



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 03:29 PM UTC

PDB ID : 8DGC / pdb_00008dgc
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 wwPDB EM Validation Summary 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:

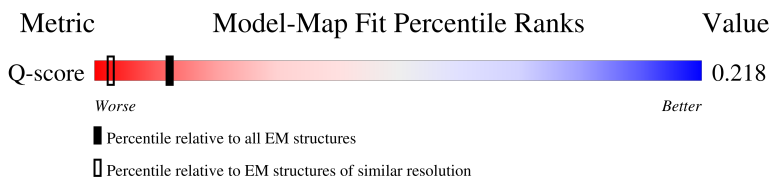
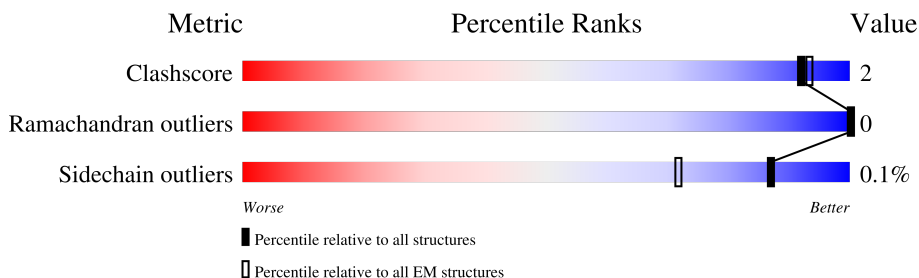
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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% 94% ..
1	B	2092	65% 91% ..
1	C	2092	66% 94% ..
1	D	2092	65% 91% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	586	92% 87% 5% 8%
2	F	586	92% 87% 5% 8%
2	G	586	92% 86% 5% 8%
2	H	586	92% 86% 5% 8%

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.

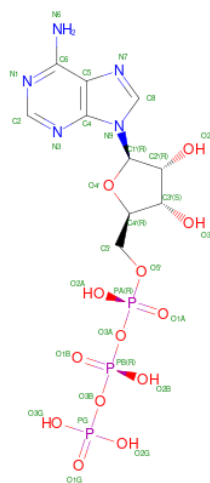
- Molecule 1 is a protein called SeAvs3.

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 (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

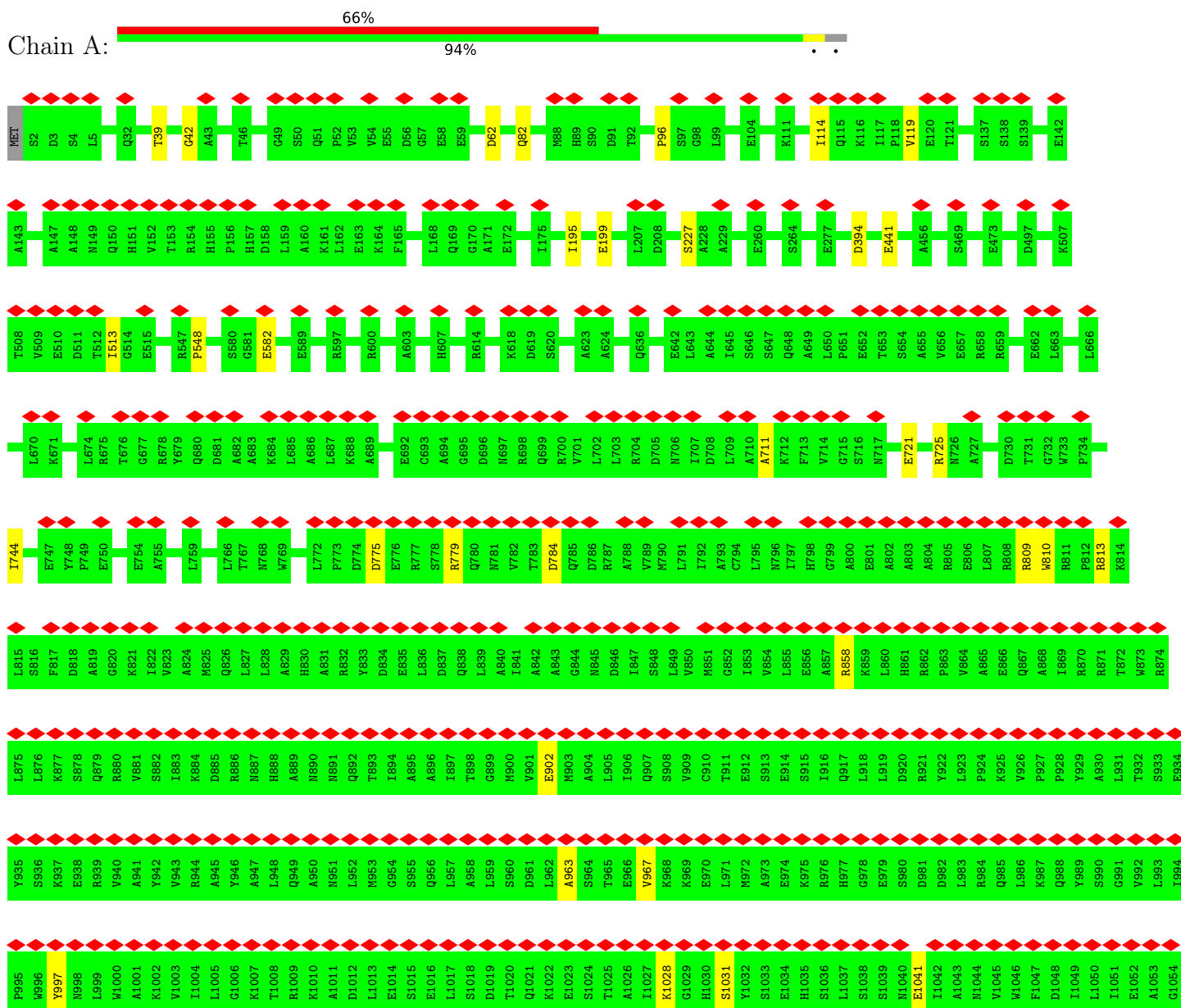
Continued from previous page...

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

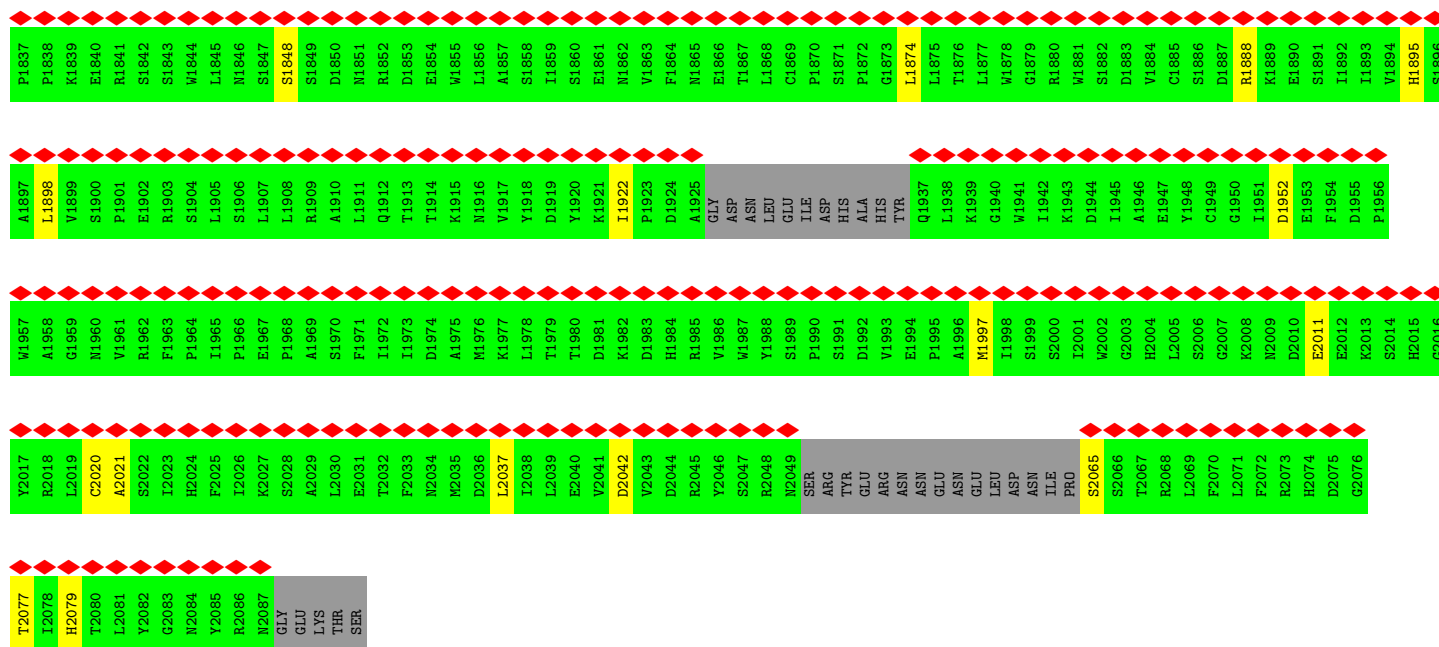
3 Residue-property plots

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.

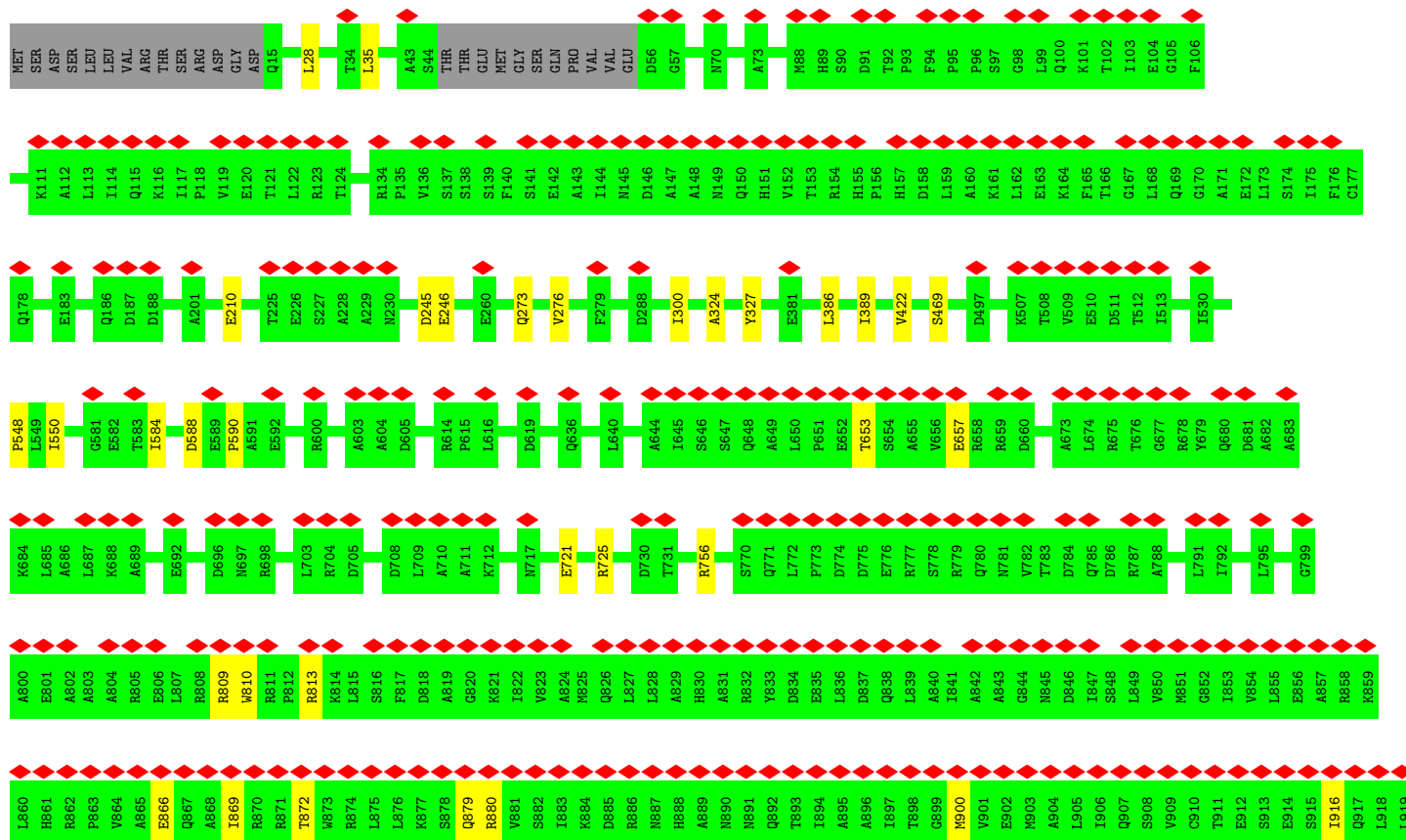
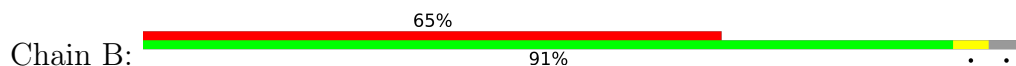
• Molecule 1: SeAvs3



