



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:09 AM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

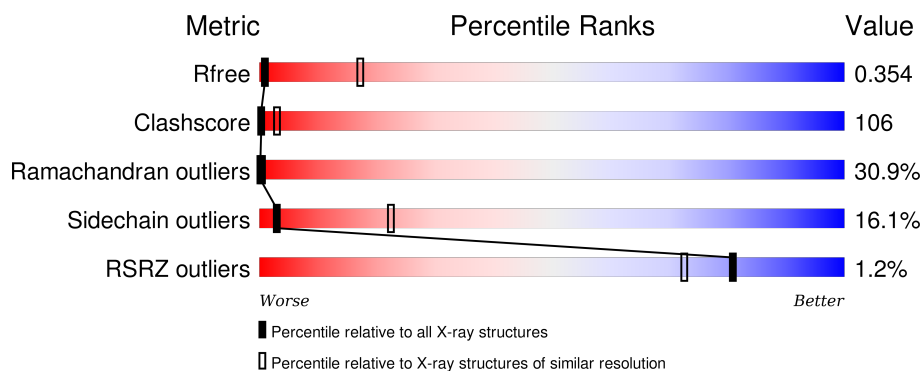
1 Overall quality at a glance

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}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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 on the lower 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 $\leq 5\%$. 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	<div> <div></div> <div>27% 46% 22% 5%</div> </div>
1	D	1688	<div> <div></div> <div>27% 46% 22% 5%</div> </div>
1	G	1688	<div> <div></div> <div>27% 46% 22% 5%</div> </div>
2	B	2006	<div> <div>%</div> <div>34% 54% 11% .</div> </div>
2	E	2006	<div> <div>%</div> <div>34% 54% 11% .</div> </div>

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

2 Entry composition

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
1	A	1683	Total	C	N	O	S	0	0	0
			11319	7070	2007	2205	37			
1	D	1683	Total	C	N	O	S	0	0	0
			11319	7070	2007	2205	37			
1	G	1683	Total	C	N	O	S	0	0	0
			11319	7070	2007	2205	37			

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

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

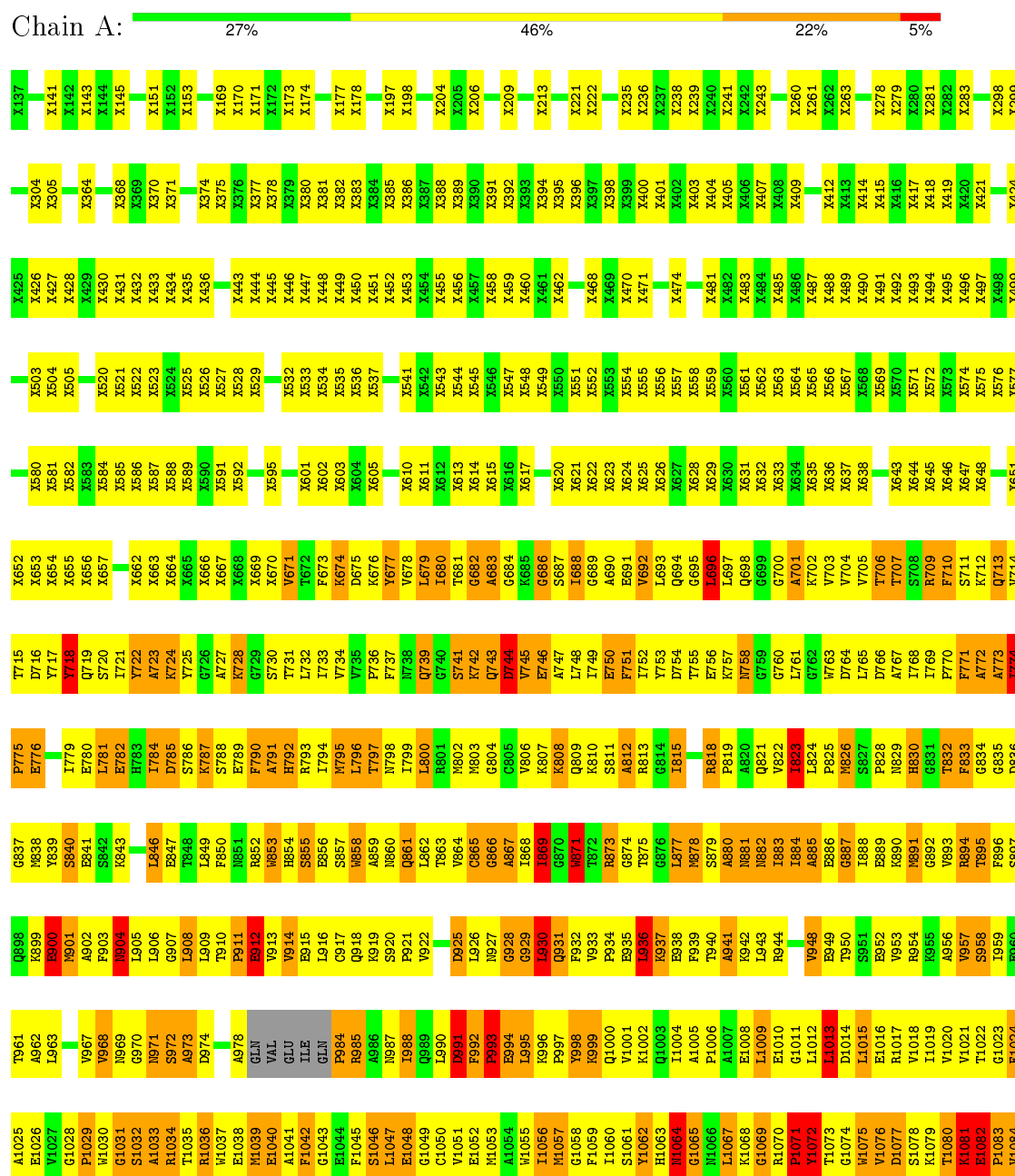
- Molecule 3 is a protein called Tail protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	65	Total	C	N	O	0	0	0
			325	195	65	65			
3	F	65	Total	C	N	O	0	0	0
			325	195	65	65			
3	I	65	Total	C	N	O	0	0	0
			325	195	65	65			

