



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2023 – 06:59 AM EDT

PDB ID : 1I6V
Title : THERMUS AQUATICUS CORE RNA POLYMERASE-RIFAMPICIN COMPLEX
Authors : Campbell, E.A.; Korzheva, N.; Mustaev, A.; Murakami, K.; Goldfarb, A.; Darst, S.A.
Deposited on : 2001-03-05
Resolution : 3.30 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

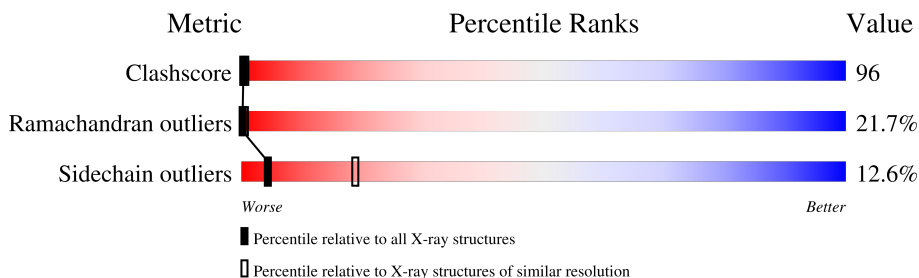
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	12% 40% 15% • 29%
1	B	314	11% 46% 16% • 27%
2	C	1118	14% 60% 24% •
3	D	1264	18% 52% 21% • 7%
4	E	99	19% 62% 18% •

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 21292 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	Total	C	N	O	S	0	0	0
			1741	1109	299	330	3			
1	B	230	Total	C	N	O	S	0	0	0
			1761	1122	299	337	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	VAL	GLY	conflict	UNP Q9KWU8
A	232	SER	LEU	conflict	UNP Q9KWU8
B	112	VAL	GLY	conflict	UNP Q9KWU8
B	232	SER	LEU	conflict	UNP Q9KWU8

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1113	Total	C	N	O	S	12	0	0
			8508	5386	1514	1585	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LYS	GLU	conflict	UNP Q9KWU7
C	?	-	GLU	deletion	UNP Q9KWU7
C	1111	VAL	ILE	conflict	UNP Q9KWU7

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1174	Total	C	N	O	S	17	0	0
			8502	5329	1550	1596	27			

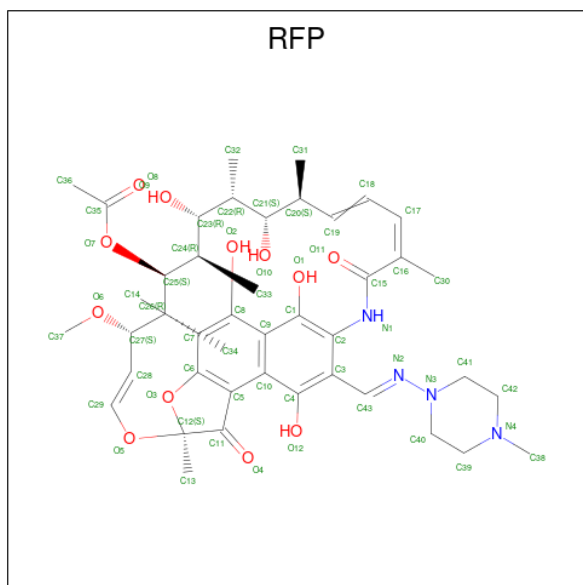
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	ALA	GLY	conflict	UNP Q9KWU6
D	77	ALA	GLY	conflict	UNP Q9KWU6
D	91	ALA	GLY	conflict	UNP Q9KWU6
D	113	ALA	GLY	conflict	UNP Q9KWU6
D	139	ALA	GLY	conflict	UNP Q9KWU6
D	144	ALA	GLY	conflict	UNP Q9KWU6
D	863	THR	VAL	conflict	UNP Q9KWU6
D	866	THR	VAL	conflict	UNP Q9KWU6
D	1009	ASN	LYS	conflict	UNP Q9KWU6

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				S
4	E	98	719	453	132	130	4	0	0	0

- Molecule 5 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	59	43	4	12	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

