



## wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 02:44 AM UTC

PDB ID : 9CMO / pdb\_00009cmo  
EMDB ID : EMD-45751  
Title : Cryo-EM model derived from localized reconstruction of Ad657-hexon-FII complex at 4.14Å resolution  
Authors : Reddy, V.S.; Ma, O.X.  
Deposited on : 2024-07-15  
Resolution : 4.17 Å(reported)  
Based on initial model : 6BIT

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

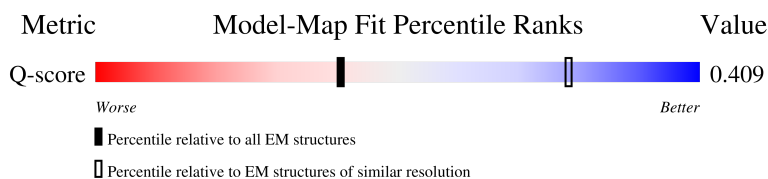
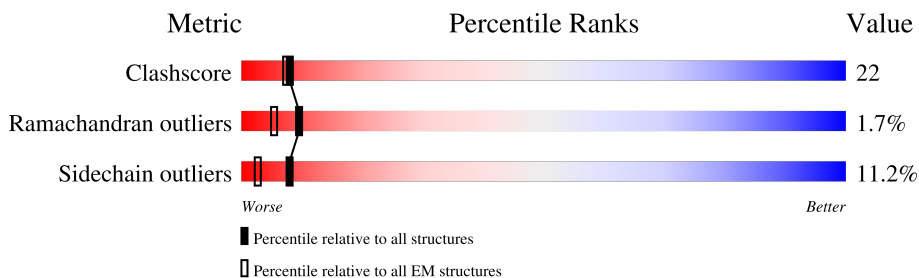
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.17 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	5438 ( 3.67 - 4.67 )

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  $\geq 3$ , 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	J	959	<p>54% 35% 7% ..</p>
1	K	959	<p>55% 34% 7% ..</p>
1	L	959	<p>56% 32% 7% ..</p>
2	Z	622	<p>85% 56% 33% . 7%</p>

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

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	CGU	Z	19	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26791 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	931	7402	4685	1259	1420	38	0	0
1	K	929	7393	4680	1258	1417	38	0	0
1	L	927	7374	4670	1252	1414	38	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	291	LEU	VAL	conflict	UNP A0A348FV85
J	827	ILE	LEU	conflict	UNP A0A348FV85
J	853	VAL	PHE	conflict	UNP A0A348FV85
K	291	LEU	VAL	conflict	UNP A0A348FV85
K	827	ILE	LEU	conflict	UNP A0A348FV85
K	853	VAL	PHE	conflict	UNP A0A348FV85
L	291	LEU	VAL	conflict	UNP A0A348FV85
L	827	ILE	LEU	conflict	UNP A0A348FV85
L	853	VAL	PHE	conflict	UNP A0A348FV85

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Z	579	4615	2868	805	910	32	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	L	1	Total	Ca	0
			1	1	

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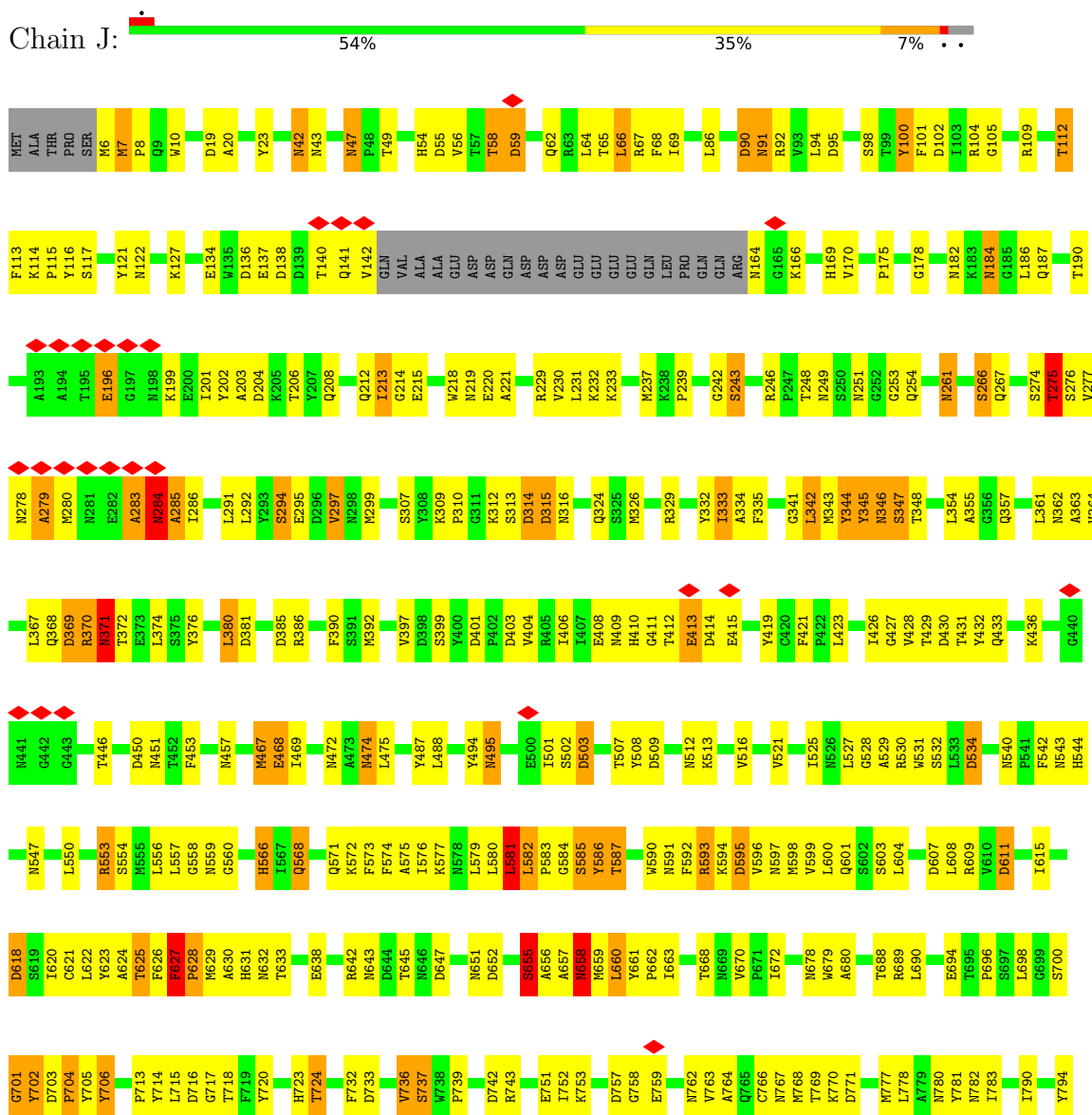
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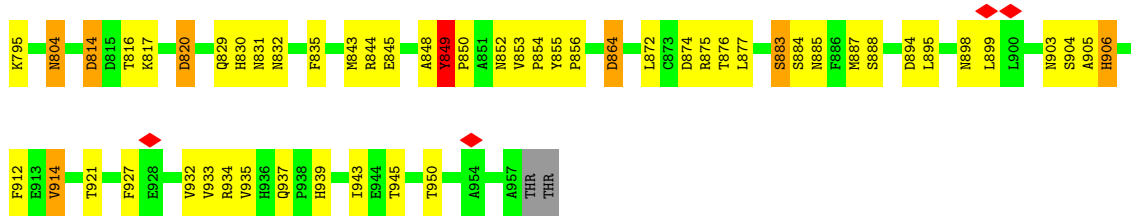
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
3	Z	6	6	6	0