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 errors 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 ($\text{RSRZ} > 2$). 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



X435	X436	X437	X438	X443	X444	X445	X446	X447	X448	X449	X450	X451	X452	X453	X454	X455	X456	X457	X458	X459	X460	X461	X462	X468	X469	X470	X471	X474	X481	X482	X483	X484	X485	X486	X487	X488	X489	X490	X491	X492	X493	X494	X495	X496	X497	X498	X499	X503	X504	X505	X520	X521	X522																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
X374	X375	X376	X377	X378	X379	X380	X381	X382	X383	X384	X385	X386	X387	X388	X389	X390	X391	X392	X393	X394	X395	X396	X397	X398	X399	X400	X401	X402	X403	X404	X405	X406	X407	X408	X409	X412	X413	X414	X415	X416	X417	X418	X419	X420	X421	X424	X425	X426	X427	X428	X429	X430	X431	X432	X433	X434																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
X137	X141	X142	X143	X144	X145	X169	X170	X171	X172	X173	X174	X177	X178	X179	X181	X182	X183	X184	X185	X186	X187	X188	X189	X197	X198	X204	X205	X206	X209	X213	X235	X236	X239	X241	X260	X261	X262	X263	X278	X279	X280	X281	X282	X283	X298	X299	X304	X305	X365	X368	X369	X370	X371																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
D1085	D1086	D1087	D1088	D1089	D1090	D1091	D1092	D1093	D1094	D1095	D1096	D1097	D1098	D1099	D1100	D1101	D1102	D1103	D1104	D1105	D1106	D1107	D1108	D1109	D1110	D1111	D1112	D1113	D1114	D1115	D1116	D1117	D1118	D1119	D1120	D1121	D1122	D1126	D1127	D1128	D1129	D1130	D1131	D1132	D1133	D1134	D1135	D1136	D1137	D1138	D1139	D1140	D1141	D1142	D1143	D1144	D1145	D1146																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
Q1147	Q1148	Q1149	Q1150	Q1151	Q1152	Q1153	Q1154	Q1155	Q1156	Q1157	Q1158	Q1159	Q1160	Q1161	Q1162	Q1163	Q1164	Q1165	Q1166	Q1167	Q1168	Q1169	Q1170	Q1171	Q1172	Q1173	Q1174	Q1175	Q1176	Q1177	Q1178	Q1179	Q1180	Q1181	Q1182	Q1183	Q1184	Q1185	Q1186	Q1187	Q1188	Q1189	Q1190	Q1191	Q1192	Q1193	Q1194	Q1195	Q1196	Q1197	Q1198	Q1199	Q1200	Q1201	Q1202	Q1203	Q1204	Q1205	Q1206																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
R1207	R1208	R1209	R1210	R1211	R1212	R1213	R1214	R1215	R1216	R1217	R1218	R1219	R1220	R1221	R1222	R1223	R1224	R1225	R1226	R1227	R1228	R1229	R1230	R1231	R1232	R1233	R1234	R1235	R1236	R1237	R1238	R1239	R1240	R1241	R1242	R1243	R1244	R1245	R1246	R1247	R1248	R1249	R1250	R1251	R1252	R1253	R1254	R1255	R1256	R1257	R1258	R1259	R1260	R1261	R1262	R1263	R1264	R1265	R1266																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
D1267	D1268	D1269	D1270	D1271	D1272	D1273	D1274	D1275	D1276	D1277	D1278	D1279	D1280	D1281	D1282	D1283	D1284	D1285	D1286	D1287	D1288	D1289	D1290	D1291	D1292	D1293	D1294	D1295	D1296	D1297	D1298	D1299	D1300	D1301	D1302	D1303	D1304	D1305	D1306	D1307	D1308	D1309	D1310	D1311	D1312	D1313	D1314	D1315	D1316	D1317	D1318	D1319	D1320	D1321	D1322	D1323	D1324	D1325	D1326	D1327																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
G1327	G1328	G1329	G1330	G1331	G1332	G1333	G1334	G1335	G1336	G1337	G1338	G1339	G1340	G1341	G1342	G1343	G1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
M1388	M1389	M1390	M1391	M1392	M1393	M1394	M1395	M1396	M1397	M1398	M1399	M1400	M1401	M1402	M1403	M1404	M1405	M1406	M1407	M1408	M1409	M1410	M1411	M1412	M1413	M1414	M1415	M1416	M1417	M1418	M1419	M1420	M1421	M1422	M1423	M1424	M1425	M1426	M1427	M1428	M1429	M1430	M1431	M1432	M1433	M1434	M1435	M1436	M1437	M1438	M1439	M1440	M1441	M1442	M1443	M1444	M1445	M1446	M1447																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
R1448	R1449	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460	R1461	R1462	R1463	R1464	R1465	R1466	R1467	R1468	R1469	R1470	R1471	R1472	R1473	R1474	R1475	R1476	R1477	R1478	R1479	R1480	R1481	R1482	R1483	R1484	R1485	R1486	R1487	R1488	R1489	R1490	R1491	R1492	R1493	R1494	R1495	R1496	R1497	R1498	R1499	R1500	R1501	R1502	R1503	R1504	R1505	R1506	R1507	R1508																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
G1509	G1510	G1511	G1512	G1513	G1514	G1515	G1516	G1517	G1518	G1519	G1520	G1521	G1522	G1523	G1524	G1525	G1526	G1527	G1528	G1529	G1530	G1531	G1532	G1533	G1534	G1535	G1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	G1544	G1545	G1546	G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
H1570	H1571	H1572	H1573	H1574	H1575	H1576	H1577	H1578	H1579	H1580	H1581	H1582	H1583	H1584	H1585	H1586	H1587	H1588	H1589	H1590	H1591	H1592	H1593	H1594	H1595	H1596	H1597	H1598	H1599	H1600	H1601	H1602	H1603	H1604	H1605	H1606	H1607	H1608	H1609	H1610	H1611	H1612	H1613	H1614	H1615	H1616	H1617	H1618	H1619	H1620	H1621	H1622	H1623	H1624	H1625	H1626	H1627	H1628	H1629																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
T1630	T1631	T1632	T1633	T1634	T1635	T1636	T1637	T1638	T1639	T1640	T1641	T1642	T1643	T1644	T1645	T1646	T1647	T1648	T1649	T1650	T1651	T1652	T1653	T1654	T1655	T1656	T1657	T1658	T1659	T1660	T1661	T1662	T1663	T1664	T1665	T1666	T1667	T1668	T1669	T1670	T1671	T1672	T1673	T1674	T1675	T1676	T1677	T1678	T1679	T1680	T1681	T1682	T1683	T1684	T1685	T1686	T1687	T1688	T1689																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
M1690	M1691	M1692	M1693	M1694	M1695	M1696	M1697	M1698	M1699	M1700	M1701	M1702	M1703	M1704	M1705	M1706	M1707	M1708	M1709	M1710	M1711	M1712	M1713	M1714	M1715	M1716	M1717	M1718	M1719	M1720	M1721	M1722	M1723	M1724	M1725	M1726	M1727	M1728	M1729	M1730	M1731	M1732	M1733	M1734	M1735	M1736	M1737	M1738	M1739	M1740	M1741	M1742	M1743	M1744	M1745	M1746	M1747	M1748	M1749	M1750	M1751	M1752																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
X1761	X1762	X1773	X1778	X1779	X1780	X1781	X1782	X1783	X1784	X1793	X1794	X1795	X1799	X1811	X1812	X1813	X1826	X1827	X1853	X1857	X1860	X1861	X1862	X1863	X1864	X1865	X1868	X1872	X1881	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	X2



