



Full wwPDB EM Validation Report ⓘ

Feb 4, 2024 – 10:45 AM 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)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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:

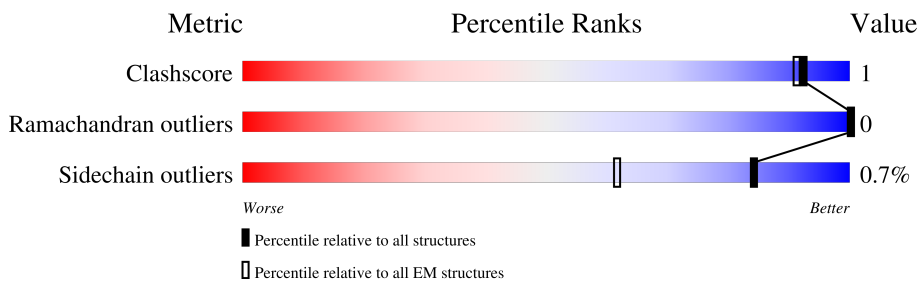
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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	66% (Upper red bar), 93% (Green), 5% (Yellow), 8% (Grey)
1	B	2092	65% (Upper red bar), 91% (Green), 5% (Yellow), 8% (Grey)
1	C	2092	66% (Upper red bar), 93% (Green), 5% (Yellow), 8% (Grey)
1	D	2092	65% (Upper red bar), 91% (Green), 5% (Yellow), 8% (Grey)
2	E	586	92% (Upper red bar), 87% (Green), 5% (Yellow), 8% (Grey)
2	F	586	92% (Upper red bar), 87% (Green), 5% (Yellow), 8% (Grey)
2	G	586	92% (Upper red bar), 87% (Green), 5% (Yellow), 8% (Grey)
2	H	586	92% (Upper red bar), 86% (Green), 5% (Yellow), 8% (Grey)

2 Entry composition [i](#)

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
			Total	C	N	O	S		
1	A	2028	16152	10199	2840	3056	57	0	0
1	B	2004	15974	10095	2809	3014	56	0	0
1	C	2028	16152	10199	2840	3056	57	0	0
1	D	2004	15974	10095	2809	3014	56	0	0

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

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

- 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	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	

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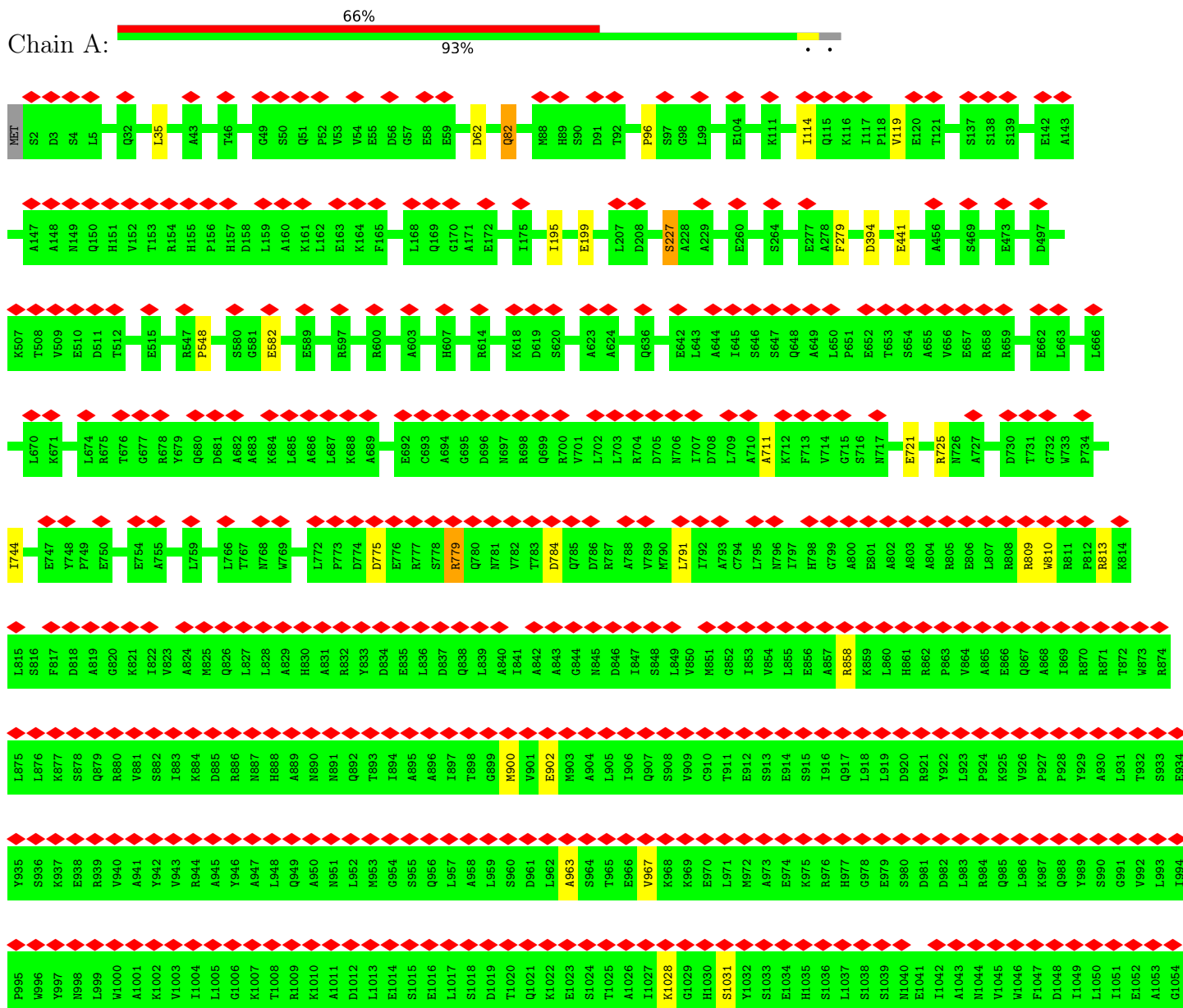
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Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0
4	G	1	Total 1	Mg 1	0
4	H	1	Total 1	Mg 1	0

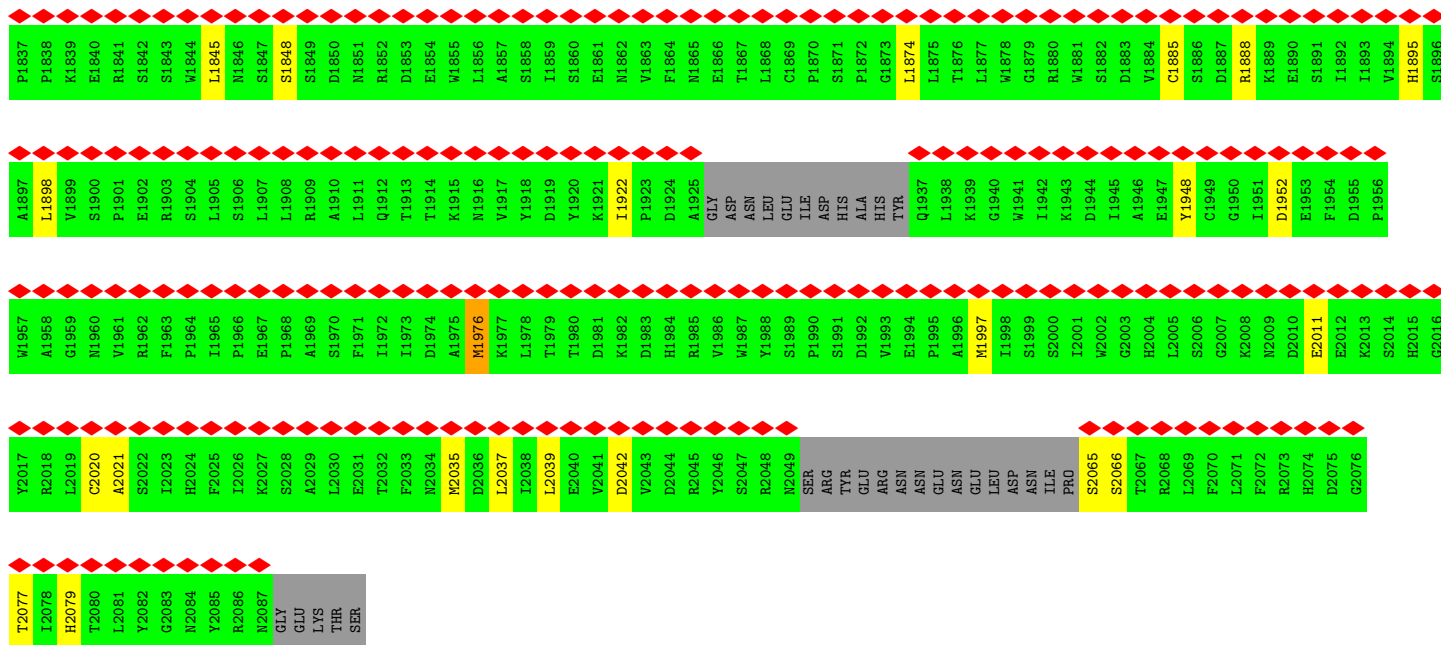
3 Residue-property plots

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.

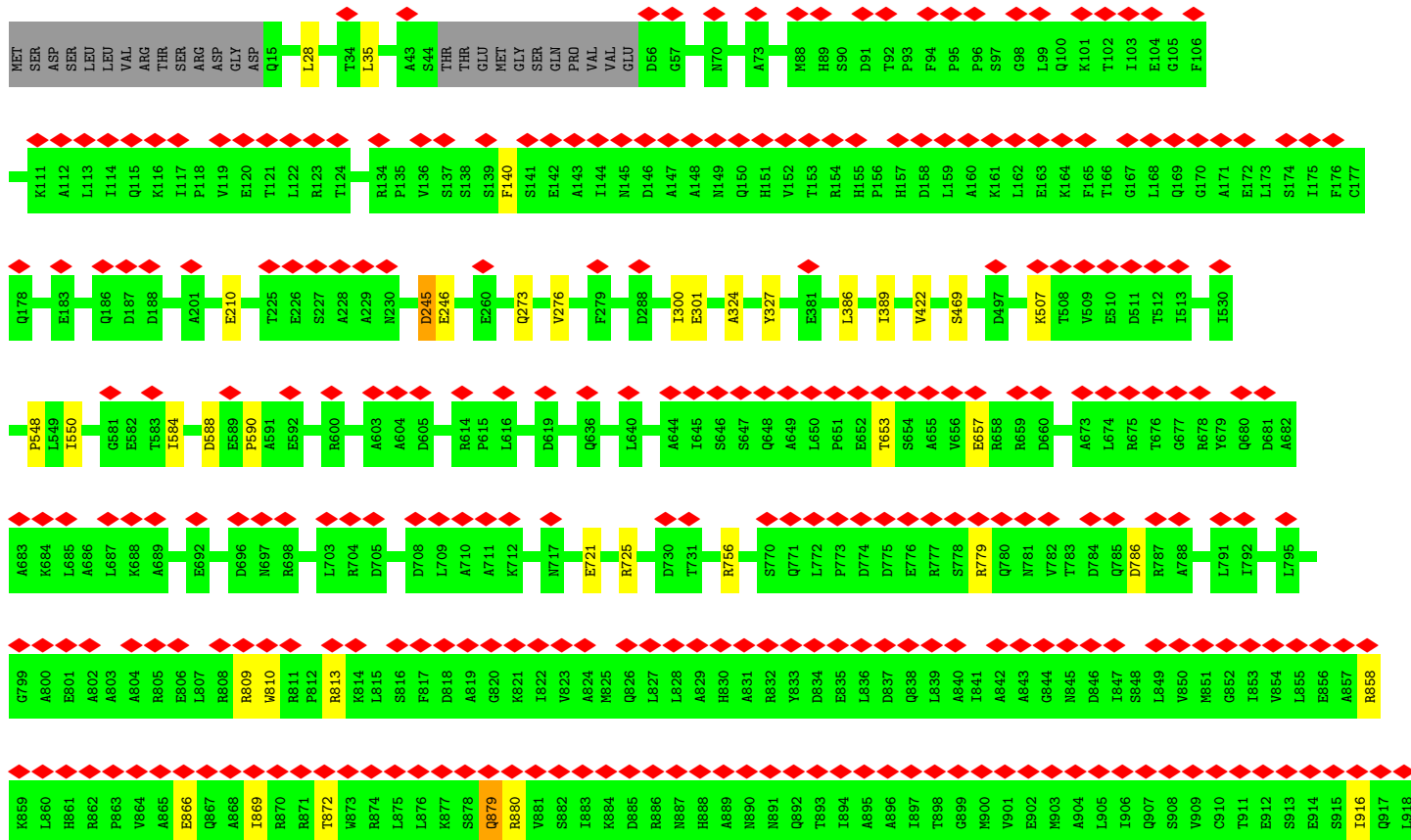
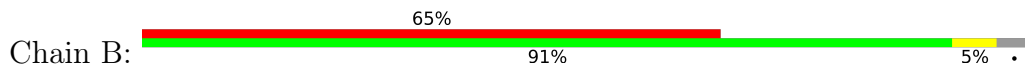
• Molecule 1: SeAvs3



M1055	V1056	S1057	K1058	D1059	D1060	V1061	E1062	M1063	M1064	L1065	K1066	M1067	S1068	Q1069	H1070	K1071	G1072	M1073	R1074	V1075	F1076	T1077	P1078	T1079	L1080	H1081	F1082	S1084	S1085	V1086	K1087	M1088	M1089	I1090	S1091	G1092	L1093	G1094	E1095	L1096	S1097	V1098	H1099	F1100	A1101	E1102	L1103	A1104	L1105	S1106	L1107	M1108	R1109	D1110	E1111	H1112	S1113	D1114	
A1115	Q1116	I1117	K1118	A1119	D1120	G1121	Y1122	I1123	D1124	L1125	S1126	R1127	S1128	L1129	I1130	S1131	L1132	D1133	E1134	P1135	E1136	A1137	K1138	E1139	Y1140	F1141	N1142	Q1143	A1144	E1146	N1149	K1150	L1151	G1152	D1153	E1154	N1155	L1156	S1157	R1158	W1159	E1160	A1161	I1162	L1163	D1164	L1165	A1166	E1167	Y1168	V1169	A1170	G1171	K1172	T1173	Q1174	V1175		
P1176	P1177	E1178	I1179	S1180	Y1181	K1182	L1183	A1184	R1185	C1186	A1187	E1188	L1189	L1190	R1191	E1192	Y1193	V1194	D1195	L1196	D1197	K1198	H1199	F1200	A1201	W1202	S1203	D1204	L1205	V1206	E1207	L1208	I1209	A1210	E1211	L1212	C1213	P1214	S1215	S1216	R1217	L1218	A1219	I1220	I1221	L1222	S1223	R1224	W1225	D1226	R1227	L1228	F1229	G1230	M1231	H1232	R1233	S1234	I1235
L1236	A1237	W1238	T1239	I1240	E1241	H1242	L1243	V1244	R1245	K1246	M1247	K1248	I1249	M1250	A1251	L1252	D1253	A1254	L1255	L1256	P1257	I1258	T1259	F1260	E1261	M1262	D1263	W1264	H1265	K1266	C1267	D1268	I1269	L1270	D1271	S1272	V1273	L1274	S1275	S1276	S1277	T1278	D1279	K1280	A1281	I1282	D1283	I1284	M1285	A1286	F1287	E1288	V1289	V1290	Y1291	H1292	Y1293	T1294	K1295
F1296	N1297	V1298	Q1299	M1300	I1301	Q1302	M1303	L1304	K1305	K1306	L1307	D1308	A1309	I1310	S1311	L1312	S1313	L1314	G1315	I1316	E1317	H1318	T1319	E1320	L1321	K1322	D1323	W1324	I1325	S1326	G1327	L1328	Q1329	H1330	THR	GLU	THR	VAL	SER	LYS	SER	SER	LEU	SER	ASN	ASP	GLN	G1348	H1349	D1350	Q1351	W1352	W1353	E1354	S1355				
I1356	F1357	K1358	D1359	C1360	D1361	L1362	S1363	S1364	I1365	D1366	G1367	L1368	S1369	A1370	A1371	Y1372	E1373	K1374	F1375	R1376	I1377	V1378	P1379	E1380	F1381	Y1382	S1383	K1384	E1385	T1386	F1387	L1388	K1389	K1390	A1391	I1392	S1393	R1394	V1395	L1396	R1397	G1398	K1399	E1400	C1401	S1402	F1403	I1404	T1405	A1406	I1407	G1408	A1409	I1410	F1411	H1412	W1413	G1414	L1415
Y1416	D1417	F1418	K1419	I1420	I1421	L1422	E1423	I1424	I1425	P1426	D1427	E1428	Y1429	T1430	S1431	R1432	L1433	S1434	I1435	K1436	L1437	A1440	G1441	L1442	I1443	K1444	E1445	Y1446	C1447	Q1448	R1449	F1450	C1451	M1452	R1453	L1454	R1455	K1456	S1457	R1458	V1459	Y1460	E1461	I1462	P1463	F1464	F1465	S1466	L1467	A1468	S1469	R1470	L1471	S1472	E1533	D1534	I1474	S1475	E1476
K1477	E1478	I1479	F1480	G1481	T1482	T1483	L1484	E1485	A1486	I1487	A1488	E1489	S1490	P1491	E1492	P1493	A1494	M1495	S1496	D1497	A1498	F1500	S1501	L1502	P1503	G1504	L1505	L1506	V1507	S1508	K1509	L1510	E1511	S1512	M1513	E1514	A1515	L1516	D1517	V1518	L1519	S1520	Y1521	A1522	L1523	D1524	L1525	F1526	D1527	E1528	V1529	L1530	K1531	D1532	E1533	D1534	D1535	D1536	
G1537	P1538	W1539	M1540	E1541	K1542	L1543	S1544	P1545	P1546	T1547	H1548	V1549	E1550	D1551	S1552	L1553	A1554	G1555	Y1556	I1557	W1558	A1559	R1560	L1561	G1562	S1563	P1564	E1565	A1566	E1567	M1568	L1569	W1570	Q1571	A1572	A1573	H1574	A1575	V1576	L1577	A1578	L1579	C1580	L1581	M1582	S1583	R1584	L1585	C1586	V1587	I1588	Q1589	I1590	I1591	E1592	Q1593	H1594	A1595	I1596
M1597	A1598	T1599	T1600	L1601	P1602	F1603	C1604	L1605	R1606	M1607	L1608	P1609	F1610	Y1611	T1612	L1613	H1614	A1615	Q1616	L1617	W1618	M1619	M1620	I1621	A1622	A1623	A1624	R1625	V1626	A1627	L1628	D1629	D1630	G1631	K1632	S1633	L1634	I1635	P1636	M1637	I1638	I1639	Y1640	F1641	F1642	H1643	Y1644	A1645	T1646	T1647	D1648	Q1649	P1650	H1651	V1652	L1653	I1654	R1655	H1656
F1657	A1658	A1659	R1660	T1661	L1662	A1664	L1665	H1666	D1667	S1668	P1669	L1670	I1671	S1672	I1673	P1674	A1675	Q1676	E1677	E1678	N1679	K1680	L1681	L1682	M1683	I1684	Q1685	Q1686	S1687	T1688	L1689	L1690	P1691	L1692	LEU	ASP	LYS	VAL	GLU	ASP	HTS	ARG	GLY	E1702	D1703	S1704	Y1705	T1706	F1707	F1708	I1709	D1710	F1711	G1712	P1713	W1714	W1715	L1716	
K1717	P1718	L1719	G1720	R1721	C1722	G1724	V1725	H1726	Q1727	K1728	Q1729	L1730	E1731	P1732	E1733	M1734	L1735	R1736	I1737	I1738	R1739	D1740	V1741	L1742	G1743	F1744	K1745	G1746	S1747	R1748	M1749	W1750	D1751	E1752	D1753	E1754	R1755	M1756	K1757	R1758	R1759	Y1760	Y1761	Q1762	D1763	R1764	D1765	M1766	H1767	H1768	S1769	H1770	G1771	R1833	R1834	D1835	I1836		
D1777	D1778	Y1779	H1780	F1781	Y1782	S1784	Y1785	H1786	A1787	M1788	F1789	M1790	T1791	A1792	G1793	Q1794	L1795	L1796	A1797	I1798	K1799	P1800	L1801	V1802	G1803	SER	ASP	TYR	ASP	VAL	E1810	D1811	V1812	F1813	Q1814	D1815	W1816	L1817	R1818	R1819	H1820	I1821	I1822	S1823	R1824	N1825	D1826	H1827	R1828	W1829	L1830	A1831	D1832	R1833	R1834	D1835	I1836		