### 3 Residue-property plots

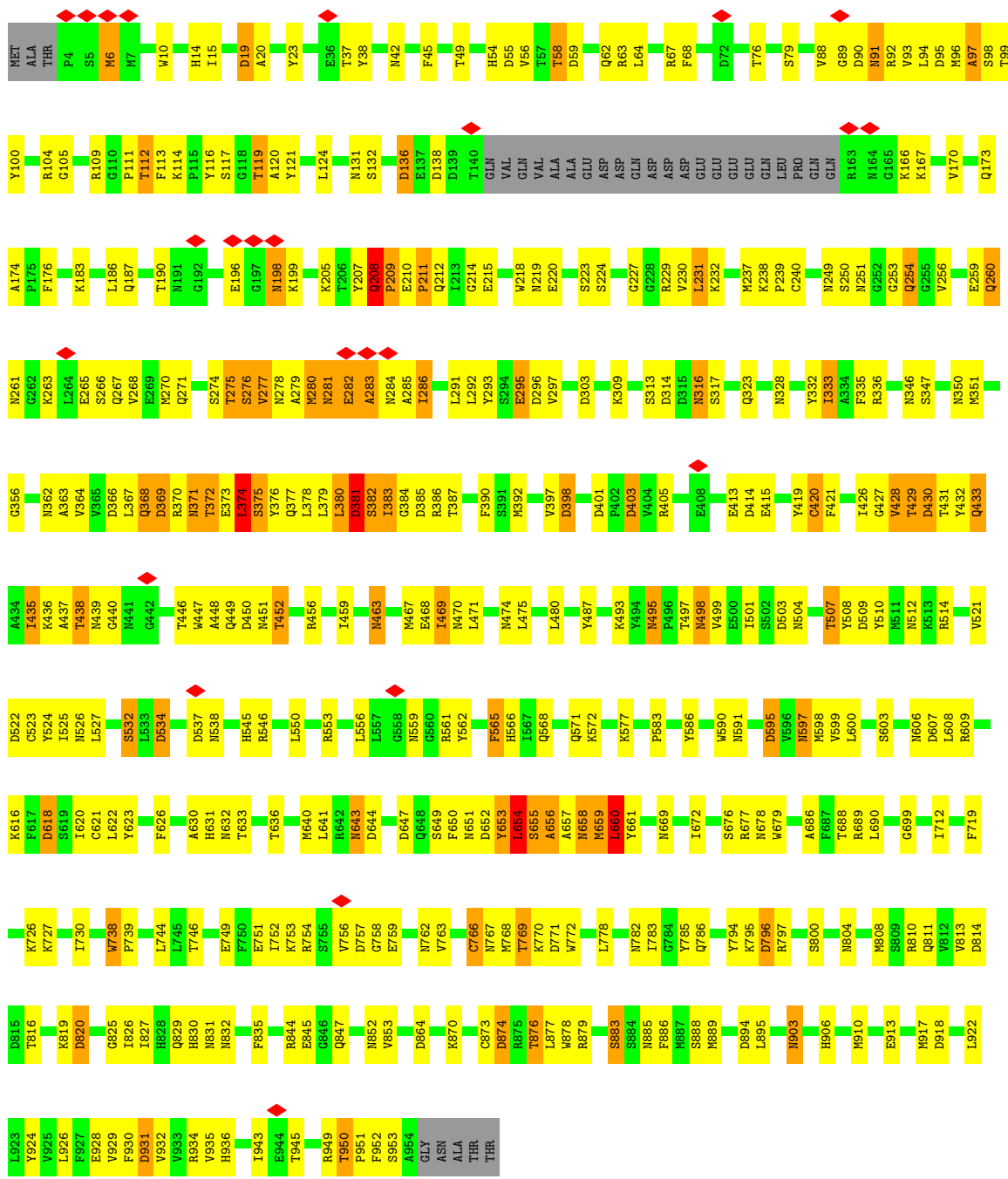
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Hexon protein

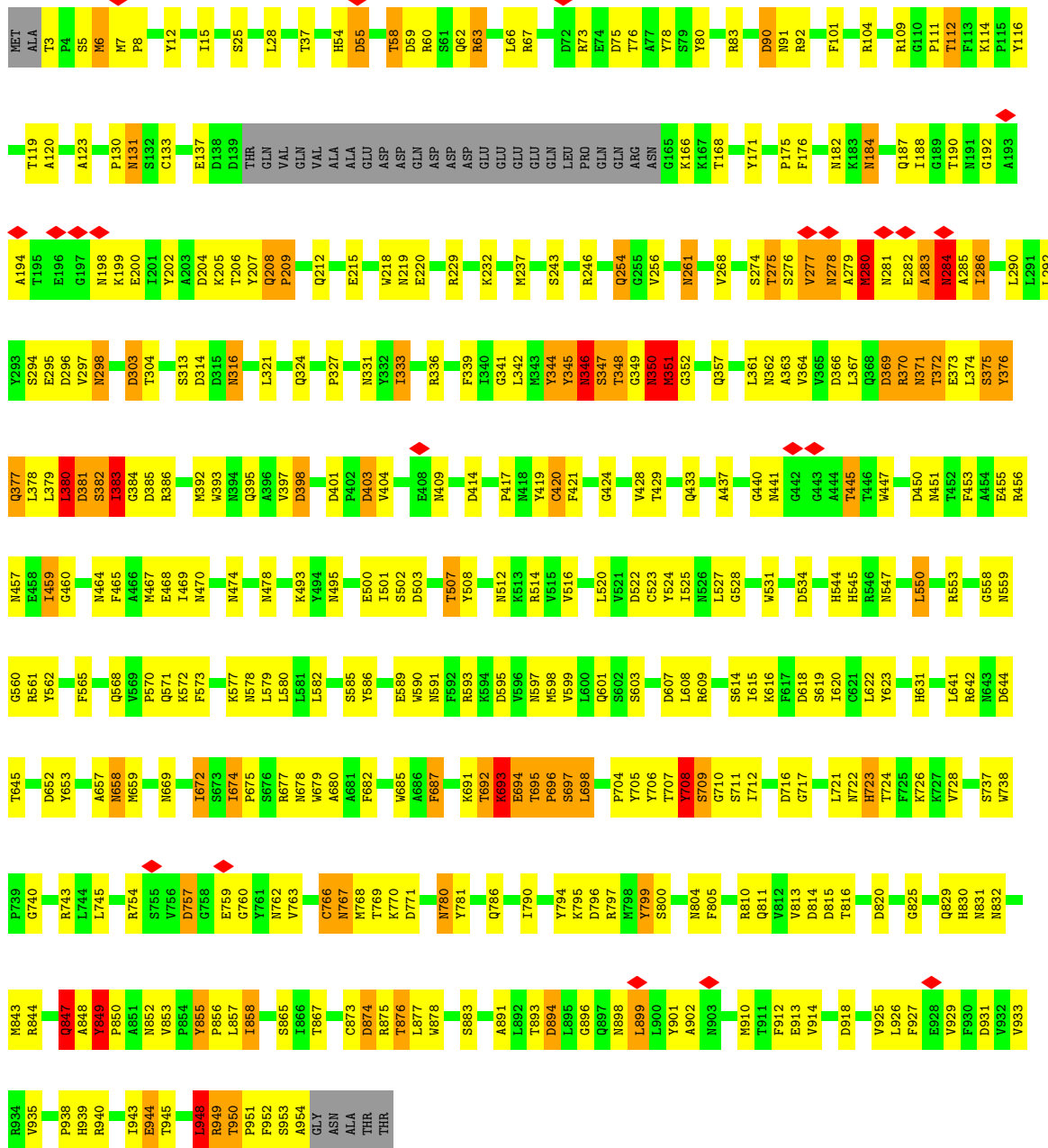




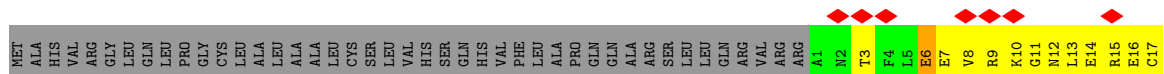
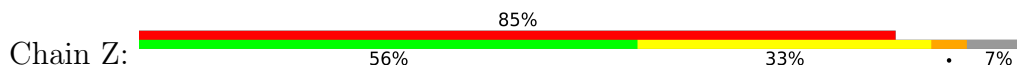
• Molecule 1: Hexon protein