D1777	K1717	F1657	M1597	G1537	K1477	Y1416	I1356	F1296	L1236	P1176	M1055
D1778	P1718	A1658	A1598	P1538	E1478	D1417	F1357	N1297	A1237	P1177	V1056
Y1779	L1719	A1659	T1599	W1539	I1479	F1418	K1358	V1298	W1238	E1178	S1057
H1780	G1720	R1660	T1600	W1540	F1480	K1419	D1359	Q1299	T1239	I1179	K1058
F1781	R1721	L1661	L1601	E1541	G1481	Y1420	C1360	M1300	I1240	S1180	D1059
Y1782	C1722	T1662	P1602	K1542	T1482	I1421	D1361	I1301	E1241	Y1181	D1060
L1783	F1723	L1663	F1603	L1543	T1483	L1422	L1362	Q1302	H1242	K1182	V1061
G1784	G1724	A1664	C1604	S1544	L1484	E1423	S1363	M1303	L1243	L1183	E1062
Y1785	V1725	L1665	P1605	P1545	E1485	S1424	S1364	L1304	V1244	A1184	M1063
H1786	S1726	H1666	R1606	P1546	A1486	I1425	L1365	K1305	K1245	R1185	I1064
Q1727	Q1727	D1667	M1607	T1547	I1487	P1426	D1366	K1306	K1246	C1186	I1065
K1728	L1728	S1668	L1608	H1548	A1488	D1427	G1367	L1307	N1247	A1187	K1066
F1729	P1609	D1669	P1609	E1549	E1489	E1428	L1368	D1308	E1248	K1067	W1067
L1730	F1610	Y1670	F1610	E1550	S1490	W1429	S1369	A1309	L1189	S1128	S1068
E1731	Y1611	I1671	E1611	D1551	P1491	T1430	A1370	I1310	N1250	T1190	Q1069
P1732	T1612	S1672	S1552	S1552	E1492	S1431	A1371	S1311	A1251	R1191	H1070
E1733	L1613	L1673	L1553	L1553	P1493	R1432	Y1372	L1252	E1192	S1131	K1071
M1734	H1614	P1674	A1554	A1554	A1494	L1433	E1373	S1313	Y1193	L1132	G1072
L1735	A1615	A1675	G1555	G1555	M1496	S1434	K1374	L1314	A1254	V1194	M1073
R1736	Q1616	Q1676	Y1556	Y1556	S1496	I1435	F1375	G1315	L1255	D1195	R1074
I1737	L1617	E1677	L1498	I1557	D1497	K1436	R1376	I1316	P1256	P1136	F1075
L1738	W1618	E1678	L1499	W1558	L1498		N1377	E1317	L1257	A1137	V1076
R1739	L1619	A1559	F1500	A1559	F1500	L1439	V1378	H1318	I1258	K1138	T1077
D1740	M1620	R1560	S1501	R1560	S1501	A1440	P1379	E1320	T1259	E1139	P1078
V1741	I1621	L1561	L1502	L1561	L1502	G1441	E1380	E1321	F1200	Y1140	T1079
L1742	A1622	G1562	P1503	G1562	P1503	I1442	F1381	L1321	E1261	F1141	L1080
G1743	A1623	S1563	G1504	S1563	G1504	I1443	Y1382	K1322	M1262	N1142	H1081
F1744	A1624	P1564	L1505	P1564	L1505	K1444	S1383	E1323	D1263	Q1143	F1082
K1745	R1625	A1565	L1506	A1565	L1506	E1445	E1384	R1324	W1264	A1144	S1084
G1746	V1626	A1566	V1507	A1566	V1507	Y1446	E1385	I1325	H1265	I1145	S1085
S1747	A1627	E1567	S1508	E1567	S1508	C1447	T1386	S1326	K1266	V1206	V1086
R1748	L1628	M1568	K1509	M1568	K1509	Q1448	F1387	G1327	G1267	E1207	C1087
M1749	D1629	R1569	L1510	R1569	L1510	R1449	I1388	L1328	D1268	I1208	A1088
W1750	D1630	W1570	E1511	W1570	E1511	F1450	K1389	Q1329	L1269	L1209	L1151
D1751	G1631	Q1571	S1512	Q1571	S1512	C1451	K1390	H1330	A1210	A1210	E1089
E1752	K1632	A1572	E1514	A1572	E1514	M1452	A1391	THR	E1211	E1211	I1090
D1753	S1633	H1574	A1515	H1574	A1515	R1453	L1392	THR	S1272	D1153	S1091
F1754	L1634	A1575	L1516	A1575	L1516	I1454	S1393	VAL	E1154	G1152	G1092
R1755	I1635	V1576	D1517	V1576	D1517	R1455	R1394	SER	L1212	L1156	L1093
N1756	N1637	L1577	V1518	L1577	V1518	K1456	V1395	LYS	S1275	S1215	G1094
K1757	I1638	A1578	L1519	A1578	L1519	S1457	K1396	SER	S1276	S1216	E1095
R1758	G1639	L1579	S1520	L1579	S1520	R1458	T1397	SER	G1277	A1217	L1096
Y1759	Y1640	C1580	Y1521	C1580	Y1521	V1459	Q1398	LEU	T1278	L1218	S1097
Y1760	F1641	R1581	A1522	R1581	A1522	E1461	K1399	SER	D1279	A1219	Y1098
Y1761	F1642	M1582	L1523	M1582	L1523	I1462	C1401	ASN	I1280	I1220	H1099
Q1762	H1643	S1583	D1524	S1583	D1524	F1463	S1402	ASP	K1281	I1162	F1100
D1763	Y1644	R1584	L1525	R1584	L1525	P1464	S1402	ASN	E1282	L1163	A1101
R1764	Y1645	T1585	F1526	T1585	F1526	F1465	F1403	GLU	W1224	D1164	E1102
D1765	T1646	C1586	D1527	C1586	D1527	S1466	I1404	GLN	K1283	L1165	L1103
H1766	T1647	E1587	E1528	E1587	E1528	L1467	T1405	M1285	A1286	A1166	A1104
H1767	D1648	I1588	V1529	I1588	V1529	A1468	A1406	D1350	E1287	E1167	L1105
H1768	Q1649	Q1589	L1530	Q1589	L1530	S1469	I1407	Q1351	F1287	Y1168	S1106
S1769	P1650	H1590	K1531	H1590	K1531	R1470	G1408	E1352	T1228	V1169	L1107
G1770	H1651	I1591	D1532	I1591	D1532	L1471	A1409	W1353	A1170	A1170	W1108
D1771	V1652	F1592	E1533	F1592	E1533	S1472	I1410	E1354	V1289	G1171	R1109
Y1772	L1653	Q1593	D1534	Q1593	D1534	G1473	F1411	E1355	V1290	K1172	D1110
P1773	I1654	H1594	D1536	H1594	D1536	I1474	H1412		Y1291	T1173	E1111
R1774	A1655	A1595	I1536	A1595	I1536	S1475	W1413		H1292	Q1174	H1112
H1775	H1656	I1596		I1596		E1476	G1414		T1294	S1234	S1113
							L1415		K1295	I1235	D1114
D1810	E1810	T1688	L1628	M1568	K1509	Q1448	F1387	G1327	C1267	E1207	V1086
D1811	D1811	T1689	D1629	R1569	L1510	R1449	I1388	L1328	D1268	I1208	C1087
V1812	V1812	L1690	D1630	W1570	E1511	F1450	K1389	Q1329	L1269	L1209	A1088
F1813	F1813	P1691	G1631	Q1571	S1512	C1451	K1390	H1330	A1210	A1210	E1089
Q1814	Q1814	V1692	K1632	A1572	E1514	M1452	A1391	THR	E1211	E1211	I1090
D1815	D1815	A1573	S1633	H1574	A1515	R1453	L1392	THR	S1272	D1153	S1091
W1816	W1816	A1575	L1634	H1574	A1515	I1454	S1393	VAL	E1154	G1152	G1092
L1817	L1817	V1576	I1635	V1576	D1517	R1455	R1394	SER	L1212	L1156	L1093
R1818	R1818	L1577	P1636	L1577	V1518	K1456	V1395	LYS	S1275	S1215	G1094
R1819	R1819	A1578	N1637	L1577	V1518	S1457	K1396	SER	S1276	S1216	E1095
H1820	H1820	H1578	I1638	A1578	L1519	R1458	T1397	SER	G1277	A1217	L1096
D1821	D1821	L1579	G1639	L1579	S1520	V1459	Q1398	LEU	T1278	L1218	S1097
T1822	T1822	Y1760	Y1640	C1580	Y1521	E1461	K1399	SER	D1279	A1219	Y1098
S1823	S1823	Y1761	F1641	R1581	A1522	I1462	C1401	ASN	I1280	I1220	H1099
R1824	R1824	Q1762	F1642	M1582	L1523	F1463	S1402	ASP	K1281	I1162	F1100
N1825	N1825	Y1705	H1643	S1583	D1524	P1464	S1402	ASN	E1282	L1163	A1101
D1826	D1826	T1706	Y1644	R1584	L1525	F1465	F1403	GLU	W1224	D1164	E1102
H1827	H1827	F1707	Y1645	T1585	F1526	F1465	I1404	K1283	K1283	L1165	L1103
R1828	R1828	G1708	T1646	C1586	D1527	S1466	T1405	M1285	A1286	A1166	A1104
W1829	W1829	H1707	T1647	E1587	E1528	L1467	A1406	D1350	E1287	E1167	L1105
L1830	L1830	I1709	D1648	I1588	V1529	A1468	A1406	Q1351	F1287	Y1168	S1106
A1831	A1831	F1711	Q1649	Q1589	L1530	S1469	I1407	E1352	T1228	V1169	L1107
D1832	D1832	G1712	P1650	H1590	K1531	R1470	G1408	W1353	A1170	A1170	W1108
R1833	R1833	P1713	H1651	I1591	D1532	L1471	A1409	E1354	V1289	G1171	R1109
R1834	R1834	P1714	V1652	F1592	E1533	S1472	I1410	E1354	V1290	K1172	D1110
D1835	D1835	W1715	L1653	Q1593	D1534	G1473	F1411	S1355	Y1291	T1173	E1111
		L1716	I1654	H1594	D1536	I1474	H1412		H1292	Q1174	H1112
						S1475	W1413		T1294	S1234	S1113
							G1414		K1295	I1235	D1114



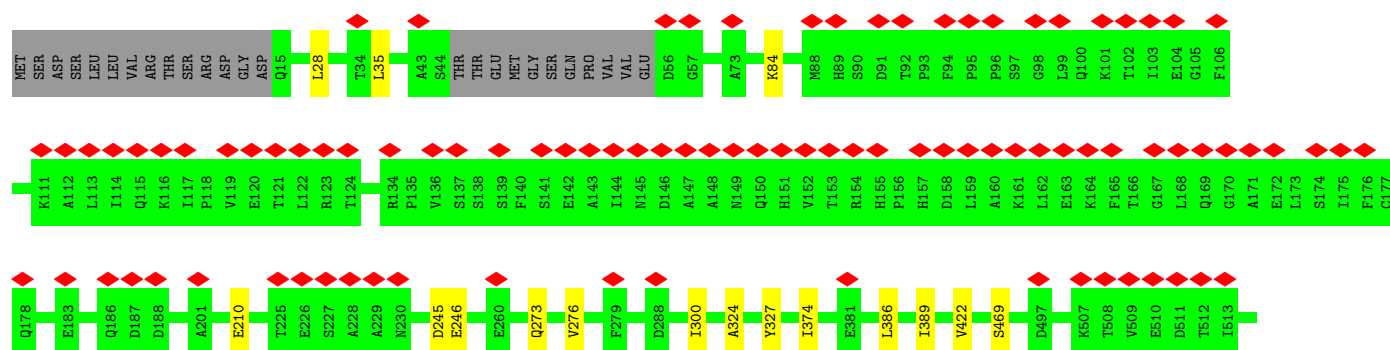
• Molecule 1: SeAvs3



Y1644	R1584	D1524	P1464	F1403	ASN	K1283	L1163	F1100	N1040	S980	D920
A1645	T1585	L1525	F1465	I1404	ASP	I1284	D1164	A1101	E1041	D981	R921
T1646	C1586	F1526	S1466	T1405	ASN	M1285	L1165	E1102	I1042	D982	Y922
T1647	V1587	D1527	L1467	A1406	GLN	A1286	A1166	L1103	A1043	L983	L923
D1648	I1588	E1528	A1468	I1407	G1348	F1287	E1167	A1104	N1044	R984	P924
Q1649	Q1589	V1529	S1469	G1408	H1349	E1288	Y1168	L1105	V1045	Q985	K925
P1650	L1530	L1530	R1470	A1409	D1350	V1289	V1169	S1106	W1046	L986	V926
H1651	K1531	K1531	L1471	I1410	Q1351	V1290	A1170	L1107	F1047	K987	P927
V1652	D1532	D1532	S1472	F1411	E1352	Y1291	G1171	W1108	I1048	Q988	P928
L1653	G1533	G1533	G1473	H1412	W1353	Y1292	K1172	R1109	I1049	Y989	Y929
I1654	I1474	I1474	I1474	W1413	E1354	Y1293	T1173	D1110	L1050	S990	A930
R1655	S1475	G1535	S1475	G1414	S1355	T1294	Q1174	E1111	I1051	G991	L931
H1656	E1476	D1536	E1476	L1415	L1356	K1295	V1175	H1112	E1052	V992	T932
P1657	K1477	G1537	K1477	Y1416	F1357	F1296	P1176	S1113	A1053	L993	S933
A1658	E1478	P1538	E1478	D1417	K1358	M1287	P1177	D1114	G1054	I994	E934
A1659	W1539	W1539	I1479	F1418	D1359	V1298	E1178	A1115	N1055	P995	Y935
R1660	F1480	K1540	F1480	K1419	C1360	Q1299	Q1116	Q1117	V1056	W996	S936
T1661	G1481	E1541	G1481	Y1420	D1361	W1300	I1179	I1117	S1057	Y997	K937
L1662	I1482	I1542	I1482	I1421	L1362	I1301	S1180	K1118	K1058	N998	E938
L1663	L1483	L1543	L1483	L1422	S1363	Q1302	K1182	A1119	D1059	L999	R939
A1664	L1484	L1544	E1485	E1423	S1364	M1303	L1183	W1000	D1060	V1000	V940
L1665	E1485	P1544	A1486	S1424	I1365	I1304	A1184	A1001	I1061	A1001	A941
H1666	I1486	P1546	A1486	I1425	D1366	K1305	R1185	K1002	E1062	K1002	Y942
D1667	I1487	T1547	I1487	P1426	G1367	K1306	C1186	V1003	V1063	V1003	V943
S1668	A1488	D1548	A1488	D1427	I1368	L1307	A1187	I1004	I1064	I1004	R944
D1669	E1489	E1549	E1489	E1428	S1369	D1308	E1188	L1005	I1065	L1005	A945
L1670	S1490	P1491	S1490	W1429	A1370	A1309	L1189	G1006	K1066	G1006	Y946
I1671	E1492	E1491	E1492	T1430	A1371	I1310	T1190	K1007	W1067	K1007	A947
S1672	P1493	L1552	P1493	S1430	Y1372	S1311	E1192	T1008	S1068	T1008	L948
L1673	A1494	L1553	A1494	R1432	E1373	T1312	R1191	R1009	Q1069	R1009	Q949
P1674	N1495	A1554	N1495	L1433	K1374	S1313	Y1193	K1010	H1070	K1010	A950
A1675	S1496	G1555	S1496	S1434	F1375	L1314	D1194	A1011	D1012	A1011	N951
Q1676	D1497	I1556	D1497	I1435	F1376	G1315	V1195	L952	G1072	L952	M952
P1677	R1498	I1557	R1498	K1436	R1377	L1316	D1196	L1013	N1073	L1013	M953
E1678	L1499	W1558	L1499	T1437	V1378	E1317	D1197	E1014	R1074	E1014	G954
N1679	A1559	A1559	F1500	T1438	P1379	H1318	K1198	S1015	V1075	S1015	S955
K1680	S1501	R1560	S1501	L1439	E1380	T1319	H1199	E1016	F1077	E1016	Q956
L1681	L1502	L1561	F1381	A1440	F1381	E1320	F1200	L1017	T1077	L1017	L957
R1682	P1503	G1562	Y1382	I1443	Y1382	L1321	A1201	S1018	P1078	S1018	A958
N1683	G1504	S1563	S1383	K1444	S1383	K1322	W1202	D1019	T1079	D1019	L959
I1684	L1505	P1564	K1394	E1445	K1394	E1323	S1203	T1020	L1080	T1020	S960
N1685	L1506	E1565	E1385	Y1446	E1385	R1324	D1204	Q1021	H1081	Q1021	D961
Q1686	V1507	A1566	T1386	Y1446	T1386	I1325	T1205	K1022	F1082	K1022	L962
S1687	S1508	C1447	F1387	C1447	F1387	S1326	V1206	E1145	F1083	E1023	A963
T1688	K1509	E1567	I1388	Q1448	I1388	G1327	E1207	S1085	S1085	S1024	S964
L1689	L1510	R1568	K1389	R1449	K1389	L1328	I1208	V1086	C1087	T1025	T965
T1689	E1511	R1569	K1390	F1450	K1390	Q1329	L1209	A1026	V1087	A1026	E966
L1690	C1451	W1570	C1451	C1451	C1451	H1330	E1210	I1027	I1027	I1027	V967
P1691	M1452	Q1571	M1452	M1452	A1391	L1330	A1088	K1028	A1088	K1028	K968
V1692	N1513	A1572	N1513	A1453	I1392	THR	D1153	G1029	I1089	G1029	K969
LEU	E1514	A1573	E1514	R1454	S1393	GLU	L1212	H1030	I1090	H1030	E970
ASP	A1515	L1574	A1515	R1455	R1394	THR	C1213	S1031	S1091	S1031	L971
LVS	V1516	A1575	V1395	K1456	V1395	VAL	P1214	G1092	G1092	G1092	M972
GLU	D1517	A1576	K1396	K1456	K1396	LVS	S1215	L1093	L1093	L1093	A973
ASP	V1518	L1577	T1397	S1457	T1397	LVS	S1216	G1094	G1094	G1094	A974
HIS	L1519	A1578	R1458	R1457	R1458	SER	A1217	E1095	E1095	E1034	K975
ARG	L1520	V1459	G1398	V1459	G1398	SER	L1218	L1096	L1096	H1035	K976
GLY	Y1521	Y1460	K1399	Y1460	K1399	LEU	A1161	S1097	S1097	S1036	H977
E1702	A1522	E1461	E1400	I1461	E1400	SER	I1220	H1098	H1098	S1038	G978
D1703	C1401	I1462	C1401	I1462	C1401	SER	I1221	S1222	S1222	S1039	E979
		F1463	S1402	F1463	S1402						