• Molecule 1: SeAvs3

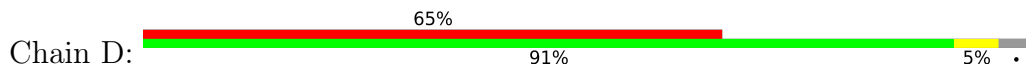


H1643	S1583	L1523	F1463	S1402	SER	D1282	S1222	I1162	H1099	N1039	E979	L919
Y1644	R1584	D1524	P1464	F1403	ASN	K1283	R1223	L1163	F1100	N1040	S980	D920
A1645	T1585	L1525	F1465	I1404	ASP	I1284	W1224	D1164	A1101	E1041	D981	R921
T1646	C1586	F1526	S1466	T1405	ASN	M1285	R1225	L1165	E1102	I1042	D982	Y922
T1647	L1587	D1527	S1467	A1406	GLU	A1286	R1226	A1166	L1103	A1043	L983	L923
L1648	V1588	E1528	A1468	I1407	GLN	F1287	R1227	E1167	A1104	N1044	R984	P924
Q1649	Q1589	E1529	S1469	G1408	G1348	H1288	T1228	Y1168	L1105	V1045	Q985	K925
P1650	G1590	L1530	R1470	A1409	H1349	V1289	F1229	V1169	S1106	V1046	L986	V926
H1651	K1591	K1531	L1471	F1410	D1350	V1290	G1230	A1170	K987	F1047	Q988	P927
L1652	F1592	D1532	S1472	F1411	E1352	Y1291	H1231	W1108	Q989	D1048	Y929	Y928
L1653	Q1593	E1533	G1473	H1412	H1292	H1292	H1232	R1109	Y989	I1049	Y929	Y929
L1654	H1594	D1534	I1474	W1413	Y1293	T1294	R1233	D1110	S990	L1050	A930	A930
R1655	A1595	E1535	S1475	G1414	S1355	L1294	S1234	H1111	G991	I1051	L931	L931
H1656	I1596	D1536	E1476	L1415	I1356	K1295	I1235	H1112	V992	E1052	S932	S932
F1657	M1597	G1537	K1477	Y1416	F1357	F1296	L1236	S1113	V993	A1053	S933	S933
A1658	A1598	P1538	E1478	D1417	K1358	F1298	A1237	D1114	L993	G1054	E934	E934
A1659	T1599	M1539	I1479	F1418	N1297	N1298	W1238	A1115	P995	N1055	S935	S935
R1660	T1600	M1540	F1480	K1419	C1360	Q1299	T1239	Q1116	W996	V1056	S936	S936
T1661	L1601	E1541	G1481	Y1420	D1361	M1300	I1240	I1117	Y997	S1057	K937	K937
L1662	P1602	I1542	I1482	I1421	L1362	I1301	E1241	K1118	R998	K1058	E938	E938
L1663	F1603	K1543	T1483	L1422	S1363	Q1302	H1242	A1119	L999	D1059	R939	R939
A1664	C1604	L1544	L1484	E1423	S1364	M1303	L1243	W1000	W1000	D1060	V940	V940
L1665	D1605	P1545	E1485	S1424	I1365	L1304	V1244	V1061	A1001	V1061	A941	A941
H1666	R1606	P1546	A1486	I1425	D1366	K1305	K1245	E1062	I1002	E1062	Y942	Y942
D1667	M1607	T1547	I1487	F1426	G1367	K1306	K1246	C1186	V1003	N1063	V943	V943
S1668	L1608	H1548	A1488	D1427	I1368	L1307	M1247	S1126	I1004	I1064	R944	R944
D1669	P1609	V1549	E1489	E1428	S1369	D1308	K1248	E1188	L1005	I1065	A945	A945
L1670	F1610	E1550	P1491	W1429	A1370	A1309	I1249	L1189	G1006	K1066	Y946	Y946
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S1672	T1612	S1552	P1493	S1431	S1311	R1191	A1251	R1191	T1008	S1068	L948	L948
L1673	L1613	L1553	A1494	R1432	T1312	L1192	L1252	E1192	R1009	Q1069	Q949	Q949
P1674	H1614	A1554	L1495	L1433	S1313	D1253	D1253	I1193	K1010	K1069	A950	A950
A1675	A1615	G1555	N1496	S1434	L1314	A1254	A1254	D1133	A1011	H1070	N951	N951
Q1676	A1616	V1556	D1497	I1435	G1315	D1195	L1255	E1134	D1012	G1072	L952	L952
E1677	L1617	I1557	R1498	K1436	I1316	D1196	P1256	R1196	L1013	N1073	M953	M953
M1678	W1618	W1558	T1437	F1437	E1317	L1316	L1257	E1136	E1014	R1074	G954	G954
N1679	L1619	L1559	L1438	T1438	H1318	H1318	L1258	A1137	S1015	V1075	S955	S955
K1680	M1620	A1560	L1439	L1439	F1319	H1199	T1259	K1138	E1016	F1076	Q956	Q956
L1681	I1621	L1561	A1440	A1440	E1320	F1200	F1260	Y1140	L1017	T1077	L957	L957
R1682	A1622	P1562	P1503	I1443	L1321	A1201	E1261	F1141	S1018	P1078	A958	A958
N1683	A1623	G1563	G1504	K1444	K1322	W1201	M1262	M1142	D1019	T1079	L959	L959
I1684	A1624	L1564	L1505	E1445	E1323	S1203	D1263	Q1143	T1020	L1080	S960	S960
N1685	R1625	E1565	L1506	Y1446	R1324	D1204	W1264	A1144	Q1021	H1081	D961	D961
Q1686	V1626	A1566	V1507	C1447	T1325	T1205	H1265	I1145	K1022	R1082	L962	L962
S1687	A1627	E1567	S1508	C1447	S1326	V1206	K1266	E1146	E1023	F1083	A963	A963
T1688	L1628	M1568	K1509	Q1448	G1327	E1207	C1267	S1084	S1024	S1084	S964	S964
T1689	D1629	R1569	L1510	R1449	K1389	L1328	D1268	S1085	T1025	S1085	T965	T965
L1690	D1630	W1570	E1511	F1450	K1390	Q1329	L1269	V1086	A1026	E1086	E966	E966
P1691	G1631	Q1571	M1512	C1451	A1391	H1330	L1270	C1087	I1027	C1087	V967	V967
V1692	K1632	R1572	M1513	R1452	I1392	D1271	D1271	A1088	K1028	K1028	K968	K968
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ASP	S1633	L1574	L1454	R1394	THR	T1272	S1272	I1090	H1030	H1030	E970	E970
VAL	L1634	R1455	R1455	V1395	VAL	V1273	V1273	S1091	S1031	S1031	M972	M972
GLU	I1635	K1456	K1456	K1396	SER	L1274	L1274	L1092	Y1032	Y1032	A973	A973
GLU	M1636	D1517	S1457	T1397	LYS	S1275	S1275	G1094	S1033	S1033	E974	E974
ASP	M1637	V1518	R1458	G1398	LYS	S1276	S1276	E1095	E1034	E1034	E974	E974
ASP	H1638	L1519	R1458	G1398	SER	C1277	C1277	L1096	H1035	H1035	R976	R976
ARG	L1639	A1578	V1459	K1399	LEU	T1278	T1278	L1097	S1036	S1036	H977	H977
GLY	E1640	Y1521	F1460	K1399	SER	D1279	D1279	Y1098	L1037	L1037	G978	G978
E1702	F1641	A1522	E1461	E1400	C1401	D1280	D1280	Y1098	S1038	S1038	G978	G978
	Y1642	I1462	I1462	I1462	I1462	I1221	I1221					

L807	R808	R809	W810	R811	P812	R813	K814	L815	S816	F817	D818	A819	G820	K821	I822	V823	A824	M825	Q826	L827	L828	A829	H830	A831	R832	Y833	D834	E835	L836	D837	L838	L839	A840	I841	A842	A843	G844	N845	D846	I847	S848	V850	M851	G852	I853	V854	L855	E856	A857	R858	K859	L860	H861	R862	P863	V864	A865	E866		
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C1949	G1950	I1951	D1952	E1953	F1954	D1955	P1956	M1957	A1958	G1959	M1960	V1961	R1962	F1963	P1964	I1965	P1966	E1967	P1968	A1969	S1970	F1971	I1972	I1973	D1974	A1975	M1976	K1977	L1978	T1979	T1980	D1981	K1982	D1983	H1984	R1985	V1986	W1987	Y1988	S1989	S1990	S1991	R1992	GLU	ARG	GLU	ARG	ASN	ASN	ASN	ASN	GLU	LEU	ASP	ASN	ILE	PRO	S2065	W2002	G2003	H2004	L2005	G2007	K2008
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L2069	F2070	L2071	F2072	R2073	H2074	D2075	G2076	L2077	I2078	H2079	T2080	L2081	Y2082	G2083	N2084	Y2085	R2086	N2087	GLY	GLU	LYS	THR	SER																																									

● Molecule 1: SeAvs3

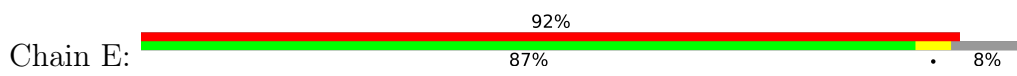


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D681	A682	A683	K684	L685	A686	L687	K688	A689	E692	D696	N697	R698	L703	R704	D705	D708	L709	A710	A711	K712	W717	E721	R725	D730	I645	S646	S647	Q648	A649	L650	P651	E652	T653	S654	A655	V656	R658	R659	A673	L674	R675	T676	G677	R678	L679	Q680																																																																								
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S1097	Y1098	H1099	F1100	A1101	E1102	L1103	A1104	L1105	S1106	L1107	W1108	H1109	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	W1147	K1150	L1151	D1152	D1153	E1154	N1155	L1156	S1157	R1158	W1159	E1160	A1161	I1162	L1163	D1164	L1165	A1166	E1167	V1168	Y1169	A1170	G1171	K1172	T1173	Q1174	W1175	P1176	E1177	E1178	I1179	S1180	K1181	K1182	L1183	A1184	R1185	C1186	E1187	E1188	L1189	T1190	R1191	E1192	Y1193	V1194	D1195	R1196	D1197	K1198	H1199	F1200	F1201	A1202	W1202	S1203	D1204	T1205	E1206	E1207	L1208	L1209	A1210	E1211	L1212	C1213	P1214	S1215	S1216	A1217	L1218	A1219
E1160	A1161	I1162	L1163	D1164	L1165	A1166	E1167	V1168	Y1169	A1170	G1171	K1172	T1173	Q1174	W1175	P1176	E1177	E1178	I1179	S1180	K1181	K1182	L1183	A1184	R1185	C1186	E1187	E1188	L1189	T1190	R1191	E1192	Y1193	V1194	D1195	R1196	D1197	K1198	H1199	F1200	F1201	A1202	W1202	S1203	D1204	T1205	E1206	E1207	L1208	L1209	A1210	E1211	L1212	C1213	P1214	S1215	S1216	A1217	L1218	A1219																																																										
I1220	I1221	S1222	R1223	W1224	R1225	D1226	R1227	T1228	F1229	G1230	N1231	H1232	R1233	S1234	I1235	L1236	W1238	T1239	I1240	E1241	H1242	L1243	V1244	K1245	K1246	N1247	K1248	I1249	N1250	A1251	L1252	D1253	A1254	L1255	P1256	L1257	I1258	T1259	F1260	E1261	N1262	E1263	W1264	H1265	K1266	C1267	D1268	L1269	L1270	D1271	S1272	V1273	L1274	S1275	C1276	T1277	D1279																																																													
D1280	K1281	D1282	K1283	I1284	M1285	A1286	F1287	E1288	V1289	Y1290	Y1291	H1292	Y1293	T1294	K1295	F1296	M1297	V1298	Q1299	N1300	I1301	M1303	L1304	K1305	K1306	L1307	D1308	A1309	I1310	S1311	S1312	S1313	L1314	G1315	L1316	E1317	H1318	T1319	E1320	L1321	K1322	E1323	A1324	I1325	S1326	G1327	L1328	Q1329	H1330	THR	GLU	THR	VAL	SER	LYS	SER	SER	L1339																																																												
LEU	SER	ASN	ASP	ASN	GLU	GLN	G1348	H1349	D1350	Q1351	E1352	W1353	E1354	S1355	I1356	F1357	K1358	D1359	C1360	D1361	L1362	S1363	I1365	D1366	G1367	I1368	S1369	A1370	A1371	E1373	K1374	F1375	R1376	N1377	V1378	P1379	E1380	F1381	Y1382	S1383	K1384	E1385	T1386	F1387	I1388	K1389	L1390	A1391	I1392	S1393	R1394	V1395	K1396	T1397	G1398	K1399																																																														
E1400	C1401	S1402	F1403	I1404	T1405	A1406	I1407	G1408	A1409	I1410	F1411	H1412	W1413	G1414	L1415	Y1416	D1417	F1418	K1419	Y1420	I1421	L1422	E1423	S1424	I1425	P1426	D1427	E1428	W1429	T1430	S1431	E1432	L1433	S1434	I1435	K1436	T1437	L1438	L1439	A1440	I1443	K1444	E1445	Y1446	C1447	Q1448	R1449	F1450	C1451	M1452	R1453	I1454	R1455	K1456	S1457	R1458	V1459																																																													

