



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 1, 2018 – 10:33 AM EST

PDB ID : 5NP0
EMDB ID: : EMD-3669
Title : Closed dimer of human ATM (Ataxia telangiectasia mutated)
Authors : Baretic, D.; Pollard, H.K.; Fisher, D.I.; Johnson, C.M.; Santhanam, B.; Truman, C.M.; Kouba, T.; Fersht, A.R.; Phillips, C.; Williams, R.L.
Deposited on : 2017-04-13
Resolution : 5.70 Å(reported)
Based on PDB ID : 4JSP

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

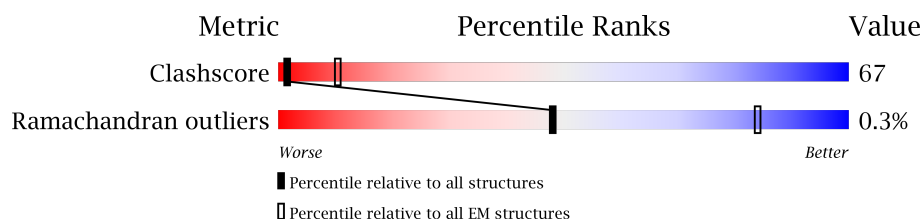
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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	125131	1336
Ramachandran outliers	121729	1120

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	3066	
1	B	3066	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25074 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 Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2528	Total	C	N	O	0	0
