



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 2, 2017 – 02:16 PM EST

PDB ID : 5TBZ
Title : E. Coli RNA Polymerase complexed with NusG
Authors : Liu, B.; Steitz, T.A.
Deposited on : 2016-09-13
Resolution : 7.00 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

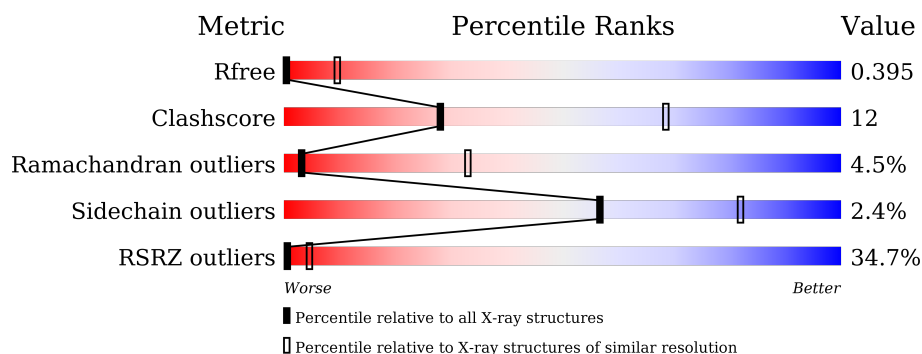
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 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	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	242	<div> <div>26%</div> <div> <div>73%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	B	242	<div> <div>47%</div> <div> <div>69%</div> <div>18%</div> <div>• 11%</div> </div> </div>
1	F	242	<div> <div>23%</div> <div> <div>72%</div> <div>20%</div> <div>• 7%</div> </div> </div>
1	G	242	<div> <div>38%</div> <div> <div>71%</div> <div>17%</div> <div>• 11%</div> </div> </div>
2	C	1342	<div> <div>32%</div> <div> <div>77%</div> <div>20%</div> <div>••</div> </div> </div>
2	H	1342	<div> <div>34%</div> <div> <div>75%</div> <div>21%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div></div><div>29%63%26%•7%</div></div>
3	I	1407	<div><div></div><div>35%64%25%•7%</div></div>
4	J	181	<div><div></div><div>27%61%18%•19%</div></div>
4	K	181	<div><div></div><div>33%56%22%••19%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50147 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	225	Total	C	N	O	S	0	0	0
			1740	1082	309	343	6			
1	B	215	Total	C	N	O	S	0	0	0
			1657	1034	291	326	6			
1	F	225	Total	C	N	O	S	0	0	0
			1740	1082	309	343	6			
1	G	216	Total	C	N	O	S	0	0	0
			1667	1040	294	327	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP P0A7Z6
A	-5	HIS	-	expression tag	UNP P0A7Z6
A	-4	HIS	-	expression tag	UNP P0A7Z6
A	-3	HIS	-	expression tag	UNP P0A7Z6
A	-2	HIS	-	expression tag	UNP P0A7Z6
A	-1	HIS	-	expression tag	UNP P0A7Z6
A	0	HIS	-	expression tag	UNP P0A7Z6
B	-6	ALA	-	expression tag	UNP P0A7Z6
B	-5	HIS	-	expression tag	UNP P0A7Z6
B	-4	HIS	-	expression tag	UNP P0A7Z6
B	-3	HIS	-	expression tag	UNP P0A7Z6
B	-2	HIS	-	expression tag	UNP P0A7Z6
B	-1	HIS	-	expression tag	UNP P0A7Z6
B	0	HIS	-	expression tag	UNP P0A7Z6
F	-6	ALA	-	expression tag	UNP P0A7Z6
F	-5	HIS	-	expression tag	UNP P0A7Z6
F	-4	HIS	-	expression tag	UNP P0A7Z6
F	-3	HIS	-	expression tag	UNP P0A7Z6
F	-2	HIS	-	expression tag	UNP P0A7Z6
F	-1	HIS	-	expression tag	UNP P0A7Z6
F	0	HIS	-	expression tag	UNP P0A7Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	ALA	-	expression tag	UNP P0A7Z6
G	-5	HIS	-	expression tag	UNP P0A7Z6
G	-4	HIS	-	expression tag	UNP P0A7Z6
G	-3	HIS	-	expression tag	UNP P0A7Z6
G	-2	HIS	-	expression tag	UNP P0A7Z6
G	-1	HIS	-	expression tag	UNP P0A7Z6
G	0	HIS	-	expression tag	UNP P0A7Z6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1319	Total	C	N	O	S	0	1	0
			10401	6524	1814	2020	43			
2	H	1319	Total	C	N	O	S	0	1	0
			10401	6524	1814	2020	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1302	Total	C	N	O	S	0	0	0
			10085	6326	1800	1911	48			
3	I	1306	Total	C	N	O	S	0	0	0
			10126	6353	1809	1916	48			

