



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:07 PM GMT

PDB ID : 4WQT
Title : Thermus thermophilus RNA polymerase complexed with an RNA cleavage stimulating factor (a GreA/Gfh1 chimeric protein)
Authors : Murayama, Y.; Sekine, S.; Yokoyama, S.
Deposited on : 2014-10-22
Resolution : 4.40 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

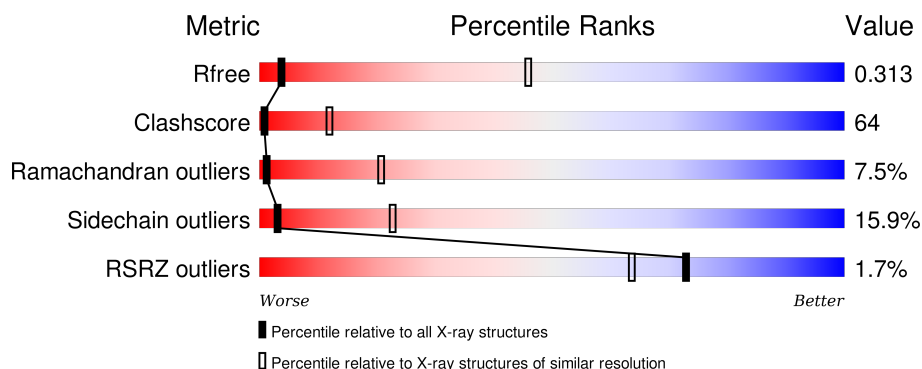
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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.



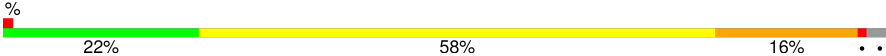
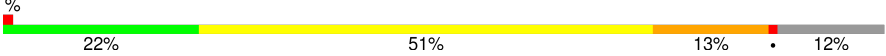
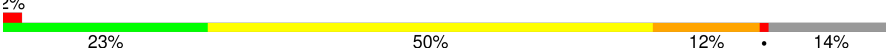
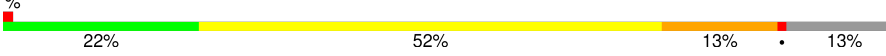

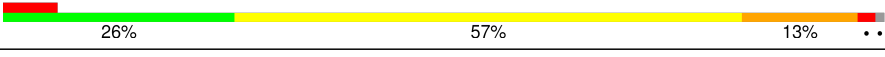
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1067 (5.20-3.60)
Clashscore	102246	1175 (5.20-3.60)
Ramachandran outliers	100387	1114 (5.20-3.60)
Sidechain outliers	100360	1096 (5.20-3.60)
RSRZ outliers	91569	1071 (5.20-3.60)

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	315	<div> <div>17%</div> <div>43%</div> <div>10%</div> <div>29%</div> </div>
1	B	315	<div> <div>17%</div> <div>44%</div> <div>10%</div> <div>29%</div> </div>
1	F	315	<div> <div>19%</div> <div>39%</div> <div>12%</div> <div>29%</div> </div>
1	G	315	<div> <div>20%</div> <div>39%</div> <div>11%</div> <div>29%</div> </div>
1	K	315	<div> <div>19%</div> <div>43%</div> <div>10%</div> <div>29%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	L	315	
2	C	1119	
2	H	1119	
2	M	1119	
3	D	1524	
3	I	1524	
3	N	1524	
4	E	99	
4	J	99	
4	O	99	
5	X	156	
5	Y	156	
5	Z	156	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 73369 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			
1	F	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	G	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	K	225	Total	C	N	O	S	0	0	0
			1769	1129	308	330	2			
1	L	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1080	Total	C	N	O	S	0	0	0
			8521	5392	1520	1585	24			
2	H	1081	Total	C	N	O	S	0	0	0
			8530	5398	1522	1586	24			
2	M	1080	Total	C	N	O	S	0	0	0
			8521	5392	1520	1585	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1334	Total	C	N	O	S	0	0	0
			10513	6654	1864	1965	30			
3	I	1318	Total	C	N	O	S	0	0	0
			10396	6583	1842	1942	29			
3	N	1323	Total	C	N	O	S	0	0	0
			10440	6613	1849	1949	29			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			
4	J	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			
4	O	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			

- Molecule 5 is a protein called RNA cleavage stimulating factor (GreA/Gfh1 chimeric protein Gre-C1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	154	Total	C	N	O	S	0	0	0
			1200	736	218	242	4			
5	Y	154	Total	C	N	O	S	0	0	0
			1200	736	218	242	4			
5	Z	154	Total	C	N	O	S	0	0	0
			1200	736	218	242	4			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	Zn	0	0
			1	1		
6	D	1	Total	Zn	0	0
			1	1		
6	N	1	Total	Zn	0	0
			1	1		

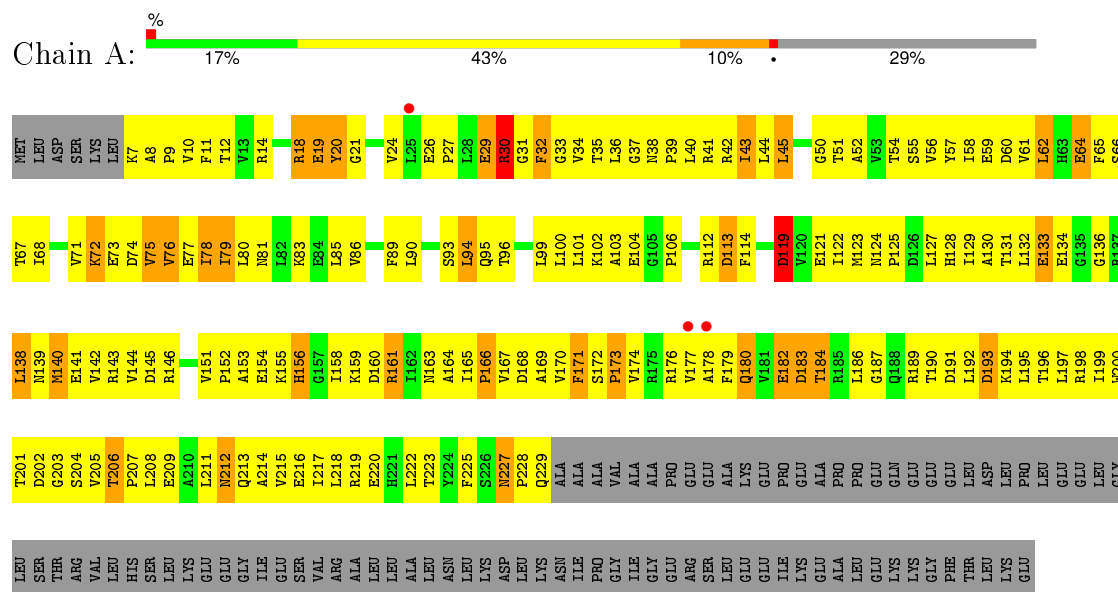
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	N	1	Total	Mg	0	0
			1	1		