E1461	I1462	F1463	P1464	F1465	S1466	L1467	A1468	S1469	R1470	L1471	S1472	G1473	I1474	S1475	E1476	K1477	E1478	I1479	F1480	G1481	I1482	T1483	L1484	E1485	A1486	I1487	A1488	E1489	S1490	P1491	E1492	P1493	A1494	M1495	S1496	D1497	R1498	L1499	F1500	S1501	P1503	G1504	L1505	L1506	V1507	S1508	K1509	L1510	E1511	S1512	M1513	E1514	L1516	D1517	L1518	L1519	S1520			
Y1521	A1522	L1523	D1524	F1525	F1526	D1527	E1528	V1529	L1530	K1531	D1532	E1533	D1534	G1535	D1536	G1537	P1538	W1539	M1540	E1541	K1542	L1543	S1544	P1545	P1546	T1547	H1548	V1549	E1550	D1551	S1552	L1553	A1554	G1555	V1556	I1557	W1558	A1559	R1560	L1561	S1562	S1563	P1564	E1565	E1567	M1568	R1569	V1570	Q1571	M1572	A1573	H1574	A1575	V1576	L1577	A1578	L1579	C1580		
R1581	M1582	S1583	R1584	C1585	V1587	I1588	Q1589	L1590	I1591	F1592	Q1593	H1594	A1595	I1596	M1597	A1598	T1599	T1600	L1601	P1602	F1603	C1604	D1605	P1606	M1607	L1608	P1609	F1610	Y1611	T1612	L1613	H1614	A1615	Q1616	L1617	W1618	L1619	M1620	I1621	A1622	A1623	A1624	M1625	V1626	A1627	L1628	D1629	D1630	G1631	K1632	S1633	L1634	I1635	P1636	M1637	I1638	G1639	Y1640		
F1641	Y1642	H1643	Y1644	A1645	T1646	T1647	D1648	Q1649	D1650	H1651	V1652	L1653	I1654	R1655	H1656	F1657	A1658	A1659	R1660	T1661	L1662	L1663	A1664	L1665	L1666	D1667	S1668	D1669	L1670	I1671	S1672	L1673	P1674	A1675	Q1676	E1677	I1678	M1679	K1680	L1681	L1682	M1683	I1684	M1685	M1686	V1687	T1688	T1689	L1690	P1691	L1692	LEU	ASP	LYS	VAL	GLU	ASP	HIS	ARG	
GLY	E1702	D1703	S1704	Y1705	T1706	F1707	G1708	I1709	D1710	F1711	G1712	P1713	Y1714	W1715	L1716	K1717	P1718	L1719	G1720	R1721	C1722	F1723	G1724	V1725	S1726	Q1727	K1728	Q1729	L1730	E1731	P1732	E1733	M1734	L1735	R1736	I1737	R1738	R1739	D1740	V1741	L1742	G1743	F1744	K1745	G1746	S1747	R1748	M1749	W1750	D1751	E1752	D1753	E1754	R1755	M1756	K1757	R1758	R1759	Y1760	
Y1761	Q1762	D1763	R1764	D1765	H1766	H1767	H1768	S1769	H1770	G1771	S1772	Y1773	P1774	R1775	V1776	D1777	D1778	H1779	H1780	F1781	Y1782	L1783	S1784	L1785	Y1786	A1787	M1788	F1789	D1790	M1791	L1792	G1793	Q1794	L1795	L1796	A1797	L1798	K1799	P1800	L1801	V1802	G1803	SER	ASP	TYR	ASP	ASP	VAL	E1810	D1811	V1812	F1813	Q1814	D1815	W1816	L1817	R1818	R1819	H1820	
D1821	I1822	S1823	R1824	M1825	H1827	R1828	L1830	A1831	D1832	R1833	R1834	D1835	I1836	P1837	P1838	K1839	E1840	R1841	S1842	S1843	W1844	L1845	M1846	S1847	S1848	S1849	D1850	M1851	R1852	D1853	E1854	W1855	L1856	A1857	S1858	I1859	S1860	E1861	M1862	V1863	F1864	M1865	E1866	T1867	L1868	C1869	P1870	S1871	P1872	G1873	L1874	L1875	T1876	L1877	W1878	G1879	R1880			
W1881	S1882	D1883	Y1884	C1885	S1886	D1887	R1888	K1889	E1890	S1891	I1892	I1893	V1894	H1895	S1896	A1897	L1898	V1899	S1900	E1902	R1903	S1904	L1905	P1906	L1907	L1908	R1909	A1910	L1911	Q1912	T1913	L1914	K1915	M1916	V1917	Y1918	D1919	Y1920	K1921	I1922	P1923	D1924	A1925	GLY	ASP	ASN	LEU	GLU	ILE	ASP	HIS	ALA	HIS	TYR	Q1937	L1938	K1939	G1940		
Y1941	I1942	K1943	D1944	I1945	A1946	E1947	Y1948	C1949	G1950	I1951	D1952	E1953	F1954	D1955	P1956	W1957	A1958	G1959	M1960	V1961	R1962	F1963	P1964	I1965	P1966	E1967	P1968	A1969	S1970	F1971	I1972	I1973	D1974	A1975	M1976	K1977	L1978	T1979	T1980	D1981	K1982	D1983	H1984	R1985	V1986	W1987	Y1988	S1989	P1990	S1991	D1992	V1993	E1994	P1995	A1996	M1997	I1998	S1999	S2000	
I2001	W2002	G2003	H2004	L2005	S2006	G2007	K2008	M2009	D2010	E2011	E2012	K2013	S2014	H2015	G2016	Y2017	R2018	L2019	C2020	A2021	S2022	I2023	H2024	F2025	I2026	K2027	S2028	A2029	L2030	E2031	T2032	F2033	M2034	M2035	D2036	L2037	I2038	L2039	E2040	V2041	D2042	V2043	D2044	R2045	T2046	S2047	R2048	M2049	SER	ARG	TYR	GLU	ARG	GLU	ASN	GLU	ASN	GLU	GLU	LEU
ASP	ASN	ILE	PRO	S2065	S2066	T2067	R2068	L2069	F2070	L2071	F2072	R2073	H2074	D2075	G2076	T2077	H2078	I2079	T2080	L2081	Y2082	G2083	M2084	Y2085	R2086	M2087	GLY	GLU	LYS	THR	SER																													

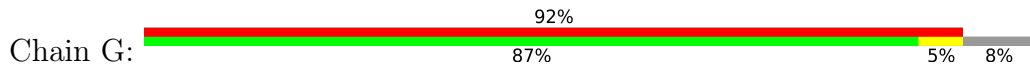
• Molecule 2: Terminase, large subunit



MET	S2	Q3	S4	Q5	E6	A7	R8	N9	A10	L11	I12	I13	A14	Q15	L16	K17	G18	D19	F20	V21	A22	F23	L24	F25	V26	L27	W28	K29	A30	L31	R32	L33	F34	K35	F36	T37	K38	C39	Q40	I41	D42	M43	A44	R45	T46	L47	A48	N49	G50	D51	H52	K53	K54	F55	I56	L57	Q58	A59	F60
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R241	L242	A243	P244	M245	L246	K247	A248	E249	Y250	D251	E252	G253	F254	E255	L256	L257	R258	G259	Q260	P261	T262	D263	P264	V265	R266	F267	D268	M269	D270	D271	L272	R273	E274	R275	E276	L277	E278	Y279	G280	K281	A282	G283	Y284	T285	L286	Q287	F288	M289	L290	N291	P292	N293	L294	S295	D296	A297	E298	K299	Y300
P301	L302	R303	L304	R305	D306	A307	I308	V309	C310	A311	V312	D313	P314	E315	R316	A317	P318	L319	S320	Y321	Q322	W323	L324	P325	N326	R327	Q328	N329	R330	N331	E332	E333	L334	P335	N336	V337	G338	L339	K340	G341	D342	D343	I344	H345	T346	A347	K348	T349	C350	S351	S352	R353	T354	A355	E356	Y357	Q358	S359	K360
I361	L362	V363	I364	D365	P366	S367	G368	R369	G370	K371	D372	E373	F374	G375	Y376	A377	V378	L379	Y380	S381	Q382	W383	G384	P385	N386	R387	L388	N389	E390	V391	G392	G393	F394	R395	G396	G397	E398	D399	D400	A401	T402	L403	E404	K405	L406	A407	K408	K409	A410	K411	Q412	W413	K414	V415	Q416	T417	V418	V419	H420
E421	S422	M423	F424	G425	D426	G427	M428	F429	G430	K431	I432	F433	S434	P435	I436	A437	L438	K439	H440	H441	K442	C443	A444	L445	I446	E447	I448	R449	A450	K451	G452	M453	E454	E455	M456	R457	I458	C459	D460	T461	I462	E463	P464	L465	M466	G467	A468	H469	K470	L471	V472	I473	R474	D475	E476	V477	I478	R479	E480
D481	Y482	Q483	T484	A485	R486	D487	L488	D489	G490	K491	H492	D493	V494	R495	Y496	S497	A498	F499	Y500	Q501	M502	T503	R504	M505	T506	R507	E508	R509	G510	A511	V512	S513	H514	D515	D516	R517	I518	D519	A520	I521	A522	L523	G524	E525	I526	Y527	L528	R529	A530	G531	M532	L533	V534	D535	S536	R537	V538	G539	GLU
GLU	GLU	MET	THR	LEU	GLU	PHE	LEU	HIS	HIS	MET	GLU	LYS	GLN	THR	THR	ILE	GLY	GLY	ASP	GLN	ILE	HIS	HIS	SER	PHE	ASP	VAL	GLY	GLY	VAL	ASP	ILE	TYR	TYR	GLU	GLU	ASP	ASP	GLY	GLY	SER	SER	PHE	ILE	LEU	GLU	TRP												

• Molecule 2: Terminase, large subunit



MET	S2	Q3	S4	Q5	E6	A7	K8	N9	A10	L11	I12	I13	A14	Q15	L16	K17	G18	D19	F20	V21	A22	F23	L24	R25	V26	L27	W28	K29	A30	L31	N32	L33	P34	K35	P36	T37	K38	C39	Q40	I41	D42	M43	A44	R45	T46	L47	A48	N49	G50	D51	K52	K53	K54	F55	I56	L57	Q58	A59	F60	
R61	G62	I63	G64	K65	S66	F67	I68	T69	C70	A71	F72	V73	V74	W75	V76	L77	G78	R79	D80	P81	T82	L83	K84	R85	L86	I87	V88	S89	A90	S91	K92	E93	R94	A95	D96	A97	N98	S99	I100	F101	I102	K103	N104	I105	I106	D107	L108	L109	P110	F111	L112	S113	E114	L115	K116	P117	R118	P119	G120	
Q121	R122	D123	S124	I125	V126	I127	F128	L129	V130	G131	L132	A133	K134	P135	D136	H137	S138	P139	S140	G201	V141	K142	S143	L144	G145	H146	T147	G148	Q149	L150	T151	G152	S153	R154	A155	D156	I157	I158	L159	A160	D161	D162	V163	E164	V165	P166	G167	N168	S169	R170	T171	S172	A173	A174	R175	E176	K177	L178	W179	T180
L181	V182	T183	E184	F185	A186	A187	L188	L189	K190	P191	L192	P193	T194	S195	R196	I197	I198	Y199	L200	G201	T202	P203	Q204	T205	M206	M207	T208	L209	Y210	K211	E212	L213	E214	D215	N216	K217	G218	Y219	S220	T221	V222	I223	W224	P225	A226	Q227	Y228	P229	R230	N231	D232	A233	E234	A235	L236	Y237	Y238	G239	D240	
R241	L242	A243	P244	M245	L246	K247	A248	E249	Y250	D251	E252	G253	F254	E255	L256	L257	R258	G259	Q260	P261	T262	D263	P264	V265	R266	F267	D268	M269	D270	D271	L272	R273	E274	R275	E276	L277	E278	Y279	G280	K281	A282	G283	Y284	T285	L286	Q287	F288	M289	L290	N291	P292	N293	L294	S295	D296	A297	E298	K299	Y300	
P301	L302	R303	L304	R305	D306	A307	I308	V309	C310	A311	V312	D313	P314	E315	R316	A317	P318	L319	S320	Y321	Q322	W323	L324	P325	N326	R327	Q328	N329	R330	N331	E332	E333	L334	P335	N336	V337	G338	L339	K340	G341	D342	D343	I344	H345	T346	A347	K348	T349	C350	S351	S352	R353	T354	A355	E356	Y357	Q358	S359	K360	
I361	L362	V363	I364	D365	P366	S367	G368	R369	G370	K371	D372	E373	F374	G375	Y376	A377	V378	L379	Y380	S381	Q382	W383	G384	P385	N386	R387	L388	M389	E390	V391	G392	G393	F394	R395	G396	G397	E398	D399	D400	A401	T402	L403	E404	K405	L406	A407	K408	K409	A410	K411	Q412	W413	K414	V415	Q416	T417	V418	V419	H420	

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 i

5.1 Standard geometry i

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.

All (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
2	H	191	PRO	CA-N-CD	-8.27	99.93	111.50
2	G	191	PRO	CA-N-CD	-8.26	99.94	111.50
2	E	191	PRO	CA-N-CD	-8.23	99.98	111.50
2	F	123	ASP	CB-CG-OD2	8.07	125.56	118.30
2	H	123	ASP	CB-CG-OD2	8.04	125.54	118.30
1	A	96	PRO	N-CD-CG	-7.22	92.38	103.20
1	C	96	PRO	N-CD-CG	-7.20	92.41	103.20
2	E	123	ASP	CB-CG-OD2	6.98	124.58	118.30
2	E	162	ASP	CB-CG-OD1	6.94	124.55	118.30
2	G	389	MET	CG-SD-CE	-6.91	89.15	100.20
2	G	162	ASP	CB-CG-OD1	6.89	124.50	118.30
2	E	389	MET	CG-SD-CE	-6.87	89.20	100.20
2	F	389	MET	CG-SD-CE	-6.87	89.21	100.20
1	D	1845	LEU	CA-CB-CG	6.62	130.53	115.30
1	B	1845	LEU	CA-CB-CG	6.61	130.49	115.30
1	D	245	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	245	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	1845	LEU	CA-CB-CG	5.37	127.64	115.30
1	D	1923	PRO	N-CD-CG	-5.35	95.17	103.20
1	B	1923	PRO	N-CD-CG	-5.34	95.19	103.20
1	C	35	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	35	LEU	CA-CB-CG	5.34	127.57	115.30
1	C	1730	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	1845	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	1730	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	791	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	791	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	1976	MET	CB-CG-SD	5.09	127.67	112.40
1	C	1976	MET	CB-CG-SD	5.08	127.64	112.40
2	E	319	LEU	CA-CB-CG	5.05	126.92	115.30
2	E	191	PRO	N-CD-CG	-5.05	95.63	103.20
2	G	319	LEU	CA-CB-CG	5.04	126.89	115.30
2	G	191	PRO	N-CD-CG	-5.02	95.67	103.20

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

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Mol	Chain	Res	Type	Group
1	D	548	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
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.