			12537	7481	2528	2528		
1	B	2528	Total	C	N	O	0	0
			12537	7481	2528	2528		

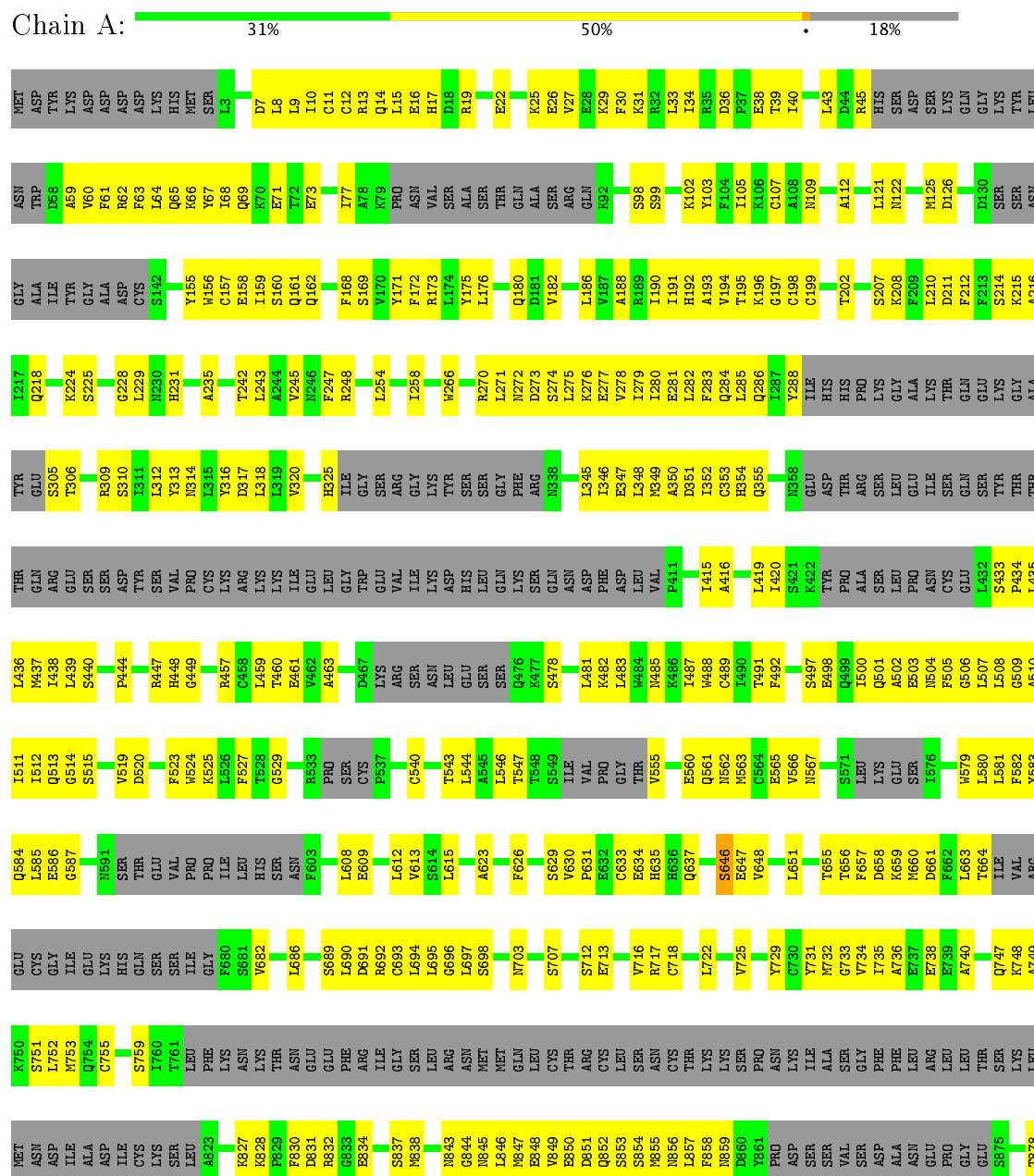
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP Q13315
A	-8	ASP	-	expression tag	UNP Q13315
A	-7	TYR	-	expression tag	UNP Q13315
A	-6	LYS	-	expression tag	UNP Q13315
A	-5	ASP	-	expression tag	UNP Q13315
A	-4	ASP	-	expression tag	UNP Q13315
A	-3	ASP	-	expression tag	UNP Q13315
A	-2	ASP	-	expression tag	UNP Q13315
A	-1	LYS	-	expression tag	UNP Q13315
A	0	HIS	-	expression tag	UNP Q13315
B	-9	MET	-	initiating methionine	UNP Q13315
B	-8	ASP	-	expression tag	UNP Q13315
B	-7	TYR	-	expression tag	UNP Q13315
B	-6	LYS	-	expression tag	UNP Q13315
B	-5	ASP	-	expression tag	UNP Q13315
B	-4	ASP	-	expression tag	UNP Q13315
B	-3	ASP	-	expression tag	UNP Q13315
B	-2	ASP	-	expression tag	UNP Q13315
B	-1	LYS	-	expression tag	UNP Q13315
B	0	HIS	-	expression tag	UNP Q13315

