



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 07:02 AM EDT

PDB ID : 5M59
Title : Crystal structure of Chaetomium thermophilum Brr2 helicase core in complex with Prp8 Jab1 domain
Authors : Absmeier, E.; Becke, C.; Wollenhaupt, J.; Santos, K.F.; Wahl, M.C.
Deposited on : 2016-10-20
Resolution : 3.20 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

<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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

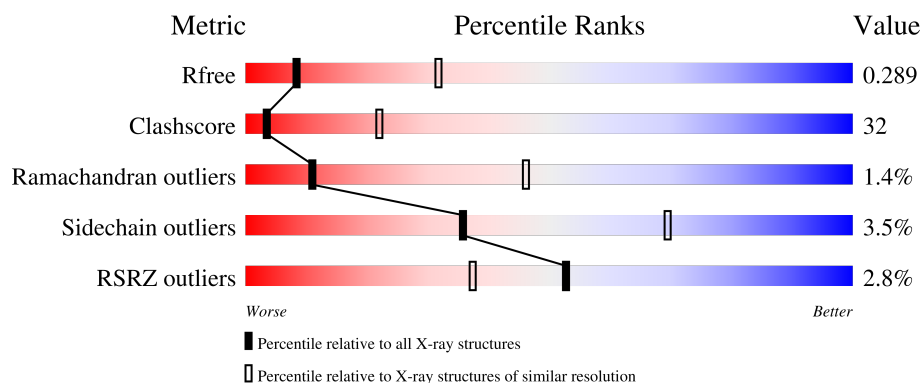
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 ≥ 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	B	276	<div> <div>%</div> <div> <div></div> <div>45%</div> <div>48%</div> <div>• •</div> </div> </div>
1	D	276	<div> <div>50%</div> <div>42%</div> <div>• 5%</div> </div>
1	F	276	<div> <div>%</div> <div> <div></div> <div>50%</div> <div>44%</div> <div>• •</div> </div> </div>
1	H	276	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>47%</div> <div>• •</div> </div> </div>
2	A	1772	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>49%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	C	1772	
2	E	1772	
2	G	1772	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	E	2201	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 63679 atoms, of which 12 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 Putative pre-mRNA splicing factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	266	Total	C	N	O	S	0	0	0
			2116	1352	362	392	10			
1	D	263	Total	C	N	O	S	0	0	0
			2093	1339	359	385	10			
1	F	265	Total	C	N	O	S	0	0	0
			2116	1353	362	391	10			
1	H	267	Total	C	N	O	S	0	0	0
			2125	1358	364	393	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2034	GLY	-	expression tag	UNP G0SFL3
B	2035	ALA	-	expression tag	UNP G0SFL3
B	2036	MET	-	expression tag	UNP G0SFL3
D	2034	GLY	-	expression tag	UNP G0SFL3
D	2035	ALA	-	expression tag	UNP G0SFL3
D	2036	MET	-	expression tag	UNP G0SFL3
F	2034	GLY	-	expression tag	UNP G0SFL3
F	2035	ALA	-	expression tag	UNP G0SFL3
F	2036	MET	-	expression tag	UNP G0SFL3
H	2034	GLY	-	expression tag	UNP G0SFL3
H	2035	ALA	-	expression tag	UNP G0SFL3
H	2036	MET	-	expression tag	UNP G0SFL3

- Molecule 2 is a protein called Pre-mRNA splicing helicase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1738	Total	C	N	O	S	0	0	0
			13917	8891	2369	2592	65			
2	C	1702	Total	C	N	O	S	0	0	0
			13628	8709	2319	2536	64			

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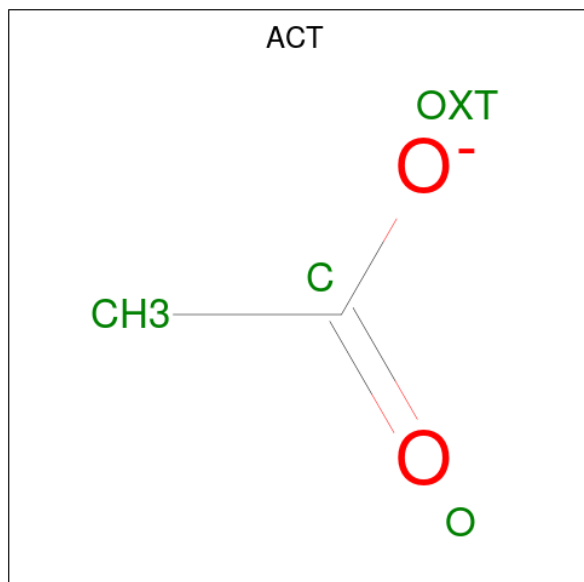
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	1740	Total	C	N	O	S	0	0	0
			13925	8896	2372	2592	65			
2	G	1710	Total	C	N	O	S	0	0	0
			13701	8753	2336	2547	65			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	expression tag	UNP G0S0B9
A	423	ALA	-	expression tag	UNP G0S0B9
A	424	GLU	-	expression tag	UNP G0S0B9
A	425	PHE	-	expression tag	UNP G0S0B9
C	422	GLY	-	expression tag	UNP G0S0B9
C	423	ALA	-	expression tag	UNP G0S0B9
C	424	GLU	-	expression tag	UNP G0S0B9
C	425	PHE	-	expression tag	UNP G0S0B9
E	422	GLY	-	expression tag	UNP G0S0B9
E	423	ALA	-	expression tag	UNP G0S0B9
E	424	GLU	-	expression tag	UNP G0S0B9
E	425	PHE	-	expression tag	UNP G0S0B9
G	422	GLY	-	expression tag	UNP G0S0B9
G	423	ALA	-	expression tag	UNP G0S0B9
G	424	GLU	-	expression tag	UNP G0S0B9
G	425	PHE	-	expression tag	UNP G0S0B9

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 7 2 3 2	0	0
3	C	1	Total C H O 7 2 3 2	0	0
3	E	1	Total C H O 7 2 3 2	0	0
3	G	1	Total C H O 7 2 3 2	0	0

