



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2023 – 02:00 PM EDT

PDB ID : 2PFF  
Title : Structural Insights of Yeast Fatty Acid Synthase  
Authors : Xiong, Y.; Lomakin, I.B.; Steitz, T.A.  
Deposited on : 2007-04-04  
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

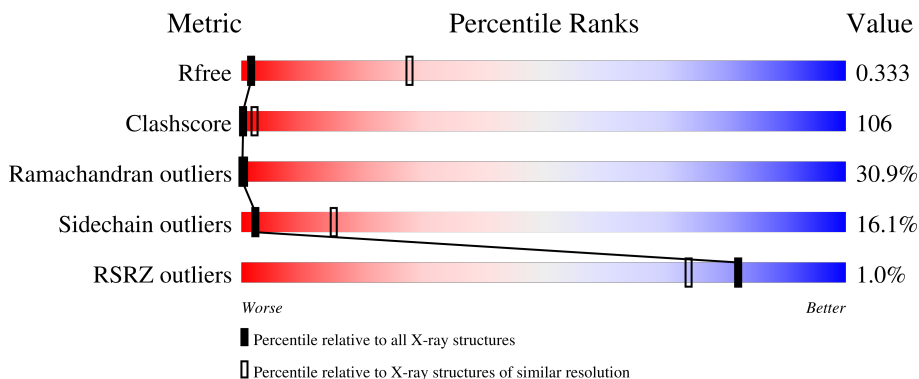
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

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.



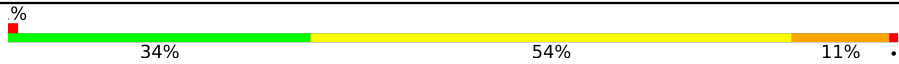



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1688	27% 46% 22% 5%
1	D	1688	27% 46% 22% 5%
1	G	1688	27% 46% 22% 5%
2	B	2006	34% 54% 11% .
2	E	2006	34% 54% 11% .

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Mol	Chain	Length	Quality of chain
2	H	2006	 <p>%</p> <p>34% 54% 11%</p>
3	C	65	 <p>48% 52%</p>
3	F	65	 <p>45% 55%</p>
3	I	65	 <p>42% 58%</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 71862 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1683	11319	7070	2007	2205	37	0	0	0
1	D	1683	11319	7070	2007	2205	37	0	0	0
1	G	1683	11319	7070	2007	2205	37	0	0	0

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	2006	12310	7625	2253	2416	16	0	0	0
2	E	2006	12310	7625	2253	2416	16	0	0	0
2	H	2006	12310	7625	2253	2416	16	0	0	0

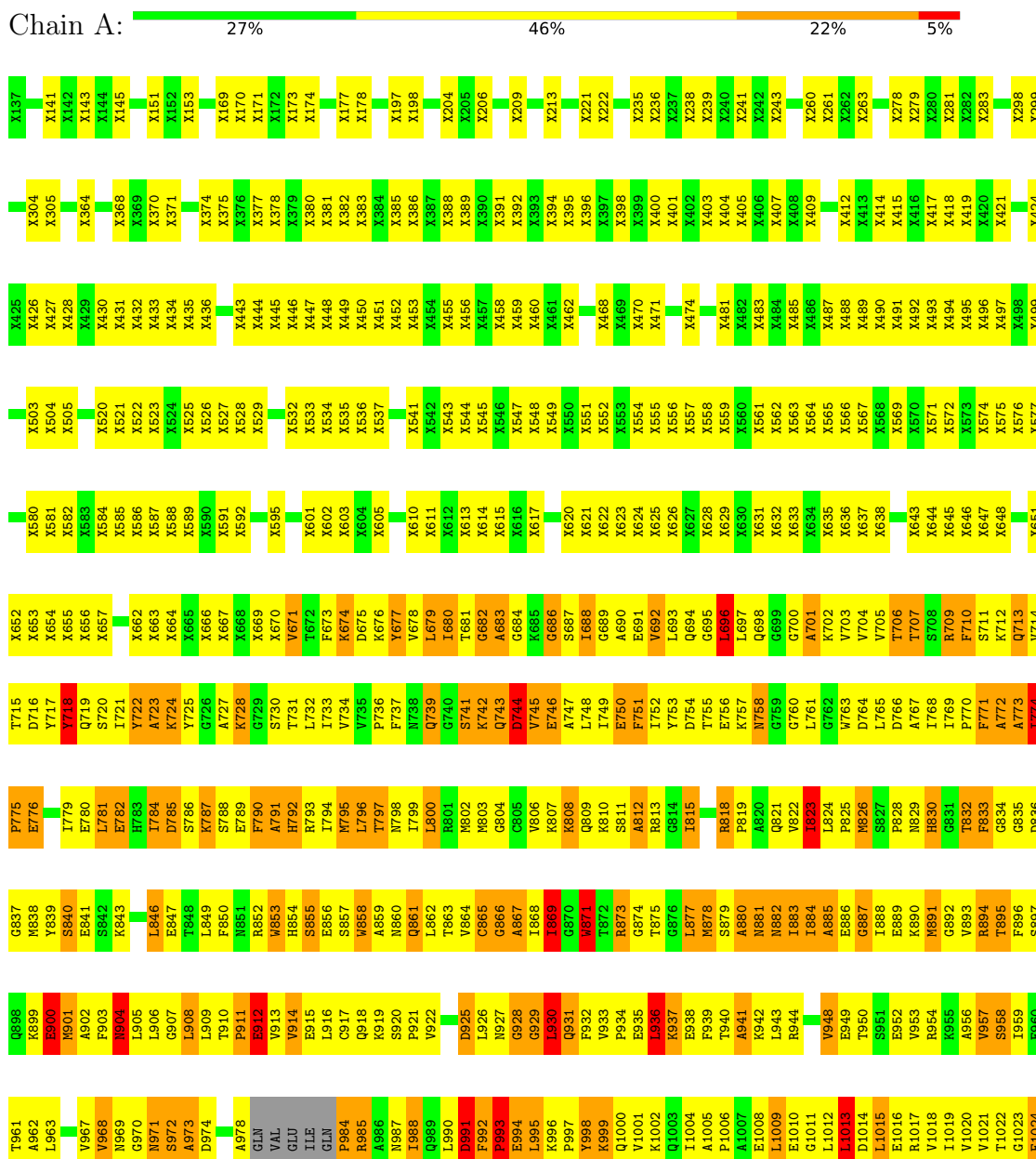
- Molecule 3 is a protein called Tail protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	65	325	195	65	65	0	0	0
3	F	65	325	195	65	65	0	0	0
3	I	65	325	195	65	65	0	0	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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Fatty acid synthase subunit alpha



