



wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 04:59 PM EST

PDB ID : 8DGC
EMDB ID : EMD-27421
Title : Avs3 bound to phage PhiV-1 terminase
Authors : Wilkinson, M.E.; Gao, L.; Strecker, J.; Makarova, K.S.; Macrae, R.K.; Koonin, E.V.; Zhang, F.
Deposited on : 2022-06-23
Resolution : 3.40 Å(reported)

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

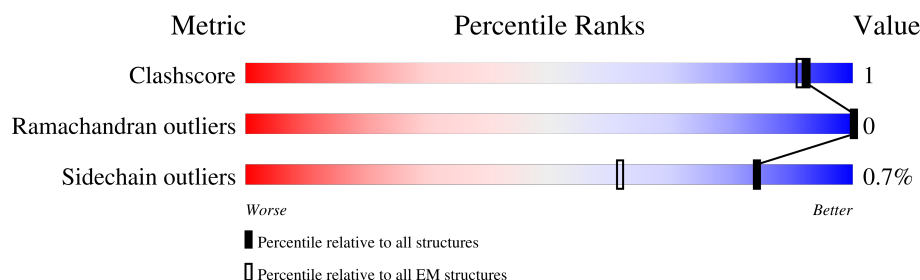
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2092	<div> <div>66%</div> <div>93%</div> <div>• •</div> </div>
1	B	2092	<div> <div>65%</div> <div>91%</div> <div>5% •</div> </div>
1	C	2092	<div> <div>66%</div> <div>93%</div> <div>• •</div> </div>
1	D	2092	<div> <div>65%</div> <div>91%</div> <div>5% •</div> </div>
2	E	586	<div> <div>92%</div> <div>87%</div> <div>• 8%</div> </div>
2	F	586	<div> <div>92%</div> <div>87%</div> <div>5% 8%</div> </div>
2	G	586	<div> <div>92%</div> <div>87%</div> <div>5% 8%</div> </div>
2	H	586	<div> <div>92%</div> <div>86%</div> <div>5% 8%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 81600 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 SeAvs3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2028	Total	C	N	O	S	0	0
			16152	10199	2840	3056	57		
1	B	2004	Total	C	N	O	S	0	0
			15974	10095	2809	3014	56		
1	C	2028	Total	C	N	O	S	0	0
			16152	10199	2840	3056	57		
1	D	2004	Total	C	N	O	S	0	0
			15974	10095	2809	3014	56		

- Molecule 2 is a protein called Terminase, large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	538	Total	C	N	O	S	0	0
			4273	2717	741	796	19		
2	F	538	Total	C	N	O	S	0	0
			4273	2717	741	796	19		
2	G	538	Total	C	N	O	S	0	0
			4273	2717	741	796	19		
2	H	538	Total	C	N	O	S	0	0
			4273	2717	741	796	19		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0
3	F	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0
3	H	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0
4	B	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0

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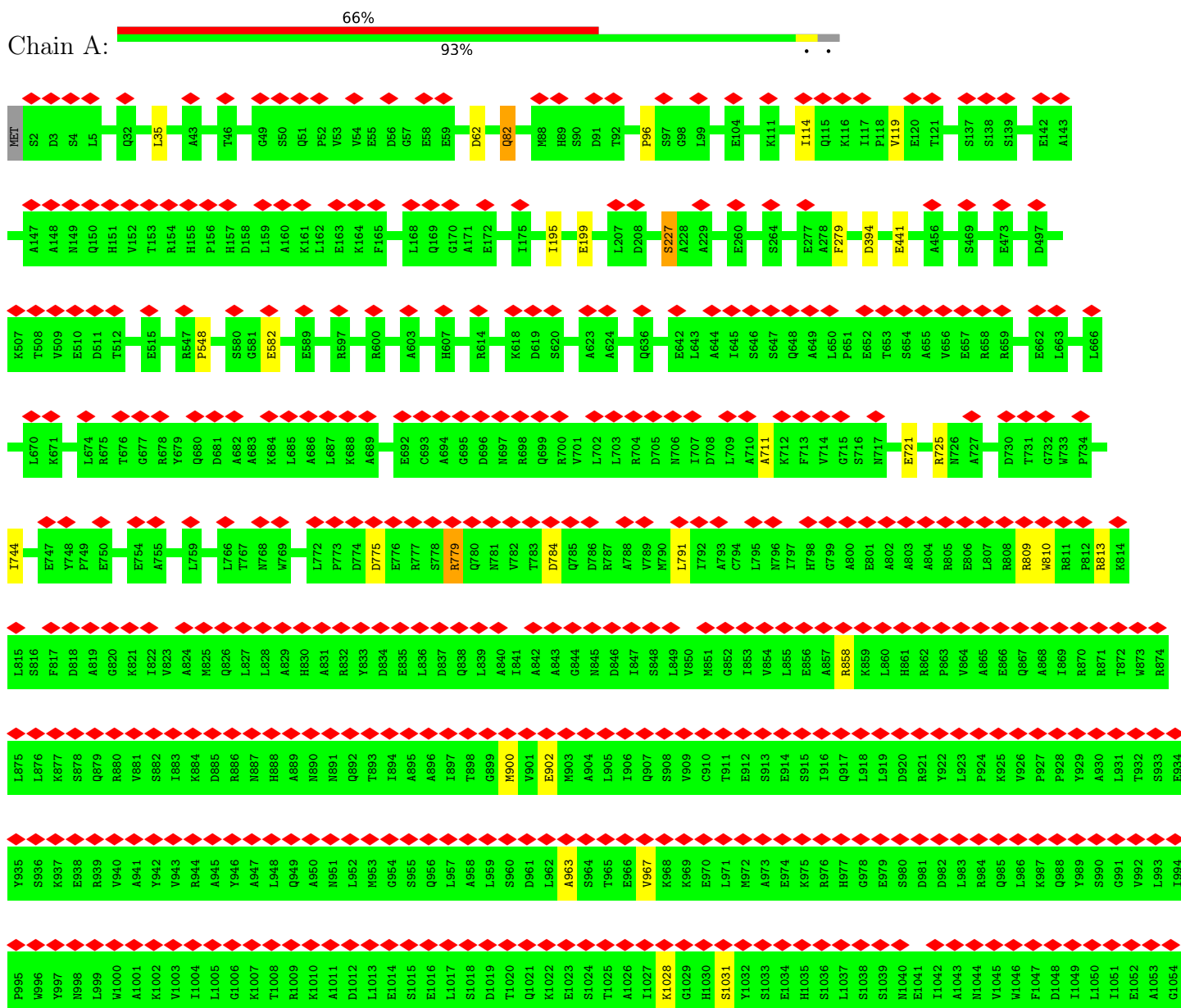
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Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0
4	G	1	Total 1	Mg 1	0
4	H	1	Total 1	Mg 1	0

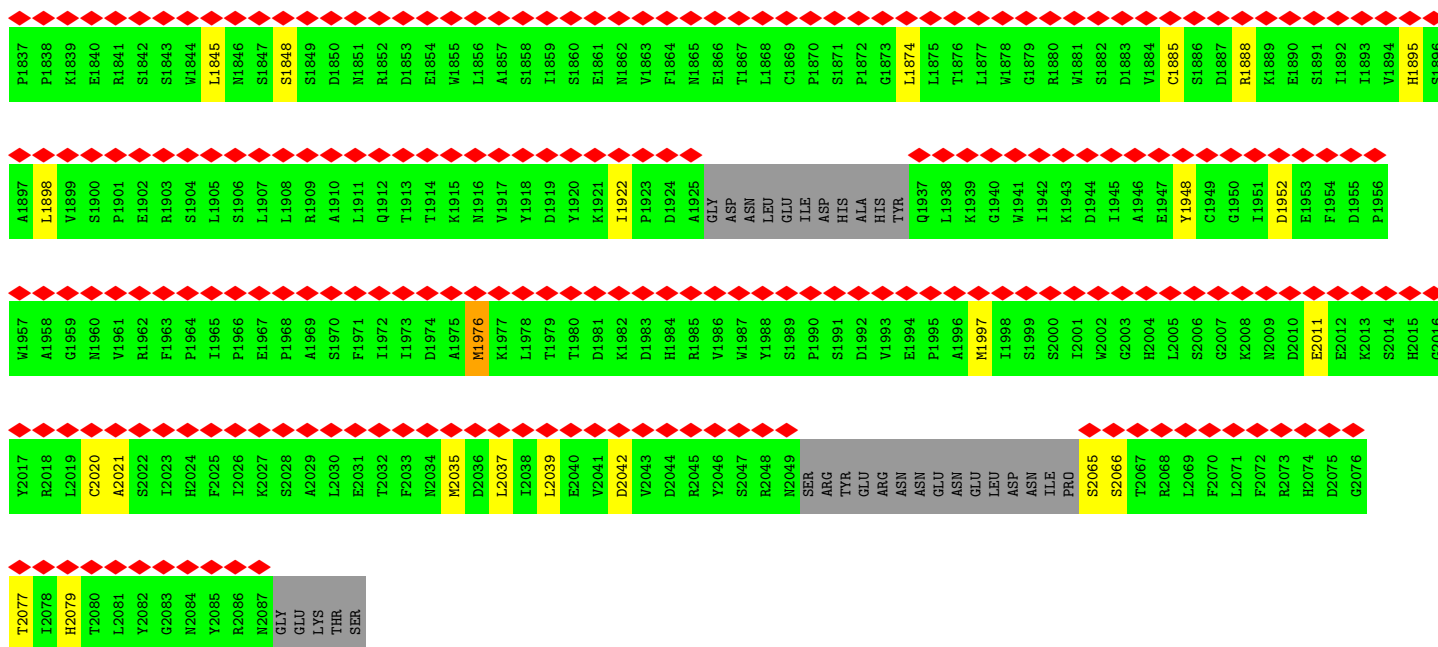
3 Residue-property plots

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

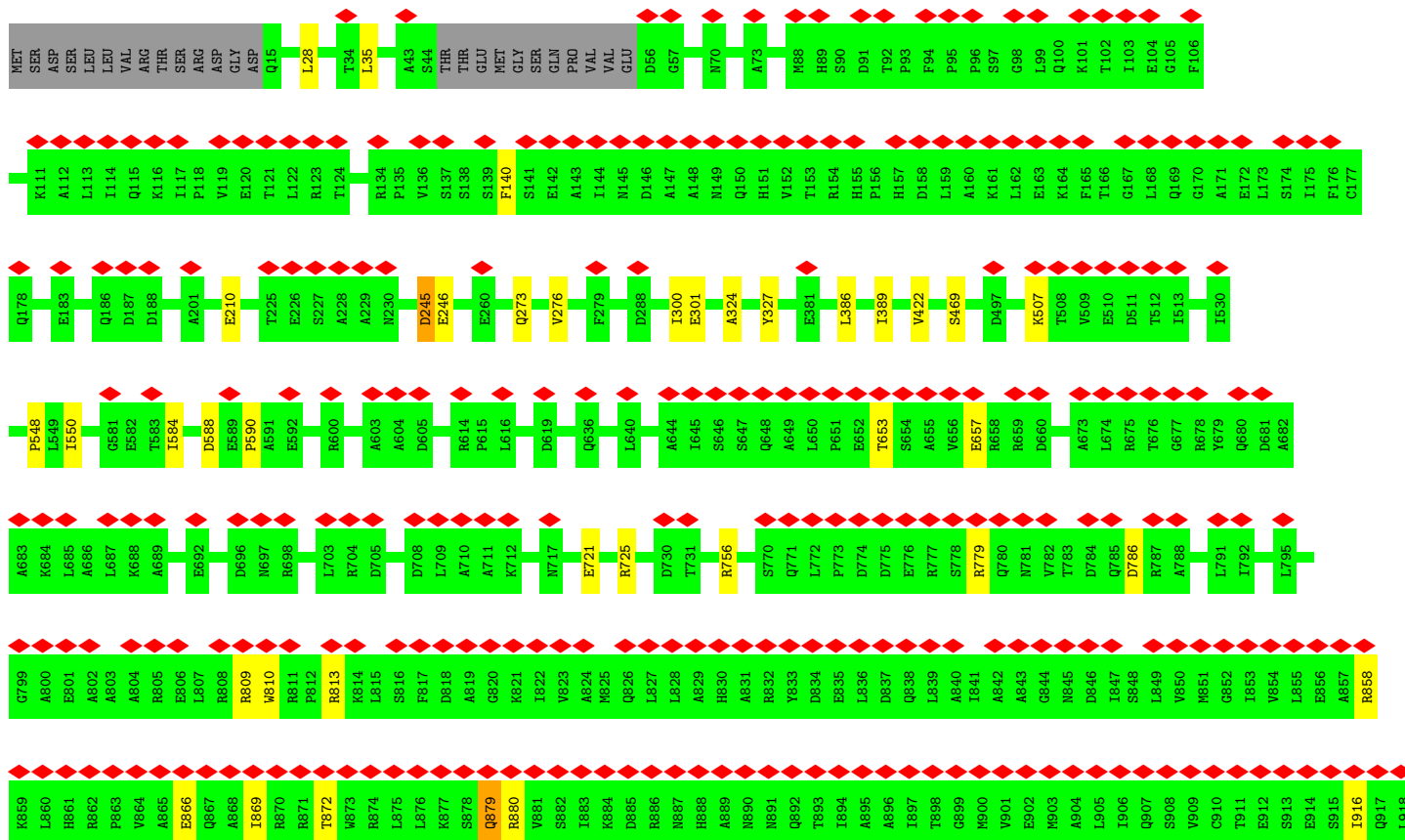
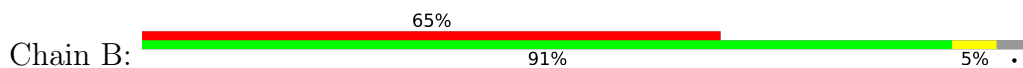
• Molecule 1: SeAvs3