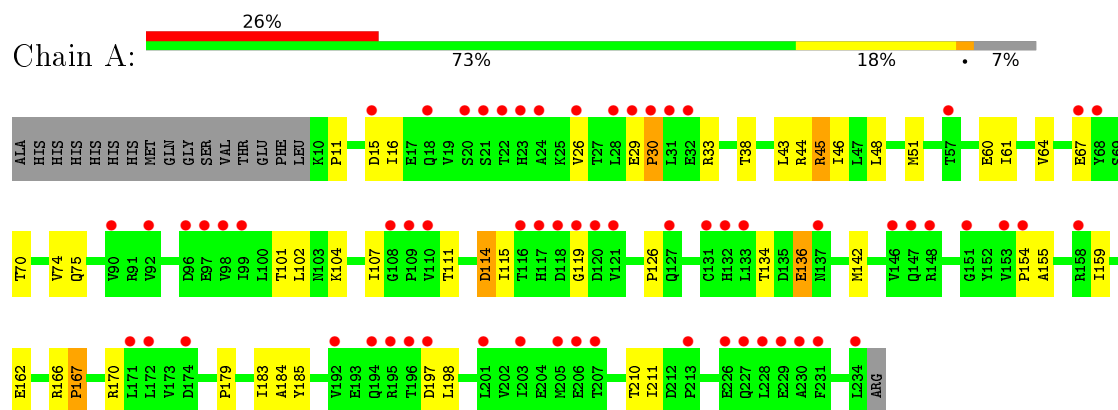
- Molecule 4 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	147	Total	C	N	O	S	0	0	0
			1165	740	201	217	7			
4	K	147	Total	C	N	O	S	0	0	0
			1165	740	201	217	7			

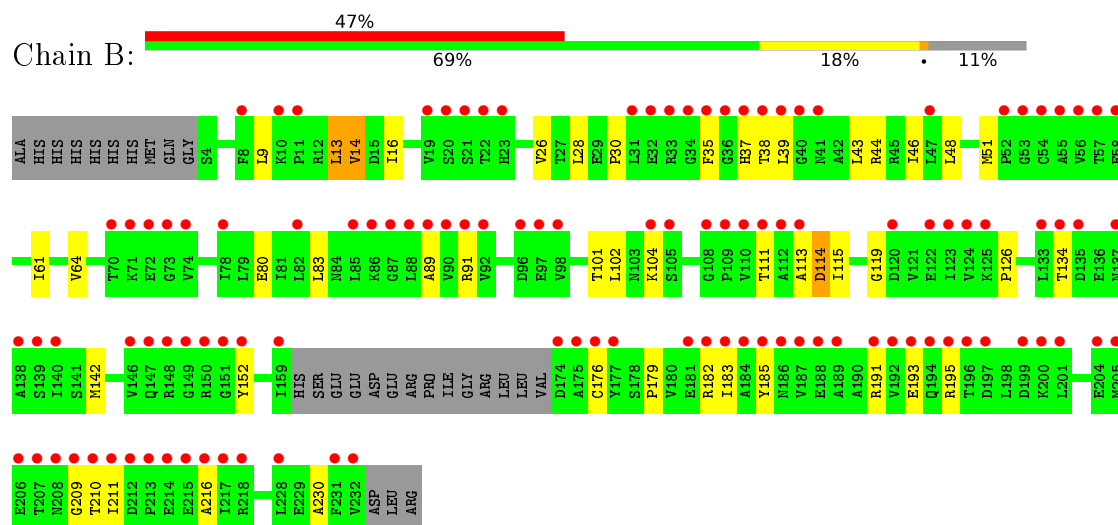
3 Residue-property plots [i](#)

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.

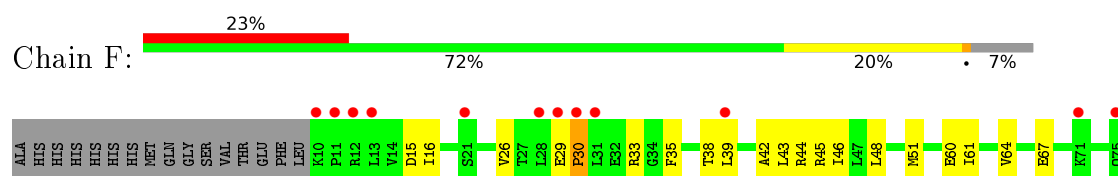
- Molecule 1: DNA-directed RNA polymerase subunit alpha

