



## wwPDB EM Validation Summary 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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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

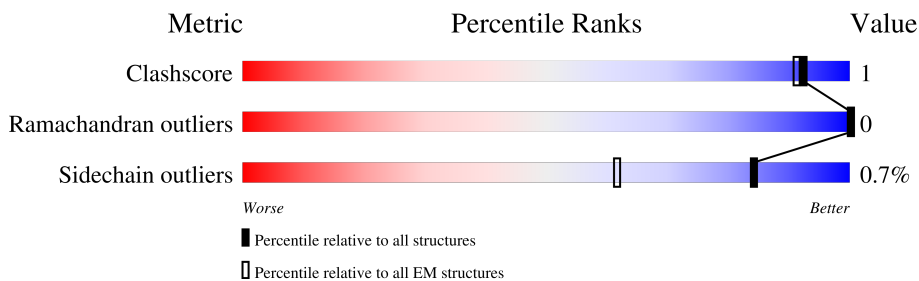
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal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

# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2092	<div style="display: flex; justify-content: space-between;"> <span>66%</span> <span>93%</span> <span>5%</span> <span>8%</span> </div>
1	B	2092	<div style="display: flex; justify-content: space-between;"> <span>65%</span> <span>91%</span> <span>5%</span> <span>8%</span> </div>
1	C	2092	<div style="display: flex; justify-content: space-between;"> <span>66%</span> <span>93%</span> <span>5%</span> <span>8%</span> </div>
1	D	2092	<div style="display: flex; justify-content: space-between;"> <span>65%</span> <span>91%</span> <span>5%</span> <span>8%</span> </div>
2	E	586	<div style="display: flex; justify-content: space-between;"> <span>92%</span> <span>87%</span> <span>5%</span> <span>8%</span> </div>
2	F	586	<div style="display: flex; justify-content: space-between;"> <span>92%</span> <span>87%</span> <span>5%</span> <span>8%</span> </div>
2	G	586	<div style="display: flex; justify-content: space-between;"> <span>92%</span> <span>87%</span> <span>5%</span> <span>8%</span> </div>
2	H	586	<div style="display: flex; justify-content: space-between;"> <span>92%</span> <span>86%</span> <span>5%</span> <span>8%</span> </div>

## 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
			Total	C	N	O	P	
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
			Total	Mg	
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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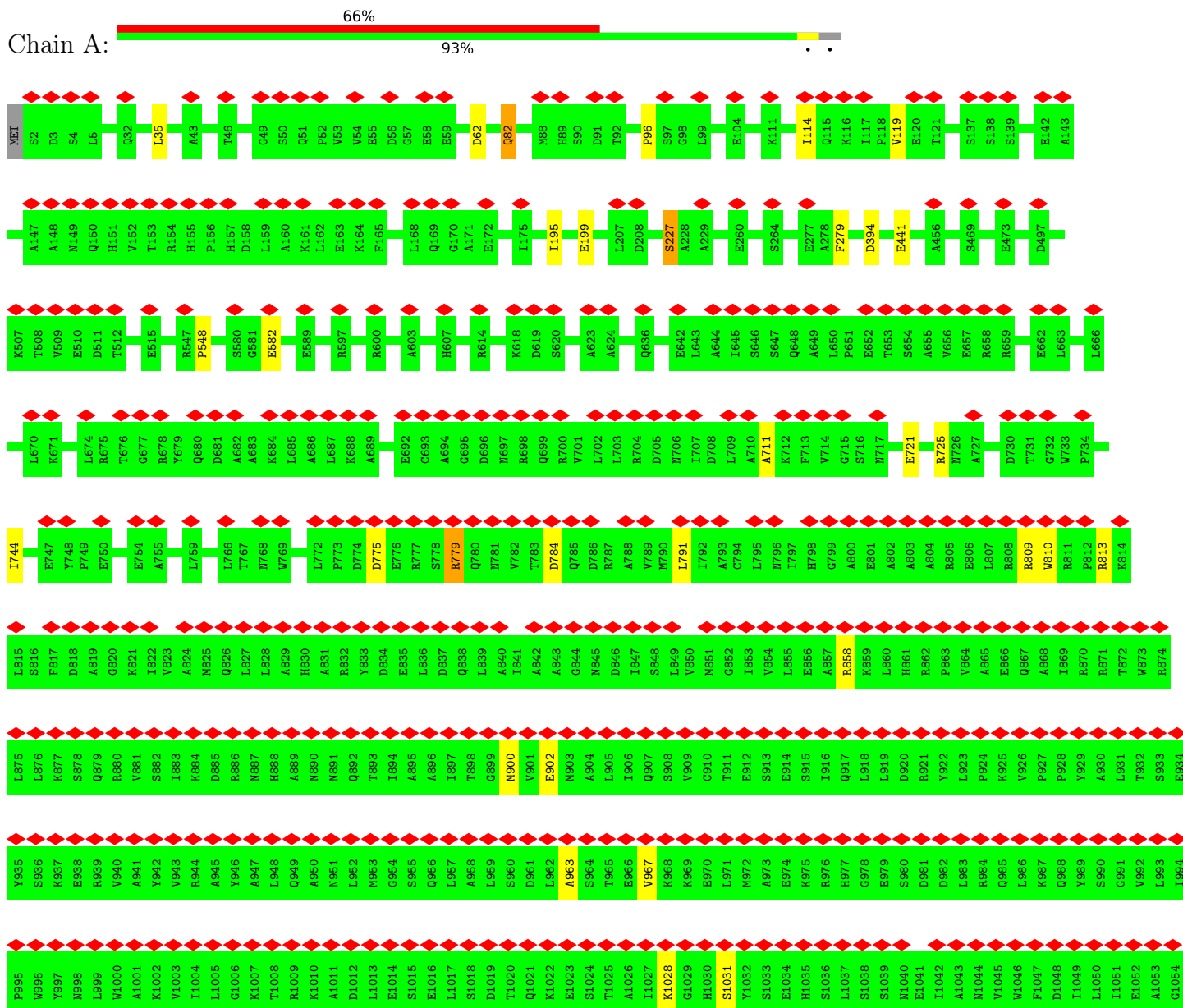
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
4	D	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0
4	G	1	Total 1	Mg 1	0
4	H	1	Total 1	Mg 1	0

### 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	L1083	S1084	S1085	V1086	C1087	A1088	L1089	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	I1122	I1123	D1124	L1125	S1126	R1127	S1128	L1129	I1130	S1131	L1132	D1133	E1134	P1135	E1136	A1137	K1138	E1139	F1140	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	S1217	R1218	A1219	I1220	I1221	S1222	R1223	W1224	D1225	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	D1282	R1283	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	E1323	R1324	I1325	S1326	G1327	L1328	Q1329	H1330	THR	GLU	THR	VAL	SER	LYS	SER	SER	LEU	SER	SER	ASN	ASP	GLU	GLN	G1348	H1349	D1350	Q1351	W1352	W1353	E1354	S1355			
I1356	F1357	K1358	D1359	C1360	D1361	L1362	S1363	S1364	L1365	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	G1413	G1414	L1415	
Y1416	D1417	F1418	K1419	I1420	I1421	L1422	E1423	I1425	P1426	D1427	E1428	Y1429	T1430	S1431	R1432	L1433	S1434	I1435	K1436	L1439	A1440	G1441	L1442	I1443	K1444	E1445	Y1446	C1447	Q1448	R1449	F1450	C1451	M1452	R1453	L1454	R1455	K1456	S1457	R1458	V1459	Y1460	E1461	I1462	F1463	F1464	F1465	S1466	L1467	A1468	S1469	R1470	L1471	S1472	E1533	D1534	D1535	D1536	E1476		
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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	F1590	I1591	E1592	Q1593	H1594	A1595	I1596	
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F1657	A1658	A1659	R1660	T1661	L1662	A1664	L1665	H1666	D1667	S1668	P1669	L1670	I1671	S1672	I1673	P1674	A1675	Q1676	E1677	E1678	N1679	K1680	L1681	F1682	N1683	I1684	N1685	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		
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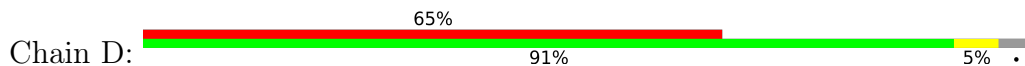
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T1647	L1587	D1527	A1467	A1406	GLN	A1286	R1226	A1166	L1103	A1043	L983	L923	
L1648	V1588	E1528	A1468	I1407	G1348	F1287	R1227	E1167	A1104	N1044	R984	P924	
Q1649	Q1589	E1529	S1469	G1408	H1349	E1288	T1228	Y1168	L1105	V1045	Q985	K925	
P1650	G1590	L1530	R1470	A1409	D1350	V1289	F1229	V1169	L1106	V1046	L986	V926	
H1651	K1591	K1531	L1471	F1410	E1352	Y1291	G1230	A1170	L1107	F1047	Q987	P927	
F1652	F1592	D1532	S1472	F1411	H1292	Y1292	H1231	W1108	Q988	D1048	Q988	P928	
L1653	Q1593	E1533	G1473	H1412	H1293	H1293	H1232	R1109	Y989	I1049	Y929	Y929	
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R1655	A1595	E1535	S1475	G1414	L1295	L1294	R1234	H1111	G991	I1051	L931	L931	
H1656	I1596	D1536	E1476	L1415	L1356	L1295	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	
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D1667	M1607	T1547	I1487	P1426	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	R1127	L1005	I1065	A945	A945	
L1670	F1610	E1550	P1491	W1429	A1370	A1309	I1249	S1128	G1006	K1066	Y946	Y946	
I1671	Y1611	D1551	E1492	T1430	I1310	I1310	M1250	L1129	K1007	S1067	A947	A947	
S1672	L1612	S1552	P1493	S1431	S1311	S1311	A1251	I1130	T1008	S1068	L948	L948	
L1673	L1613	L1553	A1494	R1432	L1312	L1312	L1252	S1131	R1009	Q1069	Q949	Q949	
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A1675	A1615	G1555	S1496	S1434	L1314	A1254	A1254	D1133	A1011	I1071	N951	N951	
Q1676	A1616	Y1556	D1497	I1435	G1315	G1315	L1255	E1134	D1012	G1072	L952	L952	
E1677	L1617	I1557	R1498	K1436	I1316	I1316	P1256	P1135	L1013	N1073	M953	M953	
M1678	W1618	W1558	T1437	T1437	E1317	E1317	L1257	E1136	E1014	R1074	G954	G954	
N1679	L1619	L1559	L1438	L1438	H1318	H1318	L1258	A1137	S1015	V1075	S955	S955	
K1680	F1620	A1560	L1439	L1439	T1319	T1319	T1259	K1138	E1016	F1076	Q956	Q956	
L1681	I1621	L1561	A1440	A1440	E1320	E1320	F1260	Y1140	L1017	T1077	L957	L957	
R1682	A1622	G1562	P1503	I1443	L1321	L1321	E1261	F1200	S1018	P1078	A958	A958	
N1683	A1623	S1563	G1504	K1444	K1322	K1322	M1262	A1201	D1019	S1079	L959	L959	
I1684	A1624	L1505	L1505	E1445	E1323	E1323	D1263	W1202	T1020	L1080	S960	S960	
N1685	R1625	E1565	L1506	E1446	R1324	R1324	W1264	Q1143	Q1021	H1081	D961	D961	
Q1686	V1626	A1566	V1507	Y1446	T1386	T1386	H1265	A1144	R1082	K1082	L962	L962	
S1687	A1627	A1567	C1447	C1447	S1325	S1325	K1266	I1145	F1083	F1083	E1023	E1023	
T1688	L1628	E1567	Q1448	Q1448	S1326	S1326	C1267	E1146	S1084	S1084	A963	A963	
T1689	M1568	M1568	K1509	R1449	I1388	G1327	K1267	E1207	S1085	S1085	S964	S964	
L1690	D1630	W1570	E1511	F1450	K1389	L1328	D1268	I1208	T1025	V1086	T965	T965	
P1691	G1631	Q1571	S1512	C1451	K1390	Q1329	L1269	L1151	A1026	E966	E966	E966	
V1692	K1632	M1513	M1513	M1452	A1391	A1391	D1270	G1152	I1027	C1087	V967	V967	
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ASP	L1634	H1574	L1454	T1454	GLU	GLU	S1272	E1154	G1029	I1090	K969	K969	
VAL	I1635	R1455	R1455	R1455	THR	THR	V1273	M1155	H1030	E970	E970	E970	
GLU	M1636	K1456	K1456	K1456	VAL	VAL	L1274	L1156	Y1032	S1091	L971	L971	
GLY	M1637	D1517	S1457	S1457	SER	SER	S1275	S1215	S1033	S1092	M972	M972	
ASP	H1638	V1518	R1458	R1458	LYS	LYS	S1276	A1217	S1033	L1093	A973	A973	
ARG	L1639	A1578	V1459	V1459	LYS	LYS	C1277	W1159	E1034	G1094	E974	E974	
GLY	Y1640	L1579	F1460	F1460	SER	SER	T1278	A1161	H1035	E1095	K975	K975	
E1702	F1641	C1580	E1461	E1461	SER	SER	D1279	A1161	S1036	L1096	R976	R976	
Y1642	Y1642	M1582	I1462	I1462	C1401	C1401	D1280	Y1098	L1037	Y1098	H977	H977	
												G978	G978