• Molecule 1: Hexon protein



• Molecule 2: Prothrombin



T561	H562	V563	F564	R565	L566	K567	X568	Y569	I570	D571	E572	F573	G574	H575	I576	J577	K578	L579	M580	N581	O582	P583	Q584	R585	S586	T587	U588	V589	W590	X591	Y592	Z593	A594	B595	C596	D597	E598	F599	G600	H601	I602	J603	K604	L605	M606	N607	O608	P609	Q610	R611	S612	T613	U614	V615	W616	X617	Y618	Z619	A620	B621	C622	D623	E624	F625	G626	H627	I628	J629	K630	L631	M632	N633	O634	P635	Q636	R637	S638	T639	U640	V641	W642	X643	Y644	Z645	A646	B647	C648	D649	E650	F651	G652	H653	I654	J655	K656	L657	M658	N659	O660	P661	Q662	R663	S664	T665	U666	V667	W668	X669	Y670	Z671	A672	B673	C674	D675	E676	F677	G678	H679	I680	J681	K682	L683	M684	N685	O686	P687	Q688	R689	S690	T691	U692	V693	W694	X695	Y696	Z697	A698	B699	C700	D701	E702	F703	G704	H705	I706	J707	K708	L709	M710	N711	O712	P713	Q714	R715	S716	T717	U718	V719	W720	X721	Y722	Z723	A724	B725	C726	D727	E728	F729	G730	H731	I732	J733	K734	L735	M736	N737	O738	P739	Q740	R741	S742	T743	U744	V745	W746	X747	Y748	Z749	A750	B751	C752	D753	E754	F755	G756	H757	I758	J759	K760	L761	M762	N763	O764	P765	Q766	R767	S768	T769	U770	V771	W772	X773	Y774	Z775	A776	B777	C778	D779	E780	F781	G782	H783	I784	J785	K786	L787	M788	N789	O790	P791	Q792	R793	S794	T795	U796	V797	W798	X799	Y800	Z801	A802	B803	C804	D805	E806	F807	G808	H809	I810	J811	K812	L813	M814	N815	O816	P817	Q818	R819	S820	T821	U822	V823	W824	X825	Y826	Z827	A828	B829	C830	D831	E832	F833	G834	H835	I836	J837	K838	L839	M840	N841	O842	P843	Q844	R845	S846	T847	U848	V849	W850	X851	Y852	Z853	A854	B855	C856	D857	E858	F859	G860	H861	I862	J863	K864	L865	M866	N867	O868	P869	Q870	R871	S872	T873	U874	V875	W876	X877	Y878	Z879	A880	B881	C882	D883	E884	F885	G886	H887	I888	J889	K890	L891	M892	N893	O894	P895	Q896	R897	S898	T899	U900	V901	W902	X903	Y904	Z905	A906	B907	C908	D909	E910	F911	G912	H913	I914	J915	K916	L917	M918	N919	O920	P921	Q922	R923	S924	T925	U926	V927	W928	X929	Y930	Z931	A932	B933	C934	D935	E936	F937	G938	H939	I940	J941	K942	L943	M944	N945	O946	P947	Q948	R949	S950	T951	U952	V953	W954	X955	Y956	Z957	A958	B959	C960	D961	E962	F963	G964	H965	I966	J967	K968	L969	M970	N971	O972	P973	Q974	R975	S976	T977	U978	V979	W980	X981	Y982	Z983	A984	B985	C986	D987	E988	F989	G990	H991	I992	J993	K994	L995	M996	N997	O998	P999	Q1000	R1001	S1002	T1003	U1004	V1005	W1006	X1007	Y1008	Z1009	A1010	B1011	C1012	D1013	E1014	F1015	G1016	H1017	I1018	J1019	K1020	L1021	M1022	N1023	O1024	P1025	Q1026	R1027	S1028	T1029	U1030	V1031	W1032	X1033	Y1034	Z1035	A1036	B1037	C1038	D1039	E1040	F1041	G1042	H1043	I1044	J1045	K1046	L1047	M1048	N1049	O1050	P1051	Q1052	R1053	S1054	T1055	U1056	V1057	W1058	X1059	Y1060	Z1061	A1062	B1063	C1064	D1065	E1066	F1067	G1068	H1069	I1070	J1071	K1072	L1073	M1074	N1075	O1076	P1077	Q1078	R1079	S1080	T1081	U1082	V1083	W1084	X1085	Y1086	Z1087	A1088	B1089	C1090	D1091	E1092	F1093	G1094	H1095	I1096	J1097	K1098	L1099	M1100	N1101	O1102	P1103	Q1104	R1105	S1106	T1107	U1108	V1109	W1110	X1111	Y1112	Z1113	A1114	B1115	C1116	D1117	E1118	F1119	G1120	H1121	I1122	J1123	K1124	L1125	M1126	N1127	O1128	P1129	Q1130	R1131	S1132	T1133	U1134	V1135	W1136	X1137	Y1138	Z1139	A1140	B1141	C1142	D1143	E1144	F1145	G1146	H1147	I1148	J1149	K1150	L1151	M1152	N1153	O1154	P1155	Q1156	R1157	S1158	T1159	U1160	V1161	W1162	X1163	Y1164	Z1165	A1166	B1167	C1168	D1169	E1170	F1171	G1172	H1173	I1174	J1175	K1176	L1177	M1178	N1179	O1180	P1181	Q1182	R1183	S1184	T1185	U1186	V1187	W1188	X1189	Y1190	Z1191	A1192	B1193	C1194	D1195	E1196	F1197	G1198	H1199	I1200	J1201	K1202	L1203	M1204	N1205	O1206	P1207	Q1208	R1209	S1210	T1211	U1212	V1213	W1214	X1215	Y1216	Z1217	A1218	B1219	C1220	D1221	E1222	F1223	G1224	H1225	I1226	J1227	K1228	L1229	M1230	N1231	O1232	P1233	Q1234	R1235	S1236	T1237	U1238	V1239	W1240	X1241	Y1242	Z1243	A1244	B1245	C1246	D1247	E1248	F1249	G1250	H1251	I1252	J1253	K1254	L1255	M1256	N1257	O1258	P1259	Q1260	R1261	S1262	T1263	U1264	V1265	W1266	X1267	Y1268	Z1269	A1270	B1271	C1272	D1273	E1274	F1275	G1276	H1277	I1278	J1279	K1280	L1281	M1282	N1283	O1284	P1285	Q1286	R1287	S1288	T1289	U1290	V1291	W1292	X1293	Y1294	Z1295	A1296	B1297	C1298	D1299	E1300	F1301	G1302	H1303	I1304	J1305	K1306	L1307	M1308	N1309	O1310	P1311	Q1312	R1313	S1314	T1315	U1316	V1317	W1318	X1319	Y1320	Z1321	A1322	B1323	C1324	D1325	E1326	F1327	G1328	H1329	I1330	J1331	K1332	L1333	M1334	N1335	O1336	P1337	Q1338	R1339	S1340	T1341	U1342	V1343	W1344	X1345	Y1346	Z1347	A1348	B1349	C1350	D1351	E1352	F1353	G1354	H1355	I1356	J1357	K1358	L1359	M1360	N1361	O1362	P1363	Q1364	R1365	S1366	T1367	U1368	V1369	W1370	X1371	Y1372	Z1373	A1374	B1375	C1376	D1377	E1378	F1379	G1380	H1381	I1382	J1383	K1384	L1385	M1386	N1387	O1388	P1389	Q1390	R1391	S1392	T1393	U1394	V1395	W1396	X1397	Y1398	Z1399	A1400	B1401	C1402	D1403	E1404	F1405	G1406	H1407	I1408	J1409	K1410	L1411	M1412	N1413	O1414	P1415	Q1416	R1417	S1418	T1419	U1420	V1421	W1422	X1423	Y1424	Z1425	A1426	B1427	C1428	D1429	E1430	F1431	G1432	H1433	I1434	J1435	K1436	L1437	M1438	N1439	O1440	P1441	Q1442	R1443	S1444	T1445	U1446	V1447	W1448	X1449	Y1450	Z1451	A1452	B1453	C1454	D1455	E1456	F1457	G1458	H1459	I1460	J1461	K1462	L1463	M1464	N1465	O1466	P1467	Q1468	R1469	S1470	T1471	U1472	V1473	W1474	X1475	Y1476	Z1477	A1478	B1479	C1480	D1481	E1482	F1483	G1484	H1485	I1486	J1487	K1488	L1489	M1490	N1491	O1492	P1493	Q1494	R1495	S1496	T1497	U1498	V1499	W1500	X1501	Y1502	Z1503	A1504	B1505	C1506	D1507	E1508	F1509	G1510	H1511	I1512	J1513	K1514	L1515	M1516	N1517	O1518	P1519	Q1520	R1521	S1522	T1523	U1524	V1525	W1526	X1527	Y1528	Z1529	A1530	B1531	C1532	D1533	E1534	F1535	G1536	H1537	I1538	J1539	K1540	L1541	M1542	N1543	O1544	P1545	Q1546	R1547	S1548	T1549	U1550	V1551	W1552	X1553	Y1554	Z1555	A1556	B1557	C1558	D1559	E1560	F1561	G1562	H1563	I1564	J1565	K1566	L1567	M1568	N1569	O1570	P1571	Q1572	R1573	S1574	T1575	U1576	V1577	W1578	X1579	Y1580	Z1581	A1582	B1583	C1584	D1585	E1586	F1587	G1588	H1589	I1590	J1591	K1592	L1593	M1594	N1595	O1596	P1597	Q1598	R1599	S1600	T1601	U1602	V1603	W1604	X1605	Y1606	Z1607	A1608	B1609	C1610	D1611	E1612	F1613	G1614	H1615	I1616	J1617	K1618	L1619	M1620	N1621	O1622	P1623	Q1624	R1625	S1626	T1627	U1628	V1629	W1630	X1631	Y1632	Z1633	A1634	B1635	C1636	D1637	E1638	F1639	G1640	H1641	I1642	J1643	K1644	L1645	M1646	N1647	O1648	P1649	Q1650	R1651	S1652	T1653	U1654	V1655	W1656	X1657	Y1658	Z1659	A1660	B1661	C1662	D1663	E1664	F1665	G1666	H1667	I1668	J1669	K1670	L1671	M1672	N1673	O1674	P1675	Q1676	R1677	S1678	T1679	U1680	V1681	W1682	X1683	Y1684	Z1685	A1686	B1687	C1688	D1689	E1690	F1691	G1692	H1693	I1694	J1695	K1696	L1697	M1698	N1699	O1700	P1701	Q1702	R1703	S1704	T1705	U1706	V1707	W1708	X1709	Y1710	Z1711	A1712	B1713	C1714	D1715	E1716	F1717	G1718	H1719	I1720	J1721	K1722	L1723	M1724	N1725	O1726	P1727	Q1728	R1729	S1730	T1731	U1732	V1733	W1734	X1735	Y1736	Z1737	A1738	B1739	C1740	D1741	E1742	F1743	G1744	H1745	I1746	J1747	K1748	L1749	M1750	N1751	O1752	P1753	Q1754	R1755	S1756	T1757	U1758	V1759	W1760	X1761	Y1762	Z1763	A1764	B1765	C1766	D1767	E1768	F1769	G1770	H1771	I1772	J1773	K1774	L1775	M1776	N1777	O1778	P1779	Q1780	R1781	S1782	T1783	U1784	V1785	W1786	X1787	Y1788	Z1789	A1790	B1791	C1792	D1793	E1794	F1795	G1796	H1797	I1798	J1799	K1800	L1801	M1802	N1803	O1804	P1805	Q1806	R1807	S1808	T1809	U1810	V1811	W1812	X1813	Y1814	Z1815	A1816	B1817	C1818	D1819	E1820	F1821	G1822	H1823	I1824	J1825	K1826	L1827	M1828	N1829	O1830	P1831	Q1832	R1833	S1834	T1835	U1836	V1837	W1838	X1839	Y1840	Z1841	A1842	B1843	C1844	D1845	E1846	F1847	G1848	H1849	I1850	J1851	K1852	L1853	M1854	N1855	O1856	P1857	Q1858	R1859	S1860	T1861	U1862	V1863	W1864	X1865	Y1866	Z1867	A1868	B1869	C1870	D1871	E1872	F1873	G1874	H1875	I1876	J1877	K1878	L1879	M1880	N1881	O1882	P1883	Q1884	R1885	S1886	T1887	U1888	V1889	W1890	X1891	Y1892	Z1893	A1894	B1895	C1896	D1897	E1898	F1899	G1900	H1901	I1902	J1903	K1904	L1905	M1906	N1907	O1908	P1909	Q1910	R1911	S1912	T1913	U1914	V1915	W1916	X1917	Y1918	Z1919	A1920	B1921	C1922	D1923	E1924	F1925	G1926	H1927	I1928	J1929	K1930	L1931	M1932	N1933	O1934	P1935	Q1936	R1937	S1938	T1939	U1940	V1941	W1942	X1943	Y1944</
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4635	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 ( $e^-/\text{\AA}^2$ )	81	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.029	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size ( $\text{\AA}$ )	129.536, 211.2, 112.64	wwPDB
Map dimensions	150, 80, 92	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.408, 1.408, 1.408	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	J	0.52	1/7595 (0.0%)	0.55	3/10330 (0.0%)
1	K	0.48	2/7587 (0.0%)	0.56	6/10318 (0.1%)
1	L	0.52	4/7568 (0.1%)	0.58	9/10294 (0.1%)
2	Z	0.17	0/4597	0.46	0/6220
All	All	0.47	7/27347 (0.0%)	0.55	18/37162 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	K	0	2
1	L	0	2
All	All	0	5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	847	GLN	CA-C	-7.75	1.49	1.53
1	L	696	PRO	CA-C	-6.84	1.44	1.52
1	J	627	PHE	C-O	-5.51	1.20	1.25
1	L	380	LEU	CA-C	-5.33	1.46	1.52
1	K	381	ASP	CA-C	-5.20	1.45	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	276	SER	N-CA-C	-12.12	97.59	112.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	697	SER	N-CA-C	-9.75	98.42	110.41
1	K	380	LEU	N-CA-C	-8.64	101.56	110.97
1	L	849	TYR	CA-C-N	-6.80	113.68	120.21
1	L	849	TYR	C-N-CA	-6.80	113.68	120.21