R1516	F1576	V1636	K1696	X1778
D1516	Q1577	R1637	L1697	X1779
P1517	K1578	A1638	F1698	X1780
R1518	F1579	V1639	V1699	X1781
L1520	L1580	S1640	K1700	X1782
A1520	T1581	I1641	K1701	X1783
P1521	G1582	T1642	E1702	X1784
L1522	H1583	S1643	H1703	
G1524	P1584	F1644	A1704	X1793
A1525	K1585	G1645	P1705	X1794
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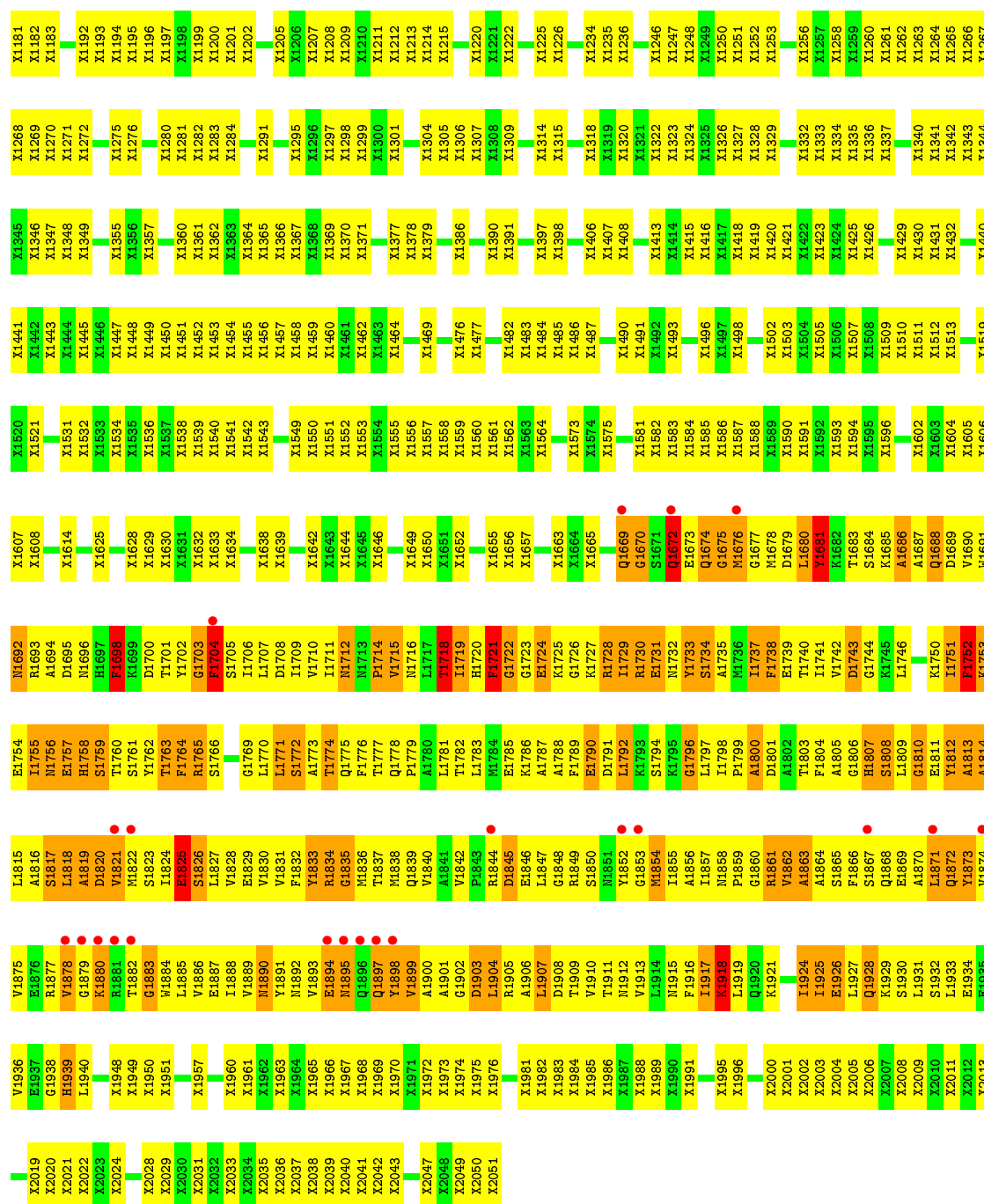
• Molecule 1: Fatty acid synthase subunit alpha