All (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
1:D:1944:ASP:OD2	1:D:1945:ILE:N	2.30	0.64
1:B:245:ASP:OD2	1:B:246:GLU:N	2.32	0.63
1:D:245:ASP:OD2	1:D:246:GLU:N	2.32	0.63
1:B:1898:LEU:HB3	1:B:2035:MET:HG2	1.81	0.63
1:D:1898:LEU:HB3	1:D:2035:MET:HG2	1.81	0.62
1:A:1028:LYS:HE3	1:A:1031:SER:HB2	1.81	0.62
1:C:1028:LYS:HE3	1:C:1031:SER:HB2	1.82	0.62
1:C:62:ASP:OD2	1:C:82:GLN:NE2	2.33	0.61
1:B:469:SER:OG	1:B:756:ARG:NH1	2.33	0.61
1:C:1635:ILE:HD11	1:C:1670:LEU:HD12	1.82	0.61
1:D:1635:ILE:HD11	1:D:1670:LEU:HD12	1.83	0.61
1:D:469:SER:OG	1:D:756:ARG:NH1	2.33	0.61
1:A:62:ASP:OD2	1:A:82:GLN:NE2	2.33	0.60
1:B:1635:ILE:HD11	1:B:1670:LEU:HD12	1.83	0.60
1:A:1635:ILE:HD11	1:A:1670:LEU:HD12	1.83	0.60
1:D:963:ALA:HB1	1:D:967:VAL:HG23	1.83	0.60
2:G:43:MET:HE1	2:G:63:ILE:HD13	1.83	0.59
1:C:1848:SER:O	1:C:1888:ARG:NH2	2.35	0.59
1:B:963:ALA:HB1	1:B:967:VAL:HG23	1.83	0.59
2:E:43:MET:HE1	2:E:63:ILE:HD13	1.83	0.59
1:A:1490:SER:OG	1:A:1492:GLU:OE1	2.21	0.58
1:A:1848:SER:O	1:A:1888:ARG:NH2	2.35	0.58
1:C:1490:SER:OG	1:C:1492:GLU:OE1	2.21	0.58
1:D:1490:SER:OG	1:D:1492:GLU:OE1	2.22	0.56
1:B:1490:SER:OG	1:B:1492:GLU:OE1	2.22	0.56
1:B:1388:ILE:HD12	1:B:1407:ILE:HD11	1.88	0.56
1:A:809:ARG:NH2	2:E:539:GLY:O	2.38	0.56
1:D:1388:ILE:HD12	1:D:1407:ILE:HD11	1.87	0.55
1:B:879:GLN:NE2	1:B:880:ARG:O	2.40	0.55
1:D:1388:ILE:O	1:D:1392:ILE:HG13	2.07	0.55
1:D:210:GLU:N	1:D:210:GLU:OE2	2.39	0.54
1:B:210:GLU:N	1:B:210:GLU:OE2	2.39	0.54
1:B:1227:ARG:NH1	1:B:1536:ASP:OD1	2.36	0.54
1:A:2077:THR:OG1	1:A:2079:HIS:NE2	2.41	0.54
1:C:1302:GLN:HA	1:C:1305:LYS:HE3	1.90	0.53
1:D:928:PRO:HD2	1:D:931:LEU:HD23	1.90	0.53
1:D:810:TRP:O	1:D:813:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1388:ILE:O	1:B:1392:ILE:HG13	2.09	0.53
1:A:227:SER:OG	1:A:227:SER:O	2.28	0.53
1:C:1227:ARG:NH1	1:C:1536:ASP:OD1	2.36	0.52
2:F:182:VAL:HG11	2:F:209:LEU:HD13	1.90	0.52
2:H:182:VAL:HG11	2:H:209:LEU:HD13	1.90	0.52
1:B:1028:LYS:HE3	1:B:1031:SER:HB2	1.92	0.52
1:A:1227:ARG:NH1	1:A:1536:ASP:OD1	2.35	0.52
1:A:1302:GLN:HA	1:A:1305:LYS:HE3	1.90	0.52
1:B:810:TRP:O	1:B:813:ARG:NH1	2.43	0.52
1:D:1762:GLN:N	1:D:1762:GLN:OE1	2.42	0.52
2:F:56:ILE:HB	2:F:221:THR:HG22	1.91	0.51
2:H:56:ILE:HB	2:H:221:THR:HG22	1.92	0.51
1:A:1997:MET:HG2	1:A:2021:ALA:HB2	1.93	0.51
2:E:56:ILE:HB	2:E:221:THR:HG22	1.92	0.51
1:A:1826:ASP:OD1	1:A:1826:ASP:N	2.35	0.51
1:C:711:ALA:HB2	1:C:744:ILE:HG13	1.92	0.51
1:D:1028:LYS:HE3	1:D:1031:SER:HB2	1.92	0.51
1:B:1952:ASP:OD1	1:B:1952:ASP:N	2.43	0.50
1:C:1997:MET:HG2	1:C:2021:ALA:HB2	1.93	0.50
1:B:809:ARG:NH2	2:F:539:GLY:O	2.44	0.50
1:A:711:ALA:HB2	1:A:744:ILE:HG13	1.93	0.50
2:G:121:GLN:HB3	2:G:123:ASP:HB3	1.93	0.50
1:A:2042:ASP:OD2	1:A:2065:SER:OG	2.23	0.50
1:A:1898:LEU:HD23	1:A:2037:LEU:HD13	1.94	0.50
1:C:1400:GLU:HB3	1:C:1429:TRP:CZ3	2.47	0.50
1:C:1898:LEU:HD23	1:C:2037:LEU:HD13	1.93	0.50
2:F:101:PHE:O	2:F:105:ILE:HG12	2.11	0.50
1:A:1400:GLU:HB3	1:A:1429:TRP:CZ3	2.47	0.50
2:F:296:ASP:O	2:F:303:ARG:NH2	2.41	0.50
2:H:101:PHE:O	2:H:105:ILE:HG12	2.12	0.50
1:C:1874:LEU:HB3	1:C:2020:CYS:SG	2.52	0.49
1:C:2042:ASP:OD2	1:C:2065:SER:OG	2.24	0.49
2:H:296:ASP:O	2:H:303:ARG:NH2	2.42	0.49
1:A:1874:LEU:HB3	1:A:2020:CYS:SG	2.52	0.49
1:A:1284:ILE:HD13	1:A:1314:LEU:HD23	1.94	0.49
1:A:1727:GLN:HA	1:A:1730:LEU:HG	1.94	0.49
1:D:653:THR:OG1	1:D:657:GLU:OE1	2.30	0.49
1:B:916:ILE:HD11	1:B:952:LEU:HB3	1.94	0.49
1:C:1284:ILE:HD13	1:C:1314:LEU:HD23	1.94	0.49
1:B:550:ILE:HB	1:B:584:ILE:HG22	1.94	0.49
1:B:653:THR:OG1	1:B:657:GLU:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:963:ALA:HB1	1:C:967:VAL:HG23	1.95	0.49
1:C:1727:GLN:HA	1:C:1730:LEU:HG	1.94	0.49
1:D:550:ILE:HB	1:D:584:ILE:HG22	1.94	0.49
1:C:227:SER:O	1:C:227:SER:OG	2.28	0.49
1:D:1952:ASP:OD1	1:D:1952:ASP:N	2.43	0.49
2:G:205:THR:OG1	2:G:207:MET:O	2.28	0.48
1:D:1227:ARG:NH1	1:D:1536:ASP:OD1	2.36	0.48
1:A:775:ASP:O	1:A:779:ARG:NE	2.42	0.48
1:B:721:GLU:OE2	1:B:725:ARG:NH2	2.46	0.48
1:D:386:LEU:HB3	1:D:422:VAL:HG12	1.96	0.48
1:D:1284:ILE:HD13	1:D:1314:LEU:HD23	1.95	0.48
2:G:56:ILE:HB	2:G:221:THR:HG22	1.95	0.48
1:D:721:GLU:OE2	1:D:725:ARG:NH2	2.46	0.48
2:F:481:ASP:OD1	2:F:517:ARG:NH1	2.47	0.48
2:G:11:LEU:O	2:G:15:GLN:HG3	2.14	0.48
2:H:453:MET:HG2	2:H:456:MET:H	1.79	0.48
1:A:721:GLU:OE2	1:A:725:ARG:NH2	2.46	0.47
1:D:916:ILE:HD11	1:D:952:LEU:HB3	1.97	0.47
1:A:963:ALA:HB1	1:A:967:VAL:HG23	1.95	0.47
1:B:1848:SER:O	1:B:1888:ARG:NH2	2.40	0.47
1:A:2011:GLU:OE1	1:A:2011:GLU:N	2.43	0.47
1:B:386:LEU:HB3	1:B:422:VAL:HG12	1.96	0.47
1:D:1401:CYS:HA	1:D:1404:ILE:HD12	1.97	0.47
1:A:195:ILE:O	1:A:199:GLU:HG2	2.15	0.47
1:B:1284:ILE:HD13	1:B:1314:LEU:HD23	1.95	0.47
1:B:1401:CYS:HA	1:B:1404:ILE:HD12	1.97	0.47
1:D:273:GLN:HA	1:D:276:VAL:HG12	1.98	0.46
1:C:195:ILE:O	1:C:199:GLU:HG2	2.15	0.46
1:B:938:GLU:N	1:B:938:GLU:OE2	2.49	0.46
1:C:721:GLU:OE2	1:C:725:ARG:NH2	2.47	0.46
2:H:178:LEU:O	2:H:182:VAL:HG12	2.16	0.46
1:C:810:TRP:O	1:C:813:ARG:NH1	2.49	0.46
2:E:11:LEU:O	2:E:15:GLN:HG3	2.14	0.46
2:F:453:MET:HG2	2:F:456:MET:H	1.80	0.46
1:A:810:TRP:O	1:A:813:ARG:NH1	2.49	0.45
1:B:273:GLN:HA	1:B:276:VAL:HG12	1.98	0.45
2:H:481:ASP:OD1	2:H:517:ARG:NH1	2.49	0.45
1:A:858:ARG:NH1	1:A:902:GLU:OE2	2.49	0.45
1:B:2027:LYS:O	1:B:2031:GLU:HG2	2.16	0.45
2:E:453:MET:HG2	2:E:456:MET:H	1.80	0.45
1:A:1711:PHE:O	1:A:1715:TRP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1711:PHE:O	1:C:1715:TRP:HB2	2.17	0.45
1:D:938:GLU:N	1:D:938:GLU:OE2	2.50	0.45
2:F:178:LEU:O	2:F:182:VAL:HG12	2.16	0.45
1:A:1952:ASP:OD1	1:A:1952:ASP:N	2.43	0.45
1:D:1727:GLN:HA	1:D:1730:LEU:HG	1.99	0.45
2:G:453:MET:HG2	2:G:456:MET:H	1.82	0.44
1:B:588:ASP:OD2	1:B:590:PRO:HD2	2.17	0.44
1:A:394:ASP:OD1	1:A:394:ASP:N	2.51	0.44
1:B:928:PRO:HD2	1:B:931:LEU:HD23	1.99	0.44
1:D:1848:SER:O	1:D:1888:ARG:NH2	2.40	0.44
1:B:1727:GLN:HA	1:B:1730:LEU:HG	1.98	0.44
1:D:1973:ILE:H	1:D:1973:ILE:HG13	1.58	0.44
2:H:29:LYS:HA	2:H:29:LYS:HD3	1.80	0.44
2:H:182:VAL:HA	2:H:185:PHE:CE1	2.53	0.44
1:A:114:ILE:HD12	1:A:119:VAL:HG22	1.99	0.44
1:C:858:ARG:NH1	1:C:902:GLU:OE2	2.50	0.44
1:A:441:GLU:N	1:A:441:GLU:OE2	2.51	0.44
1:A:582:GLU:N	1:A:582:GLU:OE1	2.50	0.43
1:B:1071:LYS:HE3	1:B:1071:LYS:HB3	1.86	0.43
1:D:588:ASP:OD2	1:D:590:PRO:HD2	2.17	0.43
1:B:1854:GLU:H	1:B:1854:GLU:CD	2.21	0.43
1:B:1855:TRP:HE3	1:B:1856:LEU:HD23	1.83	0.43
1:D:1854:GLU:H	1:D:1854:GLU:CD	2.21	0.43
2:F:182:VAL:HA	2:F:185:PHE:CE1	2.53	0.43
1:D:1711:PHE:O	1:D:1715:TRP:HB2	2.19	0.43
1:C:114:ILE:HD12	1:C:119:VAL:HG22	1.99	0.43
1:D:866:GLU:HA	1:D:869:ILE:HG22	2.01	0.43
1:D:2027:LYS:O	1:D:2031:GLU:HG2	2.18	0.43
1:C:441:GLU:OE2	1:C:441:GLU:N	2.52	0.43
1:B:1977:LYS:HB3	1:B:1990:PRO:HG3	2.01	0.43
1:B:1374:LYS:HD3	1:B:1374:LYS:HA	1.81	0.42
1:D:1977:LYS:HB3	1:D:1990:PRO:HG3	2.01	0.42
2:H:420:HIS:NE2	2:H:447:GLU:OE2	2.44	0.42
1:B:1973:ILE:H	1:B:1973:ILE:HG13	1.58	0.42
1:A:784:ASP:OD1	1:A:784:ASP:N	2.50	0.42
1:D:1855:TRP:HE3	1:D:1856:LEU:HD23	1.83	0.42
1:B:866:GLU:HA	1:B:869:ILE:HG22	2.01	0.42
1:B:1711:PHE:O	1:B:1715:TRP:HB2	2.19	0.42
1:D:869:ILE:HA	1:D:872:THR:HG22	2.02	0.42
1:C:2011:GLU:OE1	1:C:2011:GLU:N	2.43	0.42
2:E:271:ASP:O	2:E:275:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:LEU:HD23	1:B:1005:LEU:HD11	2.00	0.42
2:F:13:ILE:HD12	2:F:13:ILE:HA	1.97	0.42
2:G:182:VAL:HA	2:G:185:PHE:CE1	2.55	0.42
1:D:1709:ILE:HG23	1:D:1710:ASP:OD1	2.20	0.41
1:D:1756:ASN:O	1:D:1759:ARG:NH1	2.53	0.41
1:B:300:ILE:HG21	1:B:389:ILE:HD11	2.02	0.41
1:B:869:ILE:HA	1:B:872:THR:HG22	2.02	0.41
1:B:1874:LEU:HB3	1:B:2020:CYS:SG	2.60	0.41
1:B:324:ALA:HA	1:B:327:TYR:CZ	2.55	0.41
1:B:1709:ILE:HG23	1:B:1710:ASP:OD1	2.20	0.41
1:C:1895:HIS:HB2	1:C:1922:ILE:HD13	2.02	0.41
2:E:115:LEU:HD12	2:E:130:VAL:HG11	2.03	0.41
1:D:28:LEU:HD23	1:D:35:LEU:HG	2.01	0.41
1:D:300:ILE:HG21	1:D:389:ILE:HD11	2.02	0.41
1:D:324:ALA:HA	1:D:327:TYR:CZ	2.55	0.41
2:G:271:ASP:O	2:G:275:ARG:HG2	2.20	0.41
1:A:1895:HIS:HB2	1:A:1922:ILE:HD13	2.02	0.41
1:D:927:PRO:HA	1:D:928:PRO:HD3	1.96	0.41
1:C:1826:ASP:OD1	1:C:1826:ASP:N	2.35	0.41
2:E:182:VAL:HA	2:E:185:PHE:CE1	2.55	0.41
1:B:1283:LYS:H	1:B:1283:LYS:HG3	1.68	0.41
1:B:1756:ASN:O	1:B:1759:ARG:NH1	2.53	0.41
1:C:2077:THR:HG1	1:C:2079:HIS:CE1	2.38	0.41
2:E:214:GLU:CD	2:E:241:ARG:HH12	2.24	0.41
2:H:101:PHE:CZ	2:H:105:ILE:HD11	2.56	0.41
2:G:296:ASP:O	2:G:303:ARG:NH2	2.51	0.41
2:H:214:GLU:CD	2:H:241:ARG:HH12	2.24	0.41
1:C:552:LEU:HD21	1:C:584:ILE:HD11	2.02	0.41
1:D:84:LYS:HE2	1:D:84:LYS:HB3	1.94	0.41
1:D:1353:TRP:CD2	1:D:1390:LYS:HE2	2.56	0.41
2:G:451:LYS:O	2:G:457:ARG:NH1	2.54	0.41
2:H:177:LYS:O	2:H:181:LEU:HG	2.21	0.41
2:H:313:ASP:HA	2:H:314:PRO:HD3	1.95	0.41
1:C:1952:ASP:OD1	1:C:1952:ASP:N	2.43	0.41
2:F:29:LYS:HD3	2:F:29:LYS:HA	1.79	0.41
2:F:101:PHE:CZ	2:F:105:ILE:HD11	2.56	0.41
2:G:310:CYS:SG	2:G:311:ALA:N	2.94	0.41
1:C:530:ILE:H	1:C:530:ILE:HG12	1.74	0.40
1:C:2026:ILE:HD11	1:C:2037:LEU:HD23	2.03	0.40
1:D:374:ILE:HD12	1:D:374:ILE:HA	1.95	0.40
1:C:2075:ASP:OD1	1:C:2075:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1176:PRO:HA	1:D:1177:PRO:HD3	1.96	0.40
1:D:2020:CYS:SG	1:D:2021:ALA:N	2.94	0.40
1:C:394:ASP:OD1	1:C:394:ASP:N	2.51	0.40
1:C:1973:ILE:H	1:C:1973:ILE:HG13	1.61	0.40
2:E:310:CYS:SG	2:E:311:ALA:N	2.95	0.40
2:G:313:ASP:HA	2:G:314:PRO:HD3	1.90	0.40
1:B:28:LEU:HD23	1:B:35:LEU:HG	2.01	0.40
1:D:1388:ILE:HG22	1:D:1392:ILE:HD11	2.03	0.40
2:H:421:GLU:OE1	2:H:449:ARG:HA	2.22	0.40
1:B:1997:MET:HG2	1:B:2021:ALA:HB2	2.04	0.40
1:B:2020:CYS:SG	1:B:2021:ALA:N	2.94	0.40
1:C:1176:PRO:HA	1:C:1177:PRO:HD3	1.96	0.40
1:C:1318:HIS:O	1:C:1322:LYS:HG2	2.22	0.40
1:D:1997:MET:HG2	1:D:2021:ALA:HB2	2.04	0.40
2:F:214:GLU:CD	2:F:241:ARG:HH12	2.24	0.40

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 [i](#)

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

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	227	SER
1	A	279	PHE
1	A	779	ARG
1	A	900	MET
1	A	1195	ASP
1	A	1568	MET
1	A	1614	HIS
1	A	1759	ARG
1	A	1885	CYS
1	A	1948	TYR
1	A	1976	MET

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Mol	Chain	Res	Type
1	A	2035	MET
1	A	2039	LEU
1	A	2066	SER
1	B	140	PHE
1	B	301	GLU
1	B	507	LYS
1	B	779	ARG
1	B	786	ASP
1	B	858	ARG
1	B	879	GLN
1	B	1568	MET
1	B	1629	ASP
1	B	1885	CYS
1	B	1962	ARG
1	B	2020	CYS
1	B	2039	LEU
1	C	11	ARG
1	C	82	GLN
1	C	227	SER
1	C	279	PHE
1	C	900	MET
1	C	1195	ASP
1	C	1568	MET
1	C	1614	HIS
1	C	1759	ARG
1	C	1885	CYS
1	C	1948	TYR
1	C	1976	MET
1	C	2035	MET
1	C	2039	LEU
1	C	2066	SER
1	D	140	PHE
1	D	301	GLU
1	D	779	ARG
1	D	786	ASP
1	D	1568	MET
1	D	1629	ASP
1	D	1885	CYS
1	D	1962	ARG
1	D	2020	CYS
1	D	2039	LEU
2	F	177	LYS

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Mol	Chain	Res	Type
2	F	327	ARG
2	F	356	GLU
2	F	372	ASP
2	F	390	GLU
2	G	123	ASP
2	H	177	LYS
2	H	327	ARG
2	H	356	GLU
2	H	390	GLU

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	C	2101	4	26,33,33	0.66	0	31,52,52	0.73	1 (3%)

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	A	2101	4	26,33,33	0.66	0	31,52,52	0.73	1 (3%)
3	ATP	H	601	4	26,33,33	0.67	0	31,52,52	0.75	2 (6%)
3	ATP	D	2101	4	26,33,33	0.67	0	31,52,52	0.82	1 (3%)
3	ATP	E	601	4	26,33,33	0.68	0	31,52,52	0.74	2 (6%)
3	ATP	B	2101	4	26,33,33	0.66	0	31,52,52	0.81	1 (3%)
3	ATP	F	601	4	26,33,33	0.67	0	31,52,52	0.75	2 (6%)

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

There are no bond length outliers.