Q1589	G1590	I1591	F1592	Q1593	H1594	A1595	I1596	M1597	A1598	T1599	T1600	L1601	P1602	F1603	C1604	D1605	R1606	M1607	L1608	P1609	F1610	I1611	T1612	L1613	H1614	A1615	Q1616	L1617	M1618	L1619	M1620	I1621	A1622	A1623	A1624	R1625	V1626	A1627	L1628	D1629	D1630	G1631	K1632	S1633	L1634	I1635	P1636	M1637	I1638	G1639	Y1640	F1641	H1642	H1643	Y1644	A1645	T1646	T1647	D1648							
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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

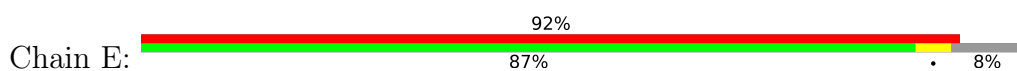


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K111	A112	L113	I114	Q115	K116	I117	P118	V119	E120	T121	L122	R123	T124	R134	P135	V136	S137	S138	S139	F140	S141	E142	A143	I144	M145	D146	A147	A148	M149	Q150	H151	V152	T153	L154	H155	P156	H157	D158	L159	A160	K161	L162	E163	K164	F165	V166	G167	L168	D169	G170	A171	E172	L173	S174	I175	F176	C177
Q178	E183	Q186	D187	D188	A201	E210	T225	E226	S227	A228	A229	M230	D245	E246	E260	Q273	V276	F279	D288	I300	E301	A324	Y327	I374	E381	L386	I389	V422	S469	D497	K507	T508	V509	E510	D511	T512	I513																				



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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	E1678	M1679	K1680	L1681	L1682	M1683	I1684	M1685	M1686	V1687	T1688	T1689	W1690	G1691	L1692	LEU	ASP	LYS	VAL	GLU	ASP	HIS	ARG
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	I1738	R1739	D1740	V1741	L1742	G1743	F1744	K1745	M1746	S1747	R1748	M1749	W1750	D1751	E1752	D1753	E1754	R1755	M1756	K1757	R1758	R1759	Y1760	
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D1821	I1822	S1823	R1824	D1825	H1827	R1828	L1830	A1831	D1832	R1833	R1834	D1835	I1836	P1837	P1838	K1839	E1840	R1841	S1842	S1843	W1844	L1845	M1846	S1847	S1848	R1849	D1850	M1851	R1852	D1853	E1854	W1855	L1856	A1857	S1858	I1859	S1860	E1861	L1862	V1863	F1864	M1865	E1866	T1867	L1868	C1869	D1870	V1871	P1872	G1873	D1874	W1875	T1876	L1877	R1878	G1879	R1880		
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I1942	K1943	D1944	I1945	A1946	Y1948	C1949	G1950	I1951	D1952	E1953	D1954	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	R2017	L2018	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	LEU
ASP	ASN	ILE	PRO	S2065	S2066	T2067	R2068	L2069	F2070	L2071	F2072	R2073	H2074	D2075	G2076	T2077	H2078	T2080	L2081	Y2082	G2083	M2084	Y2085	R2086	M2087	GLY	GLU	LYS	THR	SER																													

• Molecule 2: Terminase, large subunit

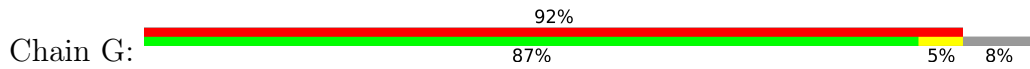


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R241	P301	I361	E421	D481	GLU
L242	L302	L362	S422	Y482	GLU
A243	R303	V363	M423	Q483	MET
P244	L304	I364	F424	T484	THR
M245	R305	D365	G425	A485	LEU
L246	D306	P366	D426	R486	PHE
K247	A307	S367	G427	D487	LEU
A248	I308	G368	M428	L488	GLU
E249	V309	R369	F429	D489	HIS
Y250	C310	G370	G430	G490	MET
D251	A311	K371	G431	K491	GLU
E252	V312	D372	I432	H492	LYS
G253	D313	E373	F433	D493	GLN
F254	P314	T374	S434	V494	THR
E255	E315	G375	P435	R495	ILE
L256	R316	Y376	I436	Y496	GLY
L257	A317	A377	L437	S497	ASP
R258	P318	V378	L438	A498	GLN
G259	L319	L379	K439	F499	HIS
Q260	S320	Y380	H440	Y500	SER
P261	Y321	S381	H441	Q501	PHE
T262	Q322	L382	K442	M502	ASP
D263	W323	N383	C443	T503	VAL
P264	L324	G384	A444	R504	GLY
V265	P325	Y385	L445	M505	VAL
R266	N326	I386	L446	T506	ASP
F267	R327	Y387	E447	R507	ILE
D268	Q328	L388	I448	E508	TYR
M269	N329	M389	R449	R509	GLU
D270	R330	E390	A450	G510	ASP
D271	N331	V391	K451	A511	GLY
L272	E332	G392	G452	V512	GLY
R273	E333	G393	M453	A513	SER
E274	L334	F394	M454	H514	PHE
R275	P335	R395	E455	D515	ILE
E276	N336	G396	M456	D516	GLU
L277	V337	G397	R457	R517	TRP
E278	G338	Y398	I458	I518	
Y279	L339	D399	C459	D519	
G280	K340	D400	D460	A520	
K281	G341	A401	T461	I521	
A282	D342	T402	I462	A522	
G283	D343	L403	E463	L523	
Y284	I344	E404	P464	G524	
T285	H345	K405	L465	I525	
L286	A346	L406	M466	E526	
Q287	F347	A407	G467	Y527	
F288	H348	K408	A468	L528	
M289	T349	K409	H469	R529	
L290	C350	A410	K470	G530	
N291	S351	K411	L471	G531	
P292	S352	Q412	V472	M532	
N293	R353	W413	I473	L533	
L294	T354	K414	R474	V534	
S295	A355	V415	D475	D535	
D296	E356	Q416	E476	S536	
A297	Y357	T417	V477	R537	
E298	Q358	V418	I478	V538	
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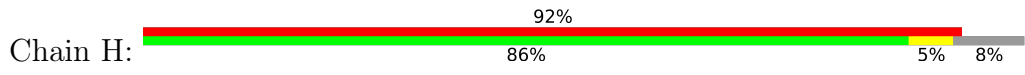


