



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:01 PM BST

PDB ID : 2VDC  
EMDB ID: : EMD-1440  
Title : THE 9.5 Å RESOLUTION STRUCTURE OF GLUTAMATE SYNTHASE FROM CRYO-ELECTRON MICROSCOPY AND ITS OLIGOMERIZATION BEHAVIOR IN SOLUTION: FUNCTIONAL IMPLICATIONS.  
Authors : Cotteville, M.; Larquet, E.; Jonic, S.; Petoukhov, M.V.; Caprini, G.; Paravisi, S.; Svergun, D.I.; Vanoni, M.A.; Boisset, N.  
Deposited on : 2007-10-04  
Resolution : 9.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

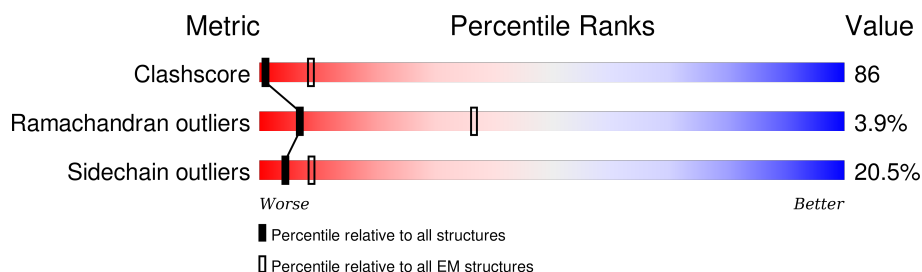
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.50 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.




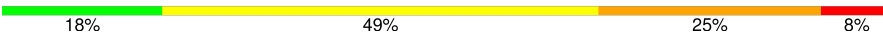

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1472	26% 52% 20% .
1	B	1472	30% 49% 17% .
1	C	1472	27% 51% 20% .
1	D	1472	30% 49% 17% .
1	E	1472	26% 51% 20% .
1	F	1472	30% 49% 17% .
2	G	456	18% 49% 25% 8%
2	H	456	17% 49% 25% 8%
2	I	456	17% 49% 25% 8%

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Mol	Chain	Length	Quality of chain
2	J	456	
2	K	456	
2	L	456	

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
6	F3S	B	2476	-	-	X	-
6	F3S	D	2476	-	-	X	-
6	F3S	E	2476	-	-	X	-
6	F3S	F	2476	-	-	X	-
7	SF4	G	483	-	-	X	-
7	SF4	H	483	-	-	X	-
7	SF4	I	483	-	-	X	-
7	SF4	J	483	-	-	X	-
7	SF4	K	483	-	-	X	-
7	SF4	L	483	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 89598 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

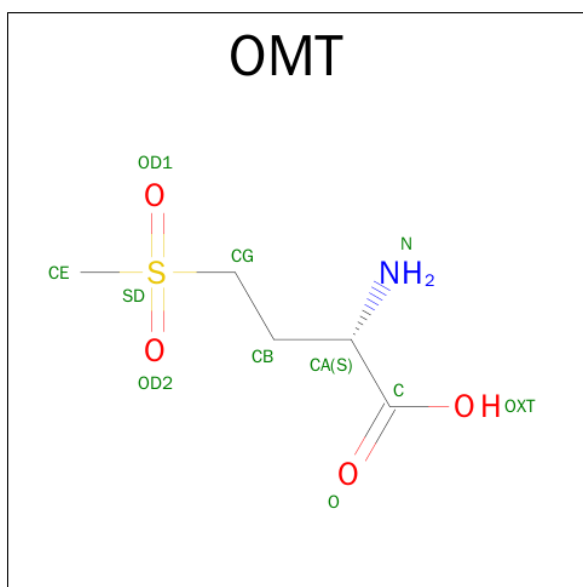
- Molecule 1 is a protein called GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		
1	B	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		
1	C	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		
1	D	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		
1	E	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		
1	F	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		

- Molecule 2 is a protein called GLUTAMATE SYNTHASE [NADPH] SMALL CHAIN.

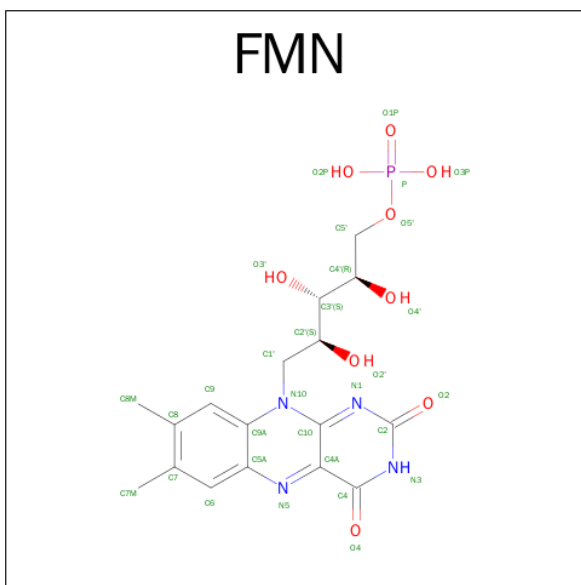
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		
2	H	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		
2	I	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		
2	J	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		
2	K	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		
2	L	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		

- Molecule 3 is S-DIOXYMETHIONINE (three-letter code: OMT) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>4</sub>S).



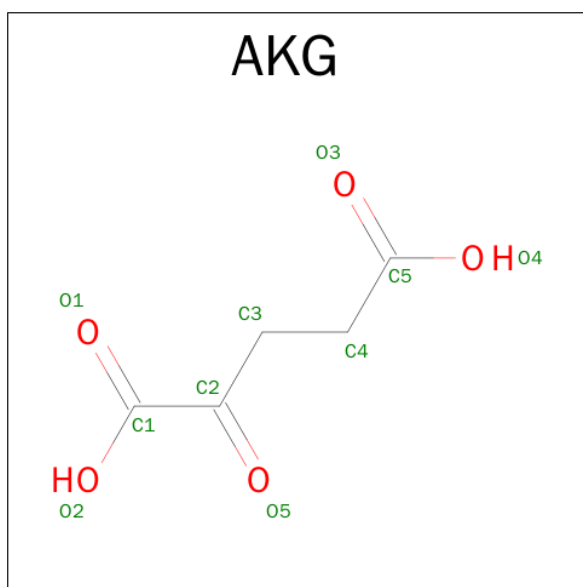
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			11	5	1	4	1	
3	B	1	Total	C	N	O	S	0
			11	5	1	4	1	
3	C	1	Total	C	N	O	S	0
			11	5	1	4	1	
3	D	1	Total	C	N	O	S	0
			11	5	1	4	1	
3	E	1	Total	C	N	O	S	0
			11	5	1	4	1	
3	F	1	Total	C	N	O	S	0
			11	5	1	4	1	

- Molecule 4 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).



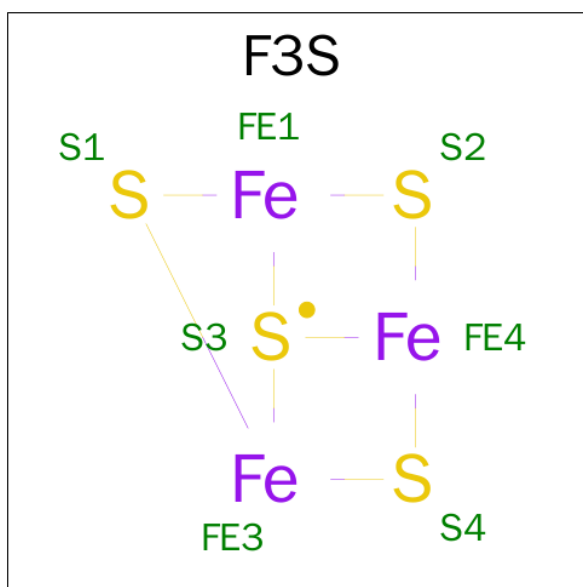
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	C	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	D	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 5 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			10	5	5	
5	B	1	Total	C	O	0
			10	5	5	
5	C	1	Total	C	O	0
			10	5	5	
5	D	1	Total	C	O	0
			10	5	5	
5	E	1	Total	C	O	0
			10	5	5	
5	F	1	Total	C	O	0
			10	5	5	

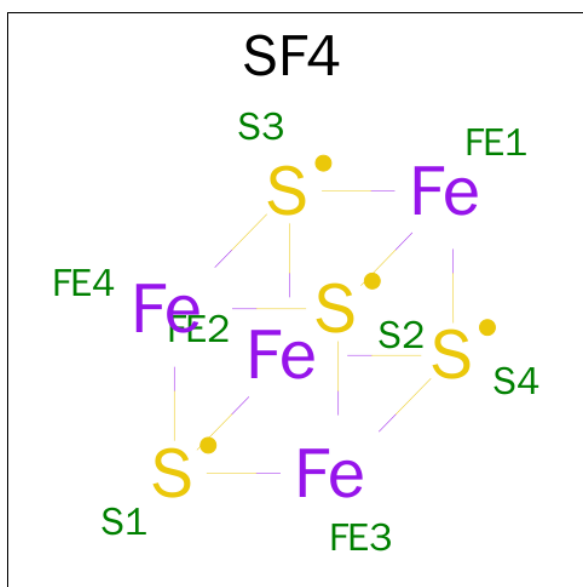
- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	Fe	S	0
			7	3	4	
6	B	1	Total	Fe	S	0
			7	3	4	
6	C	1	Total	Fe	S	0
			7	3	4	
6	D	1	Total	Fe	S	0
			7	3	4	
6	E	1	Total	Fe	S	0
			7	3	4	
6	F	1	Total	Fe	S	0
			7	3	4	

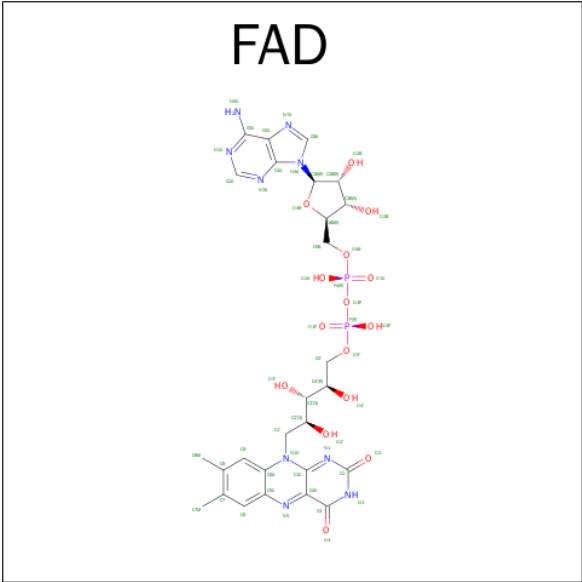
- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).