E1025	E1026	Y1027	E1028	P1029	W1030	G1031	S1032	A1033	R1034	T1035	R1036	W1037	E1038	M1039	E1040	A1041	F1042	G1043	E1044	F1045	S1046	L1047	E1048	P1049	C1050	W1051	E1052	M1053	Y1054	W1055	T1056	M1057	G1058	F1059	I1060	E1061	Y1062	H1063	N1064	G1065	N1066	L1067	K1068	G1069	R1070	Y1071	Y1072	T1073	G1074	W1075	W1076	D1077	S1078	K1079	E1080	K1081	E1082	P1083	H1084	D1085	D1086	K1087	D1088	D1089	P1090	V1091	K1092	A1093	S1094	L1095	L1096	L1097	L1098	E1099	H1100	S1101	G1102	L1103	R1104	L1105	I1106	E1107	P1108	E1109	L1110	F1111	M1112	G1113	Y1114	M1115	L1116	E1117	K1118	K1119	E1120	M1121	L1122	I1126	G1127	E1128	E1129	L1130	L1131	E1132	P1133	L1134	E1135	A1136	K1137	K1138	E1139	L1140	E1141	L1142	D1143	F1144	K1145	H1146	Q1147	H1148	G1149	D1150	V1151	W1152	D1153	L1154	L1155	E1156	L1157	S1158	E1159	T1160	E1161	F1162	Y1163	S1164	V1165	K1166	L1167	L1168	L1169	G1170	A1171	T1172	L1173	Y1174	L1175	L1176	K1177	L1178	L1179	R1180	F1181	D1182	R1183	L1184	V1185	C1186	G1187	Q1188	I1189	E1190	L1191	G1192	W1193	N1194	A1195	A1196	T1197	Y1198	E1199	M1200	S1201	L1202	D1203	I1204	L1205	S1206	V1207	P1208	P1209	P1210	L1211	T1212	L1213	F1214	V1215	L1216	L1217	L1218	S1219	V1220	E1221	A1222	F1223	L1224	A1225	S1226	G1227	L1228	T1229	P1230	P1231	Y1232	E1233	M1234	Y1235	L1236	K1237	Y1238	L1239	S1240	E1241	E1242	W1243	G1244	M1245	C1246	S1247	G1248	S1249	G1250	M1251	G1252	G1253	W1254	S1255	A1256	L1257	L1258	R1259	M1260	F1261	S1262	D1263	R1264	L1265	K1266	D1267	E1268	P1269	Q1270	Q1271	Q1272	D1273	L1274	L1275	Q1276	E1277	S1278	F1279	I1280	M1281	A1282	M1283	S1284	A1285	W1286	V1287	S1288	L1289	T1290	M1291	L1292	S1293	E1294	S1295	S1296	F1297	L1298	H1299	G1300	P1301	G1302	G1303	A1304	M1305	A1306	T1307	S1308	S1309	E1310	S1311	V1312	D1313	L1314	G1315	W1316	E1317	E1318	A1319	Q1320	G1321	A1322	L1323	Q1324	Q1325	M1326	Y1327	L1328	Q1329	L1330	D1331	D1332	D1333	D1334	P1335	Q1336	E1337	E1338	G1339	S1340	F1341	L1342	F1343	G1344	M1345	M1346	R1347	L1348	A1349	S1350	M1351	L1352	L1353	L1354	L1355	G1356	E1357	L1358	L1359	L1360	P1361	A1362	A1363	E1364	M1365	S1366	T1367	P1368	A1369	L1370	T1371	L1372	R1373	F1374	M1375	E1376	E1377	E1378	A1379	L1380	G1381	A1382	G1383	L1384	Q1385	L1386	L1387	M1388	Q1389	A1390	L1391	L1392	L1393	V1394	L1395	L1396	G1397	V1398	P1399	E1400	Y1401	G1402	L1403	V1404	M1405	M1406	A1407	E1408	A1409	L1410	L1411	D1412	K1413	L1414	E1415	E1416	L1417	S1418	P1419	A1420	P1421	K1422	K1423	G1424	L1425	L1426	T1427	L1428	A1429	R1430	E1431	H1432	H1433	H1434	S1435	V1436	K1437	Y1438	A1439	L1440	L1441	P1442	M1443	L1444	Q1445	M1446	Q1447	M1448	L1449	L1450	L1451	M1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	V1462	L1463	M1464	N1465	E1466	L1467	E1468	A1469	L1470	K1471	L1472	E1473	A1474	E1475	E1476	L1477	S1478	P1479	A1480	L1481	Q1482	F1483	L1484	L1485	L1486	L1487	E1488	R1489	T1490	R1491	E1492	L1493	H1494	E1495	A1496	L1497	E1498	S1499	Q1500	L1501	L1502	A1503	L1504	Q1505	M1506	Q1507	L1508	G1509	M1510	D1511	F1512	Y1513	Y1514	R1515	L1516	P1517	L1518	F1519	R1520	L1521	L1522	A1523	G1524	A1525	L1526	A1527	L1528	A1529	M1530	L1531	T1532	L1533	D1534	L1535	L1536	E1537	L1538	L1539	V1540	F1541	G1542	H1543	T1544	S1545	L1546	M1547	A1548	M1549	D1550	A1551	K1552	L1553	E1554	L1555	T1556	L1557	M1558	L1559	M1560	E1561	Y1562	L1563	V1564	L1565	Y1566	E1567	L1568	H1569	P1570	L1571	L1572	G1573	L1574	L1575	Q1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	A1590	W1591	M1592	L1593	L1594	G1595	A1596	L1597	L1598	Q1599	D1600	L1601	M1602	P1603	L1604	L1605	T1606	E1607	M1608	R1609	M1610	A1611	D1612	M1613	V1614	D1615	L1616	L1617	L1618	E1619	Q1620	F1621	E1622	Y1623	V1624	A1625	L1626	P1627	E1628	K1629	L1630	L1631	T1632	G1633	L1634	F1635	L1636	G1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	Q1652	A1653	L1654	Y1655	L1656	H1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	E1667	D1668	L1669	Y1670	M1671	E1672	Y1673	V1674	A1675	K1676	L1677	S1678	L1679	R1680	E1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	A1704	F1705	Y1706	L1707	D1708	E1709	L1710	L1711	E1712	D1713	V1714	L1715	L1716	L1717	P1718	L1719	L1720	A1721	L1722	K1723	S1724	L1725	L1726	L1727	L1728	G1729	S1730	L1731	L1732	F1733	M1734	L1735	K1736	M1737	L1738	Q1739	S1740	L1741	L1742	S1743	Y1744	L1745	L1746	L1747	L1748	L1749	X1750	L1751	L1752	X1753	X1754	X1755	X1756	X1757	X1758	X1759	X1760	X1761	X1762	X1763	X1764	X1765	X1766	X1767	X1768	X1769	X1770	X1771	X1772	X1773	X1774	X1775	X1776	X1777	X1778	X1779	X1780	X1781	X1782	X1783	X1784	X1785	X1786	X1787	X1788	X1789	X1790	X1791	X1792	X1793	X1794	X1795	X1796	X1797	X1798	X1799	X1800	X1801	X1802	X1803	X1804	X1805	X1806	X1807	X1808	X1809	X1810	X1811	X1812	X1813	X1814	X1815	X1816	X1817	X1818	X1819	X1820	X1821	X1822	X1823	X1824	X1825	X1826	X1827	X1828	X1829	X1830	X1831	X1832	X1833	X1834	X1835	X1836	X1837	X1838	X1839	X1840	X1841	X1842	X1843	X1844	X1845	X1846	X1847	X1848	X1849	X1850	X1851	X1852	X1853	X1854	X1855	X1856	X1857	X1858	X1859	X1860	X1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T1454	R1456	E1456	A1457	Q1458	I1459	K1460	D1461	V1462	Y1463	L1464	G1465	F1466	M1467	L1468	E1469	A1470	L1471	K1472	L1473	A1474	E1475	E1476	I1477	P1478	S1479	I1480	D1481	Q1482	F1483	L1484	L1485	L1486	L1487	A1488	R1489	T1490	R1491	E1492	I1493	H1494	N1495	T1496	A1497	A1498	Q1500	L1501	K1502	H1503	A1504	Q1505	Q1506	Q1507	W1508	M1509	M1510	D1511	V1512	F1513	Y1514	K1515																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
R1516	D1517	P1518	F1519	I1520	A1521	P1522	L1523	R1524	G1525	A1526	L1527	A1528	T1529	Y1530	A1531	L1532	T1533	I1534	D1535	E1536	G1537	V1538	A1539	S1540	F1541	H1542	K1543	T1544	S1545	T1546	K1547	A1548	M1549	D1550	K1551	M1552	E1553	S1554	N1555	T1556	I1557	M1558	E1559	M1560	M1561	K1562	H1563	L1564	G1565	R1566	G1567	G1568	T1569	P1570	V1571	K1572	T1573	D1574	Y1575	N1576																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
F1577	Q1578	L1579	F1580	T1581	G1582	H1583	P1584	L1585	G1586	A1587	L1588	G1589	A1590	M1591	L1592	M1593	L1594	G1595	V1596	L1597	Q1598	L1599	M1600	N1601	S1602	H1603	I1604	T1605	P1606	G1607	L1608	R1609	M1610	A1611	D1612	M1613	V1614	D1615	K1616	L1617	L1618	E1619	Q1620	F1621	E1622	Y1623	V1624	L1625	Y1626	P1627	S1628	L1629	T1630	L1631	K1632	T1633	D1634	N1635																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
V1636	R1637	A1638	V1639	S1640	I1641	T1642	S1643	F1644	G1645	F1646	G1647	Q1648	K1649	G1650	G1651	A1652	K1653	L1654	V1655	V1656	H1657	P1658	D1659	L1660	L1661	Y1662	G1663	I1664	L1665	T1666	E1667	D1668	A1669	Y1670	M1671	M1672	Y1673	V1674	I1675	Q1676	V1677	S1678	K1679	S1680	E1681	S1682	S1683	A1684	Y1685	K1686	F1687	F1688	H1689	M1690	G1691	M1692	L1693	Y1694	N1695																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
K1696	L1697	X1698	V1699	K1700	I1701	E1702	H1703	A1704	P1705	X1706	T1707	D1708	E1709	L1710	E1711	D1712	D1713	V1714	Y1715	L1716	D1717	P1718	L1719	A1720	R1721	V1722	K1723	I1724	G1725	S1726	L1727	S1728	G1729	S1730	L1731	T1732	F1733	M1734	S1735	K1736	I1737	Q1738	Q1739	S1740	K1741	D1742	S1743	Y1744	X1745	X1746	X1747	X1748	X1749	X1750	X1751	X1752	X1753	X1754	X1755	X1756	X1757	X1758	X1759	X1760	X1761	X1762	X1763	X1764	X1765	X1766	X1767	X1768	X1769	X1770	X1771	X1772	X1773	X1774	X1775	X1776	X1777	X1778	X1779	X1780	X1781	X1782	X1783	X1784	X1785	X1786	X1787	X1788	X1789	X1790	X1791	X1792	X1793	X1794	X1795	X1796	X1797	X1798	X1799	X1800	X1801	X1802	X1803	X1804	X1805	X1806	X1807	X1808	X1809	X1810	X1811	X1812	X1813	X1814	X1815	X1816	X1817	X1818	X1819	X1820	X1821	X1822	X1823	X1824	X1825	X1826	X1827	X1828	X1829	X1830	X1831	X1832	X1833	X1834	X1835	X1836	X1837	X1838	X1839	X1840	X1841	X1842	X1843	X1844	X1845	X1846	X1847	X1848	X1849	X1850	X1851	X1852	X1853	X1854	X1855	X1856	X1857	X1858	X1859	X1860	X1861	X1862	X1863	X1864	X1865	X1866	X1867	X1868	X1869	X1870	X1871	X1872	X1873	X1874	X1875	X1876	X1877	X1878	X1879	X1880	X1881	X1882	X1883	X1884	X1885	X1886	X1887	X1888	X1889	X1890	X1891	X1892	X1893	X1894	X1895	X1896	X1897	X1898	X1899	X1900	X1901	X1902	X1903	X1904	X1905	X1906	X1907	X1908	X1909	X1910	X1911	X1912	X1913	X1914	X1915	X1916	X1917	X1918	X1919	X1920	X1921	X1922	X1923	X1924	X1925	X1926	X1927	X1928	X1929	X1930	X1931	X1932	X1933	X1934	X1935	X1936	X1937	X1938	X1939	X1940	X1941	X1942	X1943	X1944	X1945	X1946	X1947	X1948	X1949	X1950	X1951	X1952	X1953	X1954	X1955	X1956	X1957	X1958	X1959	X1960	X1961	X1962	X1963	X1964	X1965	X1966	X1967	X1968	X1969	X1970	X1971	X1972	X1973	X1974	X1975	X1976	X1977	X1978	X1979	X1980	X1981	X1982	X1983	X1984	X1985	X1986	X1987	X1988	X1989	X1990	X1991	X1992	X1993	X1994	X1995	X1996	X1997	X1998	X1999	X2000	X2001	X2002	X2003	X2004	X2005	X2006	X2007	X2008	