Chain G:  27% 46% 22% 5%

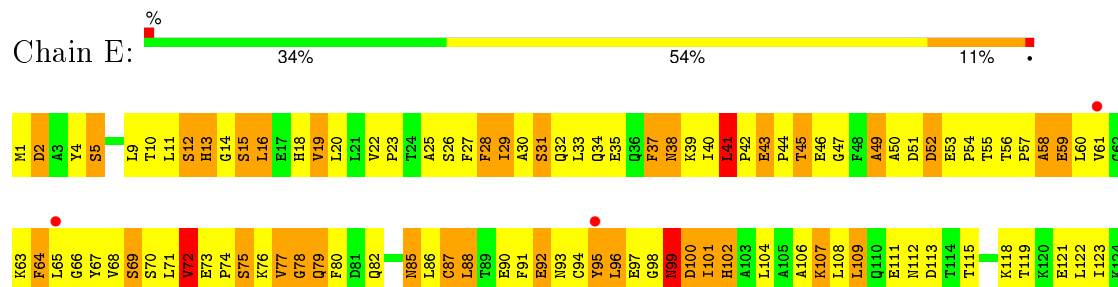
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X144	X374	X434	X522	X585	X663	A723	L784	S845	L905
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	X376	X436	X524	X587	X665	Y725	S786	E847	G907
	X377	X437	X525	X588	X666	G726	K787	T848	L908
	X378	X438	X526	X589	X667	A727	L788	L849	L909
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	X380	X440	X528	X591	X669	S730	A791	R851	R912
	X381	X441	X529	X592	X670	T731	H792	L852	R913
	X382	X442	X530	X593	X671	L732	K793	H854	Y914
	X383	X443	X531	X601	X672	I733	L794	S855	E915
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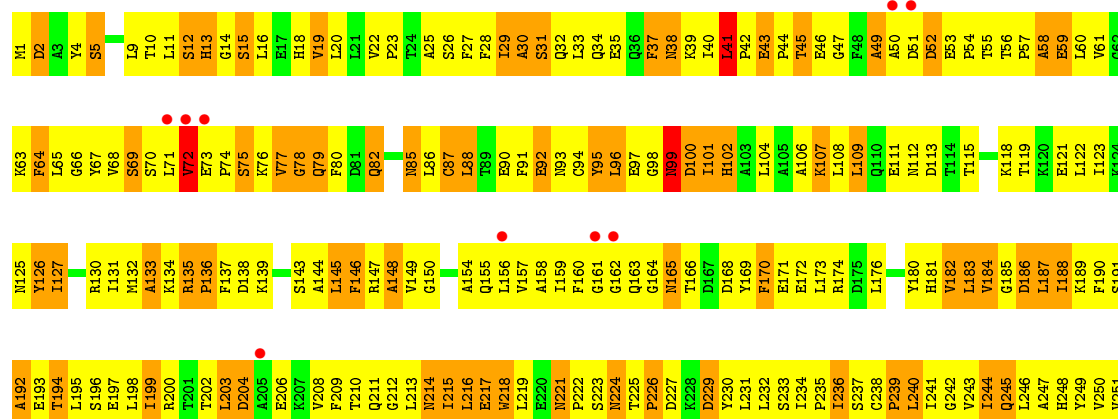
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X441	X442	X443	X444	X445	X446	X447	X448	X449	X450	X451	X452	X453	X454	X455	X456	X457	X458	X459	X460	X461	X462	X463	X464	X465	X466	X467	X468	X469	X470	X471	X472	X473	X474	X475	X476	X477	X478	X479	X480	X481	X482	X483	X484	X485	X486	X487	X488	X489	X490	X491	X492	X493	X494	X495	X496	X497	X498	X499																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
X377	X378	X379	X380	X381	X382	X383	X384	X385	X386	X387	X388	X389	X390	X391	X392	X393	X394	X395	X396	X401	X402	X403	X404	X405	X406	X407	X408	X409	X410	X411	X412	X413	X414	X415	X416	X417	X418	X419	X420	X421	X422	X423	X424	X425	X426	X427	X428	X429	X430	X431	X432	X433	X434	X435	X436	X437	X438	X439	X440	X441	X442	X443	X444	X445	X446	X447	X448	X449	X450	X451	X452	X453	X454	X455	X456	X457	X458	X459	X460	X461	X462	X463	X464	X465	X466	X467	X468	X469	X470	X471	X472	X473	X474	X475	X476	X477	X478	X479	X480	X481	X482	X483	X484	X485	X486	X487	X488	X489	X490	X491	X492	X493	X494	X495	X496	X497	X498	X499	X500	X501	X502	X503	X504	X505	X506	X507	X508	X509	X510	X511	X512	X513	X514	X515	X516	X517	X518	X519	X520	X521	X522	X523	X524	X525	X526	X527	X528	X529	X530	X531	X532	