



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:30 PM UTC

PDB ID : 7YFP / pdb_00007yfp
EMDB ID : EMD-33796
Title : The NuA4 histone acetyltransferase complex from *S. cerevisiae*
Authors : Ji, L.T.; Zhao, L.X.; Xu, K.; Gao, H.H.; Zhou, Y.; Kornberg, R.D.; Zhang, H.Q.
Deposited on : 2022-07-08
Resolution : 4.00 Å(reported)
Based on initial model : 5OJS

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
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

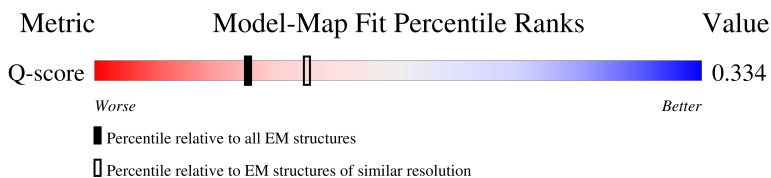
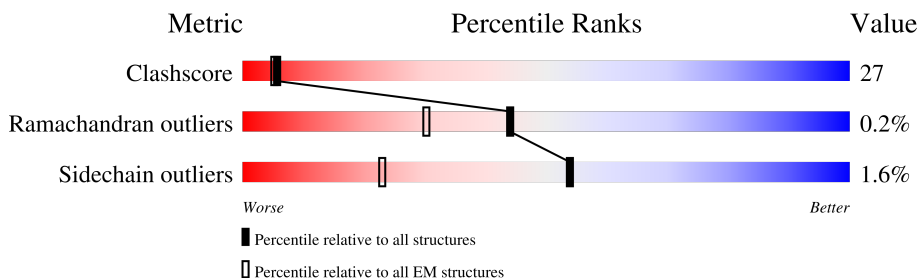
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	372	
2	B	481	
3	D	982	
4	E	476	

Continued on next page...

Mol	Chain	Length	Quality of chain
5	F	832	 9% 6% 85%
6	T	3744	 21% 47% 44% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 40949 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 Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	372	Total	C	N	O	S	0	0
			2904	1841	491	553	19		

- Molecule 2 is a protein called ARP4 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	402	Total	C	N	O	S	0	0
			3172	2024	518	619	11		

- Molecule 3 is a protein called Chromatin modification-related protein EAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	454	Total	C	N	O	S	0	0
			3777	2392	683	691	11		

- Molecule 4 is a protein called SWR1-complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	201	Total	C	N	O	S	0	0
			1668	1069	276	319	4		

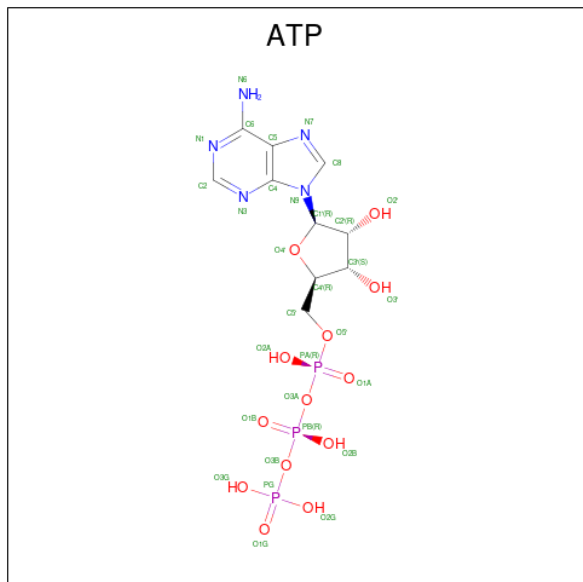
- Molecule 5 is a protein called Enhancer of polycomb-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	124	Total	C	N	O	S	0	0
			1023	653	177	190	3		

- Molecule 6 is a protein called Transcription-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	3475	Total	C	N	O	S	0	0
			28374	18368	4717	5169	120		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

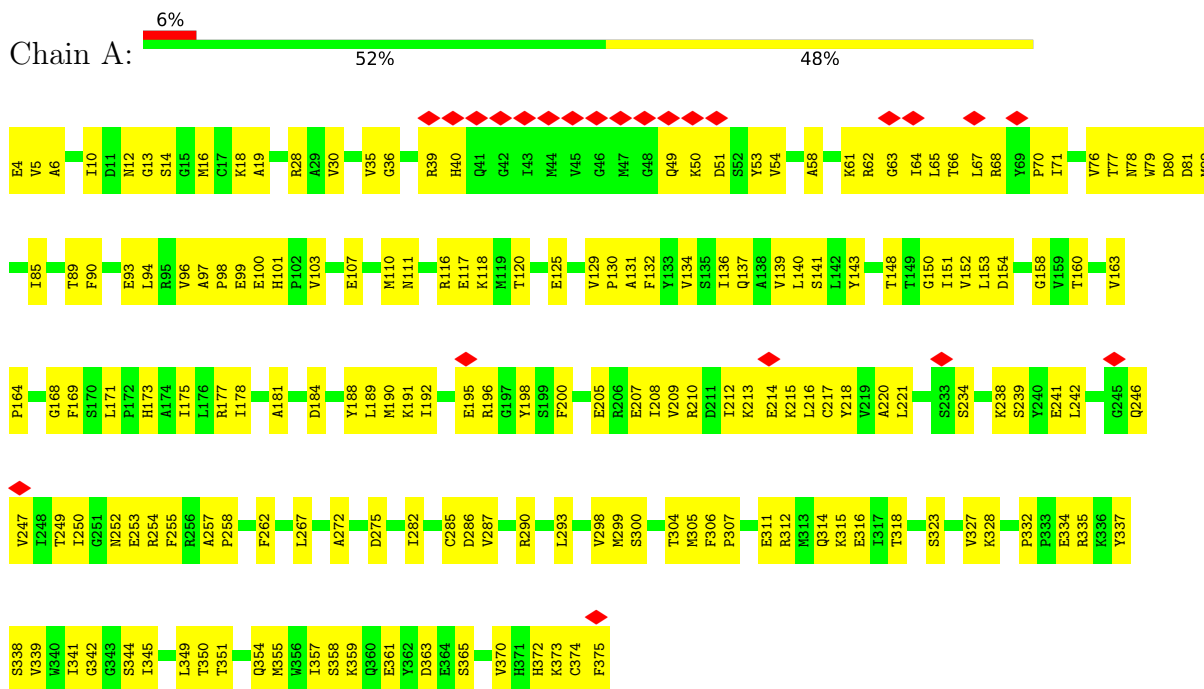


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	B	1	31	10	5	13	3	0

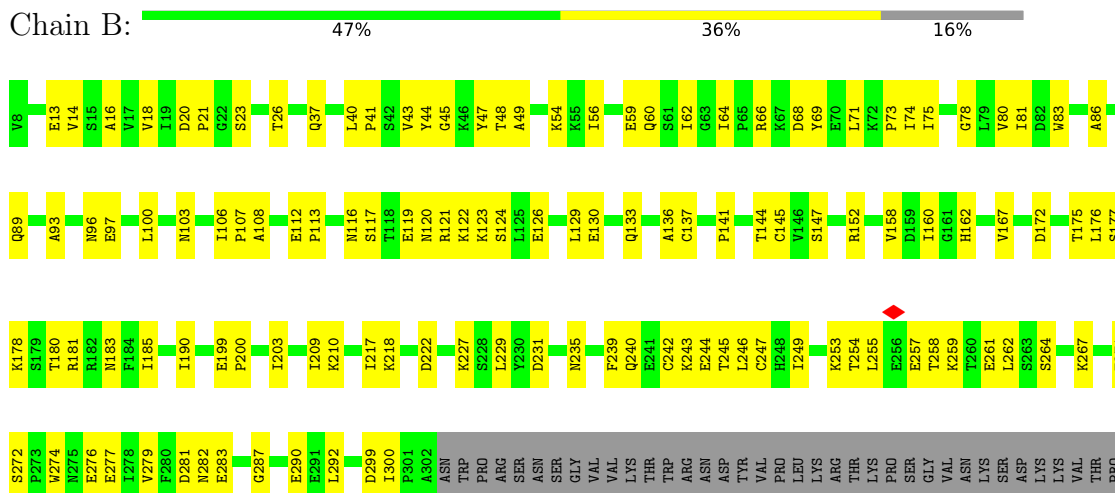
3 Residue-property plots

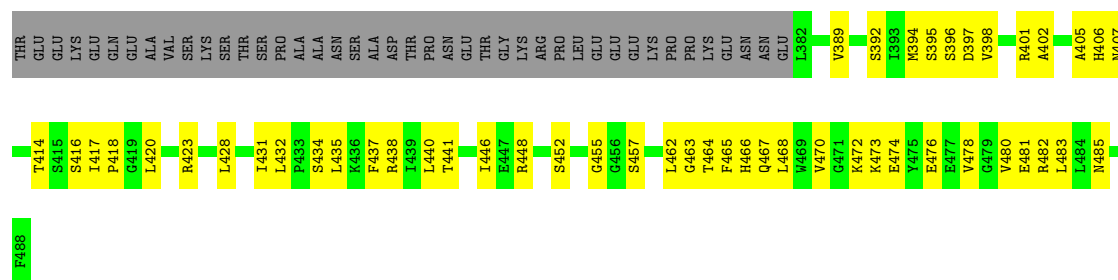
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