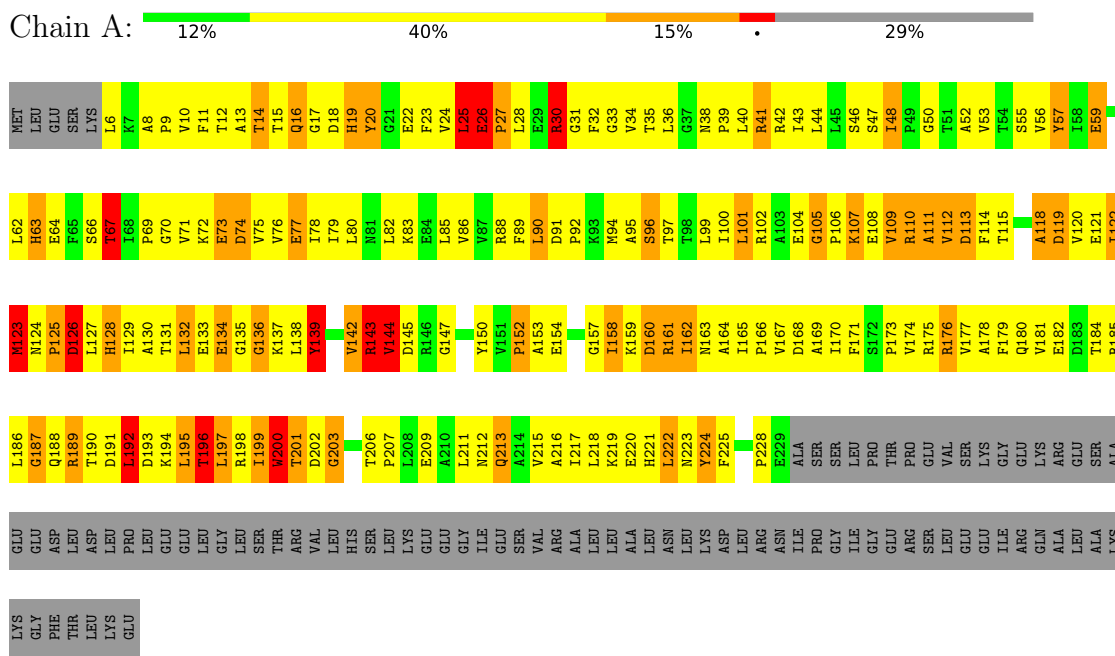
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

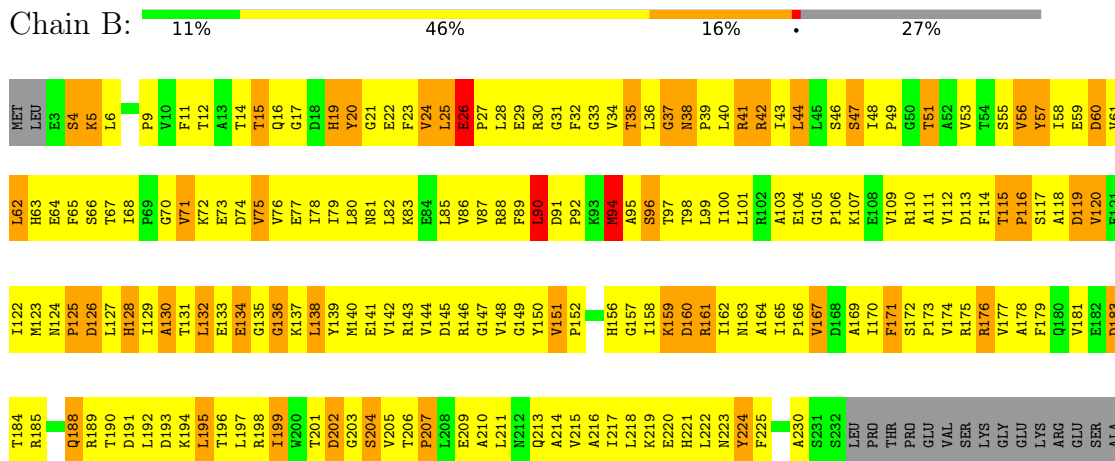
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: DNA-DIRECTED RNA POLYMERASE