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S2	G62	V182	R122	I63	I63	T183	E184	S2	G62	V182	R122
Q3	I63	T183	D123	G64	G64	E184	F185	Q3	I63	T183	D123
S4	G64	E184	S124	K65	K65	F185	A186	S4	G64	E184	S124
Q5	K65	F185	I125	E6	E6	A186	A187	Q5	K65	F185	I125
E6	E6	A186	I126	A7	A7	A187	L188	E6	E6	A186	I126
A7	F67	L188	F128	N9	N9	L188	L189	A7	F67	L188	F128
K8	I68	L189	D129	A10	A10	L189	K190	K8	I68	L189	D129
HIS	T69	L189	C70	L11	L11	K190	P191	HIS	T69	L189	C70
MET	C70	L189	V130	A71	A71	P191	L192	MET	C70	L189	V130
GLU	A71	L189	G131	F72	F72	L192	P193	GLU	A71	L189	G131
LYS	K431	L189	L132	V73	V73	P193	T194	LYS	K431	L189	L132
GLN	I432	L189	A133	W74	W74	T194	S195	GLN	I432	L189	A133
THR	D372	L189	K134	W75	W75	S195	R196	THR	D372	L189	K134
ILE	E373	L189	P135	V76	V76	R196	L197	ILE	E373	L189	P135
GLY	T374	L189	D136	L77	L77	L197	I198	GLY	T374	L189	D136
ASP	G375	L189	H137	R78	R78	I198	Y199	ASP	G375	L189	H137
GLN	Y376	L189	S138	R79	R79	Y199	L200	GLN	Y376	L189	S138
ILE	A377	L189	P139	D80	D80	L200	G201	ILE	A377	L189	P139
ASP	V378	L189	S140	P81	P81	G201	V141	ASP	V378	L189	S140
SER	L379	L189	V141	R82	R82	V141	K142	SER	L379	L189	V141
HIS	Y380	L189	K142	L83	L83	K142	S143	HIS	Y380	L189	K142
SER	S381	L189	L83	K84	K84	S143	Q144	SER	S381	L189	L83
PHE	Q322	L189	L83	R85	R85	Q144	G145	PHE	Q322	L189	L83
LEU	W323	L189	L83	V86	V86	G145	T146	LEU	W323	L189	L83
LEU	G384	L189	L83	L86	L86	T146	L147	LEU	G384	L189	L83
LEU	G384	L189	L83	L87	L87	L147	G148	LEU	G384	L189	L83
LEU	Y385	L189	L83	R88	R88	G148	Q149	LEU	Y385	L189	L83
LEU	I386	L189	L83	V88	V88	Q149	L150	LEU	I386	L189	L83
LEU	Y387	L189	L83	A90	A90	L150	T151	LEU	Y387	L189	L83
LEU	L388	L189	L83	S91	S91	T151	E152	LEU	L388	L189	L83
LEU	M389	L189	L83	K92	K92	E152	S153	LEU	M389	L189	L83
LEU	E390	L189	L83	E93	E93	S153	R154	LEU	E390	L189	L83
LEU	G392	L189	L83	R94	R94	R154	A155	LEU	G392	L189	L83
LEU	G393	L189	L83	A95	A95	A155	D156	LEU	G393	L189	L83
LEU	G394	L189	L83	D96	D96	D156	I157	LEU	G394	L189	L83
LEU	R395	L189	L83	A97	A97	I157	I158	LEU	R395	L189	L83
LEU	G396	L189	L83	N98	N98	I158	L159	LEU	G396	L189	L83
LEU	G397	L189	L83	C99	C99	L159	A160	LEU	G397	L189	L83
LEU	G398	L189	L83	Q40	Q40	A160	F101	LEU	G398	L189	L83
LEU	D999	L189	L83	I41	I41	F101	I102	LEU	D999	L189	L83
LEU	D400	L189	L83	D42	D42	I102	M43	LEU	D400	L189	L83
LEU	A401	L189	L83	A44	A44	M43	A44	LEU	A401	L189	L83
LEU	T402	L189	L83	R45	R45	A44	I105	LEU	T402	L189	L83
LEU	L403	L189	L83	T46	T46	I105	I106	LEU	L403	L189	L83
LEU	E404	L189	L83	L47	L47	I106	G167	LEU	E404	L189	L83
LEU	K405	L189	L83	M48	M48	G167	V163	LEU	K405	L189	L83
LEU	T286	L189	L83	N49	N49	V163	E164	LEU	T286	L189	L83
LEU	Q287	L189	L83	M49	M49	E164	V165	LEU	Q287	L189	L83
LEU	F288	L189	L83	P50	P50	V165	P166	LEU	F288	L189	L83
LEU	M289	L189	L83	L107	L107	P166	G167	LEU	M289	L189	L83
LEU	L289	L189	L83	L108	L108	G167	N168	LEU	L289	L189	L83
LEU	N291	L189	L83	L109	L109	N168	S169	LEU	N291	L189	L83
LEU	N291	L189	L83	P110	P110	S169	L169	LEU	N291	L189	L83
LEU	N292	L189	L83	F111	F111	L169	S170	LEU	N292	L189	L83
LEU	N293	L189	L83	L112	L112	S170	T171	LEU	N293	L189	L83
LEU	N293	L189	L83	S113	S113	T171	F111	LEU	N293	L189	L83
LEU	N294	L189	L83	L114	L114	F111	L112	LEU	N294	L189	L83
LEU	S295	L189	L83	E114	E114	L112	S113	LEU	S295	L189	L83
LEU	D296	L189	L83	K54	K54	S113	L114	LEU	D296	L189	L83
LEU	A297	L189	L83	L115	L115	E114	E114	LEU	A297	L189	L83
LEU	E297	L189	L83	K116	K116	L115	L115	LEU	E297	L189	L83
LEU	E298	L189	L83	P117	P117	K116	K116	LEU	E298	L189	L83
LEU	K299	L189	L83	L117	L117	P117	L117	LEU	K299	L189	L83
LEU	Y300	L189	L83	L118	L118	L117	L118	LEU	Y300	L189	L83
LEU		L189	L83	P119	P119	L118	L119	LEU		L189	L83
LEU		L189	L83	L120	L120	P119	L120	LEU		L189	L83
LEU		L189	L83	T180	T180	L120	L180	LEU		L189	L83



E421	S422	M423	F424	G425	D426	G427	M428	F429	G430	K431	I432	F433	S434	P435	I436	L437	L438	K439	H440	H441	K442	C443	A444	M445	L446	E447	I448	R449	A450	K451	G452	M453	K454	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	L446	T506	R507	E508	R509	G510	A511	V512	SER	SER	PHE	ILE	D515	D516	R517	I518	D519	A520	I521	A522	L523	G524	I525	E526	Y527	L528	R529	E530	G531	M532	L533	V534	D535	S536	R537	V538	G539	GLU
GLU	GLU	MET	THR	LEU	LEU	PHE	LEU	GLU	HIS	HIS	THR	THR	ILE	GLY	GLY	ASP	GLN	ILE	HIS	SER	PHE	ASP	VAL	GLY	GLY	VAL	ASP	ASP	GLU	GLU	GLY	SER	SER	PHE	ILE	ILE	D515	D516	R517	I518	D519	A520	I521	A522	L523	G524	I525	E526	Y527	L528	R529	E530	G531	M532	L533	V534	D535	S536	R537	V538	G539	GLU

● 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	F25	V26	L27	W28	K29	A30	L31	N32	L33	P34	K35	P36	T37	K38	C39	Q40	I41	D42	M43	G44	R45	I46	L47	A48	M49	G50	D51	H52	K53	K54	F55	L56	L57	Q58	A59	F60					
R61	G62	I63	G64	K65	S66	F67	I68	T69	D129	C70	A71	F72	V73	V74	W75	V76	L77	W78	R79	D80	P81	Q82	L83	K84	W85	L86	I87	W88	S89	A90	S91	K92	E93	L94	A95	D96	A97	N98	S99	I100	F101	I102	K103	M104	I105	I106	D107	L108	L109	P110	D51	F111	L112	S113	K114	K54	F55	L115	K116	L117	Q58	A59	P119	G120
Q121	R122	D123	S124	V125	I126	S127	F128	D129	V130	G131	L132	A133	K134	P135	D136	H137	S138	P139	S140	V141	K142	S143	V144	G145	L146	T147	G148	Q149	L150	T151	K152	S153	R154	A155	D156	I157	I158	I159	A160	D161	D162	V163	E164	V165	P166	G167	N168	S169	P170	T171	S172	S173	A174	R175	L176	K177	L178	W179	T180					
L181	V182	T183	E184	F185	A186	L187	L188	L189	K190	P191	L192	P193	T194	S195	R196	V197	I198	Y199	L200	G201	T202	P203	Q204	T205	E206	M207	T208	L209	Y210	K211	E212	L213	E214	D215	N216	K217	G218	Y219	S220	T221	V222	L223	W224	P225	A226	Q227	Y228	P229	R230	N231	D232	A233	E234	A235	D236	Y237	Y238	G239	D240					
R241	L242	A243	P244	M245	L246	K247	A248	E249	Y250	D251	E252	G253	P254	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	A410	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	R326	R327	Q328	N329	R330	N331	E332	E333	L334	P335	N336	V337	G338	L339	K340	G341	D342	D343	I344	H345	A346	F347	H348	T349	C350	S351	S352	R353	T354	L355	A356	E356	Y357	Q358	S359	K360				
I361	L362	V363	I364	D365	P366	S367	G368	R369	G370	K371	D372	E373	T374	G375	Y376	A377	V378	L379	S380	S381	L382	N383	G384	Y385	I386	Y387	L388	M389	E390	V391	G392	G393	F394	R395	G396	G397	Y398	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	L437	L438	K439	H440	H441	K442	C443	A444	M445	L446	E447	I448	R449	A450	K451	G452	M453	K454	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	L446	T506	R507	E508	R509	G510	A511	V512	SER	SER	PHE	ILE	D515	D516	R517	I518	D519	A520	I521	A522	L523	G524	I525	E526	Y527	L528	R529	E530	G531	M532	L533	V534	D535	S536	R537	V538	G539	GLU		
GLU	GLU	MET	THR	LEU	LEU	PHE	LEU	GLU	HIS	HIS	THR	THR	ILE	GLY	GLY	ASP	GLN	ILE	HIS	SER	PHE	ASP	VAL	GLY	GLY	VAL	ASP	ASP	GLU	GLU	GLY	SER	SER	PHE	ILE	ILE	D515	D516	R517	I518	D519	A520	I521	A522	L523	G524	I525	E526	Y527	L528	R529	E530	G531	M532	L533	V534	D535	S536	R537	V538	G539	GLU		

## 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.

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

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

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

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

## 5.2 Too-close contacts [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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 221 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:165:VAL:HG12	2:F:167:GLY:H	1.55	0.72
2:H:165:VAL:HG12	2:H:167:GLY:H	1.55	0.70
2:G:165:VAL:HG12	2:G:167:GLY:H	1.61	0.65
1:B:1944:ASP:OD2	1:B:1945:ILE:N	2.30	0.65
2:E:165:VAL:HG12	2:E:167:GLY:H	1.61	0.64

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

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

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

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [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

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

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

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	C	2101	4	26,33,33	0.66	0	31,52,52	0.73	1 (3%)
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.

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

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

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

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

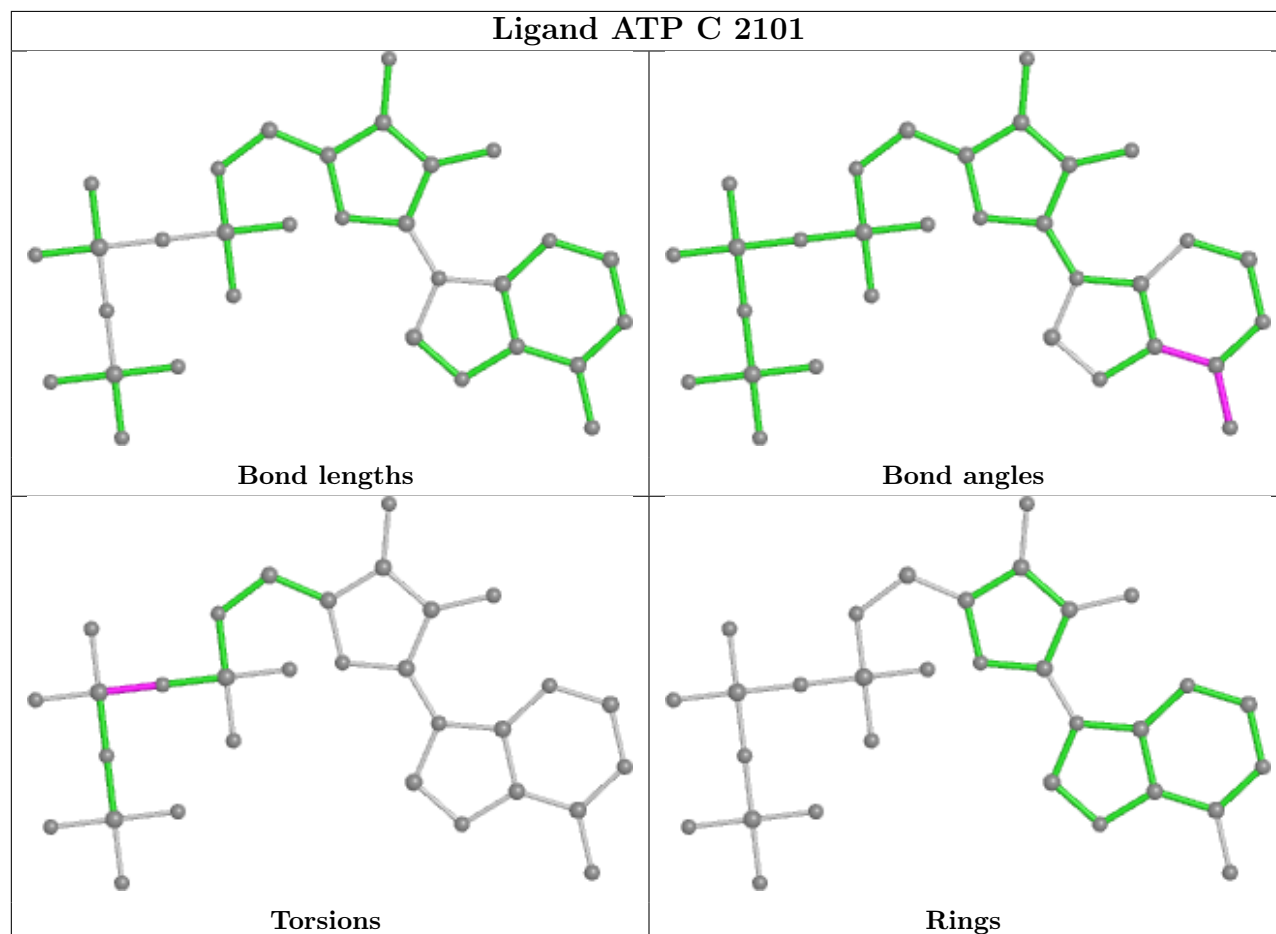
There are no ring outliers.