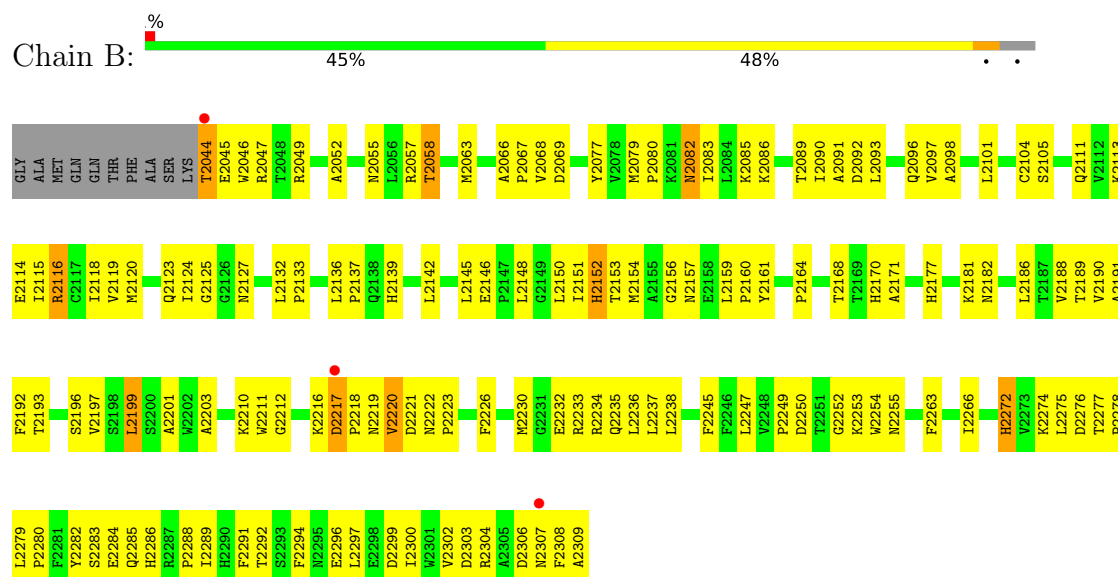
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	D	2	Total O 2 2	0	0
4	C	5	Total O 5 5	0	0
4	F	1	Total O 1 1	0	0
4	E	7	Total O 7 7	0	0
4	G	3	Total O 3 3	0	0

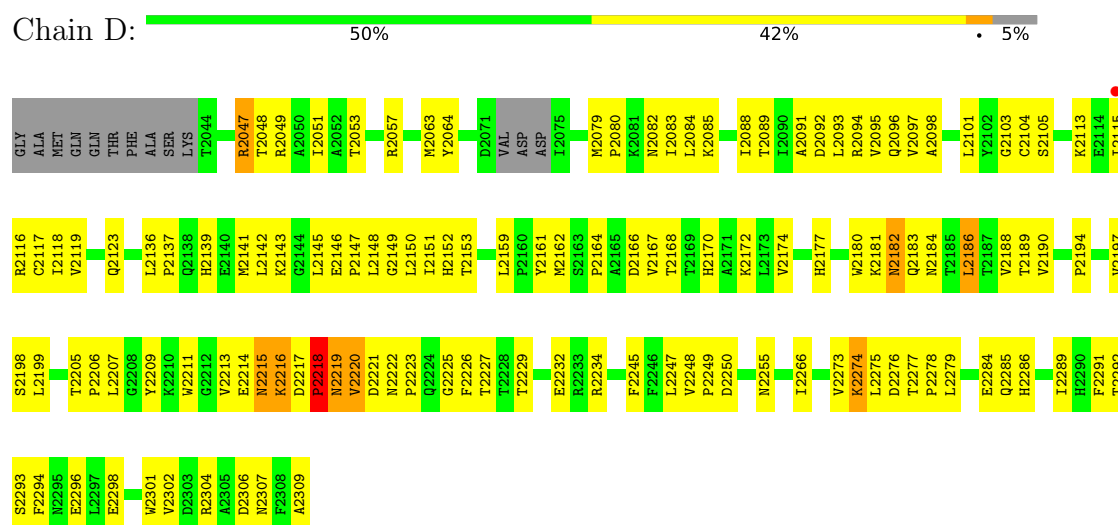
3 Residue-property plots

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.

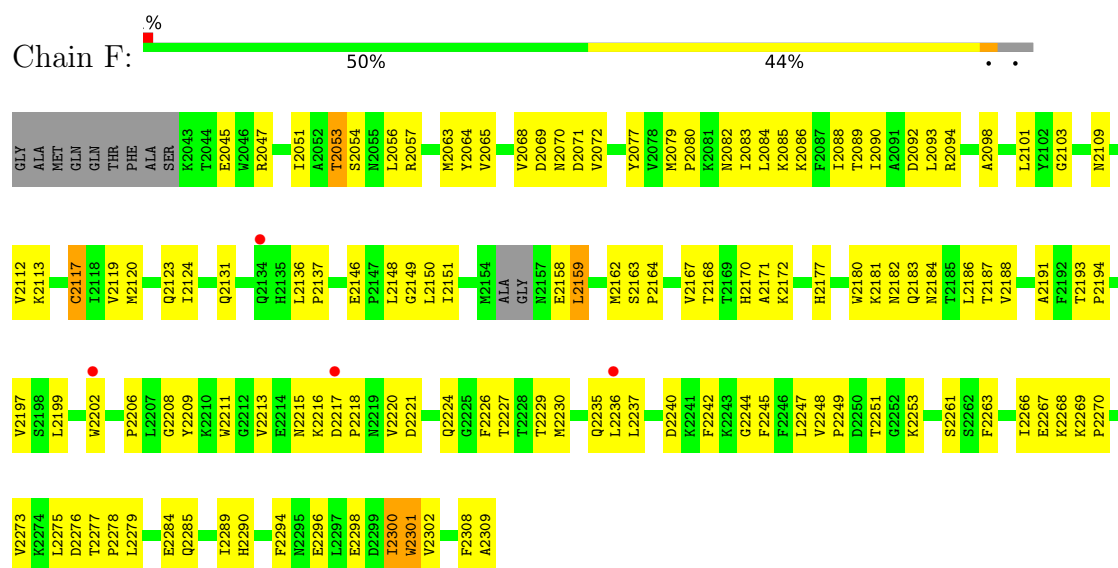
• Molecule 1: Putative pre-mRNA splicing factor



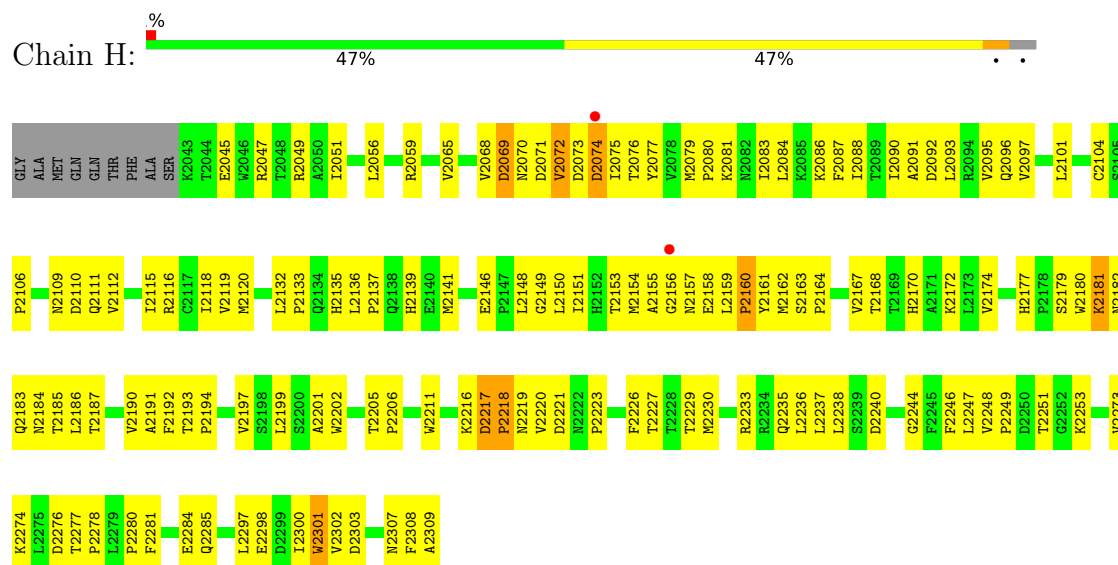
• Molecule 1: Putative pre-mRNA splicing factor