• Molecule 1: DNA-DIRECTED RNA POLYMERASE



R805	R806	R807	D810	P811	G812	E814	L815	K816	P817	G818	V819	R820	E821	R822	V823	R824	V825	F826	V827	A828	R831	K832	L833	Q834	V835	G836	D837	K838	L839	A840	N841	R842	H843	G844	N845	K846	G847	V848	A849	A850	K851	I852	L853	P854	V855	E856	D857	M858	P859	H860	L861	A921	F922	G985	N923	L924	T865	V925	F926																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
V867	D868	V869	I870	L871	N872	P873	L874	G875	V876	P877	S878	R879	M880	N881	G883	Q884	L885	L886	E887	T888	H889	L890	G891	L892	A893	G894	F895	F896	L897	E898	Q899	R900	I901	I902	S903	P904	V905	F906	D907	G908	A909	T910	E911	P912	E913	I914	K915	E916	L917	E981	P982	E920	A921	F922	G985	N923	L924	T865	V925	F926																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
G927	K928	R929	Q930	G931	E932	G933	F934	G935	V936	D937	K938	R939	E940	V943	L944	A945	R946	A947	K949	T888	L950	G951	L952	V953	S954	S958	F959	E960	E961	Q962	L963	K964	E965	L966	F967	D968	L969	G970	K971	G972	V973	L974	Y975	D976	G977	K978	T979	G980	E981	P982	E920	A921	F922	G985	N923	L924	T865	V925	F926																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G990	Q991	M992	F993	I994	M995	K996	L997	Y998	H999	M1000	V1001	L1002	E1003	K1004	M1005	H1006	R1008	S1009	T1010	G1011	P1012	Y1013	S1014	L1015	I1016	T1017	Q1018	Q1019	P1020	L1021	G1022	K1023	A1024	A1025	Q1026	F1027	G1028	G1029	Q1030	R1031	F1032	F1033	E1034	M1035	E1036	V1037	W1038	A1039	L1040	E1041	A1042	Y1043	G1044	A1045	T1048	Q1050																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
E1051	M1052	L1053	T1054	K1055	K1056	S1057	D1058	D1059	I1060	E1061	G1062	L1063	A1066	Y1067	Q1068	A1069	I1070	I1071	K1072	G1073	E1074	D1075	V1076	F1077	E1078	P1079	S1080	V1081	P1082	L1083	S1084	F1085	V1087	L1088	V1089	A1090	E1091	L1092	Q1093	A1094	L1095	A1096	L1097	D1098	V1099	Q1100	T1101	L1102	D1103	E1104	K1105	D1106	M1107	P1108	V1109	D1110	V1111																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
F1112	E1113	G1114	L1115	A1116	S1117	L1118	R1119	V1120	A1121	L1122	P1123	F1124	R1125	R1126	R1127	R1128	R1129	R1130	R1131	R1132	R1133	R1134	R1135	R1136	R1137	R1138	R1139	R1140	R1141	R1142	R1143	R1144	R1145	R1146	R1147	R1148	R1149	R1150	R1151	R1152	R1153	R1154	R1155	R1156	R1157	R1158	R1159	R1160	R1161	R1162	R1163	R1164	R1165	R1166	R1167	R1168	R1169	R1170	R1171	R1172	R1173	R1174	R1175	R1176	R1177	R1178	R1179	R1180	R1181	R1182	R1183	R1184	R1185	R1186	R1187	R1188	R1189	R1190	R1191	R1192	R1193	R1194	R1195	R1196	R1197	R1198	R1199	R1200	R1201	R1202	R1203	R1204	R1205	R1206	R1207	R1208	R1209	R1210	R1211	R1212	R1213	R1214	R1215	R1216	R1217	R1218	R1219	R1220	R1221	R1222	R1223	R1224	R1225	R1226	R1227	R1228	R1229	R1230	R1231	R1232	R1233	R1234	R1235	R1236	R1237	R1238	R1239	R1240	R1241	R1242	R1243	R1244	R1245	R1246	R1247	R1248	R1249	R1250	