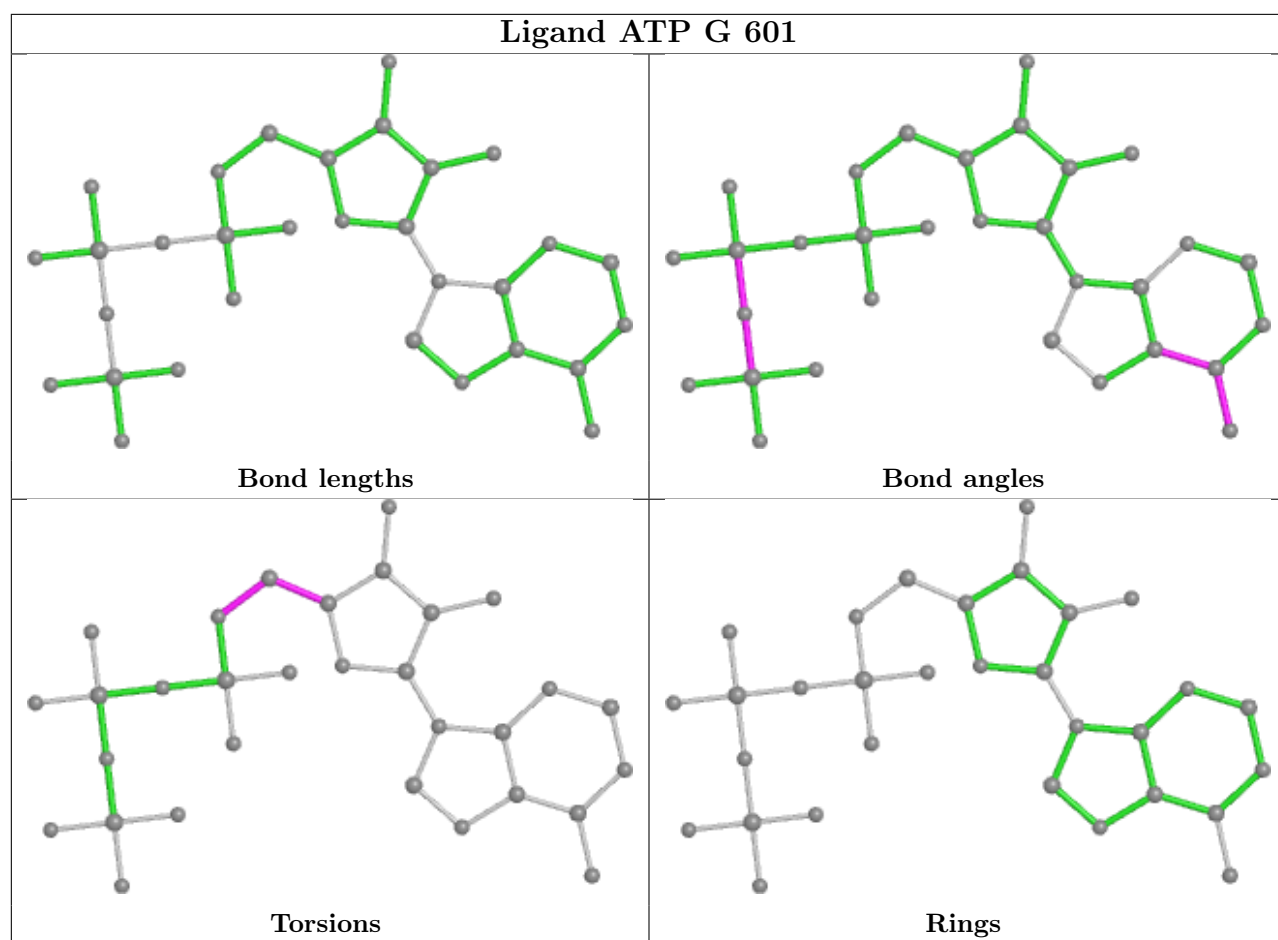
No monomer is involved in short contacts.

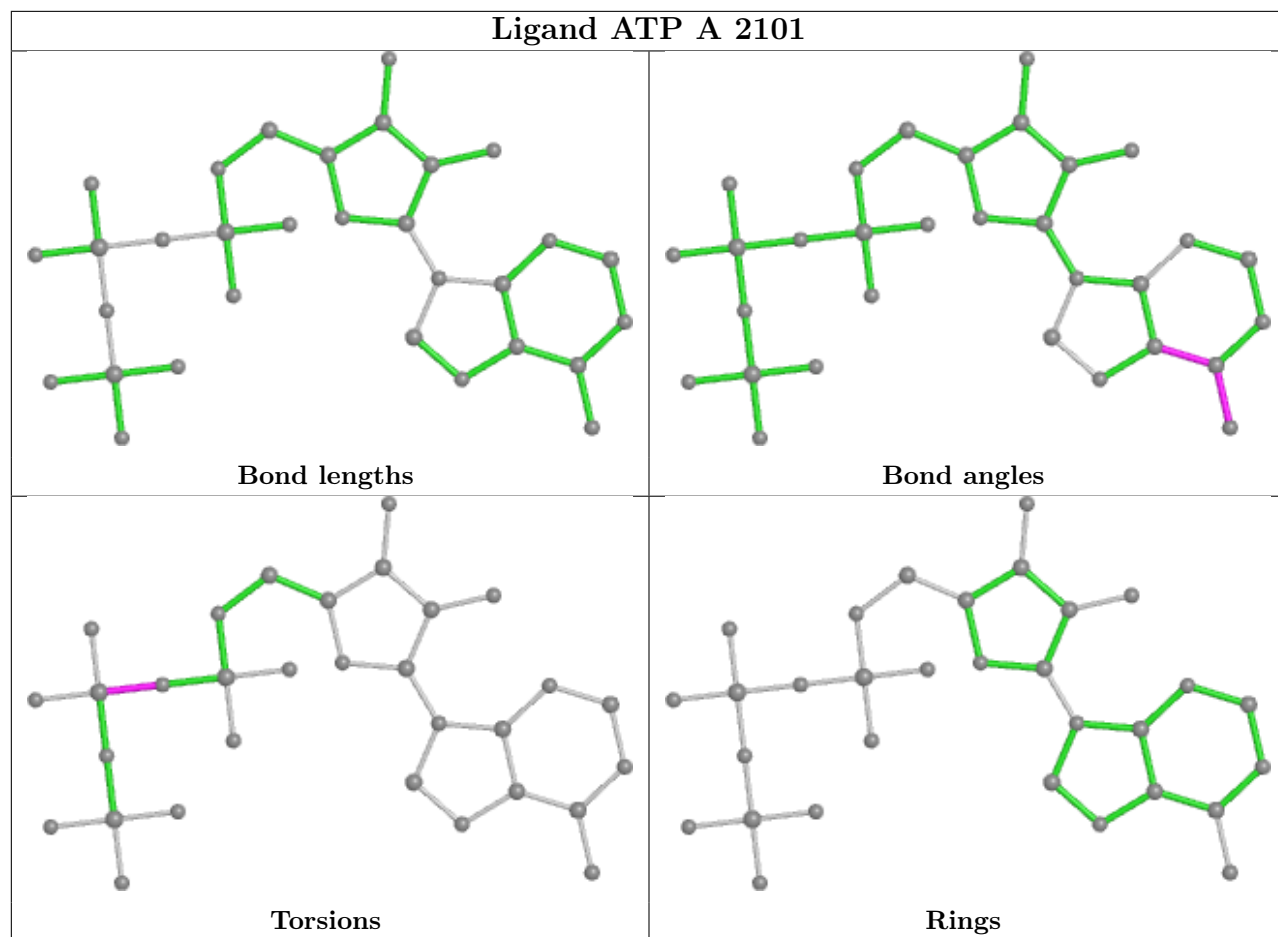
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