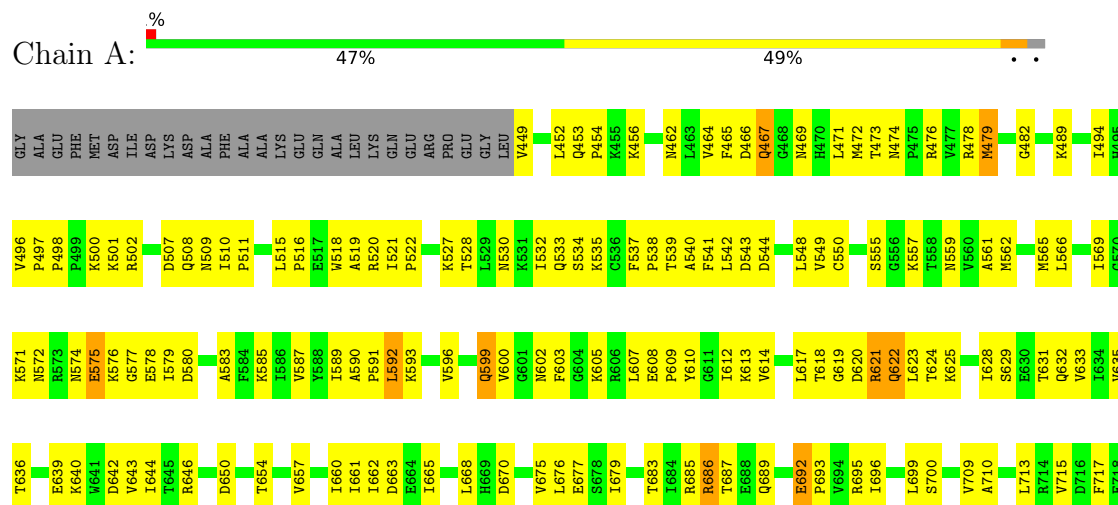
• Molecule 1: Putative pre-mRNA splicing factor



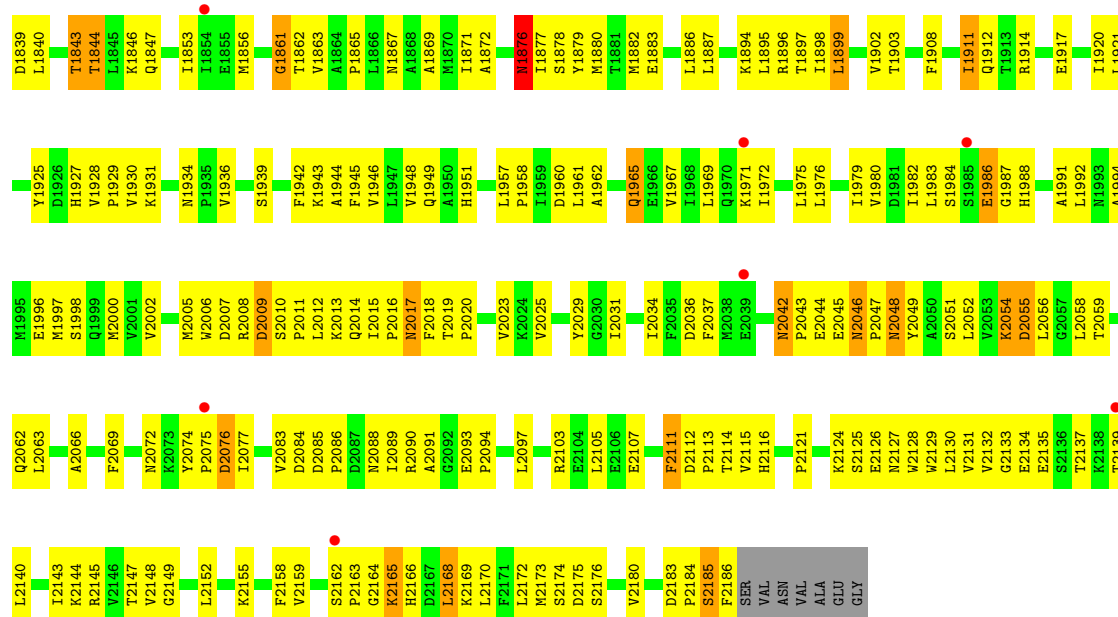
• Molecule 1: Putative pre-mRNA splicing factor



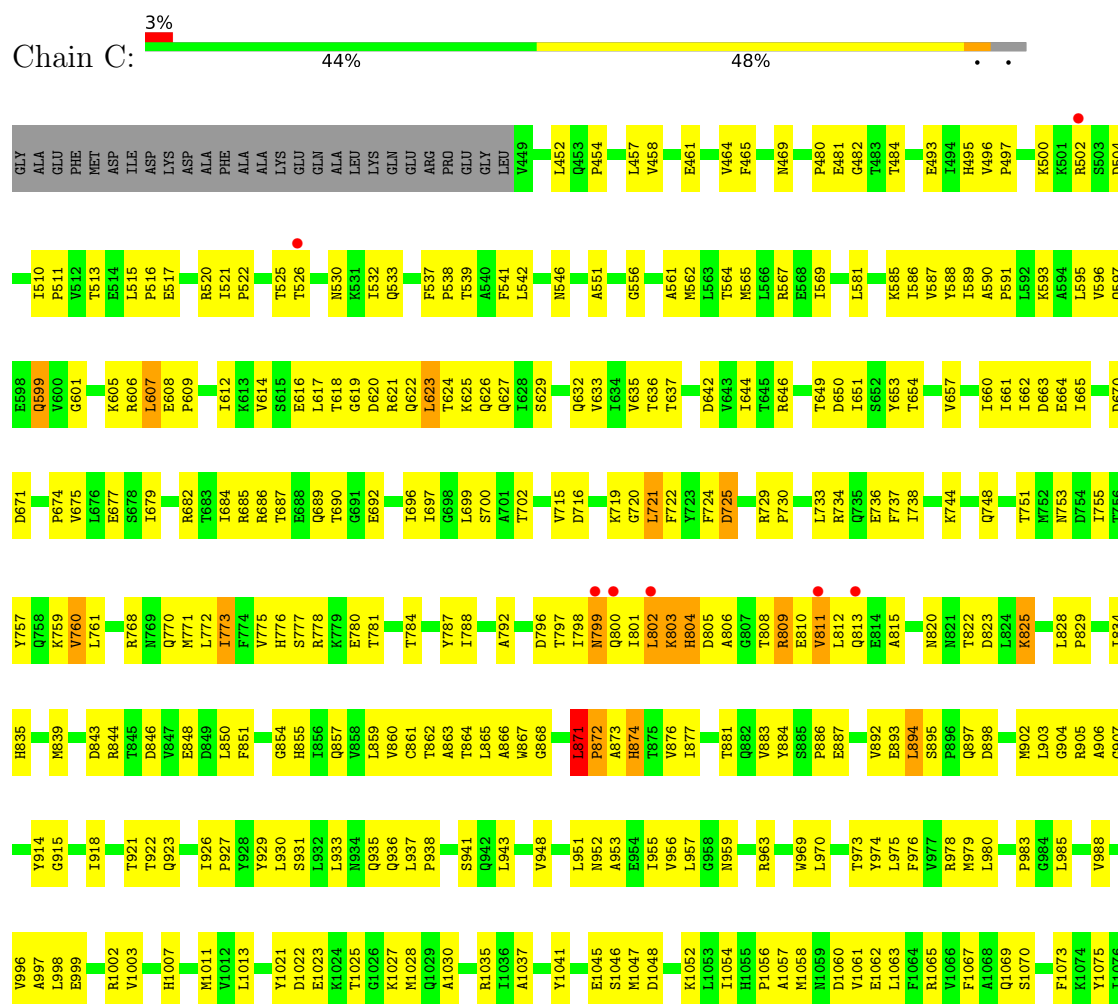
• Molecule 2: Pre-mRNA splicing helicase-like protein



