



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:46 PM GMT

PDB ID : 3UZE  
Title : Crystal structure of the dengue virus serotype 3 envelope protein domain III in complex with the variable domains of Mab 4E11  
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Deposited on : 2011-12-07  
Resolution : 2.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

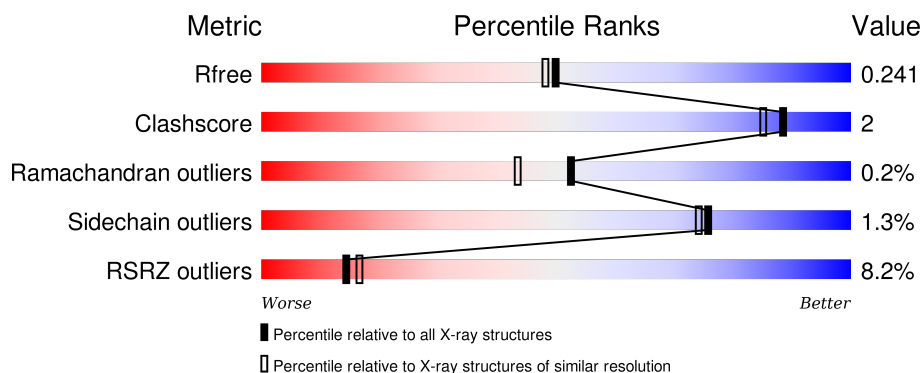
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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  $\geq 3$ , 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	253	<div> <div>2%</div> <div>83%</div> <div>8%</div> <div>9%</div> </div>
1	B	253	<div> <div>3%</div> <div>83%</div> <div>6%</div> <div>11%</div> </div>
2	C	139	<div> <div>9%</div> <div>60%</div> <div>8%</div> <div>32%</div> </div>
2	D	139	<div> <div>19%</div> <div>48%</div> <div>5%</div> <div>47%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	254	-	-	-	X
3	EDO	A	255	-	-	-	X
3	EDO	C	1	-	-	-	X
4	GOL	A	257	-	-	-	X
4	GOL	A	258	-	-	-	X
4	GOL	B	258	-	-	-	X
5	EPE	B	254	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5202 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 Variable domains of murine anti-dengue Mab 4E11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	5	0
			1790	1128	306	347	9			
1	B	226	Total	C	N	O	S	0	4	0
			1759	1111	299	340	9			

- Molecule 2 is a protein called Envelope protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	94	Total	C	N	O	S	0	0	0
			730	470	123	134	3			
2	D	74	Total	C	N	O	S	0	0	0
			581	377	92	109	3			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	396	PRO	-	EXPRESSION TAG	UNP Q7TGD1
C	397	PHE	-	EXPRESSION TAG	UNP Q7TGD1
C	398	GLU	-	EXPRESSION TAG	UNP Q7TGD1
C	399	ASP	-	EXPRESSION TAG	UNP Q7TGD1
C	400	ASP	-	EXPRESSION TAG	UNP Q7TGD1
C	401	ASP	-	EXPRESSION TAG	UNP Q7TGD1
C	402	ASP	-	EXPRESSION TAG	UNP Q7TGD1
C	403	LYS	-	EXPRESSION TAG	UNP Q7TGD1
C	404	ALA	-	EXPRESSION TAG	UNP Q7TGD1
C	405	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	406	TRP	-	EXPRESSION TAG	UNP Q7TGD1
C	407	SER	-	EXPRESSION TAG	UNP Q7TGD1
C	408	HIS	-	EXPRESSION TAG	UNP Q7TGD1
C	409	PRO	-	EXPRESSION TAG	UNP Q7TGD1
C	410	GLN	-	EXPRESSION TAG	UNP Q7TGD1
C	411	PHE	-	EXPRESSION TAG	UNP Q7TGD1