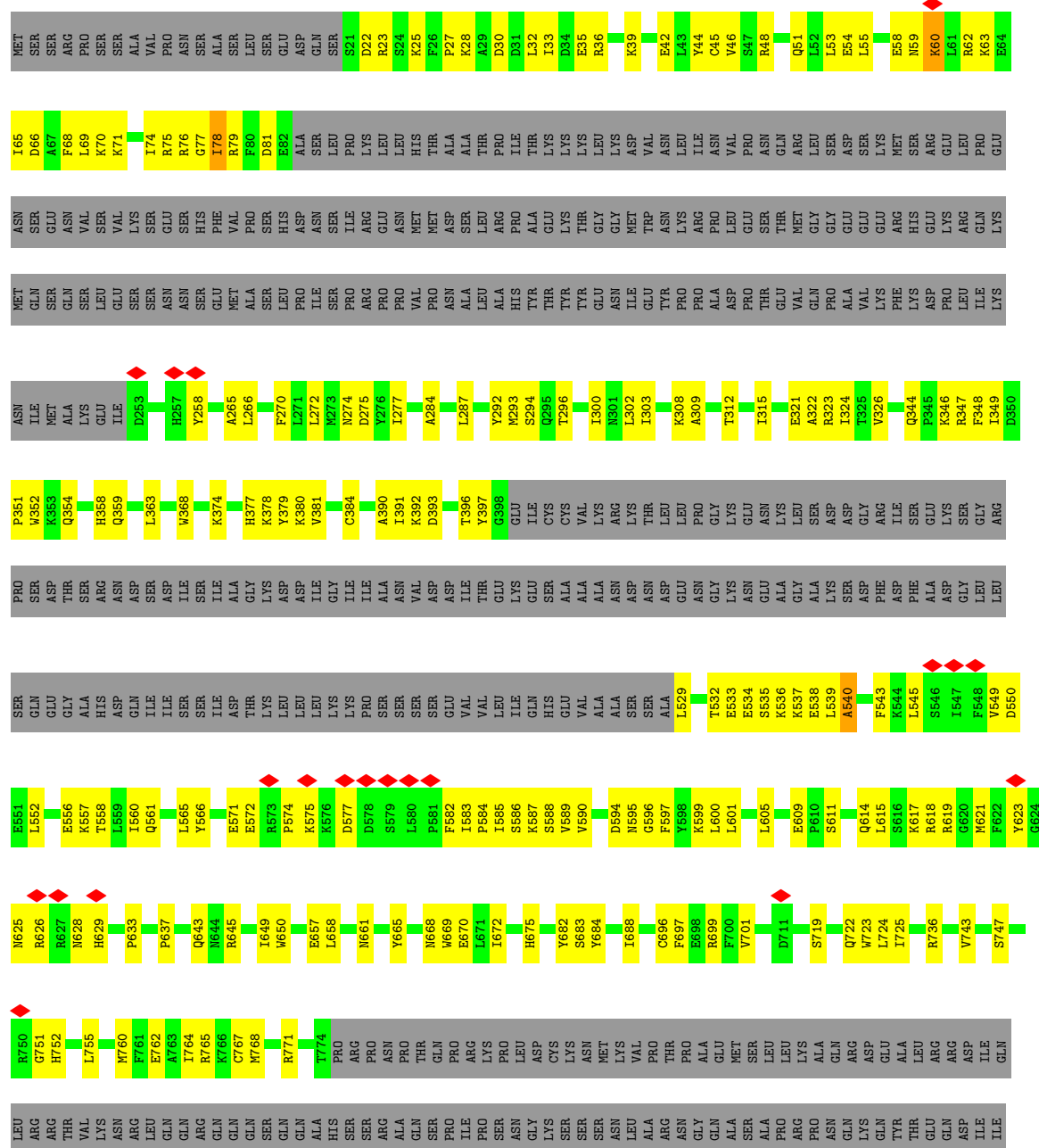
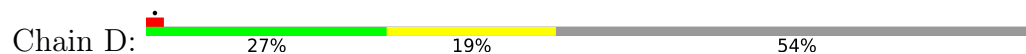


• Molecule 2: ARP4 isoform 1

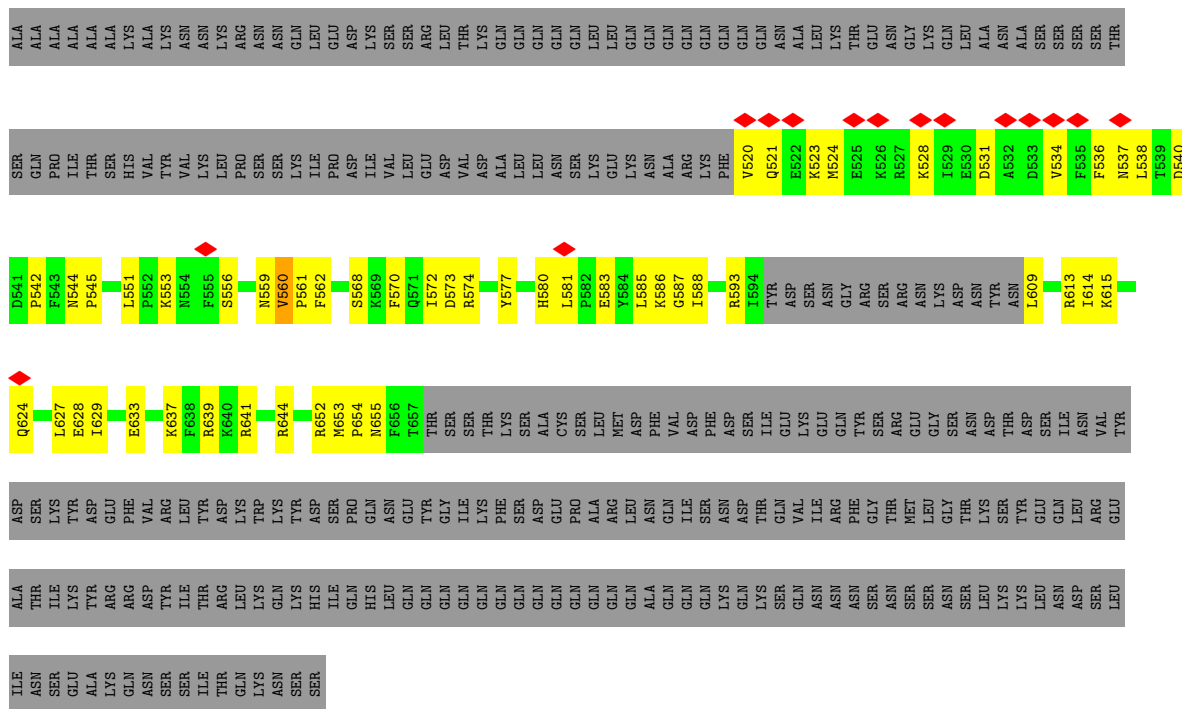




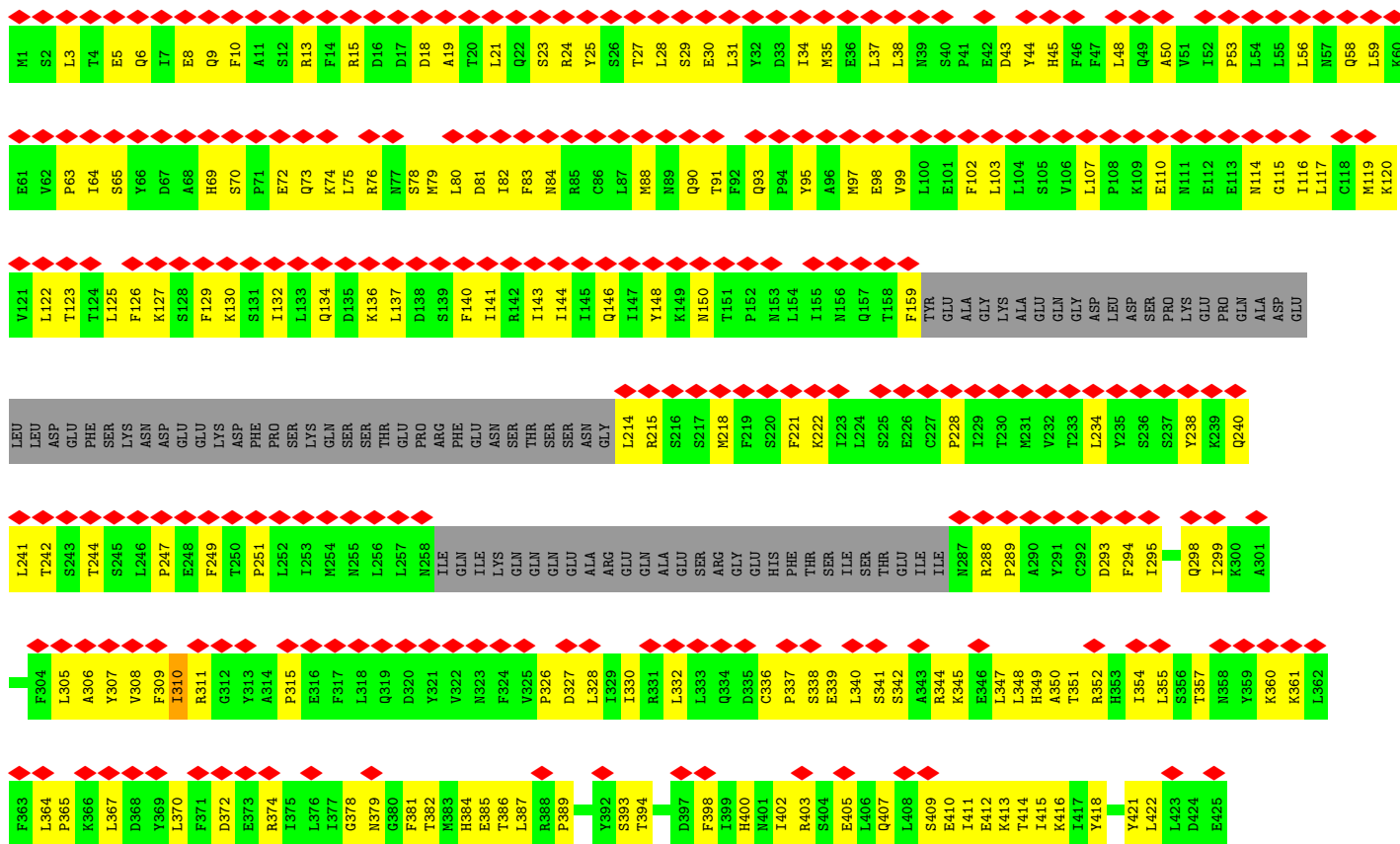
• Molecule 3: Chromatin modification-related protein EAF1