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: Serine-protein kinase ATM

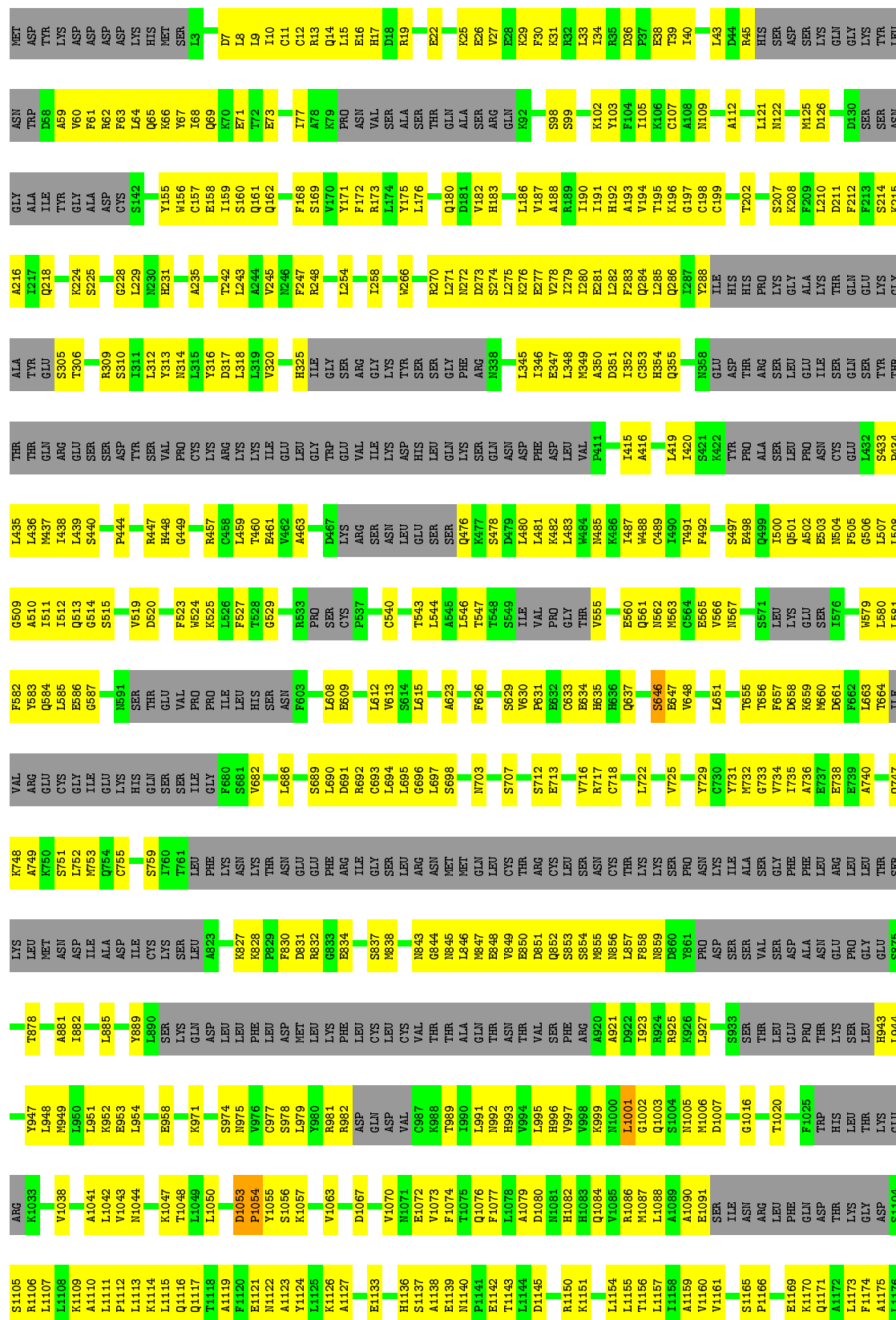


I1960	Y1961	A1962	D1963	K1964	K1965	S1966	N1967	S1968	S1969	Q1970	E1971	K1972	A1973	S1974	L1975	P1976	G1977	G1978	G1979	S1980	S1981	S1982	S1983	S1984	S1985	S1986	S1987	S1988	S1989	S1990	S1991	S1992	S1993	S1994	S1995	S1996	S1997	S1998	S1999	S2000	S2001	S2002	S2003	S2004	S2005	S2006	S2007	S2008	S2009	S2010	S2011	S2012	S2013	S2014	S2015	S2016	S2017	S2018	S2019																																																																																																																																																																																																																																																																																																																																																																															
L1824	Q1825	L1826	L1827	L1828	P1829	M1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889																																																																																																																																																																																																																																																																																																																																																																									
L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823																																																																																																																																																																																																																																																																																																																																																										
L1668	E1669	G1670	E1671	E1672	E1673	E1674	E1675	E1676	E1677	E1678	E1679	E1680	E1681	E1682	E1683	E1684	E1685	E1686	E1687	E1688	E1689	E1690	E1691	E1692	E1693	E1694	E1695	E1696	E1697	E1698	E1699	E1700	E1701	E1702	E1703	E1704	E1705	E1706	E1707	E1708	E1709	E1710	E1711	E1712	E1713	E1714	E1715	E1716	E1717	E1718	E1719	E1720	E1721	E1722	E1723	E1724	E1725	E1726	E1727	E1728	E1729	E1730	E1731	E1732	E1733	E1734	E1735	E1736	E1737	E1738	E1739	E1740	E1741	E1742																																																																																																																																																																																																																																																																																																																																																																
L1594	M1595	L1596	F1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667																																																																																																																																																																																																																																																																																																																																																																	
H1516	L1517	H1518	V1519	V1520	V1521	G1522	Q1523	E1524	E1525	E1526	E1527	E1528	E1529	E1530	E1531	E1532	E1533	E1534	E1535	E1536	E1537	E1538	E1539	E1540	E1541	E1542	E1543	E1544	E1545	E1546	E1547	E1548	E1549	E1550	E1551	E1552	E1553	E1554	E1555	E1556	E1557	E1558	E1559	E1560	E1561	E1562	E1563	E1564	E1565	E1566	E1567	E1568	E1569	E1570	E1571	E1572	E1573	E1574	E1575	E1576	E1577	E1578	E1579	E1580	E1581	E1582	E1583	E1584	E1585	E1586	E1587	E1588	E1589	E1590	E1591	E1592	E1593																																																																																																																																																																																																																																																																																																																																																													
