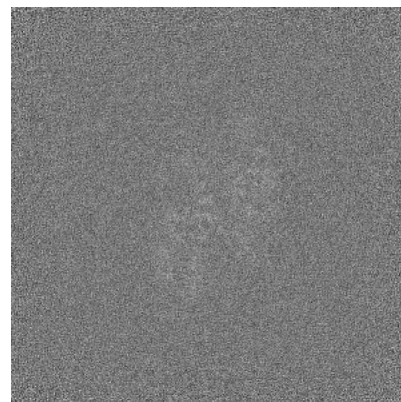
6.2.2 Raw map



X Index: 215



Y Index: 215

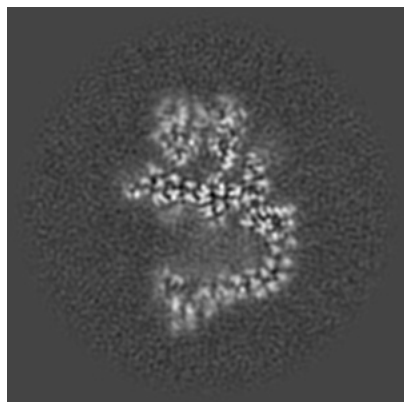


Z Index: 215

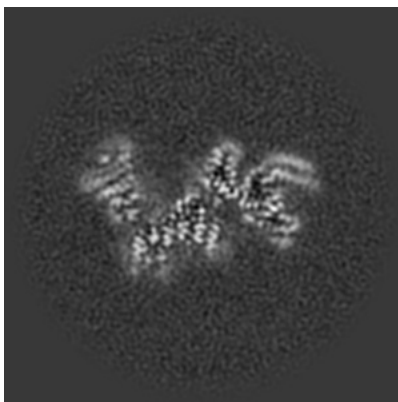
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