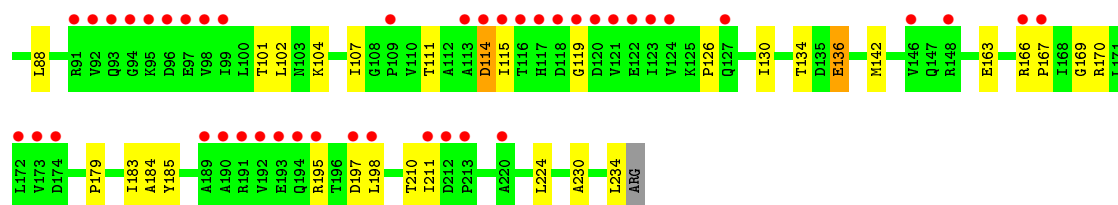


- Molecule 1: DNA-directed RNA polymerase subunit alpha

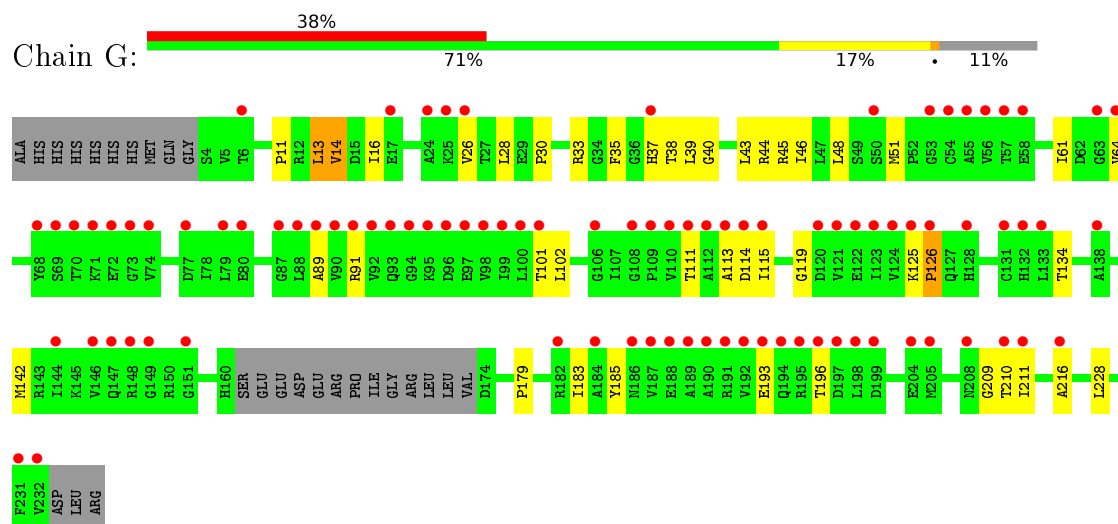


- Molecule 1: DNA-directed RNA polymerase subunit alpha