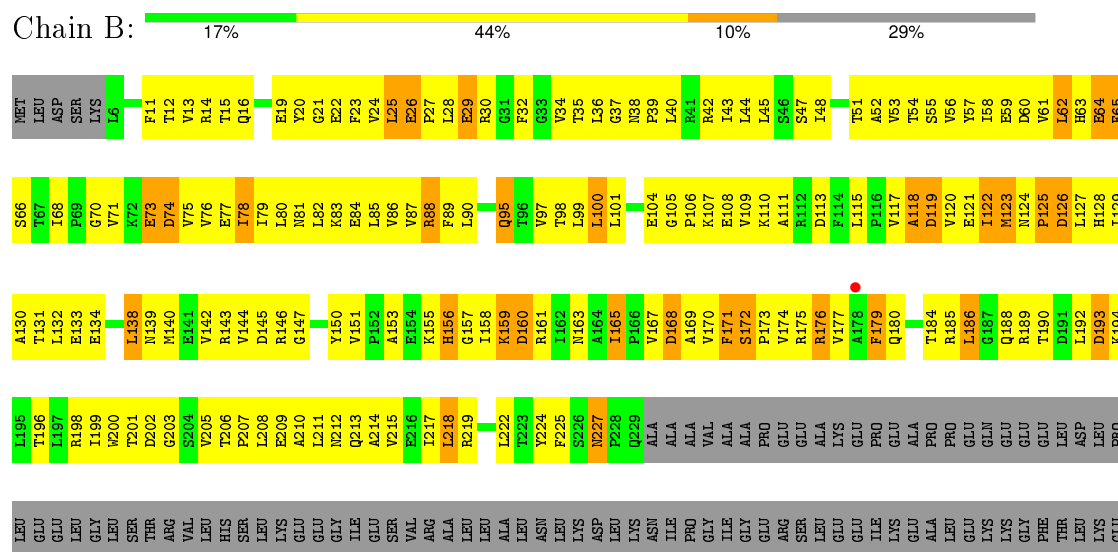
3 Residue-property plots

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 ($RSRZ > 2$). 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.

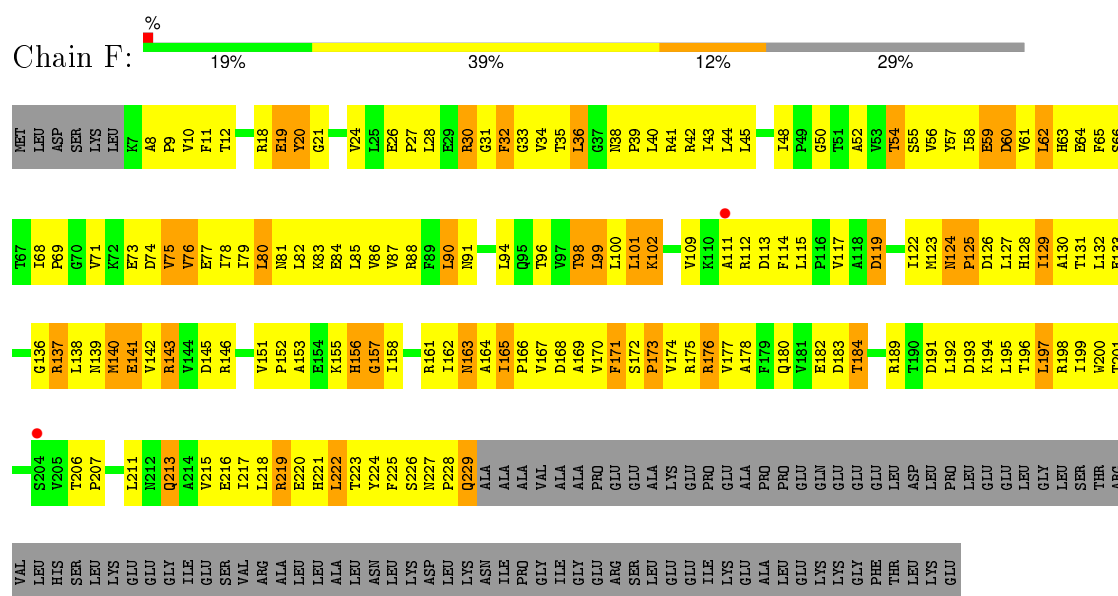
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