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	853	VAL	Peptide
1	K	208	GLN	Peptide
1	K	738	TRP	Peptide
1	L	208	GLN	Peptide
1	L	853	VAL	Peptide

## 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	J	7402	0	7067	351	0
1	K	7393	0	7062	356	0
1	L	7374	0	7040	364	0
2	Z	4615	0	4343	184	0
3	L	1	0	0	0	0
3	Z	6	0	0	0	0
All	All	26791	0	25512	1161	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 22.

The worst 5 of 1161 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:K:275:THR:HB	1:K:277:VAL:HG22	1.33	1.08
1:J:277:VAL:HB	1:J:280:MET:HG3	1.40	1.03

*Continued on next page...*

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:949:ARG:HG2	1:L:953:SER:HB2	1.52	0.90
1:J:116:TYR:HE1	1:L:858:ILE:HD11	1.36	0.89
2:Z:441:PRO:HD3	2:Z:540:TYR:HB3	1.52	0.89

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	J	927/959 (97%)	786 (85%)	124 (13%)	17 (2%)	6	34
1	K	925/959 (96%)	789 (85%)	118 (13%)	18 (2%)	6	33
1	L	923/959 (96%)	784 (85%)	119 (13%)	20 (2%)	5	29
2	Z	567/622 (91%)	520 (92%)	44 (8%)	3 (0%)	24	62
All	All	3342/3499 (96%)	2879 (86%)	405 (12%)	58 (2%)	9	35

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	283	ALA
1	J	285	ALA
1	J	346	ASN
1	J	370	ARG
1	J	585	SER

### 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	J	799/824 (97%)	699 (88%)	100 (12%)	4	18
1	K	799/824 (97%)	701 (88%)	98 (12%)	4	19
1	L	797/824 (97%)	699 (88%)	98 (12%)	4	19
2	Z	486/521 (93%)	458 (94%)	28 (6%)	18	42
All	All	2881/2993 (96%)	2557 (89%)	324 (11%)	8	21

5 of 324 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	351	MET
1	L	894	ASP
1	L	397	VAL
1	L	687	PHE
2	Z	109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	433	GLN
1	K	646	ASN
1	L	762	ASN
1	K	474	ASN
1	L	212	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](#)

10 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	CGU	Z	14	2,3	9,11,12	1.18	0	10,14,16	0.78	0
2	CGU	Z	29	2,3	9,11,12	1.36	0	10,14,16	0.83	0
2	CGU	Z	6	2,3	9,11,12	1.64	1 (11%)	10,14,16	0.92	0
2	CGU	Z	16	2,3	9,11,12	1.28	0	10,14,16	0.95	0
2	CGU	Z	19	2	9,11,12	1.56	1 (11%)	10,14,16	0.84	0
2	CGU	Z	7	2,3	9,11,12	1.74	2 (22%)	10,14,16	0.89	0
2	CGU	Z	26	2,3	9,11,12	1.41	1 (11%)	10,14,16	0.81	0
2	CGU	Z	32	2	9,11,12	1.53	1 (11%)	10,14,16	0.90	0
2	CGU	Z	20	2,3	9,11,12	1.39	1 (11%)	10,14,16	0.81	0
2	CGU	Z	25	2	9,11,12	1.72	1 (11%)	10,14,16	0.90	0

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	CGU	Z	14	2,3	-	2/13/14/16	-
2	CGU	Z	29	2,3	-	8/13/14/16	-
2	CGU	Z	6	2,3	-	3/13/14/16	-
2	CGU	Z	16	2,3	-	2/13/14/16	-
2	CGU	Z	19	2	-	3/13/14/16	-
2	CGU	Z	7	2,3	-	5/13/14/16	-
2	CGU	Z	26	2,3	-	0/13/14/16	-
2	CGU	Z	32	2	-	2/13/14/16	-
2	CGU	Z	20	2,3	-	1/13/14/16	-
2	CGU	Z	25	2	-	4/13/14/16	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	25	CGU	CG-CD2	3.54	1.56	1.52
2	Z	7	CGU	CG-CD2	3.09	1.56	1.52
2	Z	19	CGU	CG-CD1	2.97	1.55	1.52
2	Z	6	CGU	CG-CD2	2.71	1.55	1.52
2	Z	7	CGU	CG-CD1	2.12	1.54	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Z	6	CGU	C-CA-CB-CG
2	Z	6	CGU	OE21-CD2-CG-CB
2	Z	6	CGU	OE22-CD2-CG-CB
2	Z	7	CGU	N-CA-CB-CG
2	Z	14	CGU	C-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	14	CGU	2	0
2	Z	6	CGU	3	0
2	Z	16	CGU	2	0
2	Z	19	CGU	7	0
2	Z	32	CGU	1	0
2	Z	25	CGU	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

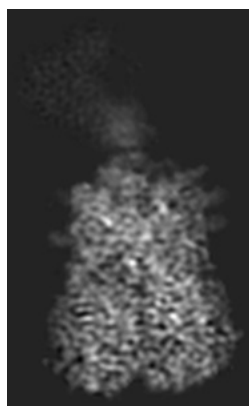
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45751. These allow visual inspection of the internal detail of the map and identification of artifacts.