Mol	Chain	Residues	Atoms			AltConf
7	G	1	Total	Fe	S	0
			16	8	8	
7	G	1	Total	Fe	S	0
			16	8	8	
7	H	1	Total	Fe	S	0
			16	8	8	
7	H	1	Total	Fe	S	0
			16	8	8	
7	I	1	Total	Fe	S	0
			16	8	8	
7	I	1	Total	Fe	S	0
			16	8	8	
7	J	1	Total	Fe	S	0
			16	8	8	
7	J	1	Total	Fe	S	0
			16	8	8	
7	K	1	Total	Fe	S	0
			16	8	8	
7	K	1	Total	Fe	S	0
			16	8	8	
7	L	1	Total	Fe	S	0
			16	8	8	
7	L	1	Total	Fe	S	0
			16	8	8	

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).

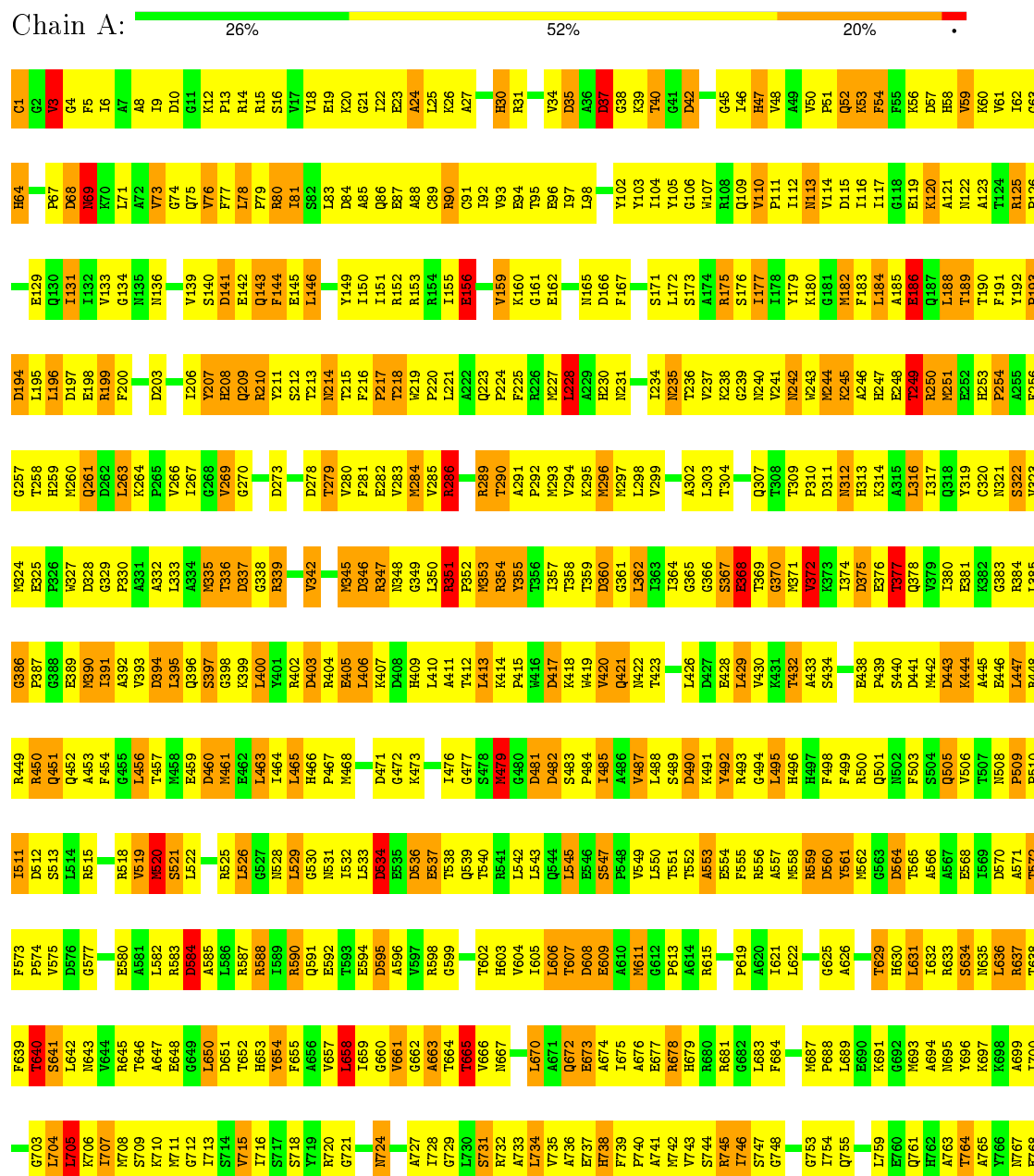


Mol	Chain	Residues	Atoms					AltConf
8	G	1	Total	C	N	O	P	0
			53	27	9	15	2	
8	H	1	Total	C	N	O	P	0
			53	27	9	15	2	
8	I	1	Total	C	N	O	P	0
			53	27	9	15	2	
8	J	1	Total	C	N	O	P	0
			53	27	9	15	2	
8	K	1	Total	C	N	O	P	0
			53	27	9	15	2	
8	L	1	Total	C	N	O	P	0
			53	27	9	15	2	

### 3 Residue-property plots

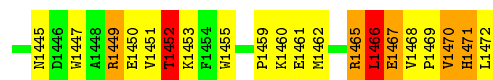
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

#### • Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN



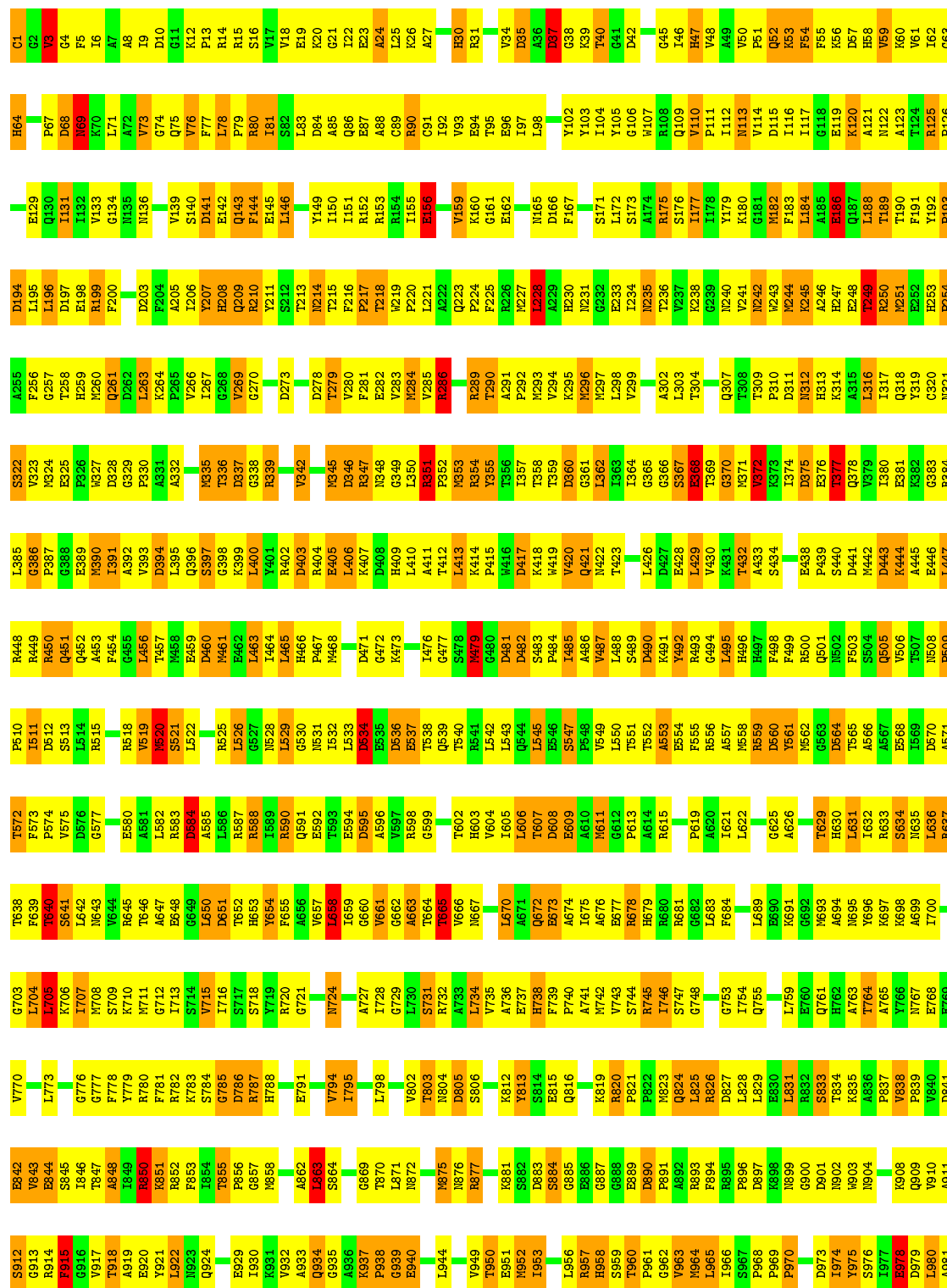


G1380	D1381	M1382	F1383	A1384	M1387	T1388	G1389	G1390	Y1393	Y1394	Y1395	D1396	L1397	D1398	I1399	G1400	L1401	P1402	L1403	Y1404	L1405	M1406	D1407	E1408	V1409	L1410	L1411	F1412	G1413	R1414	V1417	G1418	H1419	Y1420	E1421	Q1423	L1424	K1425	H1426	L1427	I1428	E1429	E1430	V1431	V1432	T1433	E1434	Q1435	L1436	R1437	L1438	F1439	A1440	A1441	E1442																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
I1081	L1082	R1147	A1217	D1218	A1219	R1220	S1221	L1222	G1226	E1227	M1228	L1229	T1230	E1231	L1232	A1233	Y1233	I1232	L1233	G1234	M1235	P1236	V1237	G1243	T1244	R1245	L1246	S1247	A1248	L1249	M1250	L1251	T1252	L1253	M1254	L1255	L1256	L1257	L1258	L1259	Q1260	G1261	H1262	I1263	L1264	L1265	L1266	L1267	L1268	L1269	Q1274	A1278	F1279	A1280	Q1282	E1289	M1290	L1291	A1292	L1293	L1294																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
R1147	A1151	G1152	L1153	G1154	F1155	L1156	S1157	L1158	M1159	E1160	V1161	L1162	G1163	R1164	T1165	D1166	L1167	L1168	H1169	Q1170	V1171	S1172	R1173	E1176	H1177	L1178	D1179	L1180	L1181	D1182	L1183	L1184	P1185	R1186	L1187	V1190	D1191	P1192	G1193	E1194	M1195	L1201	R1204	M1205	E1206	V1207	P1208	L1209	T1210	G1211	L1212	L1213	L1214	L1215	L1216																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
A1217	D1218	A1219	R1220	S1221	L1222	G1226	E1227	M1228	L1229	T1230	E1231	L1232	A1233	Y1233	I1232	L1233	G1234	M1235	P1236	V1237	G1243	T1244	R1245	L1246	S1247	A1248	L1249	M1250	L1251	T1252	L1253	M1254	L1255	L1256	L1257	L1258	L1259	Q1260	G1261	H1262	I1263	L1264	L1265	L1266	L1267	L1268	L1269	Q1274	A1278	F1279	A1280	Q1282	E1289	M1290	L1291	A1292	L1293	L1294																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
Y1295	R1298	S1301	G1302	R1308	P1309	T1310	T1311	E1316	T1317	M1318	I1322	I1323	G1324	M1325	P1326	V1327	L1328	Y1329	L1336	F1337	A1338	A1339	G1340	E1344	R1345	F1346	A1347	V1348	R1349	T1354	V1355	V1356	V1357	E1358	G1359	C1360	E1366	M1368	T1369	G1370	T1372	A1373	V1374	S1375	L1376	G1377	R1378	L1379	E1380	E1381	E1382	E1383	E1384	E1385	E1386	E1387	E1388	E1389	E1390	E1391	E1392	E1393	E1394	E1395	E1396	E1397	E1398	E1399	E1400	E1401	E1402	E1403	E1404	E1405	E1406	E1407	E1408	E1409	E1410	E1411	E1412	E1413	E1414	E1415	E1416	E1417	E1418	E1419	E1420	E1421	E1422	E1423	E1424	E1425	E1426	E1427	E1428	E1429	E1430	E1431	E1432	E1433	E1434	E1435	E1436	E1437	E1438	E1439	E1440	E1441	E1442																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
L1364	G1365	G1366	S1367	E1368	T1369	I1374	D1375	T1377	Q1378	V1379	L1380	E1381	I1382	L1383	F1384	G1385	P1387	G1388	E1389	M1390	V1393	D1394	L1395	Q1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G1437	E1438	P1439	S1440	D1441	M1442	D1443	K1444	E1445	E1446	L1447	R1448	V1449	R1450	Q1451	R1452	F1453	F1454	G1455	L1456	T1457	N1458	D1459	D1460	E1462	L1463	L1464	L1465	L1466	H1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
F1499	R1500	Q1501	N1502	S1503	F1504	Q1505	N1508	P1509	P1510	L1511	D1512	S1513	L1514	R1515	R1516	R1517	R1518	R1519	R1520	S1521	L1522	R1523	L1524	L1525	L1526	G1527	N1528	L1529	L1530	N1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960	L1961	L1962	L1963	L1964	L1965	L1966	L1967	L1968	L1969	L1970	L1971	L1972	L1973	L1974	L1975	L1976	L1977	L1978	L1979	L1980	L1981	L1982	L1983	L1984	L1985	L1986	L1987	L1988	L1989	L1990	L1991	L1992	L1993	L1994	L1995	L1996	L1997	L1998	L1999	L2000	L2001	L2002	L2003	L2004	L2005	L2006	L2007	L2008	L2009	L2010	L2011	L2012	L2013	L2014	L2015	L2016	L2017	L2018	L2019	L2020	L2021	L2022	L2023	L2024	L2025	L2026	L2027	L2028	L2029	L2030	L2031	L2032	L2033	L2034	L2035	L2036	L2037	L2038	L2039	L2040	L2041	L2042	L2043	L2044	L2045	L2046	L2047	L2048	L2049	L2050	L2051	L2052	L2053	L2054	L2055	L2056	L2057	L2058	L2059	L2060	L2061	L2062	L2063	L2064	L2065	L2066	L2067	L2068	L2069	L2070	L2071	L2072	L2073	L2074	L2075	L2076	L2077	L2078	L2079	L2080	L2081	L2082	L2083	L2084	L2085	L2086	L2087	L2088	L2089	L2090	L2091	L2092	L2093	L2094	L2095	L2096	L2097	L2098	L2099	L2100	L2101	L2102	L2103	L2104	L2105	L2106	L2107	L2108	L2109	L2110	L2111	L2112	L2113	L2114	L2115	L2116	L2117	L2118	L2119	L2120	L2121	L2122	L2123	L2124	L2125	L2126	L2127	L2128	L2129	L2130	L2131	L2132	L2133	L2134	L2135	L2136	L2137	L2138	L2139	L2140	L2141	L2142	L2143	L2144	L2145	L2146	L2147	L2148	L2149	L2150	L2151	L2152	L2153	L2154	L2155	L2156	L2157	L2158	L2159	L2160	L2161	L2162	L2163	L2164	L2165	L2166	L2167	L2168	L2169	L2170	L2171	L2172	L2173	L2174	L2175	L2176	L2177	L2178	L2179	L2180	L2181	L2182	L2183	L2184	L2185	L2186	L2187	L2188	L2189	L2190	L2191	L2192	L2193	L2194	L2195	L2196	L2197	L2198	L2199	L2200	L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	L2261	L2262	L2263	L2264	L2265	L2266	L2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	L2277	L2278	L2279	L2280	L2281	L2282	L2283	L2284	L2285	L2286	L2287	L2288	L2289	L2290	L2291	L2292	L2293	L2294	L2295	L2296	L2297	L2298	L2299	L2300	L2301	L2302	L2303	L2304	L2305	L2306	L2307	L2308	L2309	L2310	L2311	L2312



• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

Chain C: 27% 51% 20%

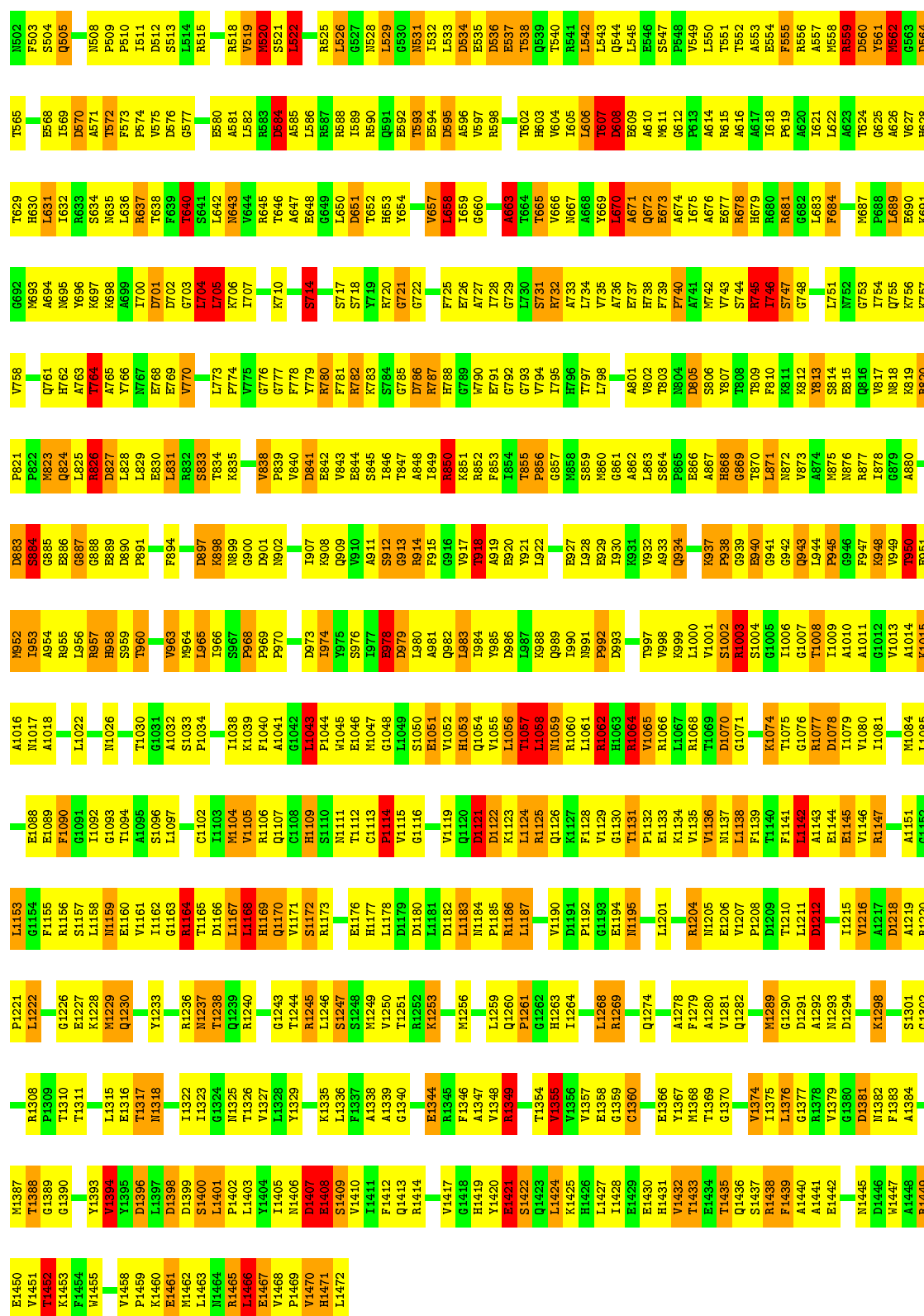


T1452	K1453	F1454	V1455	Q1456	V1457	V1458	P1459	K1460	E1461	M1462	R1465	L1466	E1467	V1468	P1469	V1470	H1471	L1472																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

Chain D:  30% 49% 17%

S440	D441	M442	D443	K444	A445	E446	L447	R448	R449	L450	Q451	A453	F454	G455	L456	T457	M458	E459	D460	M461	L463	L464	L465	H466	P467	D471	K472	K473	E474	L475	L476	G477	S478	M479	G480	D481	D482	S483	P484	A485	A486	L487	L488	S489	D490	K491	Y492	R493	G494	L495	H496	H497	F498	F499	R500	Q501		
S367	E368	T369		L374	D375	E376	L377	V379	G378	V379	L380	E381	L385	G386	P387	G388	E389	M390	V393	D394	M394	L395	G396	S397	G398	K399	D402	D403	R404	E405	L406	K407	D408	H409	L410	A411	L412	L413	K414	P415	D416	R417	N418	L419	V420	Q421	M422	L423	L426	D427	E428	L429	V430	G437	E438	R500	P439	
E296					A302	L303	T304	Q307	T308	T309	P310	D311	N312	H313	K314	K315	L316	I317	Q318	Y319	C320	N321	S322		E325	P326	K327	D328	G329	P330	D337	G338	R339		V342	G343	G344	D345	D346	R347	N348	G349	R351	P352	N353	R354	Y355	T359	D360	G361	T362	L363	I364	G365	G366			
A229	N231	G232	E233	I234	N235	T236	V237	K238	G239	N240	Y241	N242	N243	N244	K245		E248	T249	N250	E251	E252	H253	P254	A255	F256	G257	T258	H259	N260	Q261	D262	L263		V266	L267	G268	V269	G270		S274		D278	T279	V280	F281	E282	V283	N284	V285	R286	R289	G290	G291	G292	G293			
V159			E162	Q163	N165	D166		S171	L172	S173	A174	R175	I177				M182	F183	L184	A185	E186	Q187	L188	T189	F190	Y191	Y192	P193	D194	L195	L196	D197	E198	R199		D203		Y207	H208	Q209	R210	Y211	S212	T213	T215	F216	V217	T218	W219	P220	L221	A222	Q223	P224	F225	R226	I227	L228
E87	A88	C89	R90	C91	I92	V93	E94		L98	A99	F100	G101	Y102		Y105	G106	M107	R108	Q109	V110	P111	I112	N113	V114	D115	I116	I117	G118	E119	K120	A121	N122		R125		Q130	F131	M136	K137	G138	V139	S140	D141	E142	Q143	F144	E145	L146	D147	L148	Y149	I150	I151	R152	R153	R154	E155	C156
C1	G2	V3	G4	F5	A8	I9		K12	P13		A24	L25	K26			H30	R31		V34	D35	A36	D37	G38	K39	T40	G41	D42		H47		V50	P51	Q52	K53	F54	F55	K56		V59	K60	V61	I62	G63		D68		L71		G74	Q75	V76	F77	L78	P79	R80	I81	A85	Q86