D1452	L1453	K1454	S1455	G1456	L1457	G1458	G1459	A1460	A1461	A1462	F1463	F1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	Q1474	R1475	P1476	S1477	E1478	E1479	E1480	E1481	E1482	E1483	E1484	E1485	E1486	E1487	E1488	E1489	E1490	E1491	E1492	E1493	E1494	E1495	E1496	E1497	E1498	E1499	E1500	E1501	E1502	E1503	E1504	E1505	E1506	E1507	E1508	E1509	E1510	E1511	E1512	E1513																																																																																																																																																																																																																																																																																																																																																																													
S1383	H1384	V1385	K1386	K1387	L1388	L1389	P1390	S1391	S1392	S1393	S1394	S1395	S1396	H1397	K1398	H1399	K1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	E1422	E1423	E1424	E1425	E1426	E1427	E1428	E1429	E1430	E1431	E1432	E1433	E1434	E1435	E1436	E1437	E1438	E1439	E1440	E1441	E1442	E1443	E1444	E1445	E1446	E1447	E1448	E1449	E1450	E1451																																																																																																																																																																																																																																																																																																																																																																						
T1241	T1242	M1243	L1244	F1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667
S1105	R1106	L1107	L1108	K1109	A1110	L1111	L1112	L1113	K1114	L1115	Q1116	Q1117	L1118	L1119	F1120	E1121	E1122	E1123	E1124	A1125	A1126	A1127	E1128	H1129	S1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240																																																																																																																																																																																																																																																																																																			
ARG	K1033	V1034	V1035	A1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	D1051	P1052	E1053	E1054	E1055	E1056	K1057	V1058	V1059	V1060	V1061	V1062	V1063	V1064	V1065	V1066	V1067	V1068	V1069	V1070	V1071	V1072	V1073	V1074	V1075	V1076	V1077	V1078	V1079	V1080	V1081	V1082	V1083	V1084	V1085	V1086	V1087	V1088	V1089	V1090	V1091	V1092	V1093	V1094	V1095	V1096	V1097	V1098	V1099	V1100	V1101	V1102	V1103	V1104	V1105	V1106	V1107	V1108	V1109	V1110	V1111	V1112	V1113	V1114	V1115	V1116	V1117	V1118	V1119	V1120	V1121	V1122	V1123	V1124	V1125	V1126	V1127	V1128	V1129	V1130	V1131	V1132	V1133	V1134	V1135	V1136	V1137	V1138	V1139	V1140	V1141	V1142	V1143	V1144	V1145	V1146	V1147	V1148	V1149	V1150	V1151	V1152	V1153	V1154	V1155	V1156	V1157	V1158	V1159	V1160	V1161	V1162	V1163	V1164	V1165	V1166	V1167	V1168	V1169	V1170	V1171	V1172	V1173	V1174	V1175	V1176	V1177	V1178	V1179	V1180	V1181	V1182	V1183	V1184	V1185	V1186	V1187	V1188	V1189	V1190	V1191	V1192	V1193	V1194	V1195	V1196	V1197	V1198	V1199	V1200	V1201	V1202	V1203	V1204	V1205	V1206	V1207	V1208	V1209	V1210	V1211	V1212	V1213	V1214	V1215	V1216	V1217	V1218	V1219	V1220	V1221	V1222	V1223	V1224	V1225	V1226	V1227	V1228	V1229	V1230	V1231	V1232	V1233	V1234	V1235	V1236	V1237	V1238	V1239	V1240																																																																																																																																																																																																																										
L948	R949	L950	L951	R952	R953	L954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965																																																																																																																																																																																																																																																																																																																																																																																																																									