X2009	X2010	X2011	X2012	X2013	X2014	X2015	X2016	X2017	X2018	X2019	X2020	X2021	X2022	X2023	X2024	X2025	X2026	X2027	X2028	X2029	X2030	X2031	X2032	X2033	X2034	X2035	X2036	X2037	X2038	X2039	X2040	X2041	X2042	X2043	X2044	X2045	X2046	X2047	X2048	X2049	X2050	X2051	X2052	X2053	X2054	X2055	X2056	X2057	X2058	X2059	X2060	X2061	X2062	X2063	X2064	X2065	X2066	X2067	X2068	X2069	X2070	X2071	X2072	X2073	X2074	X2075	X2076	X2077	X2078	X2079	X2080	X2081	X2082	X2083	X2084	X2085	X2086	X2087	X2088	X2089	X2090	X2091	X2092	X2093	X2094	X2095	X2096	X2097	X2098	X2099	X2100	X2101	X2102	X2103	X2104	X2105	X2106	X2107	X2108	X2109	X2110	X2111	X2112	X2113	X2114	X2115	X2116	X2117	X2118	X2119	X2120	X2121	X2122	X2123	X2124	X2125	X2126	X2127	X2128	X2129	X2130	X2131	X2132	X2133	X2134	X2135	X2136	X2137	X2138	X2139	X2140	X2141	X2142	X2143	X2144	X2145	X2146	X2147	X2148	X2149	X2150	X2151	X2152	X2153	X2154	X2155	X2156	X2157	X2158	X2159	X2160	X2161	X2162	X2163	X2164	X2165	X2166	X2167	X2168	X2169	X2170	X2171	X2172	X2173	X2174	X2175	X2176	X2177	X2178	X2179	X2180	X2181	X2182	X2183	X2184	X2185	X2186	X2187	X2188	X2189	X2190	X2191	X2192	X2193	X2194	X2195	X2196	X2197	X2198	X2199	X2200	X2201	X2202	X2203	X2204	X2205	X2206	X2207	X2208	X2209	X2210	X2211	X2212	X2213	X2214	X2215	X2216	X2217	X2218	X2219	X2220	X2221	X2222	X2223	X2224	X2225	X2226	X2227	X2228	X2229	X2230	X2231	X2232	X2233	X2234	X2235	X2236	X2237	X2238	X2239	X2240	X2241	X2242	X2243	X2244	X2245	X2246	X2247	X2248	X2249	X2250	X2251	X2252	X2253	X2254	X2255	X2256	X2257	X2258	X2259	X2260	X2261	X2262	X2263	X2264	X2265	X2266	X2267	X2268	X2269	X2270	X2271	X2272	X2273	X2274	X2275	X2276	X2277	X2278	X2279	X2280	X2281	X2282	X2283	X2284	X2285	X2286	X2287	X2288	X2289	X2290	X2291	X2292	X2293	X2294	X2295	X2296	X2297	X2298	X2299	X2300	X2301	X2302	X2303	X2304	X2305	X2306	X2307	X2308	X2309	X2310	X2311	X2312	X2313	X2314	X2315	X2316	X2317	X2318	X2319	X2320	X2321	X2322	X2323	X2324	X2325	X2326	X2327	X2328	X2329	X2330	X2331	X2332	X2333	X2334	X2335	X2336	X2337	X2338	X2339	X2340	X2341	X2342	X2343	X2344	X2345	X2346	X2347	X2348	X2349	X2350	X2351	X2352	X2353	X2354	X2355	X2356	X2357	X2358	X2359	X2360	X2361	X2362	X2363	X2364	X2365	X2366	X2367	X2368	X2369	X2370	X2371	X2372	X2373	X2374	X2375	X2376	X2377	X2378	X2379	X2380	X2381	X2382	X2383	X2384	X2385	X2386	X2387	X2388	X2389	X2390	X2391	X2392	X2393	X2394	X2395	X2396	X2397	X2398	X2399	X2400	X2401	X2402	X2403	X2404	X2405	X2406	X2407	X2408	X2409	X2410	X2411	X2412	X2413	X2414	X2415	X2416	X2417	X2418	X2419	X2420	X2421	X2422	X2423	X2424	X2425	X2426	X2427	X2428	X2429	X2430	X2431	X2432	X2433	X2434	X2435	X2436	X2437	X2438	X2439	X2440	X2441	X2442	X2443	X2444	X2445	X2446	X2447	X2448	X2449	X2450	X2451	X2452	X2453	X2454	X2455	X2456	X2457	X2458	X2459	X2460	X2461	X2462	X2463	X2464	X2465	X2466	X2467	X2468	X2469	X2470	X2471	X2472	X2473	X2474	X2475	X2476	X2477	X2478	X2479	X2480	X2481	X2482	X2483	X2484	X2485	X2486	X2487	X2488	X2489	X2490	X2491	X2492	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2502	X2503	X2504	X2505	X2506	X2507	X2508	X2509	X2510	X2511	X2512	X2513	X2514	X2515	X2516	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2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M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21	M22	M23	M24	M25	M26	M27	M28	M29	M30	M31	M32	M33	M34	M35	M36	M37	M38	M39	M40	M41	M42	M43	M44	M45	M46	M47	M48	M49	M50	M51	M52	M53	M54	M55	M56	M57	M58	M59	M60	M61	M62																									
K63	F64	L65	G66	Y67	V68	S69	S70	L71	S12	E73	G14	S15	L16	E17	G18	H18	V19	F80	L20	L21	V22	P23	T24	A25	S26	F27	F28	E29	A30	F31	N32	G33	N38	N39	D100	L101	L41	H102	A103	P42	E43	P44	T45	E46	G47	F48	Q109	Q110	A49	A50	D51	D52	E53	P54	T55	K118	T119	A120	E121	L122	V123	L124																								
M125	Y126	I127	R130	L131	M132	A133	R200	K134	R135	T201	F136	F137	D204	K205	E206	S143	A144	L145	G146	R147	A148	V149	G150	A154	Q155	L156	V157	N158	E159	G162	Q163	G164	N165	T166	D167	L168	Y169	F170	A105	E171	A106	L172	L173	R174	D175	Q110	E111	N112	D113	H181	V182	L183	T184	G185	K118	D186	L187	L188	K189	F190	I191	S191																								
A192	E193	T194	L195	S196	E197	L198	L199	R200	T201	T202	E203	D204	K205	E206	R207	S143	A144	L145	G146	R147	A148	V149	G150	A154	Q155	L156	V157	N158	E159	G162	Q163	G164	N165	T166	D167	L168	Y169	F170	A105	E171	A106	L172	L173	R174	D175	Q110	E111	N112	D113	H181	V182	L183	T184	G185	K118	D186	L187	L188	K189	F190	I191	S191																								
T252	A253	K254	L255	S256	G257	F258	T259	P260	G261	E262	L263	R264	S265	Y266	L267	S330	N331	K268	F208	T210	G211	G212	L213	N214	T215	L216	E217	N218	L219	S220	E221	N222	A280	N221	P222	S223	N224	P225	T226	E227	N165	K228	D229	Y230	L231	L232	S233	L234	S235	L173	P235	L236	S237	C238	L240	T241	G242	V243	F304	F305	L306	G307	L246	V308	R309	C310	F311	E312																		
P315	N316	T317	S318	L319	P320	F321	S322	R323	L324	E325	L328	E329	N330	K268	F208	T210	G211	G212	L213	N214	T215	L216	E217	N218	L219	S220	E221	N222	A280	N221	P222	S223	N224	P225	T226	E227	N165	K228	D229	Y230	L231	L232	S233	L234	S235	L173	P235	L236	S237	C238	L240	T241	G242	V243	F304	F305	L306	G307	L246	V308	R309	C310	F311	E312																						
L377	V378	S379	L380	G381	P382	P383	Q384	S385	L386	L387	L388	N390	L391	T392	L401	L402	D403	Q404	S405	R406	L407	P408	F409	S410	E411	R412	K413	L414	K415	F416	S417	M418	R419	F420	L421	P422	V423	A424	S425	P426	F427	H428	S429	H430	L431	L432	V433	P434	A435	S436	D437	L438	I439																																	
M440	K441	D442	L443	V444	K445	M446	M447	V448	S449	F450	M451	A452	K453	L454	L455	D461	T462	F463	Q464	G465	S466	D467	L468	R469	V470	L471	S472	G473	S474	L475	N536	E477	R478	L479	V480	D481	C482	L483	L484	R485	L486	P487	V488	K489	M490	E491	L492	L493	T494	D495	F496	K497	A498	T499																																
H500	L501	D502	L503	F504	G505	P506	G507	S508	A509	S510	G511	L512	G513	V514	L515	D521	T522	F523	G524	V525	R526	E527	L528	V529	A530	G531	L532	L533	L534	L535	N536	P537	D538	D539	D540	Y541	G542	F543	K544	G545	X550	X551	X552	X553	X554	X555	X556	X557	X558	X559	X560	X561	X562	X563	X564	X565	X566	X567																												
X568	X569	X570	X571	X572	X573	X574	X575	X576	X577	X578	X579	X580	X581	X582	X583	X584	X585	X586	X587	X588	X589	X590	X591	X592	X593	X594	X595	X596	X597	X598	X599	X600	X601	X602	X603	X604	X605	X606	X607	X608	X609	X610	X611	X612	X613	X614	X615	X616	X617	X618	X619	X620	X621	X622	X623	X624	X625	X626	X627	X628	X629	X630	X631	X632	X633	X634	X635	X636	X637	X638	X639	X640	X641	X642	X643	X644	X645	X646	X647							
X648	X649	X650	X651	X652	X653	X654	X655	X656	X657	X658	X659	X660	X661	X662	X663	X664	X665	X666	X667	X668	X669	X670	X671	X672	X673	X674	X675	X676	X677	X678	X679	X680	X681	X682	X683	X684	X685	X686	X687	X688	X689	X690	X691	X692	X693	X694	X695	X696	X697	X698	X699	X700	X701	X702	X703	X704	X705	X706	X707	X708	X709	X710	X711	X712	X713	X714	X715	X716	X717	X718	X719	X720	X721	X722	X723	X724										
X725	X726	X727	X728	X729	X730	X731	X732	X733	X734	X735	X736	X737	X738	X739	X740	X741	X742	X743	X744	X745	X746	X747	X748	X749	X750	X751	X752	X753	X754	X755	X756	X757	X758	X759	X760	X761	X762	X763	X764	X765	X766	X767	X768	X769	X770	X771	X772	X773	X774	X775	X776	X777	X778	X779	X780	X781	X782	X783	X784	X785	X786	X787	X788	X789	X790	X791	X792	X793	X794	X795	X796	X797	X798	X799	X800	X801	X802	X803								
X806	X807	X808	X809	X810	X811	X812	X813	X814	X815	X816	X817	X818	X819	X820	X821	X822	X823	X824	X825	X826	X827	X828	X829	X830	X831	X832	X833	X834	X835	X836	X837	X838	X839	X840	X841	X842	X843	X844	X845	X846	X847	X848	X849	X850	X851	X852	X853	X854	X855	X856	X857	X858	X859	X860	X861	X862	X863	X864	X865	X866	X867	X868	X869	X870	X871	X872	X873	X874	X875	X876	X877	X878	X879	X880	X881	X882	X883	X884	X885	X886						
X887	X888	X889	X890	X891	X892	X893	X894	X895	X896	X897	X898	X899	X900	X901	X902	X903	X904	X905	X906	X907	X908	X909	X910	X911	X912	X913	X914	X915	X916	X917	X918	X919	X920	X921	X922	X923	X924	X925	X926	X927	X928	X929	X930	X931	X932	X933	X934	X935	X936	X937	X938	X939	X940	X941	X942	X943	X944	X945	X946	X947	X948	X949	X950	X951	X952	X953	X954	X955	X956	X957	X958	X959	X960	X961	X962	X963	X964	X965	X966	X967	X968	X969	X970	X971	X972	X973
X974	X975	X976	X977	X978	X979	X980	X981	X982	X983	X984	X985	X986	X987	X988	X989	X990	X991	X992	X993	X994	X995	X996	X997	X998	X999	X1000	X1001	X1002	X1003	X1004	X1005	X1006	X1007	X1008	X1009	X1010	X1011	X1012	X1013	X1014	X1015	X1016	X1017	X1018	X1019	X1020	X1021	X1022	X1023	X1024	X1025	X1026	X1027	X1028	X1029	X1030	X1031	X1032	X1033	X1034	X1035	X1036	X1037	X1038	X1039	X1040	X1041	X1042	X1043	X1044	X1045	X1046	X1047	X1048												