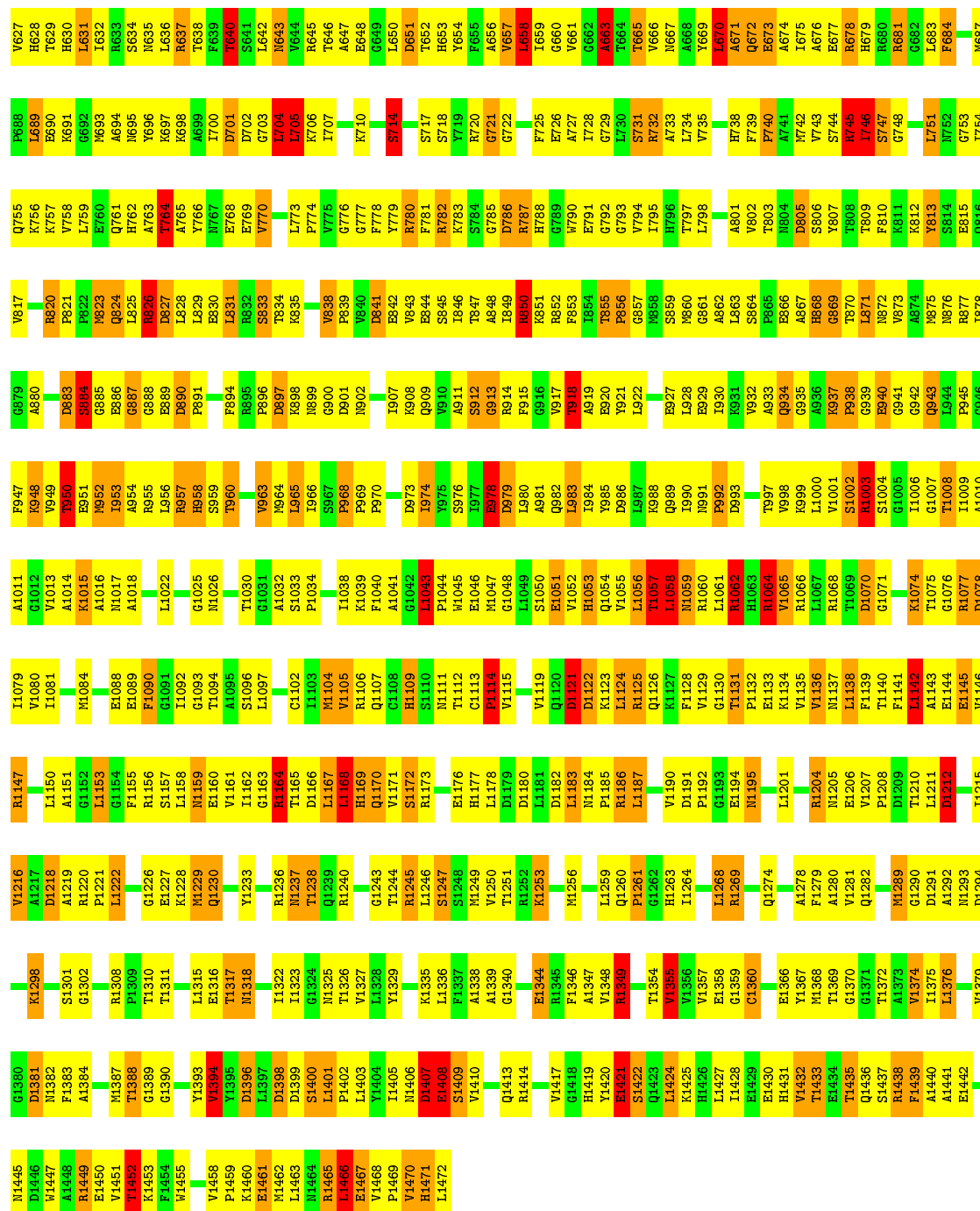




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S1050	G985	G913	E843	L773	L705	V644	G577	R515	A853	M390	K327	Q260	E199	I132	R69	G3
E1051	D986	R914	E844			V644			F454	I391	D328	Q261	R199	V133	K70	G4
H1052	L987	F915	S845	G776	I707	R845	E580	R518	G455	A392	G329	D262	F200	G134	L71	F5
H1053	G988	G916	T846	G777	I708	T846	A581	R519	G456	V393	P330	L263		H135	A72	I6
Q1054	Q889	V917	T847	F778	S709	A847	L582	R520	T457	D394	A381	K264	D203	H136	V73	A7
V1055	I990	T918	T848	F779	K710	E848	R583	S521	F458	L395	A382	V266			G74	A8
L1056	I991	R849	R850	R780	M711	G849	R584	L522	F459	Q396		V266	T206	V139	G75	I9
T1057	P992	R850	R851	F781	I713	L850	A585		D460	S397	M335	S140	Y207	S140	F76	D10
L1058	P992	R851	R852	R782	I714	L851	L586		M461	G398	T336	G268	R208	D141	F77	
M1059	D993	L922	R853	K783	G715	T852	R587	R526	E462	K399	D337	V269	Q209	E142	L78	R14
R1060		R923	R854	S784	G716	H853	R588	G527	L463	L400	G338	G270	R210	Q143	P79	R15
L1061		Q924	R854	G785	I716	T854	R589	N528	I464	Y401	K339		Y211	F144	R80	S16
V998			T855	D786	S717	A855	R590	N529		R402	V342	D273	S212	L146	I81	V17
K999			T856	R787	S718	A856	Q591	G530	R466	D403			T213	L145	S82	V18
R1063			R857	R788	S719	V857	E592	N531	R466	R404	M345		R214		L83	E19
R1064			R858	G789	R720	L858	T593	I532	M468	E405	T279		T215	Y149	D84	K20
V1065	S1002	K931	R859	G790	G721	L859	E594	L533		L406	D346	V280	F216	I150	A85	Q21
R1066	R1003	V932	R860	H790		G660	D595	D534	D471	K407	R347	F281	P217	I151	Q86	T22
L1067	S1004	A933	R861	E791		V661	A596	E535	G472	D408	K348	E282	T218	I152	E87	E23
G1068	G1005	Q934	G662		A727	G662	V597	D536	K473	H409	G349	V283	W219	R153	A88	A24
T1069	G1006	A936	G663			A663	R598	E537		L410	L350	M284	P220	R154	C89	L25
D1070	G1007	A936	T664			T664	G599	T538	I476	A411	R351	V285	L221	I155	R90	K26
G1071			T665			T665		Q539	G477	T412	P352		A222	E156	C91	A27
			V666			V666	T602	T540	S478	L413	K353		Q223		I92	
K1074			V667			V667	V603	R541	R491	K414	R354	R289	P224	V159	E93	R50
T1075			L670			L670	V604	L542	R492	P415	V355	T290	F225	K160	E94	R31
G1076			L671			L671	T605	L543	D481	M416	T356	A291	R226		T95	
R1077			A670			A670	L606	Q544	D482	D417	K357	P292	M227	E162	E96	V34
D1078			Q672			Q672	T607	L545	S483	K418	T358	M293	K228		I97	D35
I1079			E673			E673	D608	E546	P484	M419	T359	V294	L228		K36	
			A674			A674	E609	S548	L486	V420	D360	K295	A229		L98	
M1084			R675			R675	A610	P548	A486	Q422	L362	M296	M231	F167		D37
			R676			R676	G612	L550	V487	L488	L363	L298	G232		Y102	G38
A1087			R677			R677	P613	T551	S489	T423	T364	L298	T234	L172	I103	K39
E1088			R678			R678	G614	T552	D490	L426	G365	V299	M235	S173	I104	T40
E1089			R679			R679	R615	A553	K491	D427	G366		T236	A174	I105	G41
F1090			R680			R680	R615	E554	R492	E428	S367	L303	V237	R175	G106	D42
G1091			R681			R681	P619	F555	R493	L429	E368	T304	K238	S176	Q109	I46
I1092			R682			R682	A620	R556	Q494	V430	T369		G239	I177	V110	H47
G1093			R683			R683	L621	A557	L495	K431	G370	Q307	M240	H178	P111	V48
			F684			F684	L622	M558	H496	T432	K371	T308	V241	Y179	I112	L49
S1096			M687			M687	G625	R559	F497	A432	R372	T309	N242	K180	V50	
G1101			P688			P688	A626	D560	F498	A433	K373	P310	W243	G181	P51	
C1102			L689			L689	G626	Y561	F499	D442	I374	D244	M182	D115	Q52	
P1034			E890			E890	R500	M562	R500	E438	D375	N312	K245	D116	Q53	
Q1035			K691			K691	T629	G563	Q501	P439	E376	H313	A246	L184	I117	F54
V1105			G692			G692	H630	D564	N502	S440	T377	K314	E247	A185	G118	
R1106			M693			M693	L631	T565	F503	D441	Q378	A315	E248	E186	F55	
Q1107			A694			A694	L632	A566	S504	M442	V379	L316	T249	Q187	K56	
K1108			M695			M695	T632	R566	F504	D443	I380	I317	R250	Q187	D57	
F1109			G696			G696	R633	A567	Q505	K443	T380	I317	K250	L188	H58	
S1110			K697			K697	S634	E568	V506	D443	E381	Q318	M251	T189	N122	
N1111			T764			T764	R635	I569	T507	A445	K382	T319	E252	T190	A123	V59
G1043			A698			A698	L636	D570	N508	E446	G383	C320	R252	F191	K60	
T1112			R699			R699	R637	A571	P509	L447	K384	C321	P254	Y192	V61	
C1113			T700			T700	T638	T572	F509	L447	R385	S322	A255	Y192	I62	
P1114			D701			D701	F639	F373	I511	R448	G386	V323	F256	P193	G63	
V1115			E702			E702	T640	P574	D512	R450	P387	M324	G257	L195	H64	

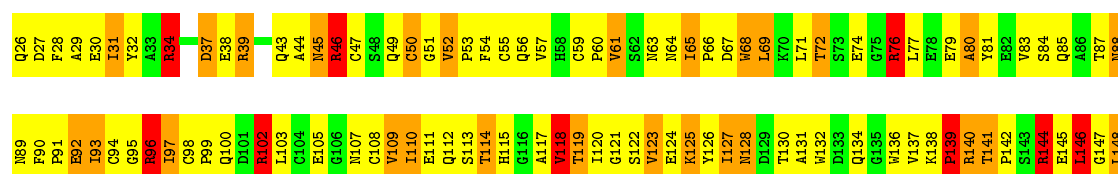


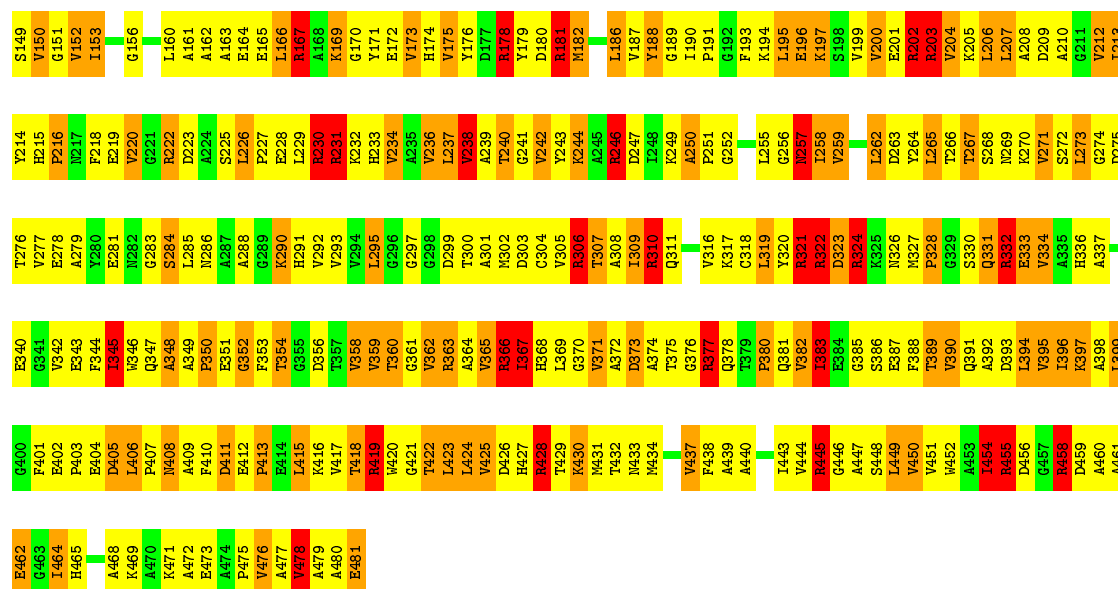
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F501	G439	G366	K296	L229	V159	E88	V3
I502	S440	S367	K297	E230	E160	C89	G4
F503	D441	C368	L298	K231	E162	R90	F5
S504	M442	T369	V299	G232	Q163	C91	
Q505	D443			E233	I164	I92	A8
	K444	I374	A302	L234	M165	V93	I9
N508	A445	D375	L303	K235	D166	E94	
F509	E446	E376	T304	T236			K12
P510	L447	F377	Q307	V237	S171	L98	P13
L511	R448	Q378	K308	K238	L172	A99	
D512	R449	F379	T308	G239	S173	F100	A24
F515	R450	I380	T309	K240	A174	G101	L26
S513	Q451	E381	P310	V241	R175	Y102	K26
R515	Q452		D311	K242	S176		
	A453	L383	N312	I243	I177	Y105	H30
	F454	G386	H313	K244		G106	R31
	G455	P387	A315	K245	M182	I107	
	L456	G388	G316	E248	F183	R108	V34
	T457	E389	L316	K249	Q109	Q109	D35
	M458	K390	I317	T250	A185	A36	D37
	E459		Q318	K250	E186	P111	
R525	D460	V393	S319	K251	Q187	I112	C38
L526	M461	D394	G320	E252	L188	M113	C39
Q527	E462	L395	N321	H253	T189	T40	T40
N528	L463	G396	S322	T254	K190	D115	G41
L529	L464	S397		A255	T190	D115	
S530	I465	G398	E325	F256	Y192	I117	D42
N531	H466	K399	P326	G257	P193	G118	H47
	P467		K327	T258	D194	E119	V48
		R402	D328	H259	L195	A49	A49
D471	G472	D403	D329	T261	L196	V50	
G473	K473	R404	P330	Q261	D197	P51	
	E474	L406		D262	E198	Q52	
	A475	K407	T336	L263	R199	K53	
	L476	D408	D337				
G477	G409	G338	R339	T267	D203	Q130	F54
S478	L410	L410			I131	F55	
M479	A411		V342	V268	T206	M136	V59
G480	T412	G343	G343	G270	H208	K137	K60
D481	L413	G344	M345		Q209	G138	V61
S482	P415	R346	D347	S274	R210	I62	
F483	P416	R347		D278	Y211	S140	G63
L485	D417	N348	T279	T279	S212	D141	
A486	K418	C349	G349	V280	T213	E142	D68
R487	M419	L350	F281	F281	N214	Q143	
L488	Q420	F282	T215	E282	T215	F144	L71
S489	Q421	P352	V283	K283	E146	E146	
D490	M422	K284	T217	V285	P217	L147	G74
K491	T423	R354	V219	K286	T218	D147	Q75
Y492		Y355			L148	V76	
					Y149	F77	
F493					L221	I150	L78
					A222	I151	P79
	L426	D427	T359	R289	Q224	R152	R80
	G494	E428	D360	T290	P224	K153	
	L429	G361	A291	K291	Q225	I81	
	H496	L429	P292	P292	F154		
	R497	V430	T293	V293	T155		A95