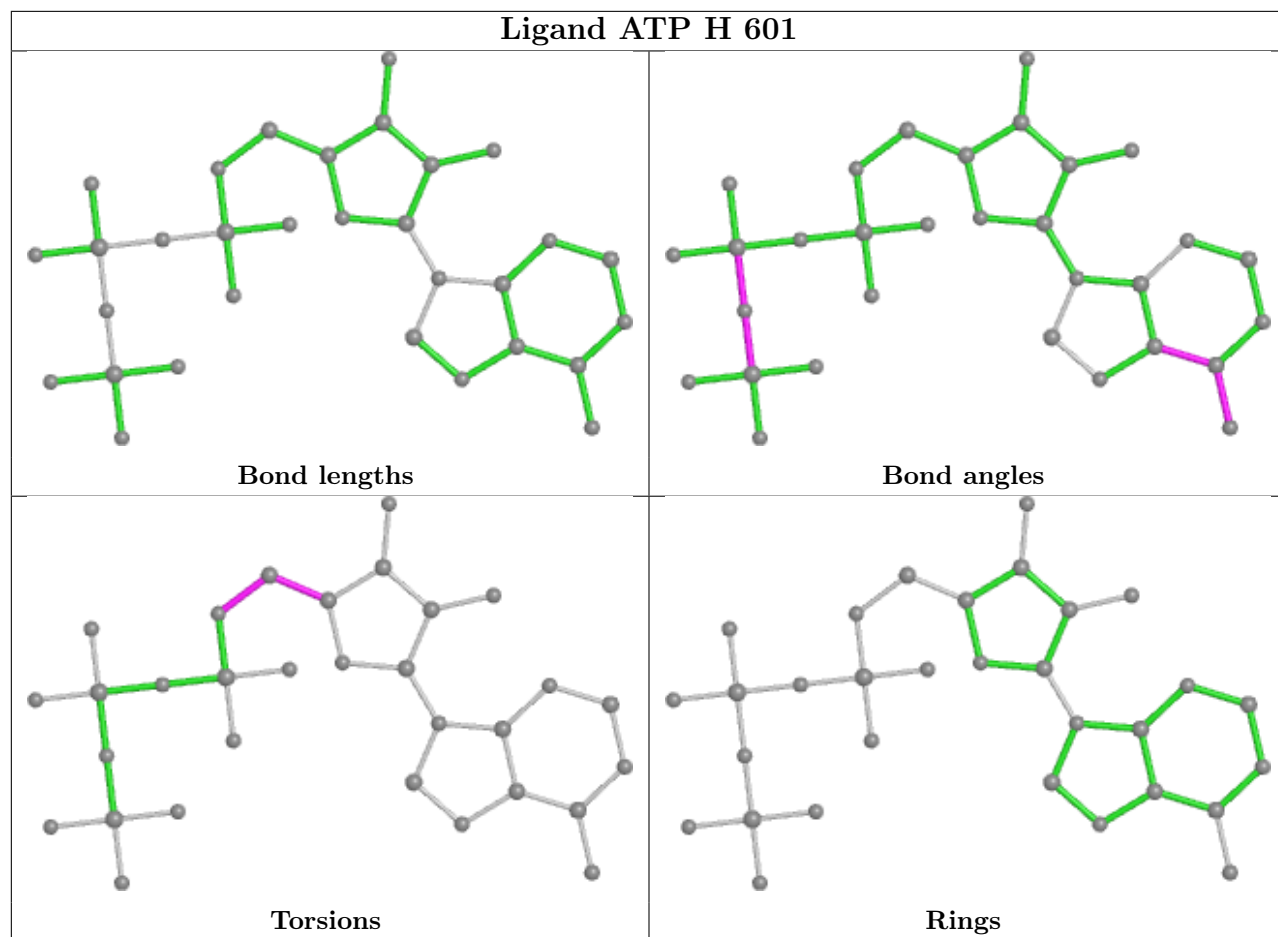


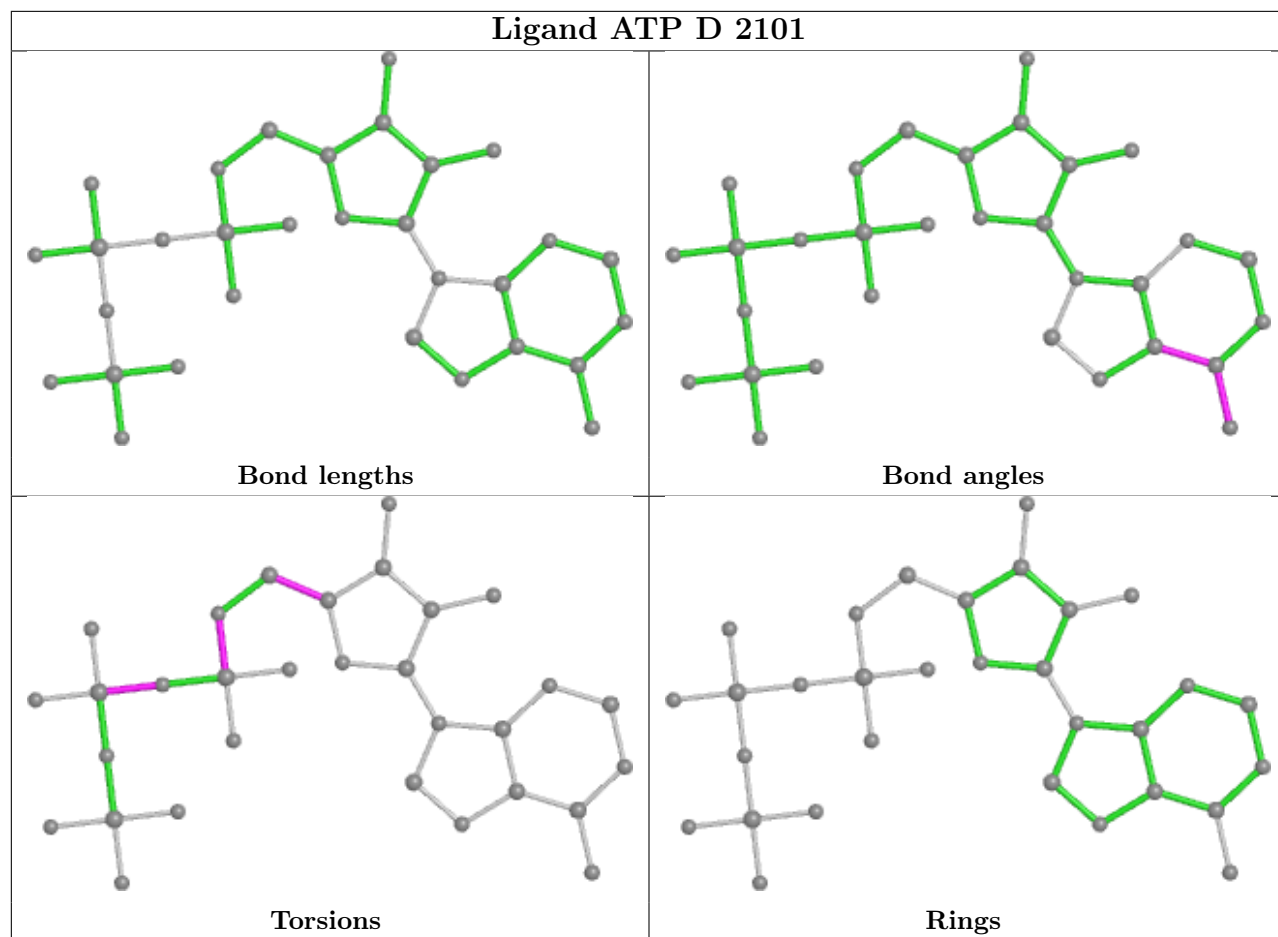
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