X1049	X1050	X1051	X1052	X1053	X1054	X1055	X1056	X1057	X1058	X1059	X1060	X1061	X1062	X1063	X1066	X1067	X1068	X1069	X1074	X1075	X1076	X1137	X1138	X1139	X1140	X1141	X1142	X1146	X1147	X1148	X1149	X1150	X1151	X1152	X1153	X1157	X1162	X1163	X1164	X1165	X1166	X1167	X1168	X1169	X1170	X1171	X1172	X1173	X1177	X1178	X1179	X1180																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
X1181	X1182	X1183	X1192	X1193	X1194	X1195	X1196	X1197	X1198	X1199	X1200	X1201	X1202	X1205	X1206	X1207	X1208	X1209	X1210	X1211	X1212	X1213	X1214	X1215	X1220	X1221	X1222	X1225	X1226	X1234	X1235	X1236	X1246	X1247	X1248	X1249	X1250	X1251	X1252	X1253	X1256	X1257	X1258	X1259	X1260	X1261	X1262	X1263	X1264	X1265	X1266																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
X1268	X1269	X1270	X1271	X1272	X1275	X1276	X1280	X1281	X1282	X1283	X1284	X1291	X1295	X1296	X1297	X1298	X1299	X1300	X1301	X1304	X1305	X1306	X1307	X1308	X1309	X1314	X1315	X1318	X1319	X1320	X1321	X1322	X1323	X1324	X1325	X1326	X1327	X1328	X1329	X1332	X1333	X1334	X1335	X1336	X1337	X1340	X1341	X1342	X1343	X1344																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
X1345	X1346	X1347	X1348	X1349	X1355	X1356	X1357	X1360	X1361	X1362	X1363	X1364	X1365	X1366	X1367	X1368	X1369	X1370	X1371	X1377	X1378	X1379	X1386	X1390	X1391	X1397	X1398	X1406	X1407	X1408	X1413	X1414	X1415	X1416	X1417	X1418	X1419	X1420	X1421	X1422	X1423	X1424	X1425	X1426	X1429	X1430	X1431	X1432	X1433	X1434	X1440																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1461	X1462	X1463	X1464	X1469	X1476	X1477	X1482	X1483	X1485	X1486	X1487	X1490	X1491	X1492	X1493	X1496	X1497	X1498	X1502	X1503	X1504	X1505	X1506	X1507	X1508	X1509	X1510	X1511	X1512	X1513	X1519																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
X1520	X1521	X1531	X1532	X1533	X1534	X1535	X1536	X1537	X1538	X1539	X1540	X1541	X1542	X1543	X1544	X1545	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1558	X1559	X1560	X1561	X1562	X1563	X1564	X1573	X1574	X1575	X1581	X1582	X1583	X1584	X1585	X1586	X1587	X1588	X1589	X1590	X1591	X1592	X1593	X1594	X1595	X1596	X1602	X1603	X1604	X1605	X1606																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
X1607	X1608	X1614	X1625	X1628	X1629	X1630	X1631	X1632	X1633	X1634	X1638	X1639	X1642	X1643	X1644	X1645	X1646	X1649	X1650	X1651	X1652	X1655	X1656	X1657	X1663	X1664	X1665	Q1669	G1670	S1671	Q1672	E1673	Q1674	G1675	M1676	G1677	M1678	D1679	L1680	Y1681	K1682	T1683	S1684	K1685	L1686	A1687	Q1688	D1689	L1690	W1691																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
M1692	R1693	A1694	D1695	A1696	H1697	F1698	L1700	L1701	F1702	G1703	F1704	S1705	L1706	L1707	D1708	L1709	V1710	L1711	L1712	M1713	P1714	L1715	L1716	L1717	L1718	L1719	L1720	F1721	M1722	G1723	G1724	L1725	G1726	L1727	R1728	L1729	L1730	E1731	N1732	Y1733	S1734	A1735	M1736	L1737	F1738	E1739	T1740	L1741	V1742	D1743	G1744	L1745	L1746	K1750	L1751	F1752	L1753																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
E1754	L1755	M1756	E1757	A1758	H1759	T1760	S1761	L1762	F1763	L1764	R1765	S1766	G1769	L1770	L1771	S1772	A1773	T1774	Q1775	F1776	T1777	Q1778	P1779	A1780	L1781	L1782	L1783	M1784	E1785	L1786	A1787	L1788	F1789	E1790	D1791	L1792	K1793	S1794	G1795	L1796	L1797	L1798	P1799	A1800	D1801	A1802	T1803	F1804	A1805	G1806	H1807	S1808	L1809	G1810	E1811	Y1812	A1813	A1814																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
L1815	A1816	L1817	L1818	A1819	D1820	V1821	M1822	S1823	L1824	E1825	S1826	L1827	L1828	E1829	V1830	F1831	L1832	Y1833	L1834	G1835	M1836	T1837	M1838	Q1839	V1840	A1841	L1842	P1843	L1844	D1845	L1846	L1847	G1848	R1849	S1850	N1851	Y1852	G1853	M1854	L1855	A1856	L1857	M1858	P1859	G1860	R1861	V1862	A1863	L1864	S1865	F1866	S1867	Q1868	S1869	L1870	L1871	Q1872	L1873	V1874																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
V1875	E1876	R1877	L1878	K1879	K1880	L1881	T1882	G1883	M1884	L1885	V1886	E1887	L1888	M1889	M1890	L1891	M1892	L1893	E1894	M1895	Q1896	Q1897	Y1898	V1899	A1900	A1901	G1902	L1903	L1904	R1905	A1906	D1907	L1908	T1909	V1910	T1911	N1912	V1913	L1914	M1915	F1916	L1917	X1918	L1919	Q1920	L1921	L1924	L1925	E1926	L1927	Q1928	L1929	S1930	L1931	L1932	L1933	E1934	E1935																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
V1936	E1937	G1938	H1939	L1940	X1948	X1949	X1950	X1951	X1957	X1960	X1961	X1962	X1963	X1964	X1965	X1966	X1967	X1968	X1969	X1970	X1971	X1972	X1973	X1974	X1975	X1976	X1981	X1982	X1983	X1984	X1985	X1986	X1987	X1988	X1989	X1990	X1991	X1996	X2000	X2001	X2002	X2003	X2004	X2005	X2006	X2007	X2008	X2009	X2010	X2011	X2012	X2013																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
X2019	X2020	X2021	X2022	X2023	X2024	X2028	X2029	X2030	X2031	X2032	X2033	X2034	X2035	X2036	X2037	X2038	X2039	X2040	X2041	X2042	X2043	X2047	X2048	X2049	X2050	X2051	X2058	X2059	X2060	X2061	X2062	X2063	X2064	X2065	X2066	X2067	X2068	X2069	X2070	X2071	X2072	X2073	X2074	X2075	X2076	X2077	X2078	X2079	X2080	X2081	X2082	X2083	X2084	X2085	X2086	X2087	X2088	X2089	X2090	X2091	X2092	X2093	X2094	X2095	X2096	X2097	X2098	X2099	X2100	X2101	X2102	X2103	X2104	X2105	X2106	X2107	X2108	X2109	X2110	X2111	X2112	X2113	X2114	X2115	X2116	X2117	X2118	X2119	X2120	X2121	X2122	X2123	X2124	X2125	X2126	X2127	X2128	X2129	X2130	X2131	X2132	X2133	X2134	X2135	X2136	X2137	X2138	X2139	X2140	X2141	X2142	X2143	X2144	X2145	X2146	X2147	X2148	X2149	X2150	X2151	X2152	X2153	X2154	X2155	X2156	X2157	X2158	X2159	X2160	X2161	X2162	X2163	X2164	X2165	X2166	X2167	X2168	X2169	X2170	X2171	X2172	X2173	X2174	X2175	X2176	X2177	X2178	X2179	X2180	X2181	X2182	X2183	X2184	X2185	X2186	X2187	X2188	X2189	X2190	X2191	X2192	X2193	X2194	X2195	X2196	X2197	X2198	X2199	X2200	X2201	X2202	X2203	X2204	X2205	X2206	X2207	X2208	X2209	X2210	X2211	X2212	X2213	X2214	X2215	X2216	X2217	X2218	X2219	X2220	X2221	X2222	X2223	X2224	X2225	X2226	X2227	X2228	X2229	X2230	X2231	X2232	X2233	X2234	X2235	X2236	X2237	X2238	X2239	X2240	X2241	X2242	X2243	X2244	X2245	X2246	X2247	X2248	X2249	X2250	X2251	X2252	X2253	X2254	X2255	X2256	X2257	X2258	X2259	X2260	X2261	X2262	X2263	X2264	X2265	X2266	X2267	X2268	X2269	X2270	X2271	X2272	X2273	X2274	X2275	X2276	X2277	X2278	X2279	X2280	X2281	X2282	X2283	X2284	X2285	X2286	X2287	X2288	X2289	X2290	X2291	X2292	X2293	X2294	X2295	X2296	X2297	X2298	X2299	X2300	X2301	X2302	X2303	X2304	X2305	X2306	X2307	X2308	X2309	X2310	X2311	X2312	X2313	X2314	X2315	X2316	X2317	X2318	X2319	X2320	X2321	X2322	X2323	X2324	X2325	X2326	X2327	X2328	X2329	X2330	X2331	X2332	X2333	X2334	X2335	X2336	X2337	X2338	X2339	X2340	X2341	X2342	X2343	X2344	X2345	X2346	X2347	X2348	X2349	X2350	X2351	X2352	X2353	X2354	X2355	X2356	X2357	X2358	X2359	X2360	X2361	X2362	X2363	X2364	X2365	X2366	X2367	X2368	X2369	X2370	X2371	X2372	X2373	X2374	X2375	X2376	X2377	X2378	X2379	X2380	X2381	X2382	X2383	X2384	X2385	X2386	X2387	X2388	X2389	X2390	X2391	X2392	X2393	X2394	X2395	X2396	X2397	X2398	X2399	X2400	X2401	X2402	X2403	X2404	X2405	X2406	X2407	X2408	X2409	X2410	X2411	X2412	X2413	X2414	X2415	X2416	X2417	X2418	X2419	X2420	X2421	X2422	X2423	X2424	X2425	X2426	X2427	X2428	X2429	X2430	X2431	X2432	X2433	X2434	X2435	X2436	X2437	X2438	X2439	X2440	X2441	X2442	X2443	X2444	X2445	X2446	X2447	X2448	X2449	X2450	X2451	X2452	X2453	X2454	X2455	X2456	X2457	X2458	X2459	X2460	X2461	X2462	X2463	X2464	X2465	X2466	X2467	X2468	X2469	X2470	X2471	X2472	X2473	X2474	X2475	X2476	X2477	X2478	X2479	X2480	X2481	X2482	X2483	X2484	X2485	X2486	X2487	X2488	X2489	X2490	X2491	X2492	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2502	X2503	X2504	X2505	X2506	X2507	X2508	X2509	X2510	X2511	X2512	X2513	X2514	X2515	X2516	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2539	X2540	X2541	X2542	X2543	X2544	X2545	X2546	X2547	X2548	X2549	X2550	X2551	X2552	X2553	X2554	X2555	X2556	X2557	X2558	X2559	X2560	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2570	X2571	X2572	X2573	X2574	X2575	X2576	X2577	X2578	X2579	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2587	X2588	X2589	X2590	X2591	X2592	X2593	X2594	X2595	X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2603	X2604	X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612	X2613	X2614	X2615	X2616	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2641	X2642	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2656	X2657	X2658	X2659	X2660	X2661	X2662	X2663	X2664	X2665	X2666	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	X2704	X2705	X2706	X2707	X2708	X2709	X2710	X2711	X2712	X2713	X2714	X2715	X2716	X2717	X2718