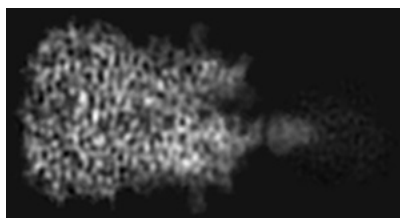
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

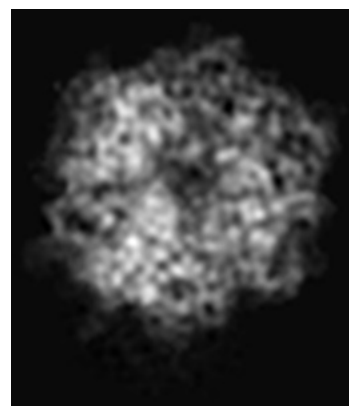
#### 6.1.1 Primary map



X

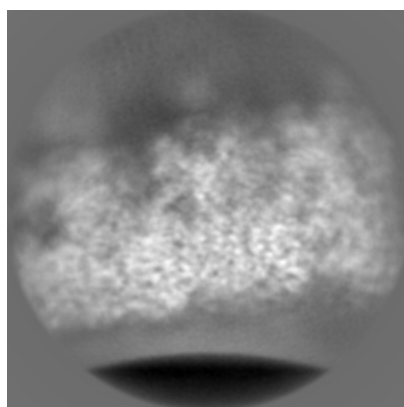


Y

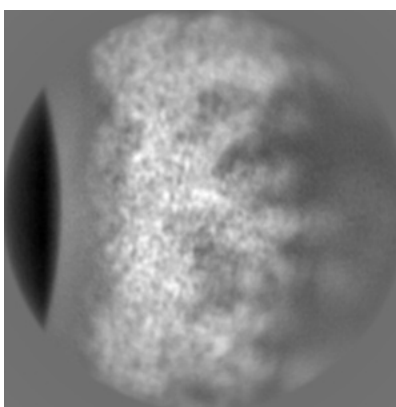


Z

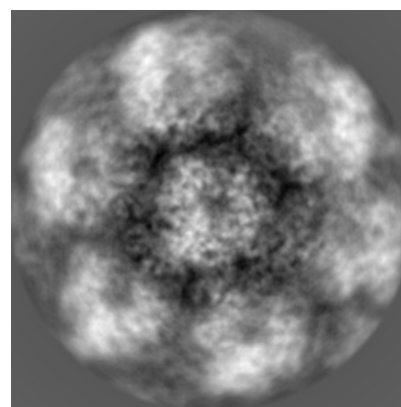
#### 6.1.2 Raw map



X



Y

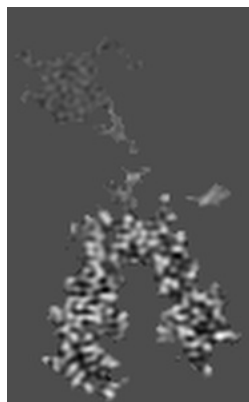


Z

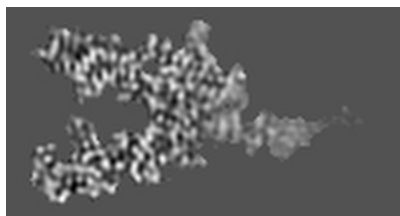
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

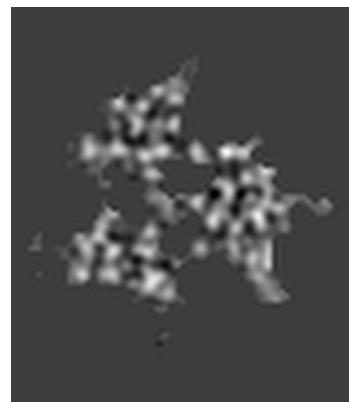
### 6.2.1 Primary map



X Index: 40

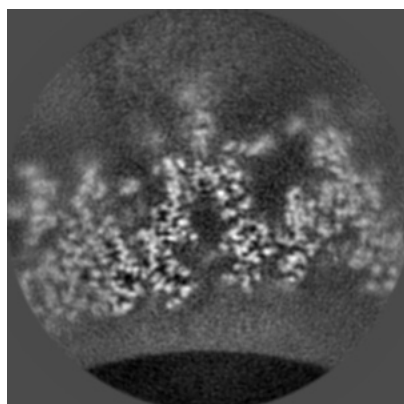


Y Index: 46

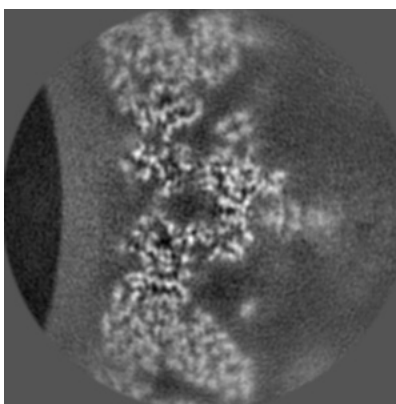


Z Index: 75

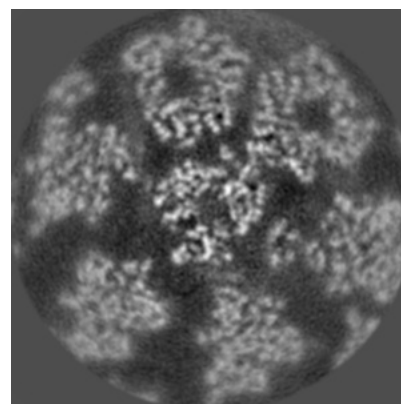
### 6.2.2 Raw map



X Index: 100



Y Index: 100

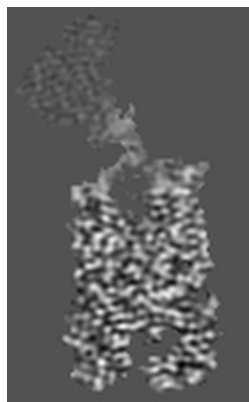


Z Index: 100

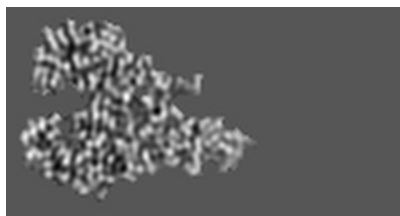
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