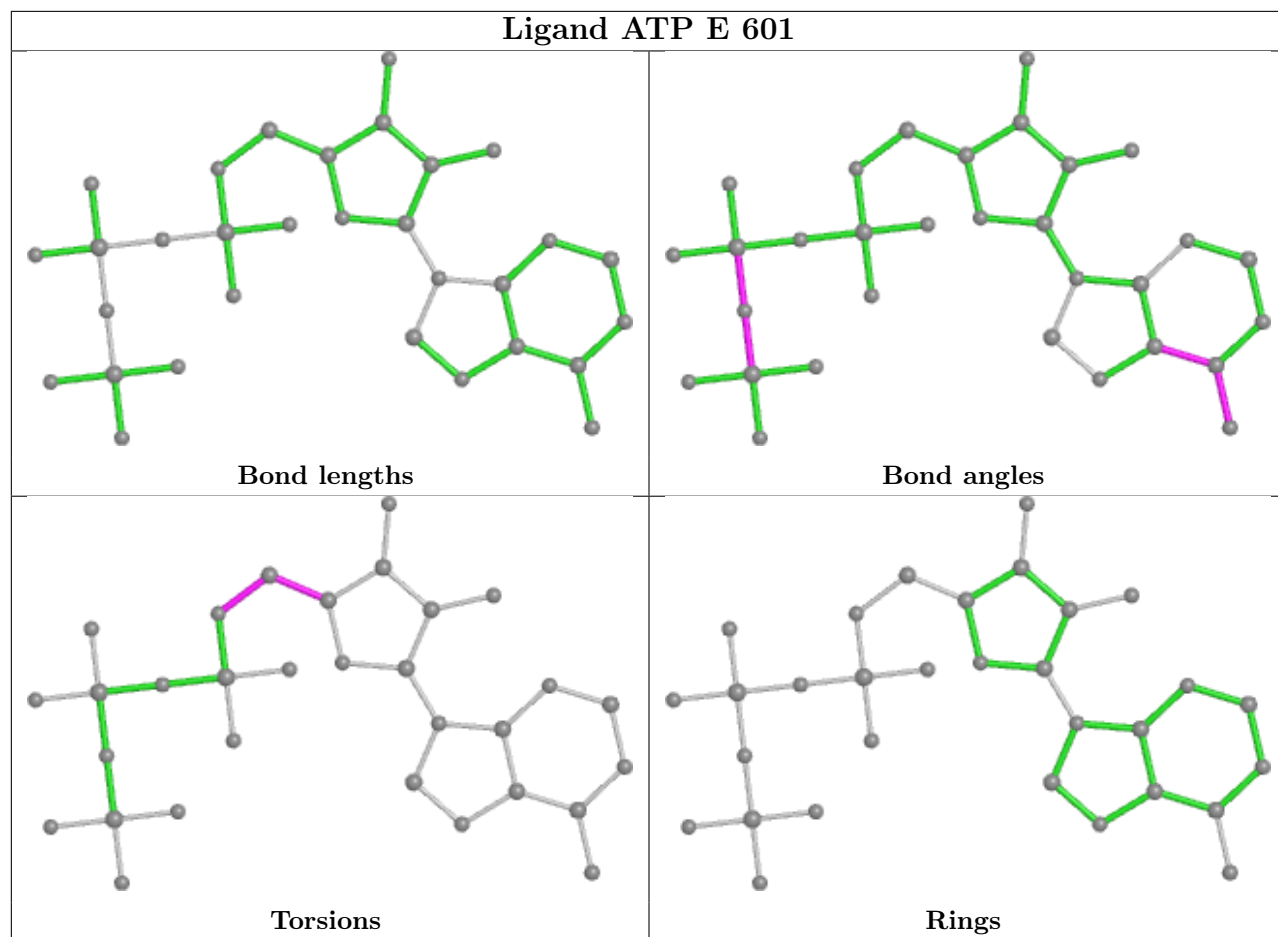


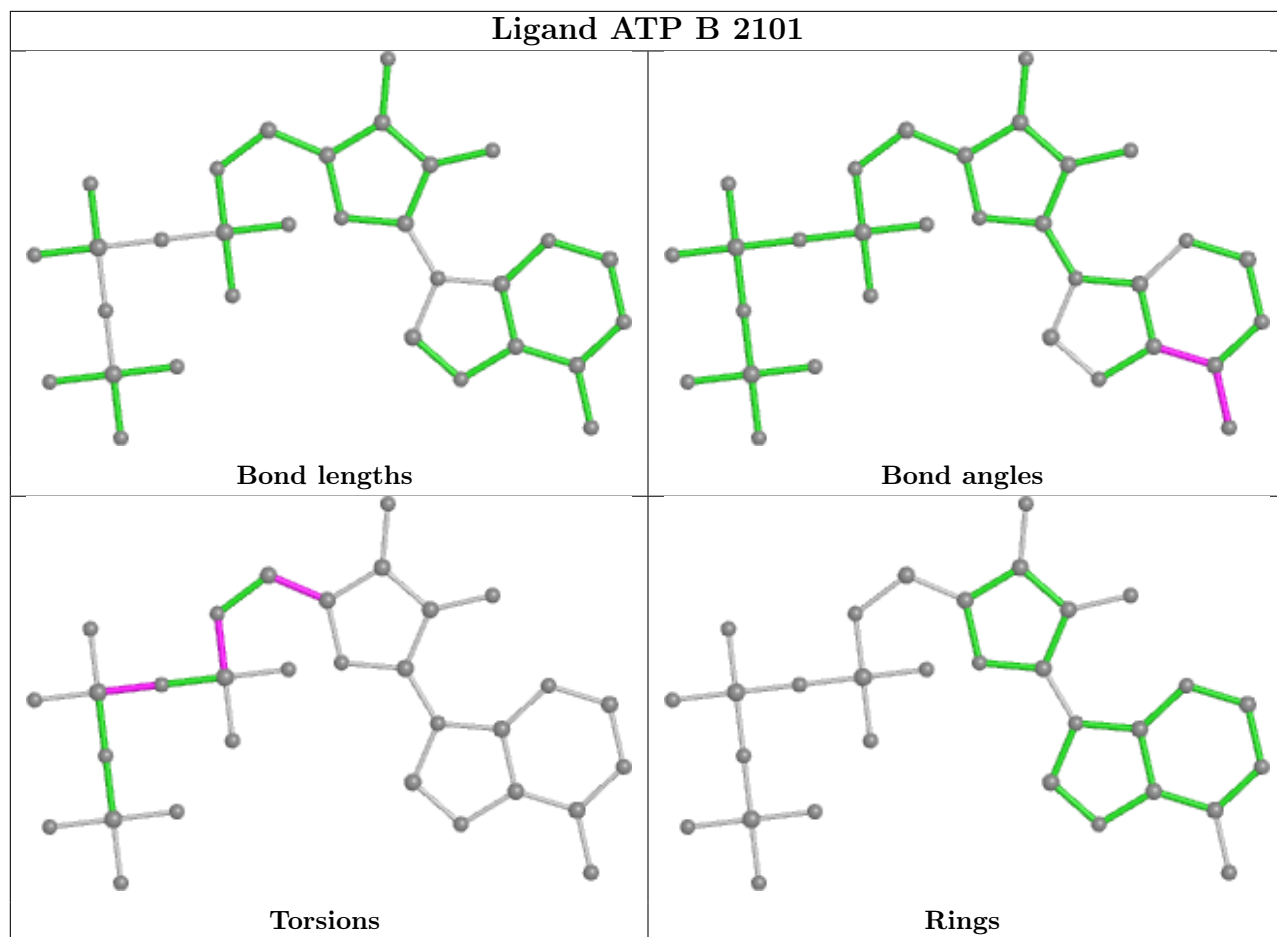


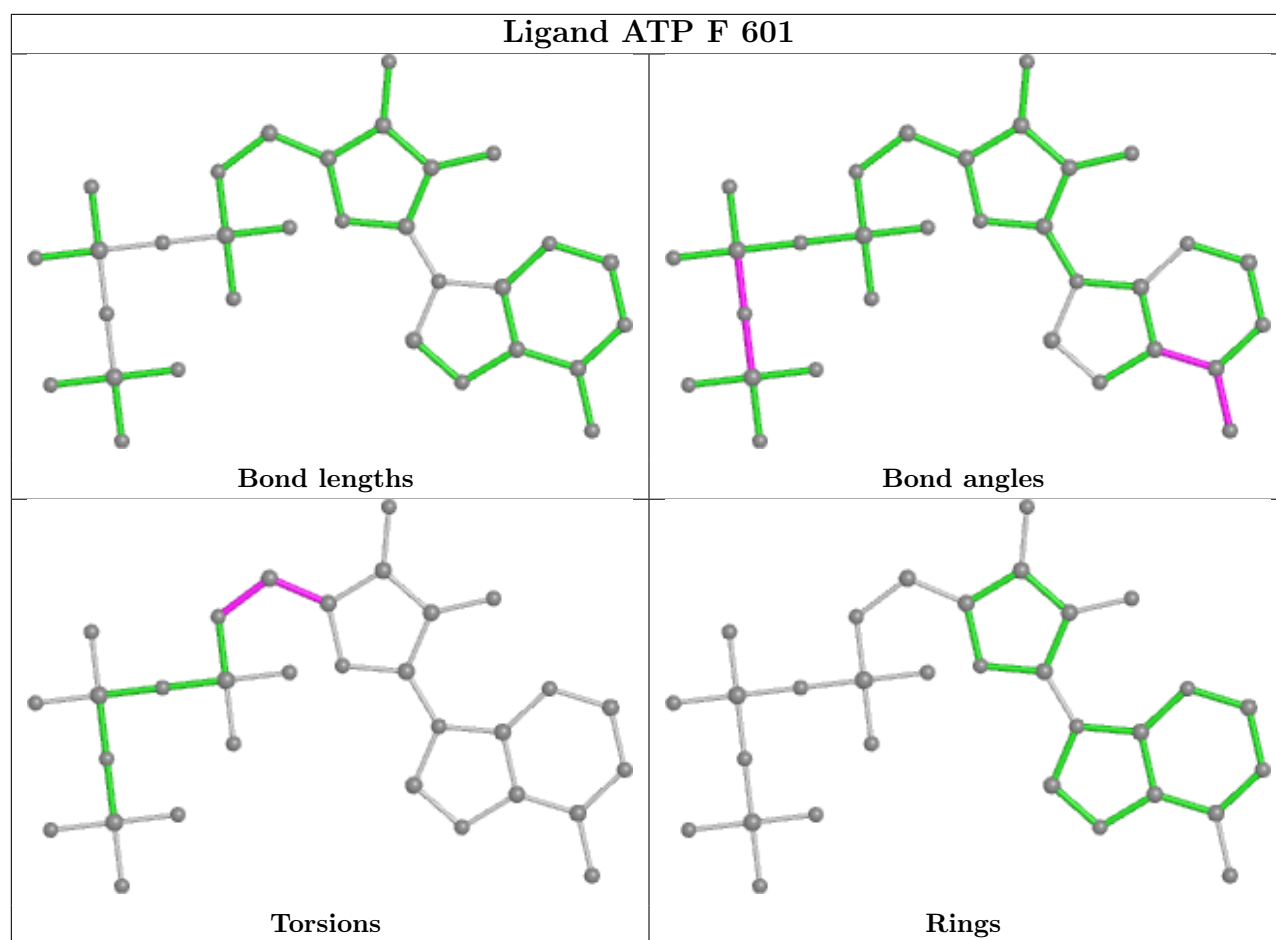












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



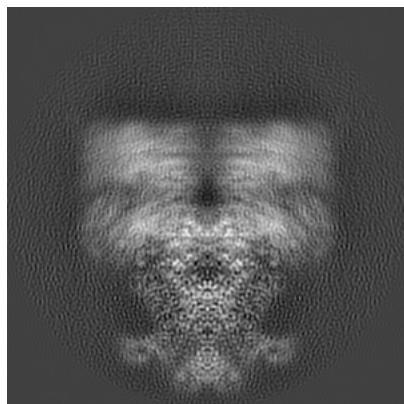
## 6 Map visualisation [i](#)

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

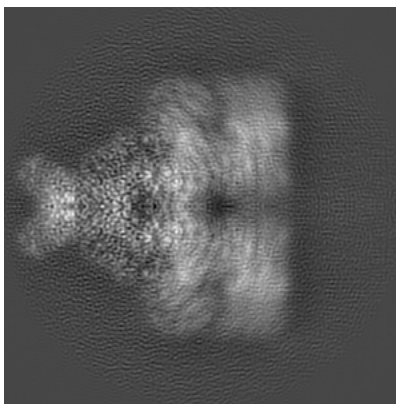
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

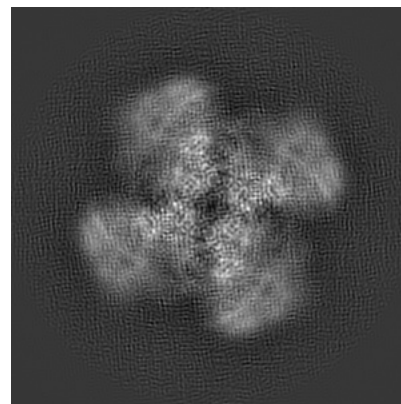
#### 6.1.1 Primary map



X

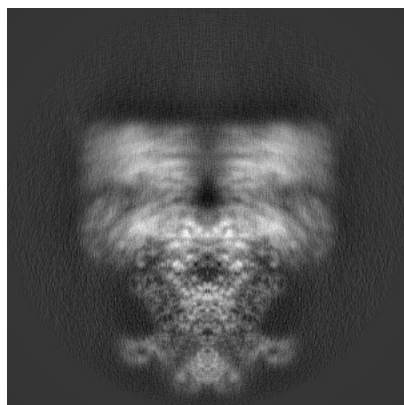


Y

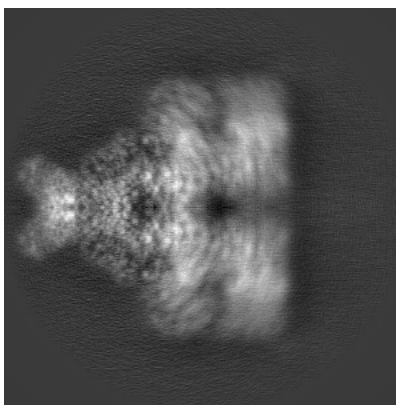


Z

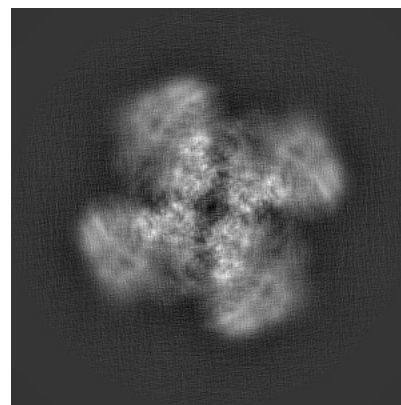
#### 6.1.2 Raw map



X



Y

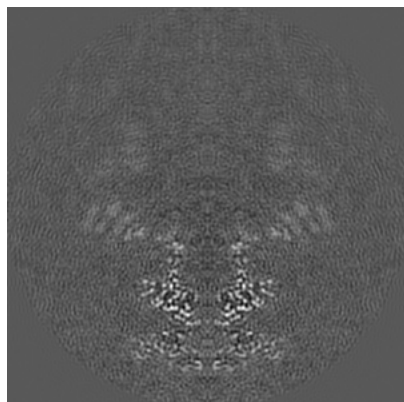


Z

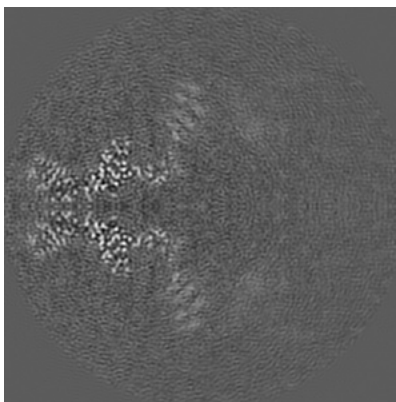
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