- Molecule 6: Transcription-associated protein 1



Q1350	I1351	G1281	P1191	L1106	I1011	D914	H837	I763	M691	E630	ASN	K496	S426
G1352	L1285	V1284	E1192	L1107	R1014	P915	L838	F766	Q692	V633	ASP	K497	L427
N1353	L1286	E1296	L1193	H1109	R1014	I916	L839	K767	M693	F634	V558	E498	A428
V1354	H1198	E1296	I1198	F1110	Y1018	E918	Q840	L768	D694	K635	M560	K499	L429
L1357	H1199	L1289	H1199	G1111	T1022	I921	L842	S769	T697	D636	F561	A500	T430
T1358	D1203	T1290	D1203	L1112	T1022	D922	H843	F770	F698	L637	D562	E501	V431
F1359	E1204	D1291	E1204	Q1114	K1030	S942	Q844	W771	H699	F638	I563	E501	Q432
L1360	T1205	T1292	T1205	V1115	S1031	H943	L846	S772	E700	H639	I563	K502	I433
L1361	Y1206	V1293	Y1206	N1116	S1031	N944	L847	V773	I701	E640	K564	L503	M434
S1362	T1117	G1294	T1207	T1117	P1036	V945	T648	W774	I702	C541	N565	K504	K437
L1363	T1118	E1295	N1208	T1118	A1046	R947	A849	L775	E705	I642	Y566	N505	L438
T1366	R1123	K1209	K1209	R1123	Y1039	F936	R850	F776	E706	G544	A567	S506	L439
F1367	T1210	R1210	R1210	E1041	T1040	F937	L851	N777	L706	G544	P568	S506	L440
L1368	V1213	V1213	V1213	T1128	E1041	S942	P852	N779	F708	K646	I569	I507	M441
T1369	L1216	L1216	L1216	L1129	L1043	H943	H853	N780	W709	F647	L570	Q508	L442
F1370	P1301	P1301	P1301	N1130	K1044	N944	E854	E781	E710	F548	L571	D509	V443
N1371	K1302	V1303	K1302	L1131	T1045	V945	R855	V782	E711	LYS	L572	N510	E444
E1372	V1303	R1304	V1303	L1132	A1046	V946	E856	L783	R712	ASP	P573	D511	R445
E1373	R1304	C1307	V1223	L1133	S1049	R947	L857	L784	M713	HIS	T574	K512	I446
L1374	C1307	C1307	V1223	K1134	S1049	I948	R858	L785	L714	ASN	P575	E513	L447
F1375	L1311	L1311	F1229	L1140	I1050	L949	H859	P786	E715	GLU	T576	S514	E452
R1376	H1312	H1312	L1230	L1144	L1052	G950	E860	H787	D716	LEU	N577	E515	P458
L1377	I1313	I1313	Q1234	I1145	L1052	K951	L861	L788	S717	PRO	L586	E516	R459
Q1379	I1314	I1314	L1237	L1146	E1053	L952	C862	N789	G718	THR	L586	E516	A460
E1380	S1315	S1315	L1237	L1146	R1054	N956	L863	D790	L719	GLU	L586	E516	K461
S1381	G1319	G1319	G1240	Y1155	I1057	R957	P866	P786	L722	THR	L586	E516	K461
I1382	I1320	I1320	G1240	I1156	E1058	R957	VAL	H787	A723	THR	L586	E516	K461
V1383	G1323	G1323	V1245	I1157	K1059	P963	LEU	L793	Q724	THR	L586	E516	K461
L1384	K1324	K1324	L1248	E1158	N1060	T964	ARG	S795	L727	THR	L586	E516	K461
A1385	L1325	L1325	T1248	P1158	F1061	D965	LEU	L796	W728	THR	L586	E516	K461
A1386	H1328	H1328	E1251	E1159	D1062	L966	VAL	S799	E729	THR	L586	E516	K461
E1388	S1329	S1329	P1253	V1160	T1066	E968	ALA	T801	I731	THR	L586	E516	K461
D1389	F1332	F1332	I1256	R1161	V1067	L972	PRO	A802	I732	THR	L586	E516	K461
E1390	L1333	L1333	T1257	E1162	V1067	D973	L876	P805	G738	THR	L586	E516	K461
S1391	L1334	L1334	D1258	V1178	K1068	K981	P877	L806	I739	THR	L586	E516	K461
L1392	S1335	S1335	S1259	I1171	R1070	F960	F878	L807	L740	THR	L586	E516	K461
S1393	P1336	P1336	E1261	K1174	Q1075	I982	L879	Y808	L741	THR	L586	E516	K461
T1394	I1337	I1337	I1261	S1175	V1086	N983	H890	L812	R742	THR	L586	E516	K461
N1395	F1338	F1338	I1265	I1179	A1089	G986	Q896	R817	E743	THR	L586	E516	K461
I1396	A1339	A1339	D1266	G1180	T1090	E987	R899	R823	L744	THR	L586	E516	K461
Q1397	K1341	K1341	L1267	E1181	S1091	K981	L876	R823	L744	THR	L586	E516	K461
K1398	L1342	L1342	L1268	L1183	D1097	I982	P877	R823	L744	THR	L586	E516	K461
T1399	R1343	R1343	S1269	L1184	Q1097	N983	H890	R823	L744	THR	L586	E516	K461
T1400	A1344	A1344	T1271	L1185	H1001	G986	Q896	R823	L744	THR	L586	E516	K461
E1401	L1345	L1345	F1272	L1187	D1101	F960	Q896	R823	L744	THR	L586	E516	K461
Y1402	P1346	P1346	K1276	H1187	L1102	I982	Q896	R823	L744	THR	L586	E516	K461
S1403	F1347	F1347	T1348	S1188	L1103	N983	Q896	R823	L744	THR	L586	E516	K461
T1404	T1348	T1348	M1349	F1189	N1104	G986	Q896	R823	L744	THR	L586	E516	K461
E1405	M1349	M1349	M1349	I1190	N1105	L1001	Q905	R823	L744	THR	L586	E516	K461
Q1407	Q1407	Q1407	Q1407	I1190	N1105	L1001	Q905	R823	L744	THR	L586	E516	K461
L1408	L1408	L1408	L1408	I1190	N1105	L1001	Q905	R823	L744	THR	L586	E516	K461
Q1410	Q1410	Q1410	Q1410	I1190	N1105	L1001	Q905	R823	L744	THR	L586	E516	K461
L1411	L1411	L1411	L1411	I1190	N1105	L1001	Q905	R823	L744	THR	L586	E516	K461

L2190	L2191	E2192	K2193	C2194	L2195	S2197	D2198	H2199	H2200	D2201	E2204	A2205	L2206	K2145	F2146	V2208	V2209	I2210	Q2211	V2212	T2213	N2214	K2215	A2216	E2217	N2158	I2159	Y2160	N2163	A2164	L2165	D2166	V2167	L2168	Y2169	V2170	F2171	K2172	K2173	N2174	K2175	T2176	K2177	N2237	K2238	L2239	T2240	S2241	M2181	E2182	N2183	L2184	Q2245	Q2246	L2247	Q2248	E2249	T2250			
ASP	SER	LYS	SER	ASP	ILE	ASN	PRO	THR	GLU	ASN	VAL	ALA	THR	ALA	ILE	ILE	ILE	VAL	ASP	ALA	ASN	ASN	PRO	ILE	S2089	L2090	H2091	L2092	R2093	E2094	C2095	T2097	A2098	F2099	L2100	T2101	R2102	Y2103	S2107	ASN	HIS	ARG	ALA	ILE	GLU	THR	E2115	L2116	Q2117	L2118	R2119	A2120	I2121	N2122	I2123	L2124					
L2127	I2128	S2129	D2130	LYS	HIS	THR	THR	ASN	ASN	VAL	ASN	ASN	THR	Y2142	F2143	E2144	F2145	F2146	LEU	ILE	PHE	GLN	ASP	LEU	S2154	E2155	N2156	I2157	L2158	Y2159	Y2160	N2163	A2164	L2165	D2166	V2167	L2168	Y2169	V2170	F2171	K2172	K2173	N2174	K2175	T2176	K2177	N2237	K2238	L2239	T2240	S2241	M2181	E2182	N2183	L2184	Q2245	Q2246	L2247	Q2248	E2249	T2250
F1997	M1998	S1999	R2000	D2001	L2002	F2003	I2004	S2005	N2006	I2007	I2008	H2009	H2010	M2011	N2012	K2013	I2014	T2015	F2016	MET	SER	ASN	PRO	ILE	S2089	L2090	H2091	L2092	R2093	E2094	C2095	T2097	A2098	F2099	L2100	T2101	R2102	Y2103	S2107	ASN	HIS	ARG	ALA	ILE	GLU	THR	E2115	L2116	Q2117	L2118	R2119	A2120	I2121	N2122	I2123	L2124					
H1935	V1936	E1937	A1938	R1939	L1940	L1941	Q1944	S1945	L1946	D1947	V1948	L1949	T1950	I1951	V1952	L1953	H1954	E1955	R1956	M1957	ASN	PRO	ILE	S2089	L2090	H2091	L2092	R2093	E2094	C2095	T2097	A2098	F2099	L2100	T2101	R2102	Y2103	S2107	ASN	HIS	ARG	ALA	ILE	GLU	THR	E2115	L2116	Q2117	L2118	R2119	A2120	I2121	N2122	I2123	L2124						
F1801	V1802	L1803	K1804	S1809	I1812	Y1813	E1814	V1815	A1816	T1817	S1818	G1819	S1820	L1821	F1822	K1823	Y1824	L1825	V1826	E1827	D1828	K1829	K1830	P1831	K1832	H1838	M1839	K1840	K1843	N1846	A1847	I1848	L1849	A1850	Y1851	D1852	V1853	L1854	D1855	H1856	H1857	L1858	L1859	R1861	F1862	E1863	L1864	L1867	I1870	F1871	I1872										
K1873	A1874	D1875	P1876	E1877	I1878	I1879	A1880	E1881	T1882	K1883	D1884	I1885	I1886	I1887	K1888	F1889	C1890	V1891	M1892	I1893	I1894	K1895	L1896	D1897	E1898	T1899	L1900	I1901	K1902	Q1903	S1904	A1905	Y1906	L1907	V1908	T1909	S1910	Y1911	F1912	I1913	S1914	K1915	F1916	D1917	F1918	P1919	I1920	K1921	V1922	V1923	T1924	F1927	L1930	L1931	R1932	S1933	S1934				
H1935	V1936	E1937	A1938	R1939	L1940	L1941	Q1944	S1945	L1946	D1947	V1948	L1949	T1950	I1951	V1952	L1953	H1954	E1955	R1956	M1957	ASN	PRO	ILE	S2089	L2090	H2091	L2092	R2093	E2094	C2095	T2097	A2098	F2099	L2100	T2101	R2102	Y2103	S2107	ASN	HIS	ARG	ALA	ILE	GLU	THR	E2115	L2116	Q2117	L2118	R2119	A2120	I2121	N2122	I2123	L2124						
F1997	M1998	S1999	R2000	D2001	L2002	F2003	I2004	S2005	N2006	I2007	I2008	H2009	H2010	M2011	N2012	K2013	I2014	T2015	F2016	MET	SER	ASN	PRO	ILE	S2089	L2090	H2091	L2092	R2093	E2094	C2095	T2097	A2098	F2099	L2100	T2101	R2102	Y2103	S2107	ASN	HIS	ARG	ALA	ILE	GLU	THR	E2115	L2116	Q2117	L2118	R2119	A2120	I2121	N2122	I2123	L2124					
ASP	SER	LYS	SER	ASP	ILE	ASN	PRO	THR	GLU	ASN	VAL	ALA	THR	ALA	ILE	ILE	VAL	ASP	ALA	ASN	ASN	PRO	ILE	S2089	L2090	H2091	L2092	R2093	E2094	C2095	T2097	A2098	F2099	L2100	T2101	R2102	Y2103	S2107	ASN	HIS	ARG	ALA	ILE	GLU	THR	E2115	L2116	Q2117	L2118	R2119	A2120	I2121	N2122	I2123	L2124						
L2127	I2128	S2129	D2130	LYS	HIS	THR	THR	ASN	ASN	VAL	ASN	ASN	THR	Y2142	F2143	E2144	F2145	F2146	LEU	ILE	PHE	GLN	ASP	LEU	S2154	E2155	N2156	I2157	L2158	Y2159	Y2160	N2163	A2164	L2165	D2166	V2167	L2168	Y2169	V2170	F2171	K2172	K2173	N2174	K2175	T2176	K2177	N2237	K2238	L2239	T2240	S2241	M2181	E2182	N2183	L2184	Q2245	Q2246	L2247	Q2248	E2249	T2250
R1412	I1413	A1414	C1415	I1416	K1417	L1418	L1419	A1420	I1421	A1422	L1423	K1424	N1425	E1426	E1427	F1428	A1429	T1430	A1431	Q1432	Q1433	G1434	N1435	I1436	R1437	I1438	I1439	I1440	L1441	A1442	V1443	F1444	F1445	K1446	T1447	M1448	L1449	K1450	T1451	S1452	P1453	E1454	I1455	I1456	N1457	T1458	T1459	Y1460	E1461	A1462	K1464	G1465	L1467	A1468	E1469	N1470	S1471				
K1472	L1473	P1474	K1475	L1476	L1477	L1478	Q1479	N1480	G1481	L1482	K1483	P1484	L1485	L1486	M1487	N1488	L1489	S1490	D1491	H1492	Q1493	G1494	L1495	T1496	V1497	P1498	G1499	L1500	D1501	A1502	P1503	P1504	Q1505	L1506	L1507	E1508	F1509	L1510	I1511	A1512	L1513	E1514	F1515	L1516	E1517	I1518	G1519	R1520	L1521	L1522	L1523	D1524	H1525	L1526	T1527	A1528	C1530	R1531			
V1532	E1533	V1534	L1535	D1536	T1537	L1538	F1539	G1540	Q1541	D1542	L1543	A1544	E1545	Q1546	M1547	P1548	K1550	I1551	I1552	V1553	S1554	I1555	I1556	M1557	I1558	F1559	H1560	L1561	L1562	P1563	P1564	Q1565	A1566	L1567	M1568	F1569	L1570	N1571	D1572	L1573	L1574	L1575	L1576	V1577	L1580	E1581	R1582	L1583	L1584	L1585	L1586	Q1587	L1588	D1589	S1590	P1591	F1592				
R1593	T1594	P1595	L1596	A1597	R1598	Y1599	M1601	R1602	F1603	H1604	M1605	P1606	A1607	T1608	E1609	Y1610	F1611	K1612	K1613	M1614	M1615	T1616	L1617	R1618	L1619	L1620	V1621	L1622	F1623	M1624	C1625	M1626	I1627	V1628	Q1629	R1630	P1631	A1632	A1633	K1634	E1635	L1636	A1637	F1640	E1641	K1642	L1643	D1644	M1645	N1646	F1647	Y1648	D1649	F1650	Y1651	M1654					
I1655	P1656	K1657	M1658	Q1659	V1660	R1661	N1662	S1663	F1664	F1665	M1669	D1670	L1671	L1672	F1673	M1674	T1675	M1676	V1677	L1678	G1681	D1682	E1683	W1684	L1685	K1686	K1687	L1688	G1689	I1692	L1695	M1698	L1699	T1702	L1703	K1704	T1705	L1706	E1707	S1710	F1711	Y1712	K1713	D1714	H1715	L1716	Q1717	L1718	N1719	Q1720	L1728										
L1735	E1736	R1737	R1738	Q1739	Q1740	N1741	F1742	L1743	L1744	L1745	F1747	L1748	D1749	F1750	S1751	F1752	S1753	N1754	G1755	I1756	K1757	A1758	S1759	Y1760	S1761	L1762	F1765	L1766	F1767	H1768	N1769	I1770	I1771	A1772	S1773	S1774	N1775	K1776	E1777	K1778	Q1779	N1780	N1781	F1789	V1790	L1791	S1792	D1793	K1794	G1795	L1796	D1797	F1799	I1800							
F1801	V1802	L1803	K1804	S1809	I1812	Y1813	E1814	V1815	A1816	T1817	S1818	G1819	S1820	L1821	F1822	K1823	Y1824	L1825	V1826	E1827	D1828	K1829	K1830	P1831	K1832	H1838	M1839	K1840	K1843	N1846	A1847	I1848	L1849	A1850	Y1851	D1852	V1853	L1854	D1855	H1856	H1857	L1858	L1859	R1861	F1862	E1863	L1864	L1867	I1870	F1871	I1872										
K1873	A1874	D1875	P1876	E1877	I1878	I1879	A1880	E1881	T1882	K1883	D1884	I1885	I1886	I1887	K1888	F1889	C1890	V1891	M1892	I1893	I1894	K1895	L1896	D1897	E1898	T1899	L1900	I1901	K1902	Q1903	S1904	A1905	Y1906	L1907	V1908	T1909	S1910	Y1911	F1912	I1913	S1914	K1915	F1916	D1917	F1918	P1919	I1920	K1921	V1922	V1923	T1924	F1927	L1930	L1931	R1932	S1933	S1934				
H1935	V1936	E1937	A1938	R1939	L1940	L1941	Q1944	S1945	L1946	D1947	V1948	L1949	T1950	I1951	V1952	L1953	H1954	E1955	R1956	M1957	ASN	PRO	ILE	S2089	L2090	H2091	L2092	R2093	E2094	C2095	T2097	A2098	F2099	L2100	T2101	R2102	Y2103	S2107	ASN	HIS	ARG	ALA	ILE	GLU	THR	E2115	L2116	Q2117	L2118	R2119	A2120	I2121	N2122	I2123	L2124						