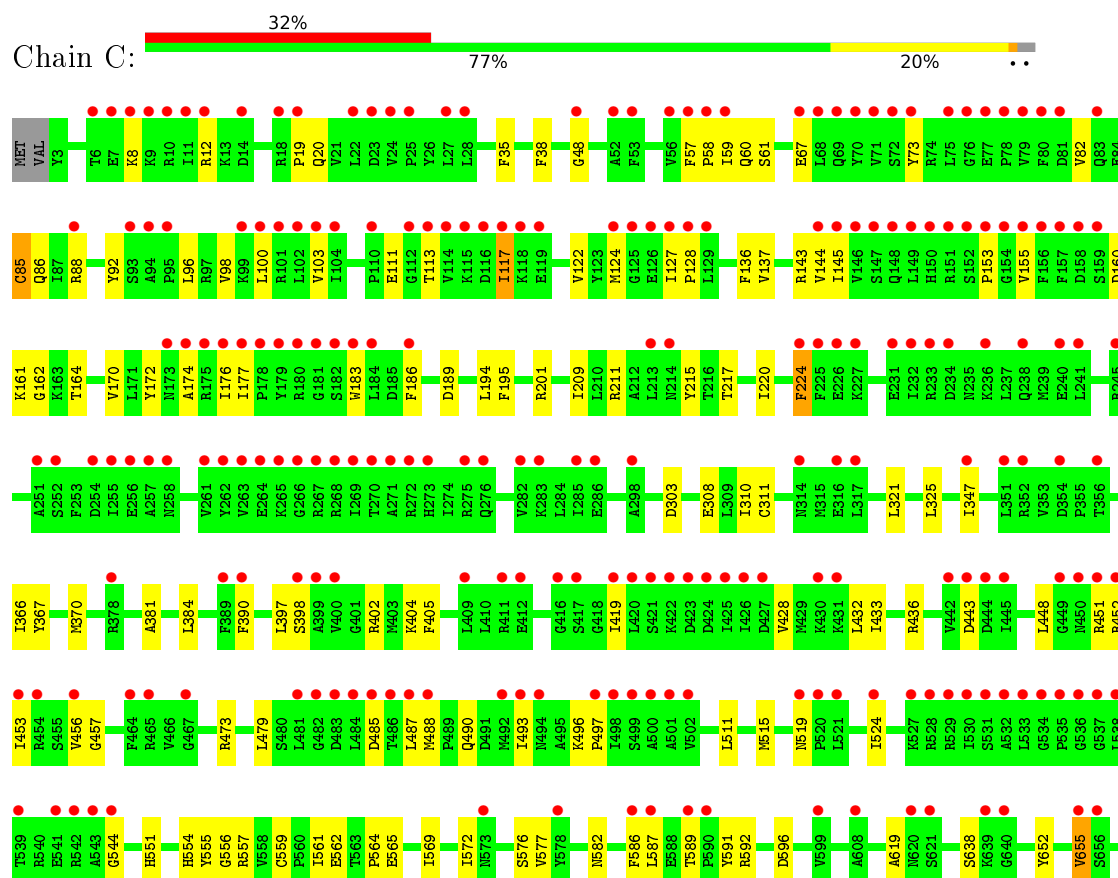


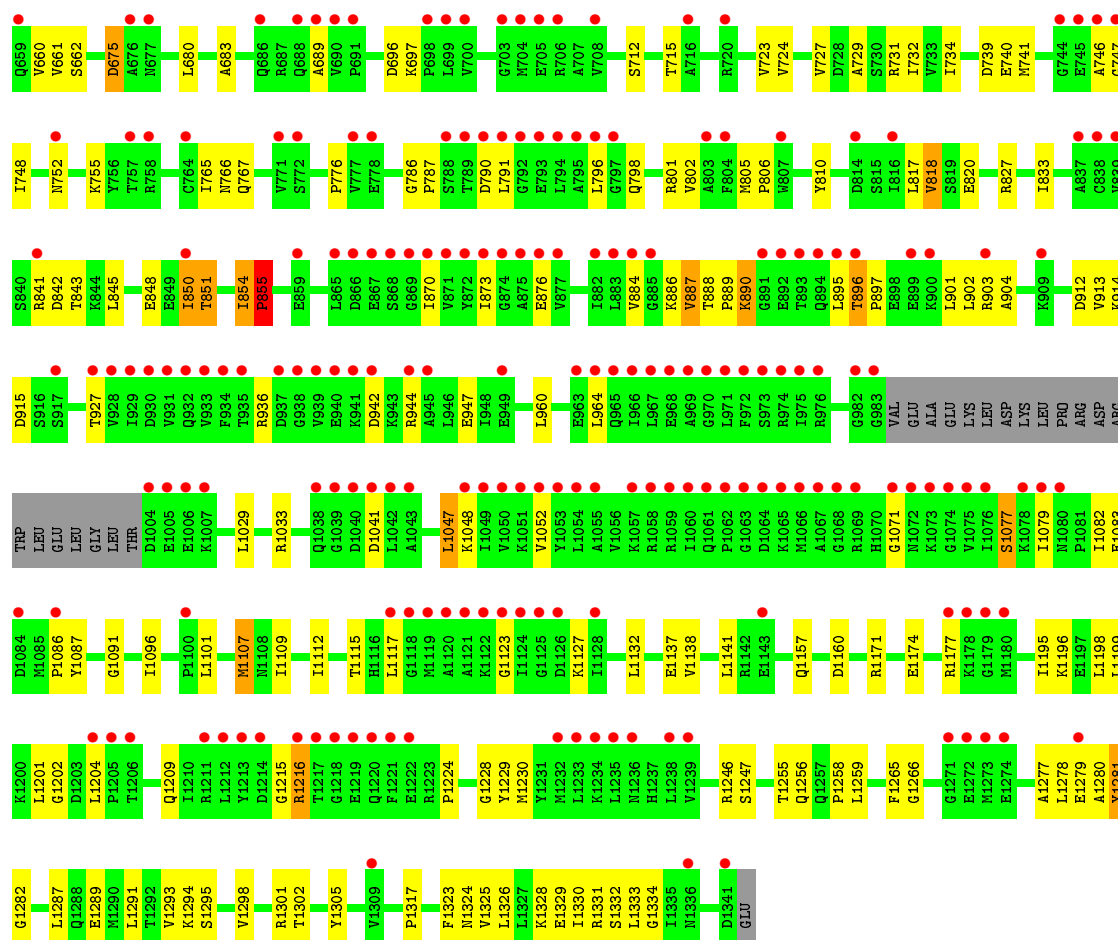


• Molecule 1: DNA-directed RNA polymerase subunit alpha

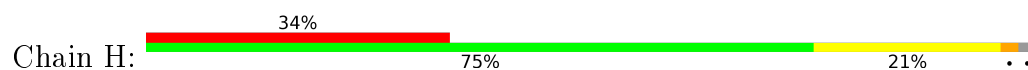


• Molecule 2: DNA-directed RNA polymerase subunit beta