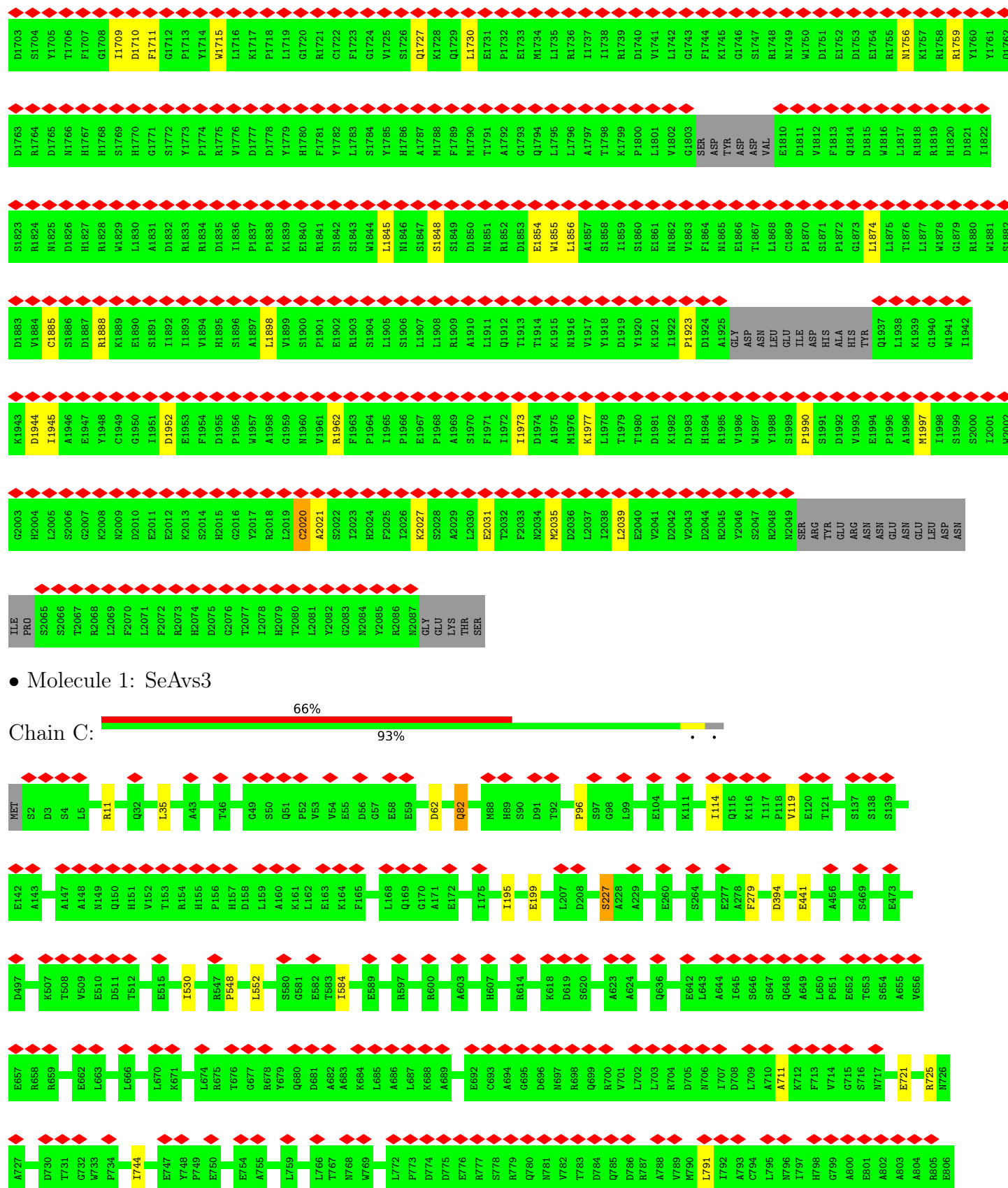
D1777	K1717	F1657	M1597	G1537	K1477	Y1416	I1356	F1296	L1236	P1176	A1115	N1055
D1778	P1718	A1658	A1598	P1538	E1478	D1417	F1367	M1297	A1237	P1177	Q1116	V1056
D1779	L1719	A1659	T1599	W1539	I1479	F1418	K1358	V1298	W1238	E1178	I1117	S1057
H1780	G1720	R1660	T1600	M1540	F1480	K1419	D1359	Q1299	T1239	I1179	K1118	K1058
F1781	R1721	T1661	L1601	E1541	G1461	Y1420	C1360	N1300	I1240	S1180	A1119	D1059
Y1782	C1722	L1662	P1602	K1542	I1482	I1421	D1361	I1301	E1241	Y1181	D1120	D1060
F1783	F1723	L1663	F1603	L1543	T1483	L1422	L1362	Q1302	H1242	K1182	G1121	L1061
S1784	G1724	A1664	C1604	S1544	L1484	E1423	S1363	M1303	L1243	L1183	Y1122	E1062
V1785	V1725	L1665	D1605	P1545	E1485	S1424	S1364	L1304	V1244	A1184	I1123	N1063
H1786	S1726	H1666	R1606	P1546	A1486	I1425	I1365	K1305	K1245	R1185	L1125	I1064
Q1727	Q1727	D1667	M1607	T1547	I1487	P1426	D1366	K1306	K1246	C1186	S1126	I1065
K1728	K1728	S1668	L1608	H1548	A1488	D1427	G1367	L1307	W1247	A1187	R1127	K1066
F1789	F1789	D1669	P1609	V1549	E1489	E1428	I1368	D1308	K1248	E1188	S1128	S1068
M1790	L1730	L1670	F1610	E1550	S1490	W1429	S1369	A1309	I1249	L1189	L1129	Q1069
T1791	E1731	I1671	Y1611	D1551	P1491	T1430	A1370	I1310	N1250	T1190	I1130	H1070
P1732	P1732	S1672	L1612	S1552	P1493	S1431	A1371	S1311	A1251	R1191	S1131	K1071
G1793	G1733	L1673	L1613	L1553	A1494	R1432	Y1372	T1312	L1252	E1192	L1132	G1072
M1794	M1734	P1674	H1614	A1554	N1495	L1433	E1373	S1313	D1253	Y1193	D1133	L1073
L1795	L1735	A1675	A1615	G1555	S1496	S1434	K1374	L1314	A1254	V1194	E1134	N1073
R1736	R1736	Q1676	Q1616	Y1556	D1497	I1435	F1375	G1315	L1255	D1195	P1135	R1074
L1796	L1737	E1677	L1617	I1557	R1498	K1436	R1376	I1316	P1256	R1196	E1136	V1075
T1798	I1738	E1678	W1618	W1558	L1499	L1439	N1377	E1317	L1257	D1197	A1137	F1076
K1799	R1739	M1679	L1619	A1559	F1500	A1440	V1378	H1318	I1258	K1198	K1138	T1077
D1740	D1740	M1680	M1620	R1560	S1501	G1441	P1379	T1319	T1259	H1199	E1139	P1078
V1741	V1741	L1681	I1621	L1561	L1502	L1442	E1381	E1320	F1260	F1201	Y1140	T1079
L1801	L1801	G1682	A1622	G1562	G1504	I1443	F1381	L1321	E1261	A1201	F1141	L1080
V1802	G1743	M1683	A1623	S1563	L1505	K1444	Y1382	K1322	N1262	W1202	N1142	H1081
G1803	F1744	I1684	A1624	P1564	L1506	E1445	S1383	E1323	D1263	S1203	Q1143	L1082
ASP	K1745	M1685	R1625	A1565	L1507	E1446	K1384	R1324	W1264	D1204	A1144	F1083
TYR	G1746	Q1686	V1626	A1566	S1508	Y1447	E1385	I1325	H1265	T1205	I1145	S1084
ASP	S1747	S1687	A1627	E1567	K1509	Q1448	T1386	S1326	K1266	V1206	E1146	S1085
VAL	R1748	T1688	L1628	M1568	K1509	L1448	F1387	G1327	C1267	E1207	N1149	V1086
E1810	N1749	R1689	D1629	R1569	L1510	R1449	I1388	L1328	D1268	T1208	C1087	C1087
D1811	W1750	M1690	D1630	W1570	E1511	F1450	K1389	Q1329	L1269	L1209	K1150	A1088
F1812	D1751	P1691	G1631	Q1571	S1512	C1451	M1391	K1329	L1270	A1210	L1151	A1089
F1813	E1752	L1692	K1632	A1572	E1514	M1452	K1390	H1330	L1271	E1211	G1152	I1090
Q1814	Q1814	LEU	A1573	A1573	R1453	R1453	A1391	THR	D1271	E1211	D1163	S1091
D1815	D1753	ASP	S1633	H1574	A1515	I1454	I1392	THR	S1272	L1212	E1154	L1091
W1816	E1754	LYS	L1634	A1575	L1516	R1455	S1393	VAL	V1273	C1213	N1155	G1092
L1817	R1755	VAL	I1635	A1575	D1517	R1456	R1394	SER	L1274	P1214	L1156	L1093
R1818	R1756	ASP	P1636	V1576	V1518	S1457	V1395	LYS	S1275	S1215	S1157	G1094
K1819	K1757	HIS	N1637	L1577	V1519	S1457	K1396	SER	S1276	S1216	E1095	E1095
R1819	R1758	ARG	I1638	A1578	S1520	R1458	T1397	SER	G1277	A1217	W1159	L1096
H1820	H1820	GLY	G1639	L1579	Y1521	V1460	G1398	LEU	T1278	L1218	E1160	S1097
R1759	R1759	GLY	G1639	C1580	Y1521	Y1460	K1399	SER	T1278	E1160	E1160	Y1098
D1821	E1760	E1702	Y1640	R1581	A1522	E1461	E1400	SER	D1279	A1219	A1161	H1099
I1822	Y1761	D1703	F1641	M1581	L1523	E1461	C1401	ASN	K1280	I1220	I1162	F1100
S1823	Q1762	S1704	Y1642	M1582	D1524	I1462	S1402	ASP	D1281	T1221	A1101	E1102
R1824	D1763	Y1705	H1643	S1583	L1525	F1463	S1402	ASN	D1282	S1222	D1164	E1102
N1825	R1764	T1706	Y1644	R1584	F1526	P1464	F1403	GLU	K1283	R1223	L1165	L1103
D1826	D1765	F1707	A1645	T1585	D1527	F1465	I1404	GLN	I1284	W1224	A1166	L1103
H1827	D1766	G1708	T1646	C1586	E1527	S1466	T1405	G1348	M1285	R1225	E1167	A1104
W1828	H1767	L1709	T1647	V1587	E1528	L1467	A1406	H1349	A1286	R1225	A1167	L1106
L1829	W1829	D1710	D1648	I1588	V1529	A1468	I1407	D1350	F1287	D1226	Y1168	S1106
L1830	H1768	D1710	D1648	I1588	L1530	S1469	I1407	Q1351	E1287	R1227	V1169	L1106
S1769	S1769	P1711	Q1649	Q1589	K1531	S1469	G1408	F1228	T1228	T1228	A1170	L1107
A1831	G1770	G1712	P1650	Q1590	D1532	R1470	I1409	E1352	E1288	F1229	G1171	W1108
D1832	G1771	P1713	H1651	I1591	D1532	L1471	I1410	W1353	V1289	G1230	R1109	D1108
R1833	R1833	Y1714	V1652	F1592	D1534	S1472	I1410	E1354	V1290	W1230	K1172	R1109
R1834	S1772	W1715	L1653	Q1593	D1534	G1473	F1411	S1355	Y1291	N1231	T1173	D1110
D1835	Y1773	L1716	I1654	H1594	G1535	I1474	H1412	S1355	H1292	H1232	Q1174	E1111
I1836	R1774	L1716	R1655	Q1595	D1536	S1475	W1413	E1476	Y1293	S1234	V1176	H1112
	V1776		H1656	I1596			L1415		K1295	I1235		D1114



• Molecule 1: SeAvs3



L1919	D1920	R1921	Y1922	P1923	K1924	V1925	P1927	P1928	Y1929	A1930	L1931	T1932	S1933	E1934	Y1935	S1936	K1937	E1938	R1939	V1940	A1941	Y1942	V1943	R1944	A1945	Y1946	A1947	L1948	Q1949	A1950	N1951	L1952	M1953	G1954	S1955	Q1956	L1957	A1958	L1959	S1960	D1961	L1962	A1963	S1964	T1965	E1966	V1967	K1968	K1969	E1970	L1971	M1972	A1973	E1974	K1975	R1976	H1977	G1978																																																												
E1979	S1980	D1981	D1982	L1983	R1984	Q1985	L1986	K1987	Q1988	Y1989	S1990	G1991	V1992	L1993	T1994	P1995	W1996	Y1997	R1998	L1999	W1000	A1001	K1002	V1003	I1004	L1005	G1006	K1007	T1008	R1009	K1010	A1011	D1012	L1013	E1014	S1015	E1016	L1017	S1018	D1019	T1020	Q1021	K1022	E1023	S1024	T1025	A1026	I1027	K1028	G1029	H1030	S1031	Y1032	S1033	E1034	H1035	S1036	L1037	S1038																																																											
S1039	N1040	E1041	I1042	A1043	N1044	V1045	W1046	F1047	D1048	I1049	L1050	I1051	E1052	A1053	G1054	N1055	Q1056	S1057	K1058	D1059	V1060	K1061	E1062	N1063	I1064	I1065	K1066	W1067	S1068	Q1069	K1070	K1071	G1072	N1073	R1074	V1075	K1076	T1077	P1078	T1079	L1080	H1081	Q1082	F1083	S1084	S1085	V1086	C1087	A1088	E1089	I1090	S1091	G1092	L1093	G1094	E1095	L1096	S1097	Y1098																																																											
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I1162	L1163	D1164	L1165	A1166	E1167	Y1168	V1169	A1170	G1171	K1172	T1173	Q1174	P1176	P1177	E1178	I1179	S1180	Y1181	K1182	L1183	A1184	R1185	C1186	A1187	E1188	L1189	T1190	R1191	E1192	Y1193	V1194	D1195	R1196	D1197	K1198	H1199	F1200	A1201	W1202	S1203	D1204	T1205	V1206	E1207	I1208	L1209	A1210	E1211	L1212	C1213	P1214	S1215	S1216	A1217	L1218	A1219	I1220	I1221																																																												
S1222	R1223	W1224	R1225	D1226	R1227	T1228	F1229	G1230	L1231	H1232	R1233	S1234	I1235	L1236	A1237	W1238	T1239	I1240	E1241	H1242	L1243	V1244	K1245	K1246	N1247	K1248	I1249	A1250	A1251	L1252	D1253	A1254	L1255	P1256	L1257	L1258	T1259	F1260	E1261	N1262	D1263	W1264	H1265	K1266	C1267	D1268	L1269	L1270	D1271	S1272	V1273	P1274	S1275	S1276	C1277	L1278	D1279	K1280																																																												
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S1402	F1403	I1404	T1405	S1406	I1407	G1408	A1409	F1410	F1411	H1412	W1413	L1414	L1415	Y1416	D1417	F1418	K1419	Y1420	I1421	L1422	E1423	S1424	I1425	P1426	D1427	E1428	W1429	T1430	S1431	R1432	L1433	S1434	T1435	K1436	T1437	T1438	L1439	A1440	T1443	K1444	E1445	Y1446	C1447	Q1448	R1449	C1451	M1452	R1453	T1454	R1455	L1456	D1457	V1458	V1459	E1461	T1462																																																														
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V1529	S1469	G1408	G1348	E1288	T1228	Y1168	L1107	F1047	K987	P927	Q867	L807
L1530	R1470	A1409	H1349	V1289	F1229	V1169	W1108	D1048	Q988	P928	A867	R808
K1531	L1471	I1410	D1350	V1290	G1230	A1170	I1109	I1049	Y989	Y929	I869	R809
D1532	S1472	F1411	Q1351	Y1291	N1231	G1171	D1110	L1050	S990	A930	R870	W810
E1533	G1473	H1412	E1352	Y1293	H1232	K1172	E1111	I1051	G991	L931	R871	R811
D1534	T1474	W1413	W1353	T1294	R1233	T1173	H1112	E1052	V992	T932	T872	R812
G1535	S1475	G1414	E1354	T1294	S1234	Q1174	S1113	A1053	L993	S933	W873	R813
D1536	L1476	L1415	S1355	K1295	I1235	V1175	D1114	G1054	T994	E934	R874	K814
G1537	K1477	Y1416	I1356	P1176	A1237	P1177	A1115	N1055	W996	Y935	L875	L815
P1538	E1478	D1417	F1357	E1178	L1236	E1179	I1117	V1056	Y997	S936	L876	S816
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W1540	F1480	K1419	D1359	T1239	T1239	S1180	A1119	D1059	N999	E939	S878	D818
E1541	G1481	Y1420	C1360	I1240	I1240	Y1181	D1120	L999	W1000	R940	R879	A819
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D1551	E1491	S1431	A1370	I1311	A1251	R1191	S1131	H1070	K1010	A950	H830	H830
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F1500	S1501	A1440	P1379	T1319	T1259	H1199	Y1139	P1078	S1018	A958	Q838	Q838
L1502	P1503	G1441	E1380	E1320	F1260	F1200	I1140	T1079	D1019	L959	L839	L839
G1504	G1504	L1442	F1381	L1321	E1261	A1201	F1141	L1080	T1020	S960	A840	A840
L1505	K1444	I1443	Y1382	K1322	N1262	W1202	N1142	H1081	Q1021	D961	I841	I841
L1506	E1445	E1323	S1383	E1323	D1263	S1203	Q1143	R1082	K1022	L962	A842	A842
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L1510	R1449	G1327	F1387	G1327	C1267	E1207	N1149	V1086	A1026	V967	I847	I847
E1511	F1450	L1328	I1388	L1328	D1268	L1208	K1150	A1088	G1029	K968	Q907	Q907
S1512	C1451	Q1329	K1389	Q1329	L1269	L1209	L1151	E1089	H1030	K969	S908	S908
N1513	M1452	H1330	K1390	H1330	L1270	A1210	G1152	I1090	H1031	E970	V909	V909
E1514	R1453	THR	A1391	THR	D1271	E1211	D1153	S1091	Y1032	L971	C910	M851
A1515	I1454	THR	I1392	VAL	S1272	L1212	E1154	G1092	S1031	L972	T911	G852
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V1518	S1457	LYS	V1395	LYS	S1275	S1215	S1157	E1095	E1034	E974	E914	L855
L1519	R1458	SER	K1396	SER	S1276	S1216	N1158	L1096	H1035	K975	S915	E856
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C1580	Y1460	SER	E1399	SER	T1279	A1219	A1161	H1099	S1038	G978	L918	K859
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L1522	I1462	ASN	C1401	ASP	K1281	T1221	L1163	F1100	N1040	S980	D920	H861
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L1525	P1464	GLU	F1403	GLU	D1283	R1223	L1165	E1102	A1043	D982	Y922	P863
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F2070	D2010	G1950	E1890	L1830	H1770	D1710	P1650	G1590
L2071	E2011	I1951	S1891	A1831	G1771	F1711	H1651	I1591
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R2073	K2013	E1953	I1893	R1833	Y1773	P1713	L1653	Q1593
H2074	S2014	F1954	V1894	R1834	P1774	Y1714	I1654	H1594
D2075	H2015	D1955	H1895	D1835	R1775	W1715	R1655	A1595
G2076	G2016	P1956	S1896	I1836	V1776	L1716	H1656	I1596
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H2079	L2019	G1959	V1899	K1839	Y1779	L1719	A1659	T1599
T2080	C2020	M1960	S1900	E1840	H1780	G1720	R1680	T1600
L2081	A2021	V1961	P1901	R1841	F1781	R1721	T1681	L1601
Y2082	S2022	R1962	E1902	S1842	Y1782	C1722	L1682	P1602
G2083	T2023	F1963	R1903	S1843	L1783	F1723	L1663	F1603
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R2086	I2026	P1966	S1906	M1846	H1786	S1726	H1666	R1606
N2087	K2027	E1967	L1907	S1847	A1787	Q1727	D1687	M1607
GLY	S2028	P1968	L1908	S1848	M1788	K1728	S1688	L1608
GLU	A2029	A1969	R1909	S1849	F1789	Q1729	D1689	P1609
LYS	L2030	S1970	A1910	D1850	M1790	L1730	L1670	F1610
THR	E2031	F1971	L1911	M1851	T1791	E1731	I1671	T1611
SER	T2032	I1972	Q1912	R1852	A1792	P1732	S1672	T1612
	F2033	T1973	T1913	D1853	G1793	E1733	I1673	L1613
	N2034	D1974	T1914	E1854	Q1794	M1734	P1674	H1614
	M2035	A1975	K1915	W1855	L1795	L1735	A1675	A1615
	D2036	M1976	N1916	L1856	L1796	R1736	Q1676	Q1616
	L2037	K1977	V1917	A1857	A1797	I1737	E1677	L1617
	T2038	L1978	Y1918	S1858	T1798	I1738	E1678	W1618
	L2039	T1979	D1919	I1859	K1799	R1739	N1679	L1619
E2040	T1980	T1980	Y1920	S1860	P1800	D1740	K1680	M1620
V2041	D1981	D1981	K1921	E1861	L1801	V1741	L1681	I1621
D2042	K1982	K1982	I1922	M1862	V1802	L1742	R1682	A1622
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R2045	R1985	R1985	A1925	M1865	TYR	K1745	N1685	R1625
Y2046	V1986	V1986	GLY	E1866	ASP	G1746	Q1686	V1626
S2047	W1987	W1987	ASN	T1867	ASP	S1747	S1687	A1627
R2048	Y1988	Y1988	LEU	L1868	VAL	R1748	T1688	L1628
N2049	S1989	S1989	GLU	C1869	E1810	M1749	T1689	D1629
SER	ARG	ARG	ILE	P1870	D1811	W1750	L1690	D1630
THR	TYR	S1991	ASP	S1871	V1812	D1751	P1691	G1631
GLU	GLU	D1992	ALA	P1872	F1813	E1752	V1692	K1632
ARG	ARG	V1993	HIS	G1873	Q1814	D1753	LEU	S1633
ASN	ASN	E1994	TYR	L1874	D1815	E1754	ASP	L1634
ASN	ASN	P1995	Q1937	L1875	W1816	R1755	LYS	I1635
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GLU	M1997	M1997	K1939	L1877	R1818	K1757	GLU	P1637
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ILE	ILE	T2001	K1943	W1881	I1822	Y1761	E1702	G1640
PRO	PRO	W2002	D1944	S1882	S1823	Q1762	D1703	F1641
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T2066	T2066	H2004	A1946	V1884	N1825	R1764	Y1705	H1643
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		S2006	Y1948	S1886	H1827	M1766	F1707	A1645
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		K2008		R1888		H1768		D1648