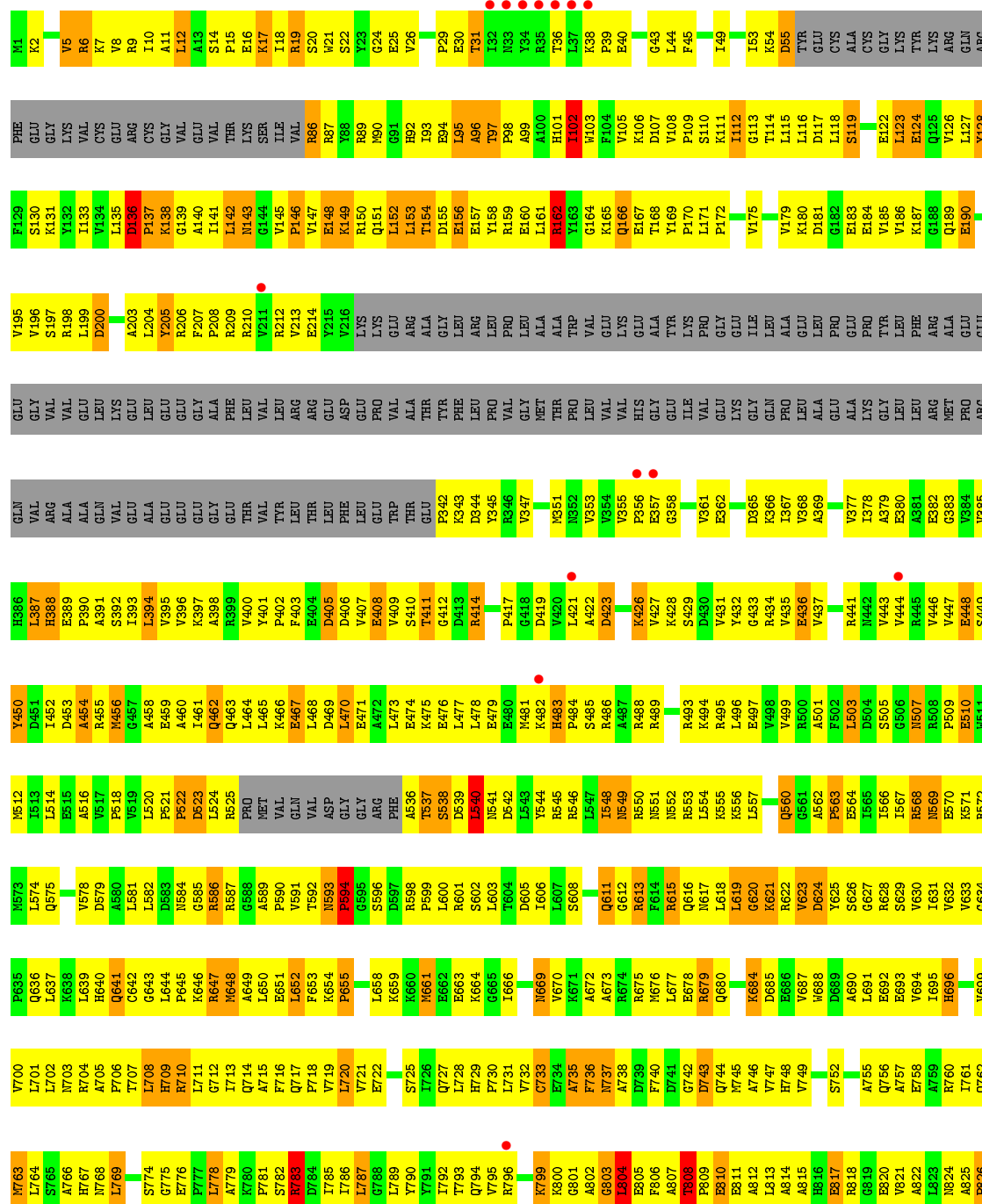
• Molecule 1: DNA-directed RNA polymerase subunit alpha