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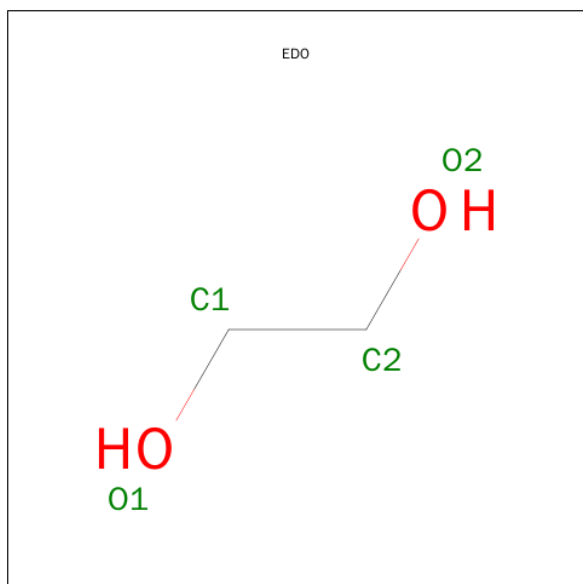
Chain	Residue	Modelled	Actual	Comment	Reference
C	412	GLU	-	EXPRESSION TAG	UNP Q7TGD1
C	413	LYS	-	EXPRESSION TAG	UNP Q7TGD1
C	414	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	415	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	416	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	417	SER	-	EXPRESSION TAG	UNP Q7TGD1
C	418	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	419	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	420	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	421	SER	-	EXPRESSION TAG	UNP Q7TGD1
C	422	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	423	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	424	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	425	SER	-	EXPRESSION TAG	UNP Q7TGD1
C	426	TRP	-	EXPRESSION TAG	UNP Q7TGD1
C	427	SER	-	EXPRESSION TAG	UNP Q7TGD1
C	428	HIS	-	EXPRESSION TAG	UNP Q7TGD1
C	429	PRO	-	EXPRESSION TAG	UNP Q7TGD1
C	430	GLN	-	EXPRESSION TAG	UNP Q7TGD1
C	431	PHE	-	EXPRESSION TAG	UNP Q7TGD1
C	432	GLU	-	EXPRESSION TAG	UNP Q7TGD1
C	433	LYS	-	EXPRESSION TAG	UNP Q7TGD1
D	396	PRO	-	EXPRESSION TAG	UNP Q7TGD1
D	397	PHE	-	EXPRESSION TAG	UNP Q7TGD1
D	398	GLU	-	EXPRESSION TAG	UNP Q7TGD1
D	399	ASP	-	EXPRESSION TAG	UNP Q7TGD1
D	400	ASP	-	EXPRESSION TAG	UNP Q7TGD1
D	401	ASP	-	EXPRESSION TAG	UNP Q7TGD1
D	402	ASP	-	EXPRESSION TAG	UNP Q7TGD1
D	403	LYS	-	EXPRESSION TAG	UNP Q7TGD1
D	404	ALA	-	EXPRESSION TAG	UNP Q7TGD1
D	405	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	406	TRP	-	EXPRESSION TAG	UNP Q7TGD1
D	407	SER	-	EXPRESSION TAG	UNP Q7TGD1
D	408	HIS	-	EXPRESSION TAG	UNP Q7TGD1
D	409	PRO	-	EXPRESSION TAG	UNP Q7TGD1
D	410	GLN	-	EXPRESSION TAG	UNP Q7TGD1
D	411	PHE	-	EXPRESSION TAG	UNP Q7TGD1
D	412	GLU	-	EXPRESSION TAG	UNP Q7TGD1
D	413	LYS	-	EXPRESSION TAG	UNP Q7TGD1
D	414	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	415	GLY	-	EXPRESSION TAG	UNP Q7TGD1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	416	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	417	SER	-	EXPRESSION TAG	UNP Q7TGD1
D	418	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	419	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	420	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	421	SER	-	EXPRESSION TAG	UNP Q7TGD1
D	422	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	423	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	424	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	425	SER	-	EXPRESSION TAG	UNP Q7TGD1
D	426	TRP	-	EXPRESSION TAG	UNP Q7TGD1
D	427	SER	-	EXPRESSION TAG	UNP Q7TGD1
D	428	HIS	-	EXPRESSION TAG	UNP Q7TGD1
D	429	PRO	-	EXPRESSION TAG	UNP Q7TGD1
D	430	GLN	-	EXPRESSION TAG	UNP Q7TGD1
D	431	PHE	-	EXPRESSION TAG	UNP Q7TGD1
D	432	GLU	-	EXPRESSION TAG	UNP Q7TGD1
D	433	LYS	-	EXPRESSION TAG	UNP Q7TGD1