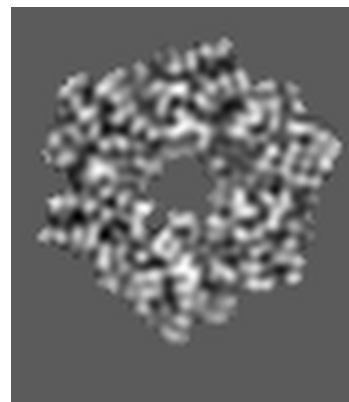
### 6.3.1 Primary map



X Index: 28

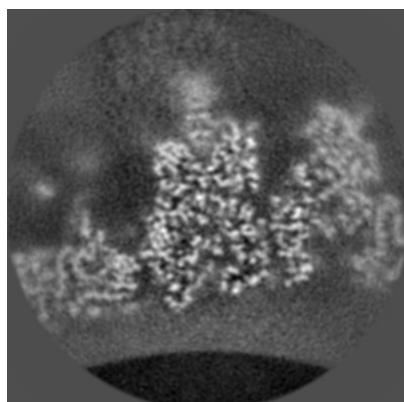


Y Index: 64

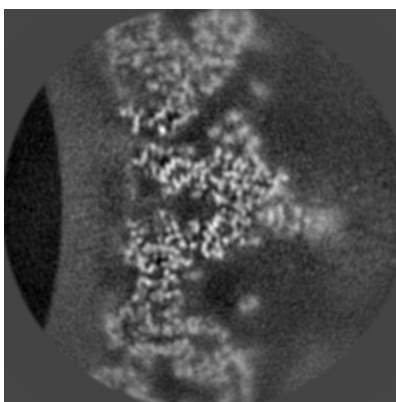


Z Index: 33

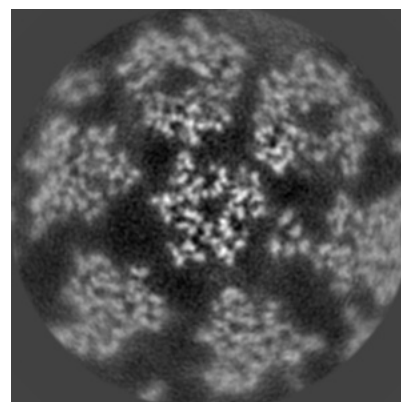
### 6.3.2 Raw map



X Index: 92



Y Index: 96

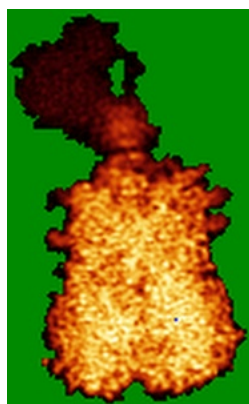


Z Index: 104

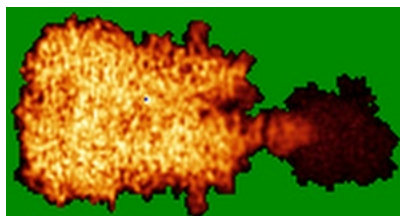
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

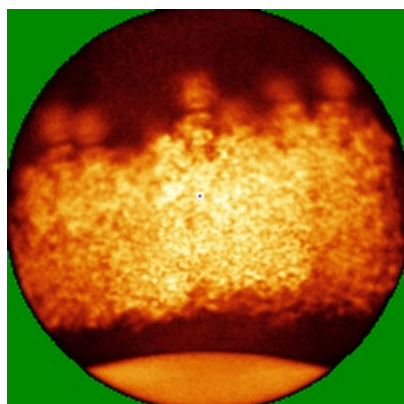


Y

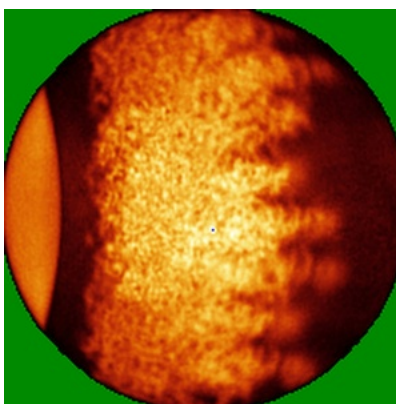


Z

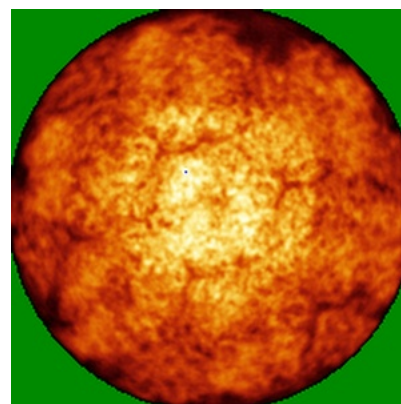
### 6.4.2 Raw map



X



Y

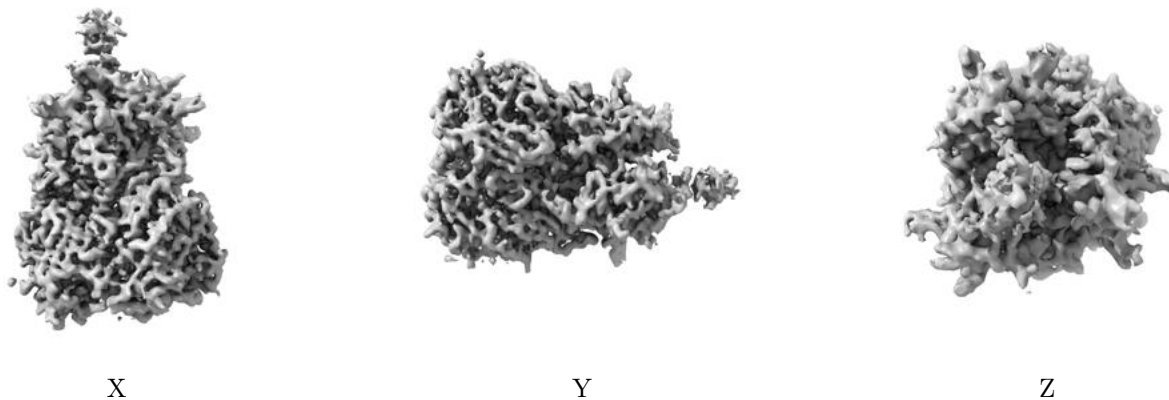


Z

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 0.007. 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.

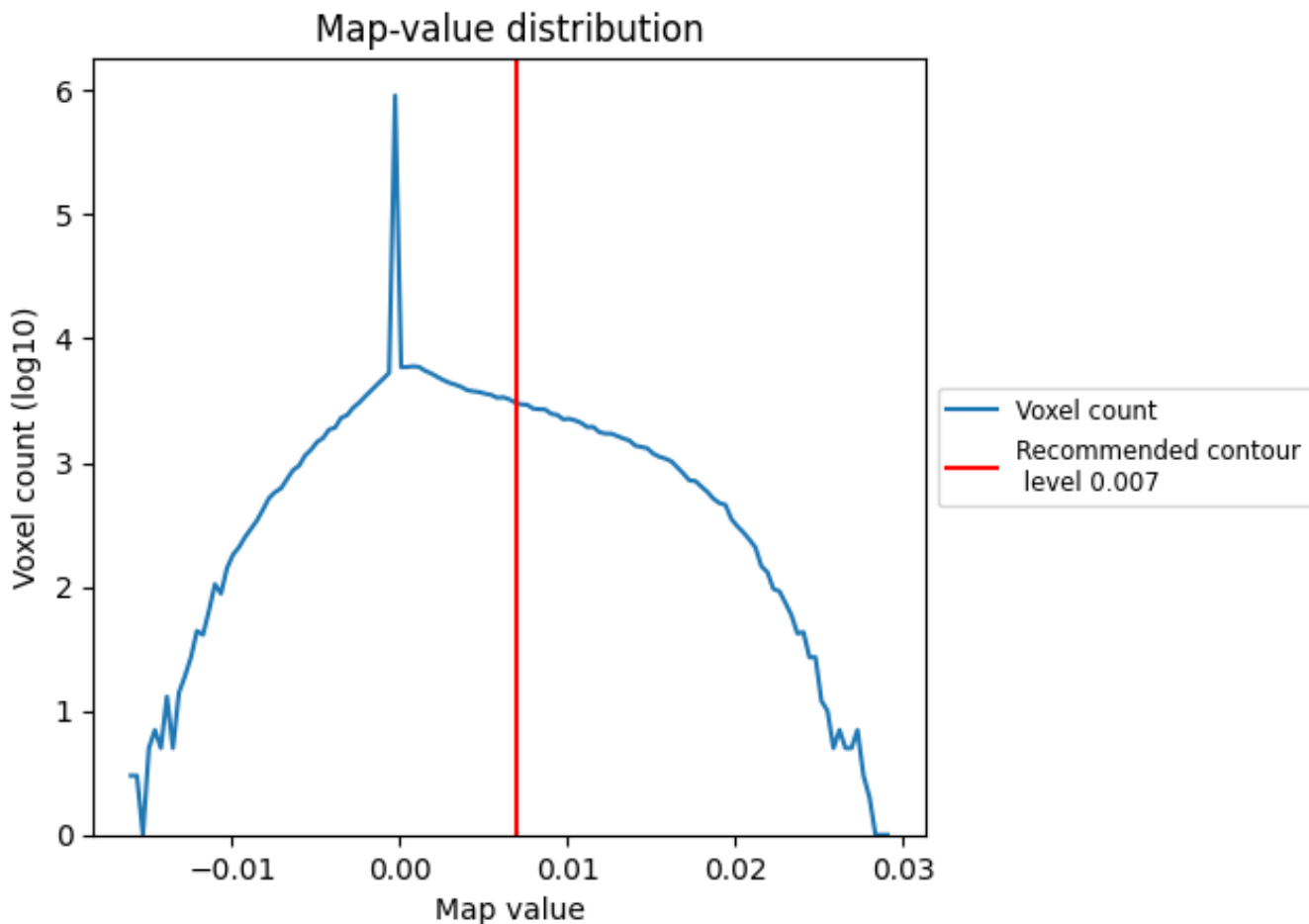
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