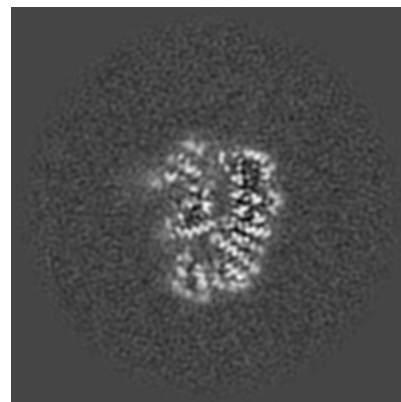
6.3.1 Primary map



X Index: 246

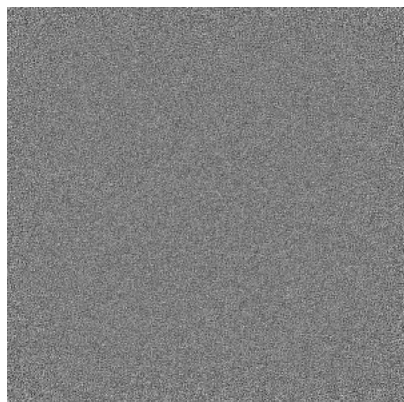


Y Index: 185

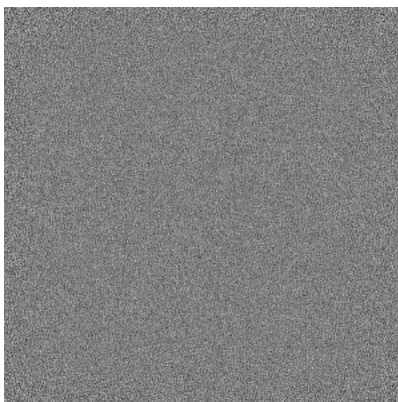


Z Index: 228

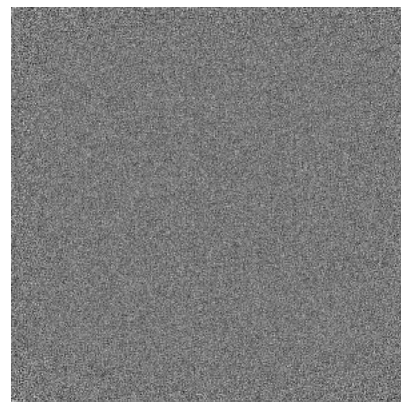
6.3.2 Raw map



X Index: 0



Y Index: 0

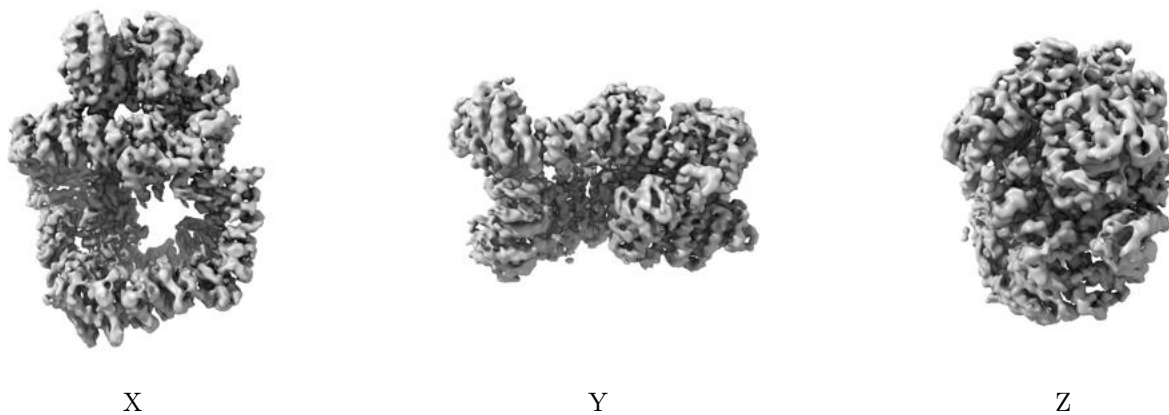


Z Index: 0

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

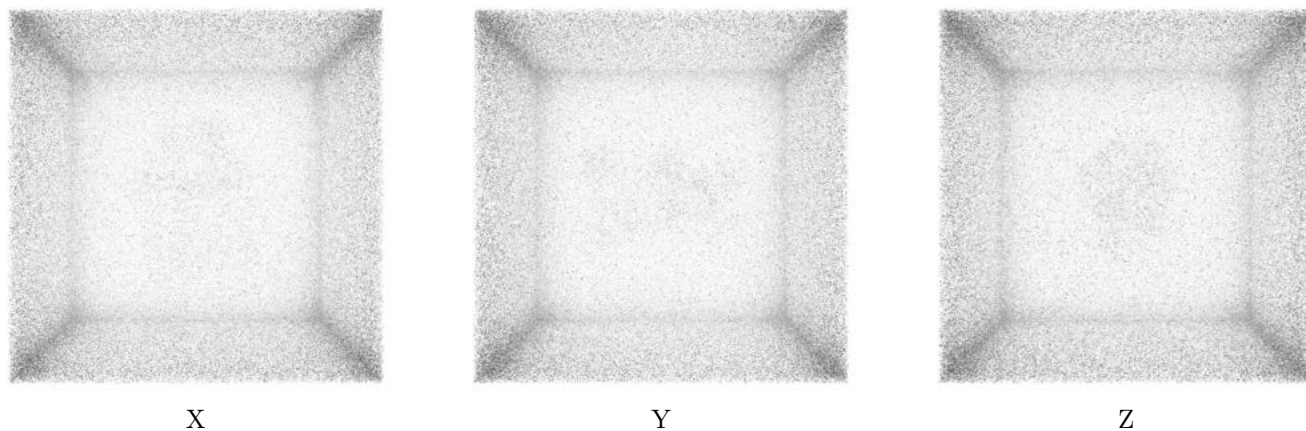
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