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



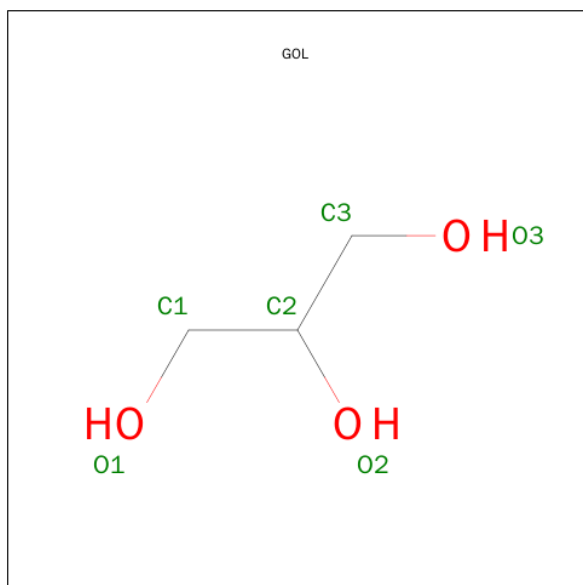
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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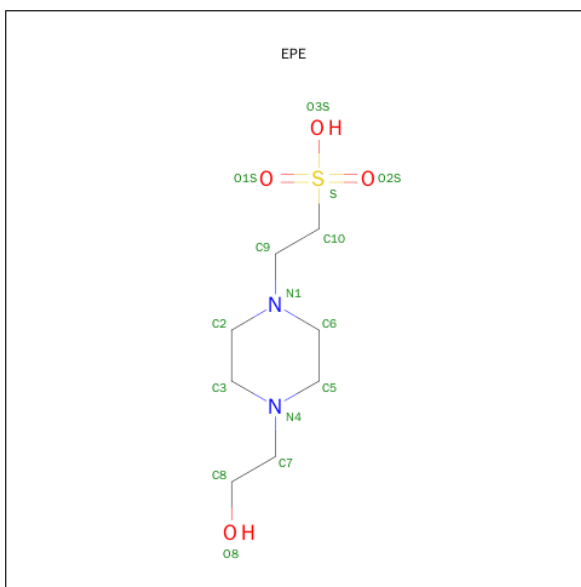
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

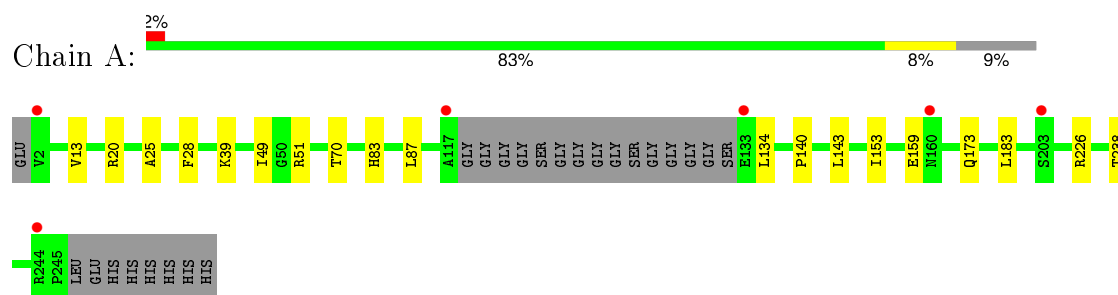
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	144	Total	O	0	0
			144	144		
6	B	90	Total	O	0	0
			90	90		
6	C	35	Total	O	0	0
			35	35		
6	D	8	Total	O	0	0
			8	8		