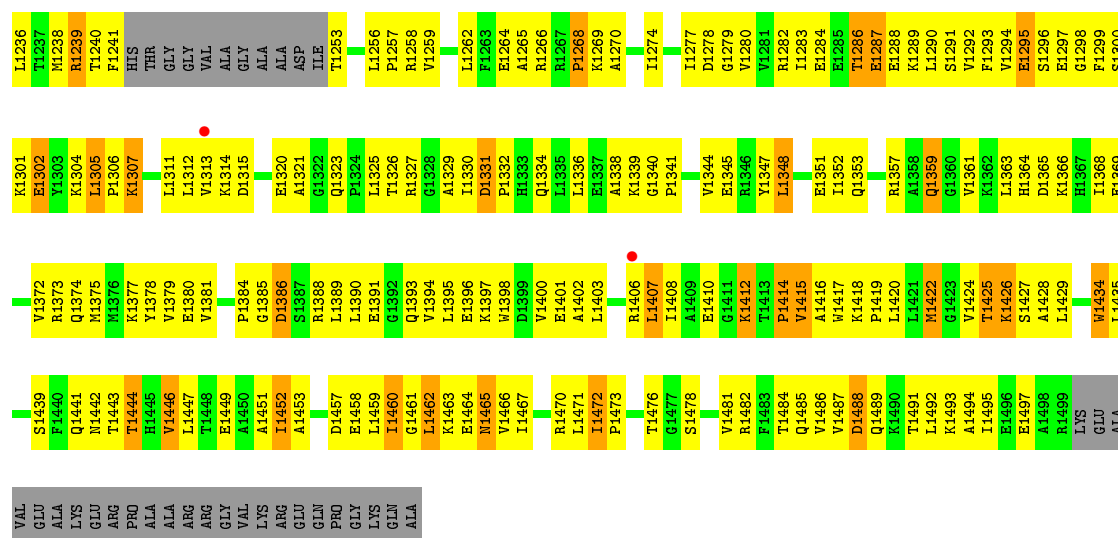


P882	K846	LYS	R721	D590	D462	K395	N330	D203	H441	P67	M1
1983	G987	ALA	I722	S591	F463	D396	R331	Q204	R142	F68	E2
E984	V848	ARG	R723	L592	L464	E397	R332	E205	S143	P69	I3
G985	V849	ASP	R724	A593	G465	T398	R333	T206	P144	E70	
P986	N663	VAL	D725	F331	F466	N399	R334	L207	G146	G7	F6
E913	K851	LVS	I726	M532	L467	P400	T335	A208	V145	R72	G7
I914	L852		P727	D633	R468		T336	R209	G147	L73	R8
K915	L853	D787	R728	V534	T469	S403	G337	E210	F148	G74	I9
E916	P854	T788	L729	S535	P470	L404	E338	L211	T149	E75	R10
A919	P855	S789	S730	F536	Y471	R405	L339	G212	P150	E11	E11
	E856	L790	E731	K537	R472	H406	M340		D151	O80	V12
F922	D857	R791	A732	Q538	R473	K407	T341	L217	P152	I13	I13
E923	M604		R733	K605	V474	R408	Q342	V218	A153	P14	P14
E924	V606		L734	V606		R409	Q343	Q219	R154	L88	L15
Y925	D607		R735	D607	G477	L410	F344	G220	P155	T89	P16
F926	G608		V736	S541	V478	S411		L221	G156	Y90	P17
G927	L668		N543	N543	V479	A412	L348	M222	R157	Q91	L18
K928	P862	V601	L737	T544	T480	A412	A349	D223	R158	T19	T19
R929	G864	R802	E738	M545	D481	G414	R350	E224	A159	A92	E20
	T865	T803	E739	I611	E482	G415	L351	S225	A160	E20	E20
V936	F676		G740	L546	E483	G416	L352	S226	S161	I21	I21
D937	F679	V616	E741	L547	V483	G417	R353	V227	I162	R97	Q22
K938	D680	R805	V742	P548	V484	G418	R354	F227	I163	L98	E23
K939	G681	L806	V743	F549	Y485	L418	L360	A228	I164	Q99	E24
R940	V682	G618	R744	N550	N486	T419	M361	M229	P164	L100	S25
E941	N683	R808	R745	E551	T487		G362	R230	L165	I101	Y26
V941	F684		G746	E552	A488	R422	E357	P231	P166	H102	
E942	E685		E747		T489	A423	R358	E232	K167	K103	A29
V943	D686	P624	E748	R557	E490	G424	M359	E233	R168	L30	L30
L944	A687	L625	V749	A558		F425	D295	A234	G169	Q31	Q31
R945	G688	R626	K750	L559	T495	D426	L360	G105	G106	T106	
E946	V689	R627	P751	M560	T496	V427	M361	L235	P170	G107	V34
	L690	F628	G752	G561	A497	R428	G362		L171	L107	
K949	S691		F753	S562	Q498	R429	S363	L238	L172	I108	
L950	E692	R630	I754	N563	A499	V430	E301	F239	D173	K109	K38
G951	E693	S631	L755	M564	N500	H431	T368	T240	E110	E110	R39
L952	L694	N632	V756	Q665	T501	R432	P369	L241	L175	D111	E40
V953	L695	Q633	G757	T566	P502	T433	A370	L242	V176	N41	
	K696	G634	R758	Q667	L503	H434	K371	R243	E177	V113	V42
	R697	T635	I759	A568	E504	Y435	L372	P244	P178	F114	G43
	D698	A636	S760	V569	G505		V373		M179	L115	I44
	F699	L637		P570	N506	I438	N374	P247	G180	G116	Q45
	T701	D638	LYS	I571	R507	C439	S375	P248	V181	H117	
	S702	Q639	GLY	I572	I508	P440	R376	K249	V182	I118	F48
	I703	R640	GLU	R573	A509	V441	P377	R250	S183	P119	R49
	R704	P641	SER	A574	A509	E442	L378	D251	M184	L120	E50
	I705	R642	GLU	Q575	E511			K252	K185	M121	T51
	E706	V643	THR	A576	R512	A447	A381	A253	V186	T122	P52
	R707	V644	PRO	V577	V514	M448	I382	V254	K189	E123	P53
		G645	GLY	V578	A515	G450	R383	A255	I54	D124	I54
	I710	Q647	GLU	V579	A516	L451	E384	V257	F191		E55
	E711	R648	ARG	M580	R517		F385	Y258	P192	I129	E56
	A712	V649	LEU	T581		S454	F386	G259	L193	N130	GLU
	R713	R650	LEU	G582	E520	L455	S387	L260	L194	ASP	
	D714	K651	LEU	E584	P521	A456	R388	L261	L195	LVS	LVS
	ARG	G652	ARG	E585	V522	A457	S389	A262	L196	D133	GLY
	L717	D653	SER	R586	I523	Y458	Q390	D263	L197	R134	LVS
	G718	L854	ILE	R587	I524	A459	L391	P264	R198	V135	GLY
	P719	R642	PHE	V588	S525	R460	S392	R265	V136	I186	G63
	E720	G658	GLU	R589	P526	V461	F394	L200	V199	Q139	L64
								Y267	L200	I140	V65
											L66