E3590	P3592	D3505	Q3406	P3305
N3691	V3596	N3506	Y3407	D3306
N3695	LYS	T3507	V3410	Y3307
N3699	PRO	I3508	R3411	E3308
N3710	LEU	L3509	H3412	T3309
N3711	LEU	T3519	S3413	L3314
N3715	LYS	V3522	R3414	N3317
N3716	ASN	P3523	R3415	N3320
N3717	HIS	F3524	E3416	L3321
T3720	ASP	S3524	E3417	E3322
L3721	LEU	N3525	R3418	D3326
L3724	SER	K3528	F3420	K3331
A3727	LEU	R3532	Q3421	E3332
V3728	PRO	T3532	L3422	N3333
S3729	I3613	S3533	Y3423	V3336
P3730	F3614	L3534	F3426	P3339
R3731	H3615	E3539	N3427	N3343
N3732	V3620	D3540	K3428	E3353
L3733	R3623	F3541	S3431	Q3357
A3734	I3624	N3542	N3432	Q3358
R3735	T3625	L3543	V3434	N3365
T3736	P3626	F3544	E3435	F3368
T3737	R3629	R3545	T3436	I3369
V3738	Q3629	Q3551	R3437	I3371
N3739	D3634	Y3552	R3438	A3372
F3740	S3635	S3553	N3439	R3373
N3743	A3636	S3554	S3440	T3377
F3744	L3637	N3558	I3441	V3378
	E3638	K3561	Q3442	R3382
	G3639	N3562	F3443	T3384
	I3648	N3563	N3444	H3385
	P3655	I3564	P3446	I3393
	N3659	N3565	L3451	D3397
	T3661	N3566	I3457	C3398
	F3666	R3567	D3460	S3399
	D3669	H3573	F3464	V3400
	H3679	V3574	T3465	H3401
	R3680	D3575	T3466	V3405
	P3681	S3578	N3472	
	I3682	N3579	K3476	
	E3683	I3580	P3482	
	E3684	V3581	L3493	
	N3685	T3582	H3497	
	P3686	L3584	D3498	
	Q3687	E3585	D3499	
	L3688	N3586		
	R3689	L3587		
		P3588		
		S3589		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	197044	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0396	Depositor
Map size ($\text{\AA}$)	330.0, 330.0, 330.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.66, 0.66, 0.66	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.18	0/2968	0.36	0/4017
2	B	0.23	0/3241	0.38	0/4398
3	D	0.25	0/3859	0.48	0/5212
4	E	0.20	0/1707	0.38	0/2300
5	F	0.24	0/1046	0.55	0/1405
6	T	0.50	0/28991	0.72	4/39278 (0.0%)
All	All	0.44	0/41812	0.64	4/56610 (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
3	D	0	3
5	F	0	1
6	T	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	3592	PRO	N-CA-CB	6.65	110.23	103.25
6	T	1960	ALA	N-CA-C	-6.22	106.33	114.04
6	T	1436	ILE	N-CA-C	-5.66	107.36	112.12
6	T	2872	SER	N-CA-C	-5.47	107.25	114.04

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	535	SER	Peptide
3	D	540	ALA	Peptide
3	D	60	LYS	Peptide
5	F	560	VAL	Peptide
6	T	1366	THR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2904	0	2874	138	0
2	B	3172	0	3125	136	0
3	D	3777	0	3763	190	0
4	E	1668	0	1630	73	0
5	F	1023	0	999	58	0
6	T	28374	0	28736	1730	0
7	B	31	0	12	5	0
All	All	40949	0	41139	2238	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 27.

The worst 5 of 2238 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:480:ARG:HD3	6:T:1760:TYR:CD1	1.17	1.60
6:T:2320:LEU:CD1	6:T:2355:MET:HB3	1.26	1.58
6:T:480:ARG:CB	6:T:1760:TYR:CZ	1.86	1.55
6:T:480:ARG:HD3	6:T:1760:TYR:CE1	1.40	1.53
6:T:2320:LEU:HD11	6:T:2355:MET:C	1.30	1.50

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/372 (100%)	346 (94%)	24 (6%)	0	100	100
2	B	398/481 (83%)	365 (92%)	33 (8%)	0	100	100
3	D	448/982 (46%)	357 (80%)	91 (20%)	0	100	100
4	E	197/476 (41%)	174 (88%)	23 (12%)	0	100	100
5	F	120/832 (14%)	93 (78%)	26 (22%)	1 (1%)	16	52
6	T	3445/3744 (92%)	3069 (89%)	366 (11%)	10 (0%)	36	70
All	All	4978/6887 (72%)	4404 (88%)	563 (11%)	11 (0%)	44	75

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	T	1796	LEU
6	T	1980	SER
5	F	542	PRO
6	T	1993	PRO
6	T	1206	TYR

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/317 (100%)	317 (100%)	0	100	100
2	B	354/428 (83%)	354 (100%)	0	100	100
3	D	414/892 (46%)	413 (100%)	1 (0%)	87	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	184/441 (42%)	184 (100%)	0	100	100
5	F	114/769 (15%)	113 (99%)	1 (1%)	70	76
6	T	3188/3452 (92%)	3117 (98%)	71 (2%)	45	65
All	All	4571/6299 (73%)	4498 (98%)	73 (2%)	54	70

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	T	2192	GLU
6	T	2556	ILE
6	T	2201	ASP
6	T	2269	ASP
6	T	1716	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
6	T	1604	HIS
6	T	3537	GLN
6	T	1998	ASN
6	T	3515	ASN
6	T	3073	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
7	ATP	B	501	-	32,33,33	1.30	5 (15%)	48,52,52	1.77	11 (22%)

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
7	ATP	B	501	-	-	3/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	ATP	C5-C4	4.34	1.46	1.39
7	B	501	ATP	C5-C6	2.51	1.48	1.41
7	B	501	ATP	C5-N7	-2.46	1.34	1.39
7	B	501	ATP	C4-N9	-2.32	1.32	1.37
7	B	501	ATP	C8-N7	2.09	1.35	1.31

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	ATP	C5-C4-N3	-5.66	118.93	126.72
7	B	501	ATP	N3-C4-N9	4.60	135.00	127.17
7	B	501	ATP	C2-N3-C4	3.58	120.57	111.83
7	B	501	ATP	C4-C5-N7	-3.28	106.83	110.58
7	B	501	ATP	N3-C2-N1	-3.05	123.97	128.58

There are no chirality outliers.