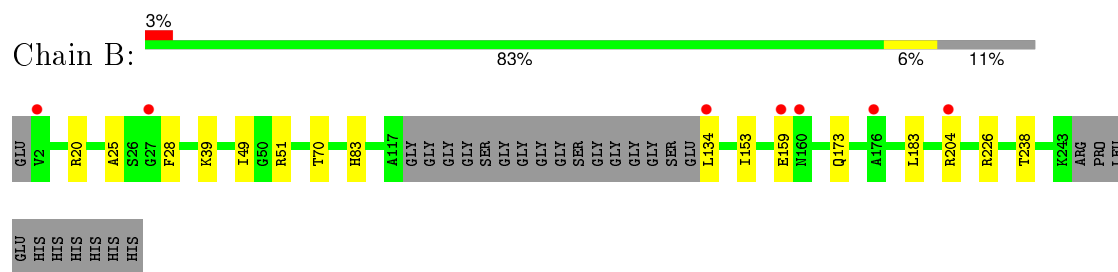
### 3 Residue-property plots [i](#)

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.

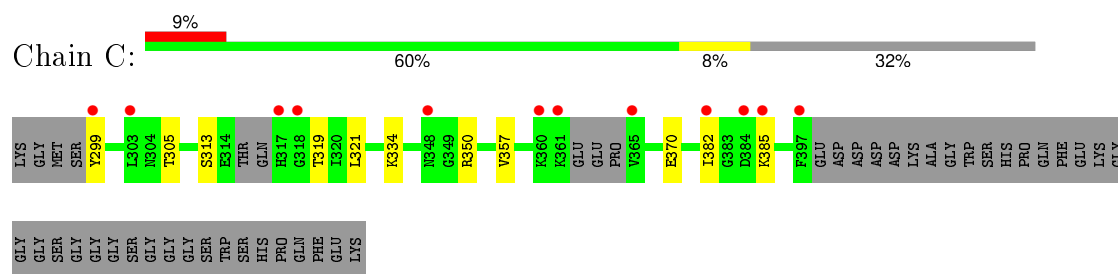
- Molecule 1: Variable domains of murine anti-dengue Mab 4E11



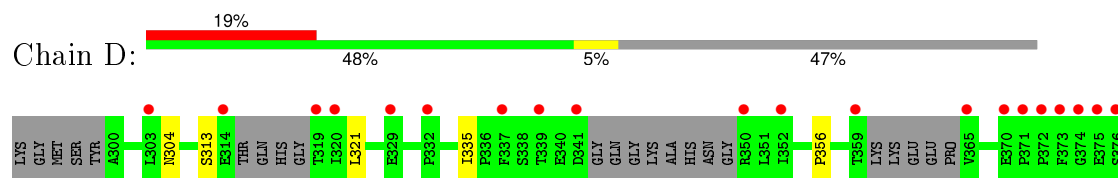
- Molecule 1: Variable domains of murine anti-dengue Mab 4E11