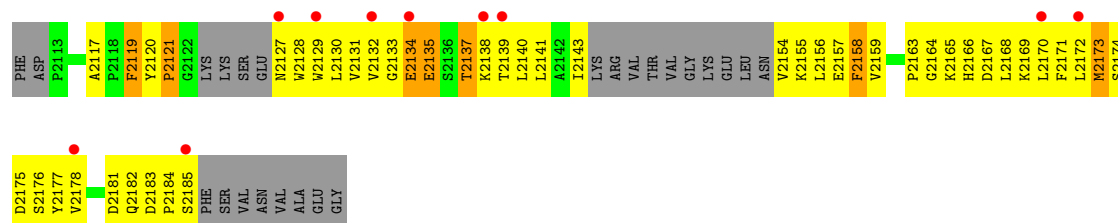
K1748	D1749	G1750	S1752	K1753	G1754	V1755	L1756	M1757	L1758	Y1688	P1759	A1760	V1761	Y1766	L1770	L1774	P1775	L1780	L1784	P1785	F1788	I1792	M1796	I1797	S1798	G1800	E1801	I1804	I1805	I1806	I1807	I1808	I1809	I1810	I1811	I1812	I1813	I1814	I1815	L1816	L1817	A1818	N1819	P1820	S1821	L1825	Q1826	D1827	K1828	A1829	H1830	L1837	S1838																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
L1676	S1677	S1678	F1679	D1680	K1681	H1682	L1683	V1684	K1685	Y1688	N1689	L1696	I1697	R1699	R1700	D1701	V1702	L1706	F1708	T1709	A1710	H1711	L1712	V1713	V1714	V1715	M1716	G1717	T1718	S1719	F1720	F1721	E1722	G1723	K1724	H1725	H1726	R1727	Y1728	Y1731	P1732	E1735	Q1736	Q1738	M1739	F1740	G1741	K1742	A1743	L1744	Q1745	P1746	S1747																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
S1581	H1586	F1587	P1588	S1589	L1590	M1591	M1594	A1595	K1596	P1597	T1598	Y1599	L1600	A1601	I1602	Q1609	P1610	V1613	F1614	V1615	R1618	K1619	Q1620	V1621	R1622	A1625	R1626	T1630	E1638	D1639	L1642	V1646	D1647	Q1648	R1650	N1653	L1658	E1658	E1663	S1666	G1670	Y1671	Y1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960	L1961	L1962	L1963	L1964	L1965	L1966	L1967	L1968	L1969	L1970	L1971	L1972	L1973	L1974	L1975	L1976	L1977	L1978	L1979	L1980	L1981	L1982	L1983	L1984	L1985	L1986	L1987	L1988	L1989	L1990	L1991	L1992	L1993	L1994	L1995	L1996	L1997	L1998	L1999	L2000	L2001	L2002	L2003	L2004	L2005	L2006	L2007	L2008	L2009	L2010	L2011	L2012	L2013	L2014	L2015	L2016	L2017	L2018	L2019	L2020	L2021	L2022	L2023	L2024	L2025	L2026	L2027	L2028	L2029	L2030	L2031	L2032	L2033	L2034	L2035	L2036	L2037	L2038	L2039	L2040	L2041	L2042	L2043	L2044	L2045	L2046	L2047	L2048	L2049	L2050	L2051	L2052	L2053	L2054	L2055	L2056	L2057	L2058	L2059	L2060	L2061	L2062	L2063	L2064	L2065	L2066	L2067	L2068	L2069	L2070	L2071	L2072	L2073	L2074	L2075	L2076	L2077	L2078	L2079	L2080	L2081	L2082	L2083	L2084	L2085	L2086	L2087	L2088	L2089	L2090	L2091	L2092	L2093	L2094	L2095	L2096	L2097	L2098	L2099	L2100	L2101	L2102	