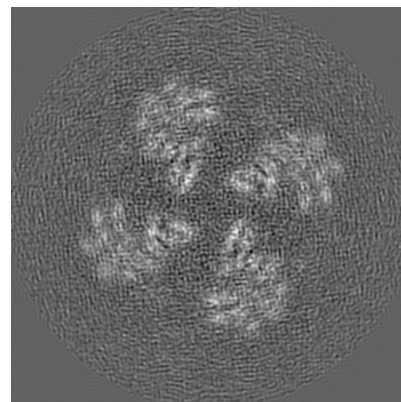
### 6.2.1 Primary map



X Index: 180

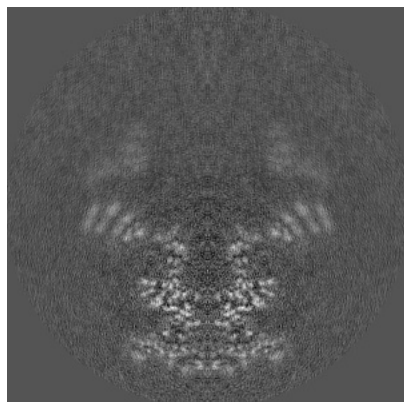


Y Index: 180

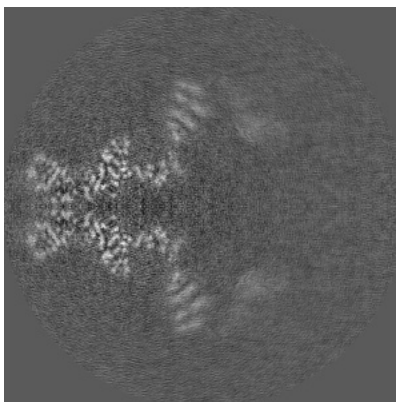


Z Index: 180

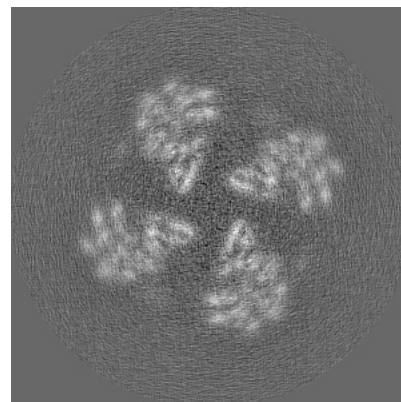
### 6.2.2 Raw map



X Index: 180



Y Index: 180

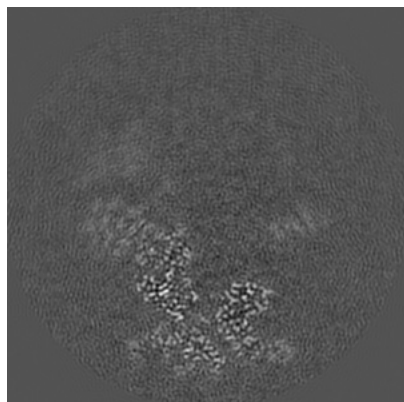


Z Index: 180

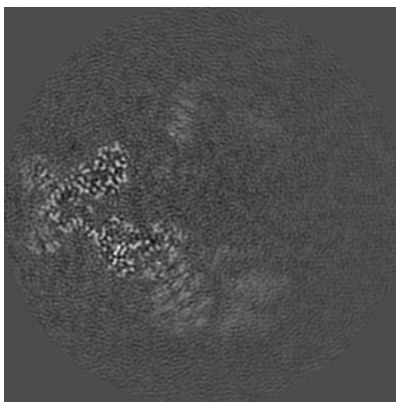
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

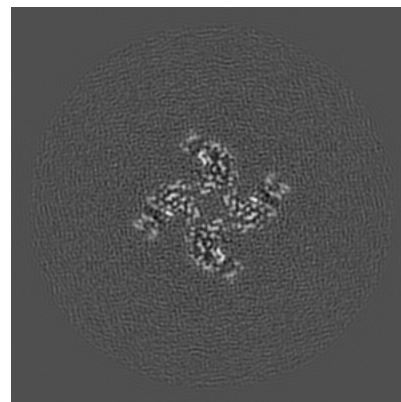
### 6.3.1 Primary map



X Index: 187

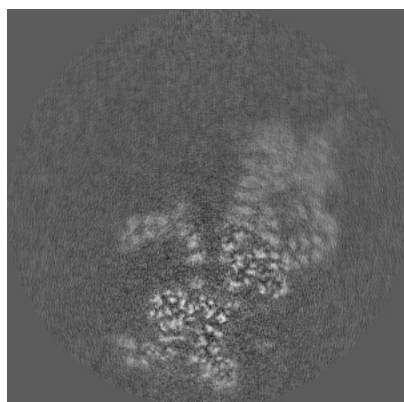


Y Index: 173

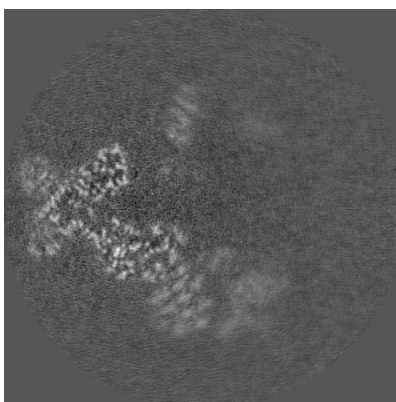


Z Index: 102

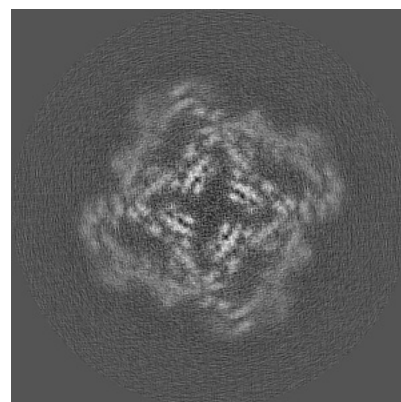
### 6.3.2 Raw map



X Index: 163



Y Index: 173

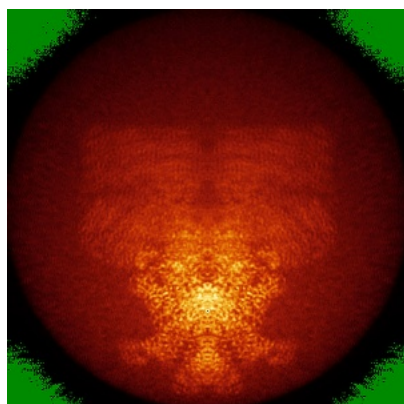


Z Index: 155

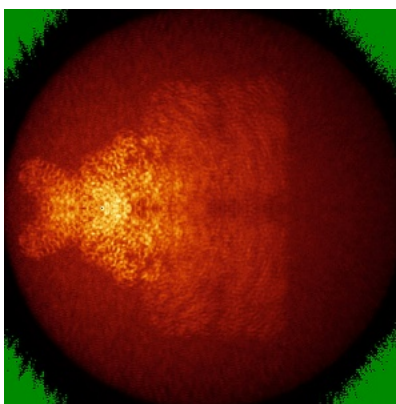
The images above show the largest variance slices of the map in three orthogonal directions.

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

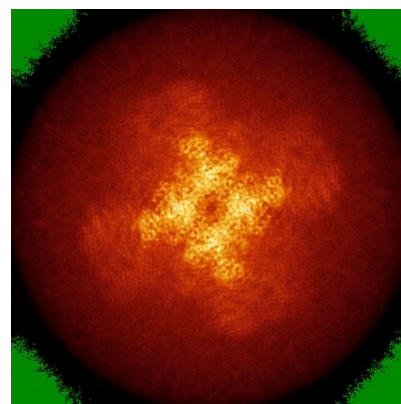
### 6.4.1 Primary map



X

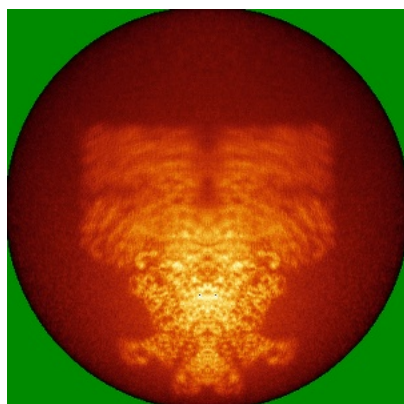


Y

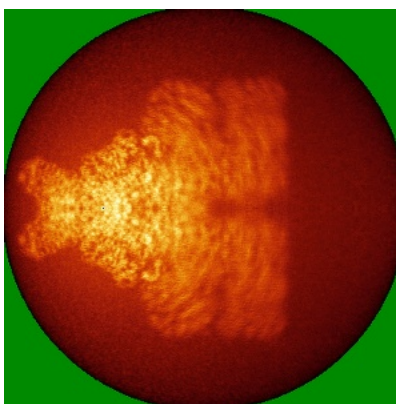


Z

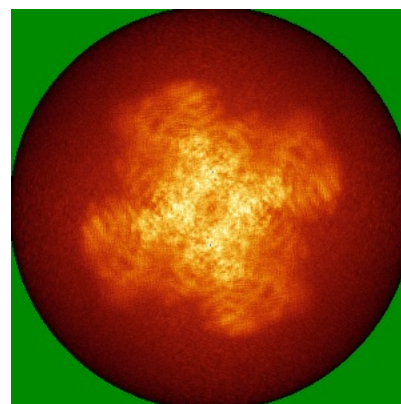
### 6.4.2 Raw map



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.

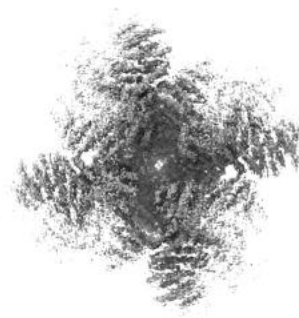
### 6.5.2 Raw map



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.

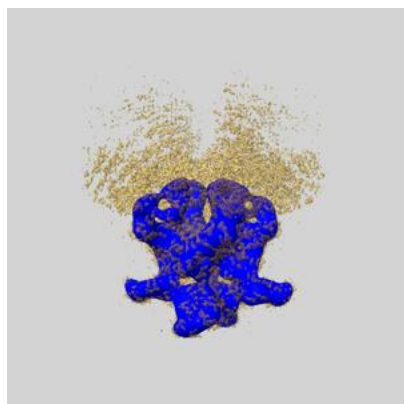
## 6.6 Mask visualisation [i](#)

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

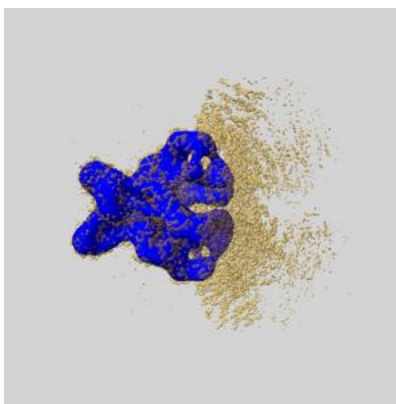
A mask typically either:

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

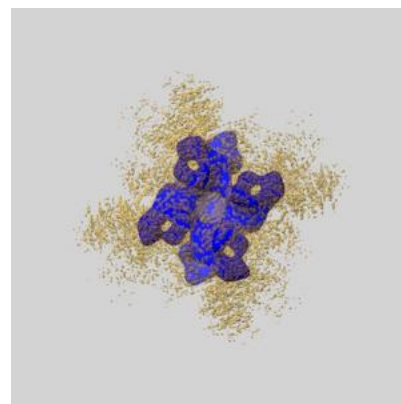
### 6.6.1 emd\_27421\_msk\_1.map [i](#)



