



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2024 – 06:12 pm BST

PDB ID : 1EA0  
Title : Alpha subunit of A. brasilense glutamate synthase  
Authors : Binda, C.; Bossi, R.T.; Vanoni, M.A.; Mattevi, A.  
Deposited on : 2000-11-02  
Resolution : 3.00 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](mailto: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>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (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)	:	2.36.2

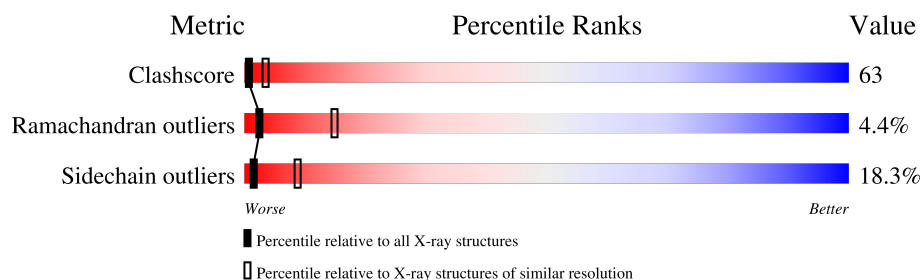
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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  $\geq 3$ , 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	1479	<div> <div>26%</div> <div>50%</div> <div>19%</div> <div>..</div> </div>
1	B	1479	<div> <div>31%</div> <div>47%</div> <div>16%</div> <div>..</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
2	OMT	A	2473	-	X	-	-
2	OMT	B	2473	-	X	-	-
5	F3S	A	2476	-	-	X	-
5	F3S	B	2476	-	-	X	-

## 2 Entry composition [i](#)

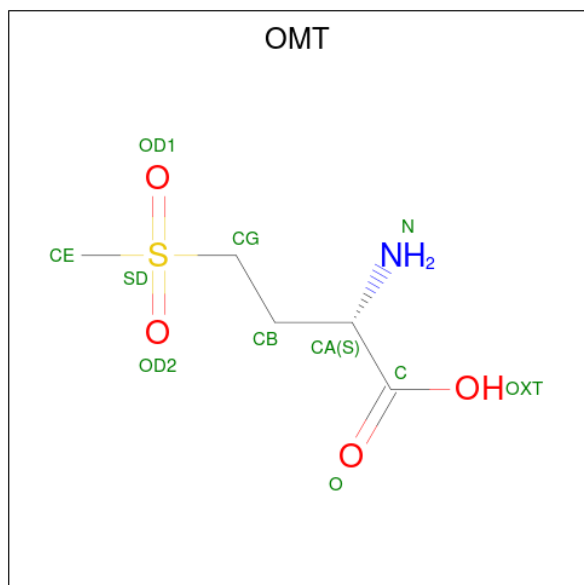
There are 5 unique types of molecules in this entry. The entry contains 22478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1452	Total	C	N	O	S	0	0	0
			11180	7018	2005	2098	59			
1	B	1452	Total	C	N	O	S	0	0	0
			11180	7018	2005	2098	59			

- Molecule 2 is S-DIOXYMETHIONINE (three-letter code: OMT) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>4</sub>S).



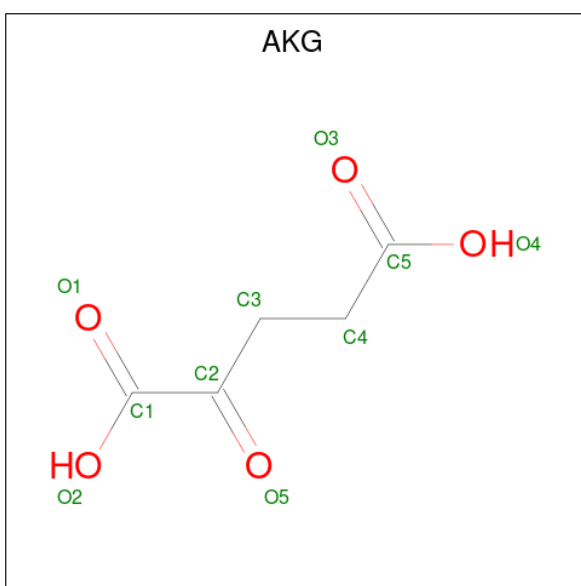
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			11	5	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			11	5	1	4	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



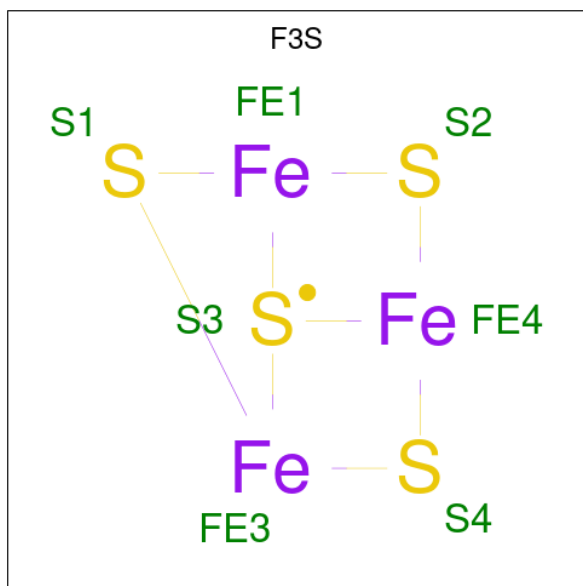
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula:  $C_5H_6O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