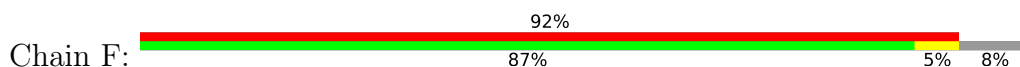
• Molecule 1: SeAvs3



MET	SER	ASP	ASP	LEU	LEU	VAL	ARG	THR	SER	ARG	ASP	GLY	ASP	Q15	L28	T34	L35	A43	S44	THR	THR	GLU	MET	GLY	SER	GLN	PRO	VAL	VAL	GLU	D56	G57	A73	K84	M88	H89	S90	D91	T92	P93	F94	P95	P96	S97	G98	L99	Q100	K101	T102	I103	E104	G105	F106				
K111	A112	L113	I114	Q115	K116	T117	P118	V119	E120	T121	L122	R123	T124	R134	P135	V136	S137	S138	S139	F140	S141	E142	A143	I144	M145	D146	A147	A148	N149	Q150	H151	V152	T153	R154	H155	P156	H157	D158	L159	A160	K161	L162	E163	K164	F165	T166	G167	L168	Q169	G170	A171	E172	L173	S174	I175	F176	C177
Q178	E183	Q186	D187	D188	A201	E210	T225	E226	S227	A228	A229	M230	D245	E246	E260	Q273	V276	F279	D288	I300	E301	A324	Y327	I374	E381	L386	I389	V422	S469	D497	K507	T508	V509	E510	D511	T512	I513																				

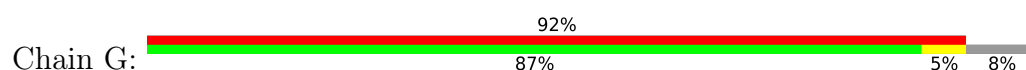
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D1280	K1281	D1282	K1283	I1284	M1285	A1286	F1287	E1288	V1289	V1290	Y1291	H1292	Y1293	T1294	K1295	F1296	M1297	V1298	Q1299	N1300	I1301	Q1302	M1303	L1304	K1305	K1306	L1307	D1308	A1309	I1310	S1311	T1312	S1313	L1314	G1315	I1316	F1317	H1318	T1319	E1320	L1321	K1322	E1323	R1324	I1325	S1326	Q1327	L1328	Q1329	THR	GLU	THR	VAL	SER	LYS	SER				
I1220	I1221	S1222	R1223	W1224	R1225	D1226	I1227	T1228	F1229	G1230	N1231	H1232	R1233	S1234	I1235	L1236	A1237	W1238	I1239	I1240	E1241	H1242	L1243	V1244	K1245	K1246	N1247	K1248	I1249	N1250	A1251	L1252	D1253	A1254	L1255	P1256	L1257	I1258	T1259	F1260	E1261	N1262	D1263	W1264	H1265	K1266	C1267	D1268	L1269	L1270	D1271	S1272	V1273	L1274	S1275	C1276	C1277	D1278	I1279	
D1280	K1281	D1282	K1283	I1284	M1285	A1286	F1287	E1288	V1289	V1290	Y1291	H1292	Y1293	T1294	K1295	F1296	M1297	V1298	Q1299	N1300	I1301	Q1302	M1303	L1304	K1305	K1306	L1307	D1308	A1309	I1310	S1311	T1312	S1313	L1314	G1315	I1316	F1317	H1318	T1319	E1320	L1321	K1322	E1323	R1324	I1325	S1326	Q1327	L1328	Q1329	THR	GLU	THR	VAL	SER	LYS	SER				
L1400	L1401	S1402	F1403	I1404	T1405	A1406	I1407	G1408	A1409	I1410	F1411	H1412	H1413	G1414	L1415	Y1416	D1417	F1418	K1419	Y1420	I1421	L1422	A1423	S1424	I1425	P1426	D1427	A1428	W1429	T1430	S1431	L1432	L1433	S1434	I1435	K1436	T1437	T1438	L1439	A1440	I1443	K1444	E1445	Y1446	C1447	Q1448	R1449	F1450	C1451	M1452	R1453	I1454	R1455	K1456	T1457	L1458	V1459	Y1460		
D681	A682	A683	K684	L685	L686	L687	K688	A689	E692	D696	N697	R698	L703	R704	D705	D708	L709	A710	A711	K712	N717	E721	R725	D730	T731	R756	S770	Q771	L772	P773	D774	D775	E776	R777	S778	R779	Q780	N781	W782	T783	D784	Q785	D786	R787	A788	L791	I792													
I530	P548	L549	I550	G581	E582	T583	I584	D588	E589	P590	A591	E592	R600	A603	A604	D605	R614	P615	L616	D619	Q636	L640	A644	I645	S646	S647	Q648	A649	L650	P651	E652	T653	S654	A655	V656	E657	R658	R659	D660	A673	L674	R675	T676	G677	R678	Y679	Q680													
L795	G799	A800	E801	A802	A803	A804	R805	E806	L807	R808	R809	W810	R811	P812	R813	K814	L815	S816	D818	A819	G820	K821	I822	V823	A824	M825	Q826	L827	L828	A829	H830	A831	R832	Y833	D834	E835	L836	D837	Q838	L839	A840	I841	A842	A843	G844	N845	D846	I847	S848	L849	V850	M851	G852	I853	V854	L855	E856			
A857	R858	K859	L860	H861	R862	P863	V864	E865	E866	Q867	A868	T869	R870	R871	T872	W873	R874	L875	L876	K877	S878	Q879	R880	V881	I882	S883	I884	D885	R886	N887	H888	A889	N890	N891	Q892	T893	I894	A895	A896	I897	T898	G899	N900	V901	E902	L903	A904	L905	I906	Q907	S908	V909	C910	T911	E912	S913	E914	S915	T916	
Q917	L918	L919	D920	R921	Y922	L923	P924	K925	V926	P927	P928	Y929	A930	L931	T932	S933	E934	Y935	S936	K937	E938	R939	V940	A941	Y942	V943	R944	A945	Y946	A947	L948	H949	Q949	A950	N951	L952	N953	G954	S955	Q956	L957	A958	L959	S960	D961	L962	A963	S964	T965	E966	V967	K968	K969	E970	L971	M972	A973	E974	K975	R976
H977	Q978	E979	S980	D981	D982	L983	R984	Q985	L986	K987	Q988	Y989	S990	G991	V992	L993	I994	P995	W996	Y997	N998	L999	W1000	A1001	K1002	V1003	I1004	L1005	G1006	K1007	T1008	L1009	K1010	A1011	D1012	L1013	E1014	S1015	E1016	L1017	S1018	D1019	T1020	Q1021	K1022	E1023	S1024	T1025	A1026	I1027	K1028	G1029	H1030	S1031	Y1032	S1033	E1034	H1035	S1036	
L1037	S1038	S1039	N1040	E1041	I1042	A1043	N1044	W1045	V1046	F1047	D1048	I1049	L1050	I1051	E1052	A1053	G1054	N1055	V1056	S1057	K1058	D1059	D1060	V1061	E1062	N1063	I1064	L1065	K1066	W1067	S1068	Q1069	H1070	K1071	E1072	L1073	R1074	V1075	F1076	T1077	P1078	T1079	L1080	H1081	R1082	F1083	S1084	S1085	V1086	C1087	A1088	E1089	T1090	N1091	L1092	L1093	G1094	E1095	L1096	
S1097	Y1098	H1099	F1100	E1101	E1102	L1103	A1104	L1105	S1106	L1107	W1108	R1109	D1110	E1111	H1112	S1113	D1114	A1115	Q1116	I1117	K1118	A1119	I1123	D1124	L1125	S1126	R1127	S1128	L1129	I1130	S1131	L1132	D1133	E1134	P1135	E1136	A1137	K1138	E1139	Y1140	F1141	N1142	Q1143	A1144	I1145	E1146	V1147	K1150	L1151	D1153	E1154	N1155	L1156	S1157	R1158	W1159				
E1160	A1161	I1162	L1163	D1164	L1165	A1166	E1167	V1168	V1169	A1170	G1171	K1172	T1173	Q1174	W1175	P1176	P1177	E1178	I1179	S1180	Y1181	K1182	L1183	A1184	R1185	C1186	A1187	E1188	L1189	T1190	R1191	E1192	Y1193	V1194	D1195	R1196	D1197	K1198	H1199	F1200	A1201	W1202	S1203	D1204	T1205	V1206	E1207	I1208	L1209	A1210	E1211	L1212	C1213	P1214	L1215	S1216	A1217	L1218	A1219	
I1220	I1221	S1222	R1223	W1224	R1225	D1226	I1227	T1228	F1229	G1230	N1231	H1232	R1233	S1234	I1235	L1236	A1237	W1238	I1239	I1240	E1241	H1242	L1243	V1244	K1245	K1246	N1247	K1248	I1249	N1250	A1251	L1252	D1253	A1254	L1255	P1256	L1257	I1258	T1259	F1260	E1261	N1262	D1263	W1264	H1265	K1266	C1267	D1268	L1269	L1270	D1271	S1272	V1273	L1274	S1275	C1276	C1277	D1278	I1279	
D1280	K1281	D1282	K1283	I1284	M1285	A1286	F1287	E1288	V1289	V1290	Y1291	H1292	Y1293	T1294	K1295	F1296	M1297	V1298	Q1299	N1300	I1301	Q1302	M1303	L1304	K1305	K1306	L1307	D1308	A1309	I1310	S1311	T1312	S1313	L1314	G1315	I1316	F1317	H1318	T1319	E1320	L1321	K1322	E1323	R1324	I1325	S1326	Q1327	L1328	Q1329	THR	GLU	THR	VAL	SER	LYS	SER				
L1400	L1401	S1402	F1403	I1404	T1405	A1406	I1407	G1408	A1409	I1410	F1411	H1412	H1413	G1414	L1415	Y1416	D1417	F1418	K1419	Y1420	I1421	L1422	A1423	S1424	I1425	P1426	D1427	A1428	W1429	T1430	S1431	L1432	L1433	S1434	I1435	K1436	T1437	T1438	L1439	A1440	I1443	K1444	E1445	Y1446	C1447	Q1448	R1449	F1450	C1451	M1452	R1453	I1454	R1455	K1456	T1457	L1458	V1459	Y1460		

- Molecule 2: Terminase, large subunit

[illegible]