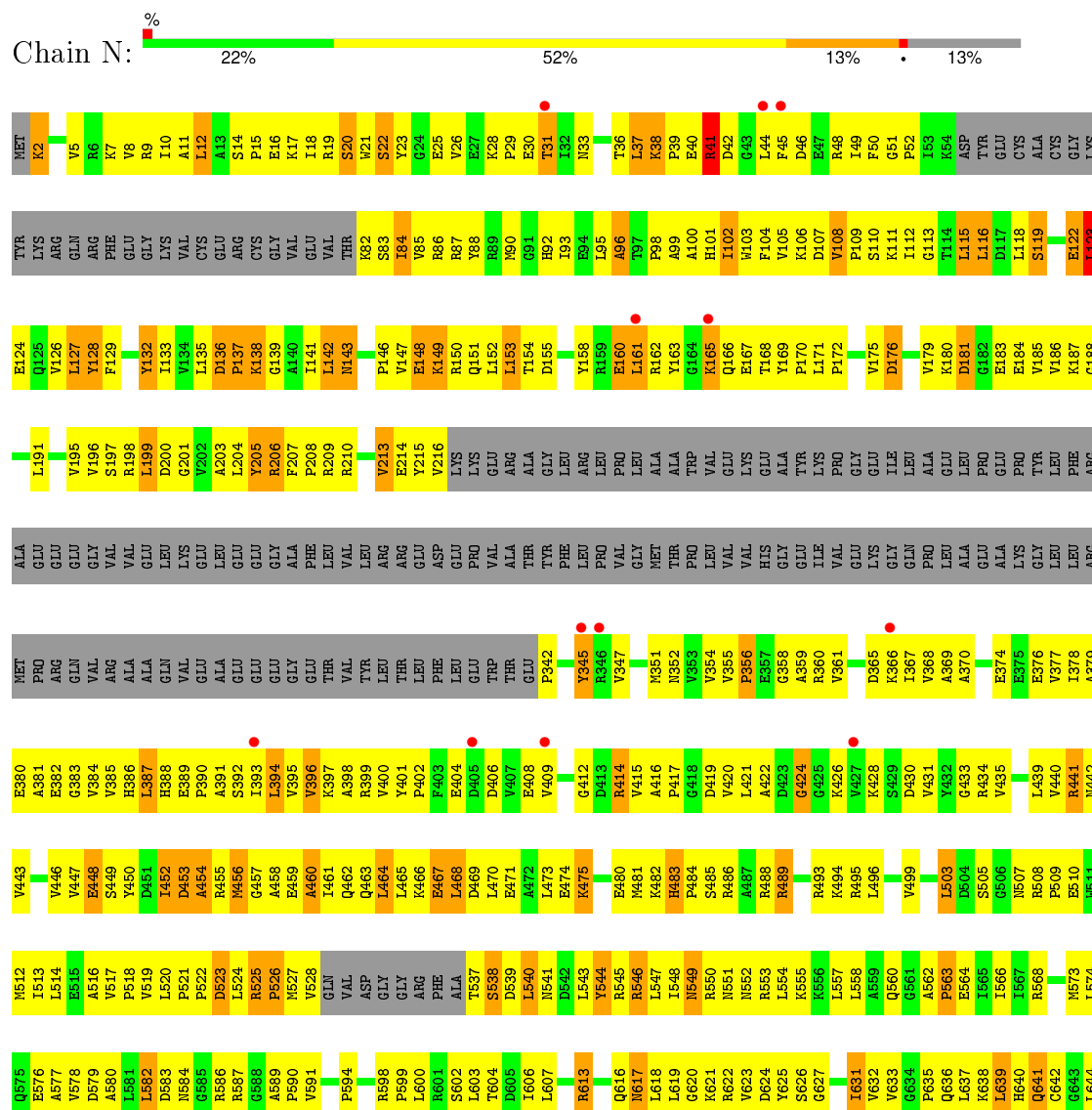


L128	P129	S130	K131	Y132	I133	V134	L135	D136	P137	K138	G139	A140	I141	N143	P146	V147	E148	K149	R150	Q151	R152	L153	T154	E157	V158	R159	E160	L161	R162	K165	Q166	E167	T168	V169	P170	L171	P172	V175	D176	A177	L178	V179	K180	D181	G182	E183	E184	V185	T186	K187	G188	Q189	E190	L191																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
ARG	GLN	ARG	ARG	PHE	GLU	GLY	LYS	VAL	CYS	GLU	ARG	ARG	GLY	VAL	THR	K82	S83	R84	G85	R86	R87	Y88	R89	R90	E91	H92	A96	T97	A100	H101	I102	W103	F104	V105	K106	D107	V108	P109	S110	K111	I112	L115	L116	P51	D117	L118	S119	T120	G121	CYS	ALA	CYS	GLY	LYS	T127																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
G1477	S1478	V1481	F1482	F1483	T1484	Q1485	V1486	D1488	I1489	K1490	T1491	L1492	K1493	L1494	L1495	E1496	E1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	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	L2462	L2463	L2464	L2465	L2466	L2467	L2468	L2469	L2470	L2471	L2472	L2473	L2474	L2475	L2476	L2477	L2478	L2479	L2480	L2481	L2482	L2483	L2484	L2485	L2486	L2487	L2488	L2489	L2490	L2491	L2492	L2493	L2494	L2495	L2496	L2497	L2498	L2499	L2500	L2501	L2502	L2503	L2504	L2505	L2506	L2507	L2508	L2509	L2510	L2511	L2512	L2513	L2514	L2515	L2516	L2517	L2518	L2519	L2520	L2521	L2522	L2523	L2524	L2525	L2526	L2527	L2528	L2529	L2530	L2531	L2532	L2533	L2534	L2535	L2536	L2537	L2538	L2539	L2540	L2541	L2542	L2543	L2544	L2545	L2546	L2547	L2548	L2549	L2550	L2551	L2552	L2553	L2554	L2555	L2556	L2557	L2558	L2559	L2560	L2561	L2562	L2563	L2564	L2565	L2566	L2567	L2568	L2569	L2570	L2571	L2572	L2573	L2574	L2575	L2576	L2577	L2578	L2579	L2580	L2581	L2582	L2583	L2584	L2585	L2586	L2587	L2588	L2589	L2590	L2591	L2592	L2593	L2594	L2595	L2596	L2597	L2598	L2599	L2600	L2601	L2602	L2603	L2604	L2605	L2606	L2607	L2608	L2609	L2610	L2611	L2612	L2613	L2614	L2615	L2616	L2617	L2618	L2619	L2620	L2621	L2622	L2623	L2624	L2625	L2626	L2627	L2628	L2629	L2630	L2631	L2632	L2633	L2634	L2635	L2636	L2637	L2638	L2639	L2640	L2641	L2642	L2643	L2644	L2645	L2646	L2647	L2648	L2649	L2650	L2651	L2652	L2653	L2654	L2655	L2656	L2657	L2658	L2659	L2660	L2661	L2662	L2663	L2664	L2665	L2666	L2667	L2668	L2669	L2670	L2671	L2672	L2673	L2674	L2675	L2676	L2677	L2678	L2679	L2680	L2681	L2682	L2683	L2684	L2685	L2686	L2687	L2688	L2689	L2690	L2691	L2692	L2693	L2694	L2695	L2696	L2697	L2698	L2699	L2700	L2701	L2702	L2703	L2704	L2705	L2706	L2707	L2708	L2709	L2710	L2711	L2712	L2713	L2714	L2715	L2716	L2717	L2718	L2719	L2720	L2721	L2722	L2723	L2724	L2725	L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745