- Molecule 2: Envelope protein



- Molecule 2: Envelope protein



1377	1378	1379	1380	1381	1382	1383	1384	1385	1386	1387	1388	1389	1390	1391	1392	1393	1394	1395	1396	1397	1398	1399	1400	1401	1402	1403	1404	1405	1406	1407	1408	1409	1410	1411	1412	1413	1414	1415	1416	1417	1418	1419	1420	1421	1422	1423	1424	1425	1426	1427	1428	1429	1430	1431	1432	1433	1434	1435	1436	1437	1438	1439	1440	1441	1442	1443	1444	1445	1446	1447	1448	1449	1450	1451	1452	1453	1454	1455	1456	1457	1458	1459	1460	1461	1462	1463	1464	1465	1466	1467	1468	1469	1470	1471	1472	1473	1474	1475	1476	1477	1478	1479	1480	1481	1482	1483	1484	1485	1486	1487	1488	1489	1490	1491	1492	1493	1494	1495	1496	1497	1498	1499	1500	1501	1502	1503	1504	1505	1506	1507	1508	1509	1510	1511	1512	1513	1514	1515	1516	1517	1518	1519	1520	1521	1522	1523	1524	1525	1526	1527	1528	1529	1530	1531	1532	1533	1534	1535	1536	1537	1538	1539	1540	1541	1542	1543	1544	1545	1546	1547	1548	1549	1550	1551	1552	1553	1554	1555	1556	1557	1558	1559	1560	1561	1562	1563	1564	1565	1566	1567	1568	1569	1570	1571	1572	1573	1574	1575	1576	1577	1578	1579	1580	1581	1582	1583	1584	1585	1586	1587	1588	1589	1590	1591	1592	1593	1594	1595	1596	1597	1598	1599	1600	1601	1602	1603	1604	1605	1606	1607	1608	1609	1610	1611	1612	1613	1614	1615	1616	1617	1618	1619	1620	1621	1622	1623	1624	1625	1626	1627	1628	1629	1630	1631	1632	1633	1634	1635	1636	1637	1638	1639	1640	1641	1642	1643	1644	1645	1646	1647	1648	1649	1650	1651	1652	1653	1654	1655	1656	1657	1658	1659	1660	1661	1662	1663	1664	1665	1666	1667	1668	1669	1670	1671	1672	1673	1674	1675	1676	1677	1678	1679	1680	1681	1682	1683	1684	1685	1686	1687	1688	1689	1690	1691	1692	1693	1694	1695	1696	1697	1698	1699	1700	1701	1702	1703	1704	1705	1706	1707	1708	1709	1710	1711	1712	1713	1714	1715	1716	1717	1718	1719	1720	1721	1722	1723	1724	1725	1726	1727	1728	1729	1730	1731	1732	1733	1734	1735	1736	1737	1738	1739	1740	1741	1742	1743	1744	1745	1746	1747	1748	1749	1750	1751	1752	1753	1754	1755	1756	1757	1758	1759	1760	1761	1762	1763	1764	1765	1766	1767	1768	1769	1770	1771	1772	1773	1774	1775	1776	1777	1778	1779	1780	1781	1782	1783	1784	1785	1786	1787	1788	1789	1790	1791	1792	1793	1794	1795	1796	1797	1798	1799	1800	1801	1802	1803	1804	1805	1806	1807	1808	1809	1810	1811	1812	1813	1814	1815	1816	1817	1818	1819	1820	1821	1822	1823	1824	1825	1826	1827	1828	1829	1830	1831	1832	1833	1834	1835	1836	1837	1838	1839	1840	1841	1842	1843	1844	1845	1846	1847	1848	1849	1850	1851	1852	1853	1854	1855	1856	1857	1858	1859	1860	1861	1862	1863	1864	1865	1866	1867	1868	1869	1870	1871	1872	1873	1874	1875	1876	1877	1878	1879	1880	1881	1882	1883	1884	1885	1886	1887	1888	1889	1890	1891	1892	1893	1894	1895	1896	1897	1898	1899	1900	1901	1902	1903	1904	1905	1906	1907	1908	1909	1910	1911	1912	1913	1914	