X533	X534	X535	X536	X537	X538	X539	X540	X541	X542	X543	X544	X545	X546	X547	X548	X549	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	X804	X805	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	X1064	X1065	X1066	X1067	X1068	X1069	X1070	X1071	X1072	X1073	X1074	X1075	X1076	X1077	X1078	X1079	X1080	X1081	X1082	X1083	X1084	X1085	X1086	X1087	X1088	X1089	X1090	X1091	X1092	X1093	X1094	X1095	X1096	X1097	X1098	X1099	X1100	X1101	X1102	X1103	X1104	X1105	X1106	X1107	X1108	X1109	X1110	X1111	X1112	X1113	X1114	X1115	X1116	X1117	X1118	X1119	X1120	X1121	X1122	X1123	X1124	X1125	X1126	X1127	X1128	X1129	X1130	X1131	X1132	X1133	X1134	X1135	X1136	X1137	X1138	X1139	X1140	X1141	X1142	X1143	X1144	X1145	X1146	X1147	X1148	X1149	X1150	X1151	X1152	X1153	X1154	X1155	X1156	X1157	X1158	X1159	X1160	X1161	X1162	X1163	X1164	X1165	X1166	X1167	X1168	X1169	X1170	X1171	X1172	X1173	X1174	X1175	X1176	X1177	X1178	X1179	X1180	X1181	X1182	X1183	X1184	X1185	X1186	X1187	X1188	X1189	X1190	X1191	X1192	X1193	X1194	X1195	X1196	X1197	X1198	X1199	X1200	X1201	X1202	X1203	X1204	X1205	X1206	X1207	X1208	X1209	X1210	X1211	X1212	X1213	X1214	X1215	X1216	X1217	X1218	X1219	X1220	X1221	X1222	X1223	X1224	X1225	X1226	X1227	X1228	X1229	X1230	X1231	X1232	X1233	X1234	X1235	X1236	X1237	X1238	X1239	X1240	X1241	X1242	X1243	X1244	X1245	X1246	X1247	X1248	X1249	X1250	X1251	X1252	X1253	X1254	X1255	X1256	X1257	X1258	X1259	X1260	X1261	X1262	X1263	X1264	X1265	X1266	X1267	X1268	X1269	X1270	X1271	X1272	X1273	X1274	X1275	X1276	X1277	X1278	X1279	X1280	X1281	X1282	X1283	X1284	X1285	X1286	X1287	X1288	X1289	X1290	X1291	X1292	X1293	X1294	X1295	X1296	X1297	X1298	X1299	X1300	X1301	X1302	X1303	X1304	X1305	X1306	X1307	X1308	X1309	X1310	X1311	X1312	X1313	X1314	X1315	X1316	X13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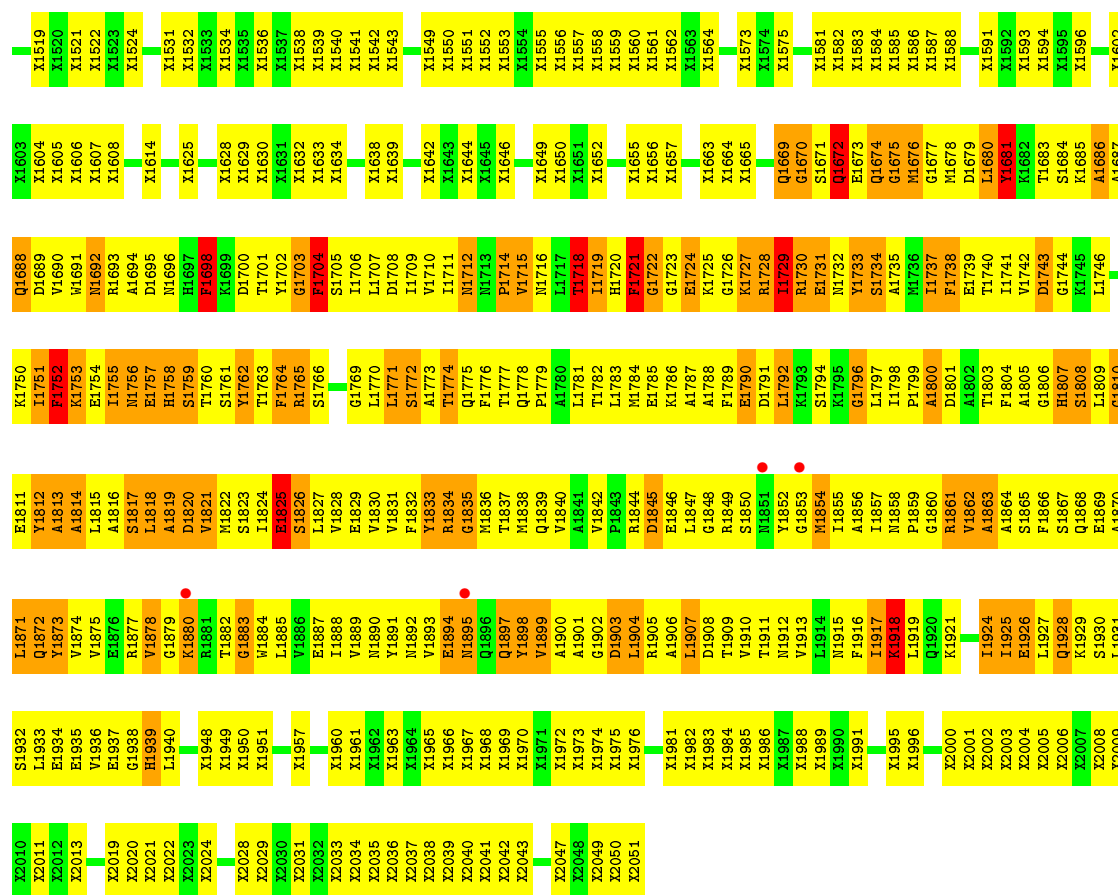
• Molecule 2: Fatty acid synthase subunit beta