L2103	L2104	L2105	L2106	L2107	L2108	L2109	L2110	L2111	L2112	L2113	L2114	L2115	L2116	L2117	L2118	L2119	L2120	L2121	L2122	L2123	L2124	L2125	L2126	L2127	L2128	L2129	L2130	L2131	L2132	L2133	L2134	L2135	L2136	L2137	L2138	L2139	L2140	L2141	L2142	L2143	L2144	L2145	L2146	L2147	L2148	L2149	L2150	L2151	L2152	L2153	L2154	L2155	L2156	L2157	L2158	L2159	L2160	L2161	L2162	L2163	L2164	L2165	L2166	L2167	L2168	L2169	L2170	L2171	L2172	L2173	L2174	L2175	L2176	L2177	L2178	L2179	L2180	L2181	L2182	L2183	L2184	L2185	L2186	L2187	L2188	L2189	L2190	L2191	L2192	L2193	L2194	L2195	L2196	L2197	L2198	L2199	L2200	L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	L2261	L2262	L2263	L2264	L2265	L2266	L2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	L2277	L2278	L2279	L2280	L2281	L2282	L2283	L2284	L2285	L2286	L2287	L2288	L2289	L2290	L2291	L2292	L2293	L2294	L2295	L2296	L2297	L2298	L2299	L2300	L2301	L2302	L2303	L2304	L2305	L2306	L2307	L2308	L2309	L2310	L2311	L2312	L2313	L2314	L2315	L2316	L2317	L2318	L2319	L2320	L2321	L2322	L2323	L2324	L2325	L2326	L2327	L2328	L2329	L2330	L2331	L2332	L2333	L2334	L2335	L2336	L2337	L2338	L2339	L2340	L2341	L2342	L2343	L2344	L2345	L2346	L2347	L2348	L2349	L2350	L2351	L2352	L2353	L2354	L2355	L2356	L2357	L2358	L2359	L2360	L2361	L2362	L2363	L2364	L2365	L2366	L2367	L2368	L2369	L2370	L2371	L2372	L2373	L2374	L2375	L2376	L2377	L2378	L2379	L2380	L2381	L2382	L2383	L2384	L2385	L2386	L2387	L2388	L2389	L2390	L2391	L2392	L2393	L2394	L2395	L2396	L2397	L2398	L2399	L2400	L2401	L2402	L2403	L2404	L2405	L2406	L2407	L2408	L2409	L2410	L2411	L2412	L2413	L2414	L2415	L2416	L2417	L2418	L2419	L2420	L2421	L2422	L2423	L2424	L2425	L2426	L2427	L2428	L2429	L2430	L2431	L2432	L2433	L2434	L2435	L2436	L2437	L2438	L2439	L2440	L2441	L2442	L2443	L2444	L2445	L2446	L2447	L2448	L2449	L2450	L2451	L2452	L2453	L2454	L2455	L2456	L2457	L2458	L2459	L2460	L2461	L2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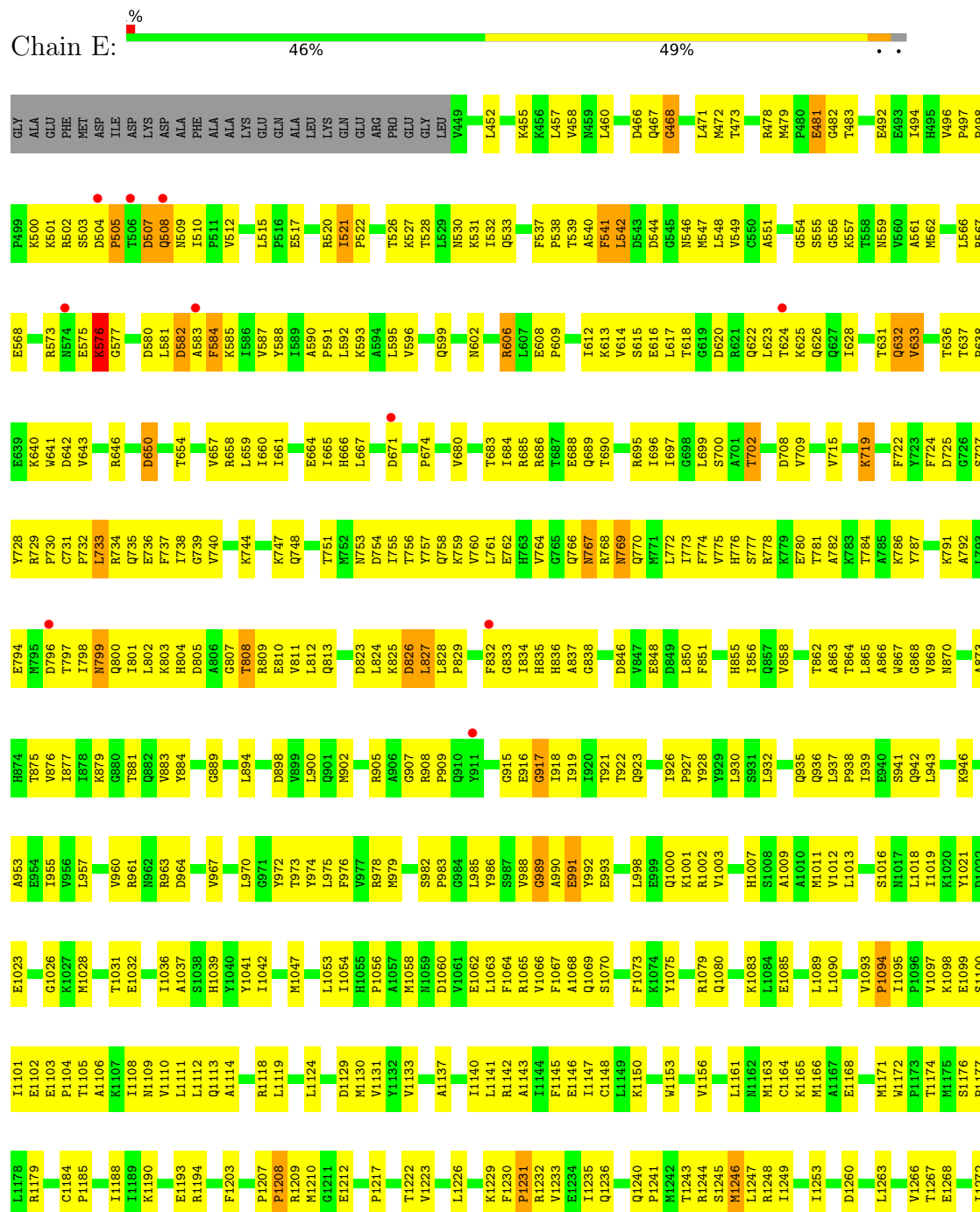
• Molecule 2: Pre-mRNA splicing helicase-like protein