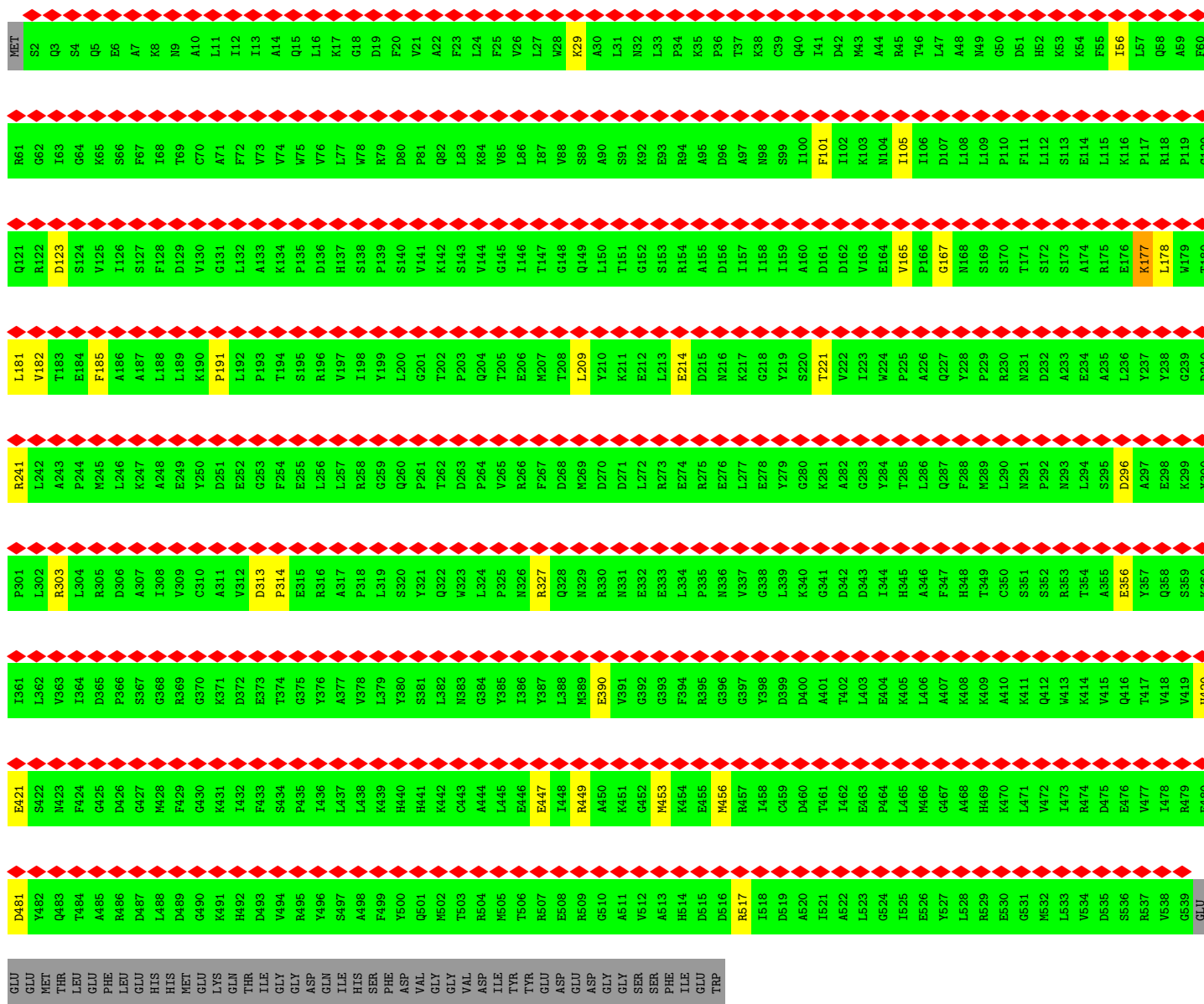
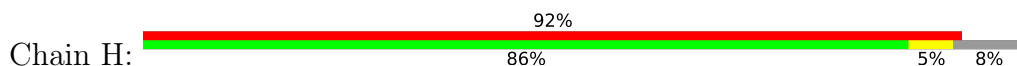
R241	P301	I361	E421	D481	GLU
L242	L302	L362	S422	Y482	GLU
A243	R303	V363	M423	Q483	MET
P244	L304	I364	F424	T484	THR
M245	R305	D365	G425	A485	LEU
L246	D306	P366	G426	R486	PHE
K247	A307	S367	G427	D487	LEU
A248	I308	G368	M428	L488	HIS
E249	V309	R369	D429	D489	HIS
Y250	C310	G370	G430	G490	MET
D251	A311	K371	K431	K491	GLU
E252	V312	D372	I432	H492	LYS
G253	D313	E373	F433	D493	GLN
F254	P314	T374	S434	V494	THR
E255	E315	G375	P435	R495	ILE
L256	R316	Y376	I436	Y496	GLY
L257	A317	A377	L437	S497	ASP
R258	P318	V378	L438	A498	GLN
G259	L319	L379	K439	F499	HIS
Q260	S320	Y380	H440	Y500	SER
P261	Y321	S381	H441	Q501	PHE
T262	Q322	L382	K442	M502	ASP
D263	W323	N383	C443	T503	VAL
P264	L324	G384	A444	R504	VAL
V265	P325	Y385	L445	M505	ASP
R266	N326	I386	L446	T506	ILE
F267	R327	Y387	E447	R507	TYR
D268	Q328	I388	I448	E508	GLU
M269	N329	M389	R449	R509	ASP
D270	R330	E390	A450	G510	ASP
D271	N331	V391	K451	A511	GLY
L272	E332	G392	G452	V512	SER
R273	E333	G393	M453	A513	SER
E274	L334	F394	K454	H514	PHE
R275	P335	R395	E455	D515	ILE
E276	N336	G396	M456	D516	GLU
L277	V337	G397	R457	R517	TRP
E278	G338	Y398	I458	I518	
Y279	L339	D399	C459	D519	
G280	K340	D400	D460	A520	
K281	G341	A401	T461	I521	
A282	D342	T402	I462	A522	
G283	D343	L403	E463	L523	
Y284	I344	E404	P464	G524	
L285	H345	K405	L465	I525	
L286	A346	L406	M466	E526	
Q287	F347	A407	G467	Y527	
F288	H348	K408	A468	L528	
M289	T349	K409	H469	R529	
L290	C350	A410	K470	E530	
N291	S351	K411	L471	G531	
P292	S352	Q412	V472	M532	
N293	R353	W413	I473	L533	
L294	T354	K414	R474	V534	
S295	A355	V415	D475	D535	
D296	E356	Q416	E476	S536	
A297	Y357	T417	V477	R537	
E298	Q358	V418	I478	V538	
K299	S359	V419	R479	G539	
Y300	K360	H420	E480	GLU	

• Molecule 2: Terminase, large subunit



MET	R61	Q121	L181	R241	P301	I361	E421	D481	GLU
S2	G62	R122	V182	L242	L302	L362	S422	Y482	GLU
Q3	I63	D123	T183	A243	R303	V363	M423	Q483	MET
S4	G64	S124	E184	P244	L304	I364	F424	T484	THR
Q5	K65	I125	F185	M245	D306	P365	G425	A485	LEU
E6	S66	I126	A186	L246	D307	P366	G426	R486	PHE
A7	F67	S127	A187	K247	I308	S367	G427	D487	LEU
K8	T68	F128	L188	A248	V309	G368	M428	L488	HIS
N9	T69	D129	L189	E249	C310	R369	D429	D489	HIS
A10	C70	V130	K190	Y250	A311	G370	G430	G490	MET
L11	A71	G131	P191	D251	V312	K371	K431	K491	GLU
I12	F72	L132	L192	E252	D313	D372	I432	H492	GLN
I13	V73	A133	P193	G253	P314	E373	F433	D493	THR
A14	V74	K134	T194	F254	E315	T374	S434	V494	ILE
Q15	W75	P135	S195	E255	R316	G375	P435	R495	GLY
L16	V76	D136	R196	L256	A317	Y376	I436	Y496	ASP
K17	L77	H137	V197	L257	P318	A377	L437	S497	GLN
G18	W78	I138	I198	R258	L319	V378	L438	A498	HIS
D19	R79	P139	Y199	G259	S320	L379	K439	F499	SER
F20	D80	S140	L200	Q260	Y321	Y380	H440	Y500	PHE
V21	P81	V141	G201	P261	Q322	S381	H441	Q501	ASP
A22	K82	K142	T202	T262	W323	L382	K442	M502	VAL
F23	L83	S143	P203	D263	L324	G384	A444	R504	VAL
L24	K84	V144	Q204	P264	P325	G385	L445	M505	ASP
F25	V85	G145	T205	V265	N326	I386	L446	T506	ILE
V26	L86	I146	E206	R266	R327	Y387	E447	R507	TYR
L27	I87	T147	M207	F267	Q328	Y388	I448	E508	GLU
W28	V88	G148	T208	D268	N329	M389	R449	R509	ASP
K29	S89	L149	L209	M269	R330	E390	A450	G510	ASP
A30	A90	L150	Y210	D270	N331	V391	K451	A511	GLY
L31	S91	T151	K211	D271	E332	G392	G452	V512	SER
N32	K92	G152	E212	L272	L334	G393	M453	A513	SER
E93	E93	S153	L213	R273	P335	F394	K454	H514	PHE
R94	R94	R154	E214	E274	N336	R395	E455	D515	ILE
A95	A95	A155	D215	R275	N337	G396	M456	D516	GLU
D96	D96	D156	N216	E276	V337	G397	R457	R517	TRP
A97	A97	I157	K217	L277	G338	Y398	I458	I518	
N98	N98	I158	G218	E278	L339	D399	C459	D519	
C39	C39	I159	Y219	Y279	K340	D400	D460	A520	
Q40	Q40	A160	S220	G280	G341	A401	T461	I521	
I41	I41	D161	T221	K281	D342	T402	I462	A522	
D42	D42	D162	V222	A282	D343	L403	E463	L523	
M43	M43	V163	I223	G283	I344	E404	P464	G524	
A44	A44	E164	W224	Y284	H345	K405	L465	I525	
R45	R45	V165	P225	L285	A346	L406	M466	E526	
T46	T46	P166	A226	L286	F347	A407	G467	Y527	
L47	L47	G167	Q227	Q287	H348	K408	A468	L528	
A48	A48	N168	Y228	F288	T349	K409	H469	R529	
N49	N49	S169	P229	M289	C350	A410	K470	E530	
P110	P110	S170	R230	L290	S351	K411	L471	G531	
F111	F111	T171	D231	N291	S352	Q412	V472	M532	
L112	L112	S172	D232	P292	R353	W413	I473	L533	
K53	K53	S173	A233	N293	L294	K414	R474	V534	
K54	K54	A174	E234	L294	S295	V415	D475	D535	
L115	L115	R175	A235	S295	D296	Q416	E476	S536	
K116	K116	E176	L236	D296	A297	T417	V477	R537	
P117	P117	K177	Y237	E297	E298	V418	I478	V538	
R118	R118	L178	Y238	E298	K299	V419	R479	G539	
P119	P119	W179	G239	K299	Y300	H420	E480	GLU	
G120	G120	T180	D240	Y300					

- Molecule 2: Terminase, large subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	44479	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	313.092, 313.092, 313.092	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8697, 0.8697, 0.8697	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG

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	0.31	0/16499	0.62	6/22369 (0.0%)
1	B	0.31	0/16319	0.62	5/22123 (0.0%)
1	C	0.31	0/16499	0.61	6/22369 (0.0%)
1	D	0.31	0/16319	0.62	5/22123 (0.0%)
2	E	0.30	0/4363	0.66	6/5899 (0.1%)
2	F	0.31	0/4363	0.65	3/5899 (0.1%)
2	G	0.30	0/4363	0.66	5/5899 (0.1%)
2	H	0.30	0/4363	0.64	2/5899 (0.0%)
All	All	0.31	0/83088	0.63	38/112580 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1923	PRO	CA-N-CD	-11.88	94.87	111.50
1	B	1923	PRO	CA-N-CD	-11.86	94.90	111.50
1	B	1153	ASP	CB-CG-OD2	8.68	126.12	118.30
1	D	1153	ASP	CB-CG-OD2	8.47	125.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	191	PRO	CA-N-CD	-8.29	99.89	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	548	PRO	Peptide
1	B	548	PRO	Peptide
1	C	548	PRO	Peptide
1	D	548	PRO	Peptide

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	16152	0	15975	34	0
1	B	15974	0	15804	49	0
1	C	16152	0	15975	37	0
1	D	15974	0	15804	49	0
2	E	4273	0	4283	11	0
2	F	4273	0	4283	14	0
2	G	4273	0	4283	13	0
2	H	4273	0	4283	16	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
3	E	31	0	12	0	0
3	F	31	0	12	0	0
3	G	31	0	12	0	0
3	H	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1	0	0	0	0
4	H	1	0	0	0	0
All	All	81600	0	80786	221	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 1.

The worst 5 of 221 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)
2:F:165:VAL:HG12	2:F:167:GLY:H	1.55	0.72
2:H:165:VAL:HG12	2:H:167:GLY:H	1.55	0.70
2:G:165:VAL:HG12	2:G:167:GLY:H	1.61	0.65
1:B:1944:ASP:OD2	1:B:1945:ILE:N	2.30	0.65
2:E:165:VAL:HG12	2:E:167:GLY:H	1.61	0.64

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	2016/2092 (96%)	1980 (98%)	36 (2%)	0	100	100
1	B	1990/2092 (95%)	1953 (98%)	37 (2%)	0	100	100
1	C	2016/2092 (96%)	1980 (98%)	36 (2%)	0	100	100
1	D	1990/2092 (95%)	1953 (98%)	37 (2%)	0	100	100
2	E	536/586 (92%)	526 (98%)	10 (2%)	0	100	100
2	F	536/586 (92%)	523 (98%)	13 (2%)	0	100	100
2	G	536/586 (92%)	526 (98%)	10 (2%)	0	100	100
2	H	536/586 (92%)	524 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	10156/10712 (95%)	9965 (98%)	191 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1754/1814 (97%)	1739 (99%)	15 (1%)	78	90
1	B	1732/1814 (96%)	1719 (99%)	13 (1%)	81	91
1	C	1754/1814 (97%)	1739 (99%)	15 (1%)	78	90
1	D	1732/1814 (96%)	1722 (99%)	10 (1%)	86	94
2	E	458/500 (92%)	458 (100%)	0	100	100
2	F	458/500 (92%)	453 (99%)	5 (1%)	73	86
2	G	458/500 (92%)	457 (100%)	1 (0%)	93	98
2	H	458/500 (92%)	454 (99%)	4 (1%)	78	90
All	All	8804/9256 (95%)	8741 (99%)	63 (1%)	84	92

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	11	ARG
2	F	356	GLU
1	C	1614	HIS
2	F	327	ARG
2	H	177	LYS

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	G	601	4	26,33,33	0.67	0	31,52,52	0.74	2 (6%)
3	ATP	D	2101	4	26,33,33	0.67	0	31,52,52	0.82	1 (3%)
3	ATP	A	2101	4	26,33,33	0.66	0	31,52,52	0.73	1 (3%)
3	ATP	B	2101	4	26,33,33	0.66	0	31,52,52	0.81	1 (3%)
3	ATP	E	601	4	26,33,33	0.68	0	31,52,52	0.74	2 (6%)
3	ATP	F	601	4	26,33,33	0.67	0	31,52,52	0.75	2 (6%)
3	ATP	H	601	4	26,33,33	0.67	0	31,52,52	0.75	2 (6%)
3	ATP	C	2101	4	26,33,33	0.66	0	31,52,52	0.73	1 (3%)

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	ATP	G	601	4	-	3/18/38/38	0/3/3/3
3	ATP	D	2101	4	-	4/18/38/38	0/3/3/3
3	ATP	A	2101	4	-	2/18/38/38	0/3/3/3
3	ATP	B	2101	4	-	4/18/38/38	0/3/3/3
3	ATP	E	601	4	-	2/18/38/38	0/3/3/3
3	ATP	F	601	4	-	3/18/38/38	0/3/3/3
3	ATP	H	601	4	-	2/18/38/38	0/3/3/3
3	ATP	C	2101	4	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2101	ATP	C5-C6-N6	2.28	123.82	120.35
3	C	2101	ATP	C5-C6-N6	2.27	123.80	120.35
3	B	2101	ATP	C5-C6-N6	2.19	123.67	120.35
3	D	2101	ATP	C5-C6-N6	2.18	123.66	120.35
3	F	601	ATP	C5-C6-N6	2.13	123.59	120.35

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

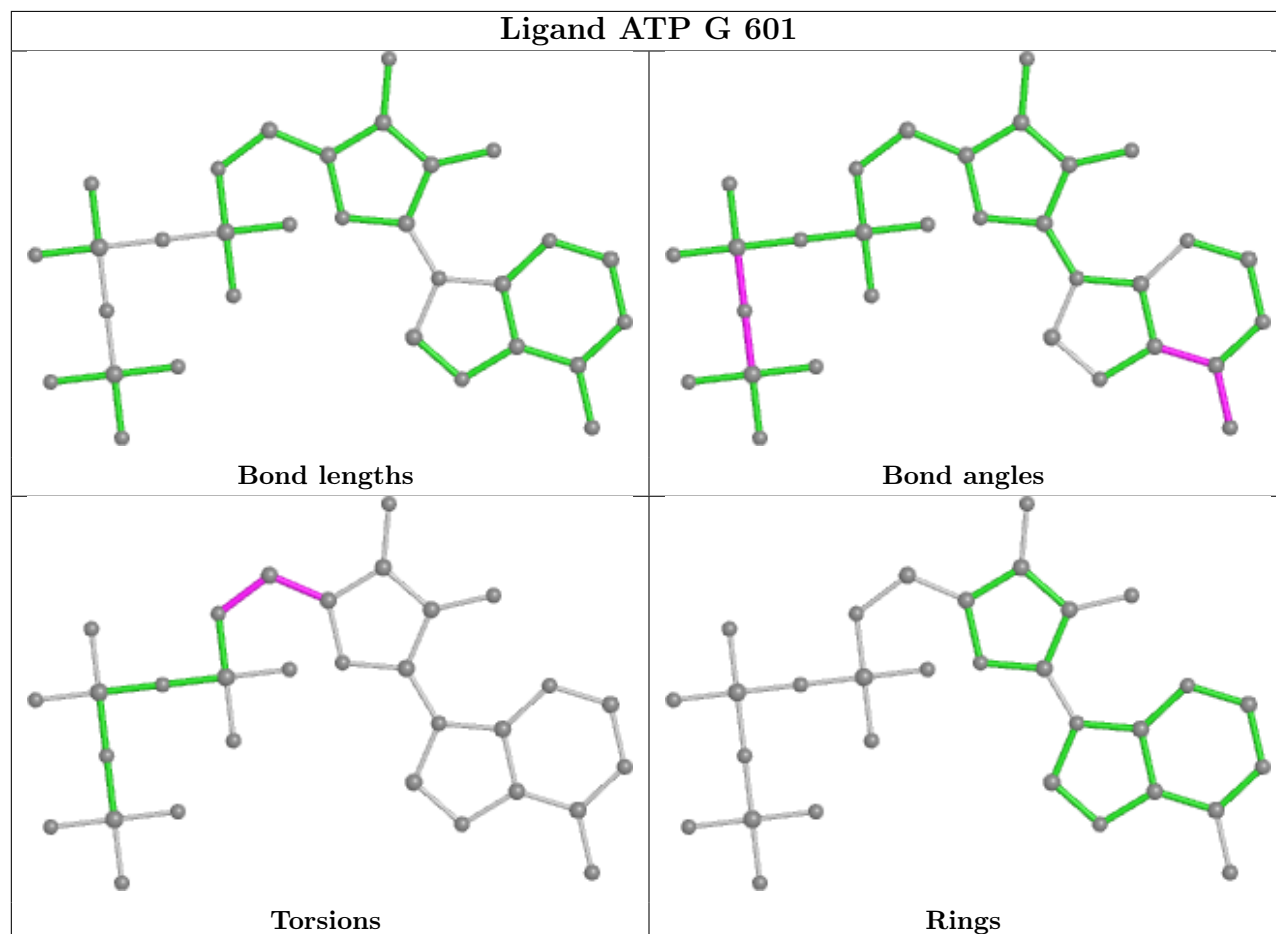
Mol	Chain	Res	Type	Atoms
3	E	601	ATP	O4'-C4'-C5'-O5'
3	H	601	ATP	O4'-C4'-C5'-O5'
3	B	2101	ATP	O4'-C4'-C5'-O5'
3	B	2101	ATP	C3'-C4'-C5'-O5'
3	D	2101	ATP	O4'-C4'-C5'-O5'