All (3) torsion outliers are listed below:

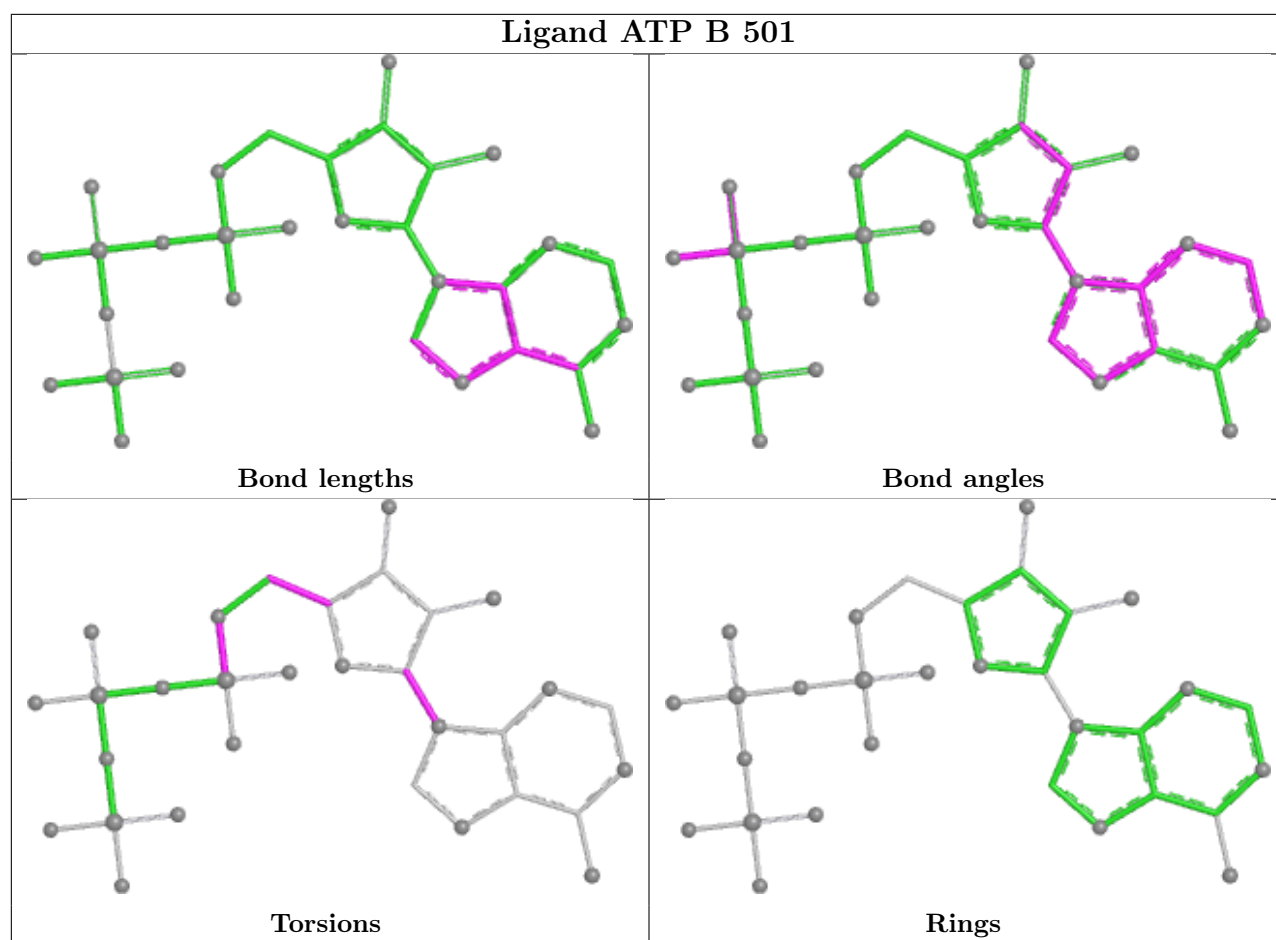
Mol	Chain	Res	Type	Atoms
7	B	501	ATP	C5'-O5'-PA-O1A
7	B	501	ATP	C2'-C1'-N9-C8
7	B	501	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	ATP	5	0

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 [i](#)

There are no chain breaks in this entry.

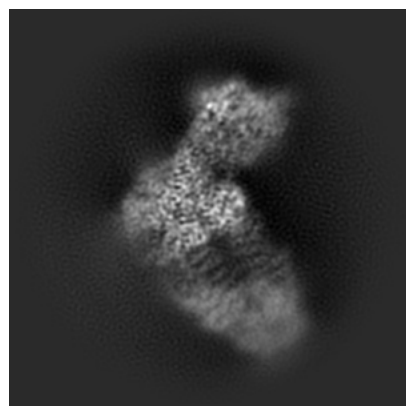
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33796. These allow visual inspection of the internal detail of the map and identification of artifacts.

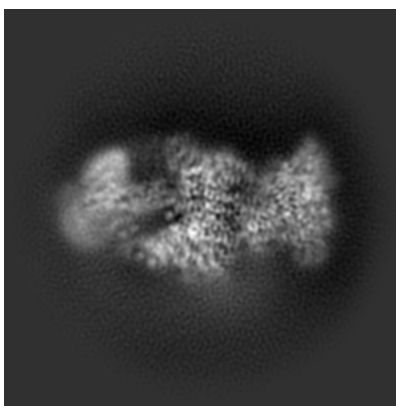
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

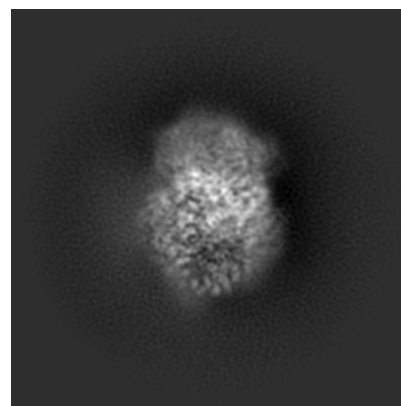
6.1.1 Primary map



X

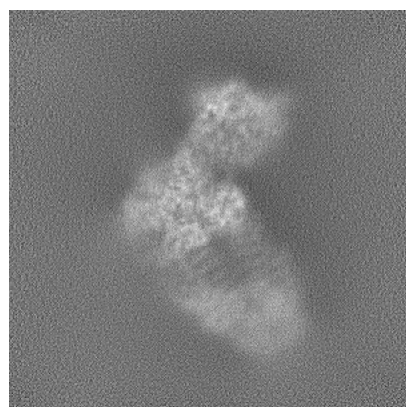


Y

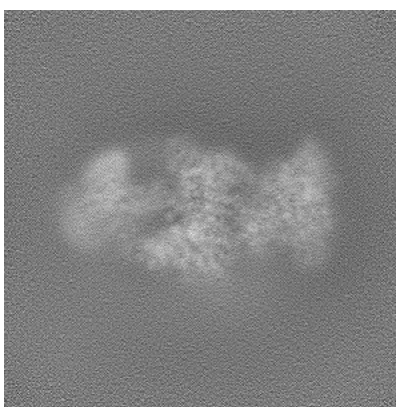


Z

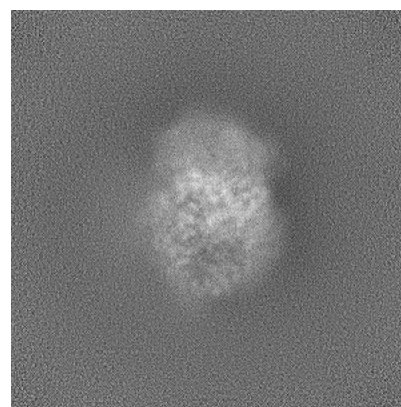
6.1.2 Raw map



X



Y

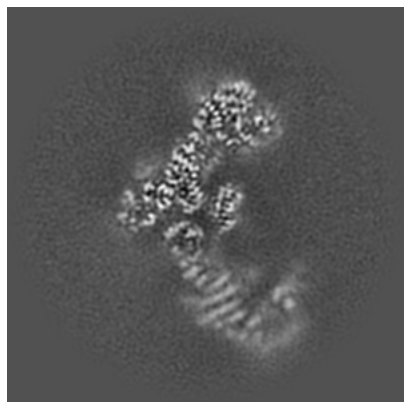


Z

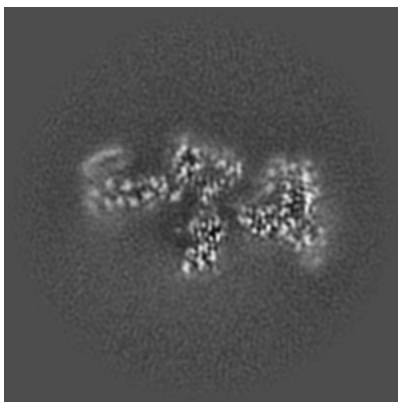
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

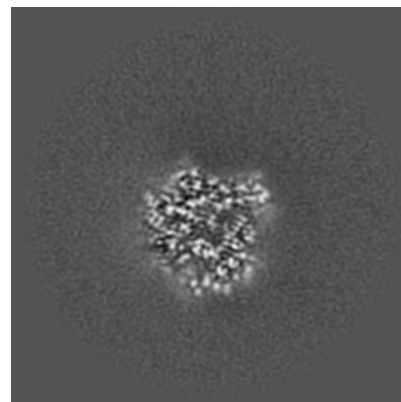
6.2.1 Primary map



X Index: 250

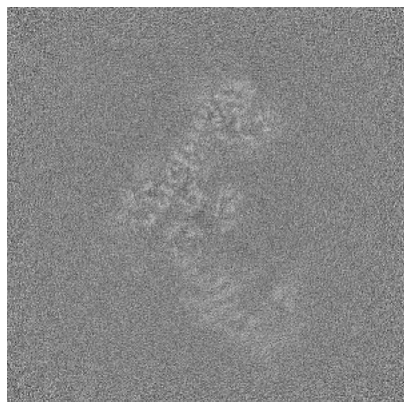


Y Index: 250

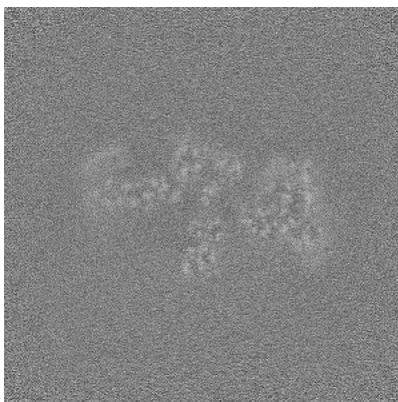


Z Index: 250

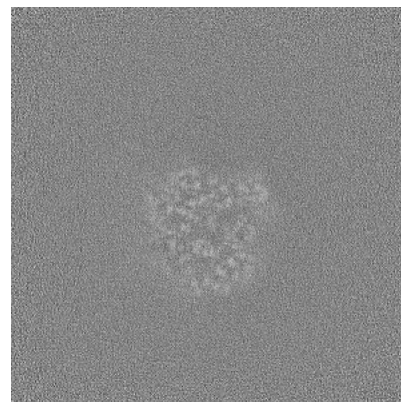
6.2.2 Raw map



X Index: 250



Y Index: 250

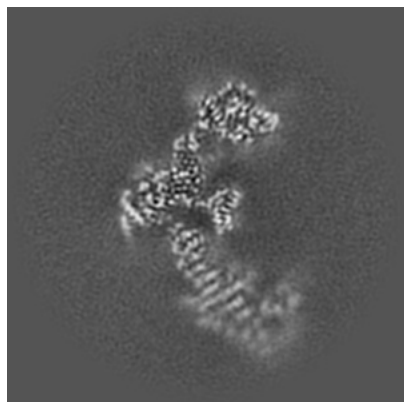


Z Index: 250

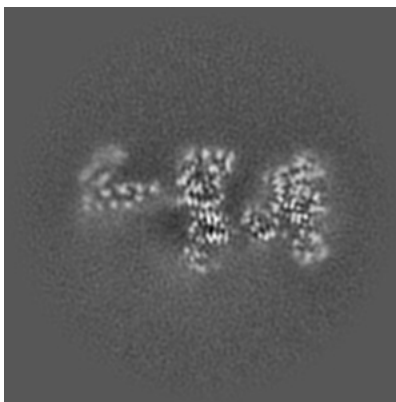
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