All (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
3	H	601	ATP	C5-C6-N6	2.11	123.56	120.35
3	E	601	ATP	C5-C6-N6	2.11	123.55	120.35
3	G	601	ATP	C5-C6-N6	2.07	123.49	120.35
3	H	601	ATP	PB-O3B-PG	2.05	139.87	132.83
3	E	601	ATP	PB-O3B-PG	2.04	139.84	132.83
3	F	601	ATP	PB-O3B-PG	2.02	139.76	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	601	ATP	PB-O3B-PG	2.01	139.73	132.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

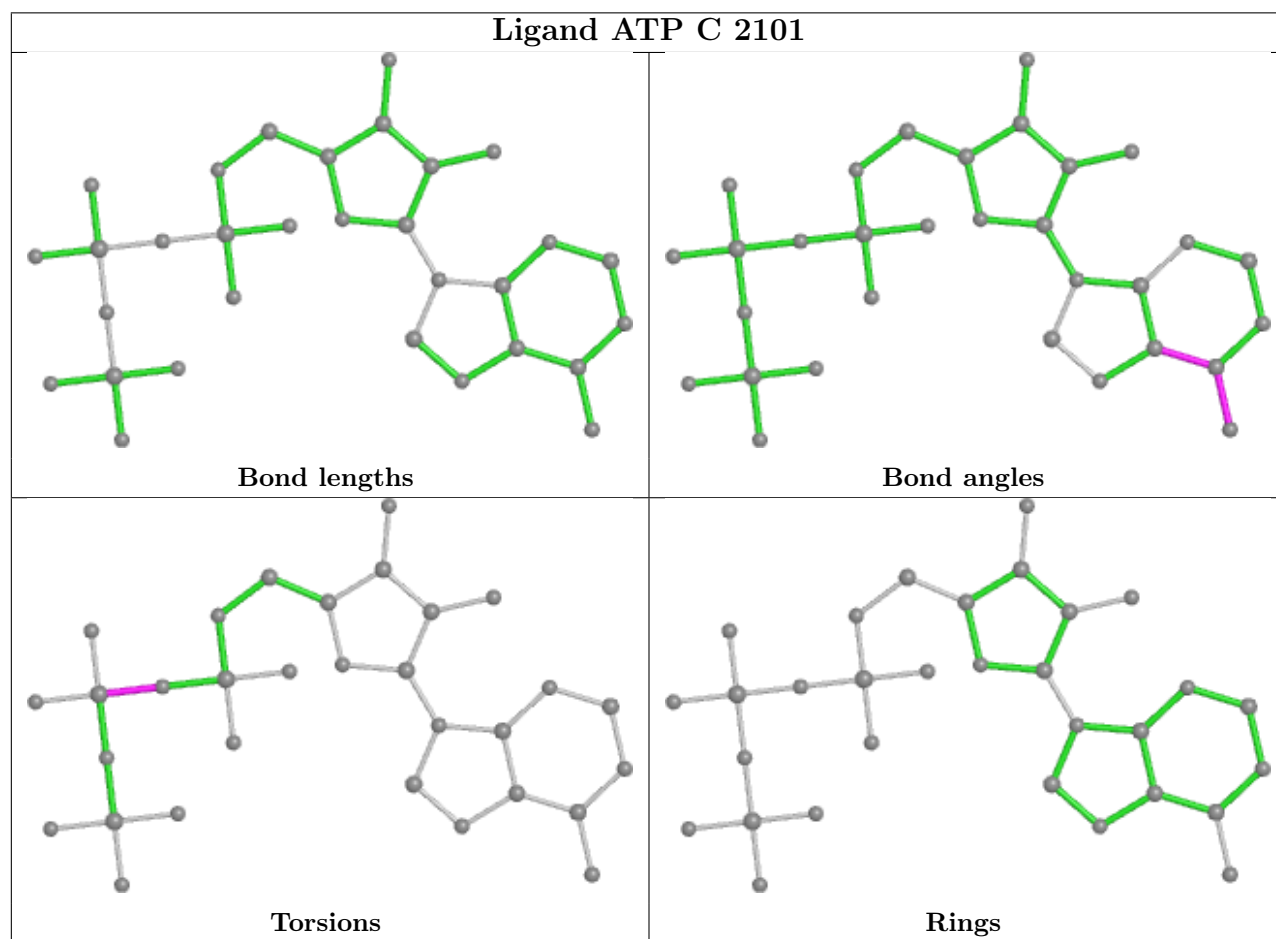
Mol	Chain	Res	Type	Atoms
3	E	601	ATP	O4'-C4'-C5'-O5'
3	H	601	ATP	O4'-C4'-C5'-O5'
3	B	2101	ATP	O4'-C4'-C5'-O5'
3	B	2101	ATP	C3'-C4'-C5'-O5'
3	D	2101	ATP	O4'-C4'-C5'-O5'
3	D	2101	ATP	C3'-C4'-C5'-O5'
3	F	601	ATP	O4'-C4'-C5'-O5'
3	G	601	ATP	O4'-C4'-C5'-O5'
3	A	2101	ATP	PA-O3A-PB-O1B
3	C	2101	ATP	PA-O3A-PB-O1B
3	F	601	ATP	C3'-C4'-C5'-O5'
3	G	601	ATP	C3'-C4'-C5'-O5'
3	F	601	ATP	C4'-C5'-O5'-PA
3	H	601	ATP	C4'-C5'-O5'-PA
3	B	2101	ATP	C5'-O5'-PA-O3A
3	D	2101	ATP	C5'-O5'-PA-O3A
3	B	2101	ATP	PA-O3A-PB-O2B
3	D	2101	ATP	PA-O3A-PB-O2B
3	E	601	ATP	C4'-C5'-O5'-PA
3	G	601	ATP	C4'-C5'-O5'-PA
3	A	2101	ATP	PA-O3A-PB-O2B
3	C	2101	ATP	PA-O3A-PB-O2B

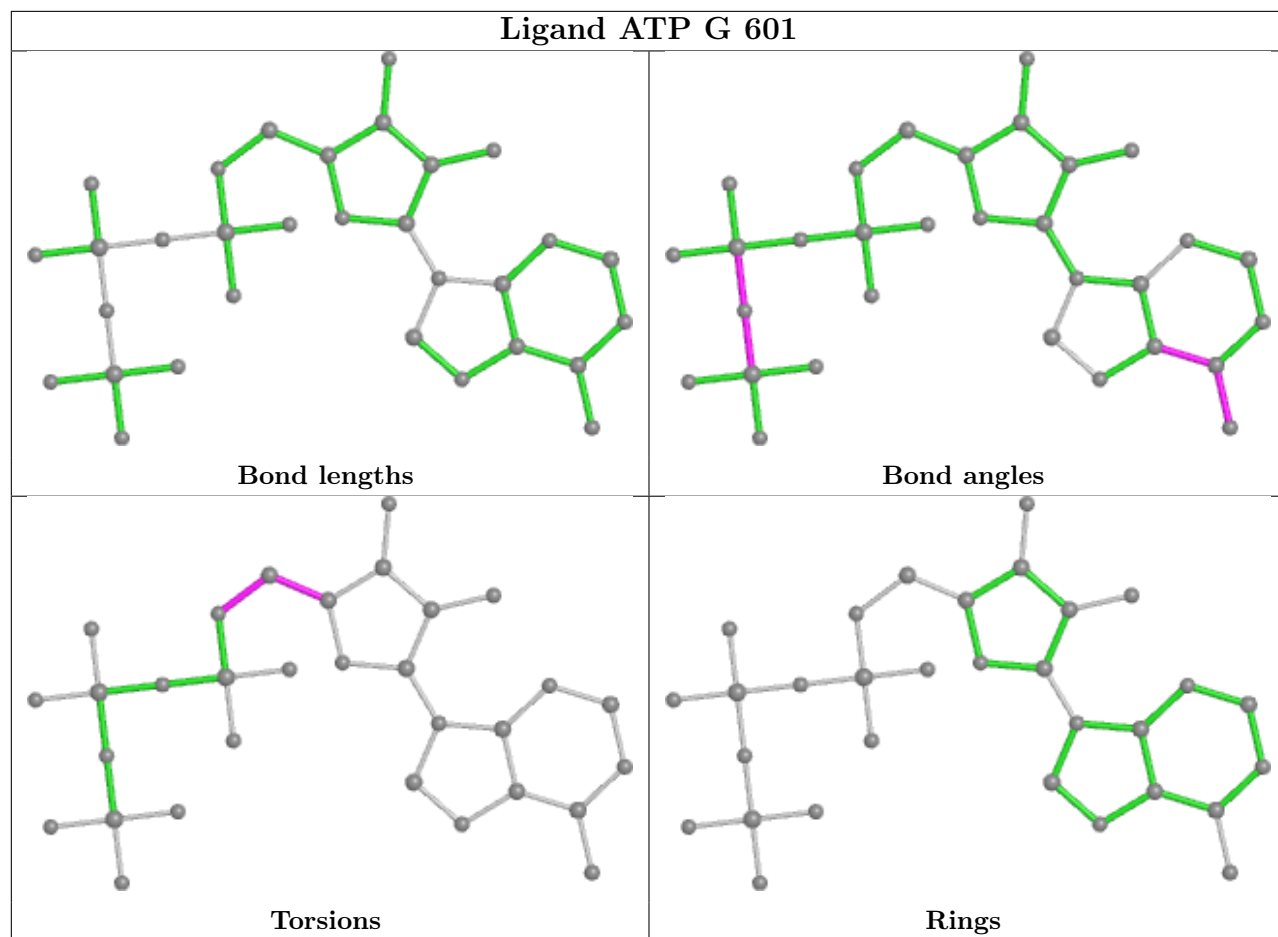
There are no ring outliers.

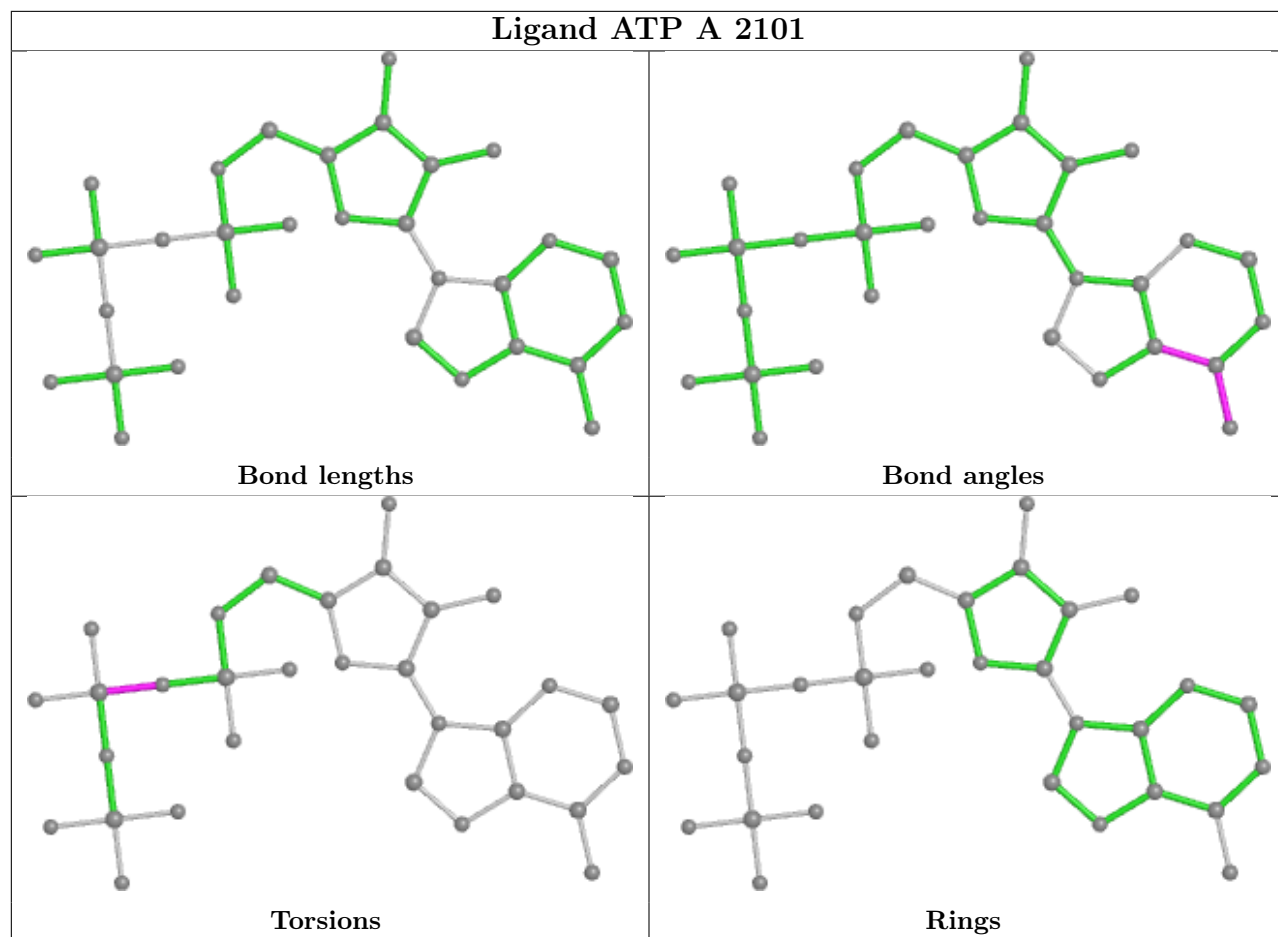
No monomer is involved in short contacts.

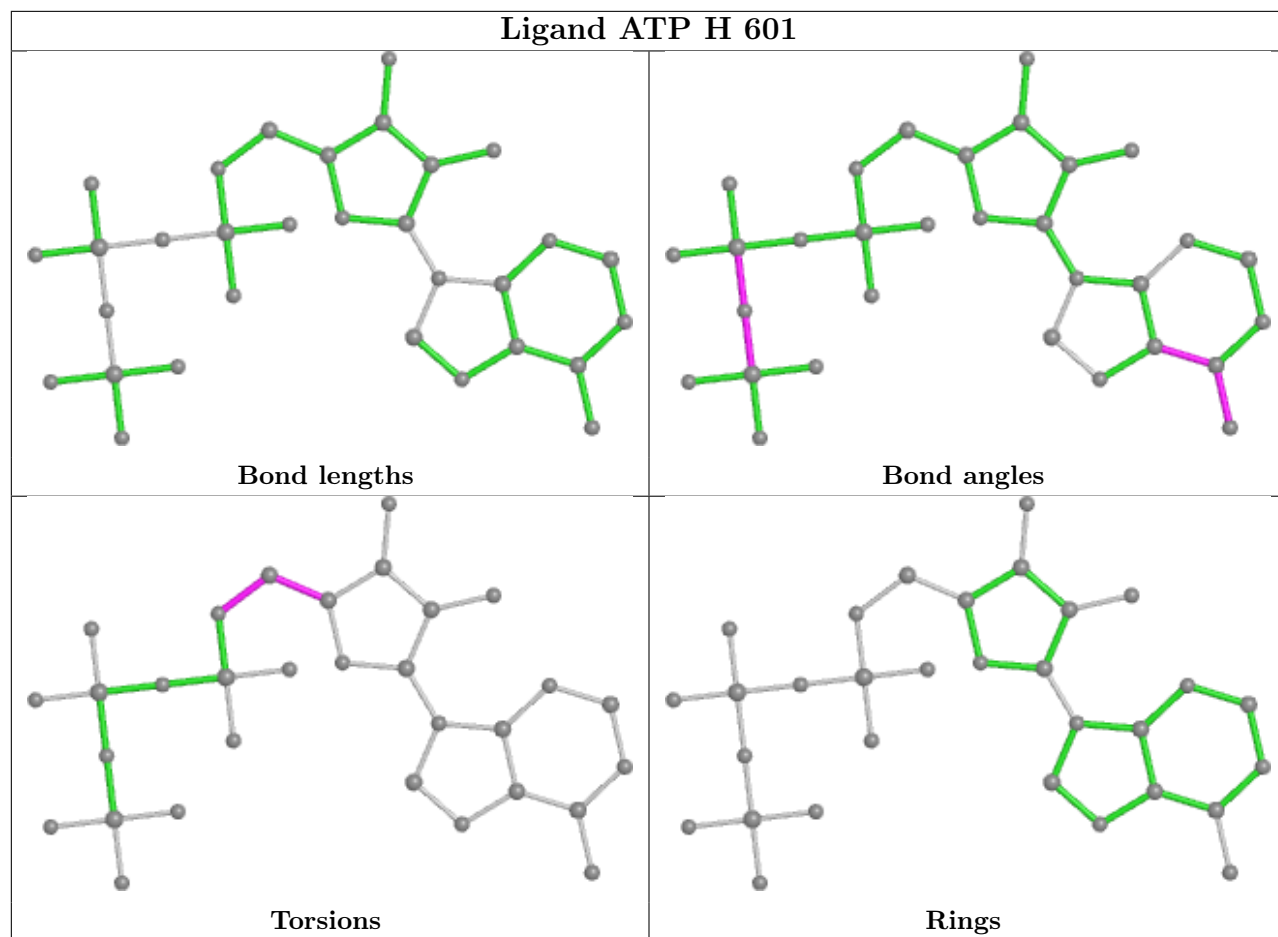
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

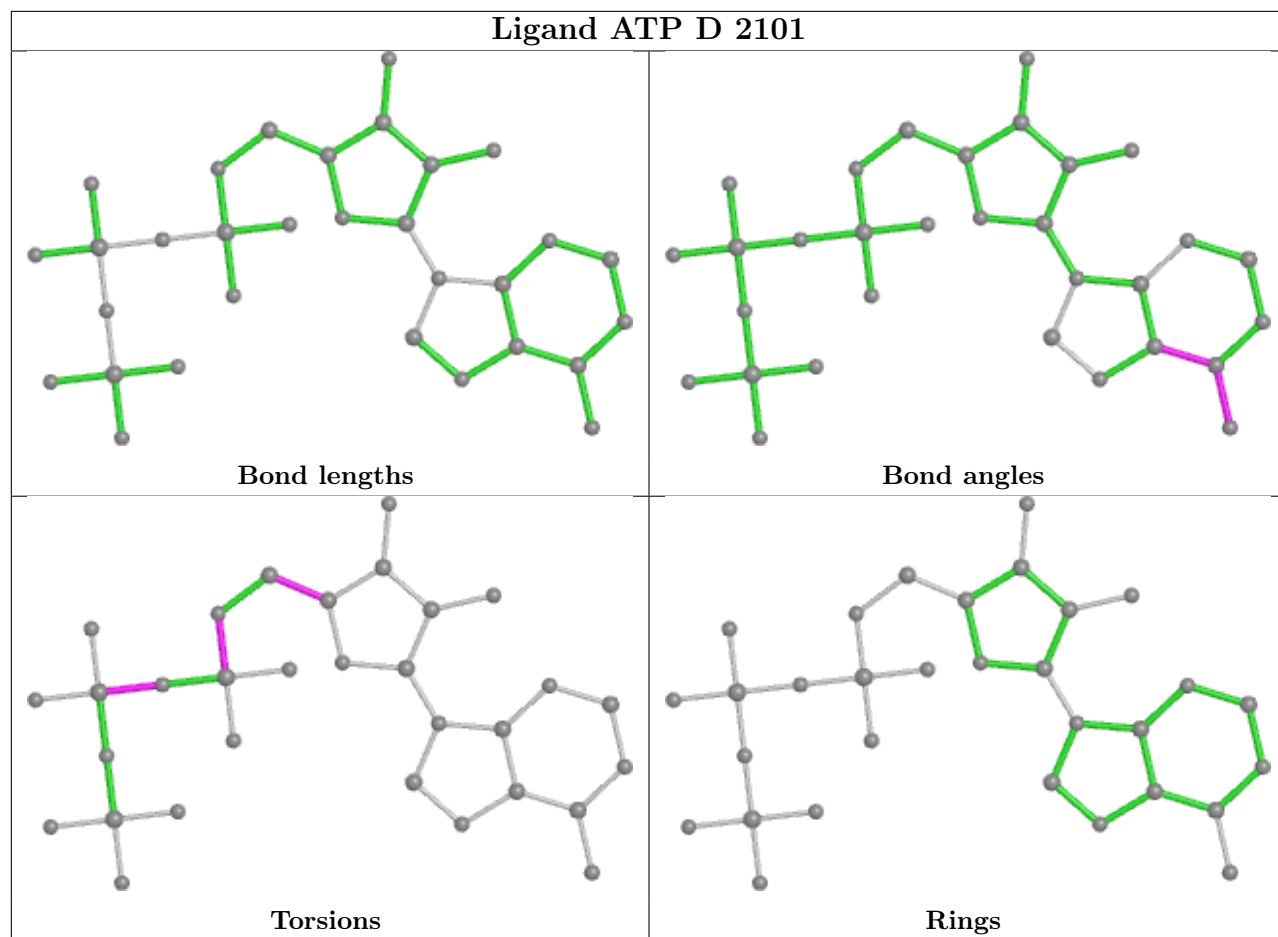
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