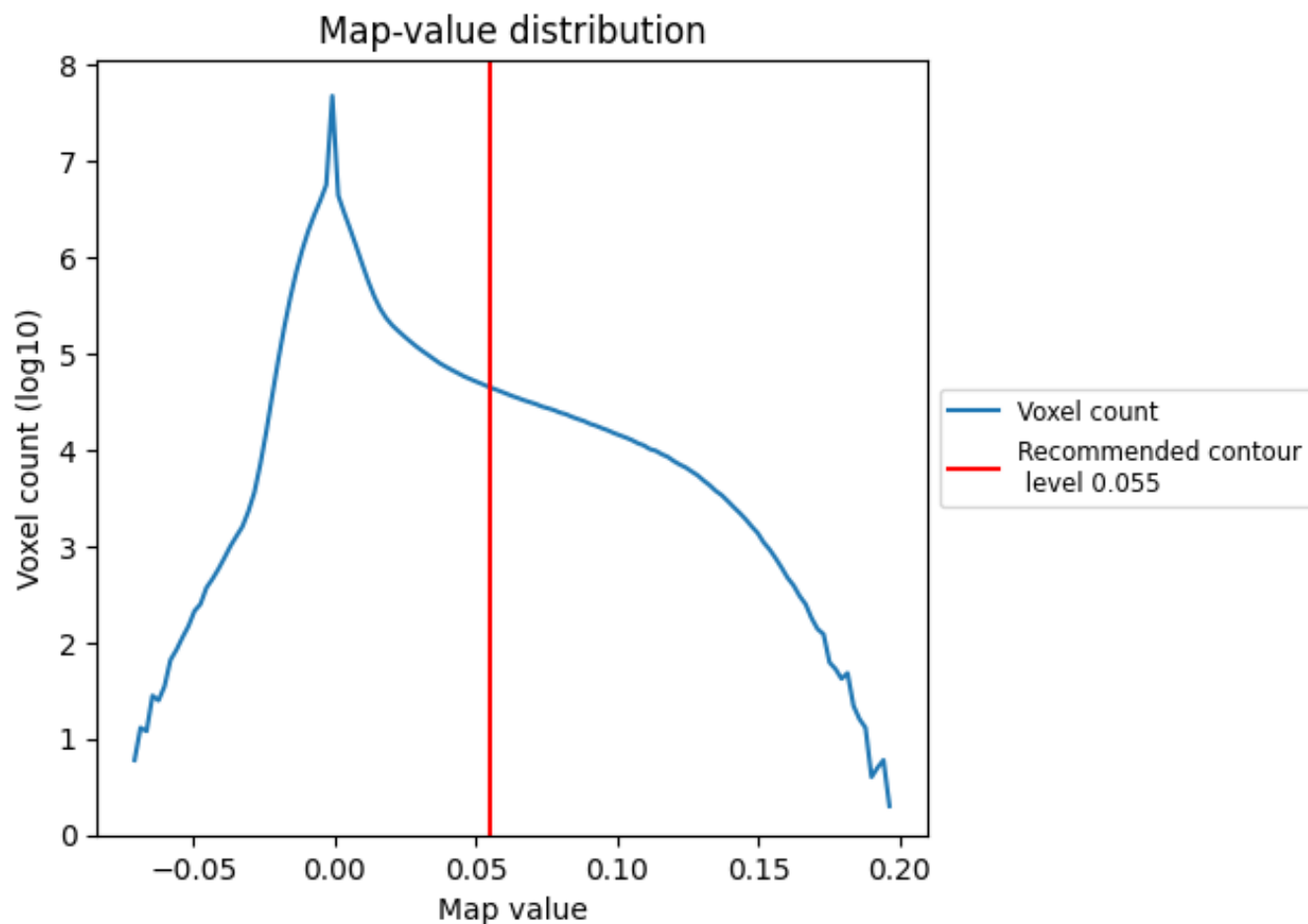
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