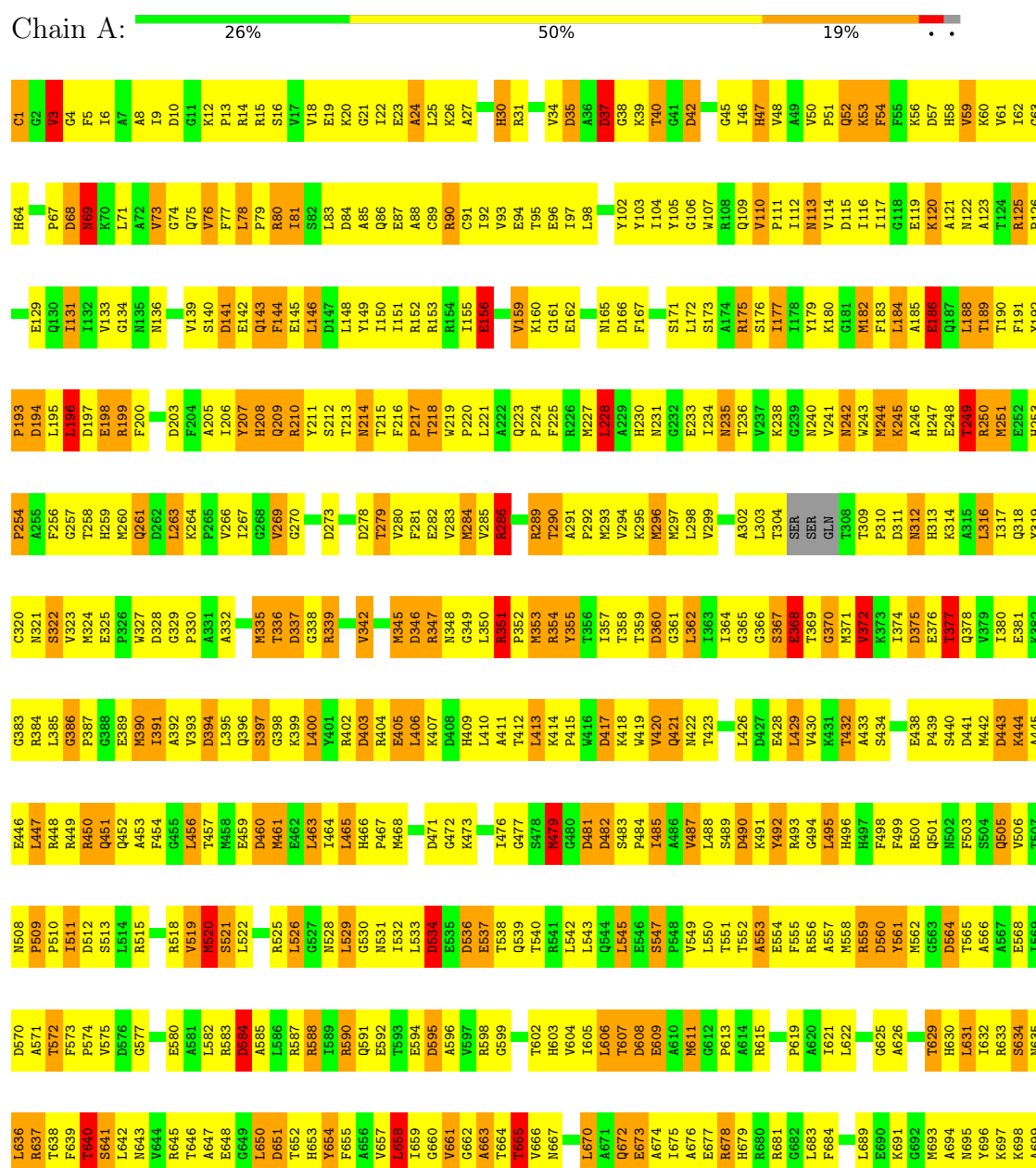
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			7	3	4		
5	B	1	Total	Fe	S	0	0
			7	3	4		