1915	1916	1917	1918	1919	1920	1921	1922	1923	1924	1925	1926	1927	1928	1929	1930	1931	1932	1933	1934	1935	1936	1937	1938	1939	1940	1941	1942	1943	1944	1945	1946	1947	1948	1949	1950	1951	1952	1953	1954	1955	1956	1957	1958	1959	1960	1961	1962	1963	1964	1965	1966	1967	1968	1969	1970	1971	1972	1973	1974	1975	1976	1977	1978	1979	1980	1981	1982	1983	1984	1985	1986	1987	1988	1989	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035	2036	2037	2038	2039	2040	2041	2042	2043	2044	2045	2046	2047	2048	2049	2050	2051	2052	2053	2054	2055	2056	2057	2058	2059	2060	2061	2062	2063	2064	2065	2066	2067	2068	2069	2070	2071	2072	2073	2074	2075	2076	2077	2078	2079	2080	2081	2082	2083	2084	2085	2086	2087	2088	2089	2090	2091	2092	2093	2094	2095	2096	2097	2098	2099	2100	2101	2102	2103	2104	2105	2106	2107	2108	2109	2110	2111	2112	2113	2114	2115	2116	2117	2118	2119	2120	2121	2122	2123	2124	2125	2126	2127	2128	2129	2130	2131	2132	2133	2134	2135	2136	2137	2138	2139	2140	2141	2142	2143	2144	2145	2146	2147	2148	2149	2150	2151	2152	2153	2154	2155	2156	2157	2158	2159	2160	2161	2162	2163	2164	2165	2166	2167	2168	2169	2170	2171	2172	2173	2174	2175	2176	2177	2178	2179	2180	2181	2182	2183	2184	2185	2186	2187	2188	2189	2190	2191	2192	2193	2194	2195	2196	2197	2198	2199	2200	2201	2202	2203	2204	2205	2206	2207	2208	2209	2210	2211	2212	2213	2214	2215	2216	2217	2218	2219	2220	2221	2222	2223	2224	2225	2226	2227	2228	2229	2230	2231	2232	2233	2234	2235	2236	2237	2238	2239	2240	2241	2242	2243	2244	2245	2246	2247	2248	2249	2250	2251	2252	2253	2254	2255	2256	2257	2258	2259	2260	2261	2262	2263	2264	2265	2266	2267	2268	2269	2270	2271	2272	2273	2274	2275	2276	2277	2278	2279	2280	2281	2282	2283	2284	2285	2286	2287	2288	2289	2290	2291	2292	2293	2294	2295	2296	2297	2298	2299	2300	2301	2302	2303	2304	2305	2306	2307	2308	2309	2310	2311	2312	2313	2314	2315	2316	2317	2318	2319	2320	2321	2322	2323	2324	2325	2326	2327	2328	2329	2330	2331	2332	2333	2334	2335	2336	2337	2338	2339	2340	2341	2342	2343	2344	2345	2346	2347	2348	2349	2350	2351	2352	2353	2354	2355	2356	2357	2358	2359	2360	2361	2362	2363	2364	2365	2366	2367	2368	2369	2370	2371	2372	2373	2374	2375	2376	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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.05Å 74.67Å 86.89Å 90.00° 104.49° 90.00°	Depositor
Resolution (Å)	40.80 – 2.04 42.06 – 2.04	Depositor EDS
% Data completeness (in resolution range)	94.6 (40.80-2.04) 94.5 (42.06-2.04)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.03Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, $R_{free}$	0.218 , 0.234 0.224 , 0.241	Depositor DCC
$R_{free}$ test set	1981 reflections (5.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 40584 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, EPE, EDO