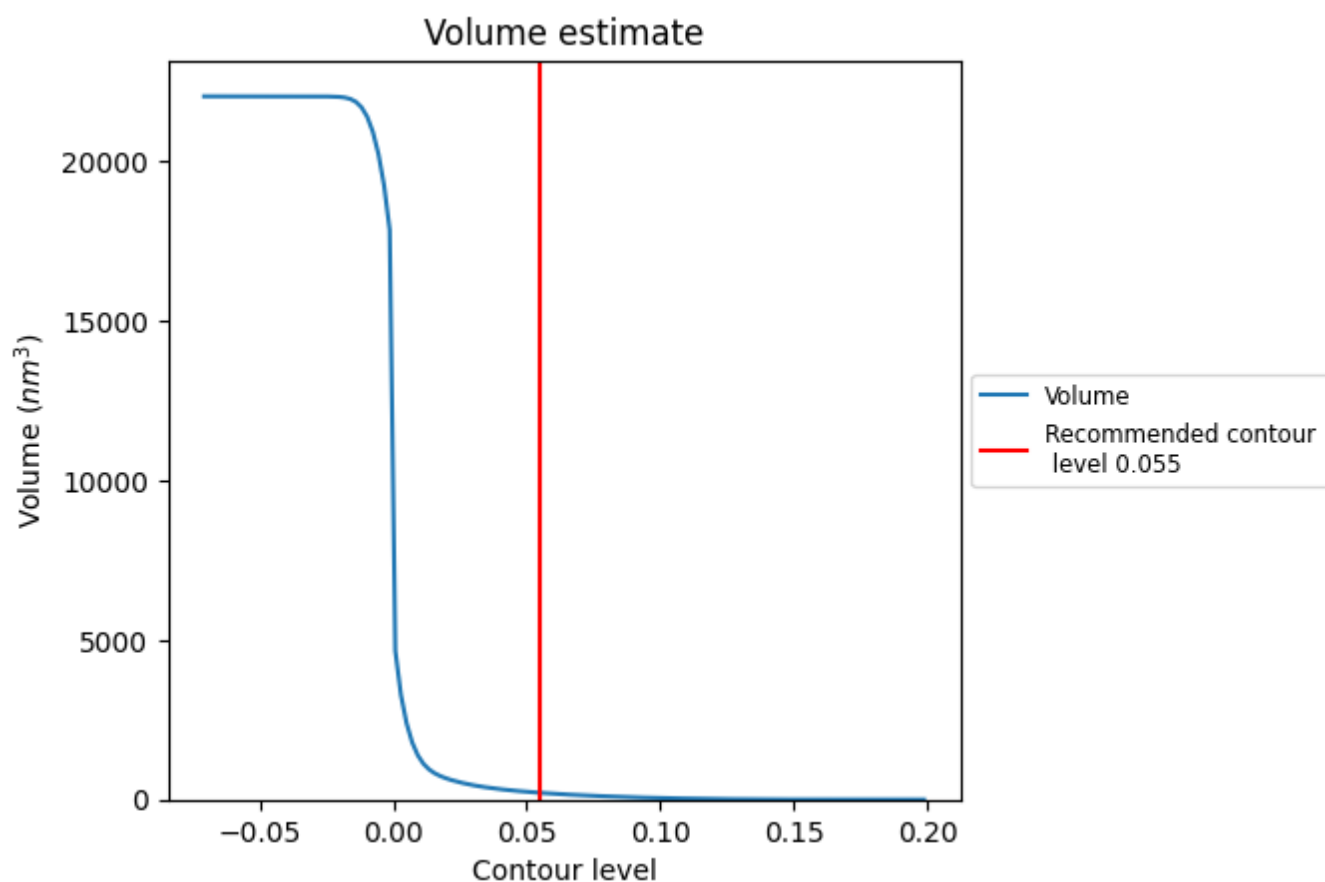
This section contains the results of statistical analysis of the map.

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.