### 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: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN



I700	I767	D701	E768	E769	V770	L773	G776	G777	F778	S709	M711	G712	I713	S714	G715	I716	S717	S718	Y719	R720	G721	N724	A727	I728	G729	L730	S731	R732	D805	S806	A733	L734	V735	A736	E737	H738	F739	F740	A741	M742	V743	S744	R745	I746	G747	G748	G753	I754	Q755	L759	E760	S761	G762	A763	P764	A765	Y766																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
N767	E768	E769	V770	L773	G776	G777	F778	S709	M711	G712	I713	S714	G715	I716	S717	S718	Y719	R720	G721	N724	A727	I728	G729	L730	S731	R732	D805	S806	A733	L734	V735	A736	E737	H738	F739	F740	A741	M742	V743	S744	R745	I746	G747	G748	G753	I754	Q755	L759	E760	S761	G762	A763	P764	A765	Y766																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
V840	D841	V842	V843	V844	S845	I846	T847	A848	R849	R850	K851	R852	F853	I854	T855	R856	G857	M858	A862	L863	S864	G869	T870	N872	M873	R874	E875	R876	R877	K881	D882	S883	H884	G885	E886	G887	G888	E889	M890	D891	A892	Q893	L894	D895	F896	D897	K898	M899	W903	Y904	S905	I906	T907	G908	Q909	V910	A911	S912																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G913	R914	F915	D986	V987	T918	Q919	E920	Y921	L922	N923	Q924	E929	I930	K931	T932	V933	A934	G935	A936	K937	P938	G939	E940	L944	V949	T950	K951	E952	L953	L956	R957	H958	S959	T960	P961	G962	V963	M964	L965	I966	S967	P969	D973	I974	Y975	S976	I977	K978	D979	L980	A981	Q982																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
L983	I984	Y985	D986	L987	K988	Q989	V990	N991	P992	D993	T997	V998	K999	L1000	V1001	S1002	R1003	S1004	G1005	T1006	D1007	G1008	I1009	A1010	A1011	A1014	K1015	A1016	M1017	L1018	D1019	L1022	H1023	S1024	G1025	N1026	S1027	G1028	G1029	T1030	S1033	P1034	Q1035	T1036	S1037	I1038	K1039	F1040	S1041	G1042	L1043	P1044	W1045	A1046	M1047																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G1048	L1049	S1050	E1051	V1052	H1053	Q1054	V1055	L1056	T1057	L1058	N1059	H1060	L1061	R1062	H1063	R1064	V1065	L1066	L1067	R1068	D1070	G1071	K1074	T1075	G1076	R1077	D1078	I1079	M1084	A1087	E1088	E1089	F1090	G1091	N1092	G1093	S1095	G1101	C1102	I1103	M1104	V1105	R1106	Q1107	C1108	H1109	S1110	N1111	T1112	C1113	P1114	V1115	G1116																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
V1117	C1118	V1119	Q1120	D1121	K1122	K1123	L1124	R1125	Q1126	T1131	P1132	E1133	K1134	V1135	V1136	F1139	T1140	F1141	L1142	A1143	E1144	E1145	V1146	E1147	E1148	L1149	L1150	L1153	G1154	F1155	R1156	S1157	L1158	M1159	E1160	V1161	G1163	R1164	T1165	D1166	L1167	H1169	Q1170	V1171	SER	ARG	GLY	ALA	GLU	HIS	LEU	ASP	D1180	L1181																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
D1182	L1183	P1184	T1185	R1186	K1187	V1190	G1193	GLU	ASN	ALA	ARG	TYR	CYS	THR	LEU	G1203	R1204	M1205	E1206	V1207	P1208	D1209	T1210	L1211	D1212	L1213	R1214	T1215	V1216	A1217	F1218	D1219	A1220	P1221	L1222	E1224	E1225	G1226	E1227	K1228	M1229	L1230	L1231	A1235	R1236	T1238	Q1239	R1240	G1243	T1244	R1245	L1246																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
M1249	T1250	T1251	R1252	K1253	F1254	G1255	M1256	L1259	Q1260	P1261	T1264	T1265	I1266	R1267	L1268	R1269	Q1274	S1275	L1276	G1277	V1281	Q1282	G1283	I1284	K1285	V1288	M1289	G1290	D1291	A1292	M1293	D1294	G1297	K1298	G1299	L1300	S1301	G1302	G1303	T1304	I1305	V1306	V1307	R1308	P1309	T1310	T1311	S1312	S1313	F1314	L1315	E1316																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
T1317	M1318	K1319	N1320	T1321	L1322	I1323	T1326	V1327	L1328	Y1329	G1334	K1335	L1336	F1337	A1338	A1339	G1340	E1344	V1348	R1349	M1350	S1351	T1354	V1355	V1356	V1357	E1358	G1359	C1360	G1361	S1362	M1363	E1366	Y1367	M1368	T1369	G1370	T1372	A1373	V1374	T1375	L1376	G1377	R1378	V1379	G1380	D1381	M1382	F1383	L1384	A1385																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
G1386	M1387	T1388	G1389	G1390	M1391	A1392	Y1393	L1394	D1395	L1397	D1398	S1400	L1401	P1402	L1403	Y1404	L1405	M1406	D1407	E1408	P1409	S1409	L1410	L1411	F1412	Q1413	L1414	T1415	E1416	V1417	H1418	H1419	L1420	E1421	S1422	Q1423	L1424	K1425	H1426	L1427	I1428	E1429	E1430	H1431	V1432	T1433	E1434	T1435	Q1436	S1437	R1438	F1439	A1440	A1441	E1442	T1443	L1444	N1445																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