X973	X897	X809	X726	X660	X570	I501	K441	L377	V951	S191	M125	K63	M1
X974	X898	X810	X727	X651	X571	I502	D442	V378	T252	A192	Y126	F64	D2
X975	X899	X811	X728	X652	X572	D503	L443	V379	K254	A193	A253	L65	A3
X976	X900	X812	X729	X653	X573	F504	V444	S380	G254	T194	G254	G66	Y4
X977	X905	X813	X730	X654	X574	G505	K445	G381	L256	L195	R130	L255	S5
X978	X906	X814	X731	X655	X575	F506	N446	P382	L256	S196	L131	V68	L9
X982	X907	X815	X732	X656	X576	G507	N447	P383	G257	E197	G257	S69	L10
X983	X911	X816	X735	X657	X580	G508	V448	Q384	F258	L198	A133	S70	T10
X989	X912	X817	X736	X660	X581	A509	S449	S385	T259	I199	K134	L71	L11
X995	X915	X818	X737	X661	X582	S510	F450	L386	G261	P200	R135	W72	S12
X996	X916	X819	X738	X662	X583	G511	N451	Y387	E261	E73	P136	E73	H13
X997	X917	X820	X739	X667	X584	L512	A452	G388	E262	T201	F137	P74	G14
X998	X918	X821	X740	X668	X585	G513	K453	L389	L263	L203	D138	S75	S15
X1002	X919	X822	X741	X669	X586	V514	D454	N390	R264	D204	K139	K76	L16
X1008	X922	X823	X742	X668	X587	L515	L455	L391	S265	A205	S143	V77	E17
X1009	X923	X824	X743	X668	X588	T516	Q456	L392	E266	E206	Y266	G78	H18
X1010	X924	X825	X744	X670	X589	H517	L457	L393	W267	K207	A144	Q79	V19
X1011	X925	X826	X745	X671	X590	R518	F458	R394	K268	E208	L145	F80	L20
X1012	X926	X827	X746	X672	X591	N519	V459	K395	G269	F209	F146	N81	L21
X1013	X927	X828	X747	X673	X592	K520	L460	A396	A270	T210	R147	Q82	V22
X1014	X928	X829	X748	X674	X593	D521	D461	P335	T271	Q211	A148	Q82	V22
X1015	X929	X830	X749	X675	X594	D522	T462	S336	G272	G212	V149	N85	T24
X1016	X930	X831	X750	X676	X595	T523	F463	P337	L277	L213	G150	L86	A25
X1017	X931	X832	X751	X677	X596	G524	D464	M338	S274	N214	A154	C87	S26
X1018	X932	X833	X752	X678	X597	V525	G465	Q403	Q275	L215	Q155	L88	F27
X1019	X933	X834	X753	X679	X598	R526	S466	S405	G276	L216	Q155	T89	F28
X1020	X934	X835	X754	X680	X600	V527	D467	R406	L277	L217	L156	E90	I29
X1021	X935	X836	X755	X681	X601	T528	L468	R407	L278	W218	V157	E90	I29
X1022	X936	X837	X756	X682	X602	V529	L469	L402	F279	L219	A30	F91	A30
X1023	X937	X838	X757	X683	X603	A530	V470	D403	T280	L219	A30	F91	A30
X1024	X938	X839	X758	X684	X604	G531	L471	Q404	A280	E220	I159	E92	S31
X1025	X939	X840	X759	X685	X605	H532	S472	S410	V281	N221	F160	C94	L33
X1026	X940	X841	X760	X686	X606	T533	S473	E411	A282	P222	G161	Y95	Q34
X1027	X941	X842	X761	X687	X607	L534	G473	R412	A283	P222	G162	L96	E36
X1028	X942	X843	X762	X688	X608	D534	S474	K415	A284	N224	Q163	E97	Q36
X1029	X943	X844	X763	X689	X609	L535	L475	K416	A285	M226	Q164	E97	Q36
X1030	X944	X845	X764	X690	X610	N536	S476	P416	T286	P226	G164	E98	F37
X1031	X945	X846	X765	X691	X611	R537	E477	S417	D287	M165	G164	E98	F37
X1032	X946	X847	X766	X692	X612	D538	R478	M418	S288	D227	T166	D100	K39
X1033	X947	X848	X767	X693	X613	D539	L479	M419	W289	W228	D167	L101	L40
X1034	X948	X849	X768	X694	X614	D540	V480	P420	N354	D229	D168	H102	L40
X1035	X949	X850	X769	X695	X615	F541	D481	L421	F292	Y230	Y169	A103	P42
X1036	X950	X851	X770	X696	X616	G542	C482	P422	F293	L231	F170	L104	P42
X1037	X951	X852	X771	X697	X617	F543	I483	V423	V294	L232	E171	A105	P44
X1038	X952	X853	X772	X698	X618	K544	L484	A424	S295	S233	N357	A106	T45
X1039	X953	X854	X773	X699	X619	Q545	R485	S425	V296	L234	L173	K107	T45
X1040	X954	X855	X774	X700	X620	L486	L486	P426	R297	P236	R174	L108	E46
X1041	X955	X856	X775	X701	X621	X551	P487	P427	K298	I236	D175	Q110	F48
X1042	X956	X857	X776	X702	X622	X552	V487	L427	K298	S237	L176	Q110	A49
X1043	X957	X858	X777	X703	X623	X553	V488	H428	A299	C238	Y177	E111	A49
X1044	X958	X859	X778	X704	X624	X554	W489	S429	A299	P239	Y177	N112	D51
X1045	X959	X860	X779	X705	X625	X555	V490	H430	T301	L240	Y180	D113	D52
X1046	X960	X861	X780	X706	X626	X556	L491	L431	V302	L241	H181	T114	E53
X1047	X961	X862	X781	X707	X627	X557	T492	L432	L303	G242	H182	T115	E53
X1048	X962	X863	X782	X708	X628	X558	V491	L433	L303	G242	H182	T115	E53
X1049	X963	X864	X783	X709	X629	X559	T493	L434	F304	V243	L183	K118	T55
X1050	X964	X865	X784	X710	X630	X560	V492	P434	S369	F304	L183	K118	T55
X1051	X965	X866	X785	X711	X631	X561	T494	P434	V305	G243	V184	L119	T56
X1052	X966	X867	X786	X712	X632	X562	V493	A435	I306	Q245	G185	T119	P57
X1053	X967	X868	X787	X713	X633	X563	T494	S436	I307	D186	G307	K120	A58
X1054	X968	X869	X788	X714	X634	X564	V495	D437	V308	E121	L187	E121	E59
X1055	X969	X870	X789	X715	X635	X565	F496	L438	R309	L222	L188	L122	L60
X1056	X970	X871	X790	X716	X636	X566	V497	L439	R309	E248	K189	L122	L60
X1057	X971	X872	X791	X717	X637	X567	T497	L440	R309	E248	K189	L122	L60
X1058	X972	X873	X792	X718	X638	X568	V498	N440	Y311	V250	F190	K124	G62