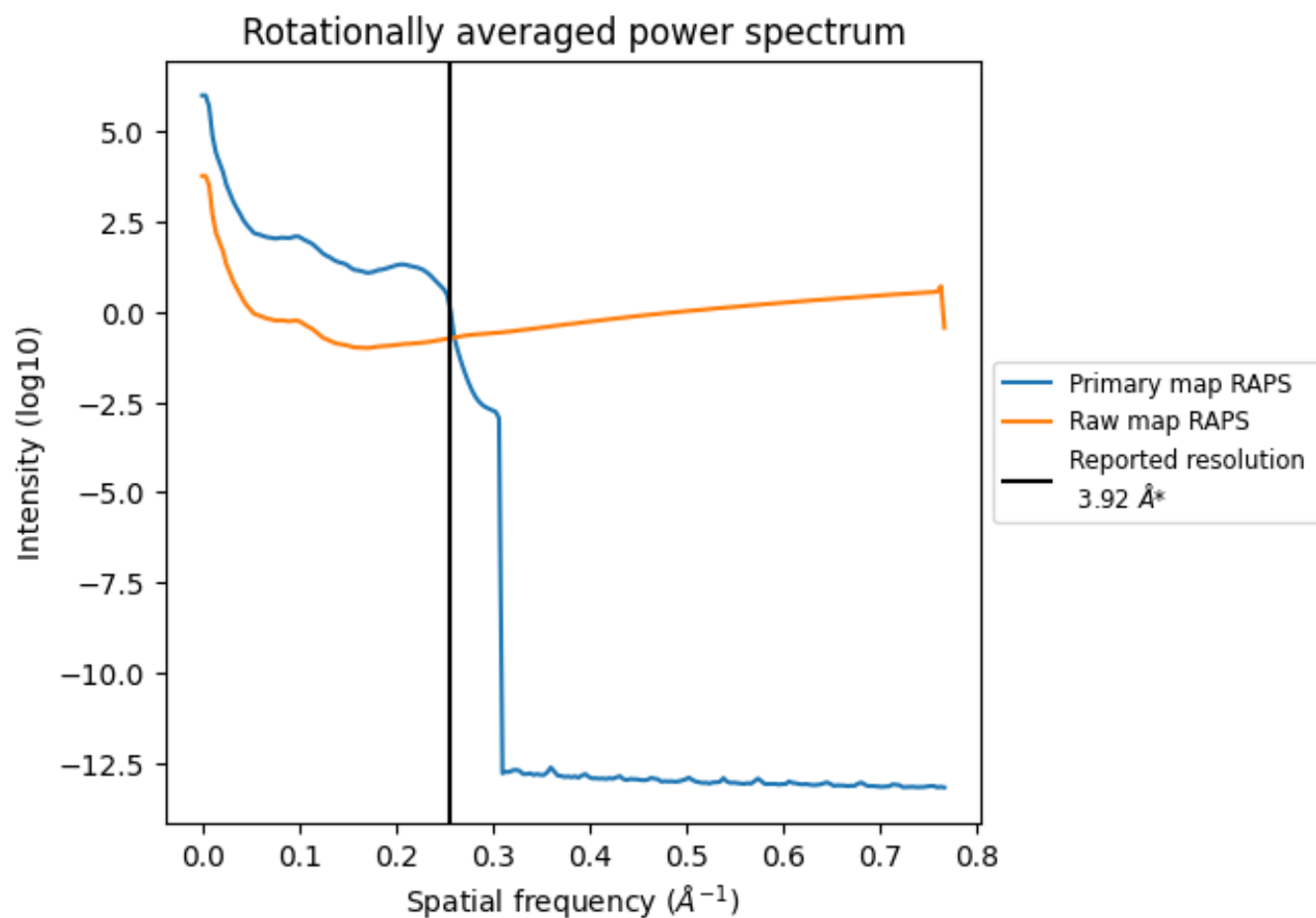
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm³; this corresponds to an approximate mass of 191 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 ⓘ