D1446	W1447	A1448	R1449	I1450	V1451	T1452	K1453	F1454	W1455	Q1456	V1457	P1458	P1459	E1460	M1461	L1463	Y1464	R1465	E1467	P1469	V1470	H1471	L1472	PRO	LYS	ALA	ILE	SER	GLU	H1478	H1479	E1480	G1481	E1482	Q1483	L1484	K1485	H1486	L1487	I1488	V1489	F1489	A1490	E1491	E1492	E1493	E1494	E1495	E1496	E1497	E1498	E1499	E1500	E1501	E1502	E1503	E1504	E1505	E1506	E1507	E1508	E1509	E1510	E1511	E1512	E1513	E1514	E1515	E1516	E1517	E1518	E1519	E1520	E1521	E1522	E1523	E1524	E1525	E1526	E1527	E1528	E1529	E1530	E1531	E1532	E1533	E1534	E1535	E1536	E1537	E1538	E1539	E1540	E1541	E1542	E1543	E1544	E1545	E1546	E1547	E1548	E1549	E1550	E1551	E1552	E1553	E1554	E1555	E1556	E1557	E1558	E1559	E1560	E1561	E1562	E1563	E1564	E1565	E1566	E1567	E1568	E1569	E1570	E1571	E1572	E1573	E1574	E1575	E1576	E1577	E1578	E1579	E1580	E1581	E1582	E1583	E1584	E1585	E1586	E1587	E1588	E1589	E1590	E1591	E1592	E1593	E1594	E1595	E1596	E1597	E1598	E1599	E1600	E1601	E1602	E1603	E1604	E1605	E1606	E1607	E1608	E1609	E1610	E1611	E1612	E1613	E1614	E1615	E1616	E1617	E1618	E1619	E1620	E1621	E1622	E1623	E1624	E1625	E1626	E1627	E1628	E1629	E1630	E1631	E1632	E1633	E1634	E1635	E1636	E1637	E1638	E1639	E1640	E1641	E1642	E1643	E1644	E1645	E1646	E1647	E1648	E1649	E1650	E1651	E1652	E1653	E1654	E1655	E1656	E1657	E1658	E1659	E1660	E1661	E1662	E1663	E1664	E1665	E1666	E1667	E1668	E1669	E1670	E1671	E1672	E1673	E1674	E1675	E1676	E1677	E1678	E1679	E1680	E1681	E1682	E1683	E1684	E1685	E1686	E1687	E1688	E1689	E1690	E1691	E1692	E1693	E1694	E1695	E1696	E1697	E1698	E1699	E1700	E1701	E1702	E1703	E1704	E1705	E1706	E1707	E1708	E1709	E1710	E1711	E1712	E1713	E1714	E1715	E1716	E1717	E1718	E1719	E1720	E1721	E1722	E1723	E1724	E1725	E1726	E1727	E1728	E1729	E1730	E1731	E1732	E1733	E1734	E1735	E1736	E1737	E1738	E1739	E1740	E1741	E1742	E1743	E1744	E1745	E1746	E1747	E1748	E1749	E1750	E1751	E1752	E1753	E1754	E1755	E1756	E1757	E1758	E1759	E1760	E1761	E1762	E1763	E1764	E1765	E1766	E1767	E1768	E1769	E1770	E1771	E1772	E1773	E1774	E1775	E1776	E1777	E1778	E1779	E1780	E1781	E1782	E1783	E1784	E1785	E1786	E1787	E1788	E1789	E1790	E1791	E1792	E1793	E1794	E1795	E1796	E1797	E1798	E1799	E1800	E1801	E1802	E1803	E1804	E1805	E1806	E1807	E1808	E1809	E1810	E1811	E1812	E1813	E1814	E1815	E1816	E1817	E1818	E1819	E1820	E1821	E1822	E1823	E1824	E1825	E1826	E1827	E1828	E1829	E1830	E1831	E1832	E1833	E1834	E1835	E1836	E1837	E1838	E1839	E1840	E1841	E1842	E1843	E1844	E1845	E1846	E1847	E1848	E1849	E1850	E1851	E1852	E1853	E1854	E1855	E1856	E1857	E1858	E1859	E1860	E1861	E1862	E1863	E1864	E1865	E1866	E1867	E1868	E1869	E1870	E1871	E1872	E1873	E1874	E1875	E1876	E1877	E1878	E1879	E1880	E1881	E1882	E1883	E1884	E1885	E1886	E1887	E1888	E1889	E1890	E1891	E1892	E1893	E1894	E1895	E1896	E1897	E1898	E1899	E1900	E1901	E1902	E1903	E1904	E1905	E1906	E1907	E1908	E1909	E1910	E1911	E1912	E1913	E1914	E1915	E1916	E1917	E1918	E1919	E1920	E1921	E1922	E1923	E1924	E1925	E1926	E1927	E1928	E1929	E1930	E1931	E1932	E1933	E1934	E1935	E1936	E1937	E1938	E1939	E1940	E1941	E1942	E1943	E1944	E1945	E1946	E1947	E1948	E1949	E1950	E1951	E1952	E1953	E1954	E1955	E1956	E1957	E1958	E1959	E1960	E1961	E1962	E1963	E1964	E1965	E1966	E1967	E1968	E1969	E1970	E1971	E1972	E1973	E1974	E1975	E1976	E1977	E1978	E1979	E1980	E1981	E1982	E1983	E1984	E1985	E1986	E1987	E1988	E1989	E1990	E1991	E1992	E1993	E1994	E1995	E1996	E1997	E1998	E1999	E2000	E2001	E2002	E2003	E2004	E2005	E2006	E2007	E2008	E2009	E2010	E2011	E2012	E2013	E2014	E2015	E2016	E2017	E2018	E2019	E2020	E2021	E2022	E2023	E2024	E2025	E2026	E2027	E2028	E2029	E2030	E2031	E2032	E2033	E2034	E2035	E2036	E2037	E2038	E2039	E2040	E2041	E2042	E2043	E2044	E2045	E2046	E2047	E2048	E2049	E2050	E2051	E2052	E2053	E2054	E2055	E2056	E2057	E2058	E2059	E2060	E2061	E2062	E2063	E2064	E2065	E2066	E2067	E2068	E2069	E2070	E2071	E2072	E2073	E2074	E2075	E2076	E2077	E2078	E2079	E2080	E2081	E2082	E2083	E2084	E2085	E2086	E2087	E2088	E2089	E2090	E2091	E2092	E2093	E2094	E2095	E2096	E2097	E2098	E2099	E2100	E2101	E2102	E2103	E2104	E2105	E2106	E2107	E2108	E2109	E2110	E2111	E2112	E2113	E2114	E2115	E2116	E2117	E2118	E2119	E2120	E2121	E2122	E2123	E2124	E2125	E2126	E2127	E2128	E2129	E2130	E2131	E2132	E2133	E2134	E2135	E2136	E2137	E2138	E2139	E2140	E2141	E2142	E2143	E2144	E2145	E2146	E2147	E2148	E2149	E2150	E2151	E2152	E2153	E2154	E2155	E2156	E2157	E2158	E2159	E2160	E2161	E2162	E2163	E2164	E2165	E2166	E2167	E2168	E2169	E2170	E2171	E2172	E2173	E2174	E2175	E2176	E2177	E2178	E2179	E2180	E2181	E2182	E2183	E2184	E2185	E2186	E2187	E2188	E2189	E2190	E2191	E2192	E2193	E2194	E2195	E2196	E2197	E2198	E2199	E2200	E2201	E2202	E2203	E2204	E2205	E2206	E2207	E2208	E2209	E2210	E2211	E2212	E2213	E2214	E2215	E2216	E2217	E2218	E2219	E2220	E2221	E2222</