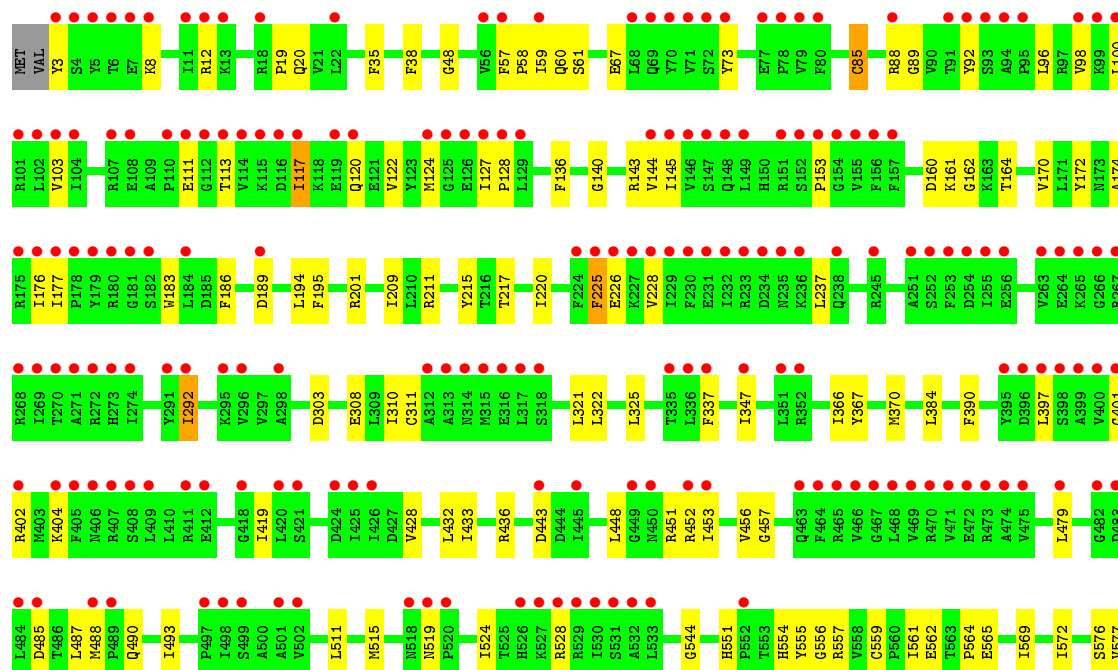


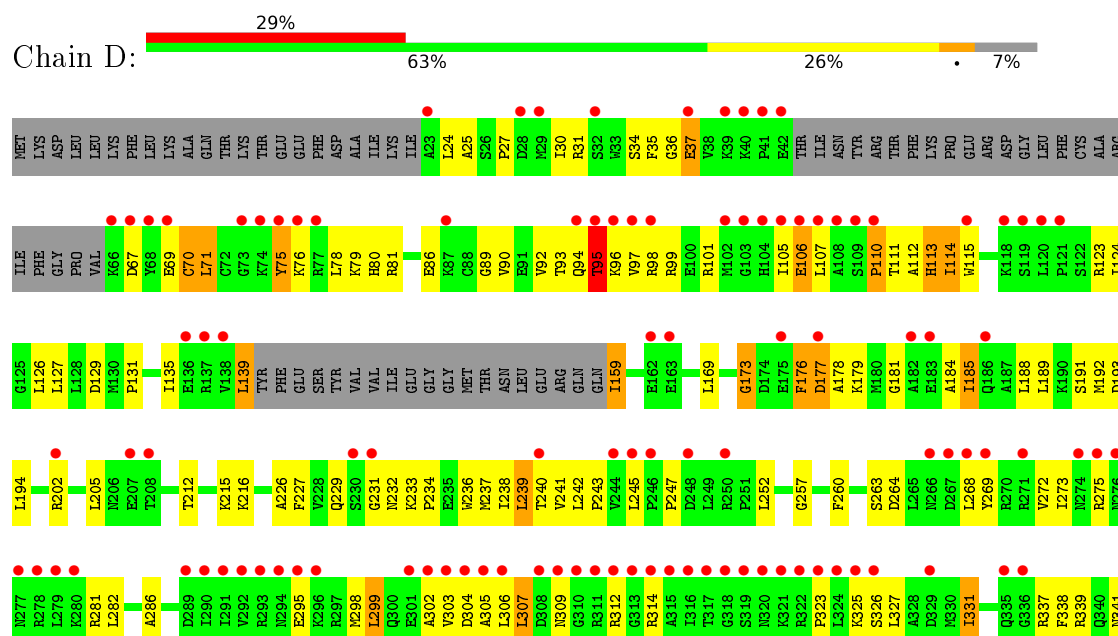


● Molecule 2: DNA-directed RNA polymerase subunit beta

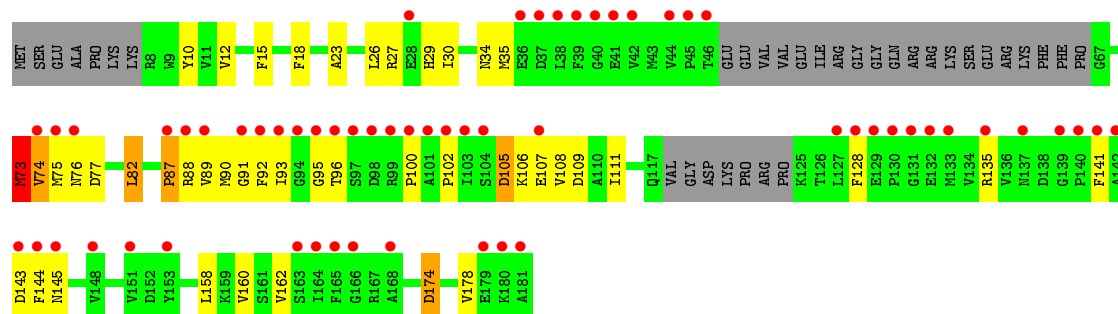


Chain H:





A1157	A1158	V1163	S1164	F1165	G1166	K1167	T1169	K1172	R1173	R1174	L1175	V1176	L1177	T1178	V1179	V1180	D1181	E1187	E1188	M1189	I1190	K1191	K1192	R1193	R1194	Q1195	L1196	M1197	F1198	V1199	E1200	G1201	V1204	S1211	D1212	G1213	P1214	E1215	A1216	P1217	H1218	D1219	L1220	L1221	F1222	L1223	R1224	G1225	V1226	V1229	V1234																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
Q1084	G1085	M1086	D1087	V1088	A1089	I1090	P1091	K1092	T1093	T1094	M1095	P1096	A1097	Q1098	Q1099	Q1100	T1101	L1102	P1103	G1104	A1105	I1106	V1107	Q1108	V1109	I1110	D1111	G1112	V1113	G1118	D1119	T1120	L1121	A1122	R1123	I1124	P1125	Q1126	E1127	L1128	G1129	G1130	T1131	K1132	I1133	I1134	P1139	F1145	R1149	P1150	P1153	A1154	I1155	A1083																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
V997	P998	V999	G1000	A1001	V1002	L1003	A1004	K1005	T1006	D1007	G1008	E1009	Q1010	V1011	A1012	G1013	V1017	A1018	R1019	W1020	P1026	V1027	I1028	T1029	E1030	S1031	F1034	V1035	R1036	F1037	L1038	D1039	M1040	T1045	T1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	S1064	R1067	D1073	L1074	R1075	P1076	A1077	L1078	K1079	I1080	D1081	I1082	A1083																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
L949	K950	D955	L957	V958	P959	R960	T961	L963	L964	H965	E966	D970	L971	M975	S976	V977	D978	A979	V980	K981	V982	V983	V984	V985	V986	V987	V988	V989	V990	V991	V992	V993	V994	V995	V996	V997	V998	V999	V1000	V1001	V1002	V1003	V1004	V1005	V1006	V1007	V1008	V1009	V1010	V1011	V1012	V1013	V1014	V1015	V1016	V1017	V1018	V1019	V1020	V1021	V1022	V1023	V1024	V1025	V1026	V1027	V1028	V1029	V1030	V1031	V1032	V1033	V1034	V1035	V1036	V1037	V1038	V1039	V1040	V1041	V1042	V1043	V1044	V1045	V1046	V1047	V1048	V1049	V1050	V1051	V1052	V1053	V1054	V1055	V1056	V1057	V1058	V1059	V1060	V1061	V1062	V1063	V1064	V1065	V1066	V1067	V1068	V1069	V1070	V1071	V1072	V1073	V1074	V1075	V1076	V1077	V1078	V1079	V1080	V1081	V1082	V1083	V1084	V1085	V1086	V1087	V1088	V1089	V1090	V1091	V1092	V1093	V1094	V1095	V1096	V1097	V1098	V1099	V1100	V1101	V1102	V1103	V1104	V1105	V1106	V1107	V1108	V1109	V1110	V1111	V1112	V1113	V1114	V1115	V1116	V1117	V1118	V1119	V1120	V1121	V1122	V1123	V1124	V1125	V1126	V1127	V1128	V1129	V1130	V1131	V1132	V1133	V1134	V1135	V1136	V1137	V1138	V1139	V1140	V1141	V1142	V1143	V1144	V1145	V1146	V1147	V1148	V1149	V1150	V1151	V1152	V1153	V1154	V1155	V1156	V1157	V1158	V1159	V1160	V1161	V1162	V1163	V1164	V1165	V1166	V1167	V1168	V1169	V1170	V1171	V1172	V1173	V1174	V1175	V1176	V1177	V1178	V1179	V1180	V1181	V1182	V1183	V1184	V1185	V1186	V1187	V1188	V1189	V1190	V1191	V1192	V1193	V1194	V1195	V1196	V1197	V1198	V1199	V1200	V1201	V1202	V1203	V1204	V1205	V1206	V1207	V1208	V1209	V1210	V1211	V1212	V1213	V1214	V1215	V1216	V1217	V1218	V1219	V1220	V1221	V1222	V1223	V1224	V1225	V1226	V1227	V1228	V1229	V1230	V1231	V1232	V1233	V1234	V1235	V1236	V1237	V1238	V1239	V1240	V1241	V1242	V1243	V1244	V1245	V1246	V1247	V1248	V1249	V1250	V1251	V1252	V1253	V1254	V1255	V1256	V1257	V1258	V1259	V1260	V1261	V1262	V1263	V1264	V1265	V1266	V1267	V1268	V1269	V1270	V1271	V1272	V1273	V1274	V1275	V1276	V1277	V1278	V1279	V1280	V1281	V1282	V1283	V1284	V1285	V1286	V1287	V1288	V1289	V1290	V1291	V1292	V1293	V1294	V1295	V1296	V1297	V1298	V1299	V1300	V1301	V1302	V1303	V1304	V1305	V1306	V1307	V1308	V1309	V1310	V1311	V1312	V1313	V1314	V1315	V1316	V1317	V1318	V1319	V1320	V1321	V1322	V1323	V1324	V1325	V1326	V1327	V1328	V1329	V1330	V1331	V1332	V1333	V1334	V1335	V1336	V1337	V1338	V1339	V1340	V1341	V1342	V1343	V1344	V1345	V1346	V1347	V1348	V1349	V1350	V1351	V1352	V1353	V1354	V1355	V1356	V1357	V1358	V1359	V1360	V1361	V1362	V1363	V1364	V1365	V1366	V1367	V1368	V1369	V1370	V1371	V1372	V1373	V1374	V1375	V1376	V1377	V1378	V1379	V1380	V1381	V1382	V1383	V1384	V1385	V1386	V1387	V1388	V1389	V1390	V1391	V1392	V1393	V1394	V1395	V1396	V1397	V1398	V1399	V1400	V1401	V1402	V1403	V1404	V1405	V1406	V1407	V1408	V1409	V1410	V1411	V1412	V1413	V1414	V1415	V1416	V1417	V1418	V1419	V1420	V1421	V1422	V1423	V1424	V1425	V1426	V1427	V1428	V1429	V1430	V1431	V1432	V1433	V1434	V1435	V1436	V1437	V1438	V1439	V1440	V1441	V1442	V1443	V1444	V1445	V1446	V1447	V1448	V1449	V1450	V1451	V1452	V1453	V1454	V1455	V1456	V1457	V1458	V1459	V1460	V1461	