- Molecule 1: Serine-protein kinase ATM

Chain B:  31% 50% . 18%






A3039	E2979	T2911	P2829	Q2762	L2692	R2612	S2549	V2484	A2415	V2355	Q2292
I3040	L2980	R2912	V2830	R2763	A2693	V2617	H2552	F2485	L2416	L2356	L2293
P3042	H2981	I2914	Y2833	S2764	V2696	R2618	H2553	L2486	L2417	Q2357	E2294
K3043	P30	V2915	Y2834	G2765	P2699	S2619	H2554	L2487	K2418	T2358	E2295
N3044	TR	V2916	C2835	L2767	P2699	E2620	H2555	C2488	R2419	T2359	A2296
L3045	LEU	G2917	C2835	E2768	K2700	E2621	T2556	S2489	E2422	Y2360	Q2297
S3046	ASN	M2918	F2839	E2768	I2701	A2622	T2557	L2490	GLU	L2361	V2298
R3047	ALA	G2919	L2840	G2772	I2702	L2623	F2558	E2362	VAL	E2363	F2299
F3049	ASP	I2920	D2841	V2773	D2703	C2624	I2559	A2301	GLY	A2364	A2301
P3050	ASP	T2921	P2842	T2774	D2703	D2625	I2560	V2365	LEU	V2365	K2302
G3051	GLN	G2922	A2843	P2775	V2705	G2626	L2561	G2496	LEU	E2366	K2303
M3052	GLU	V2923	I2844	I2776	G2706	A2626	A2562	V2497	ARG	V2367	E2304
K3053	CYS	E2924	W2845	G2777	S2707	I2628	L2563	S2498	GLU	A2368	Q2305
A3054	LYS	G2925	F2846	E2778	D2708	I2629	A2566	E2499	HIS	G2369	Q2306
W3055	ARG	V2926	E2847	F2779	L2630	L2630	A2566	V2500	ILE	N2370	L2307
V3056	ASN	F2927	K2848	V2780	K2710	D2631	D2569	N2501	ILE	TR	A2308
	LEU	R2928	R2849	V2781	E2711	N2632	E2570	G2502	THR	ASP	L2309
	SER	R2929	L2850	N2782	R2712	L2633	F2571	N2503	ASN	GLY	S2310
	ASP	C2930	A2851	N2783	K2713	D2634	F2571	M2504	ASN	GLU	I2311
	I2998	C2931	Y2852	E2784	Q2714	ALA	LEU	K2505	R2436	SER	I2312
	D2999	E2932	T2853	D2785	L2715	GLN	THR	D2506	E2444	D2377	K2313
	Q3000	K2933	R2854	G2786	V2716	THR	LYS	D2507	E2445	E2378	K2314
	S3001	T2934	S2855	A2787	R2719	TRP	PRO	G2508	E2446	L2379	M2315
	K3002	M2935	V2856	H2788	D2720	LYS	GLU	P2512	L2447	R2380	I2316
	N3003	E2936	A2857	K2789	D2721	THR	VAL	T2513	D2448	N2381	K2317
	K3004	V2937	T2858	P2793	L2722	GLN	ALA	F2516	E2449	I2382	K2318
	V3005	M2938	S2859	N2794	R2723	ARG	ARG	L2450	E2450	G2382	L2319
	A3006	R2939	S2860	D2795	Q2724	I2645	SER	L2517	L2451	K2383	D2320
	E3007	N2940	V2862	F2796	D2725	N2646	ARG	P2518	L2452	M2384	A2321
	R3008	S2941	G2863	S2797	A2726	I2647	ILE	L2519	R2453	K2385	S2322
	V3009	L2945		A2798	V2727	P2648	THR	M2520	A2454	A2386	C2323
	M3010	L2946		P2799	L2728	A2649	LYS	L2523	A2454	F2387	A2324
	R3012	T2947	G2867	Q2800	Q2729	D2650	ASN	A2524	K2455	L2388	ALA
	L3013	I2948		C2801	Q2730	T2654	VAL	A2525	K2456	S2389	ASN
	Q3014	V2949			V2731		PRO	E2526	D2458	L2390	ASN
	E3015	E2950		Q2802	F2732		LYS	E2528	R2459	R2392	S2328
	K3016	V2951		M2806	Q2733	K2657	GLN	M2527	K2460	F2393	L2330
	L3017	L2952		GLU	M2734	N2658	SER	G2528	R2461	S2394	K2331
	G3019	P2956		VAL	C2735	L2659	THR	THR	F2462	D2395	L2332
	V3020	F2957		GLN	N2736	E2660	GLN	LYS	L2463	T2396	T2333
		F2958		LYS	T2737		LEU	MET	C2464	Q2397	Y2334
				SER	L2738	P2665	D2595		E2465	Y2398	T2335
					L2739		E2596		A2466	Q2399	E2336
					Q2740	I2669	D2597		V2467	R2400	C2337
					R2741		R2598		E2468	I2401	L2338
					N2742	T2674	T2599		N2469	E2402	R2339
					T2743		E2600		Y2470	N2403	V2340
					E2744	Y2677	A2601		I2471	Y2404	C2341
					T2745		A2602		N2472	M2405	G2342
					R2746	T2682	N2603		C2473	K2406	N2343
					K2747	I2683	R2604		L2474	S2407	M2344
					R2748	Q2684	L2605		L2475	S2408	L2345
					K2749	S2685	I2606		S2476	E2409	A2346
						F2686	C2607			F2410	E2347
					V2757	E2689	T2608		H2480	E2411	T2348
					V2758	F2690	L2609		M2481	N2412	P2353
						R2691	R2610		M2482	K2413	P2353
					S2761		S2611			Q2414	A2354