S1157	L1158	F1090	A1018	A954	R820	K756	L689	H628	D564	Q501	P439	G366	M297	H230	V169
L1159	G1091	G1091	L1022	R955	P821	K757	E690	T629	T565	R502	S440	S367	L298	N231	
E1160	L1092	L1092	L1022	L956	R821	V758	K691	T629	T565	R502	S440	S367	L298	N231	
L1161	G1093	G1093	L1022	R957	R822	V759	K692	L630	E568	F503	D441	T369	V299	G232	E162
L1162	A1095	A1095	N1026	H958	R823	L759	K693	L631	L569	S504	N442	T369		G233	Q163
G1163	L1096	L1096	N1026	H959	R824	L760	K694	L632	L569	Q505	N443			I234	I164
R1164	T1030	T1030	T1030	T960	R825	H762	K695	S634	A571	N508	K444	I374	A302	N235	N165
L1165	G1031	G1031	G1031	V963	R826	H763	K696	N635	T572	P510	A445	D375	T304	T236	D166
L1166	A1032	A1032	A1032	M964	R827	V764	K697	L636	L573	P509	E446	E376	SER	V237	
L1167	S1033	S1033	P1034	L965	R828	H765	K698	L637	F573	P510	L447	T377	GLN	K238	S171
L1168	P1034	P1034	P1034	L966	R829	V766	K699	T638	P574	D512	R448	Q378	T308	G239	L172
L1169	F894	F894	F894	I967	R830	H767	K700	T639	D576	S513	R450	I380	T309	N240	S173
Q1170	R897	R897	R897	P968	R831	V768	D701	T640	G577	L514	Q451	E381	P310	N242	A174
L1171	R898	R898	R898	P969	R832	H769	D702	T641	E580	R515	Q452		D311	W243	R175
L1172	R899	R899	R899	P970	R833	V770	D703	L642	A581	R518	A453	L385	N312	W244	S176
L1173	R900	R900	R900	P971	R834	V771	L704	N643	L582	F519	F454	G386	H313	K245	I177
L1174	R901	R901	R901	P972	R835	V772	L705	N644	L583	R520	Q455	G388	A314	E248	M182
L1175	R902	R902	R902	P973	R836	V773	K706	N645	L584	R521	Q456	G388	A315	T249	F183
L1176	R903	R903	R903	P974	R837	V774	K707	N646	L585	R522	T457	E389	L316	L250	L184
L1177	R904	R904	R904	P975	R838	V775	L707	N647	L586	R523	T458	M390	I317	R251	A185
L1178	R905	R905	R905	P976	R839	V776	K708	N648	L587	R524	T459	E390	Q318	E186	
L1179	R906	R906	R906	P977	R840	V777	K709	N649	L588	R525	T460	D394	Y319	Q187	Q187
L1180	R907	R907	R907	P978	R841	V778	L710	N650	L589	R526	T461	L395	N321	H253	T189
L1181	R908	R908	R908	P979	R842	V779	K711	N651	L590	R527	T462	G396	S322	A255	P254
L1182	R909	R909	R909	P980	R843	V780	L712	N652	L591	R528	T463	G397	Y323	P256	T190
L1183	R910	R910	R910	P981	R844	V781	K713	N653	L592	R529	T464	E398	M324	G257	F191
L1184	R911	R911	R911	P982	R845	V782	L714	N654	L593	R530	T465	G399	E325	T258	P193
L1185	R912	R912	R912	P983	R846	V783	K715	N655	L594	R531	T466	K398	P326	H259	L194
L1186	R913	R913	R913	P984	R847	V784	L716	N656	L595	R532	T467	E399	W327	M260	L195
L1187	R914	R914	R914	P985	R848	V785	K717	N657	L596	R533	T468	R402	D328	Q261	L196
L1188	R915	R915	R915	P986	R849	V786	L718	N658	L597	R534	T469	D403	G329	D262	D197
L1189	R916	R916	R916	P987	R850	V787	K719	N659	L598	R535	T470	E404	D337	E198	E198
L1190	R917	R917	R917	P988	R851	V788	L720	N660	L599	R536	T471	R404	R339	R199	
L1191	R918	R918	R918	P989	R852	V789	K721	N661	L600	R537	T472	E405	G338	V266	D203
L1192	R919	R919	R919	P990	R853	V790	L722	N662	L601	R538	T473	E406	R339	I267	
L1193	R920	R920	R920	P991	R854	V791	K723	N663	L602	R539	T474	L406	G339	G268	
L1194	R921	R921	R921	P992	R855	V792	L724	N664	L603	R540	T475	E407	V269	V269	
L1195	R922	R922	R922	P993	R856	V793	K725	N665	L604	R541	T476	L410	V342	G270	
L1196	R923	R923	R923	P994	R857	V794	L726	N666	L605	R542	T477	A411	G342	Q209	Q209
L1197	R924	R924	R924	P995	R858	V795	K727	N667	L606	R543	T478	T412	G343	R210	
L1198	R925	R925	R925	P996	R859	V796	L728	N668	L607	R544	T479	G480	G344	Y211	
L1199	R926	R926	R926	P997	R860	V797	K729	N669	L608	R545	T480	L414	M345	S212	
L1200	R927	R927	R927	P998	R861	V798	L730	N670	L609	R546	T481	K414	D346	D278	
L1201	R928	R928	R928	P999	R862	V799	K731	N671	L610	R547	T482	P484	R347	T279	
L1202	R929	R929	R929	P1000	R863	V800	L732	N672	L611	R548	T483	E485	N348	V280	
L1203	R930	R930	R930	P1001	R864	V801	K733	N673	L612	R549	T484	K418	G349	F281	
L1204	R931	R931	R931	P1002	R865	V802	L734	N674	L613	V549	T485	W419	L350	T215	
L1205	R932	R932	R932	P1003	R866	V803	K735	N675	L614	L550	T486	W419	L350	E282	
L1206	R933	R933	R933	P1004	R867	V804	L736	N676	L615	T551	T487	V420	R351	V283	
L1207	R934	R934	R934	P1005	R868	V805	K737	N677	L616	T552	T488	W420	R351	P217	
L1208	R935	R935	R935	P1006	R869	V806	L738	N678	L617	T553	T489	N422	M353	T218	
L1209	R936	R936	R936	P1007	R870	V807	K739	N679	L618	T554	T490	N423	R354	V219	
L1210	R937	R937	R937	P1008	R871	V808	L740	N680	L619	T555	T491	T423	Y355	R286	
L1211	R938	R938	R938	P1009	R872	V809	K741	N681	L620	R556	T492	L426	G349	R289	
L1212	R939	R939	R939	P1010	R873	V810	L742	N682	L621	R557	T493	D427	T359	Q223	
L1213	R940	R940	R940	P1011	R874	V811	K743	N683	L622	R558	T494	E428	D360	A291	
L1214	R941	R941	R941	P1012	R875	V812	L744	N684	L623	R559	T495	L429	G361	P224	
L1215	R942	R942	R942	P1013	R876	V813	K745	N685	L624	R560	T496	W430	L362	P292	
L1216	R943	R943	R943	P1014	R877	V814	L746	N686	L625	D560	T497	V430	I363	M293	
L1217	R944	R944	R944	P1015	R878	V815	K747	N687	L626	F561	T498	G437	I364	V294	
L1218	R945	R945	R945	P1016	R879	V816	L748	N688	L627	R562	T499	E438	G365	K295	
L1219	R946	R946	R946	P1017	R880	V817	K749	N689	L628	G563	T500	E439		M296	
L1220	R947	R947	R947	P1018	R881	V818	L750	N690	L629		T501				
L1221	R948	R948	R948	P1019	R882	V819	K751	N691	L630		T502				
L1222	R949	R949	R949	P1020	R883	V820	L752	N692	L631		T503				
L1223	R950	R950	R950	P1021	R884	V821	K753	N693	L632		T504				
L1224	R951	R951	R951	P1022	R885	V822	L754	N694	L633		T505				
L1225	R952	R952	R952	P1023	R886	V823	K755	N695	L634		T506				
L1226	R953	R953	R953	P1024	R887	V824	L756	N696	L635		T507				
L1227	R954	R954	R954	P1025	R888	V825	K757	N697	L636		T508				
L1228	R955	R955	R955	P1026	R889	V826	L758	N698	L637		T509				
L1229	R956	R956	R956	P1027	R890	V827	K759	N699	L638		T510				
L1230	R957	R957	R957	P1028	R891	V828	L760	N700	L639		T511				
L1231	R958	R958	R958	P1029	R892	V829	K761	N701	L640		T512				
L1232	R959	R959	R959	P1030	R893	V830	L762	N702	L641		T513				
L1233	R960	R960	R960	P1031	R894	V831	K763	N703	L642		T514				
L1234	R961	R961	R961	P1032	R895	V832	L764	N704	L643		T515				
L1235	R962	R962	R962	P1033	R896	V833	K765	N705	L644		T516				
L1236	R963	R963	R963	P1034	R897	V834	L766	N706	L645		T517				
L1237	R964	R964	R964	P1035	R898	V835	K767	N707	L646		T518				
L1238	R965	R965	R965	P1036	R899	V836	L768	N708	L647		T519				
L1239	R966	R966	R966	P1037	R900	V837	K769	N709	L648		T520				
L1240	R967	R967	R967	P1038	R901	V838	L770	N710	L649		T521				
L1241	R968	R968	R968	P1039	R902	V839	K771	N711	L650		T522				
L1242	R969	R969	R969	P1040	R903	V840	L772	N712	L651		T523				
L1243	R970	R970	R970	P1041	R904	V841	K773	N713	L652		T524				
L1244	R971	R971	R971	P1042	R905	V842	L774	N714	L653		T525				
L1245	R972	R972	R972	P1043	R906	V843	K775	N715	L654		T526				
L1246	R973	R973	R973	P1044	R907	V844	L776	N716	L655		T527				
L1247	R974	R974	R974	P1045	R908	V845	K777	N717	L656		T528				
L1248	R975	R975	R975	P1046	R909	V846	L778	N718	L657		T529				
L1249	R976	R976	R976	P1047	R910	V847	K779	N719	L658		T530				
L1250	R977	R977	R977	P1048	R911	V848	L779	N720	L659		T531				
L1251	R978	R978	R978	P1049	R912	V849	K780	N721	L660		T532				
L1252	R979	R979	R979	P1050	R913	V850	L781	N722	L661		T533				
L1253	R980	R980	R980	P1051	R914	V851	K782	N723	L662		T534				
L1254															