R1251	R1252	R1253	R1254	R1255	R1256	R1257	R1258	R1259	R1260	R1261	R1262	R1263	R1264	R1265	R1266	R1267	R1268	R1269	R1270	R1271	R1272	R1273	R1274	R1275	R1276	R1277	R1278	R1279	R1280	R1281	R1282	R1283	R1284	R1285	R1286	R1287	R1288	R1289	R1290	R1291	R1292	R1293	R1294	R1295	R1296	R1297	R1298	R1299	R1300	R1301	R1302	R1303	R1304	R1305	R1306	R1307	R1308	R1309	R1310	R1311	R1312	R1313	R1314	R1315	R1316	R1317	R1318	R1319	R1320	R1321	R1322	R1323	R1324	R1325	R1326	R1327	R1328	R1329	R1330	R1331	R1332	R1333	R1334	R1335	R1336	R1337	R1338	R1339	R1340	R1341	R1342	R1343	R1344	R1345	R1346	R1347	R1348	R1349	R1350	R1351	R1352	R1353	R1354	R1355	R1356	R1357	R1358	R1359	R1360	R1361	R1362	R1363	R1364	R1365	R1366	R1367	R1368	R1369	R1370	R1371	R1372	R1373	R1374	R1375	R1376	R1377	R1378	R1379	R1380	R1381	R1382	R1383	R1384	R1385	R1386	R1387	R1388	R1389	R1390	R1391	R1392	R1393	R1394	R1395	R1396	R1397	R1398	R1399	R1400	R1401	R1402	R1403	R1404	R1405	R1406	R1407	R1408	R1409	R1410	R1411	R1412	R1413	R1414	R1415	R1416	R1417	R1418	R1419	R1420	R1421	R1422	R1423	R1424	R1425	R1426	R1427	R1428	R1429	R1430	R1431	R1432	R1433	R1434	R1435	R1436	R1437	R1438	R1439	R1440	R1441	R1442	R1443	R1444	R1445	R1446	R1447	R1448	R1449	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460	R1461	R1462	R1463	R1464	R1465	R1466	R1467	R1468	R1469	R1470	R1471	R1472	R1473	R1474	R1475	R1476	R1477	R1478	R1479	R1480	R1481	R1482	R1483	R1484	R1485	R1486	R1487	R1488	R1489	R1490	R1491	R1492	R1493	R1494	R1495	R1496	R1497	R1498	R1499	R1500	R1501	R1502	R1503	R1504	R1505	R1506	R1507	R1508	R1509	R1510	R1511	R1512	R1513	R1514	R1515	R1516	R1517	R1518	R1519	R1520	R1521	R1522	R1523	R1524	R1525	R1526	R1527	R1528	R1529	R1530	R1531	R1532	R1533	R1534	R1535	R1536	R1537	R1538	R1539	R1540	R1541	R1542	R1543	R1544	R1545	R1546	R1547	R1548	R1549	R1550	R1551	R1552	R1553	R1554	R1555	R1556	R1557	R1558	R1559	R1560	R1561	R1562	R1563	R1564	R1565	R1566	R1567	R1568	R1569	R1570	R1571	R1572	R1573	R1574	R1575	R1576	R1577	R1578	R1579	R1580	R1581	R1582	R1583	R1584	R1585	R1586	R1587	R1588	R1589	R1590	R1591	R1592	R1593	R1594	R1595	R1596	R1597	R1598	R1599	R1600	R1601	R1602	R1603	R1604	R1605	R1606	R1607	R1608	R1609	R1610	R1611	R1612	R1613	R1614	R1615	R1616	R1617	R1618	R1619	R1620	R1621	R1622	R1623	R1624	R1625	R1626	R1627	R1628	R1629	R1630	R1631	R1632	R1633	R1634	R1635	R1636	R1637	R1638	R1639	R1640	R1641	R1642	R1643	R1644	R1645	R1646	R1647	R1648	R1649	R1650	R1651	R1652	R1653	R1654	R1655	R1656	R1657	R1658	R1659	R1660	R1661	R1662	R1663	R1664	R1665	R1666	R1667	R1668	R1669	R1670	R1671	R1672	R1673	R1674	R1675	R1676	R1677	R1678	R1679	R1680	R1681	R1682	R1683	R1684	R1685	R1686	R1687	R1688	R1689	R1690	R1691	R1692	R1693	R1694	R1695	R1696	R1697	R1698	R1699	R1700	R1701	R1702	R1703	R1704	R1705	R1706	R1707	R1708	R1709	R1710	R1711	R1712	R1713	R1714	R1715	R1716	R1717	R1718	R1719	R1720	