X1051	X1052	X1053	X1054	X1055	X1056	X1057	X1058	X1059	X1060	X1061	X1062	X1063	X1066	X1067	X1068	X1069	X1074	X1075	X1076	X1077	X1078	X1079	X1080	X1081	X1082	X1083	X1084	X1085	X1086	X1087	X1088	X1089	X1090	X1136	X1137	X1138	X1139	X1140	X1141	X1142	X1146	X1147	X1148	X1149	X1150	X1151	X1152	X1153	X1157	X1162	X1163	X1164	X1165	X1166	X1167	X1168	X1169	X1170	X1171	X1172	X1173	X1177	X1178	X1179
X1180	X1181	X1182	X1183	X1192	X1193	X1194	X1195	X1196	X1197	X1198	X1199	X1200	X1201	X1202	X1205	X1206	X1207	X1208	X1209	X1210	X1211	X1212	X1215	X1220	X1221	X1222	X1225	X1226	X1230	X1231	X1234	X1235	X1236	X1246	X1247	X1248	X1249	X1250	X1251	X1252	X1253	X1256	X1257	X1258	X1259	X1260	X1261	X1262	X1263	X1264														
X1265	X1266	X1267	X1268	X1269	X1270	X1271	X1272	X1275	X1276	X1280	X1281	X1282	X1283	X1284	X1291	X1295	X1296	X1297	X1298	X1299	X1300	X1301	X1304	X1305	X1306	X1307	X1308	X1309	X1314	X1315	X1320	X1321	X1322	X1323	X1324	X1325	X1326	X1327	X1328	X1329	X1332	X1333	X1334	X1335	X1336	X1337	X1340	X1341	X1342	X1343														
X1344	X1345	X1346	X1347	X1348	X1349	X1355	X1356	X1357	X1360	X1361	X1362	X1369	X1370	X1371	X1377	X1378	X1379	X1386	X1390	X1391	X1397	X1398	X1407	X1408	X1413	X1414	X1415	X1416	X1418	X1419	X1420	X1421	X1422	X1423	X1424	X1425	X1426	X1429	X1430	X1431	X1432	X1433	X1441	X1442	X1443	X1444																		
X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1462	X1463	X1464	X1469	X1476	X1477	X1482	X1483	X1484	X1485	X1486	X1487	X1490	X1491	X1492	X1493	X1496	X1497	X1498	X1502	X1503	X1504	X1505	X1506	X1507	X1508	X1509	X1510	X1511	X1512	X1519	X1520	X1521	X1522	X1523	X1524													
X1531	X1532	X1533	X1534	X1535	X1536	X1537	X1538	X1539	X1540	X1541	X1542	X1543	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1558	X1559	X1560	X1561	X1562	X1563	X1564	X1573	X1574	X1575	X1581	X1582	X1583	X1584	X1585	X1586	X1587	X1588	X1589	X1590	X1591	X1592	X1593	X1594	X1595	X1602	X1603	X1604	X1605	X1606	X1607	X1608											
X1614	X1625	X1628	X1629	X1630	X1631	X1632	X1633	X1634	X1638	X1639	X1642	X1643	X1644	X1645	X1646	X1649	X1650	X1651	X1652	X1655	X1656	X1657	X1663	X1665	X1666	X1667	X1668	X1670	X1671	X1672	X1673	X1674	X1675	X1676	X1677	X1678	X1679	X1680	X1681	X1682	X1683	X1684	X1685	X1686	X1687	X1688	X1689	X1690	X1691	X1692	X1693													
A1694	D1695	H1696	H1697	F1698	D1700	T1701	Y1702	G1703	F1704	S1705	L1706	L1707	D1708	L1709	I1710	I1711	M1712	M1713	P1714	M1715	M1716	L1717	L1718	L1719	H1720	F1721	G1722	G1723	E1724	K1725	G1726	R1727	R1728	I1729	M1730	E1731	M1732	Y1733	S1734	A1735	M1736	L1737	F1738	E1739	T1740	I1741	V1742	D1743	G1744	K1745	L1746	K1750	L1751	F1752	K1753	E1754	L1755							
M1756	L1757	H1758	S1759	T1760	S1761	Y1762	T1763	F1764	S1765	S1766	G1769	L1770	L1771	S1772	S1773	A1774	R1775	Q1776	F1777	Q1778	P1779	M1780	L1781	T1782	L1783	M1784	E1785	K1786	A1787	A1788	F1789	E1790	D1791	L1792	K1793	S1794	K1795	G1796	L1797	I1798	P1799	A1800	D1801	A1802	T1803	F1804	A1805	F1806	H1807	S1808	L1809	G1810	A1811	L1812	Y1813	A1814	A1815	L1816						
S1817	L1818	A1819	D1820	M1821	M1822	S1823	L1824	E1825	L1826	L1827	E1828	V1829	V1830	V1831	F1832	R1833	R1834	G1835	M1836	T1837	M1838	Q1839	M1840	V1842	P1843	R1844	D1845	E1846	L1847	G1848	R1849	S1850	M1851	Y1852	G1853	M1854	I1855	A1856	L1857	M1858	P1859	G1860	R1861	A1862	A1863	A1864	S1865	F1866	S1867	Q1868	A1869	A1870	L1871	Q1872	Y1873	M1874	V1875	A1876	A1877					
R1877	V1878	K1879	K1880	T1881	L1882	G1883	M1884	L1885	V1886	L1887	V1888	M1889	M1890	Y1891	M1892	V1893	E1894	M1895	Q1896	Q1897	V1898	V1899	A1900	A1901	G1902	D1903	L1904	R1905	A1906	L1907	D1908	T1909	V1910	T1911	M1912	V1913	L1914	M1915	F1916	I1917	K1918	L1919	Q1920	K1921	I1922	D1923	I1924	I1925	E1926	L1927	Q1928	R1929	S1930	L1931	L1932	L1933	E1934	E1935	V1936					
E1937	G1938	H1939	L1940	X1948	X1949	X1950	X1951	X1957	X1960	X1961	X1962	X1963	X1964	X1965	X1966	X1967	X1968	X1969	X1970	X1971	X1972	X1973	X1974	X1975	X1976	X1981	X1982	X1983	X1984	X1985	X1986	X1987	X1988	X1989	X1990	X1991	X1995	X1996	X2000	X2001	X2002	X2003	X2004	X2005	X2006	X2007	X2008	X2009	X2011	X2012	X2013													
X2019	X2020	X2021	X2022	X2023	X2024	X2028	X2029	X2030	X2031	X2032	X2033	X2034	X2035	X2036	X2037	X2038	X2039	X2040	X2041	X2042	X2043	X2044	X2047	X2048	X2049	X2050	X2051																																					