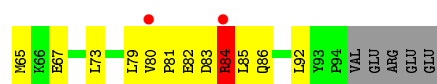
D1169	H1103	P1032	E959	V895	T834	S771	A705	C642	R572	R441	V377	PRO	GLU	A192
D1170	E1104	Q1033	E963	A896	S835	S774	P706	G643	R573	R442	I378	ARG	GLU	P193
H1171	I1105	Q1034	Y963	H897	R836	G775	I707	L644	L574	V443	A379	GLN	GLY	
H1172	V1106	I1035	L964	E898	G837	G776	L708	P645	Q675	V444		VAL	GLY	S197
	V1107	R1036	E965	L899	R838	E777	H709		E576	R445	E382	ALA	VAL	R198
K1176	R1108	Q1037	E966	I900	Y841	P777	R710	K648	A577	V446	G383	ALA	VAL	L199
A1177	E1109	L1038	E969	G903	F843	L778	L711	L649	V578	V447	V384	ALA	VAL	D200
A1178	D1111	G1040	R970	L902	R842	A779	G712	L650	D879	E448	V385	GLN	LEU	G201
	D1112	P1043	R971	P903	F843	K780	I713	E651	L581			LYS	LYS	V202
E1182	G1112	L1041	L971	V904	N844	P781	Q714	L652	L581	A580	H386	GLU	GLU	A203
I1183	G1113	R1042	L972	P905	N845	S782	A715	F653	L582	A516	L387	GLU	LEU	L204
Q1184	T1114	P1043	Q973	Q906	R846	R783	F716	K654	D583	D452	H388	ALA	LEU	
	T1115	L1044	Q973	Q907	D847	D784	Q717	P655	P518	R452	E389	GLU	GLU	Y205
V1188	M1116	M1045	Q976	K908	E848	I785	P718	F656	R586	D453	P390	GLU	GLU	R206
R1189	Y1117	Q1046	A977	I909	A849	I786	V719	L657	R587	A454	A391	GLY	GLY	F207
S1190	I1118	K1047	Y978	S910	A849	L787	V720	L658	G588	R455	S392	GLY	ALA	P208
P1191	P1048	E799	E979	L911	L851	G788	V721	K659	A589	M456	L394	PHE	PHE	R209
T1192	S1049	L1126	Q979	K912	A852	L789	E722	R660	L524		V395	VAL	VAL	R210
T1193	G1050	G981	Q981	D913	R653	V790		R661	T592	E459	V396	LEU	LEU	R211
G1194	E1051	P982	P982	L914	A854	I791	I726	E682	T593	A460	V397	LEU	LEU	R212
Q1195	T1052	L983	L983	V915	R855	I792	Q727	E683	M593	I461	K397	LEU	ARG	V213
P1196	F1053	T984	T984	Y916	G856	I793	L728	K664	P994	Q463	A398	THR	ARG	E214
R1197	E1054	D985	I857		I857	Q794	H729	G665		L464	R399	LEU	GLU	Y215
Y1198	V1055	R986	V858	F919	R858	V795	P730	T666	R601	L465	V400	PHE	ASP	
G1199	E127	P1056	D859	L920	D859	R796	L731	A667	S802	K466	Y401	LEU	PRO	LYS
V1200	T1128	V1057	E987	R921	L860	K797	V732	P688	L603	E467	P402	GLU	VAL	GLU
C1201	R1058	R1058	R989	I922	Q861	E798	C733	R669	T604		F403	TRP	VAL	
Q1202	S1131	S1059	D990	G923	D862	K799	E734	K671	G805	D469	D406	THR	ALA	ALA
K1203	L1132	S1060	Q991	N924	R663	K800	A735	K671	I606	L470	V407	GLY	THR	GLY
C1204	R1133	P1061	I992	E925	V864	G801	F736	A672	L607		E408	LYS	PHE	LEU
Y1205	L1134	R1062	L993	K926	T865	A802	N737	A673	S608	E474	V409	ASP	LEU	ARG
G1206	R1135	E1063	Q994	T927	R866	G803	A738	R674		K475	S410	TYR	PRO	LEU
Y1207	A1138	L1064	L995	A928	R867	L804	D739	R675	G612	E476	T411	ARG	VAL	PRO
D1208	D1139	T1065	K996	R929	Y868	E805			R613	L477		GLY	GLY	LEU
L1209	L1140	L1066	T997	L930	R869	F806	D743	L677	F614	L478	V415	MET	ALA	ALA
M1211	L1141	V1067	E998	L931	G870	A807	Q744	R678	R615	E479	A416	THR	ALA	ALA
A1212	Y1145	E1068	T999	D932	K871	T808	N745	R679	Q616	E490	P417	TRP	PRO	TRP
R1213	G1146	Y1070	T1000	A933	R872	P909		Q680	M817	M481	G418	LEU	VAL	VAL
P1214	R1147	F1071	E1001	L934	L873	E910	P750		L618	K482	D419	VAL	GLU	GLU
V1215	V1148	I1072	K1002	K935	T875	E911	L751	D685	G620	H483	V420	VAL	VAL	LYS
S1216	L1149	L1072	V1003	Y936	S876	L813	S752	D685	K821	P484	L421	HIS	GLY	GLY
I1217	A1150	H1075	Y1007	G938	P877	G819	S753	E686	R622	S485	A422	GLY	GLY	ALA
G1218	R1151	R1078	Y1015	F939	R878	A815	F754	V687	V623	R488	D423	GLY	TYR	TYR
E1219	V1153	T1078	F1016	T940	R879	H816	A755		D624	R489	G424	VAL	ILE	LYS
V1221	E1154	L1084	F1017	F941	L880	E917	Q756	L691	G425	A359	G425	VAL	VAL	PRO
G1222	V1155	L1084	S942	S942	L881	R818	A757	E692	K426	R360	V427	GLY	GLY	LYS
I1223	L1156	S1091	M1018	T943	F882	G819	E758	E692	K427	V361	K428	ILE	ILE	GLY
	G1157	G1092	P1019	T944	R884	E920	A759	E693	S429	E362	E362	GLN	GLN	LEU
	L1160	Y1093	L1020	T947	I885	A822	I761	V694	D430	D385	D385	PRO	PRO	ALA
I1227	E1161	L1094	Y1021	T948	V886	A825	Q762	E696	V431	R366	R366	LEU	ALA	ALA
S1228	E1162	T1095	M1023	T948	A887	P826	M763	R696	G433	I367	I367	GLY	GLY	PRO
I1229	E1163	R1096	G1023	G949	E888	A926	L764	K698	R434	V368	V368	ALA	ALA	ALA
G1230	G1163	K1097	Q1025	I951	R899	P826	S765	V699	V435	A369	A369	LYS	PRO	PRO
E1231	R1164	L1098	S1026	D952	A890	V829	A766	V700	E367	A370	A370	GLY	TYR	TYR
P1232	Y1165	V1099	G1027	D952	E891	A830	H767	L701	L567	F502	E436	LEU	LEU	LEU
G1233	L1166	D1100	A1028	T956	D892	G831	M768	L702	K638	L503	D437	LEU	LEU	LEU
T1234	S1167	P1101	E957	P957	E893	R632	L769	L702	L639	D504	D438	PHE	PHE	ARG
Q1235	M1168	T1102	M1031	E958	R894	E833	L770	R704	Q641	S505	V440	ARG	ARG	ALA



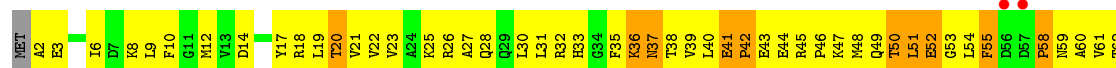
• Molecule 3: DNA-directed RNA polymerase subunit beta'