R1721	R1722	R1723	R1724	R1725	R1726	R1727	R1728	R1729	R1730	R1731	R1732	R1733	R1734	R1735	R1736	R1737	R1738	R1739	R1740	R1741	R1742	R1743	R1744	R1745	R1746	R1747	R1748	R1749	R1750	R1751	R1752	R1753	R1754	R1755	R1756	R1757	R1758	R1759	R1760	R1761	R1762	R1763	R1764	R1765	R1766	R1767	R1768	R1769	R1770	R1771	R1772	R1773	R1774	R1775	R1776	R1777	R1778	R1779	R1780	R1781	R1782	R1783	R1784	R1785	R1786	R1787	R1788	R1789	R1790	R1791	R1792	R1793	R1794	R1795	R1796	R1797	R1798	R1799	R1800	R1801	R1802	R1803	R1804	R1805	R1806	R1807	R1808	R1809	R1810	R1811	R1812	R1813	R1814	R1815	R1816	R1817	R1818	R1819	R1820	R1821	R1822	R1823	R1824	R1825	R1826	R1827	R1828	R1829	R1830	R1831	R1832	R1833	R1834	R1835	R1836	R1837	R1838	R1839	R1840	R1841	R1842	R1843	R1844	R1845	R1846	R1847	R1848	R1849	R1850	R1851	R1852	R1853	R1854	R1855	R1856	R1857	R1858	R1859	R1860	R1861	R1862	R1863	R1864	R1865	R1866	R1867	R1868	R1869	R1870	R1871	R1872	R1873	R1874	R1875	R1876	R1877	R1878	R1879	R1880	R1881	R1882	R1883	R1884	R1885	R1886	R1887	R1888	R1889	R1890	R1891	R1892	R1893	R1894	R1895	R1896	R1897	R1898	R1899	R1900	R1901	R1902	R1903	R1904	R1905	R1906	R1907	R1908	R1909	R1910	R1911	R1912	R1913	R1914	R1915	R1916	R1917	R1918	R1919	R1920	R1921	R1922	R1923	R1924	R1925	R1926	R1927	R1928	R1929	R1930	R1931	R1932	R1933	R1934	R1935	R1936	R1937	R1938	R1939	R1940	R1941	R1942	R1943	R1944	R1945	R1946	R1947	R1948	R1949	R1950	R1951	R1952	R1953	R1954	R1955	R1956	R1957	R1958	R1959	R1960	R1961	R1962	R1963	R1964	R1965	R1966	R1967	R1968	R1969	R1970	R1971	R1972	R1973	R1974	R1975	R1976	R1977	R1978	R1979	R1980	R1981	R1982	R1983	R1984	R1985	R1986	R1987	R1988	R1989	R1990	R1991	R1992	R1993	R1994	R1995	R1996	R1997	R1998	R1999	R2000	R2001	R2002	R2003	R2004	R2005	R2006	R2007	R2008	R2009	R2010	R2011	R2012	R2013	R2014	R2015	R2016	R2017	R2018	R2019	R2020	R2021	R2022	R2023	R2024	R2025	R2026	R2027	R2028	R2029	R2030	R2031	R2032	R2033	R2034	R2035	R2036	R2037	R2038	R2039	R2040	R2041	R2042	R2043	R2044	R2045	R2046	R2047	R2048	R2049	R2050	R2051	R2052	R2053	R2054	R2055	R2056	R2057	R2058	R2059	R2060	R2061	R2062	R2063	R2064	R2065	R2066	R2067	R2068	R2069	R2070	R2071	R2072	R2073	R2074	R2075	R2076	R2077	R2078	R2079	R2080	R2081	R2082	R2083	R2084	R2085	R2086	R2087	R2088	R2089	R2090	R2091	R2092	R2093	R2094	R2095	R2096	R2097	R2098	R2099	R2100	R2101	R2102	R2103	R2104	R2105	R2106	R2107	R2108	R2109	R2110	R2111	R2112	R2113	R2114	R2115	R2116	R2117	R2118	R2119	R2120	R2121	R2122	R2123	R2124	R2125	R2126	R2127	R2128	R2129	R2130	R2131	R2132	R2133	R2134	R2135	R2136	R2137	R2138	R2139	R2140	R2141	R2142	R2143	R2144	R2145	R2146	R2147	R2148	R2149	R2150	R2151	R2152	R2153	R2154	R2155	R2156	R2157	R2158	R2159	R2160	R2161	R2162	R2163	R2164	R2165	R2166	R2167	R2168	R2169	R2170	R2171	R2172	R2173	R2174	R2175	R2176	R2177	R2178	R2179	R2180	R2181	R2182	R2183	R2184	R2185	R2186	R2187	R21