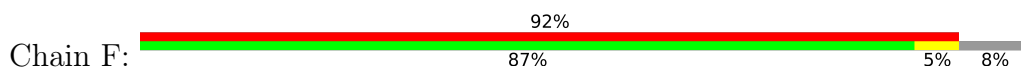
D1534	I1474	W1413	W1353	Y1293	R1233	T1173	H1112	E1052	V992	T932	T872	P812
G1535	S1475	G1414	E1354	T1294	S1234	Q1174	S1113	A1053	L993	S933	W873	R813
D1536	E1476	L1415	S1355	T1295	S1235	V1175	D1114	G1054	P994	E934	R874	K814
P1538	E1478	Y1416	I1356	F1296	L1236	P1176	A1115	N1055	P995	Y935	L875	L815
W1539	I1479	D1417	F1357	W1298	A1237	P1177	Q1116	V1056	Y996	S936	L876	S816
M1540	F1480	F1418	K1358	V1298	W1238	E1178	I1117	S1057	Y997	K937	K877	F817
E1541	G1481	K1419	D1359	Q1299	T1239	I1179	K1118	K1058	N998	E938	S878	A819
K1542	I1482	Y1420	C1360	M1300	I1240	S1180	A1119	D1059	L999	R939	Q879	G820
L1543	I1483	I1421	D1361	I1301	E1241	Y1181	D1120	D1060	W1000	V940	R880	G820
S1544	T1484	L1422	L1362	Q1302	H1242	K1182	G1121	V1061	A1001	A941	V881	K821
P1545	E1485	E1423	S1363	N1303	L1243	L1183	I1123	E1062	K1002	Y942	S882	V823
P1546	A1486	S1424	S1364	L1304	V1244	A1184	D1124	N1063	V1003	V943	I883	A824
T1547	I1487	I1425	I1365	K1305	K1245	R1185	L1125	I1064	I1004	R944	K884	M825
H1548	L1487	P1426	D1366	K1306	K1246	C1186	S1126	I1065	L1005	A945	D885	Q826
V1549	E1488	D1427	G1367	L1307	N1247	A1187	R1127	K1066	G1006	Y946	R886	Q826
E1489	A1489	E1428	I1368	D1308	K1248	E1188	S1128	W1067	K1007	A947	N887	L827
S1490	W1429	W1429	S1369	A1309	I1249	L1189	L1129	S1068	T1008	L948	H888	L828
P1491	E1492	T1430	A1370	I1310	N1250	T1190	I1130	Q1069	R1009	Q949	A889	A829
E1493	S1551	S1431	A1371	S1311	A1251	R1191	S1131	H1070	K1010	A950	N890	H830
P1493	L1553	R1432	Y1372	T1312	L1252	E1192	L1132	K1071	A1011	N951	R891	A831
A1494	N1495	L1433	E1373	S1313	D1253	Y1193	D1133	G1072	L1013	M953	T893	Y833
G1495	S1496	S1434	K1374	L1314	A1254	V1194	E1134	N1073	E1014	I894	I894	D834
Y1556	D1497	I1435	F1375	G1315	L1255	D1195	P1135	R1074	A1015	S954	A895	E835
I1557	R1376	K1436	R1376	I1316	P1256	R1196	E1136	V1075	S1015	S955	A895	L836
W1558	N1377		N1377	E1317	L1257	D1197	A1137	F1076	E1016	Q956	A896	D837
F1500	V1378		V1378	H1318	I1258	K1198	K1138	T1077	L1017	L957	I897	Q838
A1501	P1379		P1379	T1319	T1259	H1199	E1139	P1078	S1018	A958	T898	L839
L1502	S1501	A1440	E1380	E1320	F1260	F1200	Y1140	T1079	D1019	L959	G899	A840
P1503	G1504	L1442	F1381	L1321	E1261	A1201	F1141	L1080	T1020	S960	M900	I841
S1563	L1505	K1443	Y1382	K1322	N1262	W1202	Q1143	H1081	Q1021	D961	V901	A842
P1564	L1506	K1444	S1383	R1323	D1263	S1203	Q1143	R1082	K1022	L962	E902	A843
E1565	V1507	E1445	K1384	R1324	W1264	D1204	A1144	F1083	E1023	A963	M903	G844
A1566	G1447	Y1446	E1385	I1325	H1265	T1205	I1145	S1084	S1024	S964	A904	N845
E1567	S1508	G1447	T1386	S1326	K1266	V1206	E1146	S1085	T1025	T965	L905	D946
K1509	L1510	Q1449	F1387	G1327	C1267	E1207	M1149	V1086	A1026	E966	I906	I847
L1511	E1511	R1449	I1388	L1328	D1268	L1208	K1150	C1087	I1027	V967	Q907	S848
S1512	Q1571	F1450	K1389	Q1329	L1269	L1209	L1151	E1089	G1029	K968	S908	L849
G1571	N1513	C1451	I1390	H1330	L1270	A1210	G1152	I1090	H1030	K969	V909	V950
A1572	E1514	M1452	A1391	THR	D1271	E1211	D1153	S1091	S1031	L971	T911	M851
L1573	A1515	R1453	I1392	THR	S1272	L1212	E1154	G1092	Y1032	M972	E912	G952
A1575	L1516	I1454	S1393	VAL	V1273	C1213	M1155	L1093	S1033	A973	S913	V854
D1517	V1576	K1455	R1394	SER	L1274	P1214	L1156	G1094	E1034	E974	S914	L855
V1518	L1517	K1456	V1395	LYS	S1275	S1215	S1157	E1095	H1035	K975	S915	E956
L1519	L1577	S1457	K1396	LYS	S1276	S1216	R1158	L1096	S1036	R976	I916	A957
E1578	W1458	R1458	T1397	SER	C1277	A1217	W1159	S1097	S1037	H977	Q917	R558
L1579	V1459	V1459	LEU	SER	T1278	L1218	E1160	Y1098	L1037	G978	L918	K859
A1522	Y1521	E1461	R1399	ASN	D1279	A1219	A1161	H1099	S1038	E979	L919	L860
L1523	L1524	I1462	E1400	ASN	D1280	I1220	I1162	F1100	S1039	S980	D920	H961
M1582	D1524	F1463	C1401	ASP	K1281	I1221	L1163	F1100	M1040	S980	R921	R862
S1583	P1464	S1464	S1402	ASN	D1282	S1222	D1164	E1101	E1041	D981	R921	P963
L1584	F1526	F1465	F1403	GLN	K1283	R1223	L1165	E1102	I1042	D982	Y922	V864
T1585	D1527	S1466	I1404	G1348	I1284	W1224	A1166	L1103	I1043	L983	L923	P864
C1586	E1528	L1467	T1405	H1349	M1285	R1225	E1167	A1104	A1043	R984	P924	A865
V1587	E1529	A1468	A1406	D1350	A1286	W1226	Y1168	L1105	V1045	Q985	K925	E966
I1588	S1469	S1469	I1407	Q1351	F1287	D1226	V1169	S1106	W1046	L886	V926	Q867
Q1589	L1530	R1470	G1408	Q1351	E1288	R1227	A1170	L1107	F1047	K987	P927	A868
K1590	D1532	L1471	A1409	E1352	V1289	T1228	G1171	W1108	D1048	Q988	P928	I869
I1591	E1533	S1472	I1410		V1290	G1230	K1172	R1109	I1049	Y989	Y929	R870
F1592	Q1593	G1473	F1411		V1291	H1231		D1110	L1050	S990	A930	R871





- Molecule 2: Terminase, large subunit

- Molecule 2: Terminase, large subunit



MET	S2	S3	S4	S5	S6	A7	K8	N9	A10	L11	I12	I13	A14	Q15	L16	K17	G18	D19	F20	V21	A22	F23	L24	F25	V26	L27	L28	K29	A30	L31	N32	L33	P34	K35	P36	T37	K38	C39	Q40	I41	D42	M43	A44	R45	T46	L47	A48	M49	G50	D51	H52	K53	X54	F55	I56	L57	Q58	A59	F60	
	R61	G62	L63	G64	S66	F67	L68	T69	C70	A71	F72	V73	V74	W75	V76	L77	W78	R79	D80	P81	Q82	L83	K84	V85	L86	L87	V88	S89	A90	S91	K92	E93	R94	A95	D96	L97	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	V125	L126	F128	D129	V130	G131	L132	A133	K134	P135	D136	H137	S138	P139	S140	V141	K142	S143	V144	G145	L146	T147	G148	Q149	L150	T151	G152	S153	R154	A155	D156	L157	I158	T159	A160	D161	D162	V163	E164	V165	P166	G167	N168	F169	S170	T171	S172	S173	A174	R175	E176	K177	L178	V179	T180	
	L181	V182	T183	E184	F185	A186	L187	L188	L189	K190	P191	L192	P193	T194	S195	R196	V197	L198	V199	L200	G201	T202	P203	Q204	T205	E206	M207	T208	L209	Y210	K211	E212	L213	E214	D215	N216	K217	G218	Y219	S220	T221	W222	L223	W224	P225	A226	Q227	Y228	P229	R230	N231	D232	A233	E234	A235	L236	Y237	Y238	G239	L240

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: MG, ATP

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	0.25	0/16499	0.54	1/22369 (0.0%)
1	B	0.25	0/16319	0.56	2/22123 (0.0%)
1	C	0.25	0/16499	0.54	1/22369 (0.0%)
1	D	0.25	0/16319	0.56	4/22123 (0.0%)
2	E	0.23	0/4363	0.57	4/5899 (0.1%)
2	F	0.24	0/4363	0.57	2/5899 (0.0%)
2	G	0.24	0/4363	0.58	4/5899 (0.1%)
2	H	0.23	0/4363	0.57	1/5899 (0.0%)
All	All	0.25	0/83088	0.56	19/112580 (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 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1923	PRO	CA-N-CD	-12.23	94.87	112.00
1	B	1923	PRO	CA-N-CD	-12.21	94.90	112.00
2	F	191	PRO	CA-N-CD	-8.65	99.89	112.00
2	H	191	PRO	CA-N-CD	-8.62	99.93	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	191	PRO	CA-N-CD	-8.61	99.94	112.00

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	37	0
1	B	15974	0	15804	52	0
1	C	16152	0	15975	37	0
1	D	15974	0	15804	51	0
2	E	4273	0	4283	15	0
2	F	4273	0	4283	19	0
2	G	4273	0	4283	18	0
2	H	4273	0	4283	17	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

Continued on next page...

Continued from previous page...

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	244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 244 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

Continued on next page...

Continued from previous page...