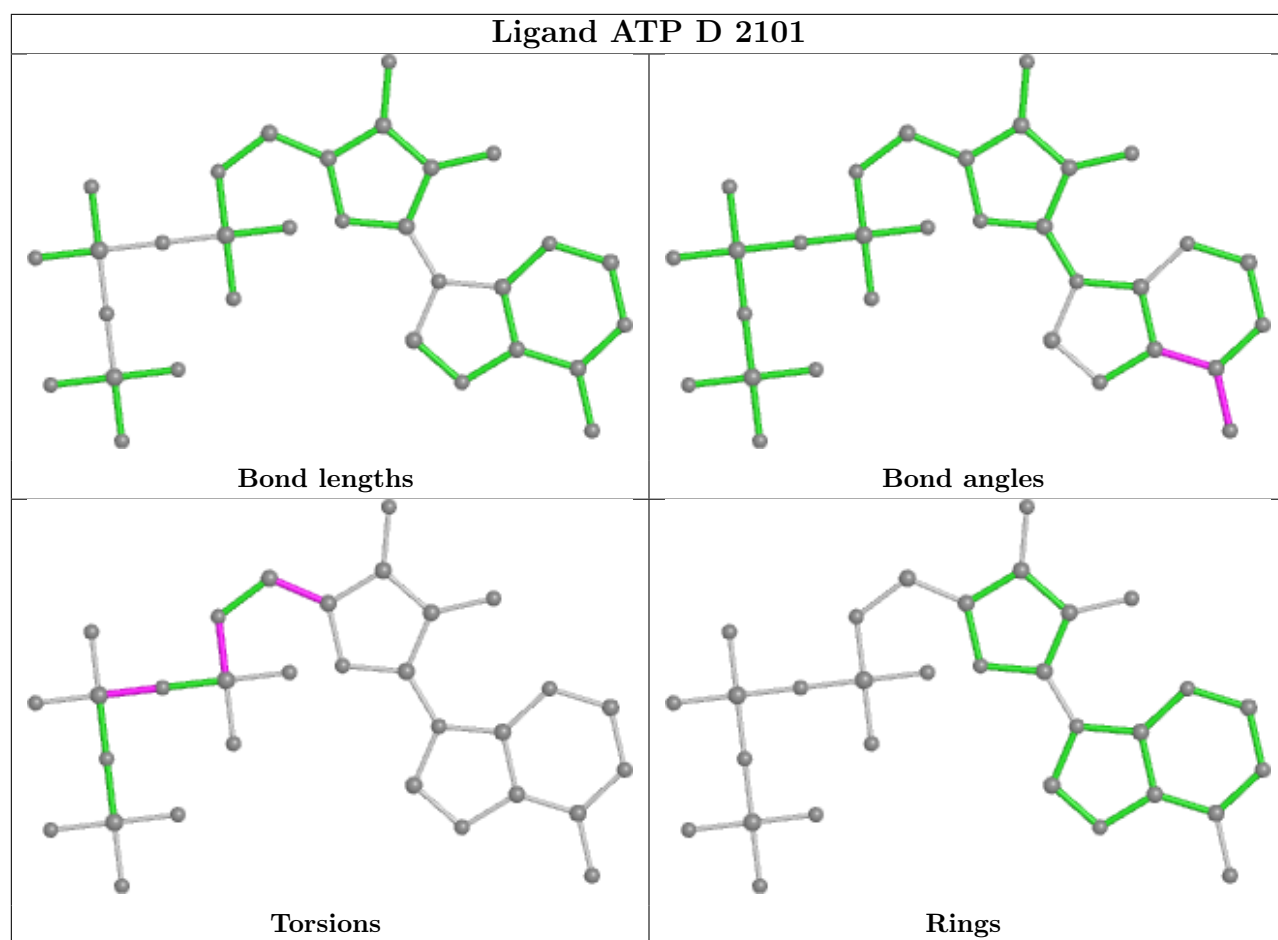
There are no ring outliers.

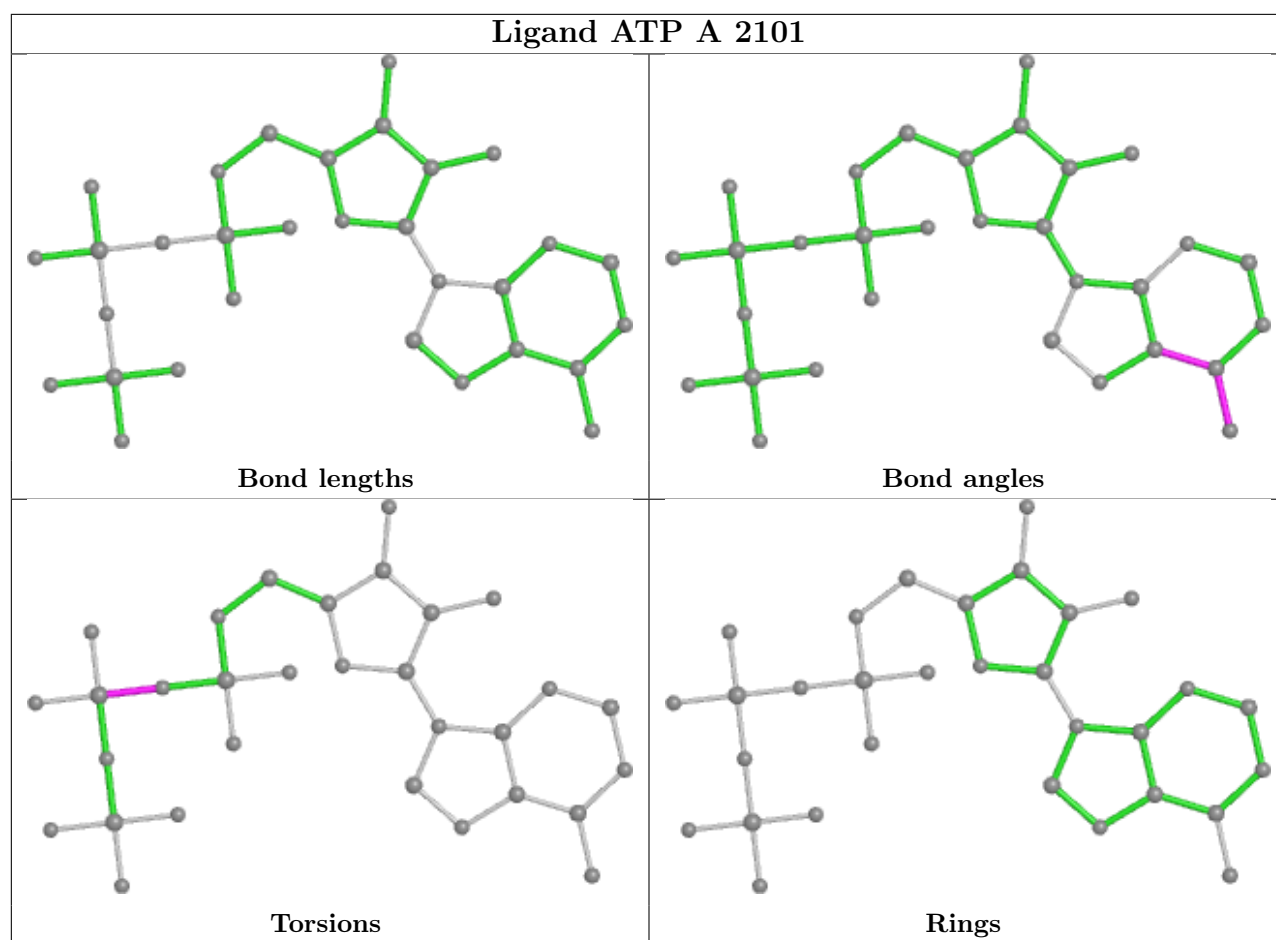
No monomer is involved in short contacts.

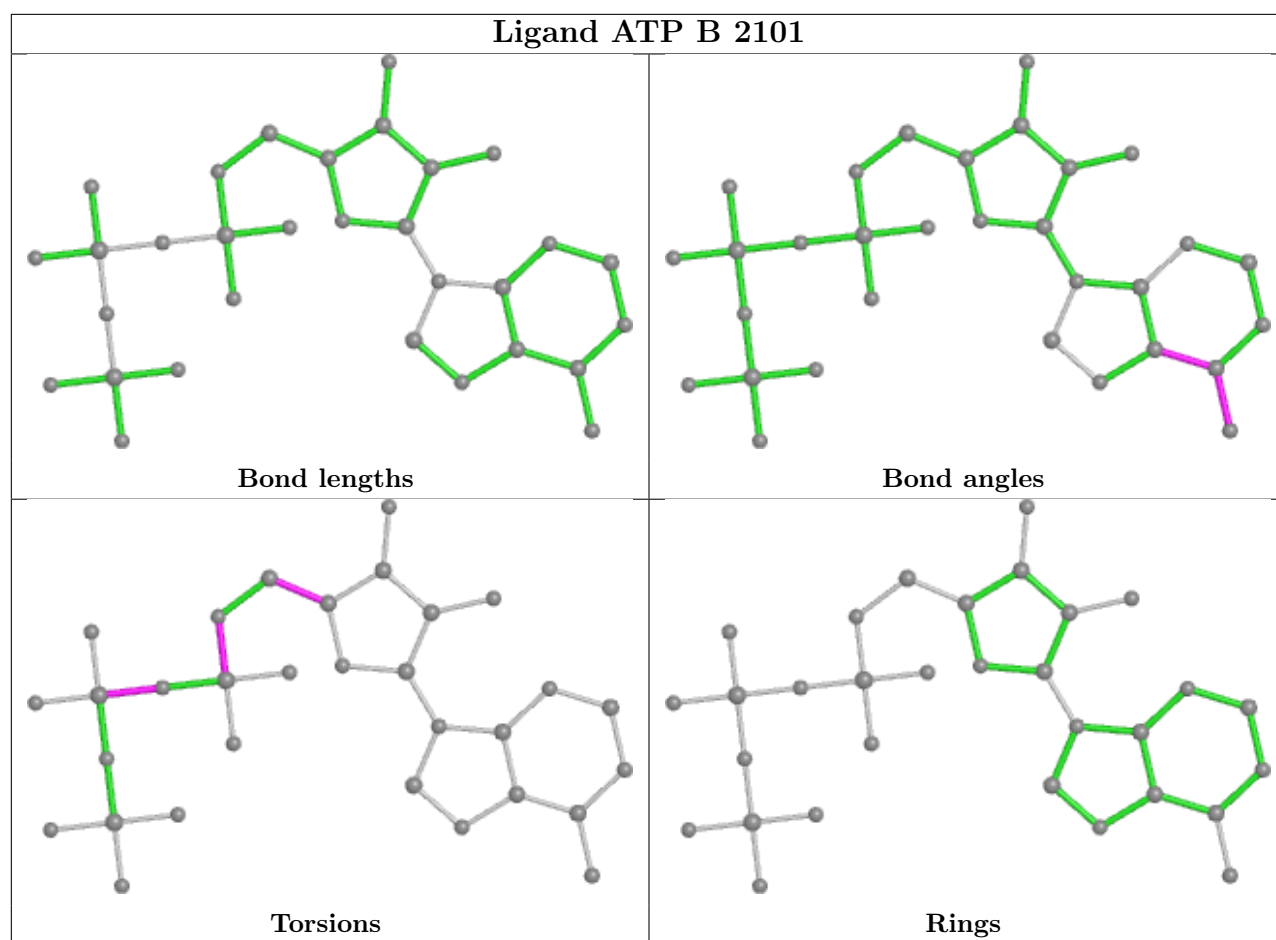
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

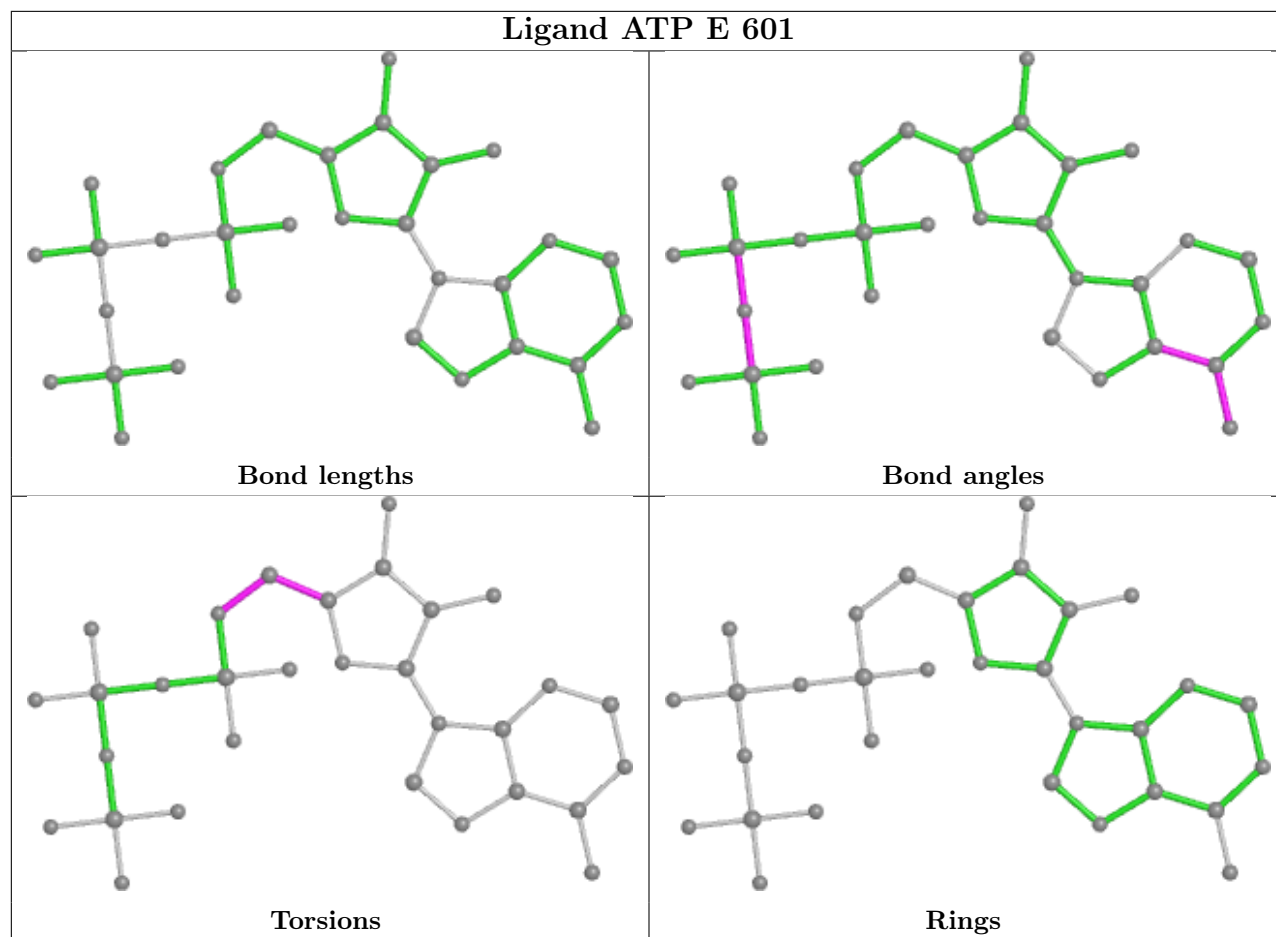
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