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	199.45Å 199.45Å 289.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.276 , 0.359	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	21292	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

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: RFP, MG, ZN

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	0.43	0/1775	0.77	1/2417 (0.0%)
1	B	0.42	1/1795 (0.1%)	0.77	1/2447 (0.0%)
2	C	0.41	0/8672	0.80	7/11752 (0.1%)
3	D	0.44	1/8439 (0.0%)	0.84	19/11447 (0.2%)
4	E	0.37	0/730	0.71	0/991
All	All	0.42	2/21411 (0.0%)	0.81	28/29054 (0.1%)

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	A	0	1
2	C	0	1
3	D	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1270	ALA	C-N	-12.09	1.06	1.34
1	B	94	MET	SD-CE	5.75	2.10	1.77

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270	ALA	O-C-N	-19.05	92.23	122.70
3	D	1270	ALA	C-N-CA	13.67	155.87	121.70
3	D	1270	ALA	CA-C-N	12.08	143.77	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	580	MET	N-CA-C	6.98	129.85	111.00
3	D	1166	LEU	CA-CB-CG	6.22	129.61	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
2	C	1013	TYR	Sidechain
3	D	1165	TYR	Sidechain
3	D	1268	PRO	Mainchain
3	D	1270	ALA	Mainchain

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	1741	0	1747	348	0
1	B	1761	0	1754	316	0
2	C	8508	0	8421	1817	0
3	D	8502	0	8002	1671	0
4	E	719	0	685	138	0
5	C	59	0	56	6	0
6	D	1	0	0	0	0
7	D	1	0	0	0	0
All	All	21292	0	20665	4041	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 96.

The worst 5 of 4041 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:MET:CE	1:B:94:MET:SD	2.10	1.39
2:C:690:ILE:HB	2:C:852:ILE:HG22	1.19	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1280:VAL:HG12	3:D:1281:VAL:HG23	1.25	1.16
2:C:491:GLU:HA	2:C:531:PHE:HA	1.29	1.15
3:D:772:PRO:HG3	3:D:778:LEU:HB2	1.28	1.14

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	222/314 (71%)	111 (50%)	61 (28%)	50 (22%)	0	0
1	B	228/314 (73%)	123 (54%)	62 (27%)	43 (19%)	0	1
2	C	1111/1118 (99%)	591 (53%)	277 (25%)	243 (22%)	0	0
3	D	1126/1264 (89%)	588 (52%)	291 (26%)	247 (22%)	0	0
4	E	96/99 (97%)	50 (52%)	24 (25%)	22 (23%)	0	0
All	All	2783/3109 (90%)	1463 (53%)	715 (26%)	605 (22%)	0	0

5 of 605 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	19	HIS
1	A	26	GLU
1	A	59	GLU
1	A	73	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/271 (70%)	161 (85%)	28 (15%)	3	13
1	B	190/271 (70%)	169 (89%)	21 (11%)	6	23
2	C	870/935 (93%)	770 (88%)	100 (12%)	5	22
3	D	782/1035 (76%)	671 (86%)	111 (14%)	3	15
4	E	67/88 (76%)	62 (92%)	5 (8%)	13	39
All	All	2098/2600 (81%)	1833 (87%)	265 (13%)	4	19