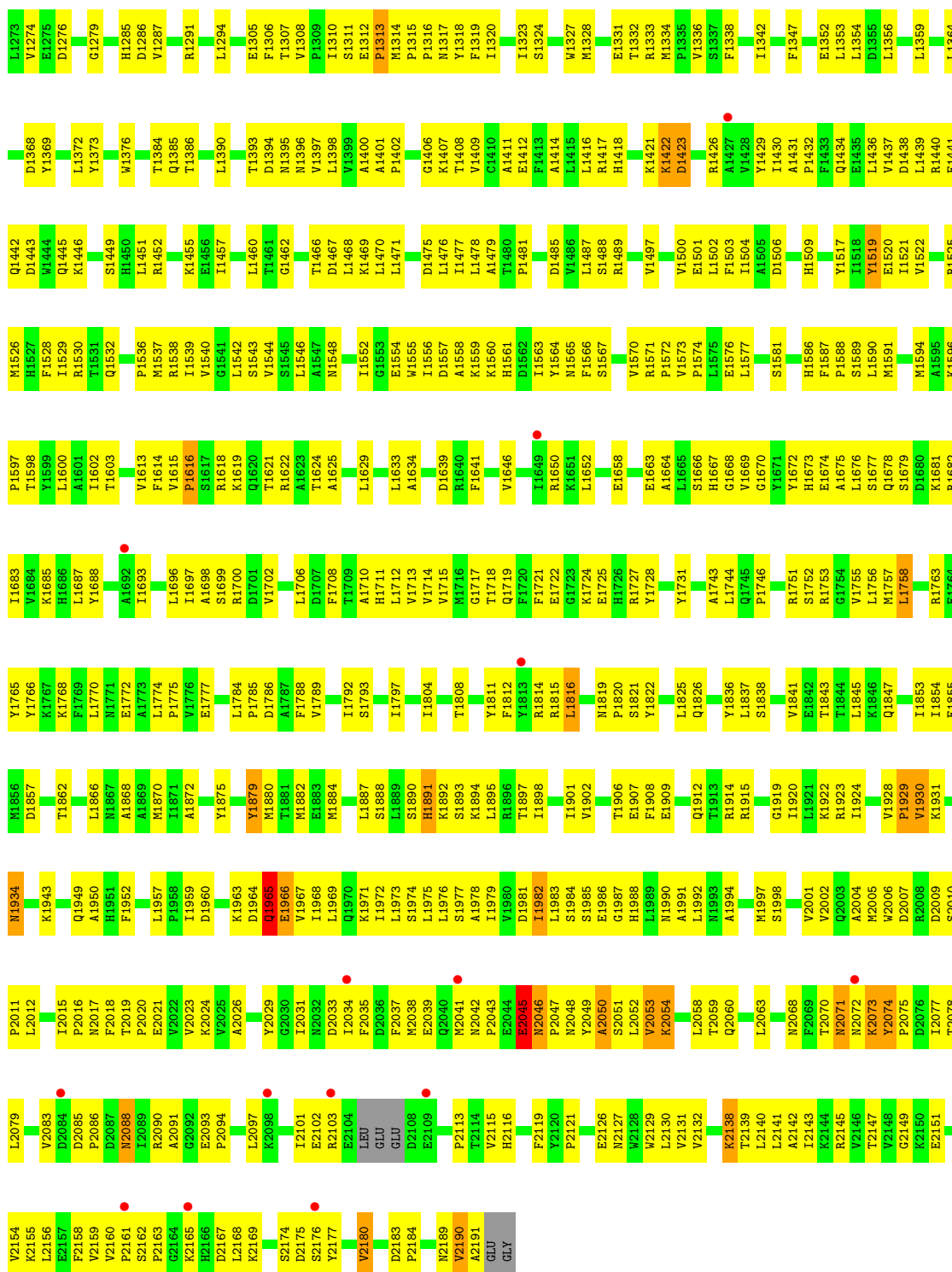






• Molecule 2: Pre-mRNA splicing helicase-like protein





• Molecule 2: Pre-mRNA splicing helicase-like protein



S1524	R1525	K1458	L1390	F1306	Y1132	P1056	E968	E887	E810	V740	T654	A583	P505
H1527	H1526	K1459	T1391	T1307	V1133	A1057	W969	E887	V811	T741	T654	F584	T506
F1528	H1527	L1460	T1393	P1309	G1138	M1058	L970	V892	Q812	D742	V657	K585	Q507
I1529	F1528	T1461	D1394	P1310	R1139	D1060	T973	E893	E814	I746	R658	I586	Q508
R1530	K1462	S1311	N1395	S1310	I1140	V1061	T974	L894	E814	I746	L659	N509	N509
T1463	T1463	M1396	V1397	P1312	L1141	E1062	L975	S895	S817	L749	T660	V512	V512
T1464	T1464	P1313	V1398	P1314	L1142	L1063	F977	D898	S818	K750	T661	T513	T513
T1465	T1465	M1314	V1399	M1314	R1143	F1064	Y976	Y919	V819	T751	T662	E514	E514
T1466	T1466	Y1318	V1399	Y1318	L1144	R1065	R978	Y919	N820	N752	L661	L515	L515
D1467	D1467	F1319	A1400	P1319	F1145	V1066	M979	N902	N821	M753	L665	P516	P516
K1468	K1468	A1401	P1402	I1320	E1146	F1067	R980	G904	T822	D754	D670	E517	E517
L1470	L1470	S1321	T1403	S1321	T1147	E1068	E981	L903	D823	I755	D671	W518	W518
L1471	L1471	G1404	G1404	V1322	C1148	Q1069	R985	R905	L824		R672	A519	A519
Q1472	Q1472	S1405	S1405	I1323	L1149	Q1069	L985	A906	K825		K673	A520	A520
Q1473	Q1473	G1406	G1406	I1323	L1149	Q1069	Y986	R908	L827		P674	P522	P522
G1474	G1474	M1328	M1328	M1328	W1153	E1072	Y986	R908	L828		F603	F523	F523
D1475	D1475	E1331	E1331	E1331	S1155	F1073	Y992	D812	L828		L679	T526	T526
L1476	L1476	E1331	E1331	E1331	V1156	Y1076	E993	T913	P829		T683	T527	T527
L1477	L1477	E1331	E1331	E1331	Q1240	P1077	E999	T914	F832		T683	T528	T528
L1478	L1478	M1334	E1412	P1335	L1159	V1078	Q1000	G917	G833		R685	T529	T529
A1479	A1479	P1335	F1413	P1335	A1160	R1079	K1001	I918	I834		R686	N530	N530
T1480	T1480	L1336	A1414	V1336	L1161	Q1080	R1002	I919	H835		T687	G611	G611
P1481	P1481	S1337	L1415	S1337	N1162	E1081	R1002	I920	H836		K613	K531	K531
L1482	L1482	F1338	L1416	F1338	M1163	E1082	V1003	I920	H836		K613	L532	L532
Q1483	Q1483	R1417	R1417	R1417	L1247	K1083	H1007	T921	M839		V614	Q533	Q533
W1484	W1484	R1418	R1418	R1418	K1165	L1084	H1007	T921	S840		S615	F537	F537
L1485	L1485	L1343	L1343	L1343	K1165	E1085	M101	T921	S840		S615	T538	T538
W1486	W1486	E1352	E1352	E1352	E1168	L1089	M101	T921	A842		E616	L617	L617
L1487	L1487	L1353	L1353	L1353	K1169	L1090	S1016	T921	A842		E616	T539	T539
S1488	S1488	L1354	L1354	L1354	R1170	L1090	M1017	T921	A842		E616	A540	A540
R1489	R1489	D1355	D1423	D1355	L1171	L1090	M1017	T921	A842		E616	F541	F541
Q1490	Q1490	L1356	G1425	L1356	W1173	P1093	L1018	T921	A842		E616	L542	L542
W1491	W1491	Q1357	G1425	Q1357	T1174	V1093	L1018	T921	A842		E616	T624	T624
K1492	K1492	P1358	R1426	P1358	T1174	K1098	Y1021	T921	A842		E616	K625	K625
R1493	R1493	L1359	A1427	L1359	M1175	E1099	Y1021	T921	A842		E616	Q626	Q626
E1494	E1494	P1360	V1428	P1360	S1176	S1100	K1027	T921	A842		E616	Q627	Q627
K1495	K1495	V1361	V1428	V1361	P1177	S1100	M1028	T921	A842		E616	L628	L628
L1496	L1496	S1362	I1430	S1362	Q1180	E1102	Q1029	T921	A842		E616	K557	K557
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V1497	V1497	L1364	P1432	L1364	Q1180	P1104	E1032	T921	A842		E616	T564	T564
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V1500	V1500	A1366	Q1434	A1366	T1183	A1106	L1033	T921	A842		E616	L566	L566
E1501	E1501	K1367	E1435	K1367	C1184	K1107	I1036	T921	A842		E616	T569	T569
L1502	L1502	D1368	L1436	D1368	P1185		A1037	T921	A842		E616	G570	G570
F1503	F1503	Y1369	V1437	Y1369	A1186	L1111	S1038	T921	A842		E616	K571	K571
I1504	I1504	Q1377	D1438	Q1377	E1187	Q1113	Y1040	T921	A842		E616	N572	N572
H1509	H1509		F1441		I1188	A1114	Y1041	T921	A842		E616	R573	R573
Q1514	Q1514	M1380	Q1442	M1380	K1191	Y1115	I1042	T921	A842		E616	D580	D580
M1515	M1515	K1381	Q1442	K1381	L1289	Y1116	I1042	T921	A842		E616	L581	L581
G1516	G1516	I1382	Q1445	I1382	L1290	L1116	M1047	T921	A842		E616	D582	D582
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Y1519	Y1519	Q1385	L1451	Q1385	R1118	L1117	M1047	T921	A842		E616	I579	I579
A1593	A1593	Q1386	G1453	Q1386	V1197	R1118	M1047	T921	A842		E616	D580	D580
A1595	A1595	T1386	G1453	T1386	D1206	L1126	M1047	T921	A842		E616	D582	D582
K1596	K1596	P1387	G1454	P1387	P1207	M1127	M1047	T921	A842		E616	D582	D582
P1597	P1597	M1388	G1454	M1388	P1208	A1128	L1053	T921	A842		E616	D582	D582
T1598	T1598	S1389	E1456	S1389	R1209	V1131	H1055	T921	A842		E616	D582	D582