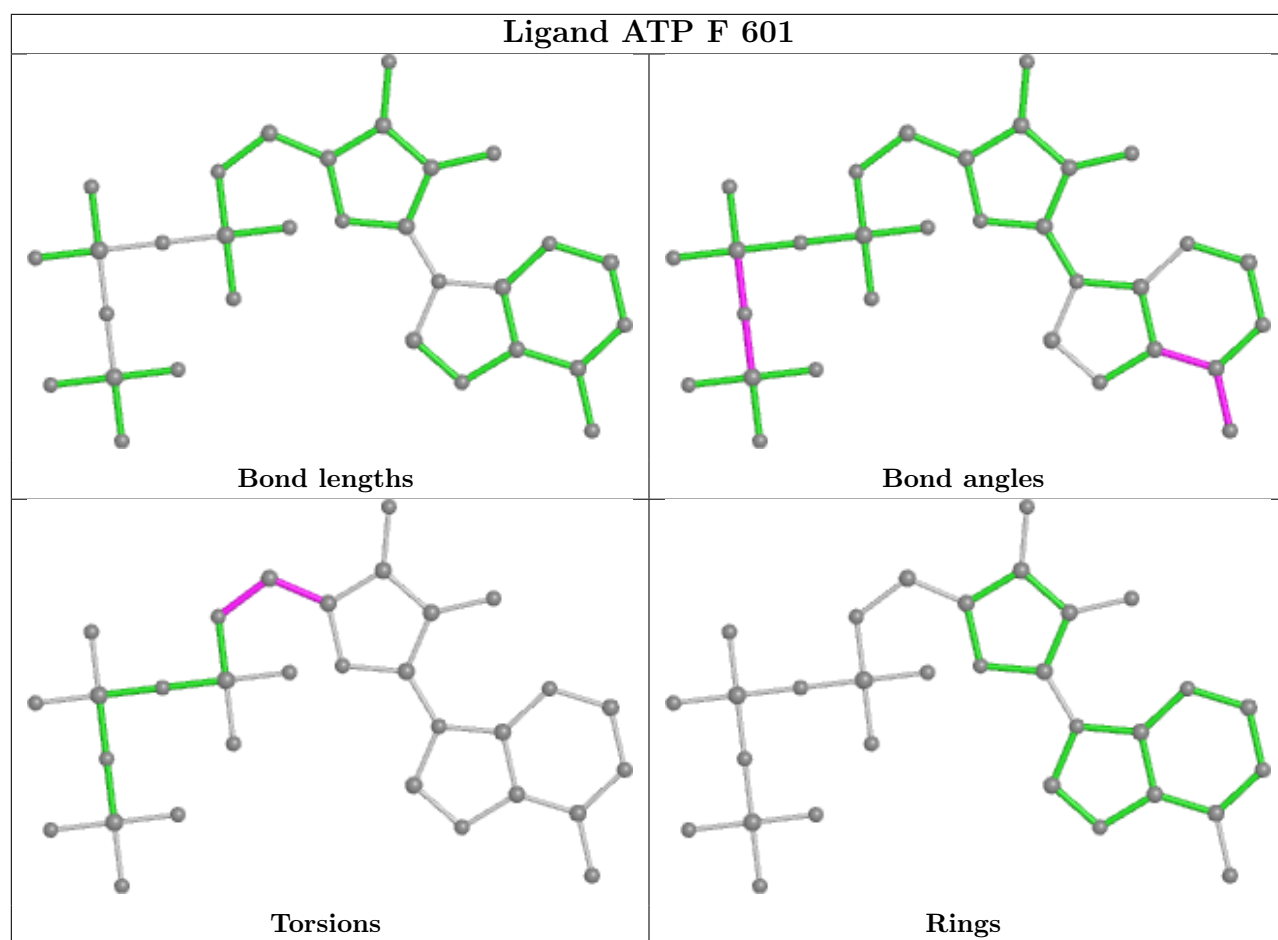


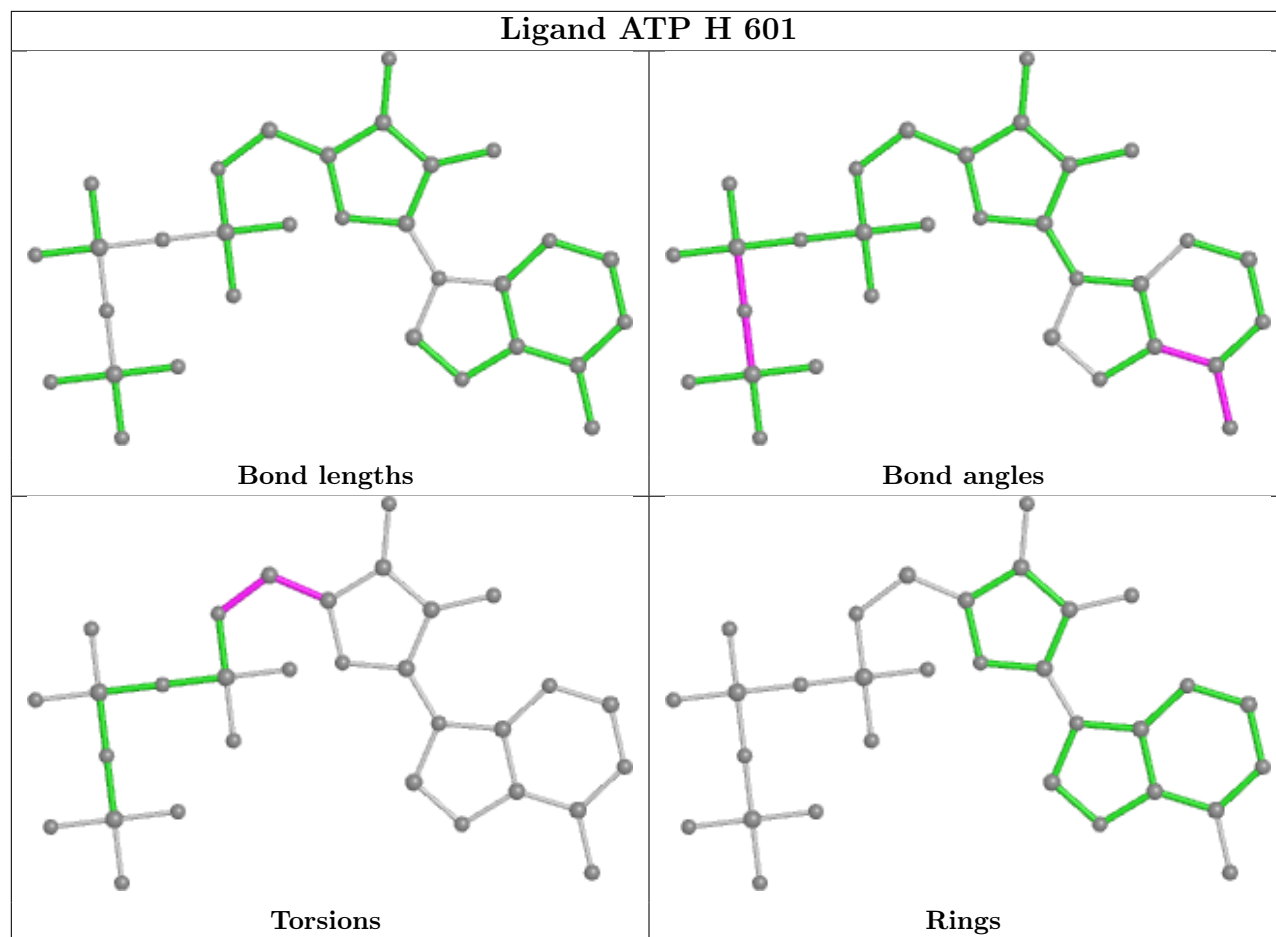


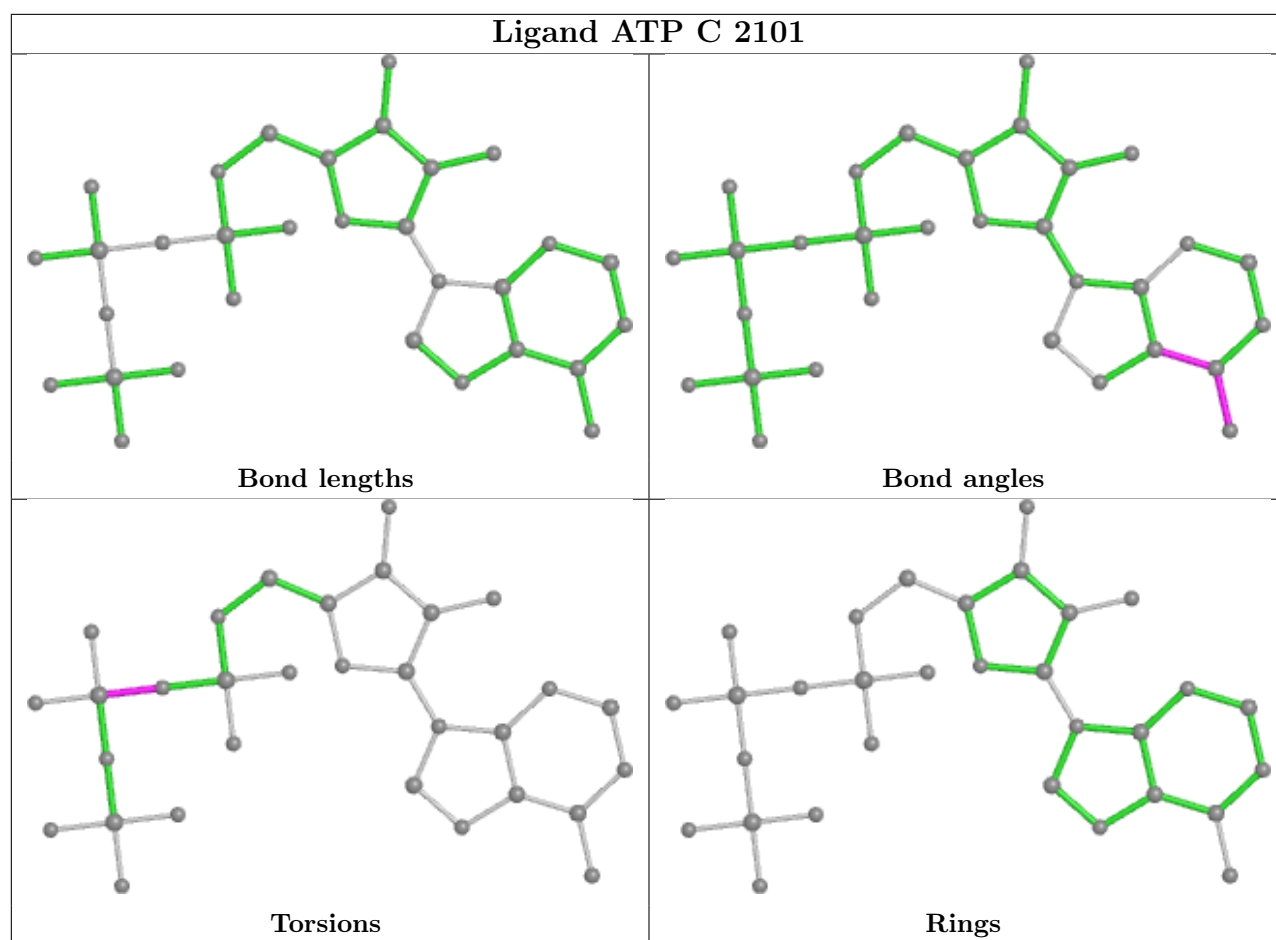












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

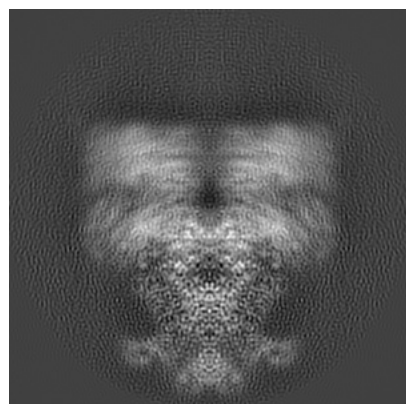
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27421. These allow visual inspection of the internal detail of the map and identification of artifacts.

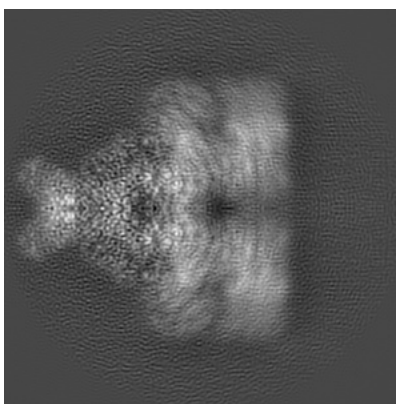
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

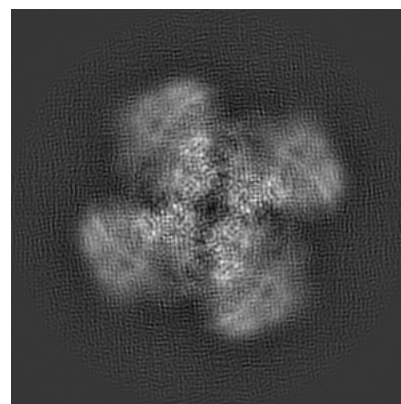
6.1.1 Primary map



X

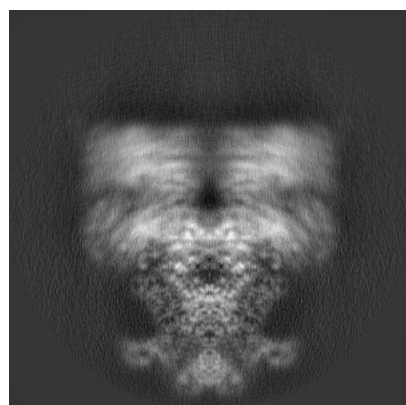


Y

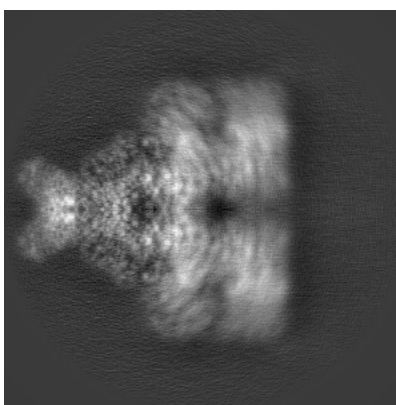


Z

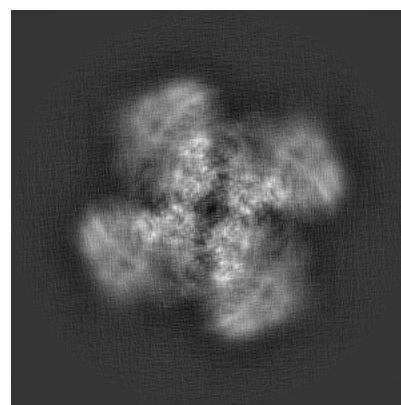
6.1.2 Raw map



X



Y

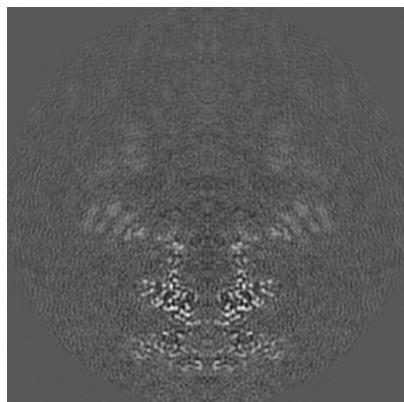


Z

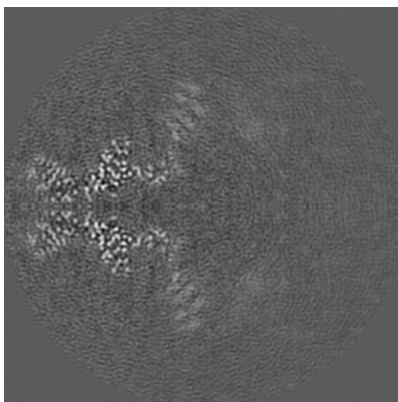
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