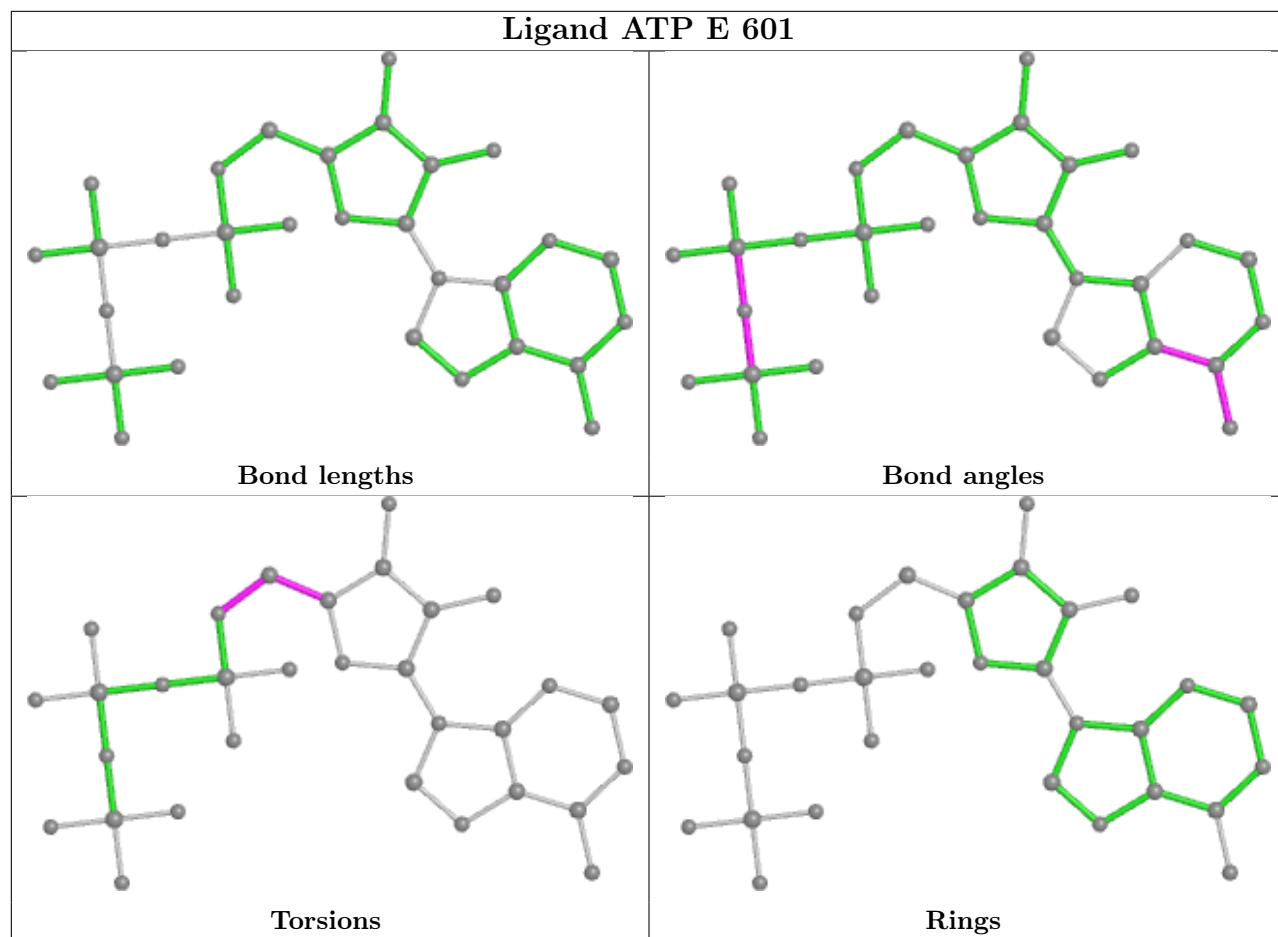


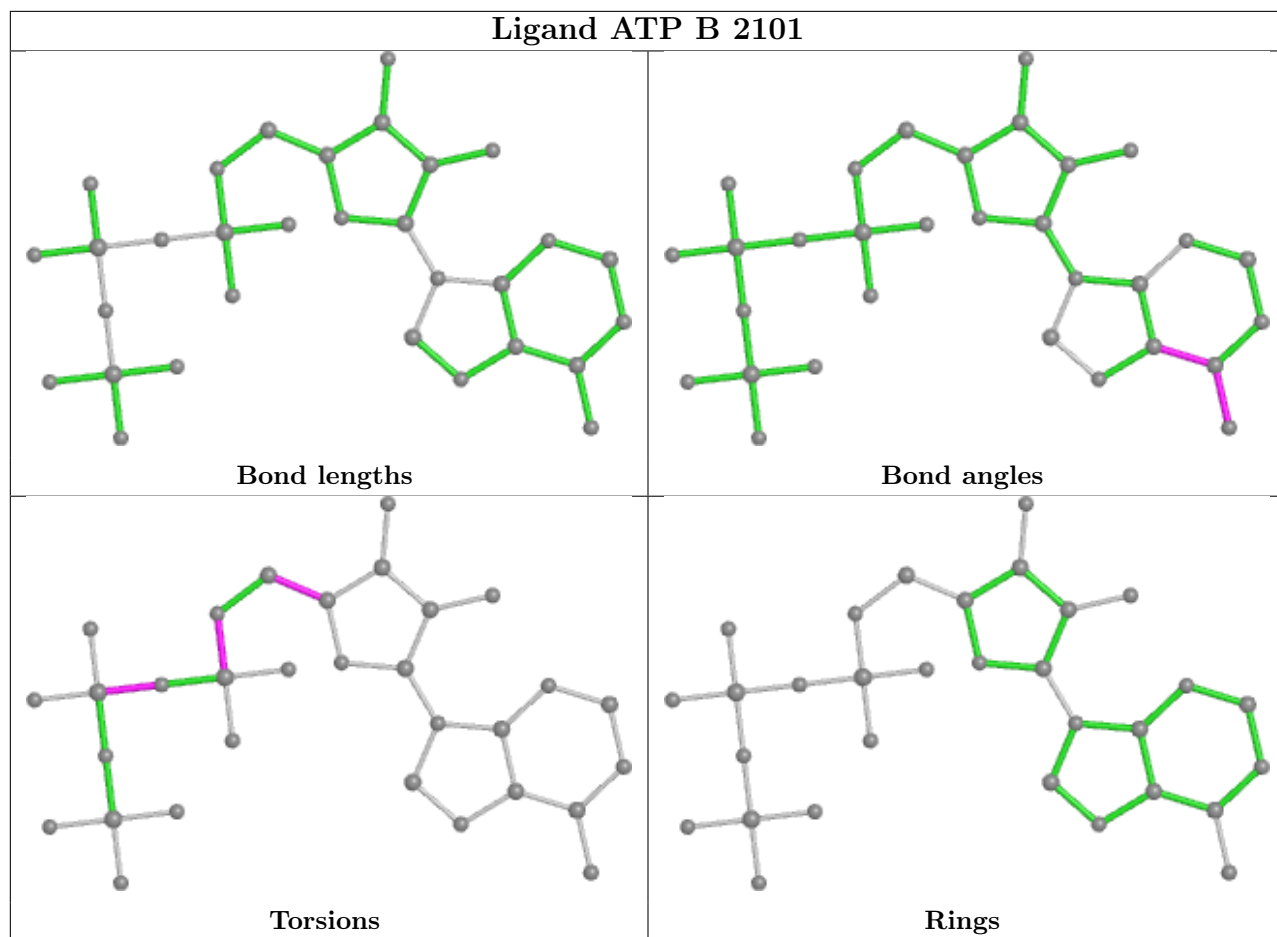


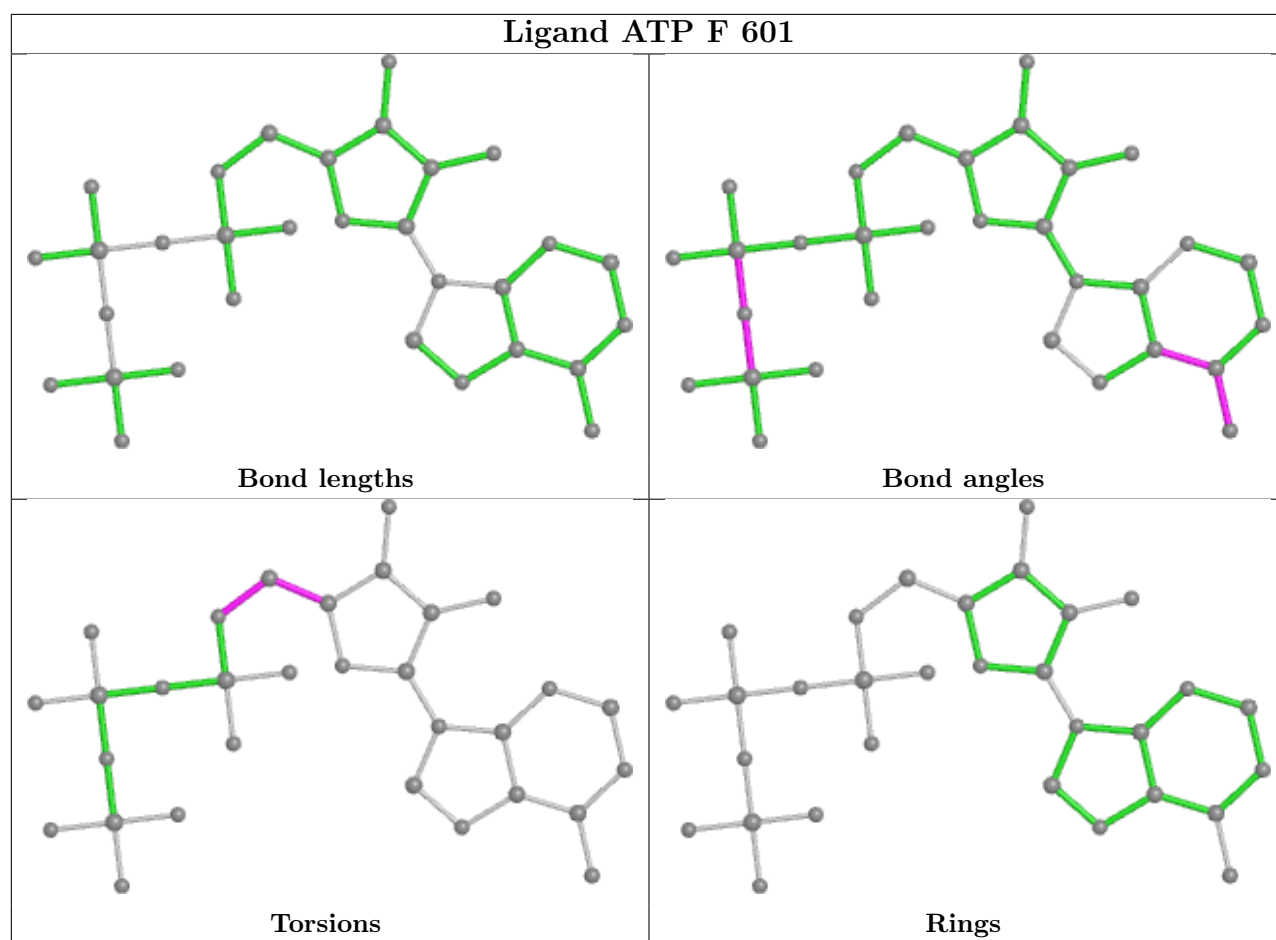












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

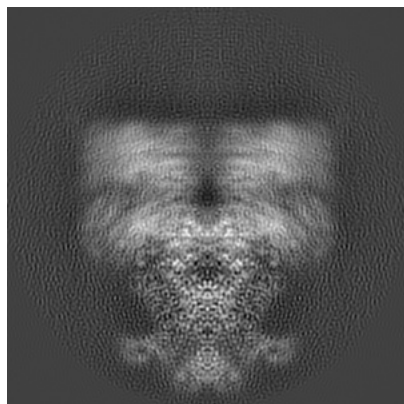
6 Map visualisation [i](#)

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.

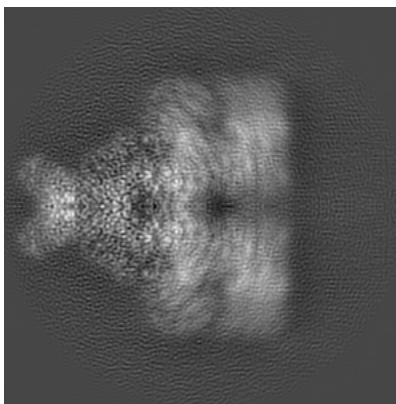
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

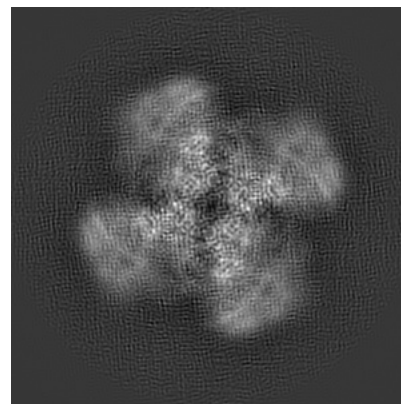
6.1.1 Primary map



X

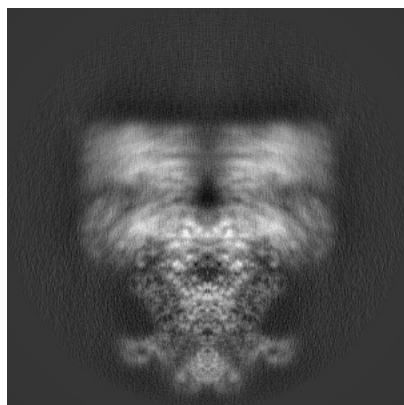


Y

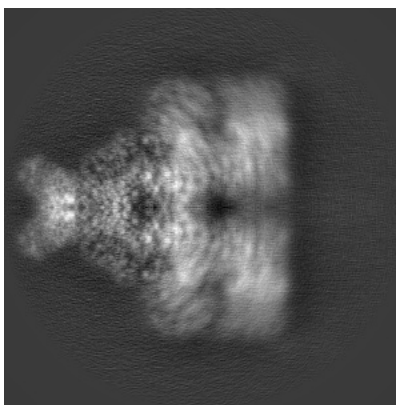


Z

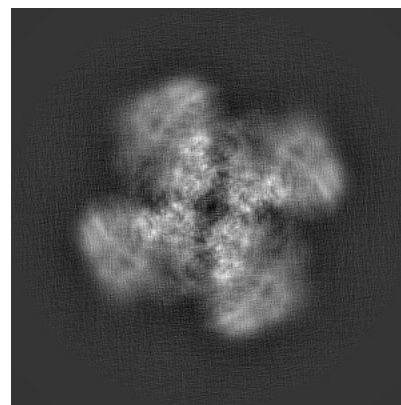
6.1.2 Raw map



X



Y

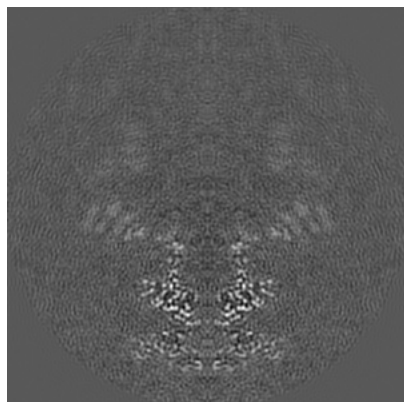


Z

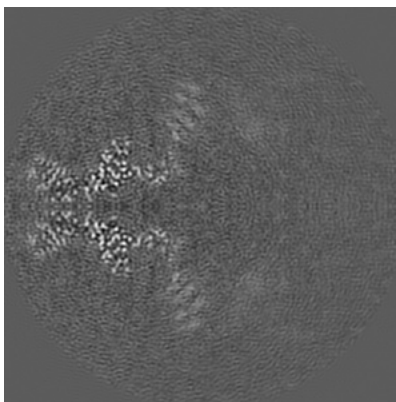
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