L2172	M2173	S2174	D2175	S2176	Y2177	D2181	Q2182	D2183	P2184	S2185	PHE	SER	VAL	ASN	VAL	ALA	GLU	GLY	L1774	L1775	P1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	F1788	L1789	F1790	E1791	L1792	S1793	L1794	L1795	K1796	M1796	L1797	F1798	S1799	G1800	E1801	D1802	A1803	L1804	M1819	P1820	S1821	Y1822	L1825	Q1826	D1827	P1828	T1829	S1834	Q1835	Y1836	L1837	S1838	D1839	L1840	V1841	E1842	T1843	K1846	Q1847	L1848	S1849	A1851	L1854	L1855	M1856	L1857	E1858	D1859	E1860	G1861	T1862	V1863	A1864	P1865	L1866	N1867	A1868	A1869	M1870	I1871	Y1874	L1875	N1876	L1877	S1878	Y1879	M1880	E1883	M1884	F1885	L1886	L1887	S1888	L1889	S1890	H1891	K1892	S1893	K1894	L1895	R1896	T1897	I1898	L1899	E1900	V1902	E1907	F1908	Q1912	T1913	R1914	E1917	G1918	G1919	K1922	L1923	L1924	Y1925	V1928	P1929	V1930	K1931	V1936	W1937	D1938	S1939	K1943	V1946	L1947	Y1948	Q1949	A1950	H1951	F1952	S1953	R1954	I1959	L1960	L1961	A1962	K1963	D1964	Q1965	E1966	V1967	I1968	L1969	Q1970	K1971	I1972	L1973	S1974	L1975	L1976	S1977	A1978	I1979	V1980	D1981	I1982	L1983	S1984	S1985	E1986	H1988	L1989	N1990	A1991	L1992	N1993	A1994	L1995	E1996	M1997	S1998	Q1999	M2000	V2001	V2002	Q2003	A2004	M2005	Z2006	D2007	R2008	D2009	S2010	P2011	L2012	Q2013	Q2014	I2015	P2016	N2017	F2018	L2019	P2020	V2023	K2024	V2025	A2026	N2027	K2028	I2031	N2032	D2033	I2034	F2035	D2036	F2037	M2038	E2039	Q2040	N2041	N2042	P2043	E2044	E2045	N2046	P2047	N2048	S2051	L2052	V2053	K2054	D2055	L2056	G2057	L2058	T2059	Q2060	A2061	Q2062	L2063	Q2064	Q2065	A2066	A2067	N2068	F2069	T2070	N2071	N2072	K2073	Y2074	PRO	ASP	ILE	THR	LEU	GLU	F2081	E2082	V2083	D2084	D2085	P2086	D2087	N2088	T2089	R2090	A2091	G2092	E2093	P2094	A2095	Y2096	L2097	K2098	I2099	H2100	E2101	E2102	R2103	E2104	L2105	E2106	E2107	ASP	GLU	L1601	T1602	T1603	Q1604	L1605	S1606	P1607	D1608	Q1609	V1613	P1616	S1617	R1618	R1622	A1625	L1629	T1630	A1631	C1632	D1639	R1640	F1641	Q1648	I1649	L1652	L1653	D1654	H1655	V1656	Q1657	E1658	G1670	Y1671	Y1672	H1673	E1674	A1675	L1676	S1677	Q1678	S1679	D1680	K1681	R1682	V1683	V1684	K1685	H1686	L1687	Y1688	M1690	T1693	Q1694	V1695	L1696	I1697	W1704	E1705	L1706	D1707	F1708	T1709	A1710	H1711	L1712	V1713	V1714	T1718	Q1719	F1720	F1721	E1722	G1723	K1724	R1727	Y1728	I1729	P1732	R1815	L1816	M1819	P1820	S1821	Y1822	L1825	Q1826	D1827	P1828	T1829	S1834	Q1835	Y1836	L1837	S1838	D1839	L1840	V1841	E1842	T1843	K1846	Q1847	L1848	S1849	A1851	L1854	L1855	M1856	L1857	E1858	D1859	E1860	G1861	T1862	V1863	A1864	P1865	L1866	N1867	A1868	A1869	M1870	I1871	Y1874	L1875	N1876	L1877	S1878	Y1879	M1880	E1883	M1884	F1885	L1886	L1887	S1888	L1889	S1890	H1891	K1892	S1893	K1894	L1895	R1896	T1897	I1898	L1899	E1900	V1902	E1907	F1908	Q1912	T1913	R1914	E1917	G1918	G1919	K1922	L1923	L1924	Y1925	V1928	P1929	V1930	K1931	V1936	W1937	D1938	S1939	K1943	V1946	L1947	Y1948	Q1949	A1950	H1951	F1952	S1953	R1954	I1959	L1960	L1961	A1962	K1963	D1964	Q1965	E1966	V1967	I1968	L1969	Q1970	K1971	I1972	L1973	S1974	L1975	L1976	S1977	A1978	I1979	V1980	D1981	I1982	L1983	S1984	S1985	E1986	H1988	L1989	N1990	A1991	L1992	N1993	A1994	L1995	E1996	M1997	S1998	Q1999	M2000	V2001	V2002	Q2003	A2004	M2005	Z2006	D2007	R2008	D2009	S2010	P2011	L2012	Q2013	Q2014	I2015	P2016	N2017	F2018	L2019	P2020	V2023	K2024	V2025	A2026	N2027	K2028	I2031	N2032	D2033	I2034	F2035	D2036	F2037	M2038	E2039	Q2040	N2041	N2042	P2043	E2044	E2045	N2046	P2047	N2048	S2051	L2052	V2053	K2054	D2055	L2056	G2057	L2058	T2059	Q2060	A2061	Q2062	L2063	Q2064	Q2065	A2066	A2067	N2068	F2069	T2070	N2071	N2072	K2073	Y2074	PRO	ASP	ILE	THR	LEU	GLU	F2081	E2082	V2083	D2084	D2085	P2086	D2087	N2088	T2089	R2090	A2091	G2092	E2093	P2094	A2095	Y2096	L2097	K2098	I2099	H2100	E2101	E2102	R2103	E2104	L2105	E2106	E2107	ASP	GLU	L2172	M2173	S2174	D2175	S2176	Y2177	D2181	Q2182	D2183	P2184	S2185	PHE	SER	VAL	ASN	VAL	ALA	GLU	GLY
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
4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.54Å 269.59Å 231.69Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	49.13 – 3.20 49.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.13-3.20) 99.0 (49.52-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.244 , 0.287 0.248 , 0.289	Depositor DCC
R_{free} test set	9222 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	93.4	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	63679	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	B	0.20	0/2175	0.38	0/2962
1	D	0.22	0/2151	0.39	0/2927
1	F	0.21	0/2174	0.39	0/2958
1	H	0.21	0/2184	0.37	0/2973
2	A	0.21	0/14227	0.37	0/19296
2	C	0.21	0/13925	0.38	0/18882
2	E	0.21	0/14234	0.38	0/19306
2	G	0.22	0/13998	0.39	0/18976
All	All	0.21	0/65068	0.38	0/88280