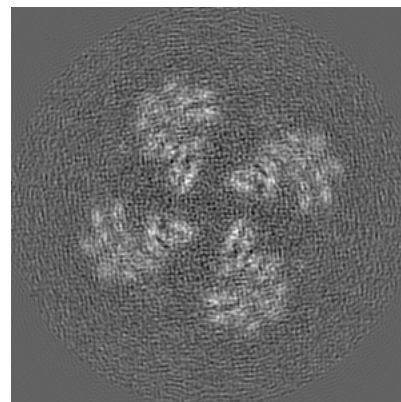
6.2.1 Primary map



X Index: 180

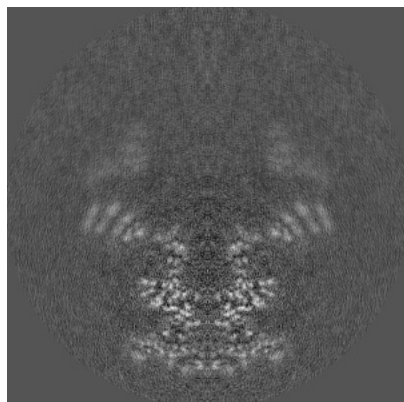


Y Index: 180

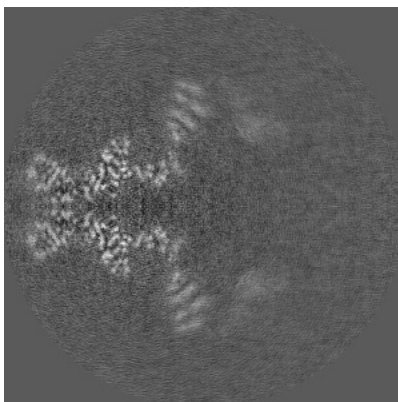


Z Index: 180

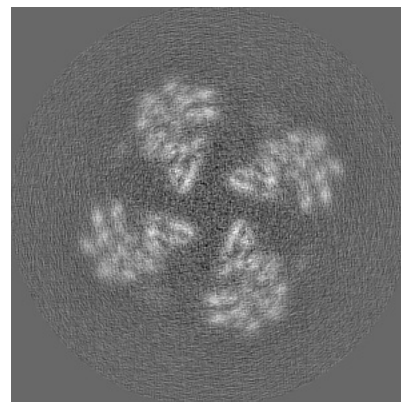
6.2.2 Raw map



X Index: 180



Y Index: 180

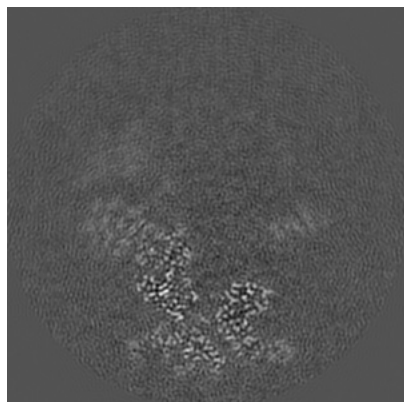


Z Index: 180

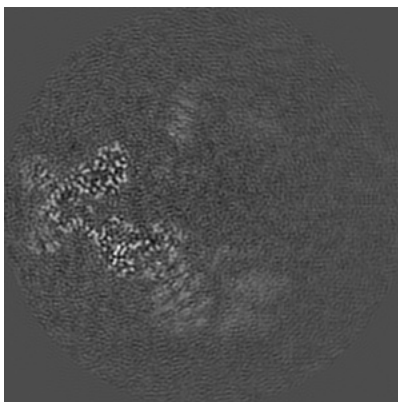
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

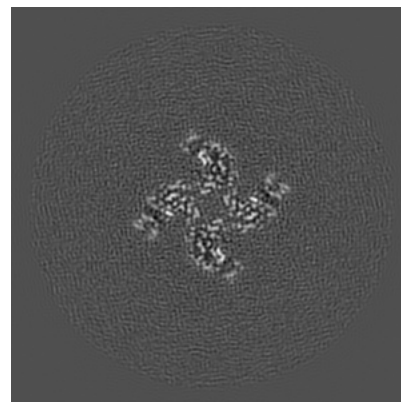
6.3.1 Primary map



X Index: 187

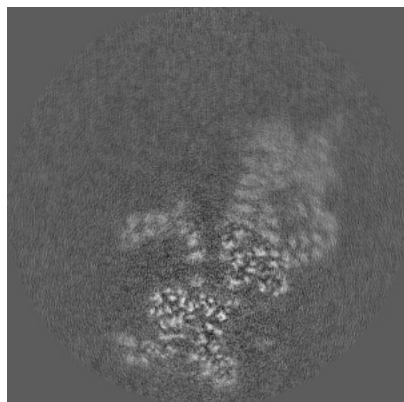


Y Index: 173

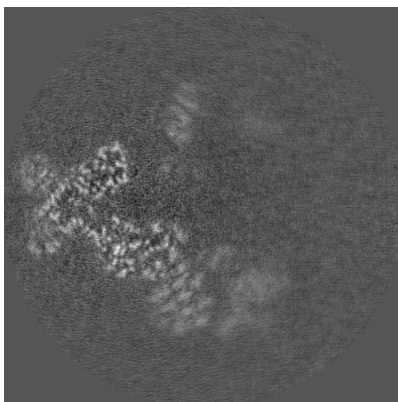


Z Index: 102

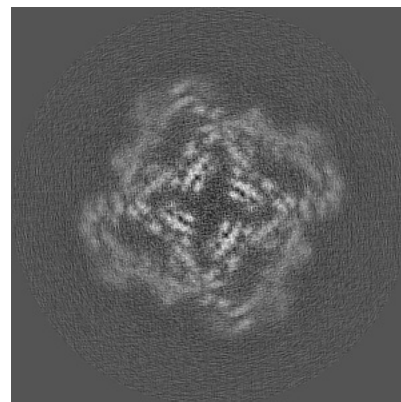
6.3.2 Raw map



X Index: 163



Y Index: 173

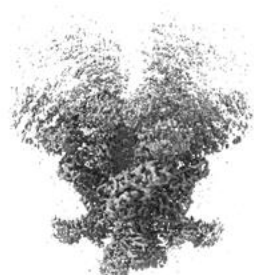


Z Index: 155

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



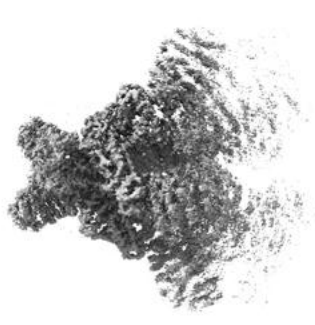
Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

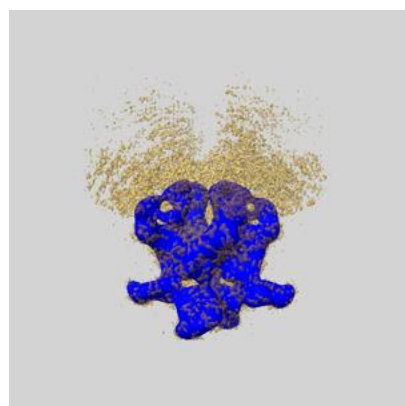
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

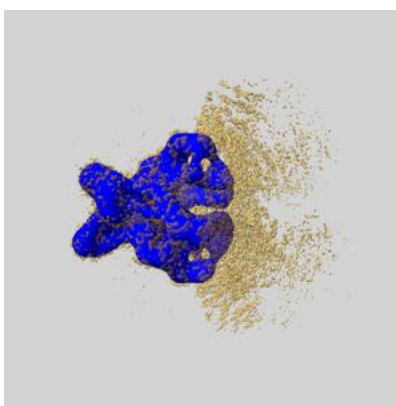
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

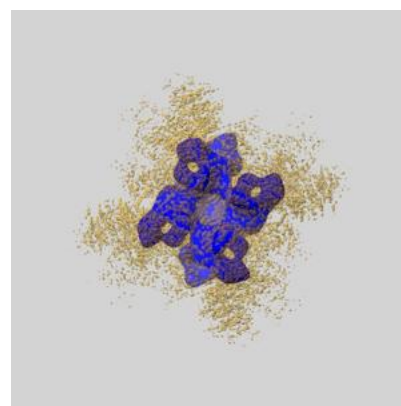
6.5.1 emd_27421_msk_1.map [i](#)



X



Y

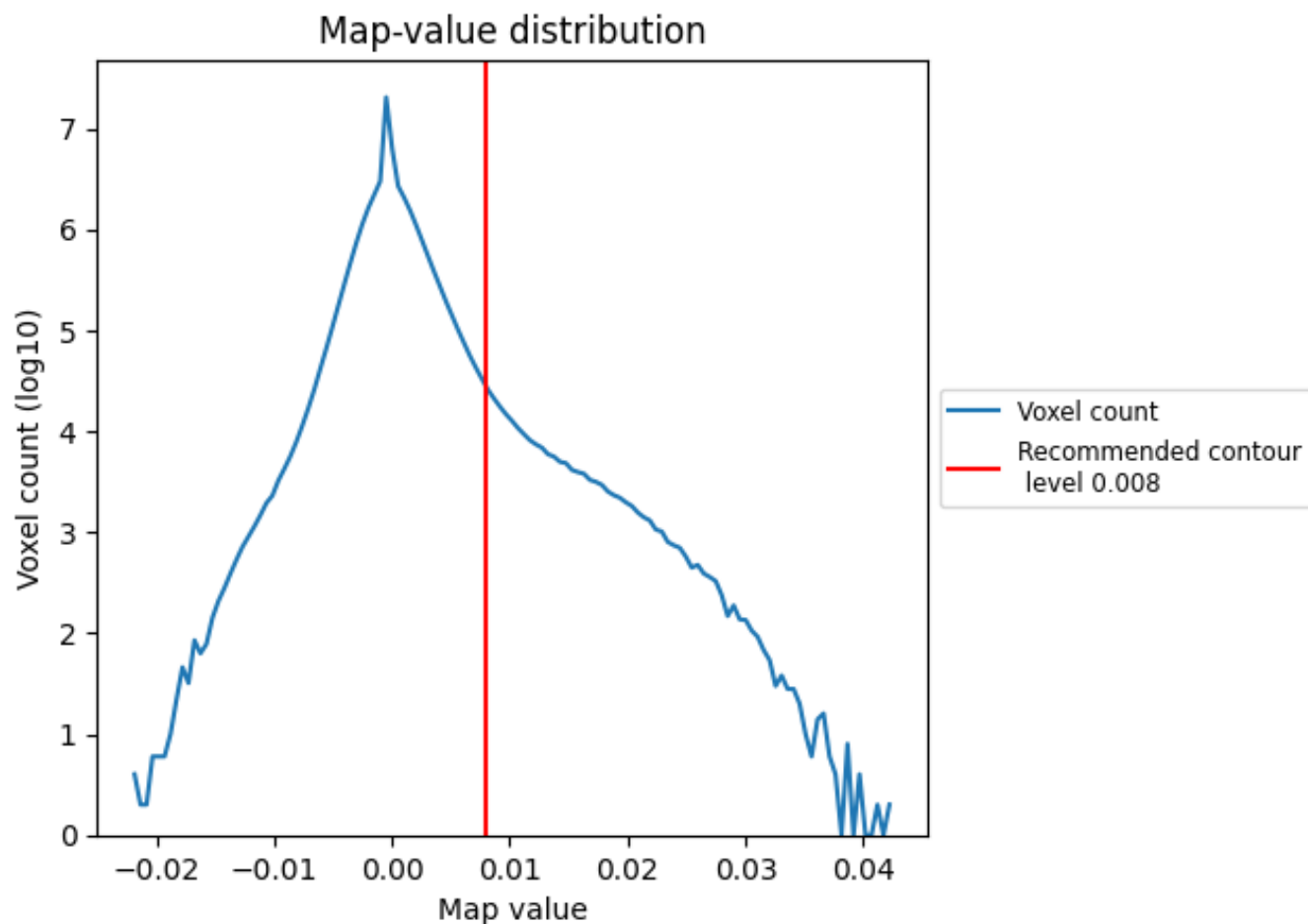


Z

7 Map analysis [i](#)

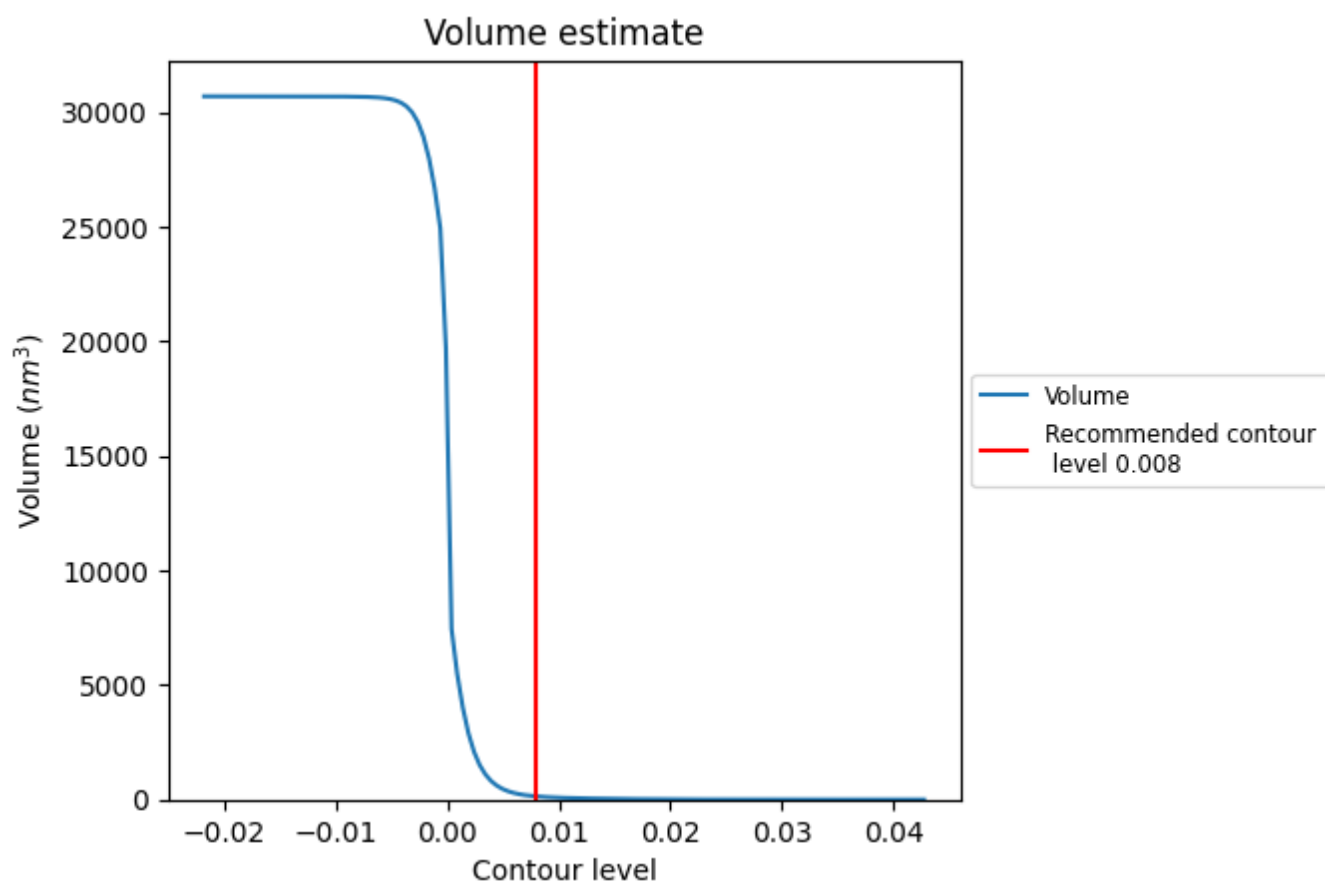
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