● Molecule 2: Fatty acid synthase subunit beta



X971	X887	X802	X722	X650	X570	L502	D442	V378	P315	T252	A192	M125	K63	M1
X972	X888	X803	X723	X651	X571	D503	L443	V379	M316	A253	E193	Y126	F64	D2
X973	X889	X804	X724	X652	X572	F504	V444	S380	T317	K254	T194	I127	L65	A3
X974	X890	X805	X725	X653	X573	G505	K445	G381	S318	L255	E195	L130	G66	Y4
X975	X891	X806	X726	X654	X574	P506	N446	P382	L319	D256	S196	R131	Y67	S5
X976	X892	X807	X727	X655	X575	G507	N447	P383	P320	G257	E197	I131	Y68	L9
X977	X893	X808	X728	X656	X576	G508	V448	Q384	P321	F258	L198	M132	S69	T10
X978	X894	X809	X729	X657	X577	A509	S449	S385	S322	T259	E199	A133	S70	L11
X989	X895	X810	X730	X658	X578	S510	F450	L386	L323	P260	R200	K134	L71	L11
X996	X896	X811	X731	X659	X579	G511	N451	G387	L324	E261	T201	R135	E72	S12
X997	X897	X812	X732	X660	X580	L512	A452	H388	L325	E262	T202	P136	E73	H13
X998	X898	X813	X733	X661	X581	G513	K453	L389	E325	E263	L203	F137	P74	G14
X999	X899	X814	X734	X662	X582	V514	D454	R390	L328	R264	D204	D138	S75	G15
X1002	X900	X815	X735	X663	X583	L515	L455	L391	E329	S265	A205	K139	K76	L16
X1008	X901	X816	X736	X664	X584	T516	Q456	T392	M330	Y266	E206	S143	V77	E17
X1009	X902	X817	X737	X665	X585	H517	L457	L393	N331	K267	K207	S144	G78	H18
X1010	X903	X818	X738	X666	X586	R518	P458	L394	E332	K268	V208	A144	Q79	V19
X1011	X904	X819	X739	X667	X587	N519	V459	R395	G333	G269	F209	L145	F80	L20
X1012	X905	X820	X740	X668	X588	K520	Y460	A396	V334	A270	T210	F146	H81	L21
X1013	X906	X821	X741	X669	X589	D521	D461	T462	P335	T271	Q211	R147	Q82	V22
X1014	X907	X822	X742	X670	X590	G522	F463	G401	S336	G272	G212	A148	Q82	P23
X1015	X908	X823	X743	X671	X591	T523	D464	L402	P337	H273	L213	V149	N85	T24
X1016	X909	X824	X744	X672	X592	G524	F465	D403	M338	S274	L214	G150	L86	A25
X1017	X910	X825	X745	X673	X593	G525	D466	D404	L339	Q275	I215	C150	C87	S26
X1018	X911	X826	X746	X674	X594	V525	G465	S405	S340	G276	L216	A154	C87	S26
X1019	X912	X827	X747	X675	X595	R526	S466	R406	I341	L277	E217	Q155	L88	F27
X1020	X913	X828	X748	X676	X596	V527	D467	R407	S342	V278	W218	Q156	T89	F28
X1021	X914	X829	X749	X677	X597	L528	L468	L407	N343	V279	L219	L156	E90	L29
X1022	X915	X830	X750	X678	X598	V529	R469	P408	M344	T279	L219	V157	F91	A30
X1023	X916	X831	X751	X679	X599	A530	V470	F409	L344	A280	E220	G150	F91	S31
X1024	X917	X832	X752	X680	X600	G531	L471	S410	T345	V281	N221	I159	N92	Q32
X1025	X918	X833	X753	X681	X601	L532	S472	E411	Q346	A282	P222	F160	C94	L33
X1028	X919	X834	X754	X682	X602	T533	G473	R412	E347	L283	S223	G161	Y95	Q34
X1029	X920	X835	X755	X683	X603	D534	S474	R413	Q348	A284	N224	Q162	L96	E36
X1030	X921	X836	X756	X684	X604	L535	L475	R414	V349	E285	T225	Q163	E97	Q37
X1031	X922	X837	X757	X685	X605	N536	S476	F416	Q350	T286	P226	Q164	G98	F36
X1034	X923	X838	X758	X686	X606	P537	E477	S417	D351	D287	D227	M165	N99	N38
X1035	X924	X839	X759	X687	X607	D538	R478	M418	V352	S288	K228	T166	D100	K39
X1036	X925	X840	X760	X688	X608	L539	L479	R419	V353	S289	D229	D167	L101	L40
X1037	X926	X841	X761	X689	X609	D540	V480	F420	M354	F168	Y230	D168	H102	L41
X1038	X927	X842	X762	X690	X610	Y541	D481	L421	K355	Y169	L231	E169	A103	P42
X1039	X928	X843	X763	X691	X611	G542	C482	P422	T356	F170	L232	F170	L104	P43
X1040	X929	X844	X764	X692	X612	F543	L483	V423	N357	E171	S233	E171	A105	P44
X1041	X930	X845	X765	X693	X613	K544	L484	A424	S358	I234	I234	E172	A106	T45
X1042	X931	X846	X766	X694	X614	Q545	P485	S425	H559	V296	P235	L173	K107	E46
X1043	X932	X847	X767	X695	X615	X546	L486	P426	L360	R297	I236	R174	L108	G47
X1044	X933	X848	X768	X696	X616	X550	V487	F427	P361	K298	S237	D175	L109	F48
X1045	X934	X849	X769	X697	X617	X551	V488	H428	Q365	A299	C238	L176	Q110	F49
X1046	X935	X850	X770	X698	X618	X552	K489	S429	I300	E300	P239	Y180	E111	A50
X1047	X936	X851	X771	X699	X619	X553	M490	H430	T301	L240	L240	H181	N112	D51
X1048	X937	X852	X772	X700	X620	X554	E491	L431	E367	V302	I241	H182	N113	D52
X1049	X938	X853	X773	X701	X621	X555	T492	L432	L368	G242	G242	V182	T114	E53
X1050	X939	X854	X774	X702	X622	X556	V493	V433	S369	F304	V243	L183	T115	P54
X1051	X940	X855	X775	X703	X623	X557	V494	P434	Q366	F305	I244	L184	T116	P55
X1052	X941	X856	X776	X704	X624	X558	K495	A435	L370	I306	Q245	K118	T117	T55
X1053	X942	X857	X777	X705	X625	X559	F496	A436	E367	G307	I246	L185	T118	T56
X1054	X943	X858	X778	X706	X626	X560	V497	D437	L368	G307	L246	D186	T119	P57
X1055	X944	X859	X779	X707	X627	X561	L498	L438	S369	V308	G247	I188	K120	A58
X1056	X945	X860	X780	X708	X628	X562	L499	L439	E367	R309	H248	I188	E121	E59
X1057	X946	X861	X781	X709	X629	X563	L499	L439	Q366	R309	H248	I188	E121	E59
X1058	X947	X862	X782	X710	X630	X564	L499	L439	L370	R309	H248	I188	E121	E59
X1059	X948	X863	X783	X711	X631	X565	L499	L439	L370	R309	H248	I188	E121	E59
X1060	X949	X864	X784	X712	X632	X566	L499	L439	L370	R309	H248	I188	E121	E59
X1061	X950	X865	X785	X713	X633	X567	L499	L439	L370	R309	H248	I188	E121	E59
X1062	X951	X866	X786	X714	X634	X568	L499	L439	L370	R309	H248	I188	E121	E59
X1063	X952	X867	X787	X715	X635	X569	L499	L439	L370	R309	H248	I188	E121	E59
X1064	X953	X868	X788	X716	X636	X570	L499	L439	L370	R309	H248	I188	E121	E59
X1065	X954	X869	X789	X717	X637	X571	L499	L439	L370	R309	H248	I188	E121	E59
X1066	X955	X870	X790	X718	X638	X572	L499	L439	L370	R309	H248	I188	E121	E59
X1067	X956	X871	X791	X719	X639	X573	L499	L439	L370	R309	H248	I188	E121	E59
X1068	X957	X872	X792	X720	X640	X574	L499	L439	L370	R309	H248	I188	E121	E59
X1069	X958	X873	X793	X721	X641	X575	L499	L439	L370	R309	H248	I188	E121	E59
X1070	X959	X874	X794	X722	X642	X576	L499	L439	L370	R309	H248	I188	E121	E59
X1071	X960	X875	X795	X723	X643	X577	L499	L439	L370	R309	H248	I188	E121	E59
X1072	X961	X876	X796	X724	X644	X578	L499	L439	L370	R309	H248	I188	E121	E59
X1073	X962	X877	X797	X725	X645	X579	L499	L439	L370	R309	H248	I188	E121	E59
X1074	X963	X878	X798	X726	X646	X580	L499	L439	L370	R309	H248	I188	E121	E59
X1075	X964	X879	X799	X727	X647	X581	L499	L439	L370	R309	H248	I188	E121	E59
X1076	X965	X880	X800	X728	X648	X582	L499	L439	L370	R309	H248	I188	E121	E59
X1077	X966	X881	X801	X729	X649	X583	L499	L439	L370	R309	H248	I188	E121	E59
X1078	X967	X882	X802	X730	X650	X584	L499	L439	L370	R309	H248	I188	E121	E59
X1079	X968	X883	X803	X731	X651	X585	L499	L439	L370	R309	H248	I188	E121	E59
X1080	X969	X884	X804	X732	X652	X586	L499	L439	L370	R309	H248	I188	E121	E59
X1081	X970	X885	X805	X733	X653	X587	L499	L439	L370	R309	H248	I188	E121	E59
X1082	X971	X886	X806	X734	X654	X588	L499	L439	L370	R309	H248	I188	E121	E59
X1083	X972	X887	X807	X735	X655	X589	L499	L439	L370	R309	H248	I188	E121	E59
X1084	X973	X888	X808	X736	X656	X590	L499	L439	L370	R309	H248	I188	E121	E59
X1085	X974	X889	X809	X737	X657	X591	L499	L439	L370	R309	H248	I188	E121	E59
X1086	X975	X890	X810	X738	X658	X592	L499	L439	L370	R309	H248	I188	E121	E59
X1087	X976	X891	X811	X739	X659	X593	L499	L439	L370	R309	H248	I188	E121	E59
X1088	X977	X892	X812	X740	X660	X594	L499	L439	L370	R309	H248	I188	E121	E59
X1089	X978	X893	X813	X741	X661	X595	L499	L439	L370	R309	H248	I188	E121	E59
X1090	X979	X894	X814	X742	X662	X596	L499	L439	L370	R309	H248	I188	E121	E59
X1091	X980	X895	X815	X743	X663	X597	L499	L439	L370	R309	H248	I188	E121	E59
X1092	X981	X896	X816	X744	X664	X598	L499	L439	L370	R309	H248	I188	E121	E59
X1093	X982	X897	X817	X745	X665	X599	L499	L439	L370	R309	H248	I188	E121	E59
X1094	X983	X898	X818	X746	X666	X600	L499	L439	L370	R309	H248	I188	E121	E59
X1095	X984	X899	X819	X747	X667	X601	L499	L439	L370	R309	H248	I188	E121	E59
X1096														