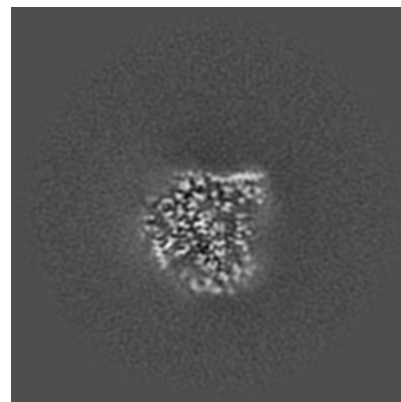
6.3.1 Primary map



X Index: 256

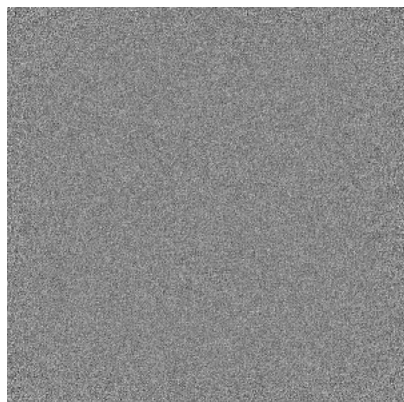


Y Index: 264

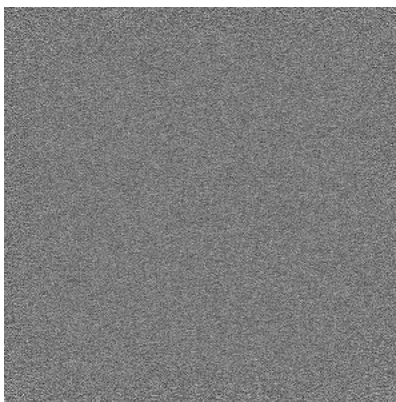


Z Index: 257

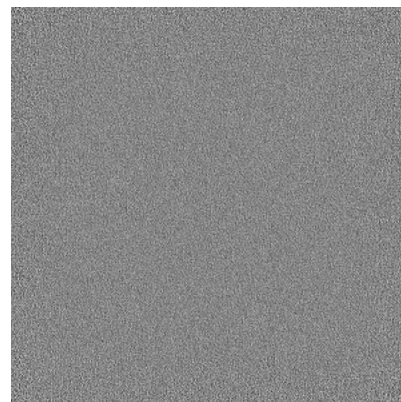
6.3.2 Raw map



X Index: 0



Y Index: 0

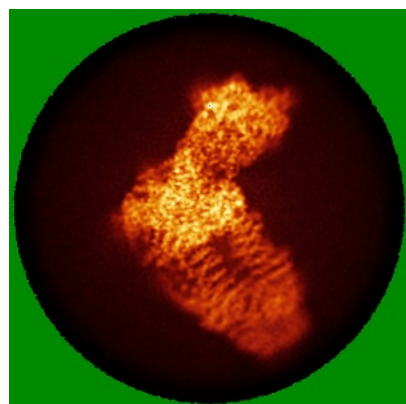


Z Index: 0

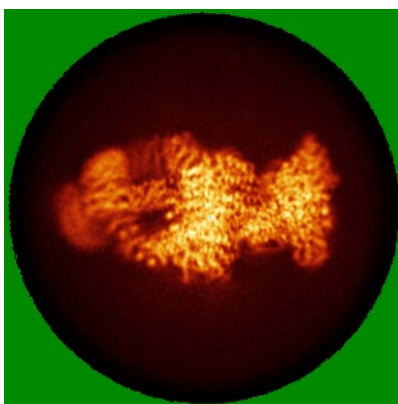
The images above show the largest variance slices of the map in three orthogonal directions.

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

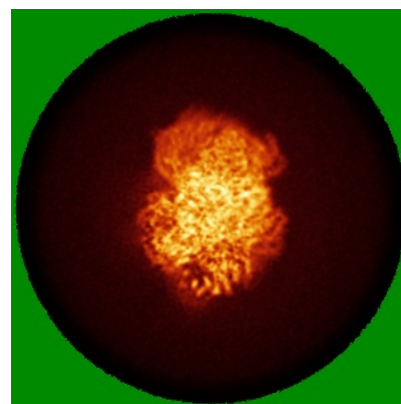
6.4.1 Primary map



X

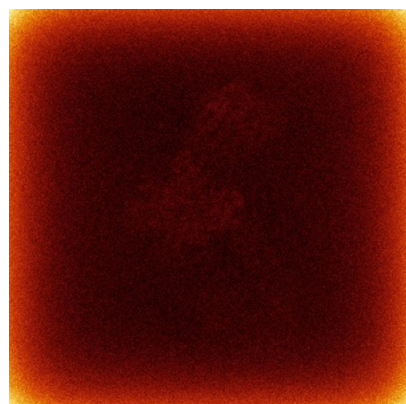


Y

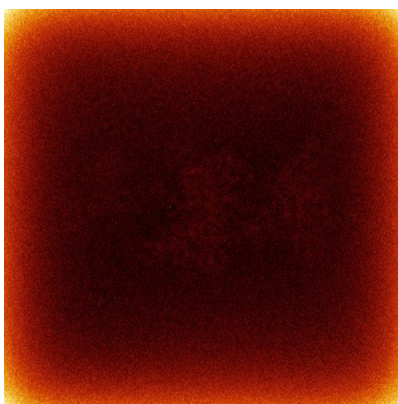


Z

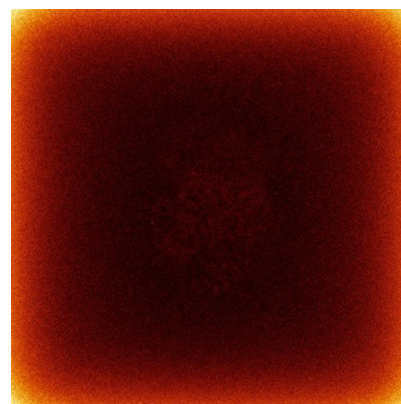
6.4.2 Raw map



X



Y

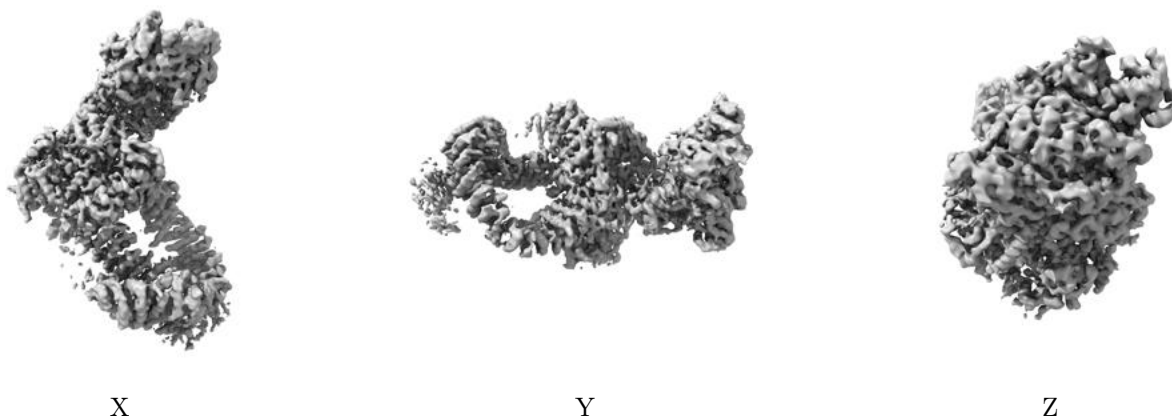


Z

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.

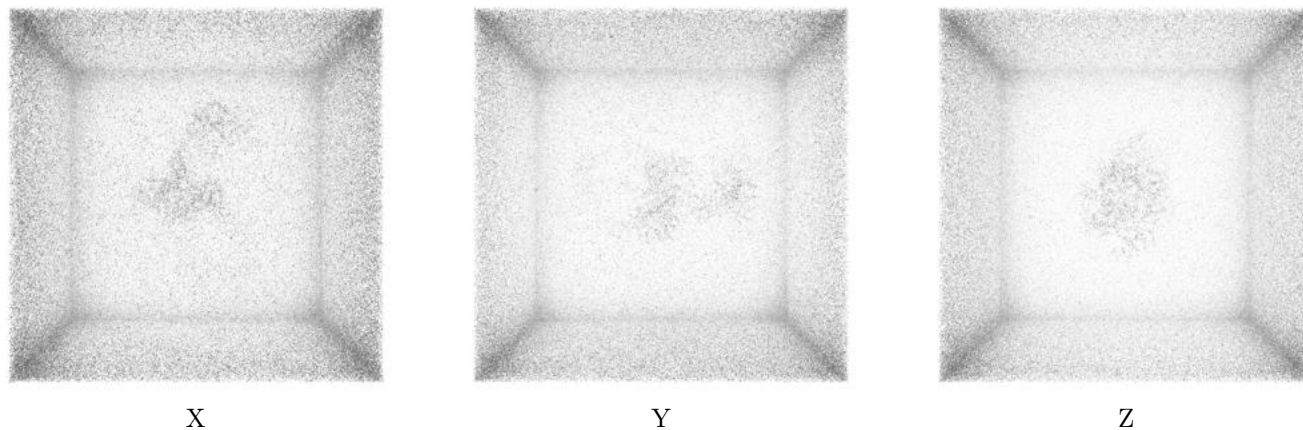
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0396. 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.