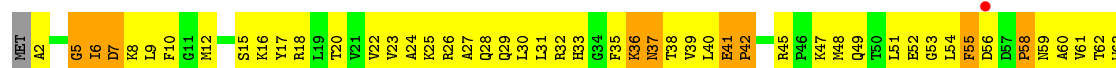




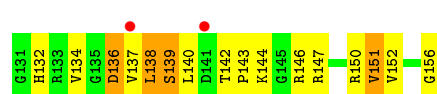
- Molecule 4: DNA-directed RNA polymerase subunit omega



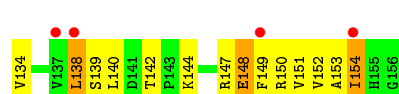
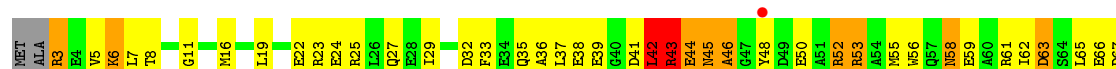
- Molecule 4: DNA-directed RNA polymerase subunit omega



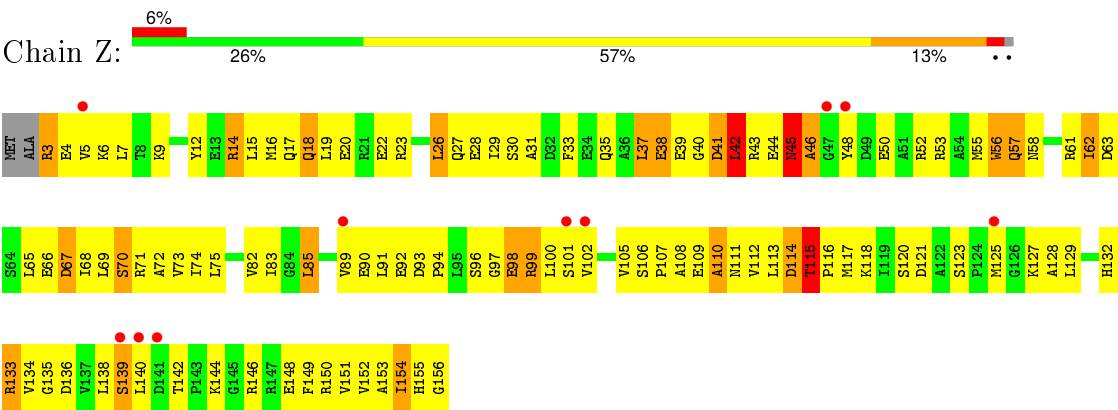
- Molecule 5: RNA cleavage stimulating factor (GreA/Gfh1 chimeric protein Gre-C1)



- Molecule 5: RNA cleavage stimulating factor (GreA/Gfh1 chimeric protein Gre-C1)



● Molecule 5: RNA cleavage stimulating factor (GreA/Gfh1 chimeric protein Gre-C1)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	189.57Å 263.77Å 195.85Å 90.00° 116.83° 90.00°	Depositor
Resolution (Å)	45.79 – 4.40 45.79 – 4.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (45.79-4.40) 96.5 (45.79-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 4.45Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.260 , 0.313 0.260 , 0.313	Depositor DCC
R_{free} test set	3149 reflections (3.01%)	DCC
Wilson B-factor (Å ²)	151.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 136.3	EDS
Estimated twinning fraction	0.129 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 104543 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	73369	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/1791	0.64	0/2436
1	B	0.51	0/1799	0.65	0/2447
1	F	0.51	0/1791	0.66	0/2436
1	G	0.51	0/1791	0.68	0/2436
1	K	0.45	0/1801	0.60	0/2450
1	L	0.51	0/1799	0.65	0/2447
2	C	0.51	0/8683	0.63	0/11747
2	H	0.53	0/8692	0.64	0/11758
2	M	0.49	0/8683	0.63	0/11747
3	D	0.52	0/10692	0.65	1/14452 (0.0%)
3	I	0.50	0/10571	0.62	0/14288
3	N	0.50	0/10617	0.63	0/14350
4	E	0.49	0/768	0.62	0/1035
4	J	0.51	0/768	0.63	0/1035
4	O	0.53	0/768	0.62	0/1035
5	X	0.68	0/1212	0.81	1/1629 (0.1%)
5	Y	0.64	0/1212	0.82	1/1629 (0.1%)
5	Z	0.62	0/1212	0.87	2/1629 (0.1%)
All	All	0.51	0/74650	0.65	5/100986 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	37	LEU	CB-CG-CD1	-6.64	99.71	111.00
5	Z	42	LEU	CA-CB-CG	5.91	128.89	115.30
5	X	40	GLY	N-CA-C	-5.23	100.03	113.10
5	Y	85	LEU	CA-CB-CG	-5.07	103.64	115.30
3	D	1242	HIS	N-CA-C	-5.02	97.45	111.00

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	1759	0	1805	257	0
1	B	1767	0	1816	262	0
1	F	1759	0	1805	253	0
1	G	1759	0	1805	236	0
1	K	1769	0	1815	236	0
1	L	1767	0	1816	230	0
2	C	8521	0	8619	1196	0
2	H	8530	0	8632	1294	0
2	M	8521	0	8619	1131	0
3	D	10513	0	10743	1508	0
3	I	10396	0	10627	1408	0
3	N	10440	0	10682	1391	0
4	E	754	0	769	86	0
4	J	754	0	769	99	0
4	O	754	0	769	124	0
5	X	1200	0	1194	142	0
5	Y	1200	0	1194	139	0
5	Z	1200	0	1194	125	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	N	1	0	0	0	0
7	D	1	0	0	0	0
7	I	1	0	0	0	0
7	N	1	0	0	0	0
All	All	73369	0	74673	9501	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 64.

The worst 5 of 9501 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)
5:Y:41:ASP:OD1	5:Y:48:TYR:HB2	1.38	1.19
1:F:54:THR:HG22	1:F:158:ILE:HG13	1.26	1.17
2:H:983:ILE:HD12	3:I:944:THR:HA	1.23	1.16
1:G:99:LEU:HD13	1:G:142:VAL:HG23	1.29	1.13
1:K:35:THR:HG21	1:L:43:ILE:HD11	1.28	1.12

There are no symmetry-related clashes.