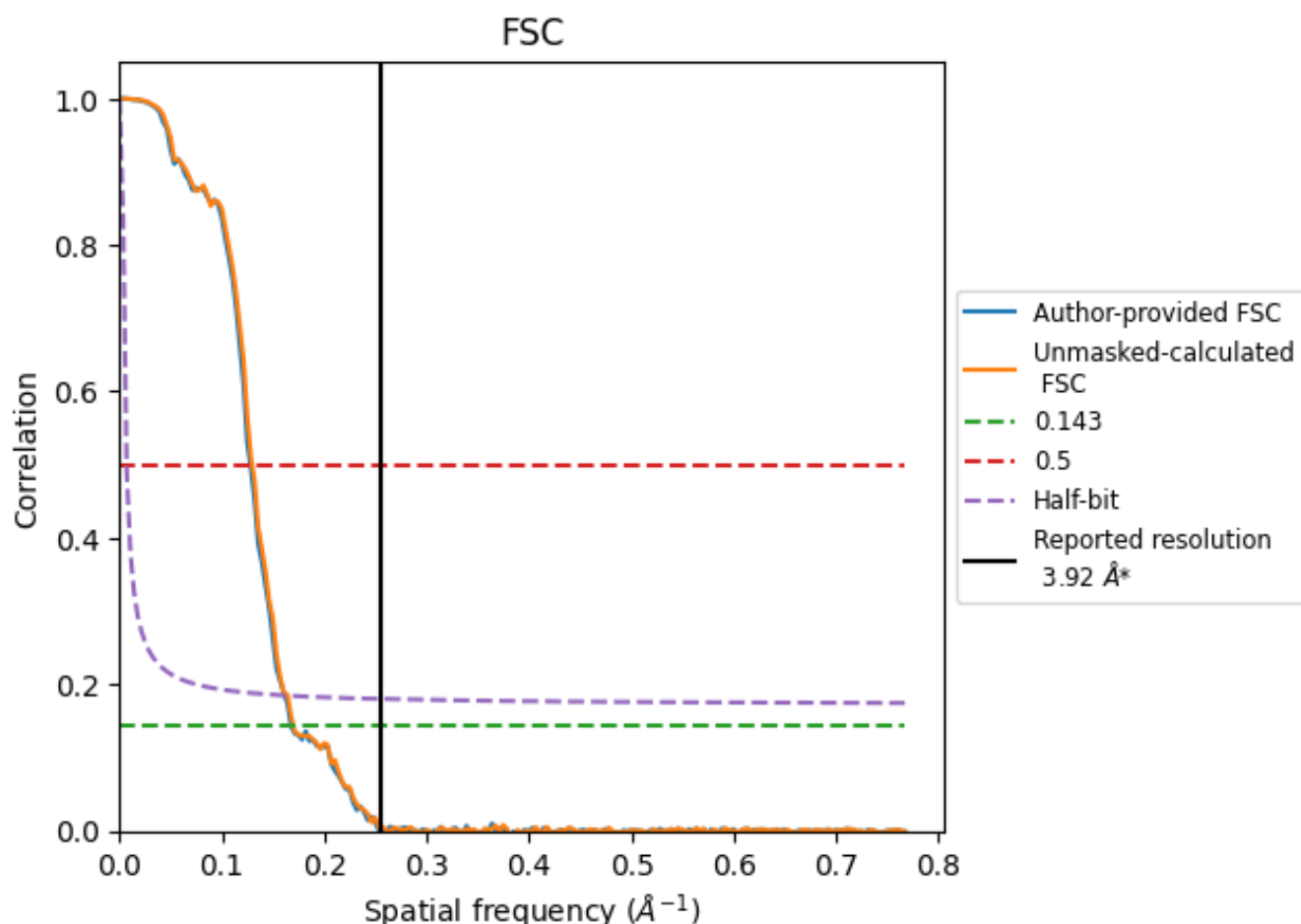


*Reported resolution corresponds to spatial frequency of 0.255 Å⁻¹

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 0.255 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.92	-	-
Author-provided FSC curve	5.97	7.82	6.20
Unmasked-calculated*	5.88	7.72	6.09

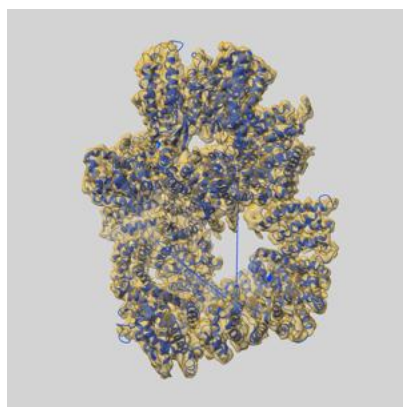
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 5.97 differs from the reported value 3.92 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.88 differs from the reported value 3.92 by more than 10 %

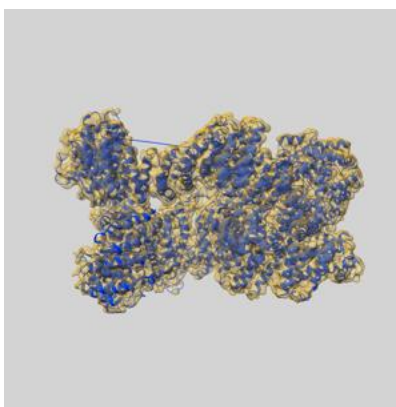
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11211 and PDB model 6ZH2. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