V1462	V1463	V1464	V1465	V1466	V1467	V1468	V1469	V1470	V1471	V1472	V1473	V1474	V1475	V1476	V1477	V1478	V1479	V1480	V1481	V1482	V1483	V1484	V1485	V1486	V1487	V1488	V1489	V1490	V1491	V1492	V1493	V1494	V1495	V1496	V1497	V1498	V1499	V1500	V1501	V1502	V1503	V1504	V1505	V1506	V1507	V1508	V1509	V1510	V1511	V1512	V1513	V1514	V1515	V1516	V1517	V1518	V1519	V1520	V1521	V1522	V1523	V1524	V1525	V1526	V1527	V1528	V1529	V1530	V1531	V1532	V1533	V1534	V1535	V1536	V1537	V1538	V1539	V1540	V1541	V1542	V1543	V1544	V1545	V1546	V1547	V1548	V1549	V1550	V1551	V1552	V1553	V1554	V1555	V1556	V1557	V1558	V1559	V1560	V1561	V1562	V1563	V1564	V1565	V1566	V1567	V1568	V1569	V1570	V1571	V1572	V1573	V1574	V1575	V1576	V1577	V1578	V1579	V1580	V1581	V1582	V1583	V1584	V1585	V1586	V1587	V1588	V1589	V1590	V1591	V1592	V1593	V1594	V1595	V1596	V1597	V1598	V1599	V1600	V1601	V1602	V1603	V1604	V1605	V1606	V1607	V1608	V1609	V1610	V1611	V1612	V1613	V1614	V1615	V1616	V1617	V1618	V1619	V1620	V1621	V1622	V1623	V1624	V1625	V1626	V1627	V1628	V1629	V1630	V1631	V1632	V1633	V1634	V1635	V1636	V1637	V1638	V1639	V1640	V1641	V1642	V1643	V1644	V1645	V1646	V1647	V1648	V1649	V1650	V1651	V1652	V1653	V1654	V1655	V1656	V1657	V1658	V1659	V1660	V1661	V1662	V1663	V1664	V1665	V1666	V1667	V1668	V1669	V1670	V1671	V1672	V1673	V1674	V1675	V1676	V1677	V1678	V1679	V1680	V1681	V1682	V1683	V1684	V1685	V1686	V1687	V1688	V1689	V1690	V1691	V1692	V1693	V1694	V1695	V1696	V1697	V1698	V1699	V1700	V1701	V1702	V1703	V1704	V1705	V1706	V1707	V1708	V1709	V1710	V1711	V1712	V1713	V1714	V1715	V1716	V1717	V1718	V1719	V1720	V1721	V1722	V1723	V1724	V1725	V1726	V1727	V1728	V1729	V1730	V1731	V1732	V1733	V1734	V1735	V1736	V1737	V1738	V1739	V1740	V1741	V1742	V1743	V1744	V1745	V1746	V1747	V1748	V1749	V1750	V1751	V1752	V1753	V1754	V1755	V1756	V1757	V1758	V1759	V1760	V1761	V1762	V1763	V1764	V1765	V1766	V1767	V1768	V1769	V1770	V1771	V1772	V1773	V1774	V1775	V1776	V1777	V1778	V1779	V1780	V1781	V1782	V1783	V1784	V1785	V1786	V1787	V1788	V1789	V1790	V1791	V1792	V1793	V1794	V1795	V1796	V1797	V1798	V1799	V1800	V1801	V1802	V1803	V1804	V1805	V1806	V1807	V1808	V1809	V1810	V1811	V1812	V1813	V1814	V1815	V1816	V1817	V1818	V1819	V1820	V1821	V1822	V1823	V1824	V1825	V1826	V1827	V1828	V1829	V1830	V1831	V1832	V1833	V1834	V1835	V1836	V1837	V1838	V1839	V1840	V1841	V1842	V1843	V1844	V1845	V1846	V1847	V1848	V1849	V1850	V1851	V1852	V1853	V1854	V1855	V1856	V1857	V1858	V1859	V1860	V1861	V1862	V1863	V1864	V1865	V1866	V1867	V1868	V1869	V1870	V1871	V1872	V1873	V1874	V1875	V1876	V1877	V1878	V1879	V1880	V1881	V1882	V1883	V1884	V1885	V1886	V1887	V1888	V1889	V1890	V1891	V1892	V1893	V1894	V1895	V1896	V1897	V1898	V1899	V1900	V1901	V1902	V1903	V1904	V1905	V1906	V1907	V1908	V1909	V1910	V1911	V1912	V1913	V1914	V1915	V1916	V1917	V1918	V1919	V1920	V1921	V1922	V1923	V1924	V1925	V1926	V1927	V1928	V1929	V1930	V1931	V1932	V1933	V1934	V1935	V1936	V1937	V1938	V1939	V1940	V1941	V1942	V1943	V1944	V1945	V1946	V1947	V1948	V1949	V1950	V1951	V1952	V1953	V1954	V1955	V1956	V1957	V1958	V1959	V1960	V1961	V1962	V1963	V1964	V1965	V1966	V1967	V1968	V1969	V1970	V1971	V1972	V1973	V1974	V1975	V1976	V1977	V1978	V1979	V1980	V1981	V1982	V1983	V1984	V1985	V1986	V1987	V1988	V1989	V1990	V1991	V1992	V1993	V1994	V1995	V1996	V1997	V1998	V1999	V2000	V2001	V2002	V2003	V2004	V2005	V2006	V2007	V2008	V2009	V2010	V2011	V2012	V2013	V2014	V2015	V2016	V2017	V2018	V2019	V2020	V2021	V2022	V2023	V2024	V2025	V2026	V2027	V2028	V2029	V2030	V2031	V2032	V2033	V2034	V2035	V2036	V2037	V2038	V2039	V2040	V2041	V2042	V2043	V2044	V2045	V2046	V2047	V2048	V2049	V2050	V2051	V2052	V2053	V2054	V2055	V2056	V2057	V2058	V2059	V2060	V2061	V2062	V2063	V2064	V2065	V2066	V2067	V2068	V2069	V2070	V2071	V2072	V2073	V2074	V2075	V2076	V2077	V2078	V2079	V2080	V2081	V2082	V2083	V2084	V2085	V2086	V2087	V2088	V2089	V2090	V2091	V2092	V2093	V2094	V2095	V2096	V2097	V2098	V2099	V2100	V2101	V2102	V2103	V2104	V2105	V2106	V2107	V2108	V2109	V2110	V2111	V2112	V2113	V2114	V2115	V2116	V2117	V2118	V2119	V2120	V2121	V2122	V2123	V2124	V2125	V2126	V2127	V2128	V2129	V2130	V2131	V2132	V2133	V2134	V2135	V2136	V2137	V2138	V2139	V2140	V2141	V2142	V2143	V2144	V2145	V2146	V2147	V2148	V2149	V2150	V2151	V2152	V2153