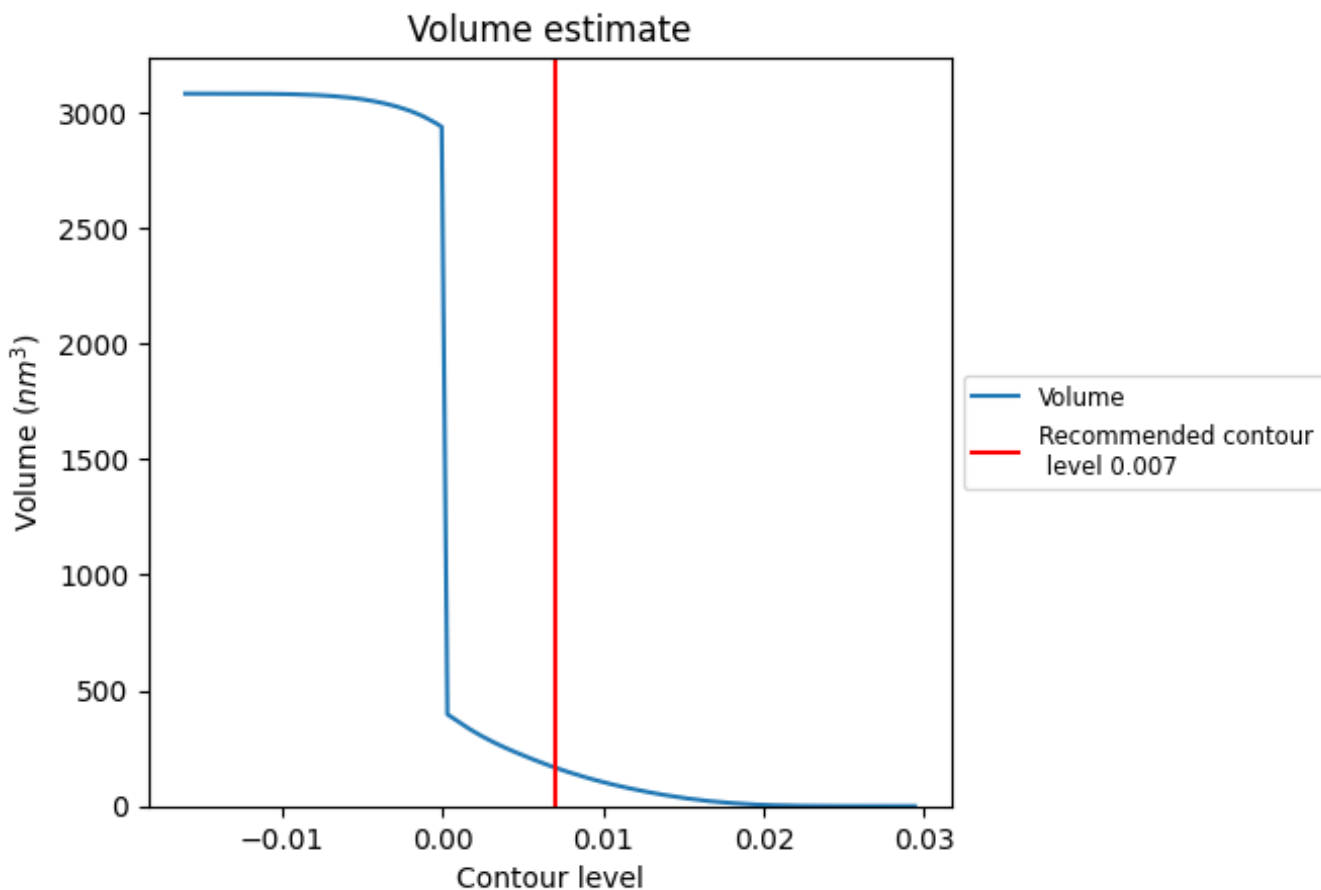
This section contains the results of statistical analysis of the map.

### 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 167 nm<sup>3</sup>; this corresponds to an approximate mass of 151 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.

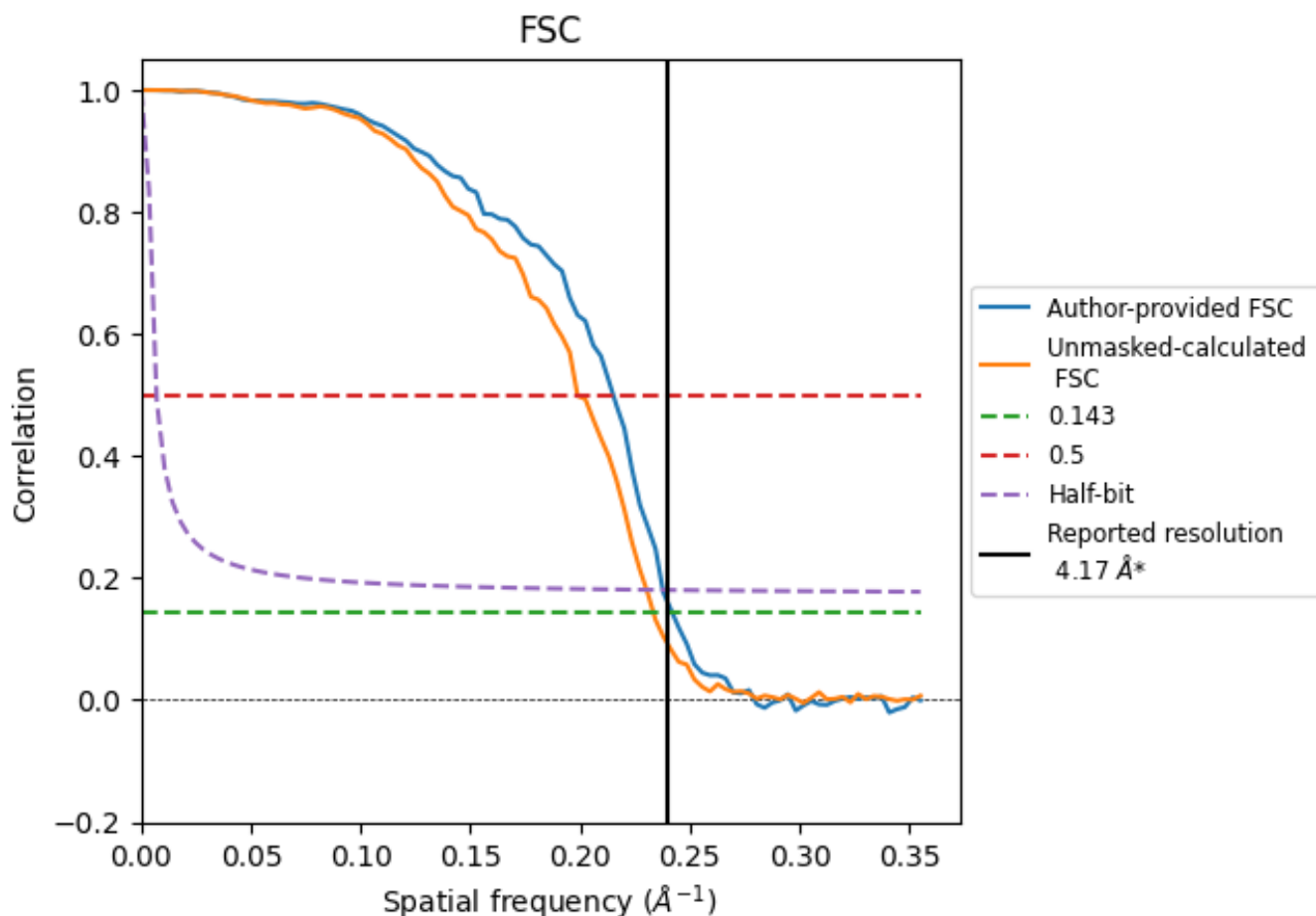
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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 0.240 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