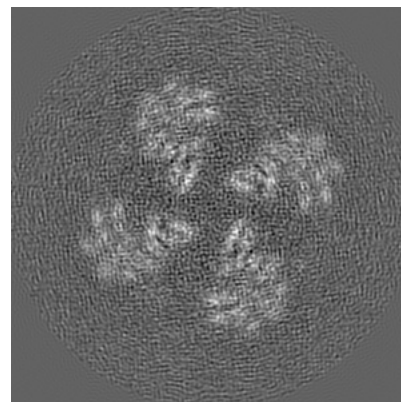
6.2.1 Primary map



X Index: 180

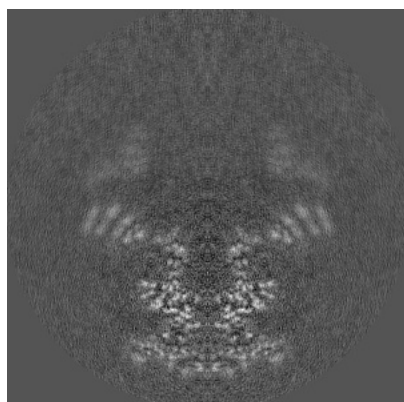


Y Index: 180

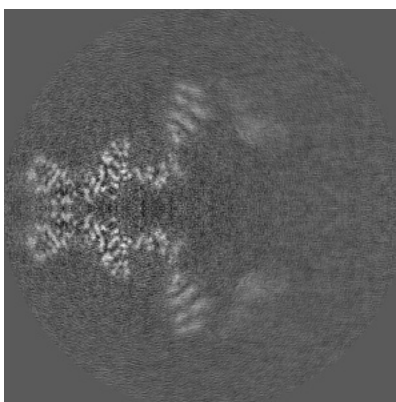


Z Index: 180

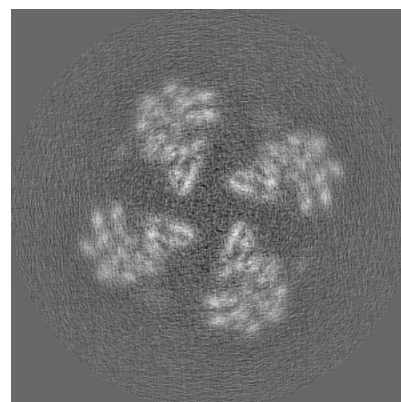
6.2.2 Raw map



X Index: 180



Y Index: 180

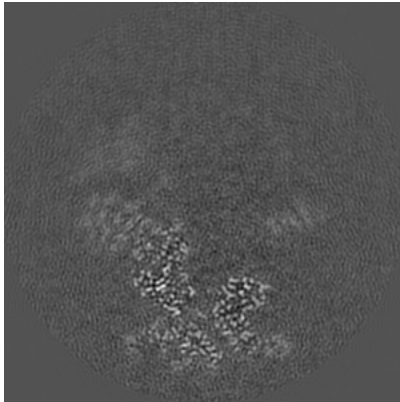


Z Index: 180

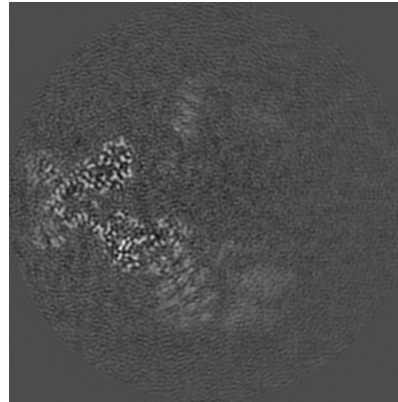
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

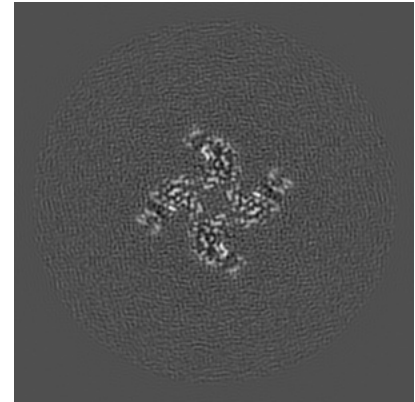
6.3.1 Primary map



X Index: 187

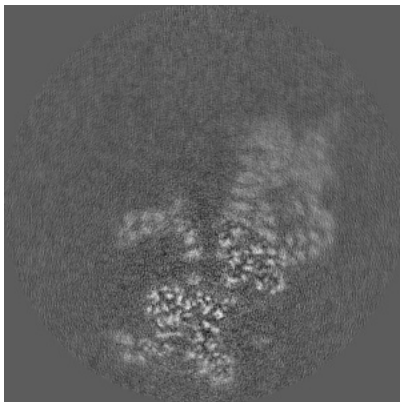


Y Index: 173

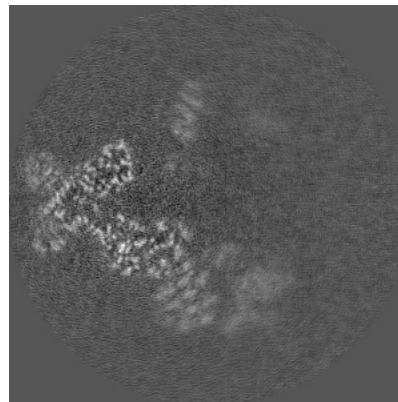


Z Index: 102

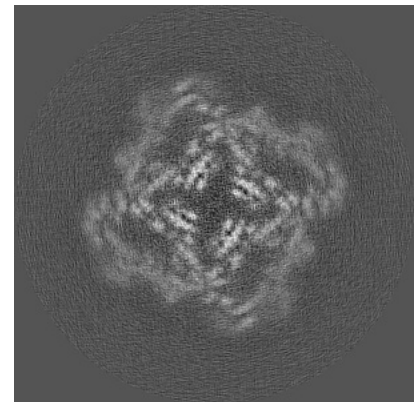
6.3.2 Raw map



X Index: 163



Y Index: 173

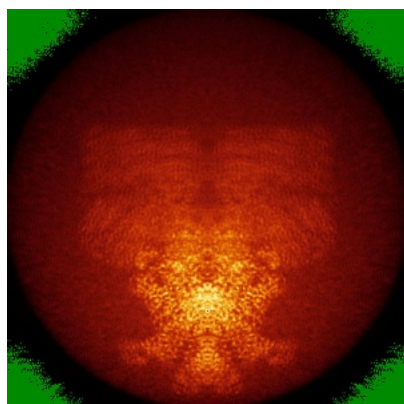


Z Index: 155

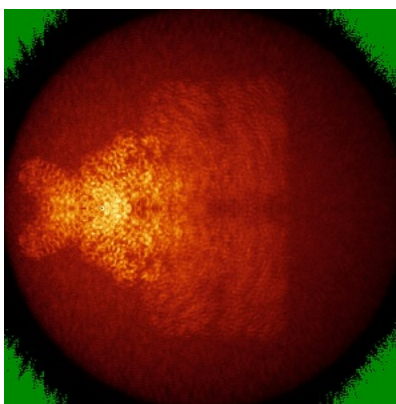
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

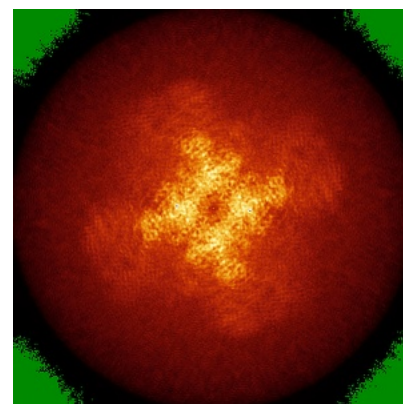
6.4.1 Primary map



X

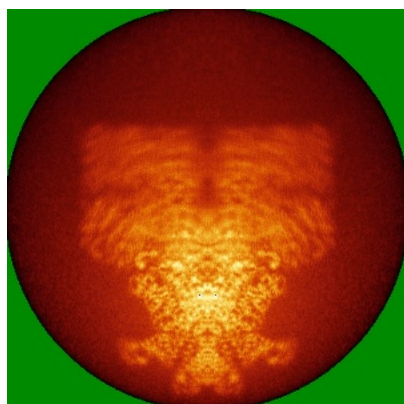


Y

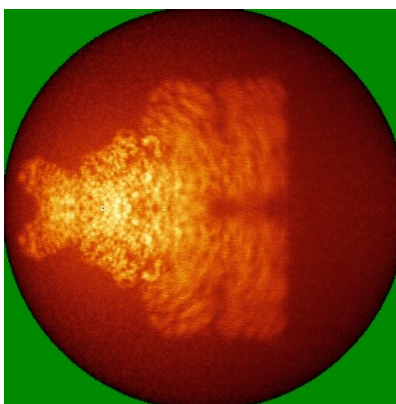


Z

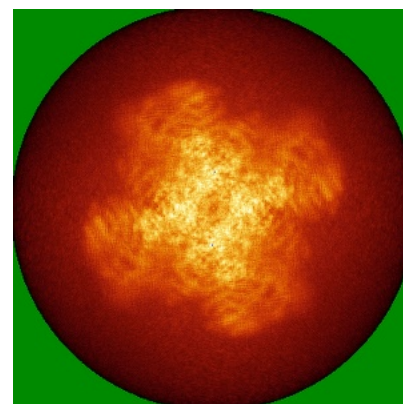
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 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.

6.5.2 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.

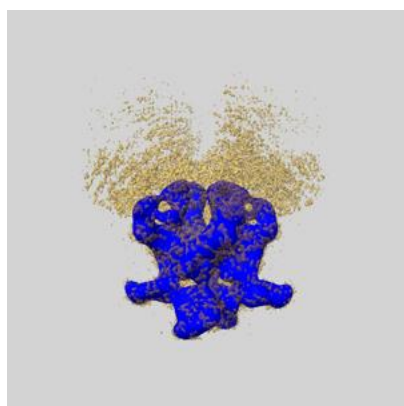
6.6 Mask visualisation [i](#)

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

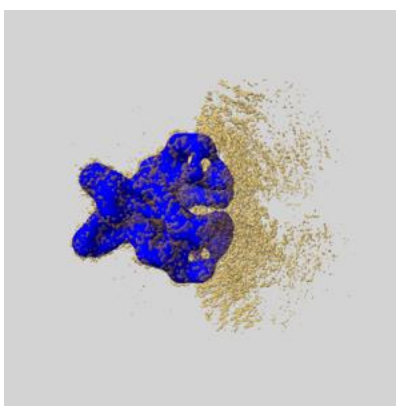
A mask typically either:

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

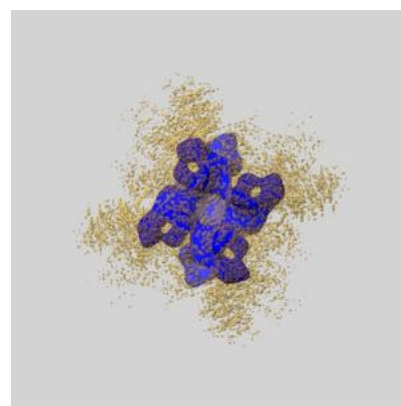
6.6.1 emd_27421_msk_1.map [i](#)



X



Y

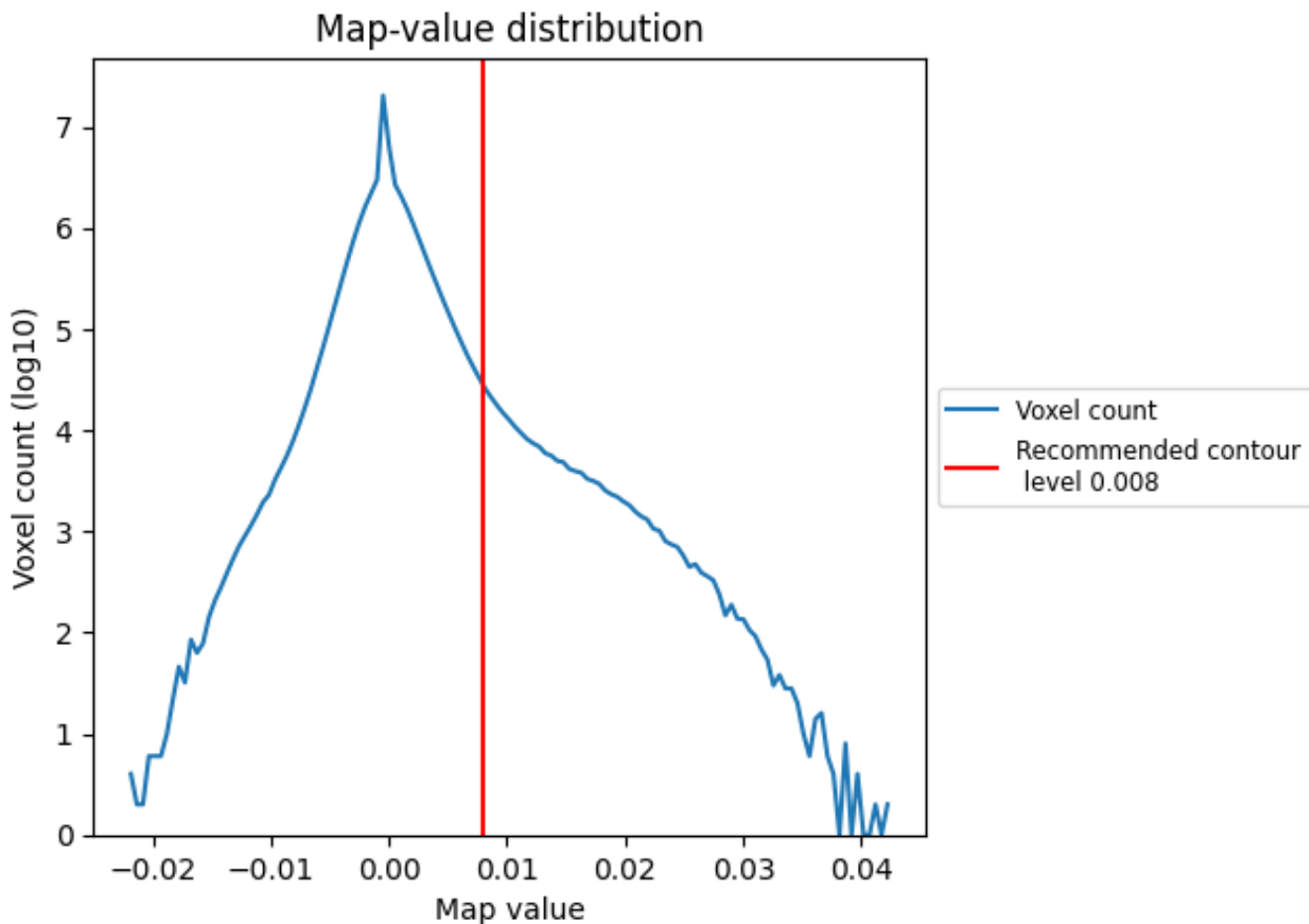


Z

7 Map analysis [i](#)

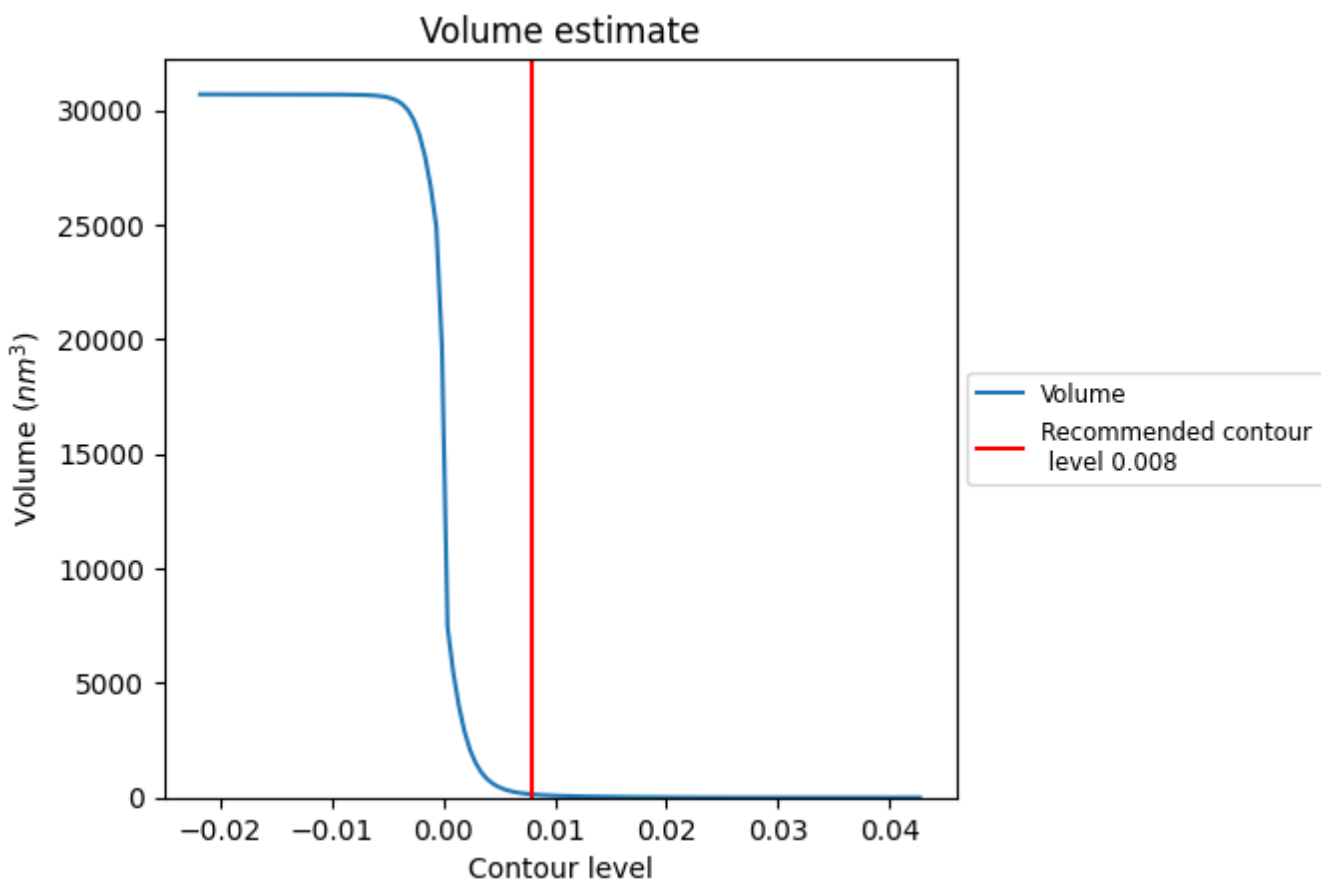
This section contains the results of statistical analysis of the map.