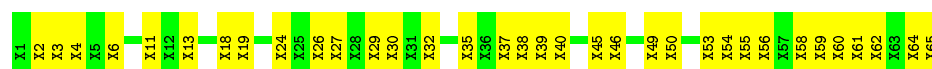


X1433	X1345	X1288	X1180	X1051	X971	X887	X802	X722	X650	X570	L502	D442	V378	P315	T252
X1441	X1346	X1269	X1181	X1052	X972	X888	X803	X723	X651	X571	D503	L443	V379	N316	A253
X1442	X1347	X1270	X1182	X1053	X973			X724	X652	X572	P504	V444	S380	N317	K254
X1443	X1348	X1271	X1183	X1054	X974		X806	X725	X653		G505	K445	G381	S318	L255
X1444	X1349	X1272		X1055	X975	X895	X807	X726	X654	X577	P506	N446	P382	L319	G256
X1445	X1355	X1275	X1192	X1056	X976	X896	X808	X727	X655	X578	G507	N447	P383	P320	G257
X1446	X1356	X1276	X1193	X1057	X977	X897	X809	X728	X656	X579	G508	V448	Q384	P321	F258
X1447	X1357	X1277	X1194	X1058	X978	X898	X810	X729	X657	X580	A509	S449	Q385	S322	T289
X1448	X1360	X1280	X1195	X1059	X979	X899	X811	X730	X658	X581	S510	L386	L386	L323	P260
X1449	X1361	X1281	X1196	X1060	X980	X899	X812	X731	X659	X582	G511	N451	G387	L324	G261
X1450	X1362	X1282	X1197	X1061	X981	X899	X813	X732	X660	X583	L512	A452	G388	G262	E262
X1451	X1363	X1283	X1198	X1062	X982		X814	X733	X661	X584	G513	K453	L389	L263	L263
X1452	X1364	X1284	X1199	X1063	X983	X905	X815	X734	X662	X585	G514	K454	L390	R264	R264
X1453	X1365		X1200		X984	X906	X816	X735		X586	G515	K455	N390	S265	S265
X1454	X1366		X1201	X1066	X985	X907	X817	X736	X667	X587	T516	Q456	T392	Y266	Y266
X1455	X1367		X1202	X1067	X986	X911	X818	X737	X668		H517	L457	L393	N331	K268
X1456	X1368		X1203	X1068	X987	X912	X819	X738	X669	X591	P458	V459	K394	E332	G269
X1457	X1369	X1295	X1204	X1069	X1002	X913	X820	X739	X670	X592	N519	V459	K395	G333	G269
X1458	X1370	X1296	X1205			X914	X821	X740	X671	X593	K520	Y460	A396	V334	A270
X1459	X1371	X1297	X1206	X1074	X1008	X915	X822	X741	X672	X594	D521	D461	G401	P335	T271
X1460	X1372	X1298	X1207	X1075	X1009	X916	X823	X742	X673	X595	G522	T462	L402	S336	G272
X1461	X1373	X1299	X1208	X1076	X1010	X917	X824	X743	X674	X596	T523	F463	L403	P337	H273
X1462	X1374	X1300	X1209	X1077	X1011	X918	X825	X744	X675	X597	G524	D464	D403	N338	S274
X1463	X1375	X1301	X1210	X1078	X1012	X919	X826	X745	X676	X598	V525	G465	Q404	L339	Q275
X1464	X1376	X1302	X1211	X1079	X1013	X920	X827	X746	X677	X599	R526	S466	S405	S340	Q275
X1465	X1377	X1303	X1212	X1080	X1014	X921	X828	X747	X678	X600	V527	D467	Q406	I341	L277
X1466	X1378	X1304	X1213	X1081	X1015	X922	X829	X748	X679	X601	V528	L468	R406		
X1467	X1379	X1305	X1214	X1082	X1016	X923	X830	X749	X680	X602	V529	L469	I407	S342	V278
X1468	X1380	X1306	X1215	X1083	X1017	X924	X831	X750	X681	X603	A530	R469	F408	N343	T279
X1469	X1381	X1307	X1216	X1084	X1018	X925	X832	X751	X682	X604	G531	V470	F409	L344	L279
X1470	X1382	X1308	X1217	X1085	X1019	X926	X833	X752	X683	X605	T532	L471	S410	T345	A280
X1471	X1383	X1309	X1218	X1086	X1020	X927	X834	X753	X684	X606	R533	S472	E411	Q346	V281
X1472	X1384	X1310	X1219	X1087	X1021	X928	X835	X754	X685	X607	R534	G473	R412	E347	A282
X1473	X1385	X1311	X1220	X1088	X1022	X929	X836	X755	X686		T535	S474	R413	E348	A283
X1474	X1386	X1312	X1221	X1089	X1023	X930	X837	X756	X687	X611	V536	L475	K415	V349	E285
X1475	X1387	X1313	X1222	X1090	X1024	X931	X838	X757	X688	X612	N537	S476	F416	Q350	T286
X1476	X1388	X1314	X1223	X1091	X1025	X932	X839	X758	X689	X613	D538	E477	S417	D351	D287
X1477	X1389	X1315	X1224	X1092	X1026	X933	X840	X759	X690	X614	D539	R478	N418	Y352	S288
X1478	X1390	X1316	X1225	X1093	X1027	X934	X841	X760	X691	X615	D540	L479	R419	V353	W289