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	233.61Å 233.61Å 305.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.6 (20.00-3.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.256 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22478	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	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: FMN, AKG, OMT, F3S

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	1.06	7/11383 (0.1%)	1.58	198/15390 (1.3%)
1	B	1.10	7/11383 (0.1%)	1.58	192/15390 (1.2%)
All	All	1.08	14/22766 (0.1%)	1.58	390/30780 (1.3%)

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	1	2
1	B	0	2
All	All	1	4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	838	VAL	CA-CB	-7.71	1.38	1.54
1	A	746	ILE	CA-CB	-7.47	1.37	1.54
1	A	848	ALA	CA-CB	-6.51	1.38	1.52
1	A	1065	VAL	CB-CG2	-6.15	1.40	1.52
1	A	3	VAL	CA-CB	-5.67	1.42	1.54

The worst 5 of 390 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1062	ARG	NE-CZ-NH1	-12.86	113.87	120.30
1	A	608	ASP	CB-CG-OD2	12.18	129.26	118.30
1	A	141	ASP	CB-CG-OD2	11.98	129.08	118.30
1	B	888	GLY	N-CA-C	-11.68	83.89	113.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	890	ASP	CB-CG-OD1	11.31	128.48	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	915	PHE	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1002	SER	Mainchain
1	A	325	GLU	Mainchain
1	B	1168	LEU	Mainchain
1	B	725	PHE	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	11180	0	11210	1498	0
1	B	11180	0	11212	1318	0
2	A	11	0	10	2	0
2	B	11	0	10	1	0
3	A	31	0	19	4	0
3	B	31	0	19	6	0
4	A	10	0	4	0	0
4	B	10	0	4	2	0
5	A	7	0	0	2	0
5	B	7	0	0	3	0
All	All	22478	0	22488	2814	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 63.