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.

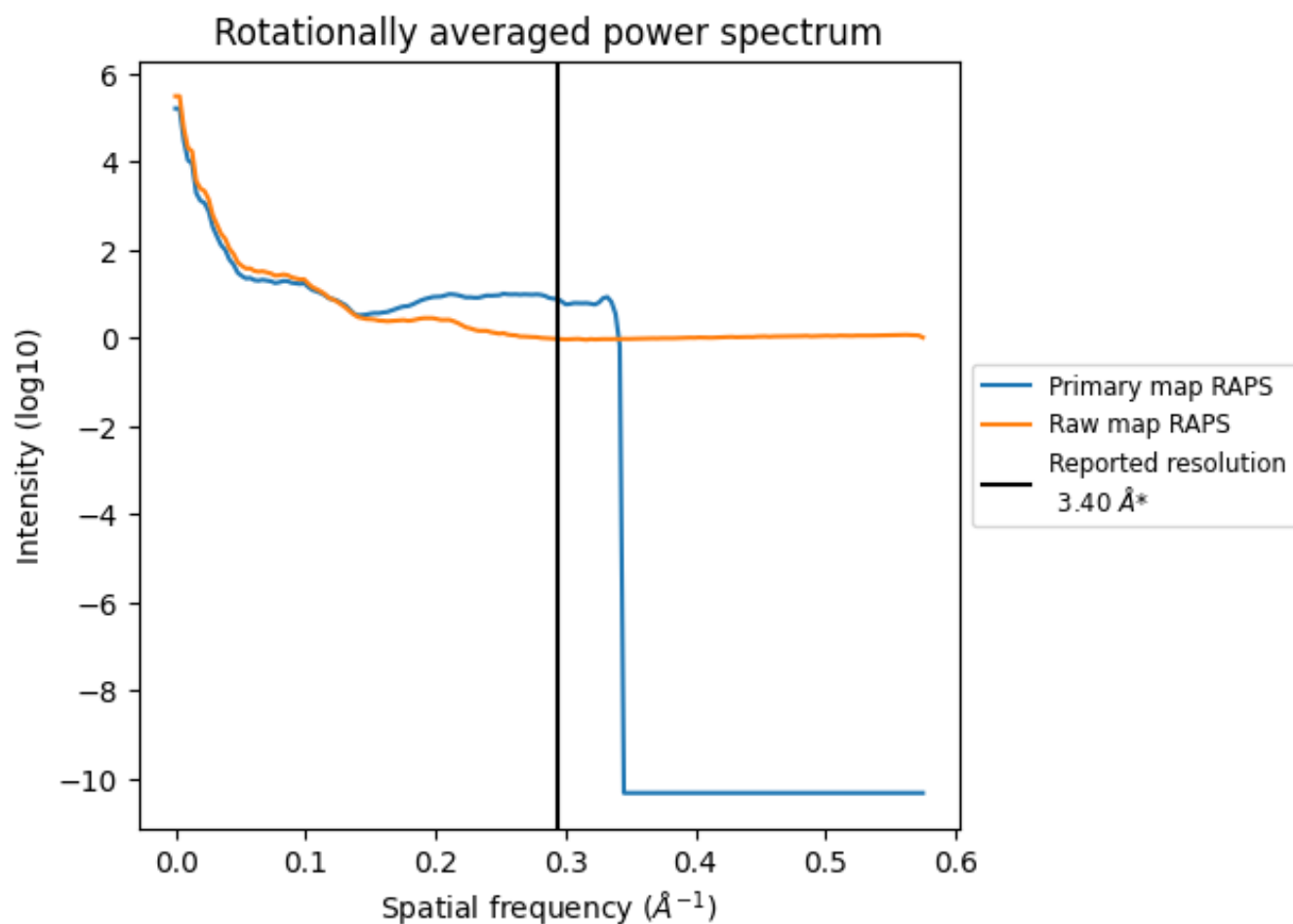
7.2 Volume estimate [\(i\)](#)



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 [i](#)

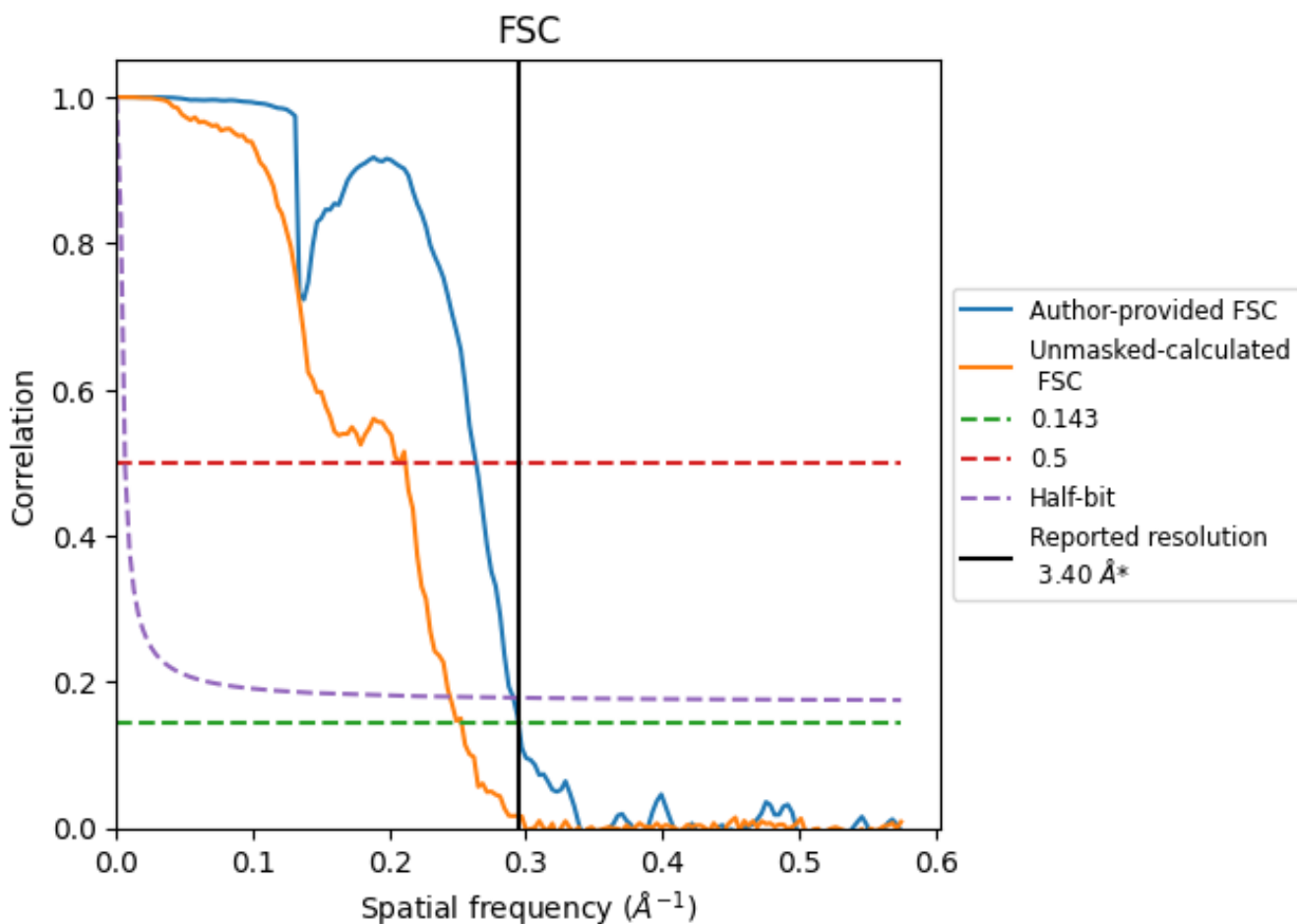


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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](#)

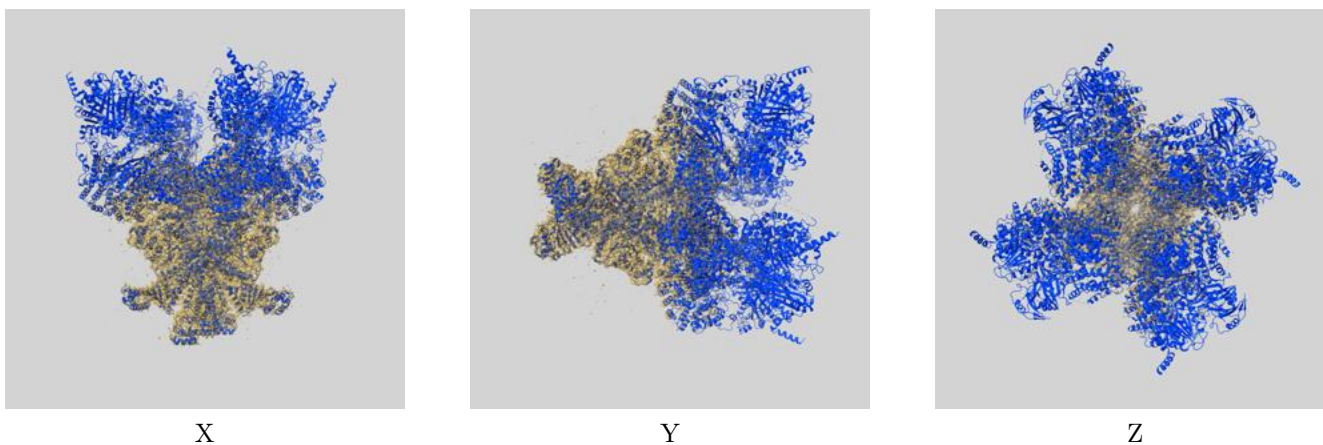
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.80	3.44
Unmasked-calculated*	3.95	4.83	4.09

*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](#)

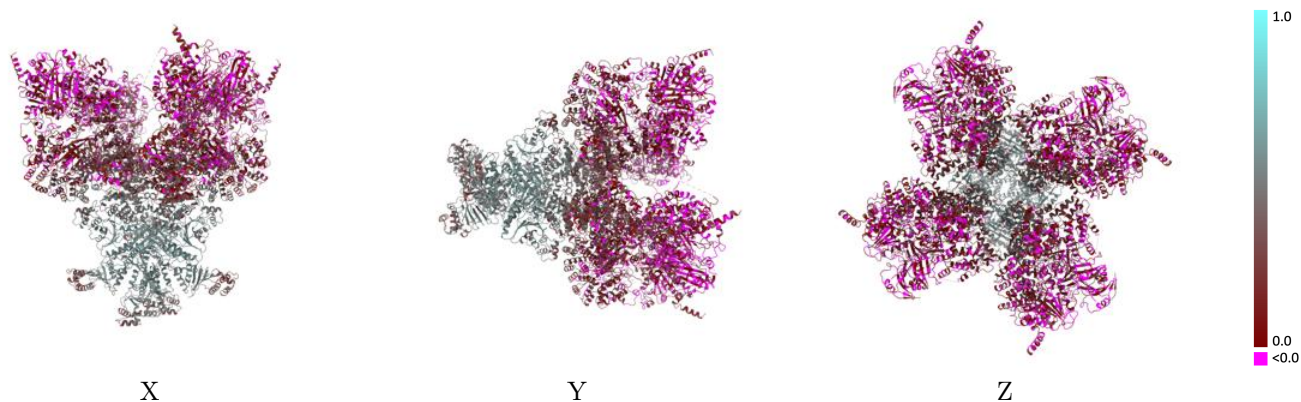
This section contains information regarding the fit between EMDB map EMD-27421 and PDB model 8DGC. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



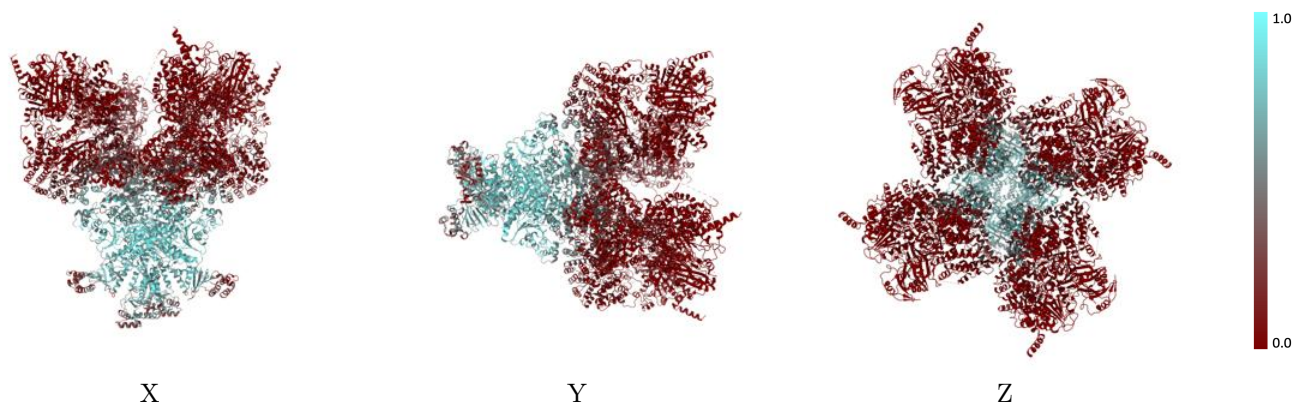
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



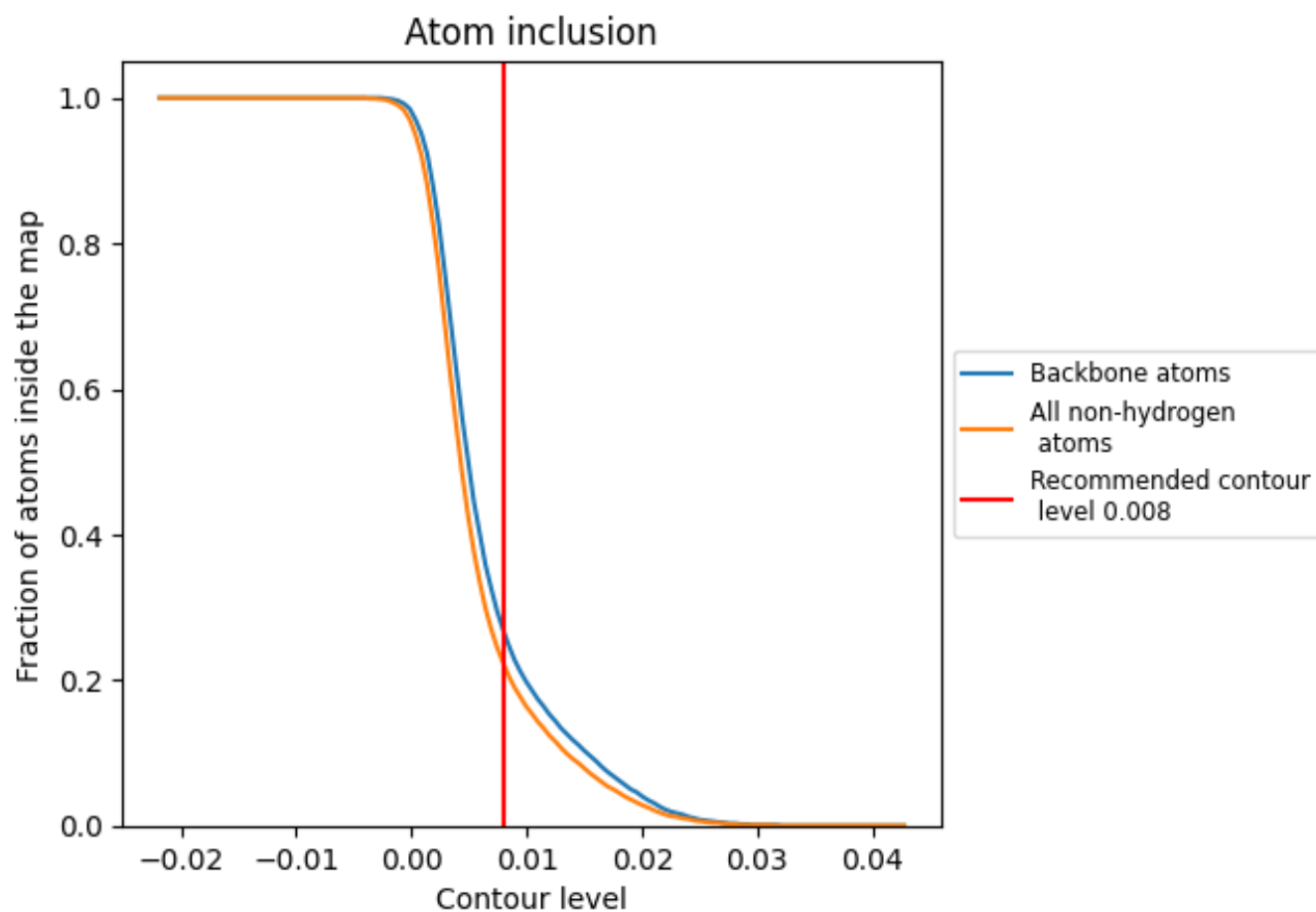
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.2220	 0.2180
A	 0.2790	 0.2510
B	 0.2790	 0.2580
C	 0.2800	 0.2470
D	 0.2790	 0.2600
E	 0.0070	 0.0760
F	 0.0090	 0.0900
G	 0.0070	 0.0720
H	 0.0090	 0.0900