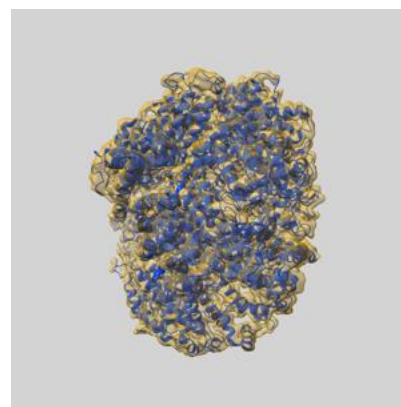
9.1 Map-model overlay [i](#)



X



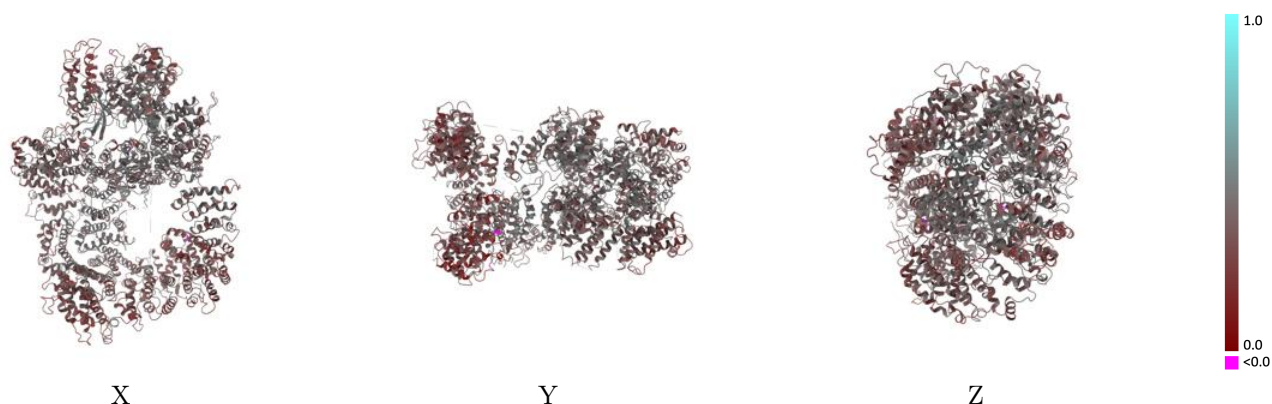
Y



Z

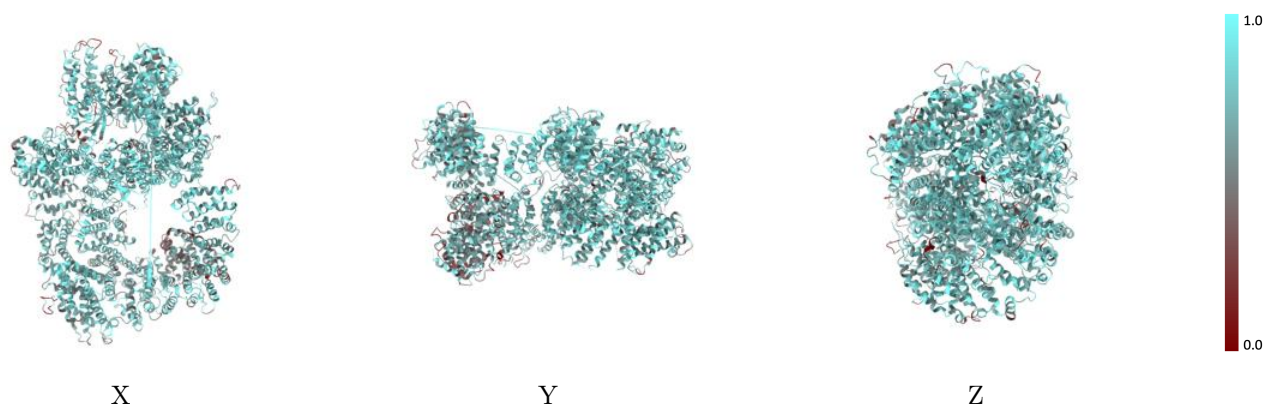
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