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2217	ASP	Peptide
2	E	1965	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2116	0	2075	139	0
1	D	2093	0	2057	120	0
1	F	2116	0	2079	124	0
1	H	2125	0	2088	127	0
2	A	13917	0	13956	862	0
2	C	13628	0	13674	959	0
2	E	13925	0	13970	867	0
2	G	13701	0	13768	973	0
3	A	4	3	3	1	0
3	C	4	3	3	1	0
3	E	4	3	3	4	0
3	G	4	3	3	0	0
4	A	12	0	0	0	0
4	C	5	0	0	0	0
4	D	2	0	0	0	0
4	E	7	0	0	0	0
4	F	1	0	0	0	0
4	G	3	0	0	1	0
All	All	63667	12	63679	4086	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

The worst 5 of 4086 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)
2:E:521:ILE:HD12	2:E:522:PRO:HD3	1.22	1.21
2:C:874:HIS:HA	2:C:907:GLY:HA2	1.28	1.13
2:G:515:LEU:HB3	2:G:516:PRO:HD2	1.18	1.10
2:A:835:HIS:HA	2:A:839:MET:HE1	1.31	1.10
2:C:2040:GLN:HA	2:C:2046:ASN:HB3	1.29	1.10

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	B	264/276 (96%)	241 (91%)	19 (7%)	4 (2%)	10	44
1	D	259/276 (94%)	239 (92%)	13 (5%)	7 (3%)	5	30
1	F	261/276 (95%)	237 (91%)	22 (8%)	2 (1%)	19	58
1	H	265/276 (96%)	243 (92%)	13 (5%)	9 (3%)	3	24
2	A	1736/1772 (98%)	1619 (93%)	105 (6%)	12 (1%)	22	61
2	C	1686/1772 (95%)	1537 (91%)	130 (8%)	19 (1%)	14	51
2	E	1736/1772 (98%)	1580 (91%)	127 (7%)	29 (2%)	9	42
2	G	1698/1772 (96%)	1537 (90%)	131 (8%)	30 (2%)	8	41
All	All	7905/8192 (96%)	7233 (92%)	560 (7%)	112 (1%)	11	46

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2217	ASP
1	B	2220	VAL
2	A	575	GLU
2	A	1748	LYS
1	D	2218	PRO

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	B	234/241 (97%)	225 (96%)	9 (4%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	231/241 (96%)	224 (97%)	7 (3%)	41	73
1	F	235/241 (98%)	227 (97%)	8 (3%)	37	70
1	H	235/241 (98%)	231 (98%)	4 (2%)	60	83
2	A	1534/1562 (98%)	1475 (96%)	59 (4%)	33	67
2	C	1503/1562 (96%)	1439 (96%)	64 (4%)	29	64
2	E	1537/1562 (98%)	1486 (97%)	51 (3%)	38	71
2	G	1511/1562 (97%)	1469 (97%)	42 (3%)	43	74
All	All	7020/7212 (97%)	6776 (96%)	244 (4%)	36	69

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1795	LYS
2	G	1501	GLU
1	F	2172	LYS
2	G	1498	GLN
2	G	2070	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	800	GLN
2	E	2071	ASN
2	G	1988	HIS
2	E	1673	HIS
2	E	2127	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	E	2201	-	3,3,3	0.77	0	3,3,3	1.35	0
3	ACT	A	2201	-	3,3,3	0.78	0	3,3,3	1.34	0
3	ACT	G	2201	-	3,3,3	0.78	0	3,3,3	1.35	0
3	ACT	C	2201	-	3,3,3	0.77	0	3,3,3	1.36	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2201	ACT	4	0
3	A	2201	ACT	1	0
3	C	2201	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 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	B	266/276 (96%)	-0.05	3 (1%) 80 69	54, 76, 110, 128	0
1	D	263/276 (95%)	-0.06	1 (0%) 92 89	56, 73, 101, 130	0
1	F	265/276 (96%)	-0.02	4 (1%) 73 61	53, 83, 117, 143	0
1	H	267/276 (96%)	-0.01	2 (0%) 87 81	54, 77, 111, 132	0
2	A	1738/1772 (98%)	0.01	25 (1%) 75 63	39, 73, 123, 171	0
2	C	1702/1772 (96%)	0.12	60 (3%) 44 28	49, 86, 159, 209	0
2	E	1740/1772 (98%)	0.06	24 (1%) 75 63	48, 80, 132, 205	0
2	G	1710/1772 (96%)	0.27	106 (6%) 20 11	48, 92, 171, 209	0
All	All	7951/8192 (97%)	0.09	225 (2%) 53 37	39, 81, 154, 209	0

The worst 5 of 225 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	2171	PHE	4.9
2	G	2142	ALA	4.6
2	C	2170	LEU	4.6
2	A	1985	SER	4.5
2	G	2088	ASN	4.5

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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACT	C	2201	4/4	0.62	0.36	80,91,97,98	0
3	ACT	E	2201	4/4	0.85	0.27	87,92,111,111	0
3	ACT	G	2201	4/4	0.85	0.24	84,89,104,104	0
3	ACT	A	2201	4/4	0.88	0.20	63,68,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.