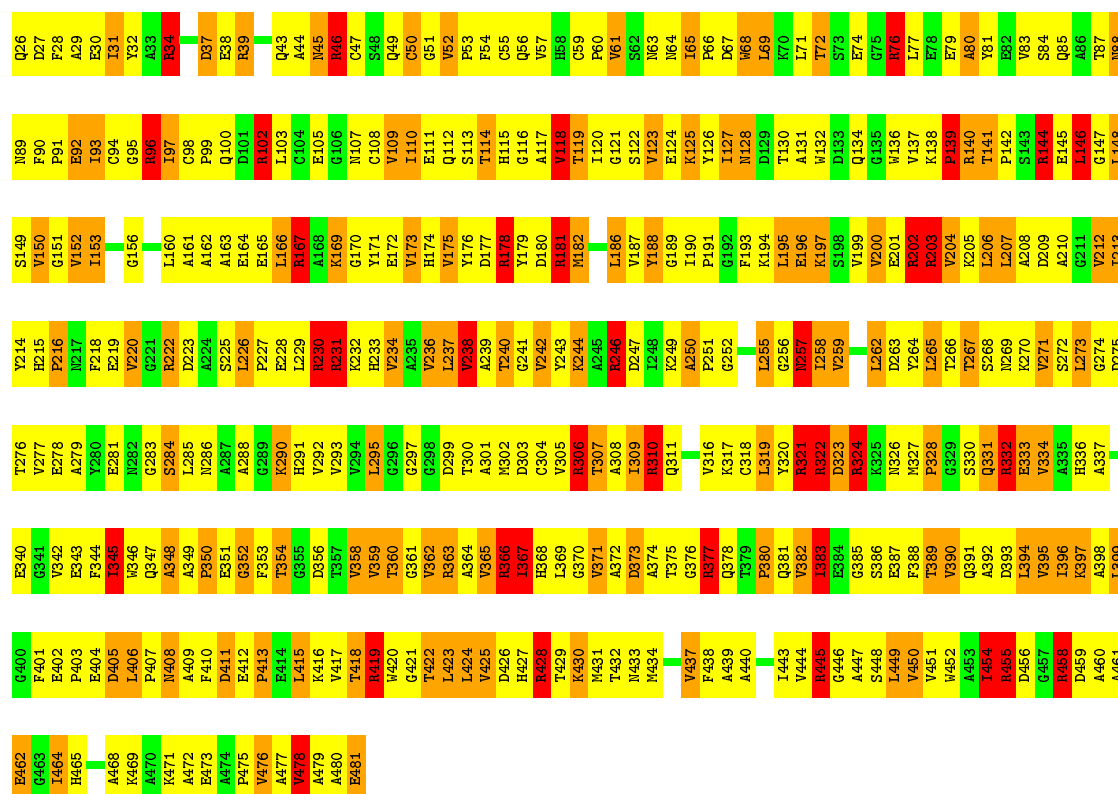


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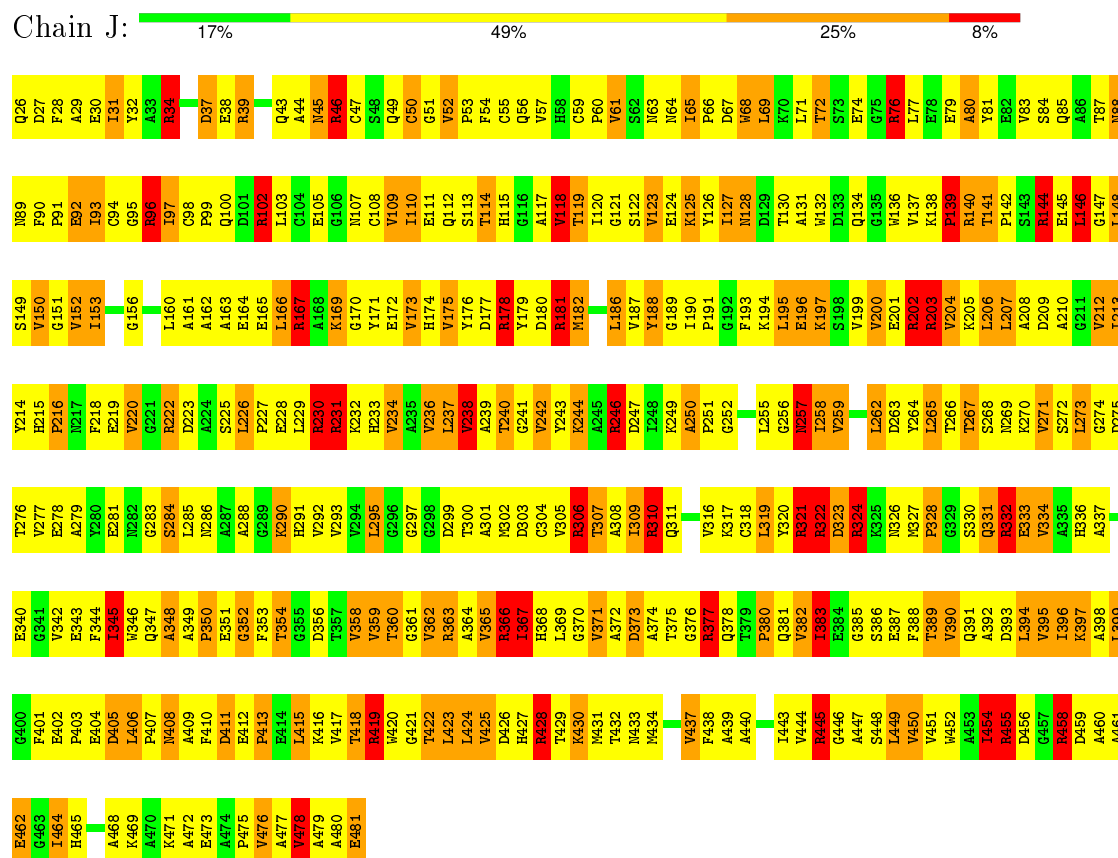
Chain G: 18% 49% 25% 8%