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%)	1753 (100%)	1 (0%)	88	89
1	B	1732/1814 (96%)	1729 (100%)	3 (0%)	87	85
1	C	1754/1814 (97%)	1752 (100%)	2 (0%)	88	89
1	D	1732/1814 (96%)	1729 (100%)	3 (0%)	87	85
2	E	458/500 (92%)	458 (100%)	0	100	100
2	F	458/500 (92%)	456 (100%)	2 (0%)	84	83
2	G	458/500 (92%)	458 (100%)	0	100	100
2	H	458/500 (92%)	456 (100%)	2 (0%)	84	83
All	All	8804/9256 (95%)	8791 (100%)	13 (0%)	87	89

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1005	LEU
1	D	1365	ILE
2	H	448	ILE
2	F	488	LEU
2	H	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	58	GLN
2	F	291	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	49	ASN
1	C	181	HIS
1	B	2004	HIS

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 oligosaccharides 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	D	2101	4	32,33,33	0.70	1 (3%)	48,52,52	0.39	0
3	ATP	G	601	4	32,33,33	0.46	0	48,52,52	0.32	0
3	ATP	C	2101	4	32,33,33	0.56	1 (3%)	48,52,52	0.32	0
3	ATP	H	601	4	32,33,33	0.44	0	48,52,52	0.32	0
3	ATP	E	601	4	32,33,33	0.44	0	48,52,52	0.32	0
3	ATP	B	2101	4	32,33,33	0.69	1 (3%)	48,52,52	0.39	0
3	ATP	A	2101	4	32,33,33	0.56	1 (3%)	48,52,52	0.31	0
3	ATP	F	601	4	32,33,33	0.46	0	48,52,52	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	D	2101	4	-	4/22/38/38	0/3/3/3
3	ATP	G	601	4	-	4/22/38/38	0/3/3/3
3	ATP	C	2101	4	-	2/22/38/38	0/3/3/3
3	ATP	H	601	4	-	2/22/38/38	0/3/3/3
3	ATP	E	601	4	-	3/22/38/38	0/3/3/3
3	ATP	B	2101	4	-	4/22/38/38	0/3/3/3
3	ATP	A	2101	4	-	2/22/38/38	0/3/3/3
3	ATP	F	601	4	-	3/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2101	ATP	PB-O3B	-2.77	1.56	1.59
3	B	2101	ATP	PB-O3B	-2.75	1.56	1.59
3	C	2101	ATP	PB-O3B	-2.31	1.57	1.59
3	A	2101	ATP	PB-O3B	-2.25	1.57	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

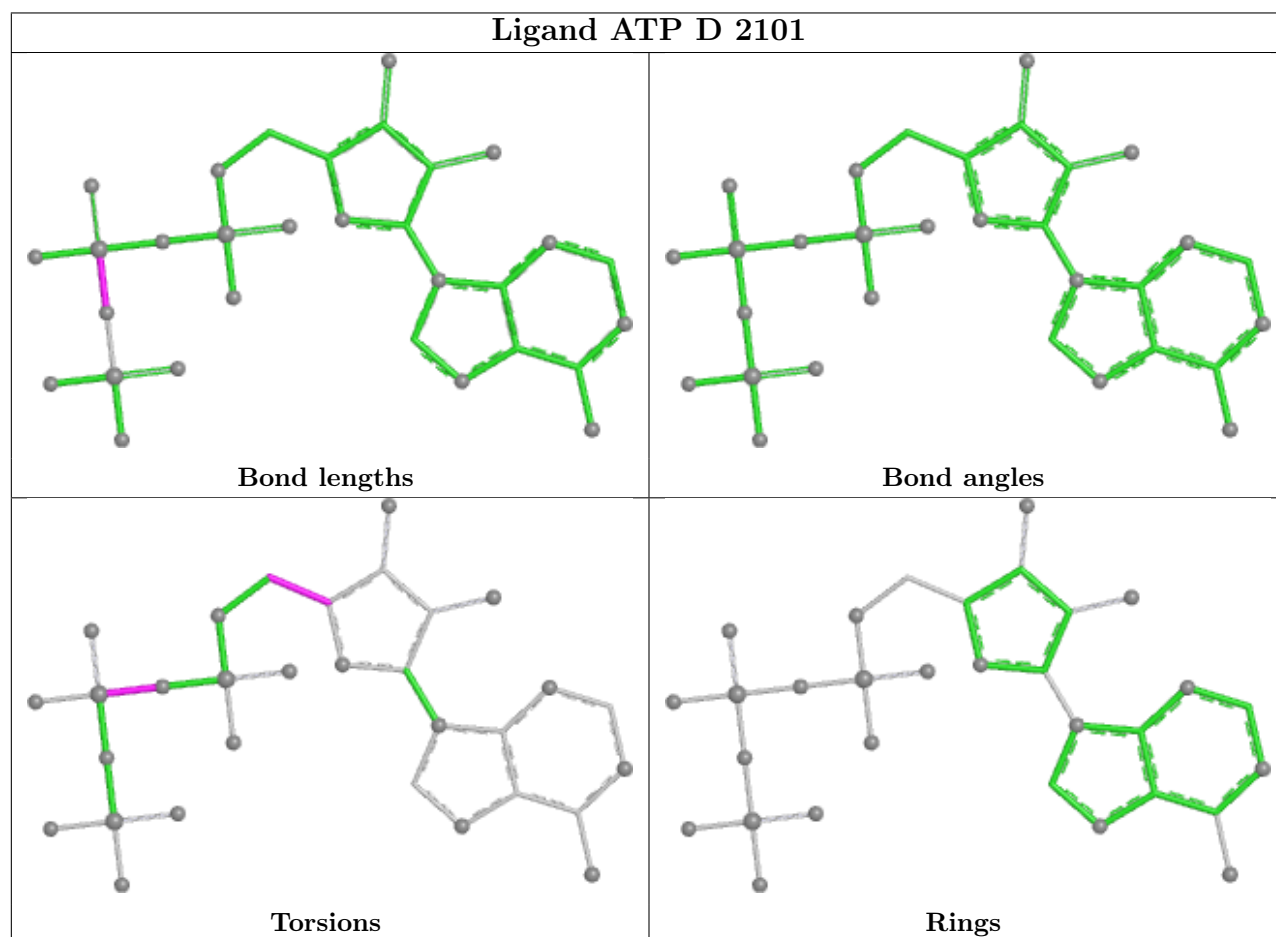
Mol	Chain	Res	Type	Atoms
3	B	2101	ATP	O4'-C4'-C5'-O5'
3	D	2101	ATP	O4'-C4'-C5'-O5'
3	F	601	ATP	O4'-C4'-C5'-O5'
3	G	601	ATP	O4'-C4'-C5'-O5'
3	B	2101	ATP	C3'-C4'-C5'-O5'

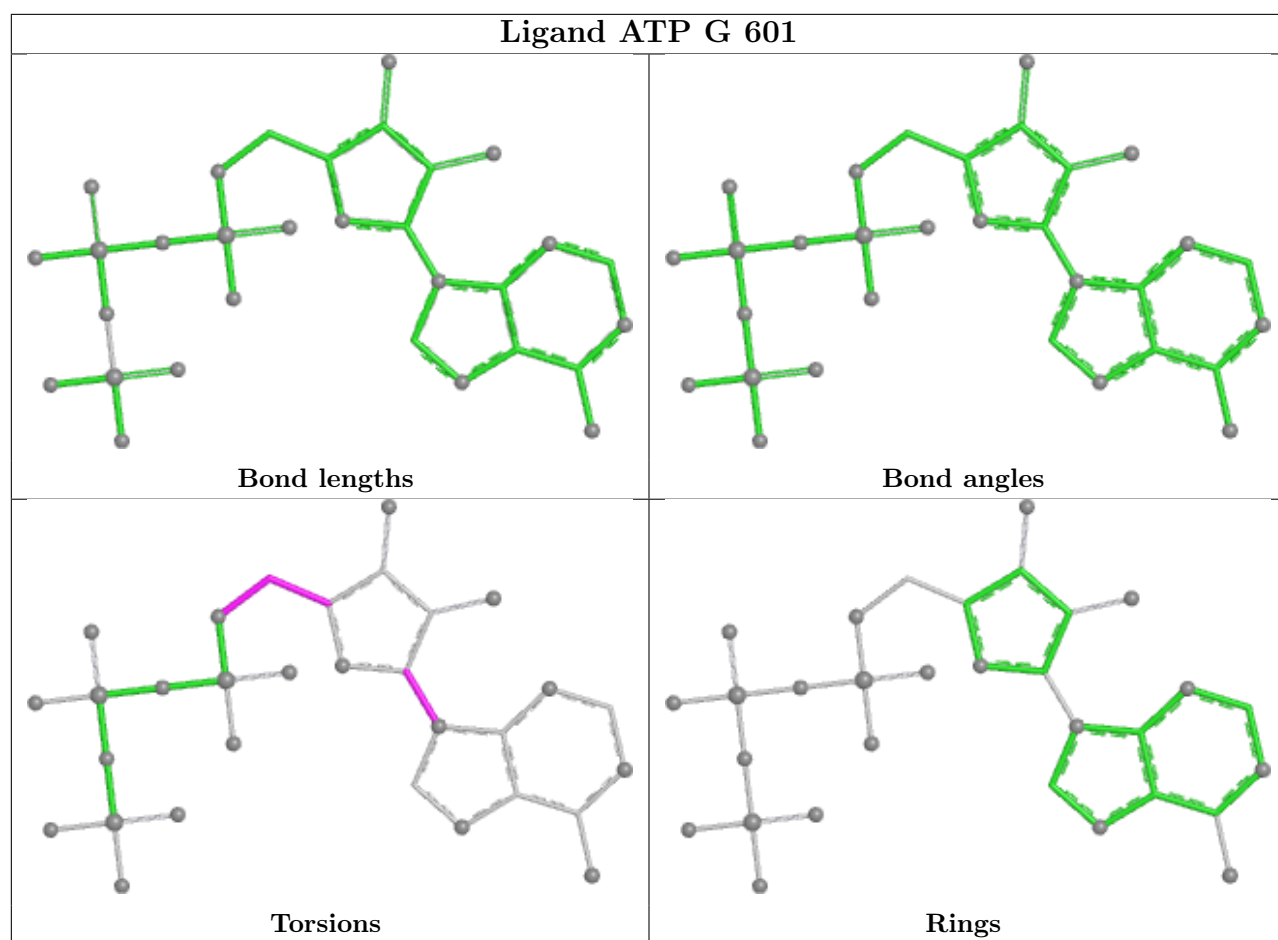
There are no ring outliers.

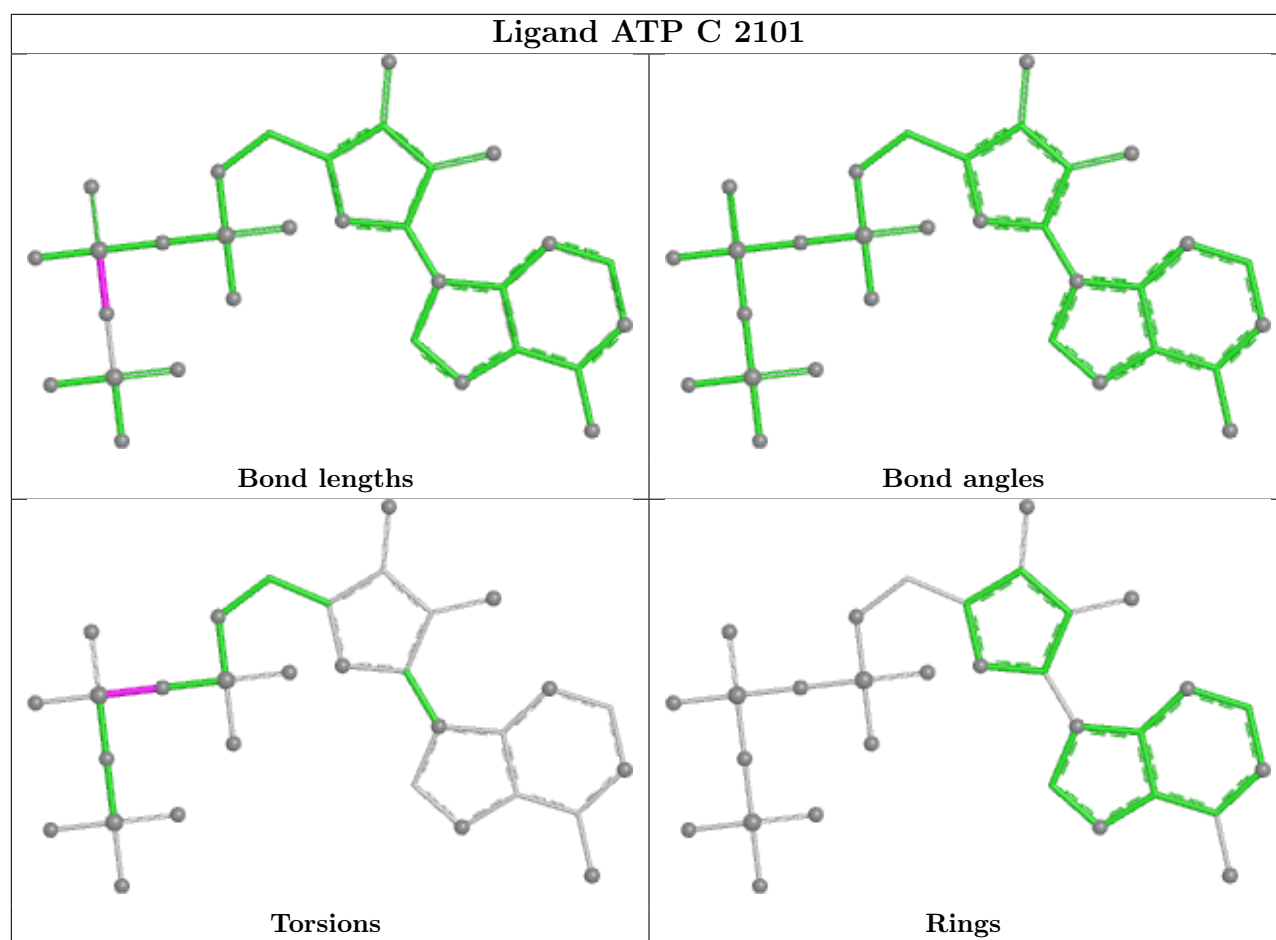
No monomer is involved in short contacts.