X1479	X1391	X1317	X1226	X1094	X1028	X935	X842	X761	X692	X616	V541	V480	F420	N354	F292
X1480	X1392	X1318	X1227	X1095	X1029	X936	X843	X762	X693	X617	G542	D481	L421	K355	F293
X1481	X1393	X1319	X1228	X1096	X1030	X937	X844	X763	X694	X618	F543	C482	V422	T356	V294
X1482	X1394	X1320	X1229	X1097	X1031	X938	X845	X764	X695	X619	G544	L484	V423	N357	V294
X1483	X1395	X1321	X1230	X1098	X1032	X939	X846	X765	X696	X620	K545	A424	A424	S295	S295
X1484	X1396	X1322	X1231	X1099	X1033	X940	X847	X766	X697	X621	K546	P485	S425	V296	V296
X1485	X1397	X1323	X1232	X1100	X1034	X941	X848	X767	X698	X622		L486	P426	R297	R297
X1486	X1398	X1324	X1233	X1101	X1035	X942	X849	X768	X699	X623	X550	P487	F427	P361	K298
X1487	X1399	X1325	X1234	X1102	X1036	X943	X850	X769	X700	X624	X551	V488	F427	A299	A299
X1488	X1400	X1326	X1235	X1103	X1037	X944	X851	X770	X701	X625	X552	H428	H428	T301	I300
X1489	X1401	X1327	X1236	X1104	X1038	X945	X852	X771	X702	X626	X553	V489	H429	E367	T301
X1490	X1402	X1328	X1237	X1105	X1039	X946	X853	X772	X703	X627	X554	T492	L431	V302	V302
X1491	X1403	X1329	X1238	X1106	X1040	X947	X854	X773	X704	X628	X555	T493	L432	L303	L303
X1492	X1404	X1330	X1239	X1107	X1041	X948	X855	X774	X705	X629	X556	T494	V433	F304	F304
X1493	X1405	X1331	X1240	X1108	X1042	X949	X856	X775	X706	X630	X557	T495	V434	L370	V294
X1494	X1406	X1332	X1241	X1109	X1043	X950	X857	X776	X707	X631	X558	Q495	A435	V371	I306
X1495	X1407	X1333	X1242	X1110	X1044	X951	X858	X777	X708	X632	X559	F496	S436	N372	G307
X1496	X1408	X1334	X1243	X1111	X1045	X952	X859	X778	X709	X633	X560	V497	D437	G373	V308
X1497	X1409	X1335	X1244	X1112	X1046	X953	X860	X779	X710	X634	X561	V498	L438	I374	R309
X1498	X1410	X1336	X1245	X1113	X1047	X954	X861	X780	X711	X635	X562	V499	I439	K375	R309
X1499	X1411	X1337	X1246	X1114	X1048	X955	X862	X781	X712	X636	X563	H500	I440	N376	G310
X1500	X1412	X1338	X1247	X1115	X1049	X956	X863	X782	X713	X637	X564	H501	K441	L377	Y311
X1501	X1413	X1339	X1248	X1116	X1050	X957	X864	X783	X714	X638	X565	H502			
X1502	X1414	X1340	X1249	X1117	X1051	X958	X865	X784	X715	X639	X566	H503			
X1503	X1415	X1341	X1250	X1118	X1052	X959	X866	X785	X716	X640	X567	H504			
X1504	X1416	X1342	X1251	X1119	X1053	X960	X867	X786	X717	X641	X568	H505			
X1505	X1417	X1343	X1252	X1120	X1054	X961	X868	X787	X718	X642	X569	H506			
X1506	X1418	X1344	X1253	X1121	X1055	X962	X869	X788	X719	X643	X570	H507			
X1507	X1419	X1345	X1254	X1122	X1056	X963	X870	X789	X720	X644	X571	H508			
X1508	X1420	X1346	X1255	X1123	X1057	X964	X871	X790	X721	X645	X572	H509			
X1509	X1421	X1347	X1256	X1124	X1058	X965	X872	X791	X722	X646	X573	H510			
X1510	X1422	X1348	X1257	X1125	X1059	X966	X873	X792	X723	X647	X574	H511			
X1511	X1423	X1349	X1258	X1126	X1060	X967	X874	X793	X724	X648	X575	H512			
X1512	X1424	X1350	X1259	X1127	X1061	X968	X875	X794	X725	X649	X576	H513			
X1513	X1425	X1351	X1260	X1128	X1062	X969	X876	X795	X726	X650	X577	H514			
X1514	X1426	X1352	X1261	X1129	X1063	X970	X877	X796	X727	X651	X578	H515			
X1515	X1427	X1353	X1262	X1130	X1064	X971	X878	X797	X728	X652	X579	H516			
X1516	X1428	X1354	X1263	X1131	X1065	X972	X879	X798	X729	X653	X580	H517			
X1517	X1429	X1355	X1264	X1132	X1066	X973	X880	X799	X730	X654	X581	H518			
X1518	X1430	X1356	X1265	X1133	X1067	X974	X881	X800	X731	X655	X582	H519			
X1519	X1431	X1357	X1266	X1134	X1068	X975	X882	X801	X732	X656	X583	H520			
X1520	X1432	X1358	X1267	X1135	X1069	X976	X883	X802	X733	X657	X584	H521			