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	248.16Å 313.78Å 162.79Å 90.00° 130.23° 90.00°	Depositor
Resolution (Å)	162.19 – 7.00 49.91 – 7.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (162.19-7.00) 93.3 (49.91-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 6.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.330 , 0.395 0.330 , 0.395	Depositor DCC
R_{free} test set	707 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	314.0	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 500.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.185 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	50147	wwPDB-VP
Average B, all atoms (Å ²)	330.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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

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	0.45	0/1761	0.72	0/2387
1	B	0.46	0/1676	0.71	0/2271
1	F	0.45	0/1761	0.74	0/2387
1	G	0.47	0/1687	0.70	0/2286
2	C	0.43	0/10569	0.67	0/14258
2	H	0.43	0/10569	0.67	0/14258
3	D	0.44	0/10233	0.76	5/13816 (0.0%)
3	I	0.44	0/10277	0.74	1/13877 (0.0%)
4	J	0.50	0/1188	0.70	0/1603
4	K	0.50	0/1188	0.74	1/1603 (0.1%)
All	All	0.44	0/50909	0.71	7/68746 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
2	H	0	2
3	D	0	1
3	I	0	1
4	K	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1194	ARG	NE-CZ-NH2	-6.82	116.89	120.30
3	D	239	LEU	CA-CB-CG	5.33	127.56	115.30
3	D	173	GLY	N-CA-C	5.30	126.36	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	117	LEU	CA-CB-CG	5.29	127.46	115.30
4	K	73	MET	C-N-CA	5.27	134.87	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	57	PHE	Peptide
2	C	855	PRO	Peptide
3	D	1178	THR	Peptide
2	H	57	PHE	Peptide
2	H	855	PRO	Peptide

5.2 Too-close contacts [i](#)

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	1740	0	1767	40	0
1	B	1657	0	1686	40	0
1	F	1740	0	1767	38	0
1	G	1667	0	1693	35	0
2	C	10401	0	10414	216	0
2	H	10401	0	10414	232	0
3	D	10085	0	10303	380	2
3	I	10126	0	10341	316	0
4	J	1165	0	1145	26	0
4	K	1165	0	1145	30	0
All	All	50147	0	50675	1182	2

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 12.

The worst 5 of 1182 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)
3:I:1001:ALA:HA	3:I:1020:TRP:HE1	1.12	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:29:HIS:HB3	4:K:82:LEU:HG	1.35	1.06
3:D:226:ALA:HB1	3:D:227:PHE:HA	1.31	1.06
3:D:1001:ALA:HA	3:D:1020:TRP:HE1	1.12	1.06
3:D:247:PRO:HB3	3:I:53:ARG:HH12	1.18	1.06

All (2) 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)
3:D:184:ALA:O	3:D:191:SER:OG[2_957]	2.03	0.17
3:D:1183:SER:OG	3:D:1183:SER:OG[2_957]	2.12	0.08

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	223/242 (92%)	182 (82%)	29 (13%)	12 (5%)	2	29
1	B	211/242 (87%)	175 (83%)	27 (13%)	9 (4%)	3	34
1	F	223/242 (92%)	183 (82%)	28 (13%)	12 (5%)	2	29
1	G	212/242 (88%)	177 (84%)	26 (12%)	9 (4%)	3	34
2	C	1316/1342 (98%)	1108 (84%)	172 (13%)	36 (3%)	6	45
2	H	1316/1342 (98%)	1110 (84%)	168 (13%)	38 (3%)	6	43
3	D	1294/1407 (92%)	1023 (79%)	190 (15%)	81 (6%)	2	25
3	I	1300/1407 (92%)	1024 (79%)	197 (15%)	79 (6%)	2	26
4	J	141/181 (78%)	123 (87%)	15 (11%)	3 (2%)	9	50
4	K	141/181 (78%)	117 (83%)	18 (13%)	6 (4%)	3	34
All	All	6377/6828 (93%)	5222 (82%)	870 (14%)	285 (4%)	3	33

5 of 285 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	67	GLU
1	A	114	ASP
1	A	155	ALA
1	B	114	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	193/208 (93%)	191 (99%)	2 (1%)	82	92
1	B	184/208 (88%)	182 (99%)	2 (1%)	80	91
1	F	193/208 (93%)	192 (100%)	1 (0%)	92	96
1	G	185/208 (89%)	183 (99%)	2 (1%)	80	91
2	C	1137/1157 (98%)	1121 (99%)	16 (1%)	74	89
2	H	1137/1157 (98%)	1120 (98%)	17 (2%)	72	88
3	D	1087/1168 (93%)	1048 (96%)	39 (4%)	42	74
3	I	1091/1168 (93%)	1054 (97%)	37 (3%)	44	75
4	J	128/158 (81%)	122 (95%)	6 (5%)	32	68
4	K	128/158 (81%)	121 (94%)	7 (6%)	27	63
All	All	5463/5798 (94%)	5334 (98%)	129 (2%)	57	82

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1347	LEU
2	H	1041	ASP
4	J	109	ASP
1	G	14	VAL
2	H	443	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	777	HIS
1	G	41	ASN
3	I	495	ASN
3	D	1249	ASN
3	D	1366	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	225/242 (92%)	1.34	64 (28%) 1 5	267, 330, 380, 416	0
1	B	215/242 (88%)	2.69	114 (53%) 0 3	266, 335, 388, 430	0
1	F	225/242 (92%)	1.26	55 (24%) 1 6	248, 320, 383, 403	0
1	G	216/242 (89%)	2.10	91 (42%) 0 4	279, 337, 380, 412	0
2	C	1319/1342 (98%)	1.62	431 (32%) 1 5	232, 313, 384, 510	0
2	H	1319/1342 (98%)	1.75	450 (34%) 0 4	231, 315, 383, 482	0
3	D	1302/1407 (92%)	1.65	415 (31%) 1 5	230, 326, 424, 473	0
3	I	1306/1407 (92%)	2.06	498 (38%) 0 4	231, 332, 431, 492	0
4	J	147/181 (81%)	1.64	49 (33%) 0 5	300, 384, 446, 483	0
4	K	147/181 (81%)	2.13	59 (40%) 0 4	324, 413, 469, 491	0
All	All	6421/6828 (94%)	1.78	2226 (34%) 0 4	230, 324, 419, 510	0

The worst 5 of 2226 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	314	ARG	18.1
3	I	989	GLY	17.0
2	H	788	SER	16.3
3	I	315	ALA	15.7
3	D	315	ALA	15.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.