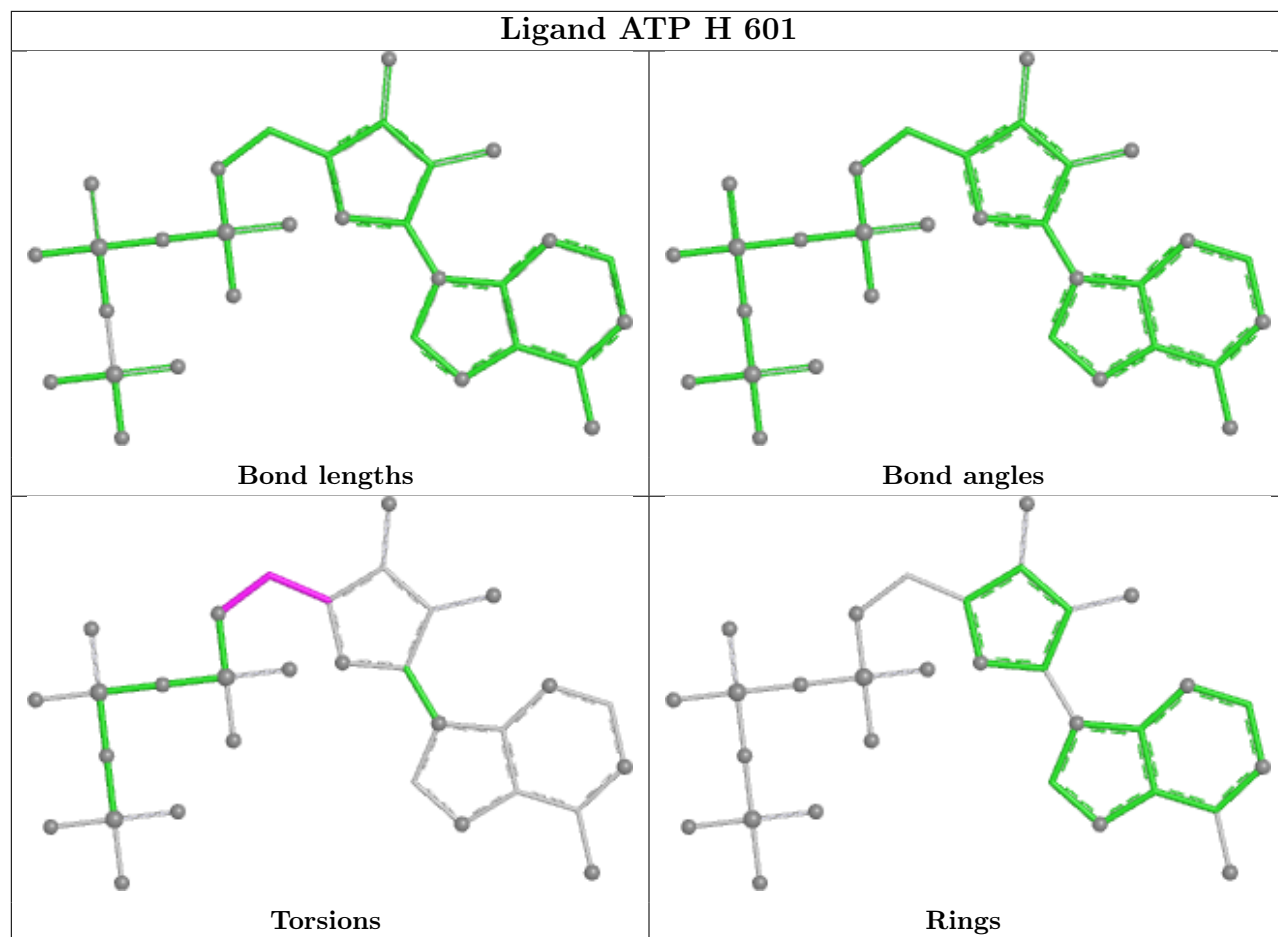
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

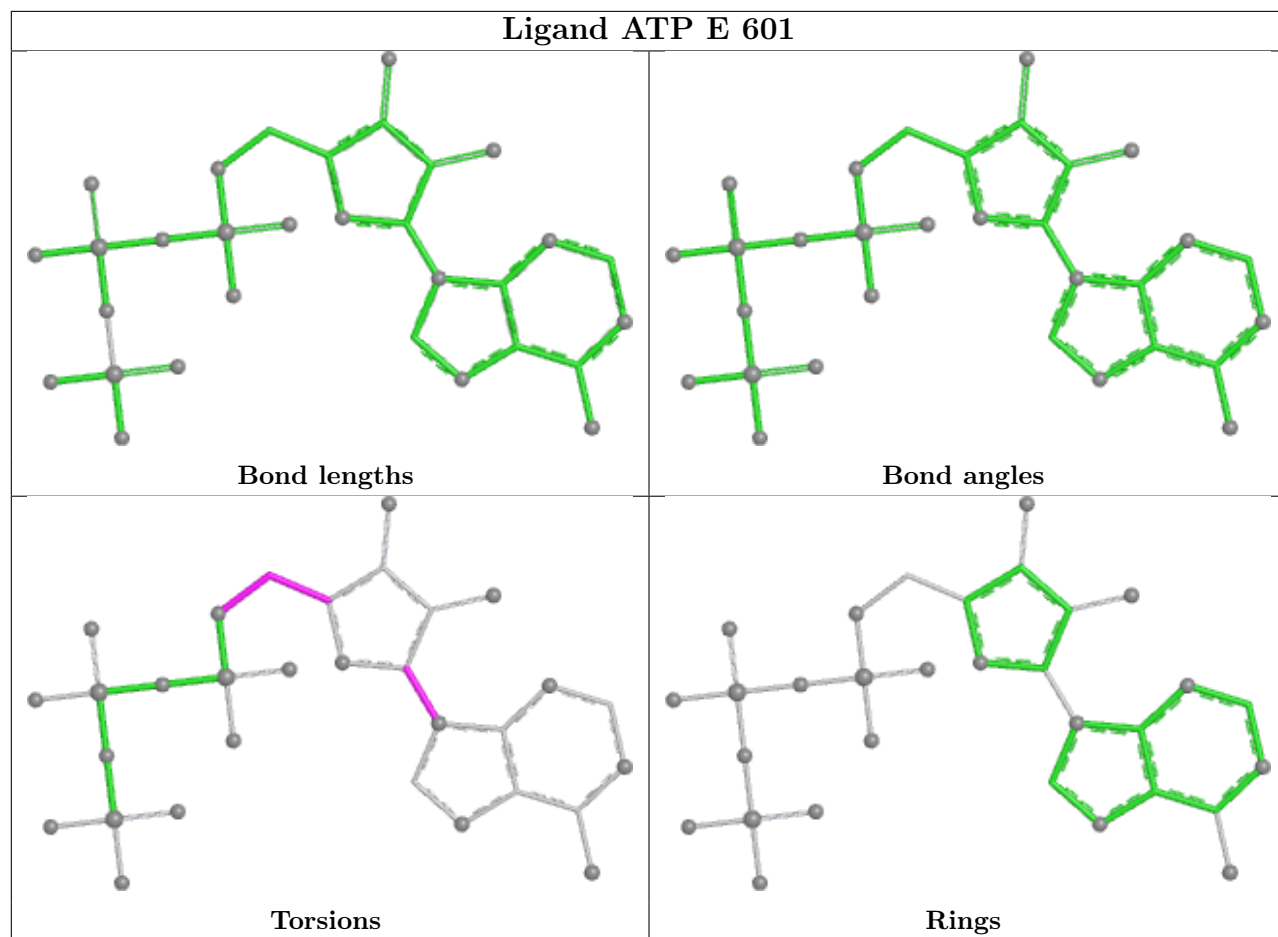
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