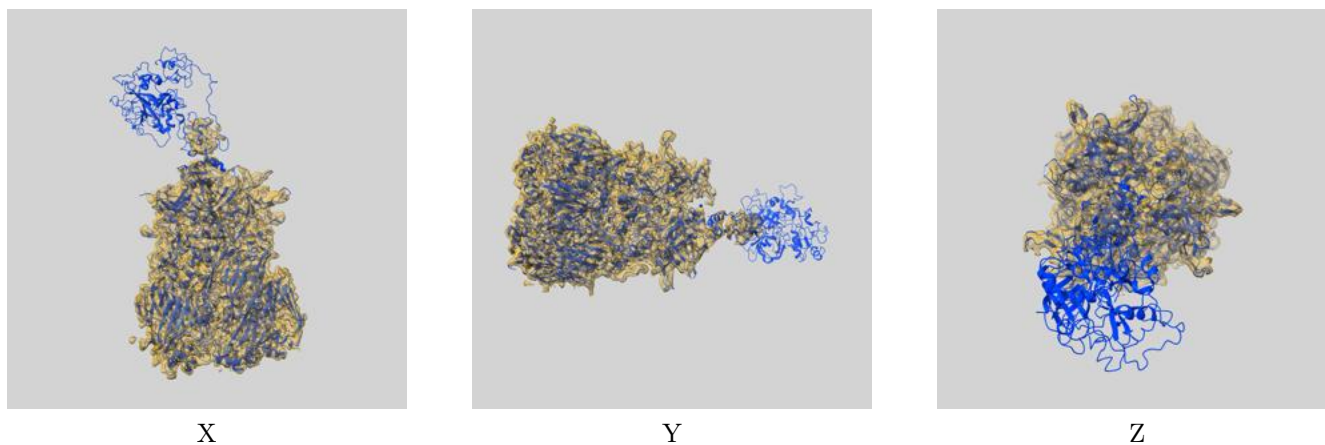
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.17	-	-
Author-provided FSC curve	4.13	4.65	4.21
Unmasked-calculated*	4.28	5.03	4.34

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

## 9 Map-model fit [i](#)

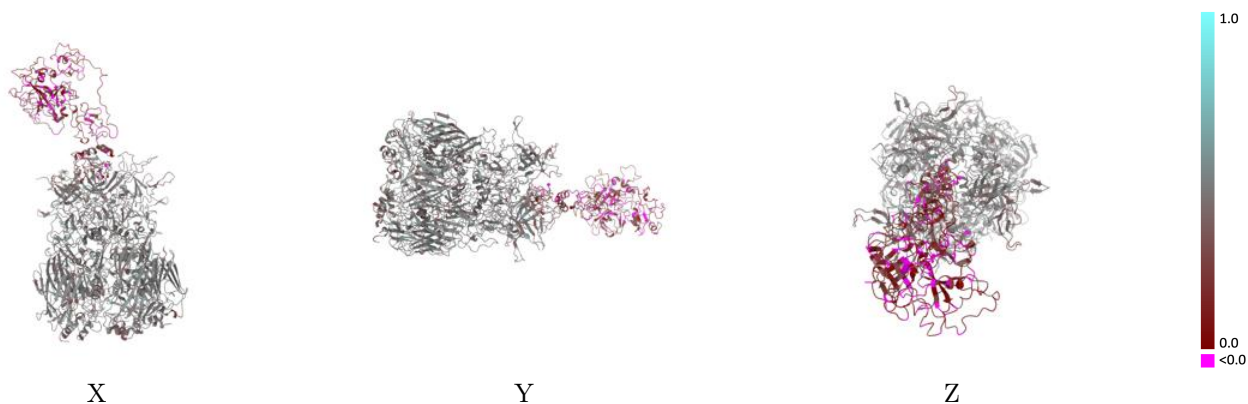
This section contains information regarding the fit between EMDB map EMD-45751 and PDB model 9CMO. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



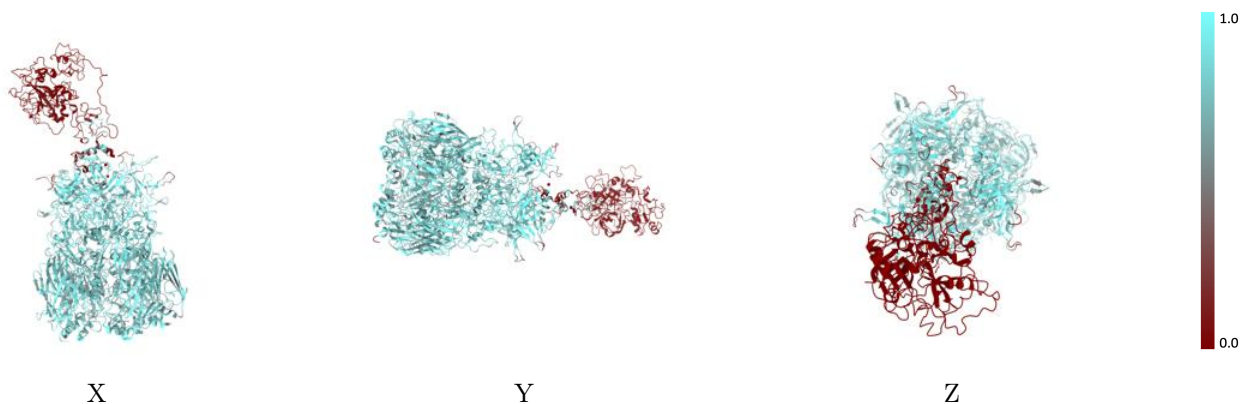
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



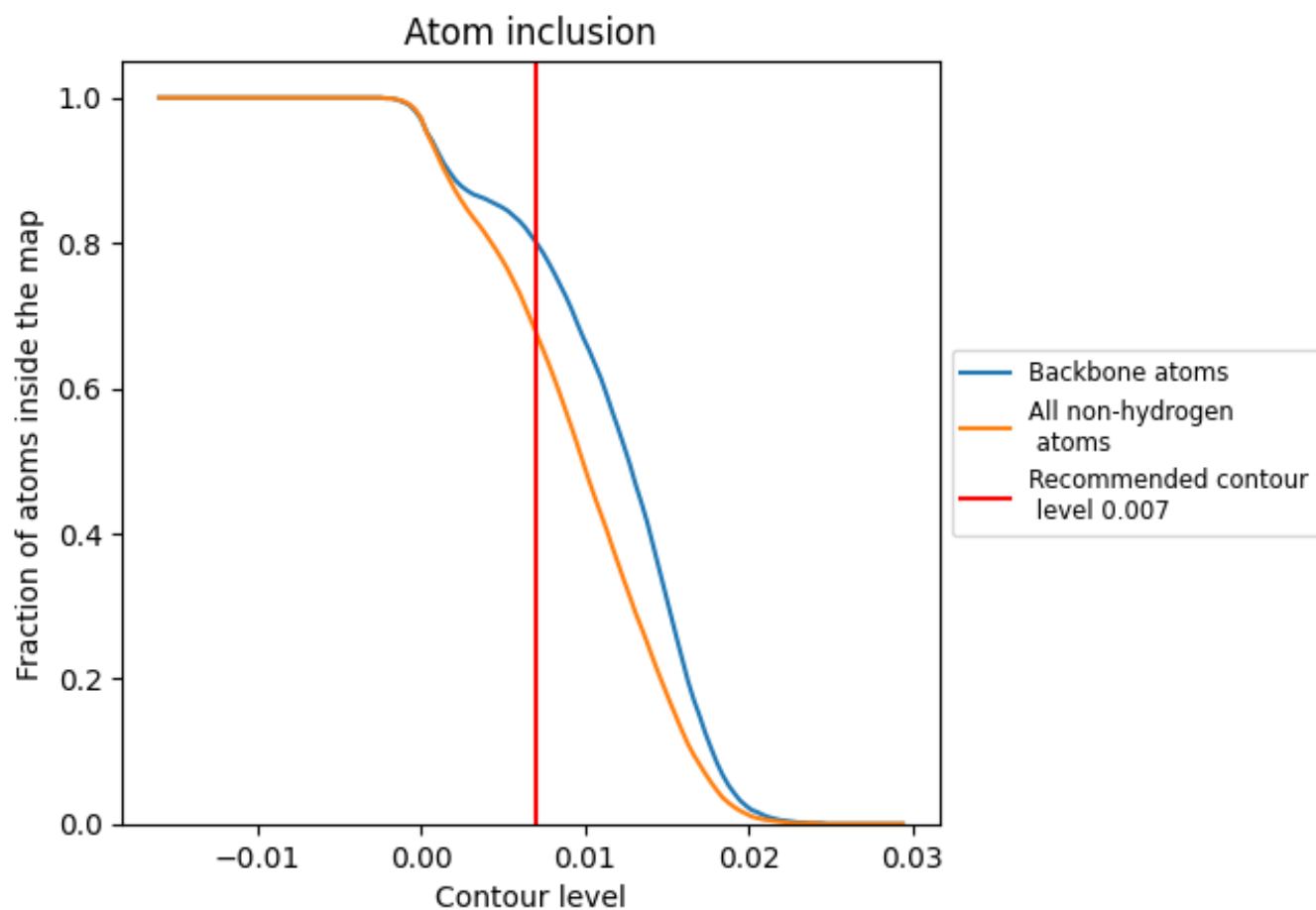
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).











## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 68% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6770	 0.4090
J	 0.7960	 0.4630
K	 0.7980	 0.4590
L	 0.8050	 0.4610
Z	 0.0860	 0.1610