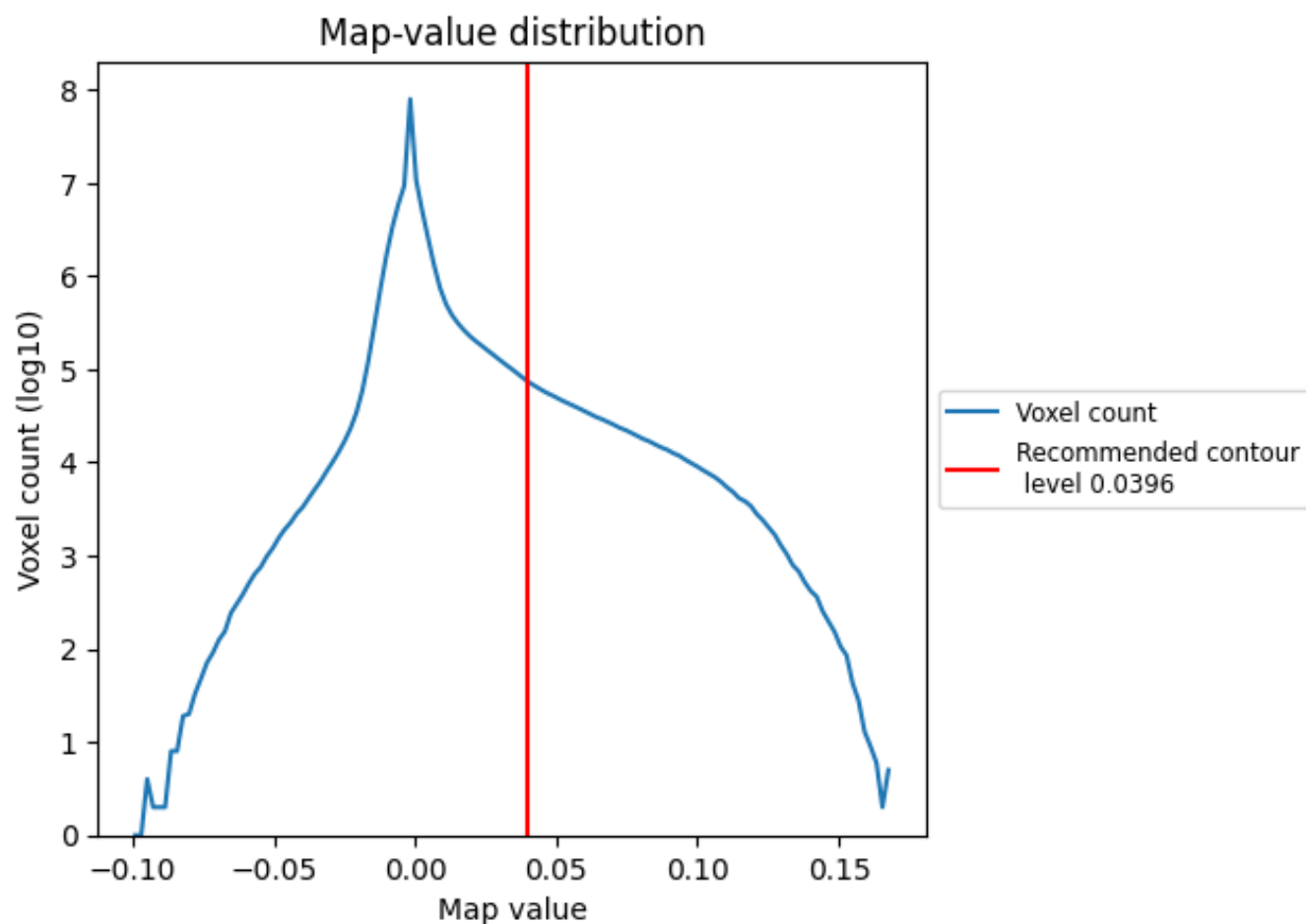
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

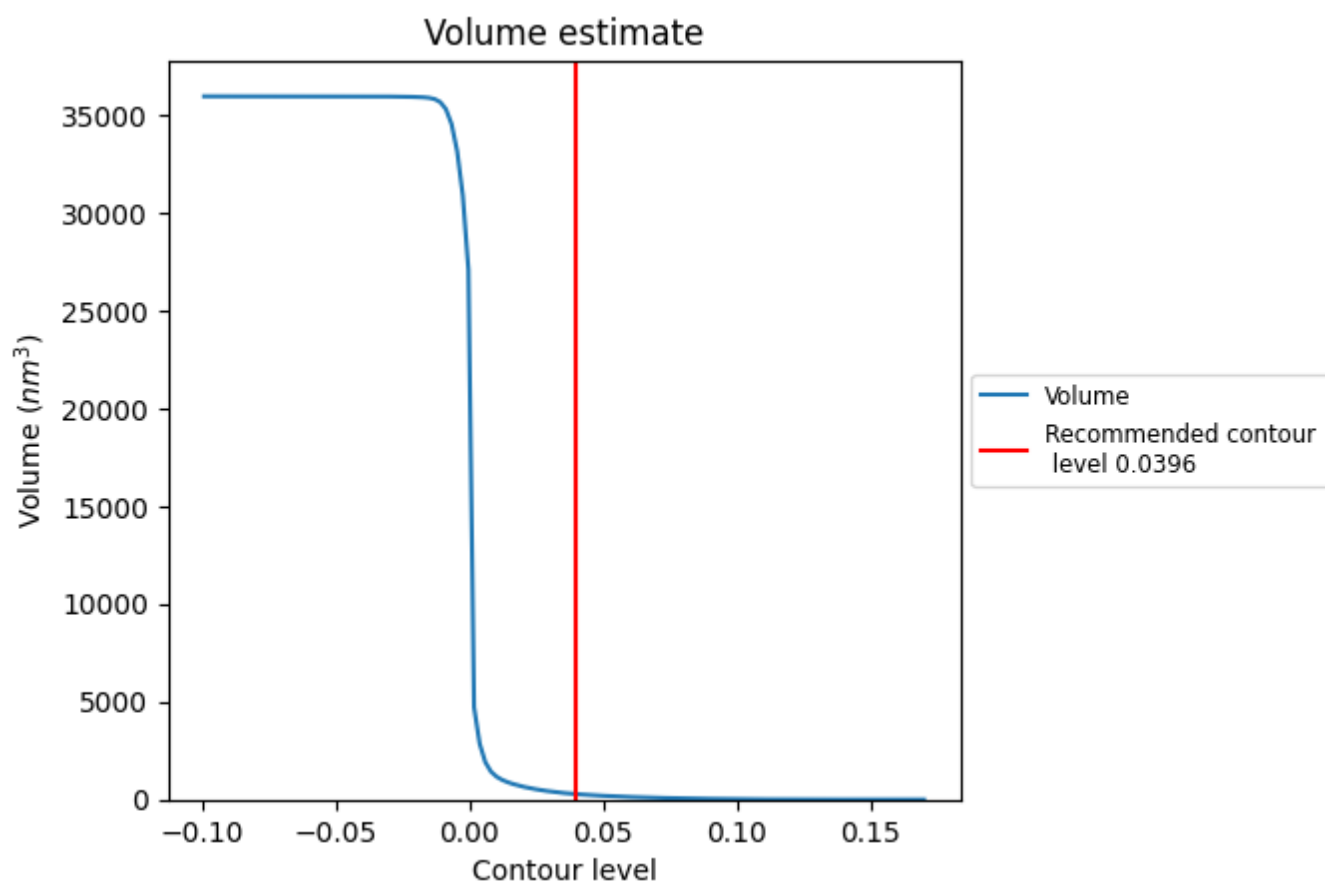
This section contains the results of statistical analysis of the map.

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.

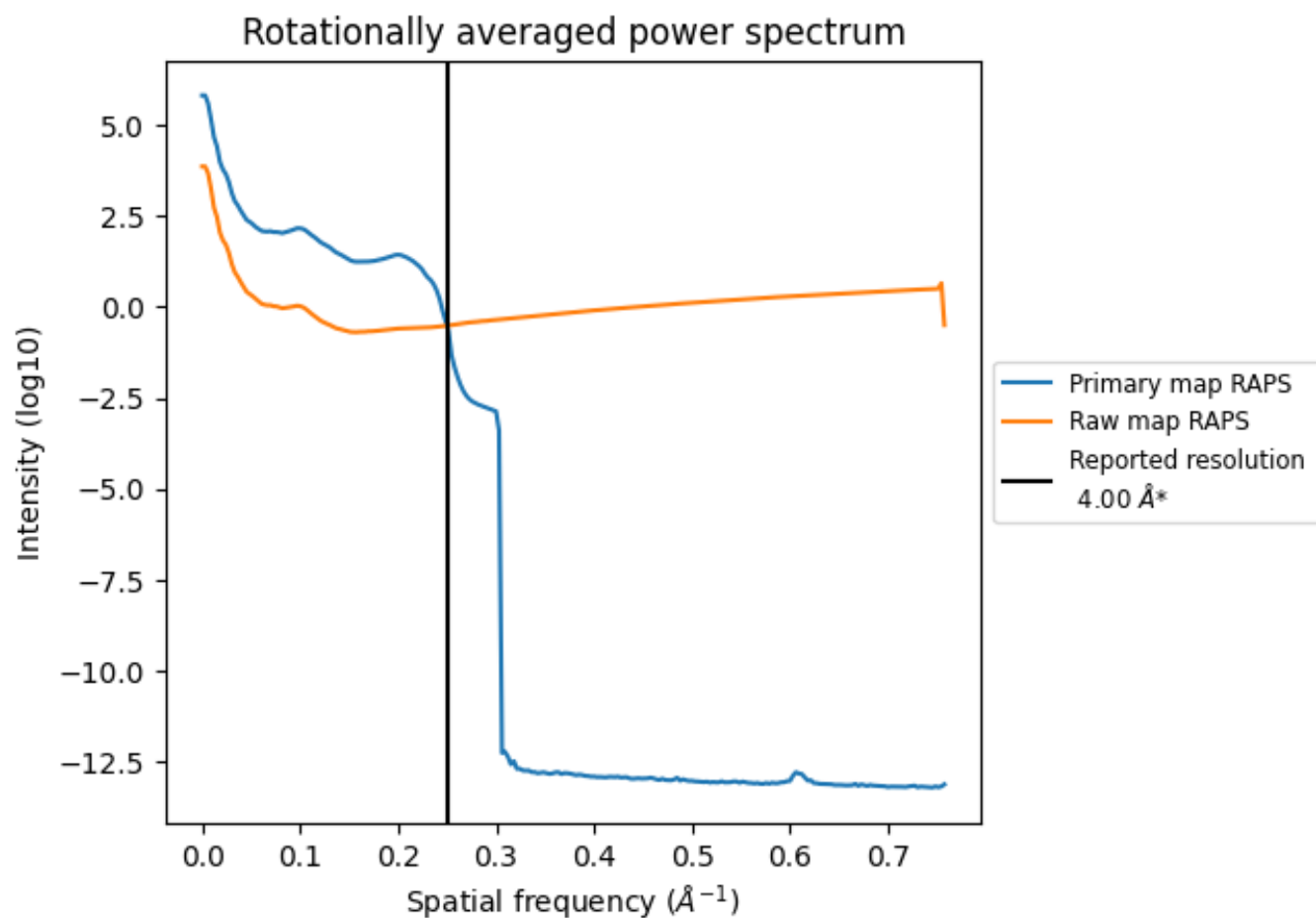
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 282 nm³; this corresponds to an approximate mass of 255 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 ⓘ