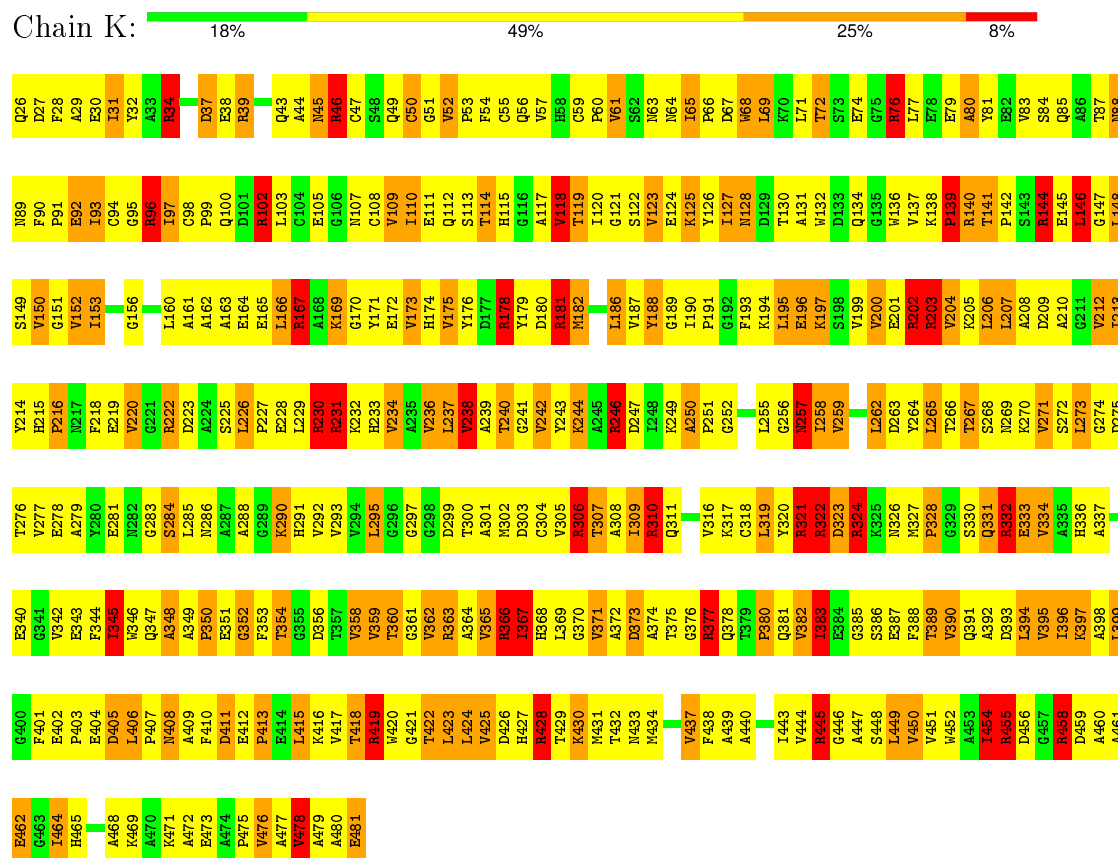




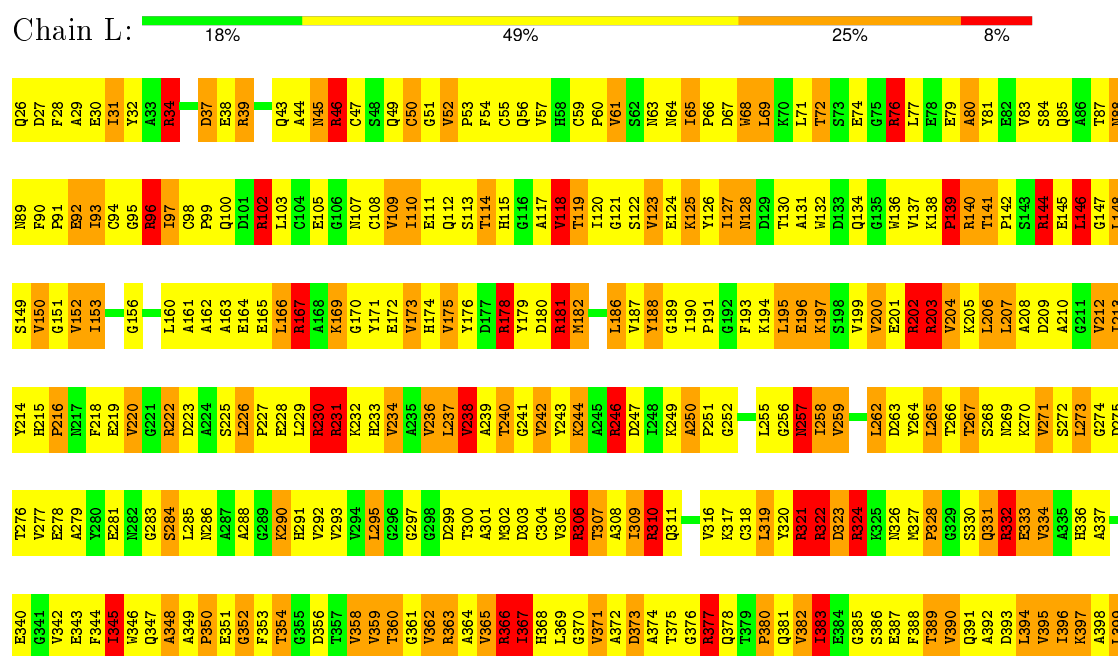
- Molecule 2: GLUTAMATE SYNTHASE [NADPH] SMALL CHAIN



• Molecule 2: GLUTAMATE SYNTHASE [NADPH] SMALL CHAIN



• Molecule 2: GLUTAMATE SYNTHASE [NADPH] SMALL CHAIN





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	WIENER FILTERING OF VOLUMES FROM FOCAL SERIES	Depositor
Microscope	JEOL 2010F UHR	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FMN, F3S, OMT, AKG, FAD

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	1.06	7/11545 (0.1%)	1.58	200/15613 (1.3%)
1	B	1.10	7/11545 (0.1%)	1.58	192/15613 (1.2%)
1	C	1.06	8/11545 (0.1%)	1.58	201/15613 (1.3%)
1	D	1.10	7/11545 (0.1%)	1.58	191/15613 (1.2%)
1	E	1.06	7/11545 (0.1%)	1.58	200/15613 (1.3%)
1	F	1.10	7/11545 (0.1%)	1.58	194/15613 (1.2%)
2	G	1.00	0/3533	1.78	76/4793 (1.6%)
2	H	1.00	0/3533	1.78	76/4793 (1.6%)
2	I	1.00	0/3533	1.78	76/4793 (1.6%)
2	J	1.00	0/3533	1.78	76/4793 (1.6%)
2	K	1.00	0/3533	1.78	76/4793 (1.6%)
2	L	1.00	0/3533	1.78	76/4793 (1.6%)
All	All	1.07	43/90468 (0.0%)	1.63	1634/122436 (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	3
1	B	0	2
1	C	1	3
1	D	0	2
1	E	1	3
1	F	0	2
2	G	0	31
2	H	0	31
2	I	0	31
2	J	0	31
2	K	0	31

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	31
All	All	3	201

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	838	VAL	CA-CB	-7.81	1.38	1.54
1	A	838	VAL	CA-CB	-7.78	1.38	1.54
1	E	838	VAL	CA-CB	-7.76	1.38	1.54
1	E	746	ILE	CA-CB	-7.49	1.37	1.54
1	A	746	ILE	CA-CB	-7.46	1.37	1.54

The worst 5 of 1634 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	45	ASN	CB-CG-OD1	-39.98	41.63	121.60
2	L	45	ASN	CB-CG-OD1	-39.98	41.63	121.60
2	G	45	ASN	CB-CG-OD1	-39.98	41.65	121.60
2	J	45	ASN	CB-CG-OD1	-39.98	41.65	121.60
2	I	45	ASN	CB-CG-OD1	-39.95	41.70	121.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	915	PHE	CA
1	C	915	PHE	CA
1	E	915	PHE	CA

5 of 201 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1002	SER	Mainchain
1	A	1171	VAL	Peptide
1	A	325	GLU	Mainchain
1	B	1168	LEU	Mainchain
1	B	725	PHE	Mainchain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11337	0	11347	1764	0
1	B	11337	0	11350	1542	0
1	C	11337	0	11347	1760	0
1	D	11337	0	11350	1536	0
1	E	11337	0	11347	1772	0
1	F	11337	0	11350	1543	0
2	G	3468	0	3397	1086	0
2	H	3468	0	3397	1079	0
2	I	3468	0	3397	1089	0
2	J	3468	0	3399	1075	0
2	K	3468	0	3399	1080	0
2	L	3468	0	3399	1078	0
3	A	11	0	10	3	0
3	B	11	0	10	0	0
3	C	11	0	10	3	0
3	D	11	0	10	0	0
3	E	11	0	10	3	0
3	F	11	0	10	1	0
4	A	31	0	19	4	0
4	B	31	0	19	7	0
4	C	31	0	19	3	0
4	D	31	0	19	7	0
4	E	31	0	19	4	0
4	F	31	0	19	6	0
5	A	10	0	4	0	0
5	B	10	0	4	2	0
5	C	10	0	4	0	0
5	D	10	0	4	2	0
5	E	10	0	4	0	0
5	F	10	0	4	1	0
6	A	7	0	0	1	0
6	B	7	0	0	3	0
6	C	7	0	0	1	0
6	D	7	0	0	3	0
6	E	7	0	0	4	0
6	F	7	0	0	3	0
7	G	16	0	0	2	0
7	H	16	0	0	2	0
7	I	16	0	0	2	0
7	J	16	0	0	2	0
7	K	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	16	0	0	2	0
8	G	53	0	31	18	0
8	H	53	0	31	18	0
8	I	53	0	31	18	0
8	J	53	0	31	18	0
8	K	53	0	31	18	0
8	L	53	0	31	17	0
All	All	89598	0	88863	15409	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 86.

The worst 5 of 15409 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:1263:HIS:CE1	1:D:900:GLY:CA	1.77	1.66
1:A:782:ARG:CG	2:J:53:PRO:HD2	1.19	1.65
1:E:782:ARG:CG	2:L:53:PRO:HD2	1.19	1.64
1:F:182:MET:CE	1:F:217:PRO:HB2	1.30	1.61
1:E:782:ARG:HG2	2:L:53:PRO:CD	1.14	1.61

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 PDB entries followed by that with respect to all EM entries.

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	1470/1472 (100%)	1174 (80%)	231 (16%)	65 (4%)	3	33
1	B	1470/1472 (100%)	1191 (81%)	215 (15%)	64 (4%)	3	33
1	C	1470/1472 (100%)	1175 (80%)	230 (16%)	65 (4%)	3	33
1	D	1470/1472 (100%)	1191 (81%)	215 (15%)	64 (4%)	3	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	1470/1472 (100%)	1174 (80%)	231 (16%)	65 (4%)	3	33
1	F	1470/1472 (100%)	1192 (81%)	214 (15%)	64 (4%)	3	33
2	G	454/456 (100%)	419 (92%)	25 (6%)	10 (2%)	8	49
2	H	454/456 (100%)	420 (92%)	24 (5%)	10 (2%)	8	49
2	I	454/456 (100%)	420 (92%)	24 (5%)	10 (2%)	8	49
2	J	454/456 (100%)	419 (92%)	25 (6%)	10 (2%)	8	49
2	K	454/456 (100%)	420 (92%)	24 (5%)	10 (2%)	8	49
2	L	454/456 (100%)	420 (92%)	24 (5%)	10 (2%)	8	49
All	All	11544/11568 (100%)	9615 (83%)	1482 (13%)	447 (4%)	7	36

5 of 447 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 ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1201/1201 (100%)	985 (82%)	216 (18%)	2	15
1	B	1201/1201 (100%)	981 (82%)	220 (18%)	2	14
1	C	1201/1201 (100%)	985 (82%)	216 (18%)	2	15
1	D	1201/1201 (100%)	981 (82%)	220 (18%)	2	14
1	E	1201/1201 (100%)	985 (82%)	216 (18%)	2	15
1	F	1201/1201 (100%)	981 (82%)	220 (18%)	2	14
2	G	358/358 (100%)	257 (72%)	101 (28%)	0	3
2	H	358/358 (100%)	257 (72%)	101 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	358/358 (100%)	257 (72%)	101 (28%)	0	3
2	J	358/358 (100%)	257 (72%)	101 (28%)	0	3
2	K	358/358 (100%)	257 (72%)	101 (28%)	0	3
2	L	358/358 (100%)	257 (72%)	101 (28%)	0	3
All	All	9354/9354 (100%)	7440 (80%)	1914 (20%)	4	10