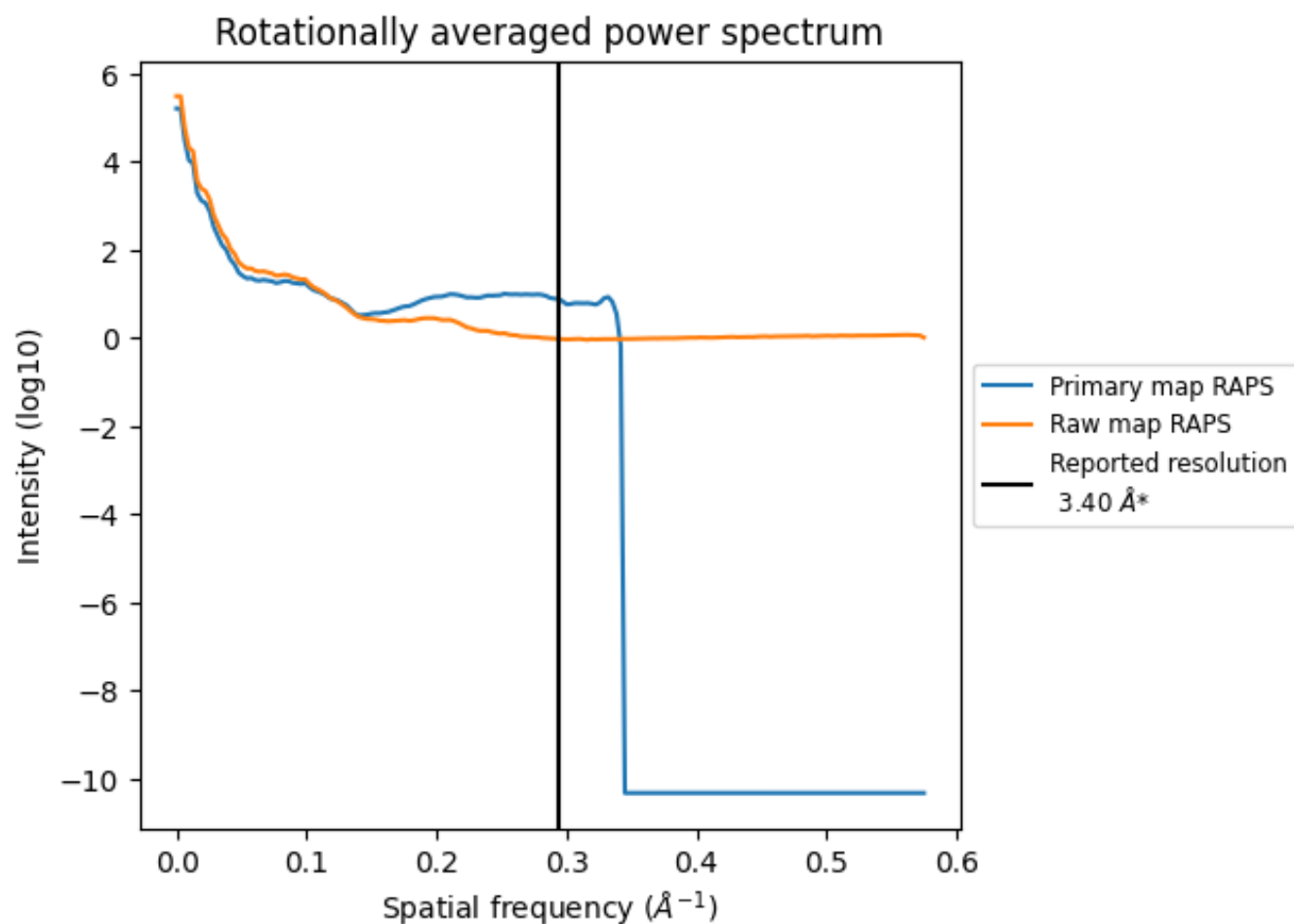
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm³; this corresponds to an approximate mass of 125 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

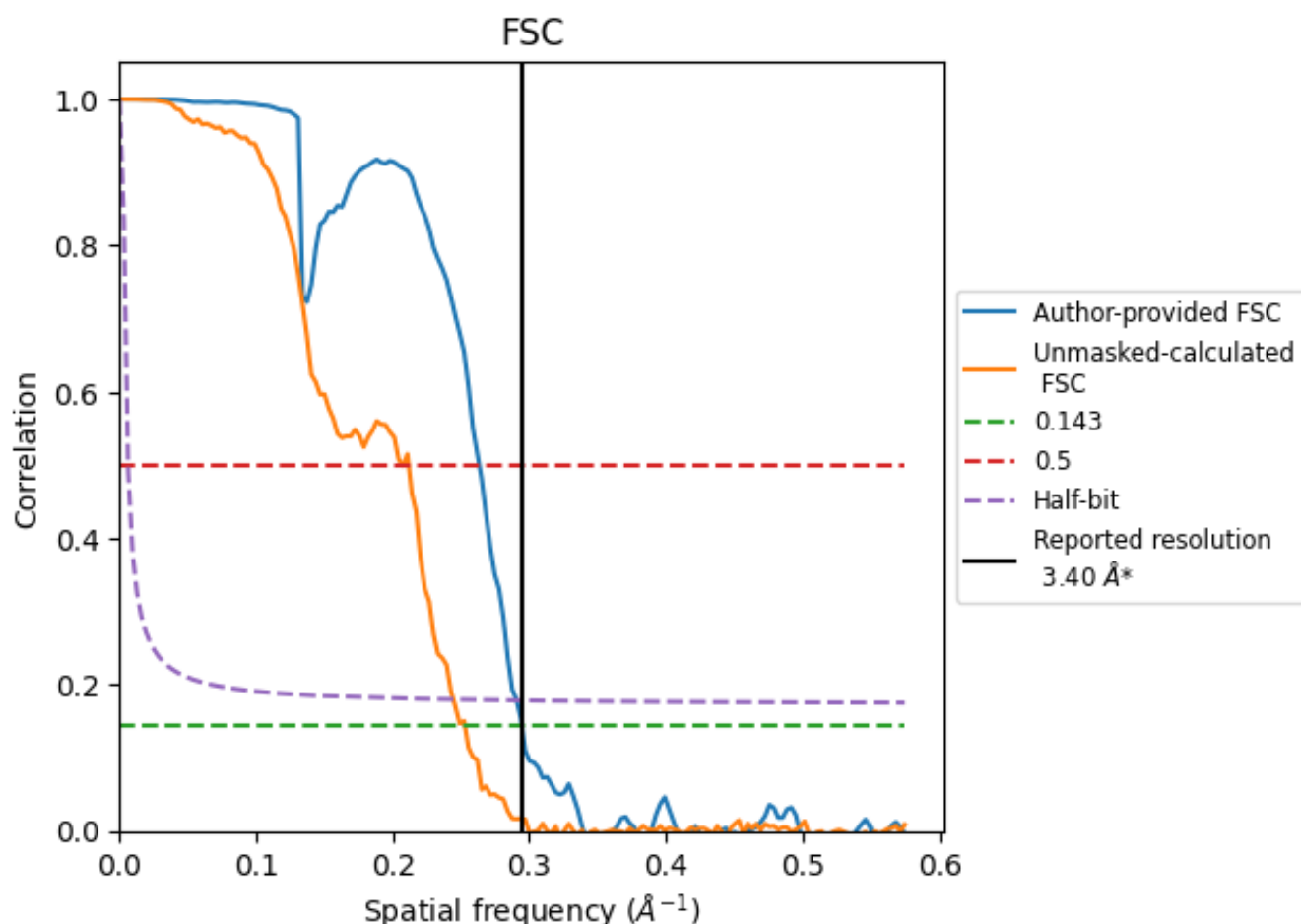


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

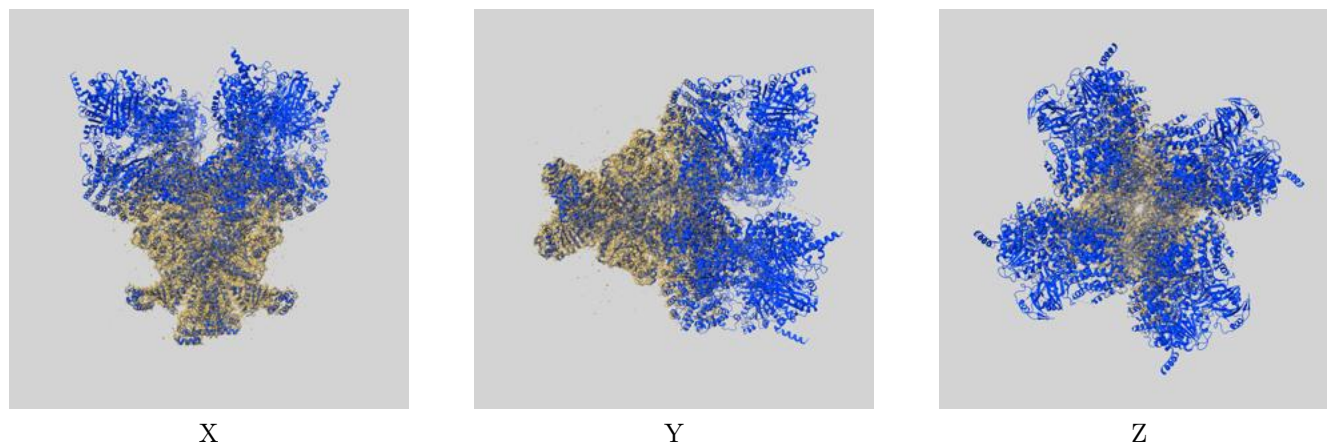
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.80	3.44
Unmasked-calculated*	3.95	4.83	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

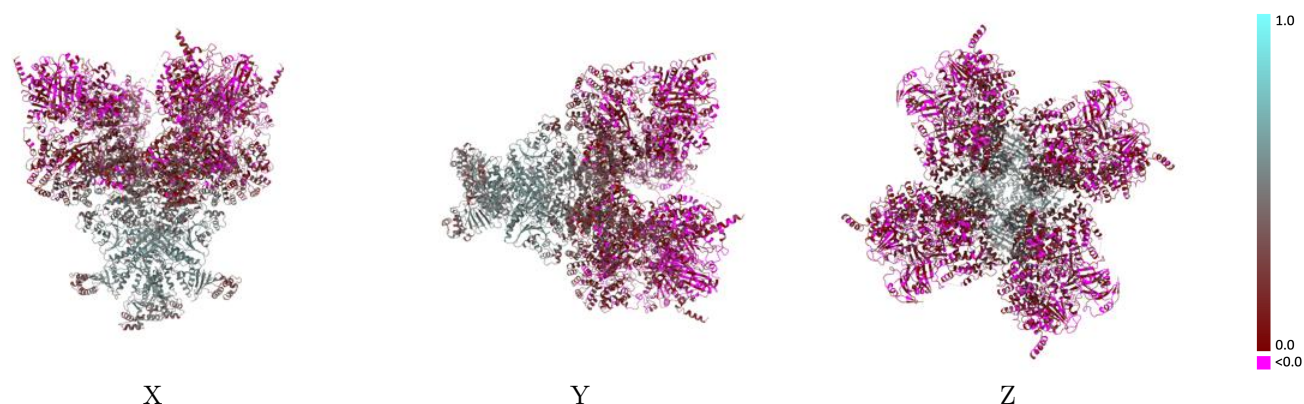
This section contains information regarding the fit between EMDB map EMD-27421 and PDB model 8DGC. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



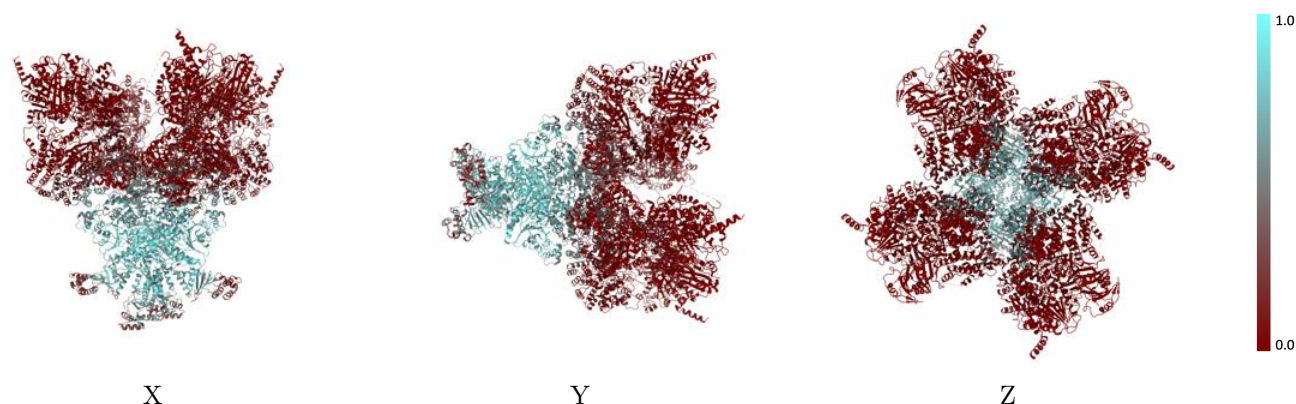
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



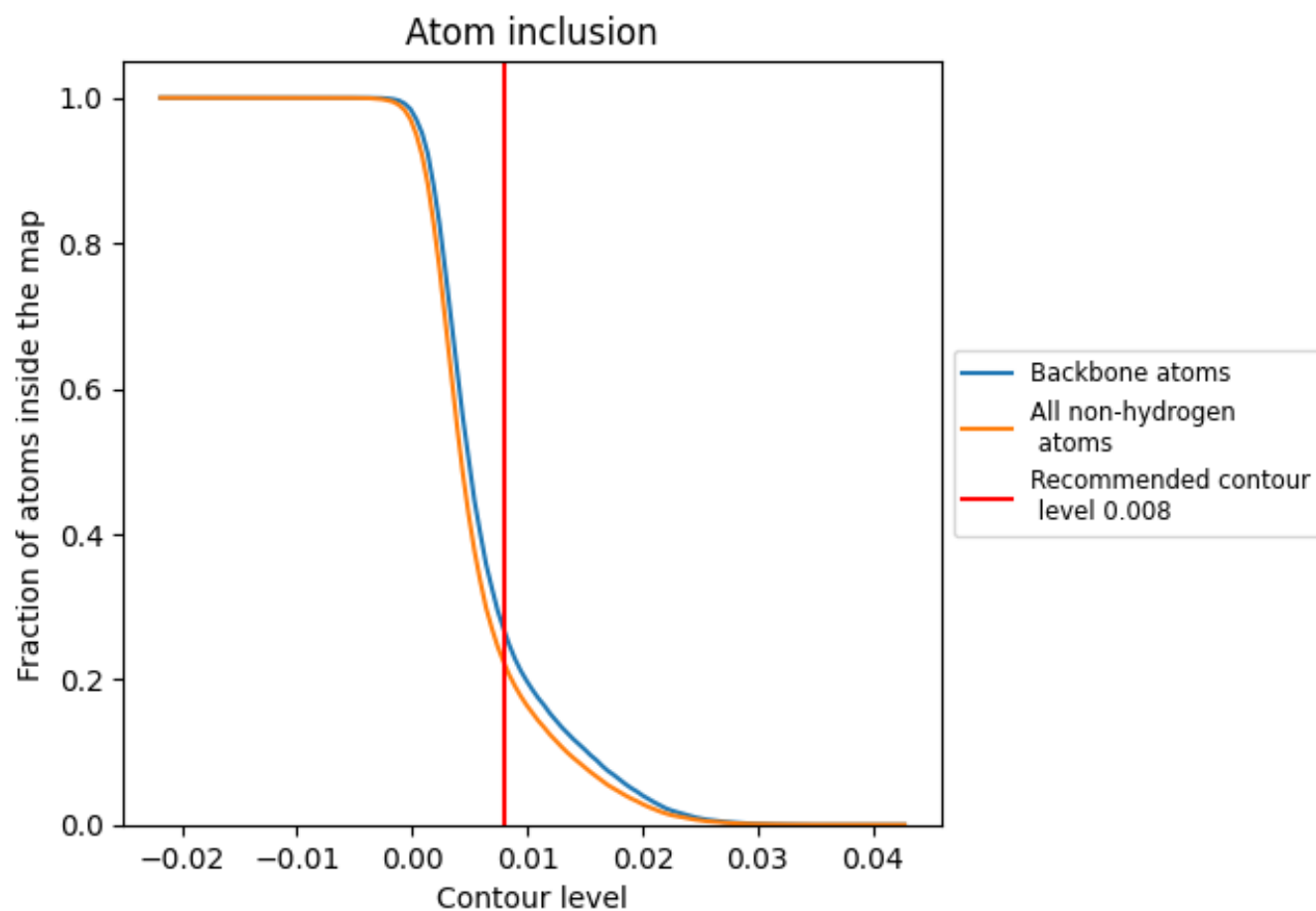
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 27% of all backbone atoms, 22% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2219	<div></div> 0.2180
A	<div></div> 0.2793	<div></div> 0.2510
B	<div></div> 0.2788	<div></div> 0.2580
C	<div></div> 0.2795	<div></div> 0.2470
D	<div></div> 0.2791	<div></div> 0.2600
E	<div></div> 0.0067	<div></div> 0.0760
F	<div></div> 0.0093	<div></div> 0.0900
G	<div></div> 0.0069	<div></div> 0.0720
H	<div></div> 0.0095	<div></div> 0.0900

1.0

0.0

<0.0