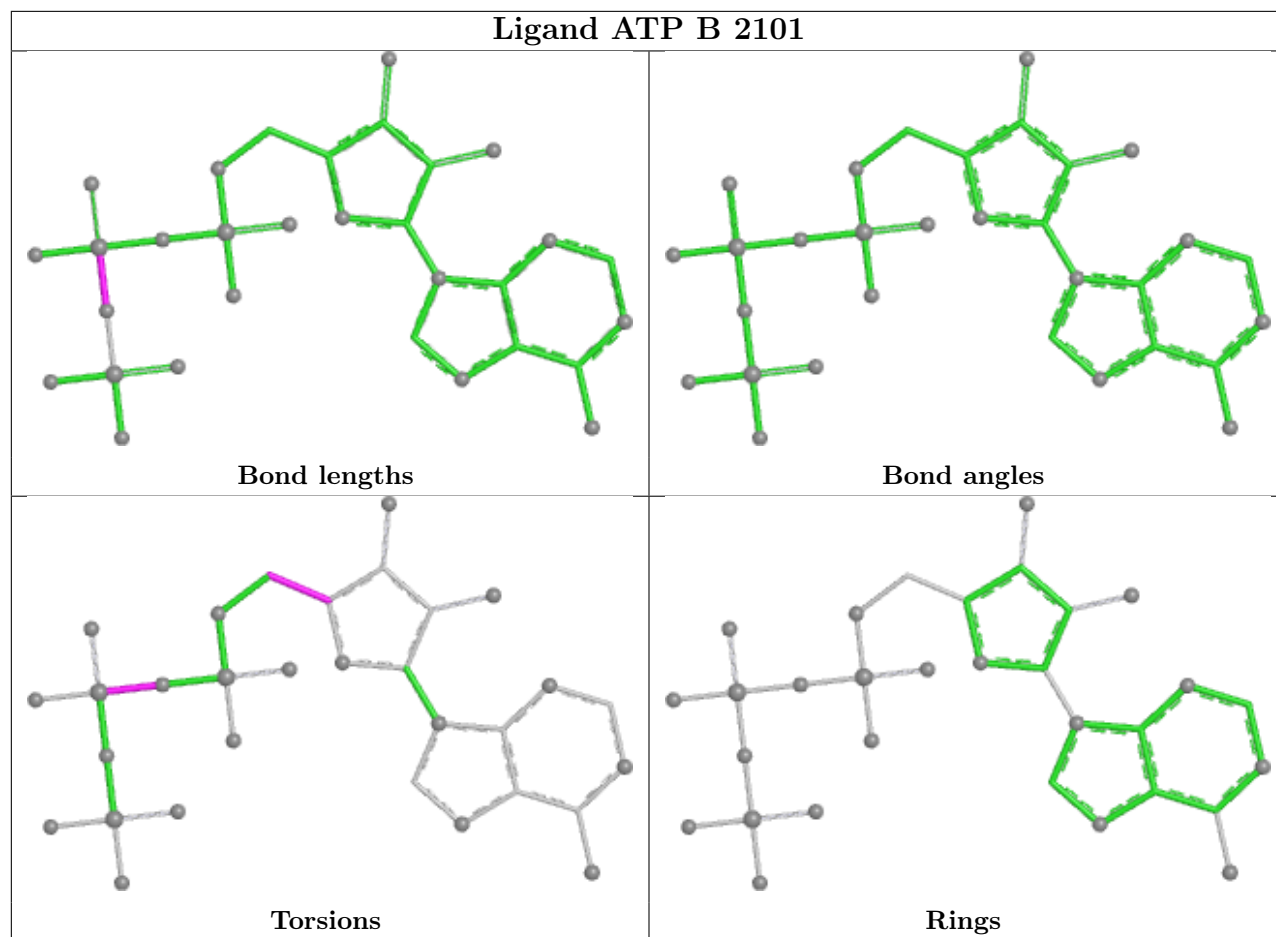


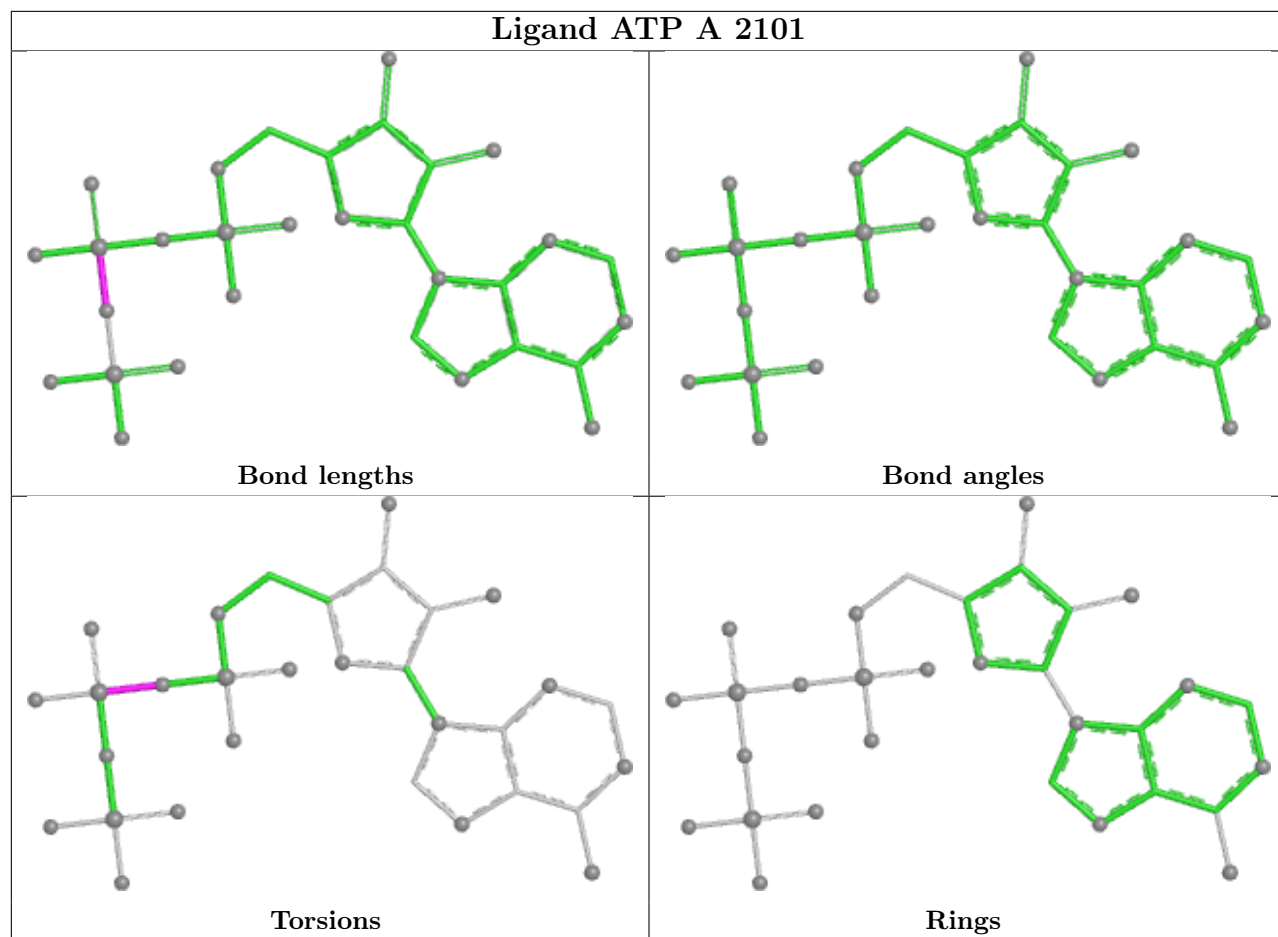


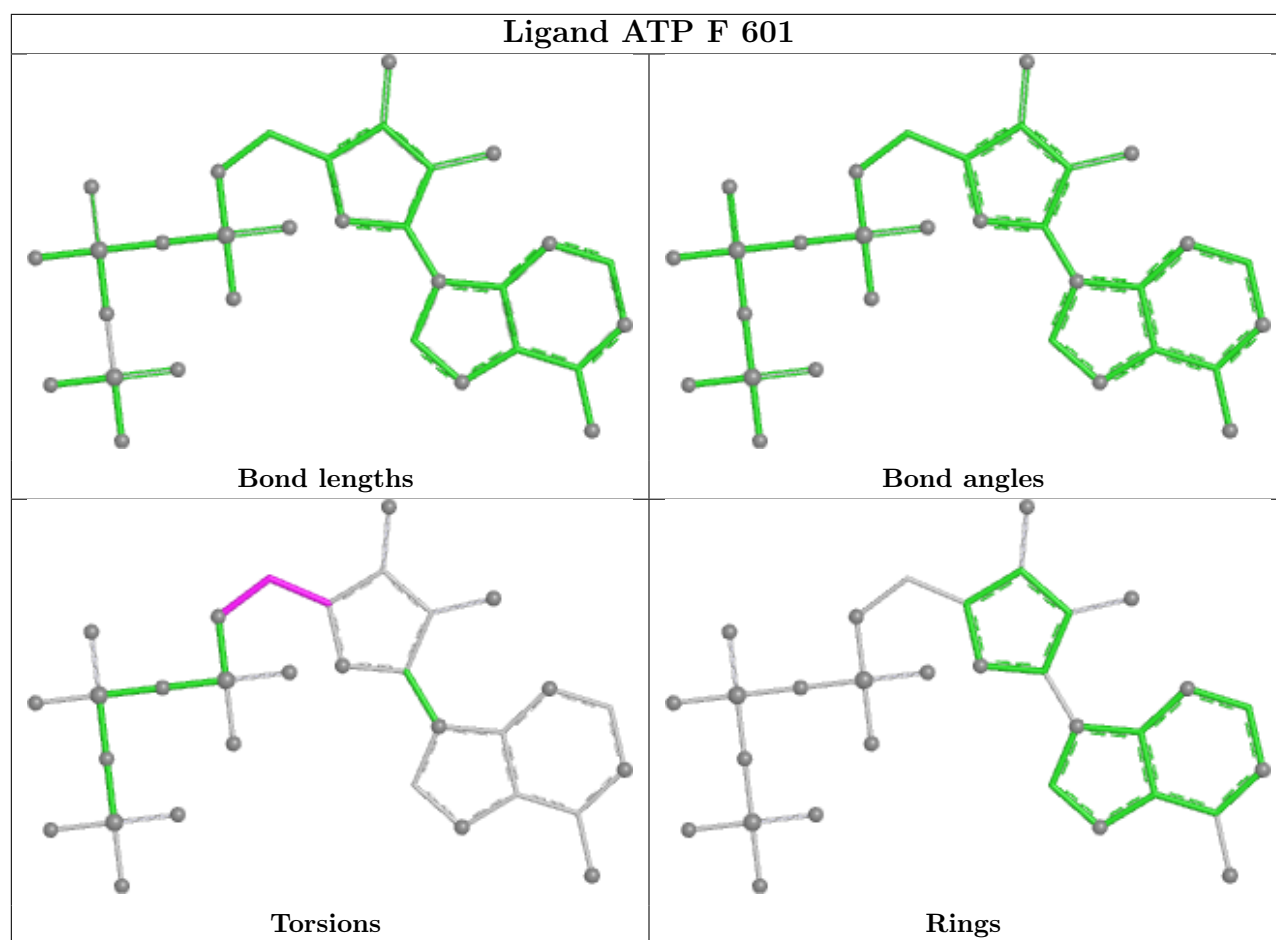












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

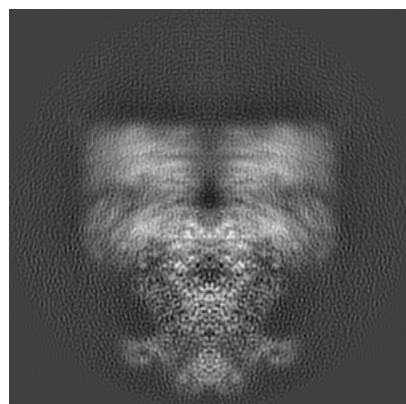
6 Map visualisation [i](#)

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.

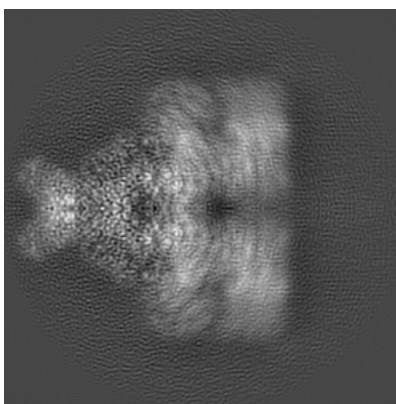
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

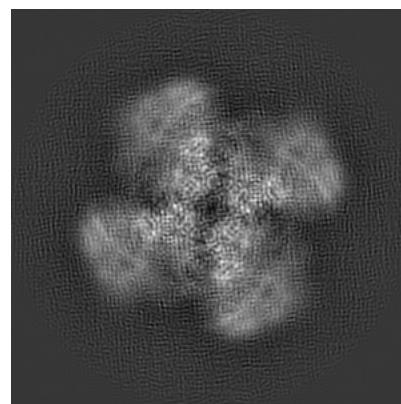
6.1.1 Primary map



X

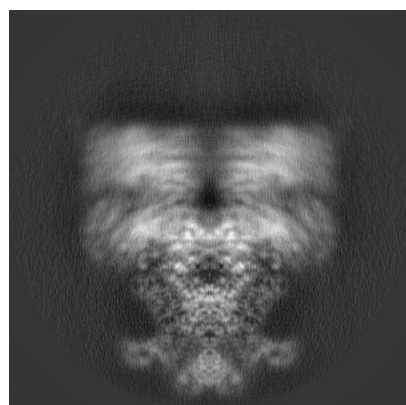


Y

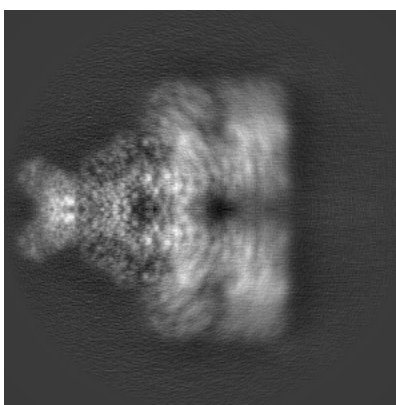


Z

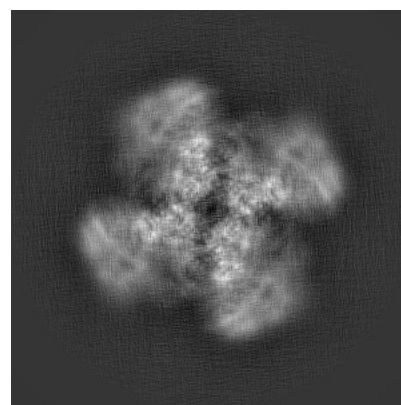
6.1.2 Raw map



X



Y

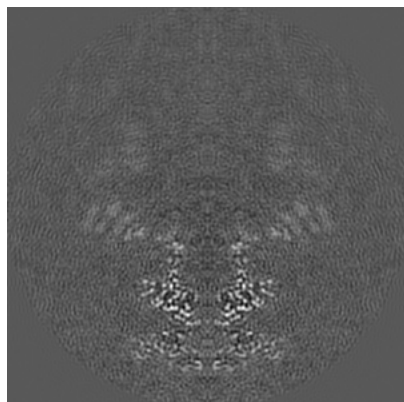


Z

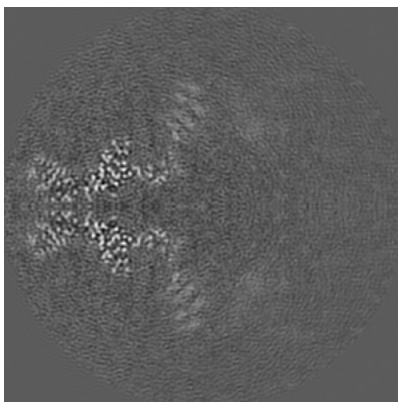
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

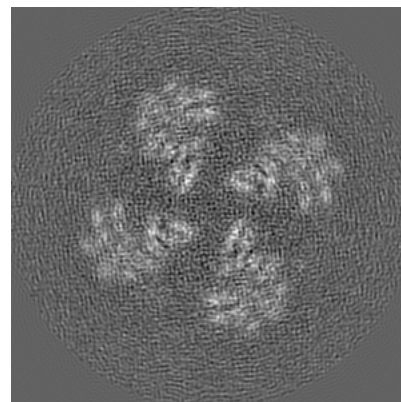
6.2.1 Primary map



X Index: 180

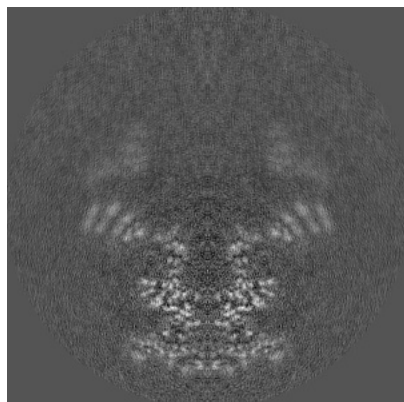


Y Index: 180

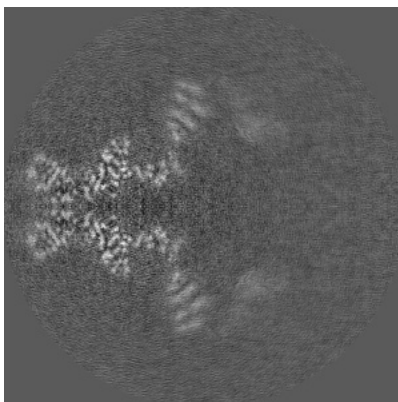


Z Index: 180

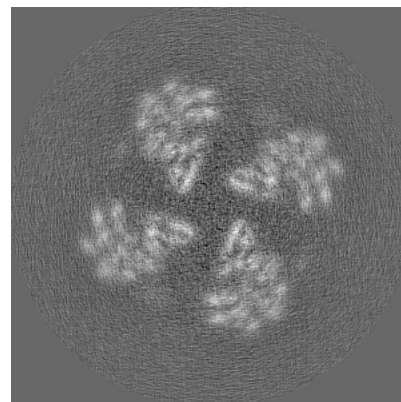
6.2.2 Raw map



X Index: 180



Y Index: 180

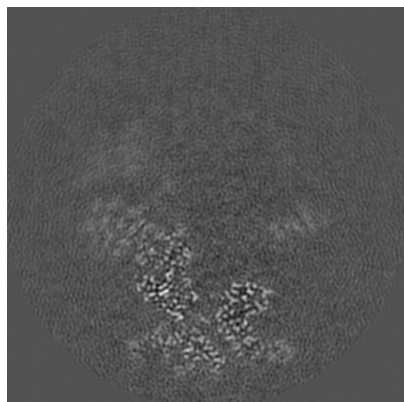


Z Index: 180

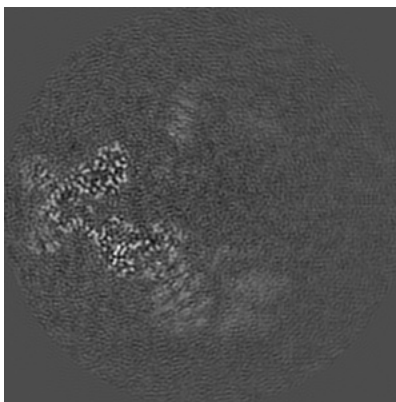
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

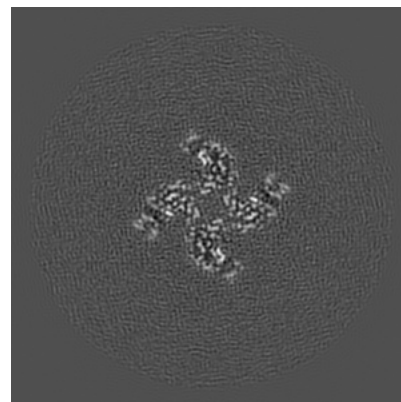
6.3.1 Primary map



X Index: 187

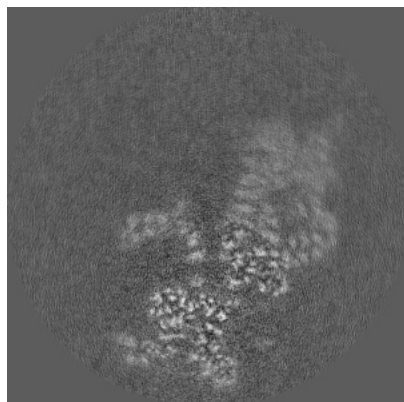


Y Index: 173

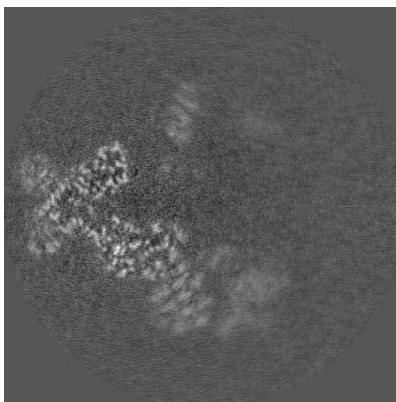


Z Index: 102

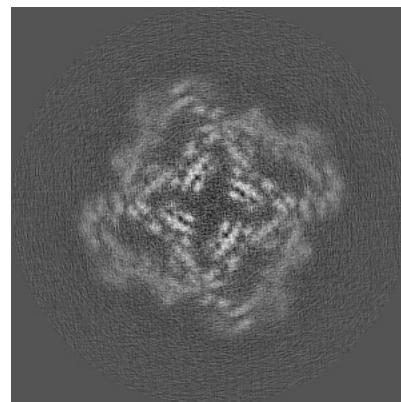
6.3.2 Raw map



X Index: 163



Y Index: 173

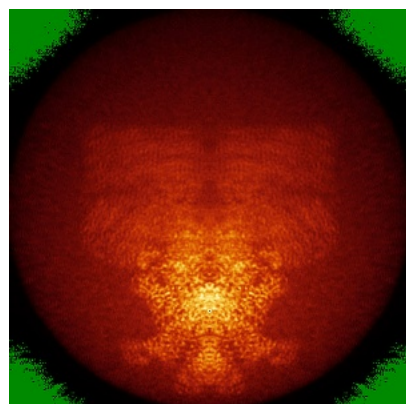


Z Index: 155

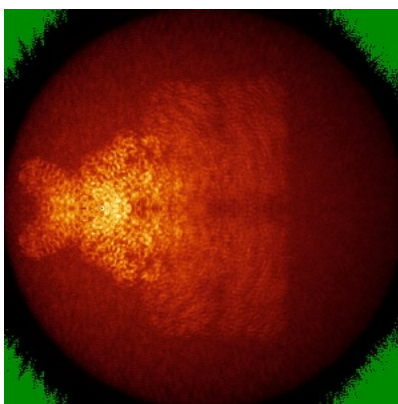
The images above show the largest variance slices of the map in three orthogonal directions.