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	0.35	0/1846	0.60	0/2504
1	B	0.35	0/1811	0.59	0/2457
2	C	0.35	0/744	0.58	0/1001
2	D	0.35	0/588	0.53	0/793
All	All	0.35	0/4989	0.58	0/6755

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1790	0	1746	9	0
1	B	1759	0	1718	7	0
2	C	730	0	740	5	0
2	D	581	0	593	3	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	4	0	6	0	0
4	A	18	0	24	1	0
4	B	12	0	16	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	15	0	18	0	0
6	A	144	0	0	0	0
6	B	90	0	0	0	0
6	C	35	0	0	0	0
6	D	8	0	0	0	0
All	All	5202	0	4885	24	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 2.

All (24) 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:A:134:LEU:HD12	1:A:159:GLU:HB2	1.80	0.62
1:B:134:LEU:HD12	1:B:159:GLU:HB2	1.81	0.61
4:A:258:GOL:H31	1:B:20:ARG:HB2	1.84	0.59
1:B:173:GLN:HB2	1:B:183:LEU:HD11	1.91	0.52
2:C:319:THR:HG22	2:C:370:GLU:HB3	1.92	0.51
1:A:70:THR:HB	1:A:83:HIS:HB2	1.93	0.51
1:A:153:ILE:HG12	1:A:238:THR:HG21	1.93	0.50
2:C:305:THR:HB	2:C:385:LYS:HB3	1.96	0.47
1:A:20:ARG:HB2	4:B:258:GOL:H11	1.96	0.47
1:B:153:ILE:HG12	1:B:238:THR:HG21	1.97	0.46
2:C:334:LYS:HA	2:C:357:VAL:HG12	1.96	0.46
2:D:379:VAL:HG22	2:D:388:LYS:HG2	1.96	0.46
1:B:39:LYS:HB2	1:B:49:ILE:HD11	1.97	0.46
1:A:173:GLN:HB2	1:A:183:LEU:HD11	1.98	0.45
1:A:13:VAL:HG21	1:A:87:LEU:HD13	1.99	0.44
2:D:313:SER:HB2	2:D:321:LEU:HB2	2.00	0.43
1:A:25:ALA:HB1	1:A:28:PHE:CE2	2.54	0.43
1:B:25:ALA:HB1	1:B:28:PHE:CE2	2.53	0.43
2:D:335:ILE:HB	2:D:356:PRO:HB2	2.01	0.43
1:B:70:THR:HB	1:B:83:HIS:HB2	2.01	0.43
2:C:313:SER:HB2	2:C:321:LEU:HB2	2.02	0.41
1:A:39:LYS:HB2	1:A:49:ILE:HD11	2.03	0.41
2:C:350:ARG:HB3	2:C:370:GLU:CG	2.52	0.40
1:A:140:PRO:HG2	1:A:143:LEU:HB2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/253 (91%)	224 (97%)	6 (3%)	0	100	100
1	B	226/253 (89%)	219 (97%)	6 (3%)	1 (0%)	39	28
2	C	88/139 (63%)	86 (98%)	2 (2%)	0	100	100
2	D	64/139 (46%)	63 (98%)	1 (2%)	0	100	100
All	All	608/784 (78%)	592 (97%)	15 (2%)	1 (0%)	52	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	ARG

### 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	194/201 (96%)	192 (99%)	2 (1%)	82	81
1	B	190/201 (94%)	188 (99%)	2 (1%)	80	79
2	C	79/112 (70%)	77 (98%)	2 (2%)	55	48
2	D	66/112 (59%)	65 (98%)	1 (2%)	72	70
All	All	529/626 (84%)	522 (99%)	7 (1%)	76	74

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	226	ARG
1	B	51	ARG
1	B	226	ARG
2	C	299	TYR
2	C	382	ILE
2	D	304	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	EDO	A	254	-	3,3,3	0.48	0	2,2,2	0.38	0
3	EDO	A	255	-	3,3,3	0.49	0	2,2,2	0.32	0
4	GOL	A	256	-	5,5,5	0.34	0	5,5,5	0.23	0
4	GOL	A	257	-	5,5,5	0.30	0	5,5,5	0.59	0
4	GOL	A	258	-	5,5,5	0.37	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EPE	B	254	-	14,15,15	0.86	0	18,20,20	2.71	8 (44%)
4	GOL	B	255	-	5,5,5	0.24	0	5,5,5	0.35	0
3	EDO	B	256	-	3,3,3	0.47	0	2,2,2	0.43	0
3	EDO	B	257	-	3,3,3	0.45	0	2,2,2	0.46	0
4	GOL	B	258	-	5,5,5	0.28	0	5,5,5	0.25	0
3	EDO	C	1	-	3,3,3	0.48	0	2,2,2	0.39	0