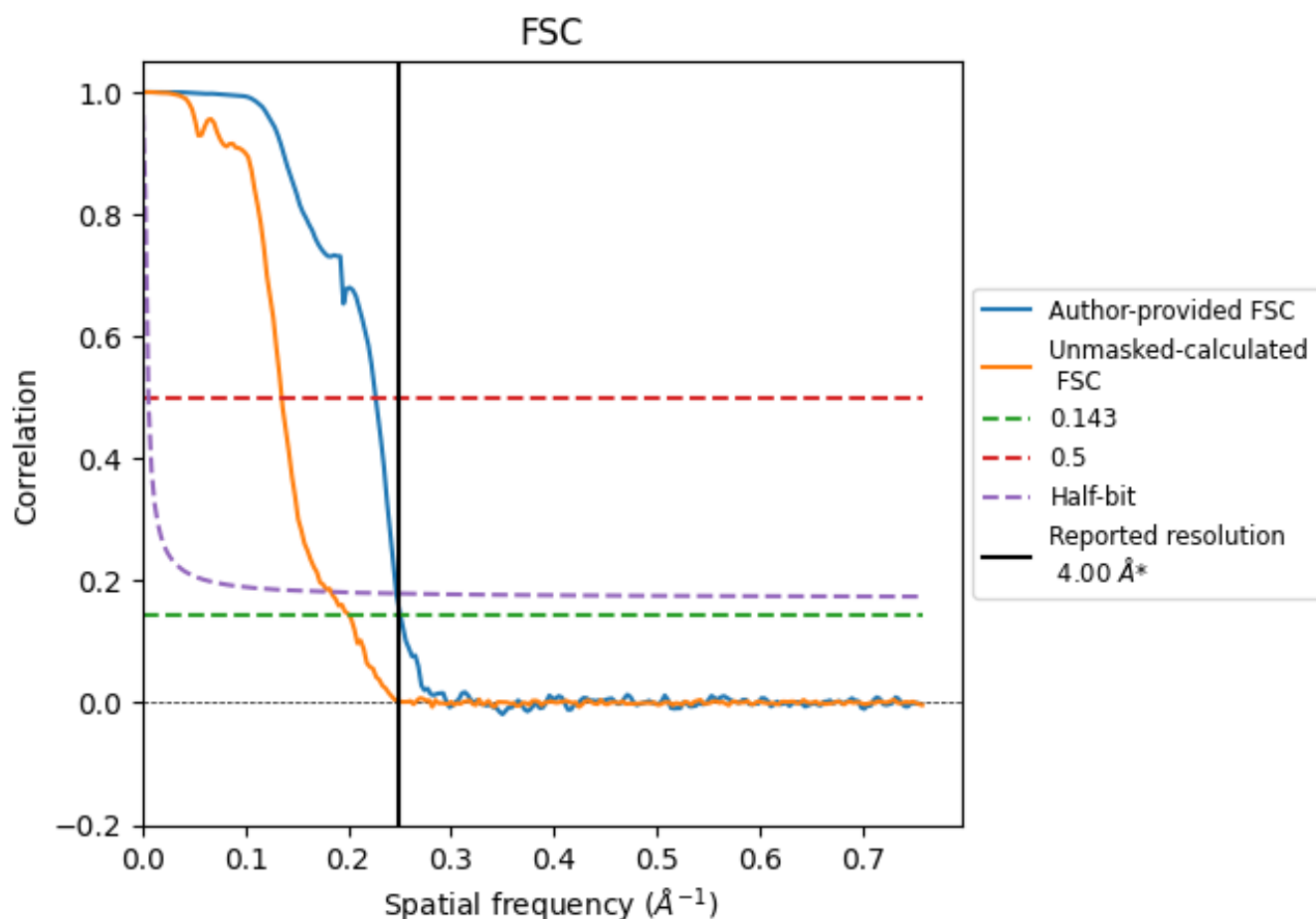


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 $0.250 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.99	4.41	4.05
Unmasked-calculated*	4.98	7.39	5.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.98 differs from the reported value 4.0 by more than 10 %

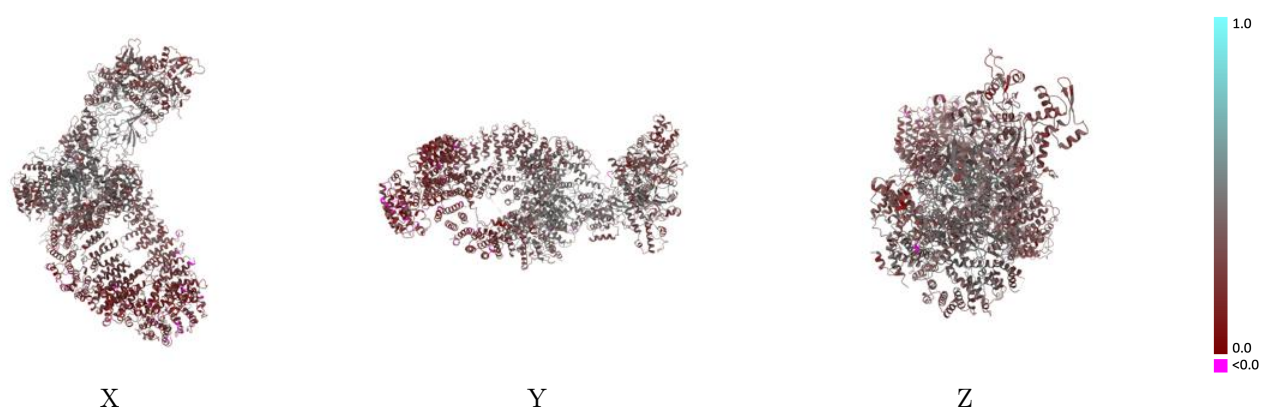
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33796 and PDB model 7YFP. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

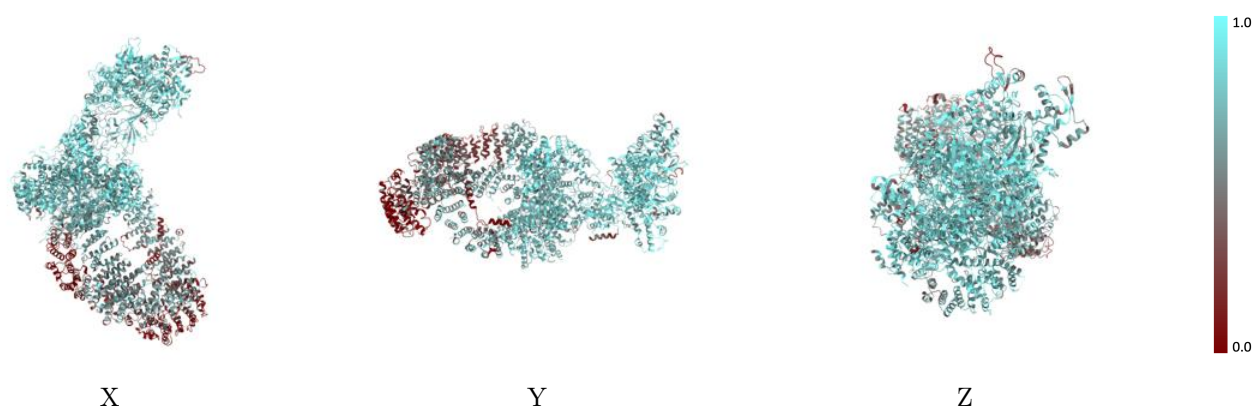
This section was not generated.

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



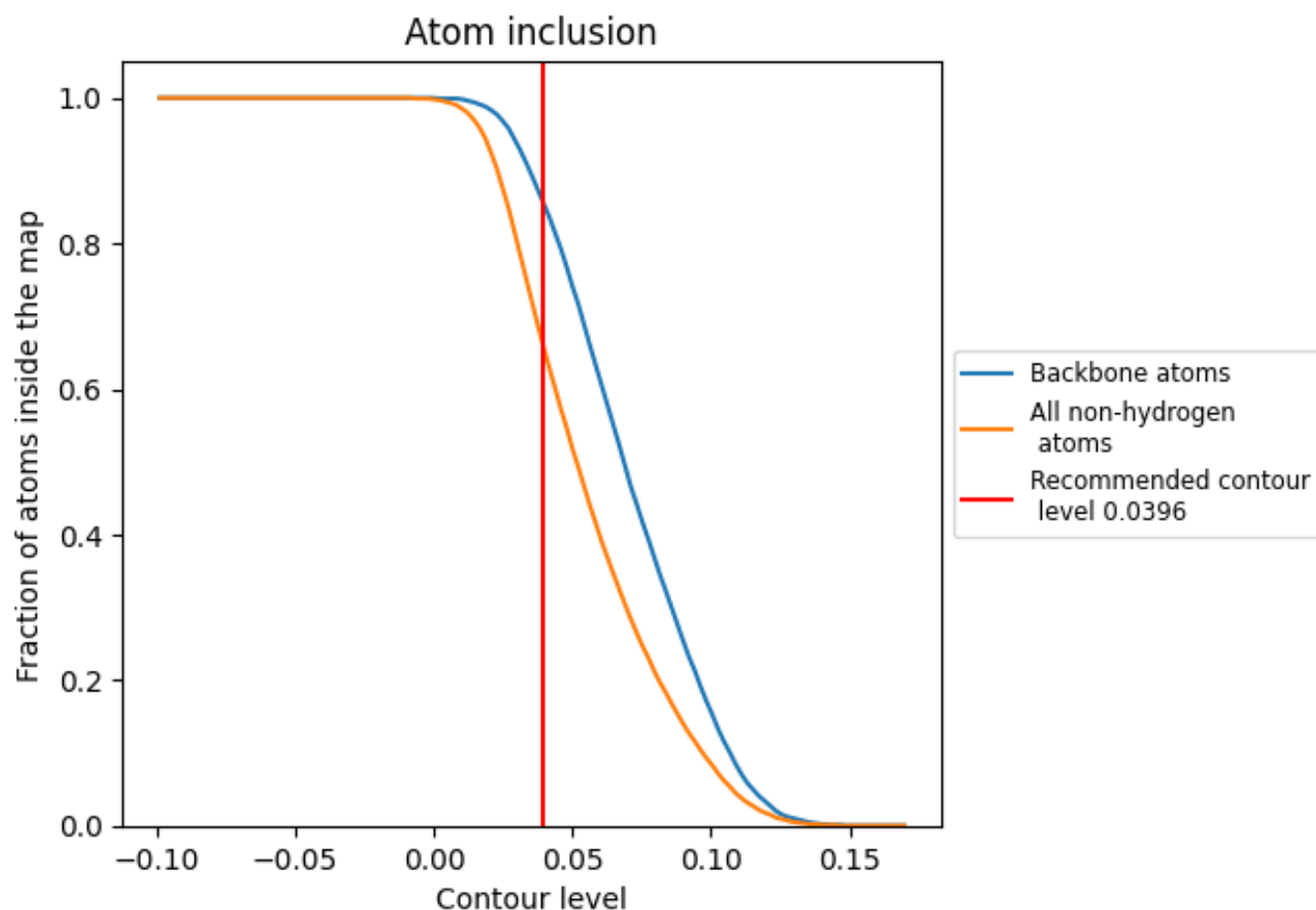
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0396).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 66% 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 (0.0396) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6570	0.3340
A	0.7470	0.3330
B	0.8340	0.3930
D	0.7720	0.3870
E	0.7870	0.3540
F	0.7500	0.4060
T	0.6020	0.3170

1.0

0.0

<0.0