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1166	LEU
3	D	1210	SER
4	E	32	ARG
2	C	438	ILE
2	C	433	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	861	GLN
3	D	909	ASN
3	D	1374	GLN
2	C	565	GLN
2	C	545	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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
5	RFP	C	1640	-	63,63,63	1.26	9 (14%)	94,94,94	0.95	4 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	RFP	C	1640	-	-	13/60/85/85	0/5/5/5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1640	RFP	O5-C29	3.47	1.48	1.39
5	C	1640	RFP	O4-C11	3.12	1.27	1.21
5	C	1640	RFP	C5-C10	2.99	1.49	1.43
5	C	1640	RFP	C39-N4	2.98	1.52	1.46
5	C	1640	RFP	C8-C9	2.77	1.51	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1640	RFP	C34-C26-C25	-2.37	107.15	111.40
5	C	1640	RFP	C5-C10-C9	-2.33	115.41	119.66
5	C	1640	RFP	O12-C4-C10	2.16	124.19	119.00
5	C	1640	RFP	C24-C23-C22	2.12	118.97	115.43

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

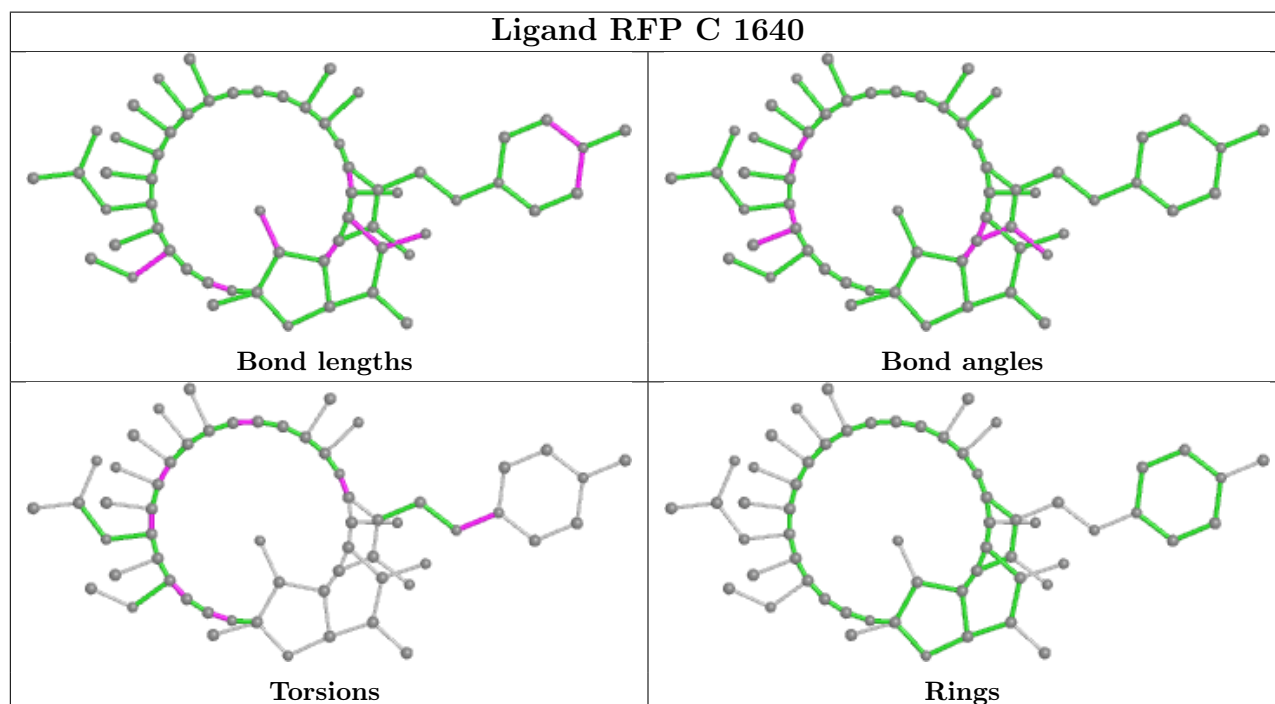
Mol	Chain	Res	Type	Atoms
5	C	1640	RFP	C17-C18-C19-C20
5	C	1640	RFP	C26-C27-C28-C29
5	C	1640	RFP	O6-C27-C28-C29
5	C	1640	RFP	C32-C22-C23-C24
5	C	1640	RFP	C21-C22-C23-C24

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1640	RFP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	155:ASP	C	2(U):UNK	N	54.72
1	D	46(U):UNK	C	452:ILE	N	47.08
1	D	10(U):UNK	C	20(U):UNK	N	15.58
1	D	1270:ALA	C	1271:LYS	N	1.06

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.