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	221/315 (70%)	167 (76%)	41 (19%)	13 (6%)	2	27
1	B	222/315 (70%)	171 (77%)	43 (19%)	8 (4%)	4	40
1	F	221/315 (70%)	166 (75%)	41 (19%)	14 (6%)	2	26
1	G	221/315 (70%)	168 (76%)	43 (20%)	10 (4%)	3	34
1	K	223/315 (71%)	173 (78%)	39 (18%)	11 (5%)	3	32
1	L	222/315 (70%)	165 (74%)	47 (21%)	10 (4%)	3	34
2	C	1074/1119 (96%)	774 (72%)	213 (20%)	87 (8%)	1	18
2	H	1075/1119 (96%)	766 (71%)	223 (21%)	86 (8%)	1	19
2	M	1074/1119 (96%)	765 (71%)	222 (21%)	87 (8%)	1	18
3	D	1326/1524 (87%)	943 (71%)	271 (20%)	112 (8%)	1	17
3	I	1308/1524 (86%)	958 (73%)	247 (19%)	103 (8%)	1	19
3	N	1313/1524 (86%)	953 (73%)	258 (20%)	102 (8%)	1	20
4	E	91/99 (92%)	66 (72%)	18 (20%)	7 (8%)	1	20
4	J	91/99 (92%)	62 (68%)	22 (24%)	7 (8%)	1	20
4	O	91/99 (92%)	58 (64%)	27 (30%)	6 (7%)	1	25
5	X	152/156 (97%)	125 (82%)	21 (14%)	6 (4%)	4	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Y	152/156 (97%)	118 (78%)	23 (15%)	11 (7%)	1	22
5	Z	152/156 (97%)	119 (78%)	24 (16%)	9 (6%)	2	27
All	All	9229/10584 (87%)	6717 (73%)	1823 (20%)	689 (8%)	1	21

5 of 689 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLU
1	A	171	PHE
1	A	228	PRO
1	B	118	ALA
1	B	126	ASP

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	196/273 (72%)	163 (83%)	33 (17%)	2	20
1	B	197/273 (72%)	161 (82%)	36 (18%)	2	16
1	F	196/273 (72%)	160 (82%)	36 (18%)	2	15
1	G	196/273 (72%)	163 (83%)	33 (17%)	2	20
1	K	196/273 (72%)	168 (86%)	28 (14%)	4	27
1	L	197/273 (72%)	160 (81%)	37 (19%)	2	15
2	C	909/941 (97%)	763 (84%)	146 (16%)	3	22
2	H	910/941 (97%)	762 (84%)	148 (16%)	3	21
2	M	909/941 (97%)	763 (84%)	146 (16%)	3	22
3	D	1124/1279 (88%)	948 (84%)	176 (16%)	3	23
3	I	1114/1279 (87%)	951 (85%)	163 (15%)	4	26
3	N	1120/1279 (88%)	946 (84%)	174 (16%)	3	24
4	E	82/88 (93%)	69 (84%)	13 (16%)	3	23
4	J	82/88 (93%)	70 (85%)	12 (15%)	4	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	82/88 (93%)	68 (83%)	14 (17%)	2	19
5	X	128/129 (99%)	111 (87%)	17 (13%)	5	30
5	Y	128/129 (99%)	108 (84%)	20 (16%)	3	23
5	Z	128/129 (99%)	104 (81%)	24 (19%)	2	15
All	All	7894/8949 (88%)	6638 (84%)	1256 (16%)	3	23

5 of 1256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	679	PHE
3	I	842	VAL
3	N	1295	GLU
2	H	799	ILE
3	I	171	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 239 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	872	ASN
3	I	845	ASN
3	N	1334	GLN
2	H	899	GLN
3	I	549	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

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	223/315 (70%)	-0.26	3 (1%) 79 71	89, 173, 228, 279	0
1	B	224/315 (71%)	-0.30	1 (0%) 93 90	108, 172, 229, 282	0
1	F	223/315 (70%)	-0.36	2 (0%) 85 80	83, 162, 225, 270	0
1	G	223/315 (70%)	-0.42	0 100 100	91, 153, 211, 230	0
1	K	225/315 (71%)	-0.12	3 (1%) 79 71	116, 192, 249, 279	0
1	L	224/315 (71%)	-0.40	0 100 100	89, 167, 217, 242	0
2	C	1080/1119 (96%)	-0.30	10 (0%) 85 80	80, 168, 245, 311	0
2	H	1081/1119 (96%)	-0.32	13 (1%) 81 73	67, 161, 239, 339	0
2	M	1080/1119 (96%)	-0.26	20 (1%) 70 61	80, 174, 247, 315	0
3	D	1334/1524 (87%)	-0.24	22 (1%) 74 65	83, 172, 251, 342	0
3	I	1318/1524 (86%)	-0.18	28 (2%) 67 57	65, 181, 280, 356	0
3	N	1323/1524 (86%)	-0.22	18 (1%) 78 69	77, 176, 260, 310	0
4	E	93/99 (93%)	-0.03	4 (4%) 39 30	115, 192, 279, 362	0
4	J	93/99 (93%)	-0.22	2 (2%) 65 56	115, 177, 268, 293	0
4	O	93/99 (93%)	-0.13	2 (2%) 65 56	88, 176, 245, 261	0
5	X	154/156 (98%)	0.17	11 (7%) 19 14	146, 228, 282, 303	0
5	Y	154/156 (98%)	0.28	13 (8%) 14 10	157, 237, 315, 379	0
5	Z	154/156 (98%)	0.12	10 (6%) 22 16	133, 219, 288, 356	0
All	All	9299/10584 (87%)	-0.23	162 (1%) 73 63	65, 175, 259, 379	0

The worst 5 of 162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	56	ASP	7.3
4	E	57	ASP	6.6
3	I	211	VAL	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	807	ARG	5.5
5	Y	129	LEU	5.2

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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	ZN	N	1601	1/1	0.95	0.06	-1.28	333,333,333,333	0
6	ZN	I	1601	1/1	0.93	0.07	-1.78	666,666,666,666	0
6	ZN	D	2001	1/1	0.98	0.07	-2.17	221,221,221,221	0
7	MG	N	1602	1/1	0.91	0.38	-	182,182,182,182	0
7	MG	D	2002	1/1	0.97	0.17	-	130,130,130,130	0
7	MG	I	1602	1/1	0.94	1.08	-	114,114,114,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.