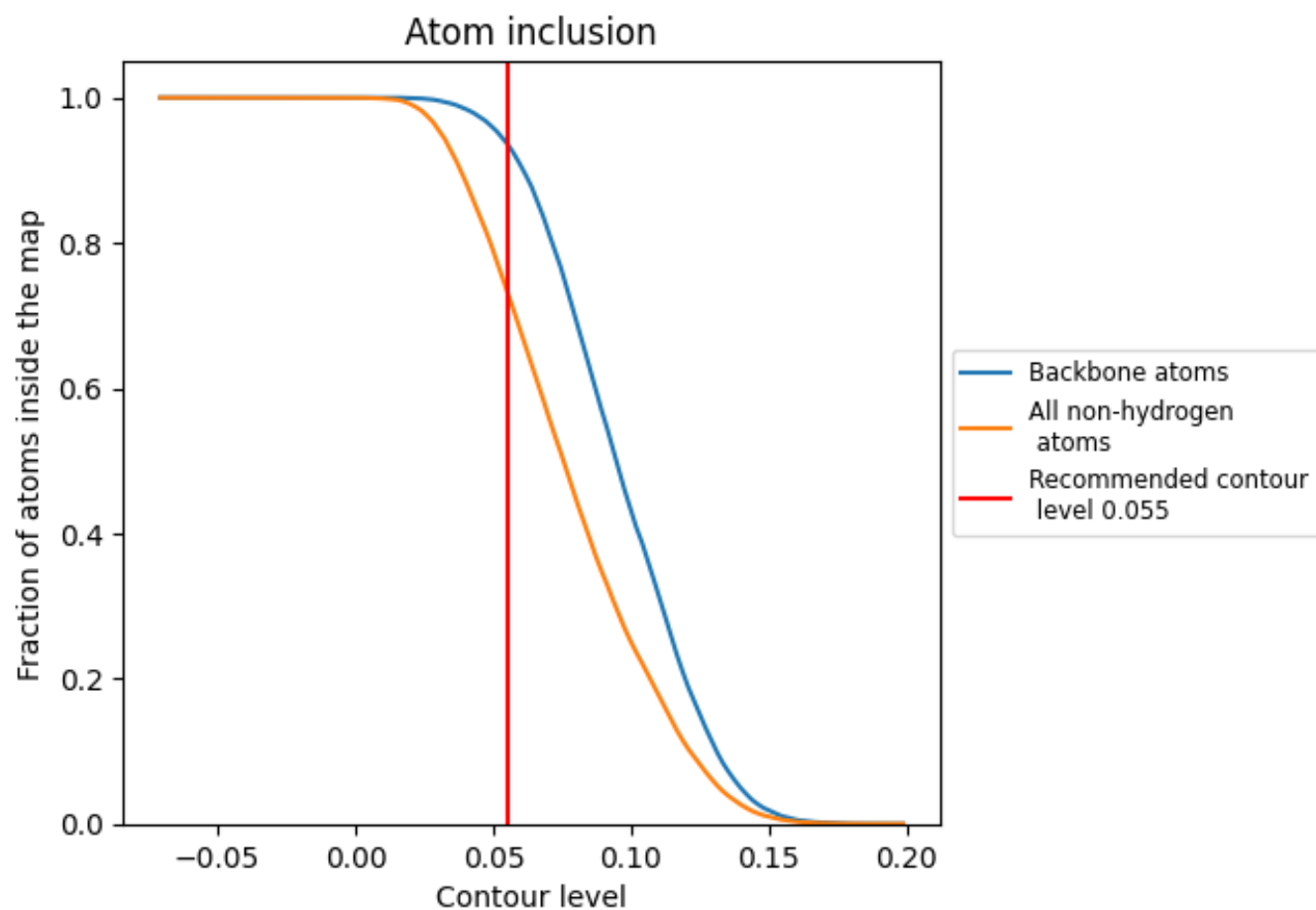
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 73% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7346	<div></div> 0.3790
A	<div></div> 0.7346	<div></div> 0.3790