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

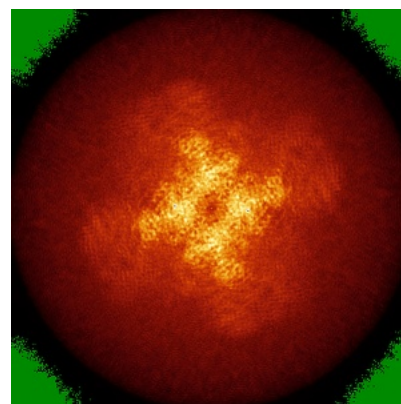
6.4.1 Primary map



X

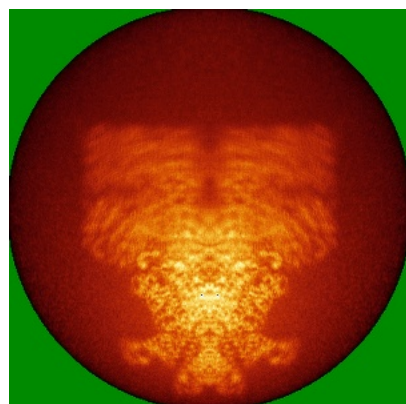


Y

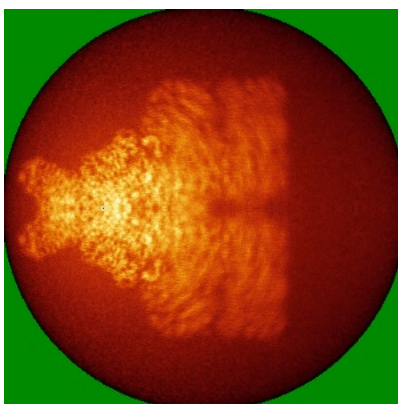


Z

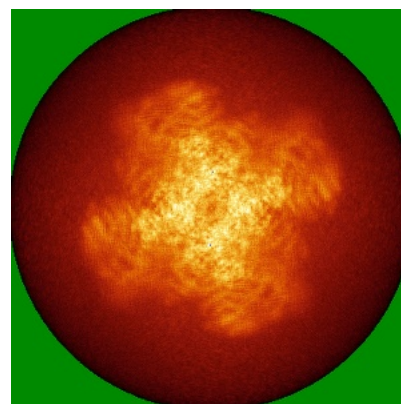
6.4.2 Raw map



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



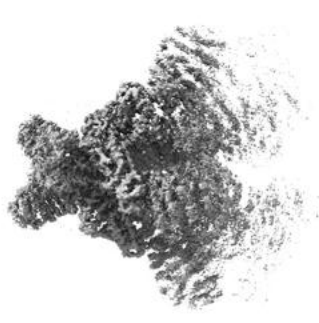
Z

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.

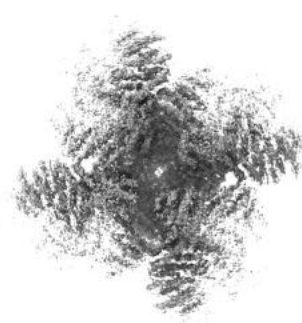
6.5.2 Raw map



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.

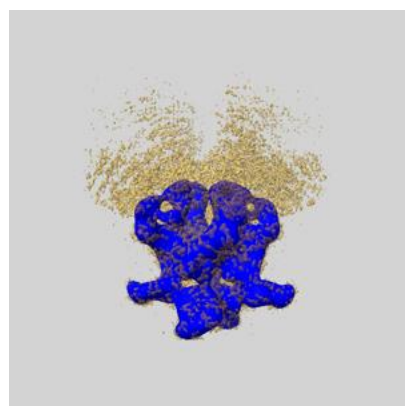
6.6 Mask visualisation [i](#)

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

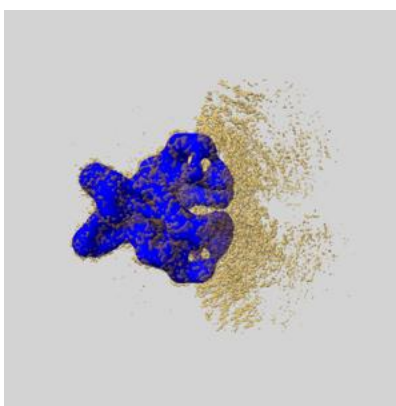
A mask typically either:

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

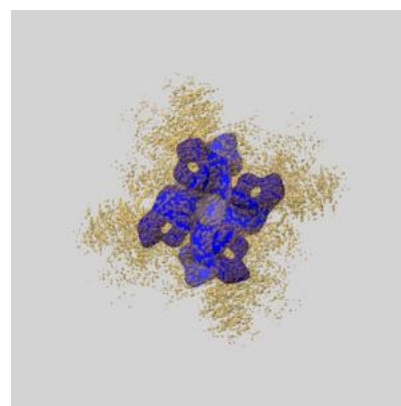
6.6.1 emd_27421_msk_1.map [i](#)



X



Y

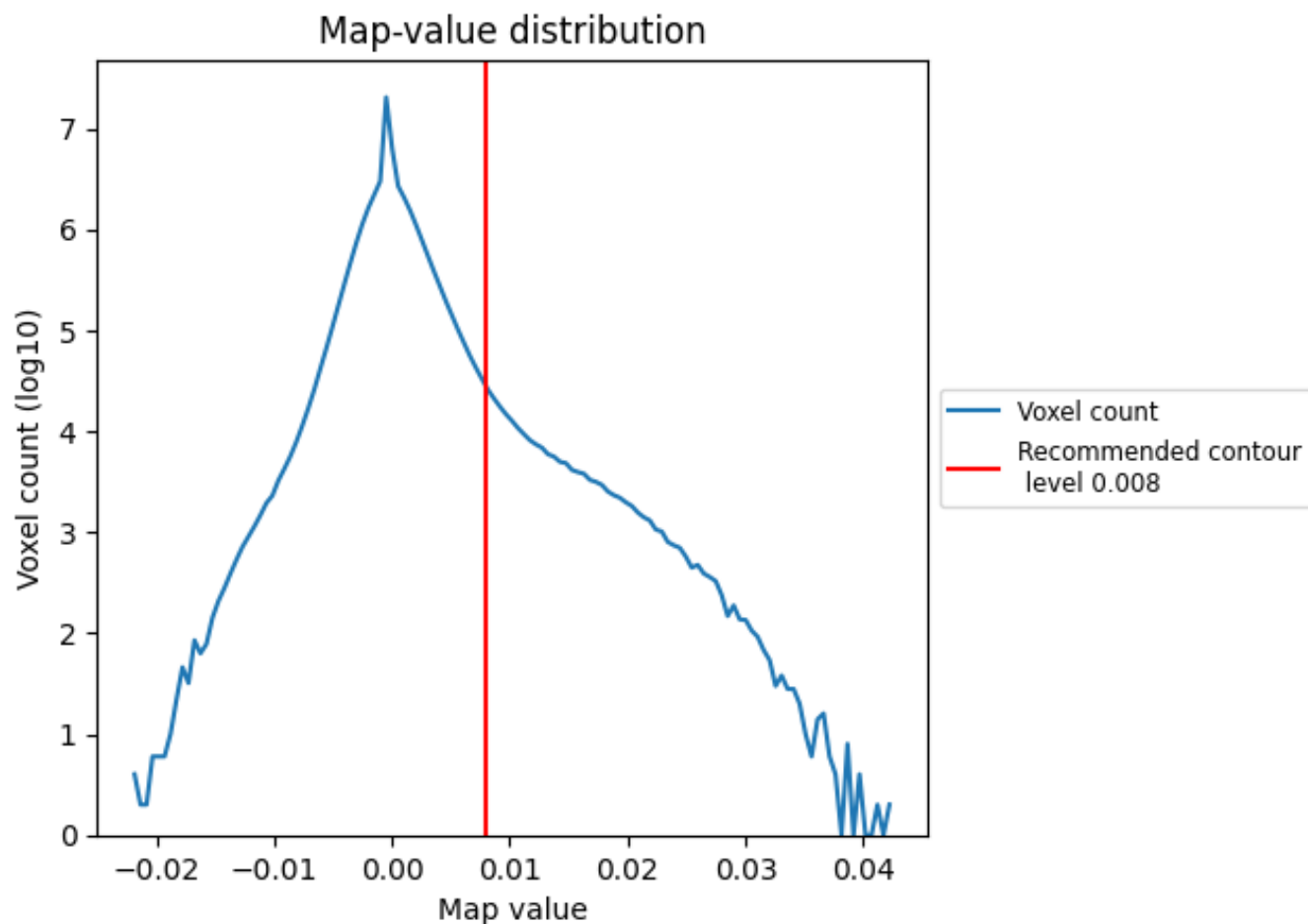


Z

7 Map analysis [i](#)

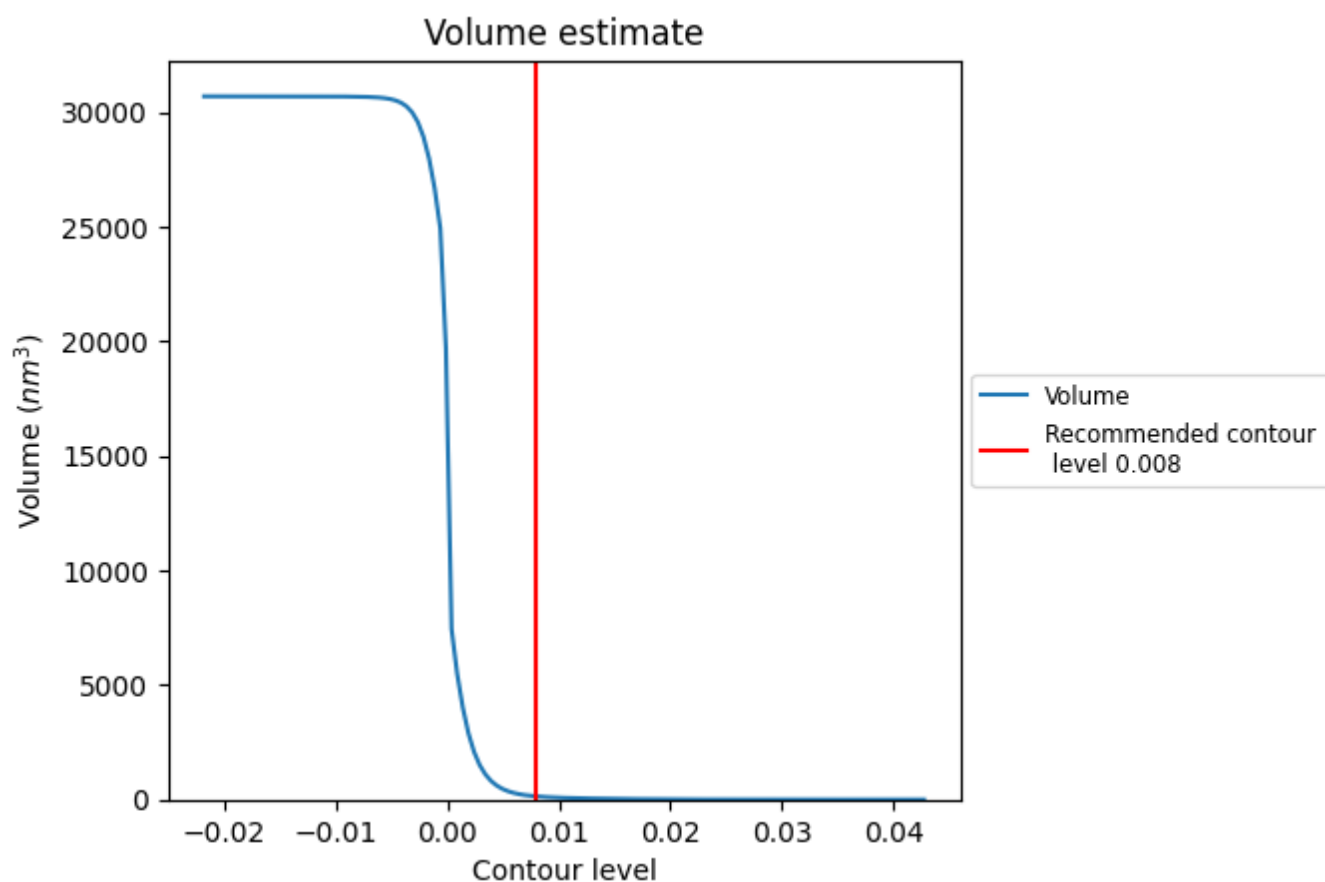
This section contains the results of statistical analysis of the map.

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.

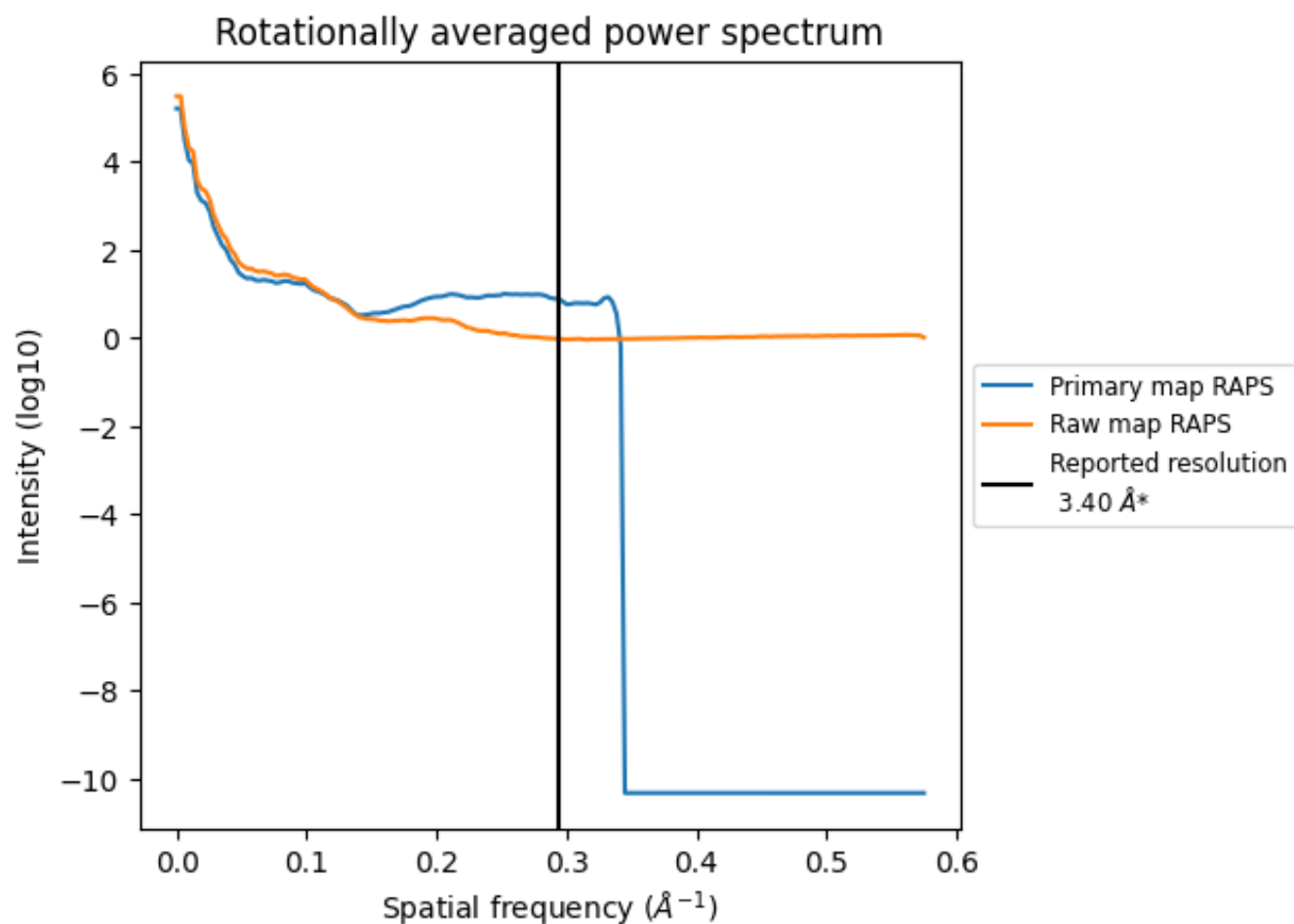
7.2 Volume estimate [i](#)