5 of 1914 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1435	THR
1	E	1402	PRO
2	K	322	ARG
1	E	120	LYS
1	E	636	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 277 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	247	HIS
1	E	52	GLN
2	J	56	GLN
1	D	321	ASN
1	D	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

42 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	OMT	A	2473	-	7,10,10	4.38	4 (57%)	8,14,14	4.85	6 (75%)
4	FMN	A	2474	-	32,33,33	1.37	5 (15%)	34,50,50	3.29	17 (50%)
5	AKG	A	2475	-	3,9,9	4.56	2 (66%)	4,11,11	2.82	2 (50%)
6	F3S	A	2476	1	0,9,9	0.00	-	0,15,15	0.00	-
3	OMT	B	2473	-	7,10,10	4.32	4 (57%)	8,14,14	7.18	5 (62%)
4	FMN	B	2474	-	32,33,33	1.23	4 (12%)	34,50,50	2.71	16 (47%)
5	AKG	B	2475	-	3,9,9	4.89	2 (66%)	4,11,11	3.33	2 (50%)
6	F3S	B	2476	1	0,9,9	0.00	-	0,15,15	0.00	-
3	OMT	C	2473	-	7,10,10	4.39	4 (57%)	8,14,14	4.86	6 (75%)
4	FMN	C	2474	-	32,33,33	1.37	5 (15%)	34,50,50	3.29	17 (50%)
5	AKG	C	2475	-	3,9,9	4.55	2 (66%)	4,11,11	2.82	2 (50%)
6	F3S	C	2476	1	0,9,9	0.00	-	0,15,15	0.00	-
3	OMT	D	2473	-	7,10,10	4.31	4 (57%)	8,14,14	7.18	5 (62%)
4	FMN	D	2474	-	32,33,33	1.23	4 (12%)	34,50,50	2.71	16 (47%)
5	AKG	D	2475	-	3,9,9	4.91	2 (66%)	4,11,11	3.33	2 (50%)
6	F3S	D	2476	1	0,9,9	0.00	-	0,15,15	0.00	-
3	OMT	E	2473	-	7,10,10	4.38	4 (57%)	8,14,14	4.85	6 (75%)
4	FMN	E	2474	-	32,33,33	1.37	5 (15%)	34,50,50	3.29	17 (50%)
5	AKG	E	2475	-	3,9,9	4.55	2 (66%)	4,11,11	2.82	2 (50%)
6	F3S	E	2476	1	0,9,9	0.00	-	0,15,15	0.00	-
3	OMT	F	2473	-	7,10,10	4.32	4 (57%)	8,14,14	7.18	5 (62%)
4	FMN	F	2474	-	32,33,33	1.23	4 (12%)	34,50,50	2.71	16 (47%)
5	AKG	F	2475	-	3,9,9	4.91	2 (66%)	4,11,11	3.33	2 (50%)
6	F3S	F	2476	1	0,9,9	0.00	-	0,15,15	0.00	-
7	SF4	G	482	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	G	483	2	0,12,12	0.00	-	0,24,24	0.00	-
8	FAD	G	484	-	52,58,58	2.12	19 (36%)	52,89,89	2.00	11 (21%)
7	SF4	H	482	2	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SF4	H	483	2	0,12,12	0.00	-	0,24,24	0.00	-
8	FAD	H	484	-	52,58,58	2.12	19 (36%)	52,89,89	2.00	11 (21%)
7	SF4	I	482	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	I	483	2	0,12,12	0.00	-	0,24,24	0.00	-
8	FAD	I	484	-	52,58,58	2.12	19 (36%)	52,89,89	2.00	11 (21%)
7	SF4	J	482	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	J	483	2	0,12,12	0.00	-	0,24,24	0.00	-
8	FAD	J	484	-	52,58,58	2.12	19 (36%)	52,89,89	2.00	11 (21%)
7	SF4	K	482	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	K	483	2	0,12,12	0.00	-	0,24,24	0.00	-
8	FAD	K	484	-	52,58,58	2.12	19 (36%)	52,89,89	2.00	11 (21%)
7	SF4	L	482	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	L	483	2	0,12,12	0.00	-	0,24,24	0.00	-
8	FAD	L	484	-	52,58,58	2.12	19 (36%)	52,89,89	2.00	11 (21%)

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	OMT	A	2473	-	-	0/6/10/10	0/0/0/0
4	FMN	A	2474	-	-	0/18/18/18	0/3/3/3
5	AKG	A	2475	-	-	0/3/9/9	0/0/0/0
6	F3S	A	2476	1	-	0/0/24/24	0/0/3/3
3	OMT	B	2473	-	-	0/6/10/10	0/0/0/0
4	FMN	B	2474	-	-	0/18/18/18	0/3/3/3
5	AKG	B	2475	-	-	0/3/9/9	0/0/0/0
6	F3S	B	2476	1	-	0/0/24/24	0/0/3/3
3	OMT	C	2473	-	-	0/6/10/10	0/0/0/0
4	FMN	C	2474	-	-	0/18/18/18	0/3/3/3
5	AKG	C	2475	-	-	0/3/9/9	0/0/0/0
6	F3S	C	2476	1	-	0/0/24/24	0/0/3/3
3	OMT	D	2473	-	-	0/6/10/10	0/0/0/0
4	FMN	D	2474	-	-	0/18/18/18	0/3/3/3
5	AKG	D	2475	-	-	0/3/9/9	0/0/0/0
6	F3S	D	2476	1	-	0/0/24/24	0/0/3/3
3	OMT	E	2473	-	-	0/6/10/10	0/0/0/0
4	FMN	E	2474	-	-	0/18/18/18	0/3/3/3
5	AKG	E	2475	-	-	0/3/9/9	0/0/0/0
6	F3S	E	2476	1	-	0/0/24/24	0/0/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMT	F	2473	-	-	0/6/10/10	0/0/0/0
4	FMN	F	2474	-	-	0/18/18/18	0/3/3/3
5	AKG	F	2475	-	-	0/3/9/9	0/0/0/0
6	F3S	F	2476	1	-	0/0/24/24	0/0/3/3
7	SF4	G	482	2	-	0/0/48/48	0/6/5/5
7	SF4	G	483	2	-	0/0/48/48	0/6/5/5
8	FAD	G	484	-	-	0/30/50/50	0/6/6/6
7	SF4	H	482	2	-	0/0/48/48	0/6/5/5
7	SF4	H	483	2	-	0/0/48/48	0/6/5/5
8	FAD	H	484	-	-	0/30/50/50	0/6/6/6
7	SF4	I	482	2	-	0/0/48/48	0/6/5/5
7	SF4	I	483	2	-	0/0/48/48	0/6/5/5
8	FAD	I	484	-	-	0/30/50/50	0/6/6/6
7	SF4	J	482	2	-	0/0/48/48	0/6/5/5
7	SF4	J	483	2	-	0/0/48/48	0/6/5/5
8	FAD	J	484	-	-	0/30/50/50	0/6/6/6
7	SF4	K	482	2	-	0/0/48/48	0/6/5/5
7	SF4	K	483	2	-	0/0/48/48	0/6/5/5
8	FAD	K	484	-	-	0/30/50/50	0/6/6/6
7	SF4	L	482	2	-	0/0/48/48	0/6/5/5
7	SF4	L	483	2	-	0/0/48/48	0/6/5/5
8	FAD	L	484	-	-	0/30/50/50	0/6/6/6

The worst 5 of 177 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2473	OMT	CG-SD	-7.14	1.69	1.78
3	F	2473	OMT	CG-SD	-7.13	1.69	1.78
3	D	2473	OMT	CG-SD	-7.11	1.69	1.78
3	E	2473	OMT	CG-SD	-6.94	1.69	1.78
3	A	2473	OMT	CG-SD	-6.89	1.69	1.78

The worst 5 of 210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2473	OMT	OD2-SD-CG	-18.10	96.68	108.26
3	F	2473	OMT	OD2-SD-CG	-18.08	96.69	108.26
3	B	2473	OMT	OD2-SD-CG	-18.06	96.70	108.26
3	C	2473	OMT	OD2-SD-CE	-10.72	97.22	108.91
3	A	2473	OMT	OD2-SD-CE	-10.70	97.24	108.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

31 monomers are involved in 180 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2473	OMT	3	0
4	A	2474	FMN	4	0
6	A	2476	F3S	1	0
4	B	2474	FMN	7	0
5	B	2475	AKG	2	0
6	B	2476	F3S	3	0
3	C	2473	OMT	3	0
4	C	2474	FMN	3	0
6	C	2476	F3S	1	0
4	D	2474	FMN	7	0
5	D	2475	AKG	2	0
6	D	2476	F3S	3	0
3	E	2473	OMT	3	0
4	E	2474	FMN	4	0
6	E	2476	F3S	4	0
3	F	2473	OMT	1	0
4	F	2474	FMN	6	0
5	F	2475	AKG	1	0
6	F	2476	F3S	3	0
7	G	483	SF4	2	0
8	G	484	FAD	18	0
7	H	483	SF4	2	0
8	H	484	FAD	18	0
7	I	483	SF4	2	0
8	I	484	FAD	18	0
7	J	483	SF4	2	0
8	J	484	FAD	18	0
7	K	483	SF4	2	0
8	K	484	FAD	18	0
7	L	483	SF4	2	0
8	L	484	FAD	17	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.