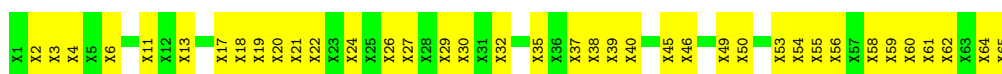




- Molecule 3: Tail protein



- Molecule 3: Tail protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.34Å 231.34Å 754.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 4.00 59.69 – 3.91	Depositor EDS
% Data completeness (in resolution range)	98.7 (60.00-4.00) 97.4 (59.69-3.91)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.88Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.319 , 0.346 0.299 , 0.333	Depositor DCC
$R_{free}$ test set	8857 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	152.3	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 180.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	71862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	151.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.80	7/8414 (0.1%)	0.95	28/11377 (0.2%)
1	D	0.80	7/8414 (0.1%)	0.95	32/11377 (0.3%)
1	G	0.82	7/8414 (0.1%)	0.96	29/11377 (0.3%)
2	B	0.41	0/6495	0.72	2/8812 (0.0%)
2	E	0.40	0/6495	0.72	3/8812 (0.0%)
2	H	0.41	0/6495	0.72	2/8812 (0.0%)
All	All	0.66	21/44727 (0.0%)	0.86	96/60567 (0.2%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1150	ASP	CB-CG	33.05	2.21	1.51
1	D	1150	ASP	CB-CG	32.65	2.20	1.51
1	A	1150	ASP	CB-CG	32.54	2.20	1.51
1	D	1181	PHE	CD2-CE2	21.08	1.81	1.39
1	G	1181	PHE	CE2-CZ	20.68	1.76	1.37

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1150	ASP	CB-CG-OD1	12.15	129.24	118.30
1	D	1150	ASP	CB-CG-OD1	12.14	129.22	118.30
1	A	1150	ASP	CB-CG-OD1	11.62	128.76	118.30
1	D	992	PHE	C-N-CD	-11.23	95.89	120.60
1	G	992	PHE	C-N-CD	-10.81	96.82	120.60

There are no chirality outliers.

There are no planarity outliers.

## 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	11319	0	8817	2535	24
1	D	11319	0	8818	2518	14
1	G	11319	0	8817	2527	24
2	B	12310	0	7819	1753	0
2	E	12310	0	7817	1770	0
2	H	12310	0	7816	1770	0
3	C	325	0	76	25	0
3	F	325	0	76	28	0
3	I	325	0	76	35	0
All	All	71862	0	50132	12923	38

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 106.

The worst 5 of 12923 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:G:1181:PHE:CE2	1:G:1181:PHE:CZ	1.76	1.71
1:A:1181:PHE:CZ	1:A:1181:PHE:CE2	1.75	1.69
1:D:1181:PHE:CE2	1:D:1181:PHE:CD2	1.81	1.68
1:G:1181:PHE:CZ	1:G:1181:PHE:CE1	1.75	1.68
1:D:1181:PHE:CD1	1:D:1181:PHE:CE1	1.78	1.66

The worst 5 of 38 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1150:ASP:OD1	1:D:1181:PHE:CE2[7_555]	1.80	0.40
1:A:1150:ASP:OD1	1:G:1181:PHE:CE2[7_555]	1.85	0.35
1:A:1181:PHE:CE2	1:G:1150:ASP:OD1[7_555]	1.85	0.35
1:A:1150:ASP:CG	1:G:1181:PHE:CE2[7_555]	1.87	0.33
1:D:1150:ASP:CG	1:D:1181:PHE:CE2[7_555]	1.87	0.33

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	1069/1688 (63%)	401 (38%)	298 (28%)	370 (35%)	0	0
1	D	1069/1688 (63%)	396 (37%)	307 (29%)	366 (34%)	0	0
1	G	1069/1688 (63%)	398 (37%)	307 (29%)	364 (34%)	0	0
2	B	817/2006 (41%)	356 (44%)	245 (30%)	216 (26%)	0	1
2	E	817/2006 (41%)	357 (44%)	244 (30%)	216 (26%)	0	1
2	H	817/2006 (41%)	352 (43%)	247 (30%)	218 (27%)	0	0
All	All	5658/11082 (51%)	2260 (40%)	1648 (29%)	1750 (31%)	0	0

5 of 1750 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	683	ALA
1	A	723	ALA
1	A	724	LYS
1	A	741	SER
1	A	742	LYS

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	871/895 (97%)	700 (80%)	171 (20%)	1	8
1	D	871/895 (97%)	697 (80%)	174 (20%)	1	8
1	G	871/895 (97%)	696 (80%)	175 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	703/703 (100%)	623 (89%)	80 (11%)	5	25
2	E	703/703 (100%)	623 (89%)	80 (11%)	5	25
2	H	703/703 (100%)	622 (88%)	81 (12%)	5	25
All	All	4722/4794 (98%)	3961 (84%)	761 (16%)	2	15

5 of 761 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	386	LEU
1	G	1185	VAL
2	E	533	LEU
2	E	372	ASN
1	G	781	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	1692	ASN
1	G	1389	GLN
2	E	1912	ASN
1	G	1063	HIS
1	G	1570	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	A	2
1	G	2

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	506:UNK	C	516:UNK	N	28.27
1	A	506:UNK	C	516:UNK	N	28.26
1	G	506:UNK	C	516:UNK	N	28.26
1	D	305:UNK	C	360:UNK	N	17.84
1	A	305:UNK	C	360:UNK	N	17.83

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1069/1688 (63%)	-0.35	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	48, 122, 192, 203	0
1	D	1069/1688 (63%)	-0.32	2 (0%) <span style="border: 1px solid blue; padding: 2px;">95</span> <span style="border: 1px solid blue; padding: 2px;">93</span>	53, 123, 194, 203	0
1	G	1069/1688 (63%)	-0.37	1 (0%) <span style="border: 1px solid blue; padding: 2px;">95</span> <span style="border: 1px solid blue; padding: 2px;">94</span>	43, 112, 190, 203	0
2	B	818/2006 (40%)	-0.12	25 (3%) <span style="border: 1px solid gray; padding: 2px;">49</span> <span style="border: 1px solid gray; padding: 2px;">38</span>	107, 177, 202, 203	0
2	E	818/2006 (40%)	-0.10	14 (1%) <span style="border: 1px solid gray; padding: 2px;">70</span> <span style="border: 1px solid gray; padding: 2px;">60</span>	111, 190, 202, 203	0
2	H	818/2006 (40%)	-0.15	17 (2%) <span style="border: 1px solid gray; padding: 2px;">63</span> <span style="border: 1px solid gray; padding: 2px;">54</span>	94, 183, 202, 203	0
3	C	0/65	-	-	-	-
3	F	0/65	-	-	-	-
3	I	0/65	-	-	-	-
All	All	5661/11277 (50%)	-0.25	59 (1%) <span style="border: 1px solid blue; padding: 2px;">82</span> <span style="border: 1px solid blue; padding: 2px;">74</span>	43, 151, 201, 203	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1895	ASN	9.5
2	H	451	ASN	4.7
2	H	51	ASP	4.3
2	E	1928	GLN	4.2
2	E	425	SER	4.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.