● Molecule 3: Tail protein

Chain C: 48% 52%



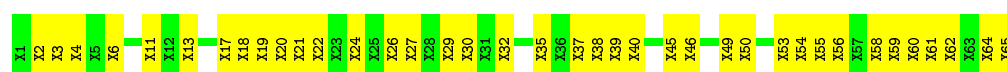
● Molecule 3: Tail protein

Chain F: 45% 55%



● Molecule 3: Tail protein

Chain I: 42% 58%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.319 , 0.346 0.320 , 0.354	Depositor DCC
R_{free} test set	8382 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	152.3	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 181.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 180567 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	71862	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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:CD2	1:D:1181:PHE:CE2	1.81	1.68
1:G:1181:PHE:CE1	1:G:1181:PHE:CZ	1.75	1.68
1:G:1181:PHE:CE2	1:G:1181:PHE:CD2	1.80	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:D:1150:ASP:CG	1:D:1181:PHE:CE2[7_555]	1.87	0.33
1:A:1150:ASP:CG	1:G:1181:PHE:CE2[7_555]	1.87	0.33

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 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	1
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

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	14
1	D	871/895 (97%)	697 (80%)	174 (20%)	1	13
1	G	871/895 (97%)	696 (80%)	175 (20%)	1	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	703/703 (100%)	623 (89%)	80 (11%)	7	36
2	E	703/703 (100%)	623 (89%)	80 (11%)	7	36
2	H	703/703 (100%)	622 (88%)	81 (12%)	7	36
All	All	4722/4794 (98%)	3961 (84%)	761 (16%)	3	22

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

Mol	Chain	Res	Type
1	D	1297	PRO
2	E	28	PHE
2	H	199	ILE
1	D	1354	GLU
1	D	1538	VAL

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

Mol	Chain	Res	Type
1	D	1351	ASN
2	E	221	ASN
2	H	331	ASN
1	D	1389	GLN
1	D	1570	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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, 95th 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 ²)	Q<0.9
1	A	1069/1688 (63%)	-0.32	0 100 100	48, 122, 192, 203	0
1	D	1069/1688 (63%)	-0.29	3 (0%) 94 92	53, 123, 194, 203	0
1	G	1069/1688 (63%)	-0.34	2 (0%) 95 94	43, 112, 190, 203	0
2	B	818/2006 (40%)	-0.08	29 (3%) 48 37	107, 177, 202, 203	0
2	E	818/2006 (40%)	-0.06	18 (2%) 65 54	111, 190, 202, 203	0
2	H	818/2006 (40%)	-0.11	18 (2%) 65 54	94, 183, 202, 203	0
3	C	0/65	-	-	-	-
3	F	0/65	-	-	-	-
3	I	0/65	-	-	-	-
All	All	5661/11277 (50%)	-0.21	70 (1%) 81 72	43, 151, 201, 203	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1895	ASN	9.8
2	H	451	ASN	4.9
2	H	51	ASP	4.5
2	E	1928	GLN	4.4
2	E	425	SER	4.2

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 carbohydrates 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.