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
3	EDO	A	254	-	-	0/1/1/1	0/0/0/0
3	EDO	A	255	-	-	0/1/1/1	0/0/0/0
4	GOL	A	256	-	-	0/4/4/4	0/0/0/0
4	GOL	A	257	-	-	0/4/4/4	0/0/0/0
4	GOL	A	258	-	-	0/4/4/4	0/0/0/0
5	EPE	B	254	-	-	0/9/19/19	0/1/1/1
4	GOL	B	255	-	-	0/4/4/4	0/0/0/0
3	EDO	B	256	-	-	0/1/1/1	0/0/0/0
3	EDO	B	257	-	-	0/1/1/1	0/0/0/0
4	GOL	B	258	-	-	0/4/4/4	0/0/0/0
3	EDO	C	1	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	254	EPE	O3S-S-O2S	-3.94	102.45	111.61
5	B	254	EPE	O3S-S-O1S	-3.17	104.22	111.61
5	B	254	EPE	C9-N1-C2	-2.79	104.12	111.27
5	B	254	EPE	C6-C5-N4	2.09	114.37	110.63
5	B	254	EPE	O2S-S-O1S	2.27	121.74	113.48
5	B	254	EPE	C3-C2-N1	2.39	114.91	110.63
5	B	254	EPE	O2S-S-C10	5.25	111.38	106.91
5	B	254	EPE	O1S-S-C10	6.33	112.31	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	258	GOL	1	0
4	B	258	GOL	1	0

## 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	229/253 (90%)	0.23	6 (2%) 59 65	16, 26, 46, 78	0
1	B	226/253 (89%)	0.32	7 (3%) 52 60	22, 33, 54, 85	0
2	C	94/139 (67%)	0.64	12 (12%) 5 5	22, 34, 59, 88	0
2	D	74/139 (53%)	2.08	26 (35%) 0 0	39, 61, 88, 105	0
All	All	623/784 (79%)	0.55	51 (8%) 14 16	16, 33, 67, 105	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	303	LEU	11.2
2	C	397	PHE	9.6
2	D	392	TYR	9.1
2	D	374	GLY	6.9
1	A	244	ARG	6.2
2	D	391	TRP	6.1
2	C	317	HIS	6.0
1	B	2	VAL	5.7
2	D	376	SER	5.6
2	C	384	ASP	5.6
2	D	375	GLU	5.1
2	D	373	PHE	4.8
2	D	370	GLU	4.7
1	A	133	GLU	4.4
2	D	372	PRO	4.3
1	A	2	VAL	4.3
2	D	393	ARG	3.9
2	D	350	ARG	3.9
2	D	319	THR	3.9
2	D	332	PRO	3.9
2	C	365	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	134	LEU	3.8
2	D	341	ASP	3.6
1	B	160	ASN	3.6
2	C	385	LYS	3.4
2	D	365	VAL	3.4
2	D	329	GLU	3.3
2	D	382	ILE	3.3
2	C	318	GLY	3.1
2	D	339	THR	3.0
1	A	160	ASN	3.0
1	B	176	ALA	2.9
2	D	377	ASN	2.8
2	D	320	ILE	2.7
1	B	27	GLY	2.7
1	B	204	ARG	2.7
2	C	299	TYR	2.7
2	D	371	PRO	2.7
2	D	359	THR	2.6
1	A	117	ALA	2.6
1	B	159	GLU	2.5
2	D	337	PHE	2.4
2	C	361	LYS	2.4
2	C	382	ILE	2.3
1	A	203	SER	2.2
2	D	314	GLU	2.2
2	C	360	LYS	2.1
2	C	348	ASN	2.1
2	D	352	ILE	2.1
2	D	378	ILE	2.0
2	C	303	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	C	1	4/4	0.77	0.41	16.78	52,54,55,57	0
4	GOL	B	258	6/6	0.52	0.28	11.39	73,74,74,75	0
5	EPE	B	254	15/15	0.90	0.26	5.97	48,50,52,55	0
4	GOL	A	258	6/6	0.63	0.27	5.06	47,48,48,49	0
4	GOL	A	257	6/6	0.88	0.18	4.64	31,33,34,34	0
3	EDO	A	254	4/4	0.74	0.24	4.63	35,37,39,39	0
3	EDO	A	255	4/4	0.67	0.19	2.35	39,40,41,43	0
4	GOL	B	255	6/6	0.91	0.18	1.00	36,36,37,37	0
3	EDO	B	257	4/4	0.91	0.15	0.21	42,44,46,47	0
4	GOL	A	256	6/6	0.73	0.20	-	55,55,55,56	0
3	EDO	B	256	4/4	0.80	0.23	-	66,68,70,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.