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25315	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.1	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.48	0/12490	0.62	6/17349 (0.0%)
1	B	0.48	0/12490	0.62	6/17349 (0.0%)
All	All	0.48	0/24980	0.62	12/34698 (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	A	0	53
1	B	0	53
All	All	0	106

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	2765	GLY	N-CA-C	9.33	136.44	113.10
1	B	2765	GLY	N-CA-C	9.31	136.38	113.10
1	A	1925	GLY	N-CA-C	-7.59	94.13	113.10
1	B	1925	GLY	N-CA-C	-7.58	94.15	113.10
1	B	2307	LEU	N-CA-C	-6.09	94.56	111.00

There are no chirality outliers.

5 of 106 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1001	LEU	Peptide
1	A	1053	ASP	Peptide
1	A	39	THR	Peptide
1	A	497	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	646	SER	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	12537	0	5446	1207	0
1	B	12537	0	5446	1207	0
All	All	25074	0	10892	2413	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 67.

The worst 5 of 2413 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:B:2095:LEU:O	1:B:2099:HIS:N	1.93	1.02
1:B:3013:LEU:O	1:B:3017:LEU:N	1.92	1.02
1:A:2068:LEU:O	1:A:2072:GLY:N	1.93	1.01
1:A:3013:LEU:O	1:A:3017:LEU:N	1.92	1.01
1:A:1955:LEU:O	1:A:1959:GLU:N	1.94	1.01

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	2435/3066 (79%)	2231 (92%)	197 (8%)	7 (0%)	44	81
1	B	2435/3066 (79%)	2232 (92%)	196 (8%)	7 (0%)	44	81
All	All	4870/6132 (79%)	4463 (92%)	393 (8%)	14 (0%)	48	81

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1367	ASP
1	A	1376	PRO
1	A	1378	PRO
1	B	1367	ASP
1	B	1376	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 carbohydrates 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3
1	A	3

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	305:SER	C	306:THR	N	6.20
1	B	305:SER	C	306:THR	N	6.20
1	A	163:GLN	C	164:TRP	N	3.12
1	B	163:GLN	C	164:TRP	N	3.12
1	A	1394:SER	C	1395:ASN	N	2.99