The worst 5 of 2814 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:182:MET:CE	1:B:217:PRO:HB2	1.30	1.59
1:A:182:MET:HE3	1:A:217:PRO:CB	1.34	1.57
1:B:1449:ARG:HH11	1:B:1449:ARG:CB	0.97	1.56
1:B:182:MET:HE3	1:B:217:PRO:CB	1.09	1.54
1:A:182:MET:CE	1:A:217:PRO:HB2	1.45	1.47

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	1444/1479 (98%)	1152 (80%)	227 (16%)	65 (4%)	2	14
1	B	1444/1479 (98%)	1170 (81%)	211 (15%)	63 (4%)	2	15
All	All	2888/2958 (98%)	2322 (80%)	438 (15%)	128 (4%)	2	15

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	444	LYS
1	A	451	GLN
1	A	705	LEU
1	A	712	GLY

### 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	1184/1206 (98%)	970 (82%)	214 (18%)	1	9
1	B	1184/1206 (98%)	965 (82%)	219 (18%)	1	8
All	All	2368/2412 (98%)	1935 (82%)	433 (18%)	1	9

5 of 433 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	144	PHE
1	B	461	MET
1	B	1245	ARG
1	B	189	THR
1	B	308	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	653	HIS
1	B	1363	ASN
1	B	755	GLN
1	B	982	GLN
1	A	943	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 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	FMN	A	2474	-	33,33,33	1.47	5 (15%)	48,50,50	2.73	20 (41%)
2	OMT	B	2473	-	9,10,10	4.16	5 (55%)	11,14,14	5.80	5 (45%)
2	OMT	A	2473	-	9,10,10	4.29	5 (55%)	11,14,14	4.49	6 (54%)
4	AKG	A	2475	-	9,9,9	3.09	4 (44%)	11,11,11	2.92	4 (36%)
3	FMN	B	2474	-	33,33,33	1.36	4 (12%)	48,50,50	2.59	20 (41%)
5	F3S	A	2476	1	0,9,9	-	-	-	-	-
4	AKG	B	2475	-	9,9,9	3.48	4 (44%)	11,11,11	2.80	4 (36%)
5	F3S	B	2476	1	0,9,9	-	-	-	-	-

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	FMN	A	2474	-	-	7/18/18/18	0/3/3/3
2	OMT	B	2473	-	-	5/10/10/10	-
2	OMT	A	2473	-	-	5/10/10/10	-
4	AKG	A	2475	-	-	2/9/9/9	-
3	FMN	B	2474	-	-	5/18/18/18	0/3/3/3
5	F3S	A	2476	1	-	-	0/3/3/3
4	AKG	B	2475	-	-	1/9/9/9	-
5	F3S	B	2476	1	-	-	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2473	OMT	CB-CG	-6.99	1.45	1.52
2	B	2473	OMT	CG-SD	-6.88	1.69	1.78
2	A	2473	OMT	CG-SD	-6.69	1.69	1.78
4	B	2475	AKG	O5-C2	6.49	1.36	1.23
2	B	2473	OMT	CB-CG	-5.99	1.46	1.52

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2473	OMT	OD2-SD-CG	-16.70	96.65	108.34
2	A	2473	OMT	OD2-SD-CE	-11.66	97.19	108.91
3	A	2474	FMN	O5'-P-O1P	-7.87	84.41	106.47
4	B	2475	AKG	C4-C3-C2	-7.64	98.63	113.03
4	A	2475	AKG	C4-C3-C2	-7.23	99.42	113.03

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2473	OMT	C-CA-CB-CG
2	A	2473	OMT	CB-CG-SD-OD1
2	A	2473	OMT	CB-CG-SD-OD2
2	B	2473	OMT	N-CA-CB-CG
2	B	2473	OMT	C-CA-CB-CG

There are no ring outliers.

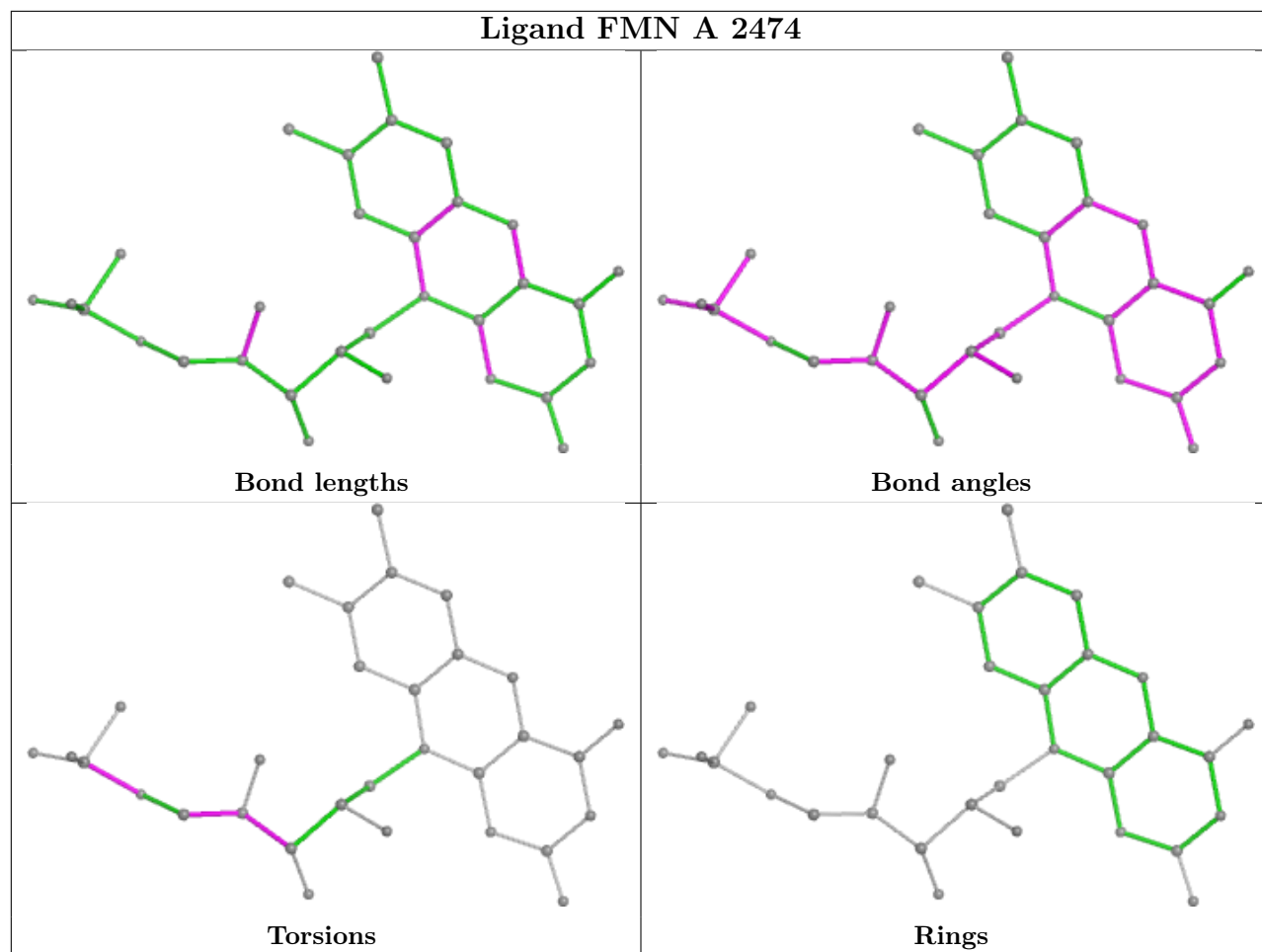
7 monomers are involved in 20 short contacts:

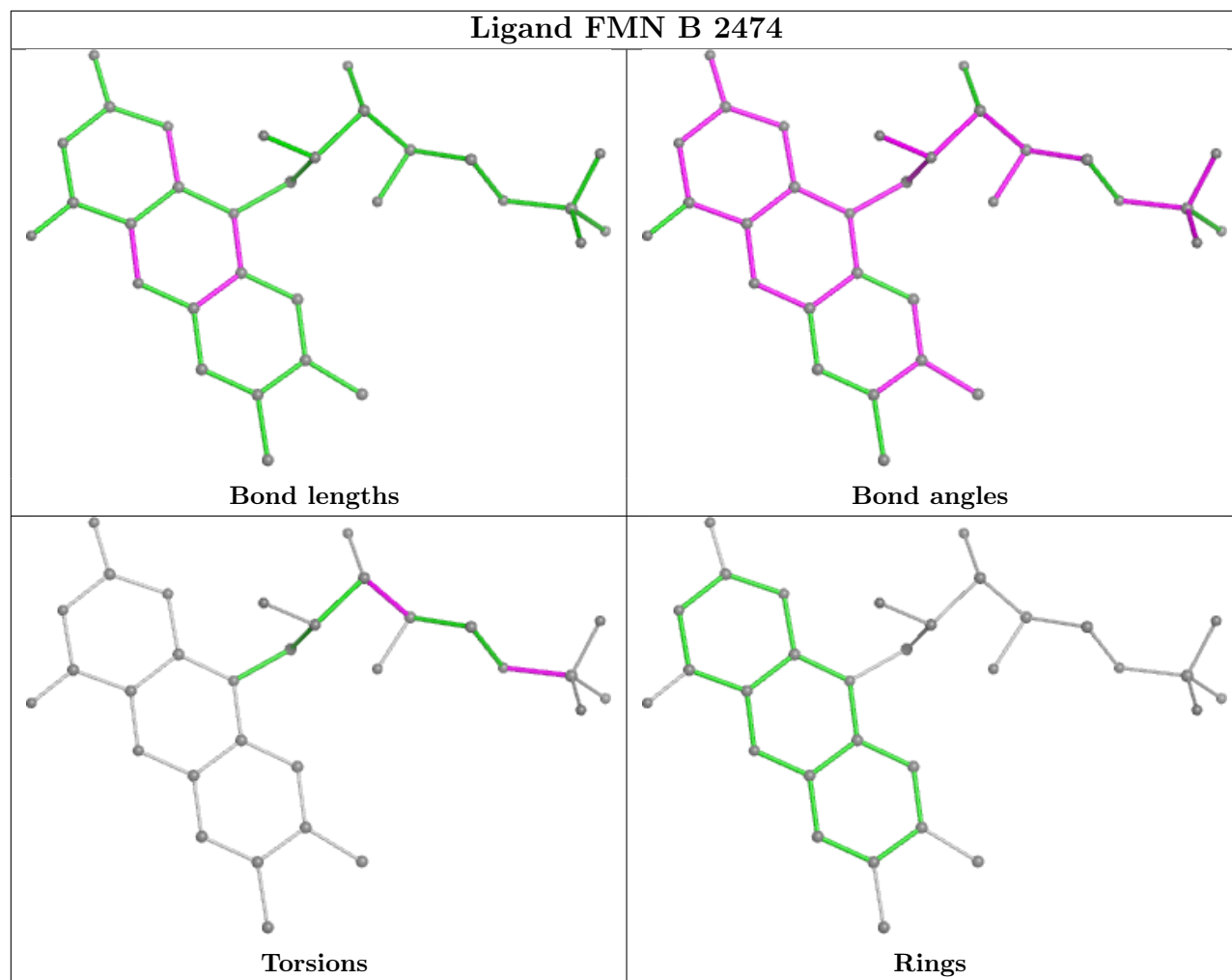
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2474	FMN	4	0
2	B	2473	OMT	1	0
2	A	2473	OMT	2	0
3	B	2474	FMN	6	0
5	A	2476	F3S	2	0
4	B	2475	AKG	2	0
5	B	2476	F3S	3	0

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.



## Ligand FMN A 2474





## 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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.