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 ⓘ

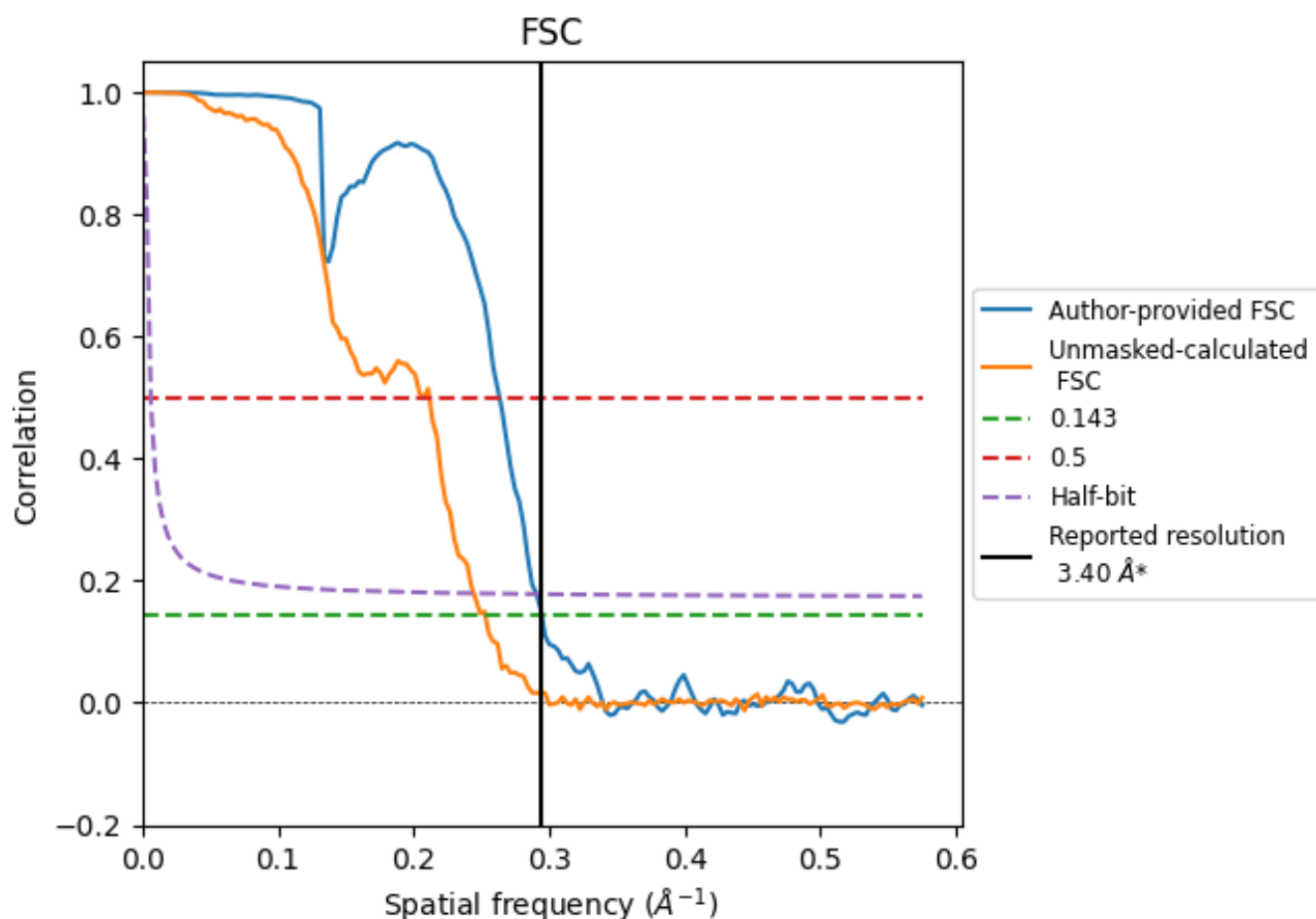


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

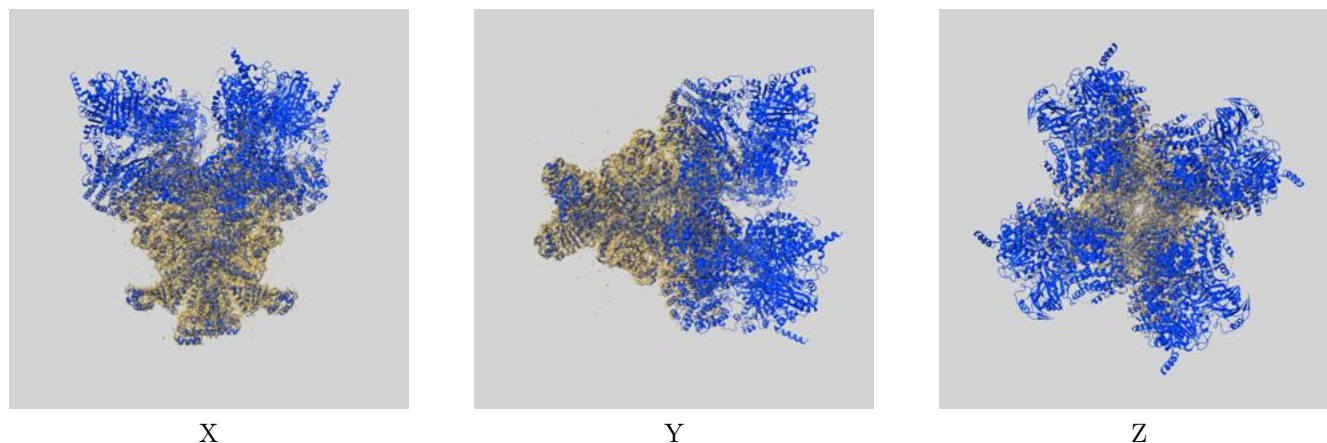
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.80	3.44
Unmasked-calculated*	3.95	4.83	4.09

*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](#)

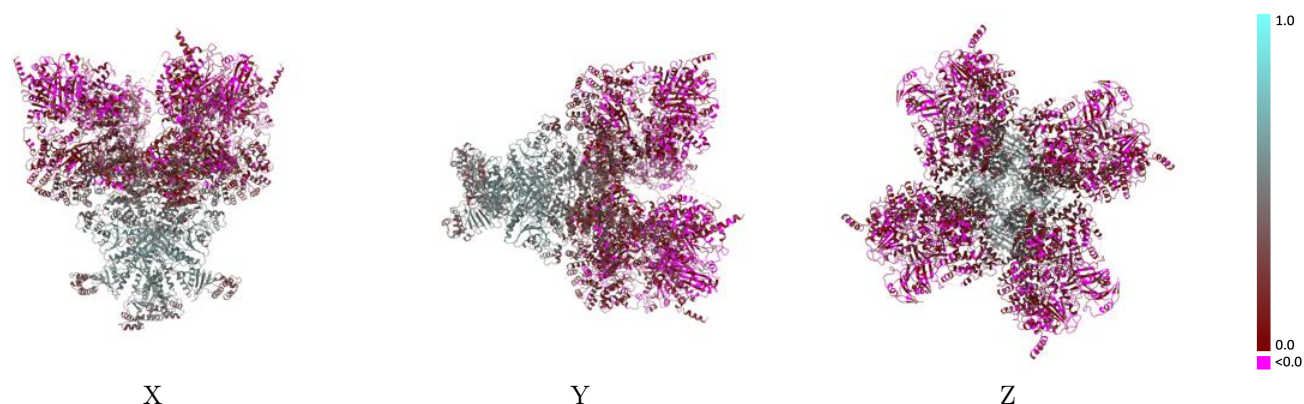
This section contains information regarding the fit between EMDB map EMD-27421 and PDB model 8DGC. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



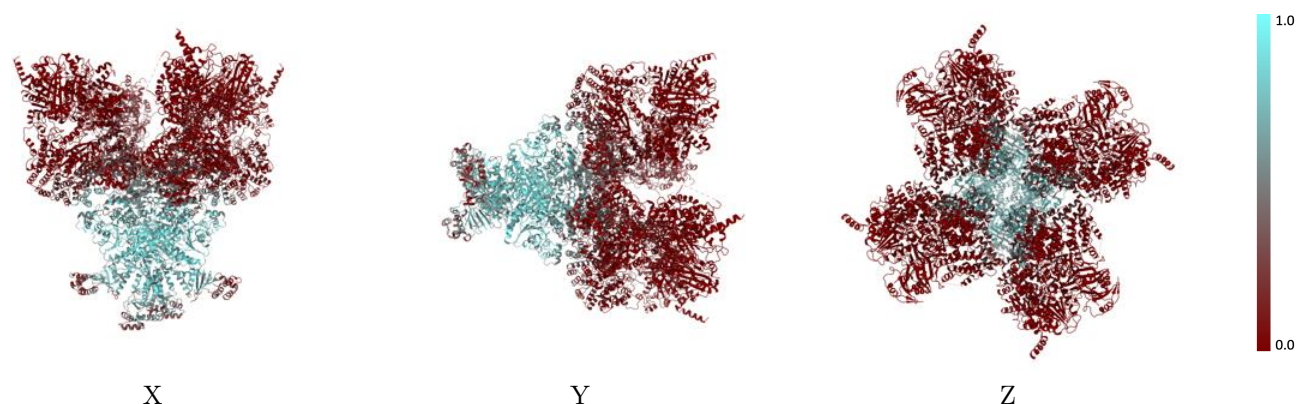
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



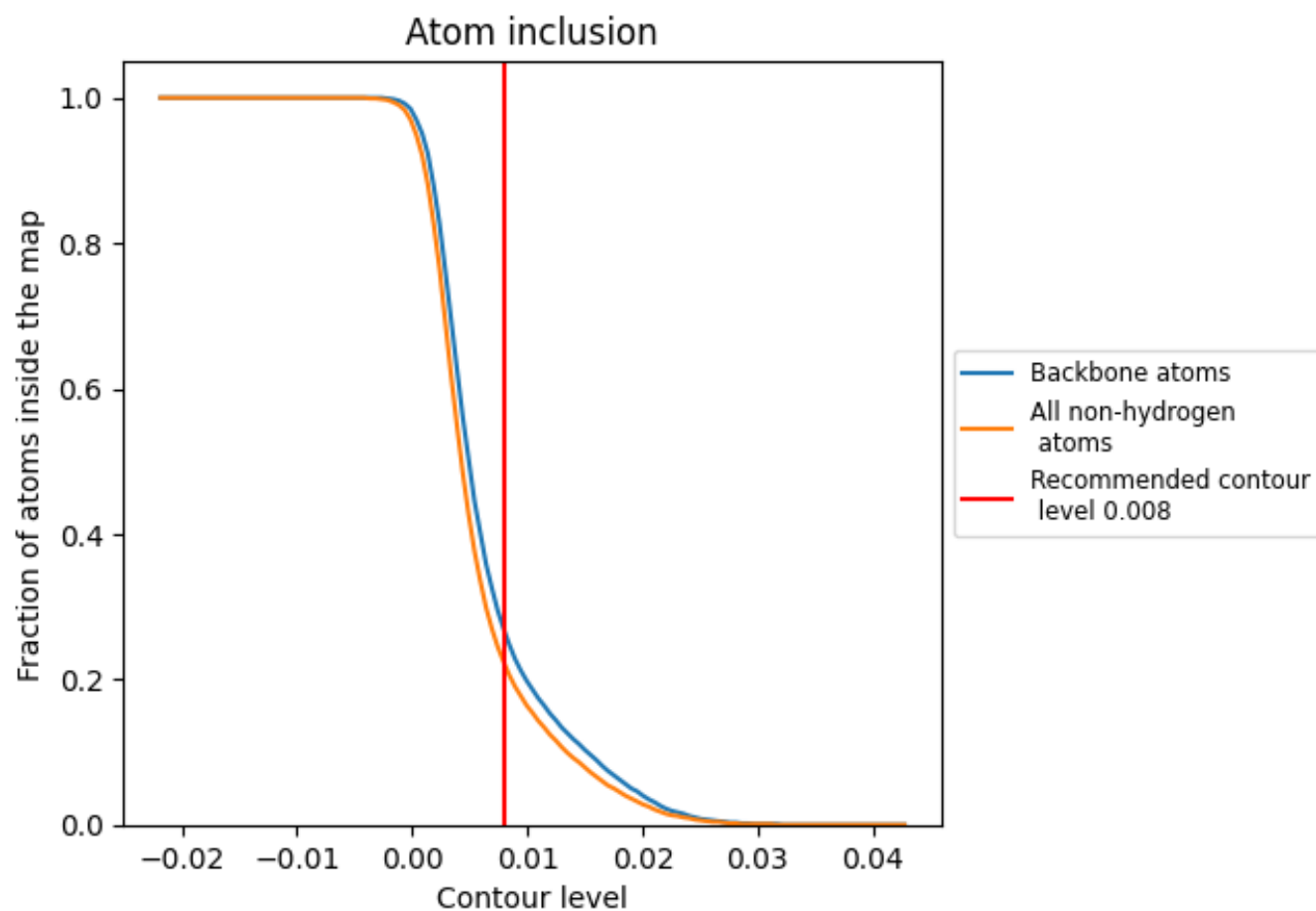
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

1.0

0.0

<0.0