X



Y

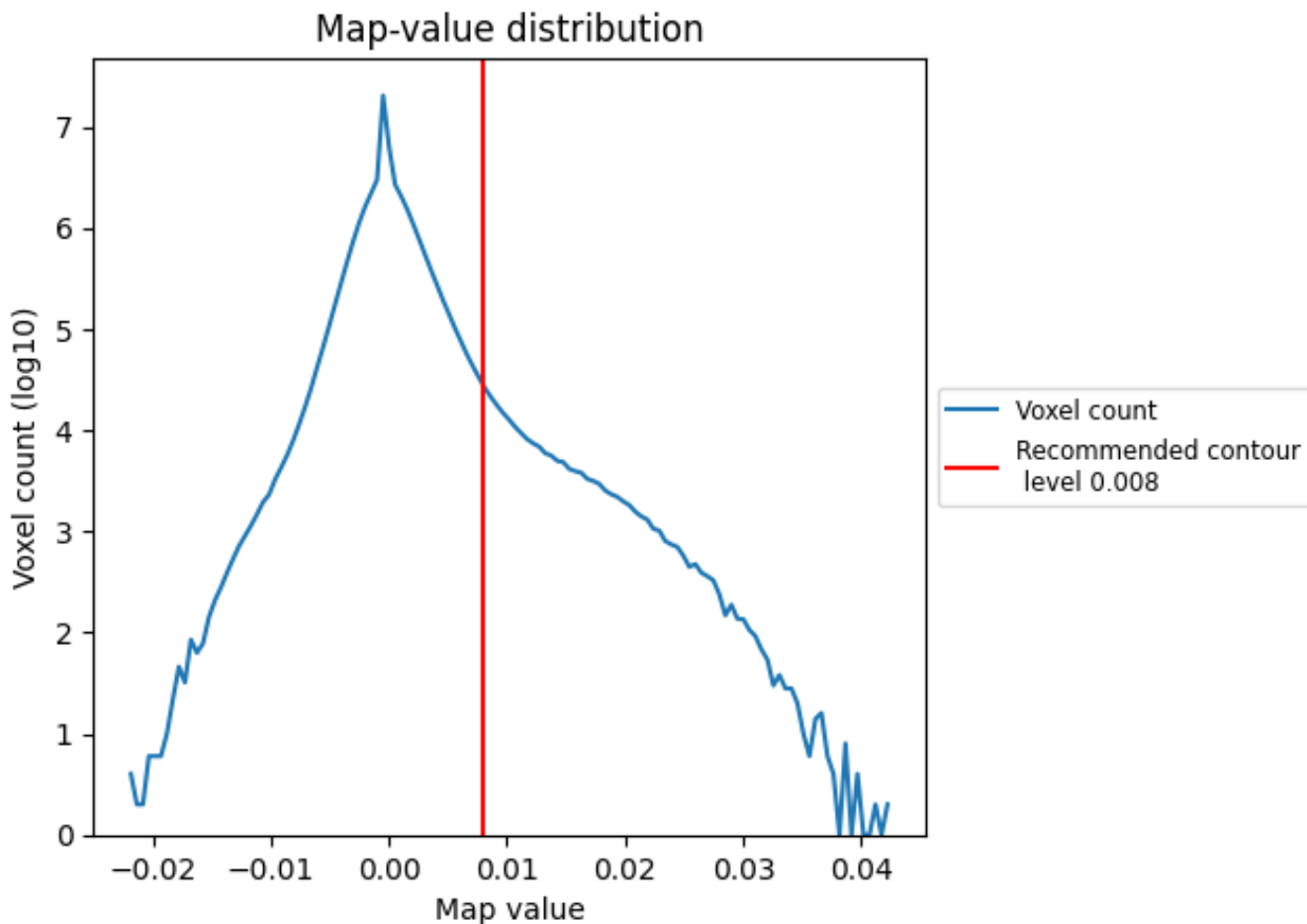


Z

## 7 Map analysis [i](#)

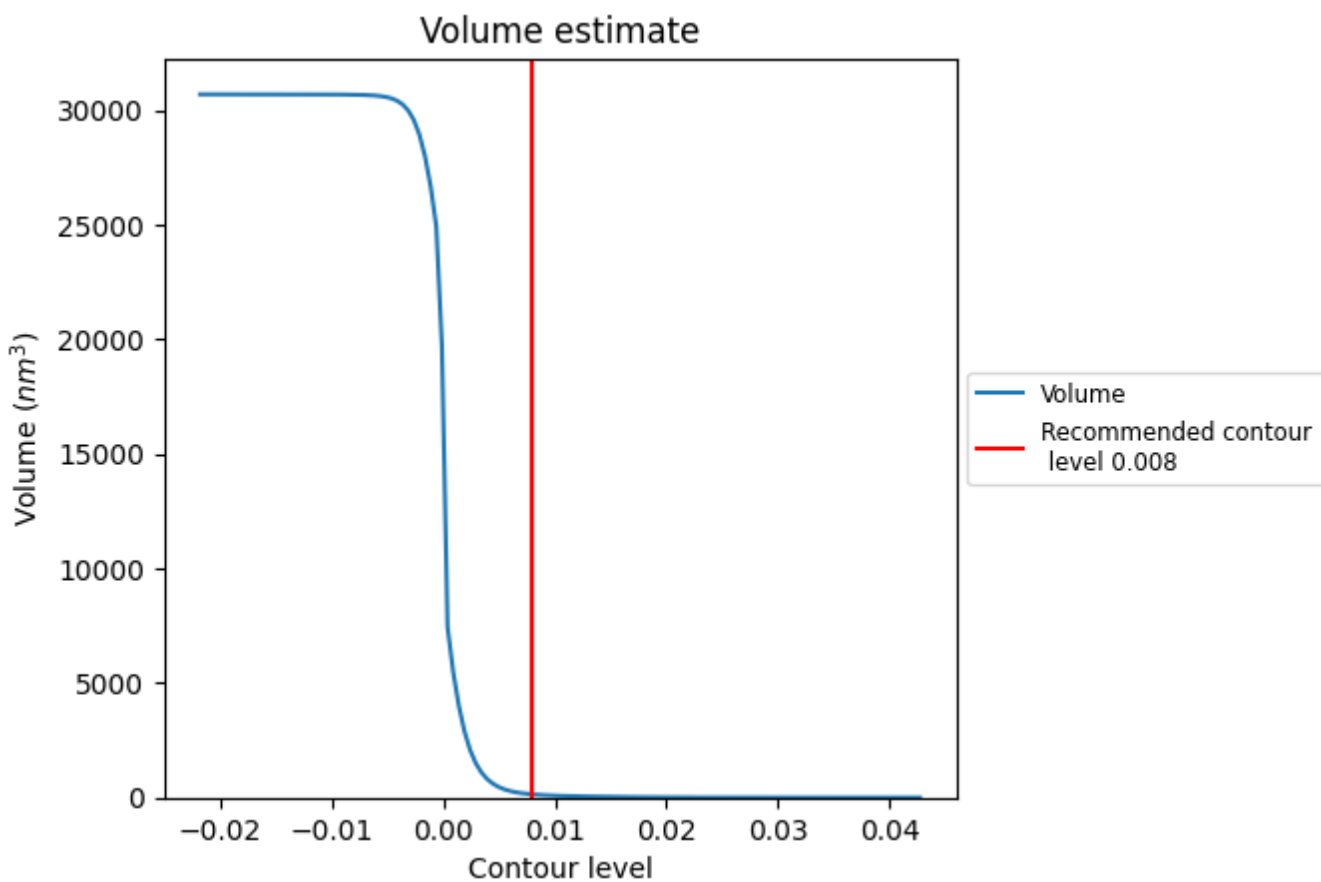
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

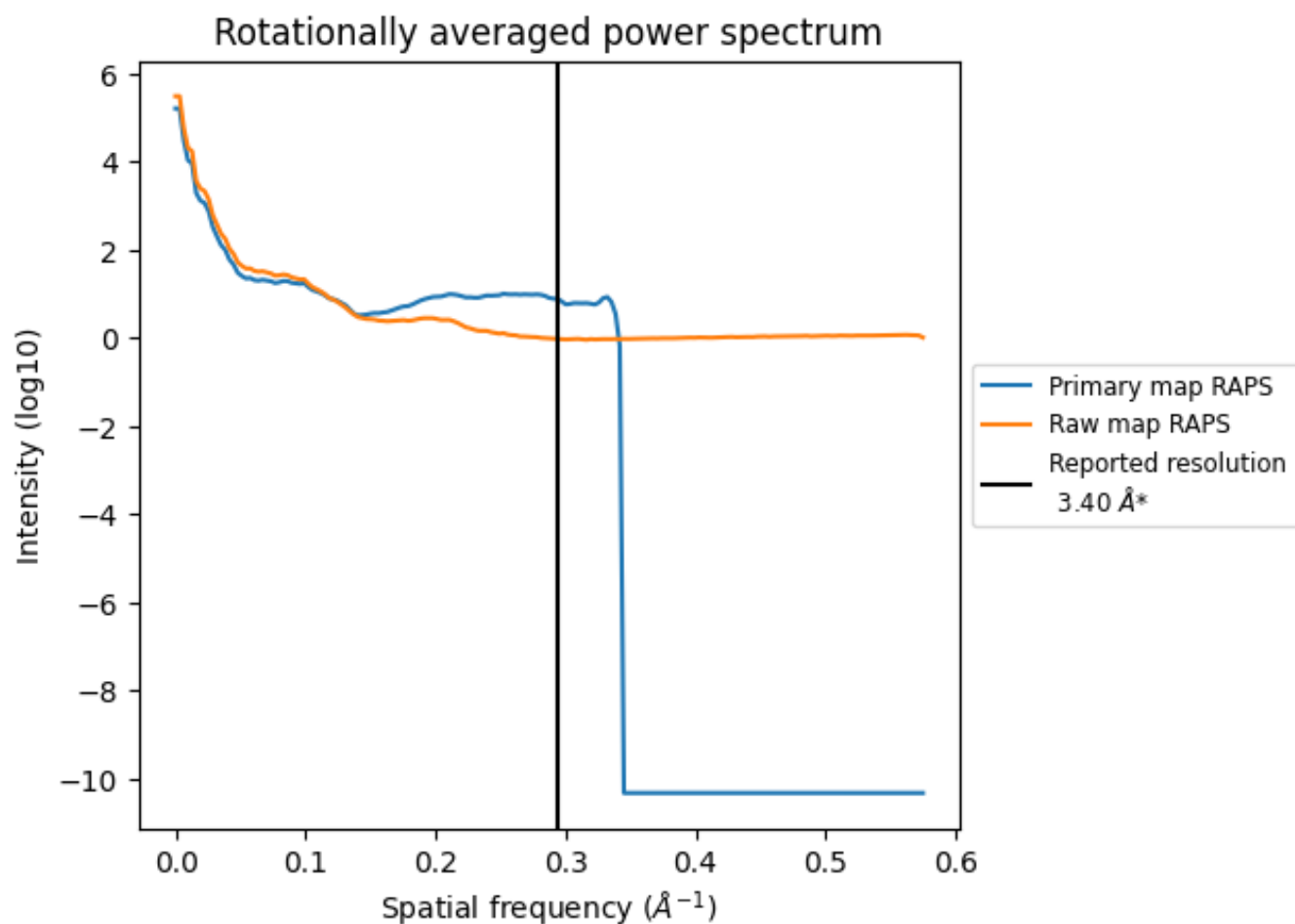


The volume at the recommended contour level is 138 nm<sup>3</sup>; this corresponds to an approximate mass of 125 kDa.

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

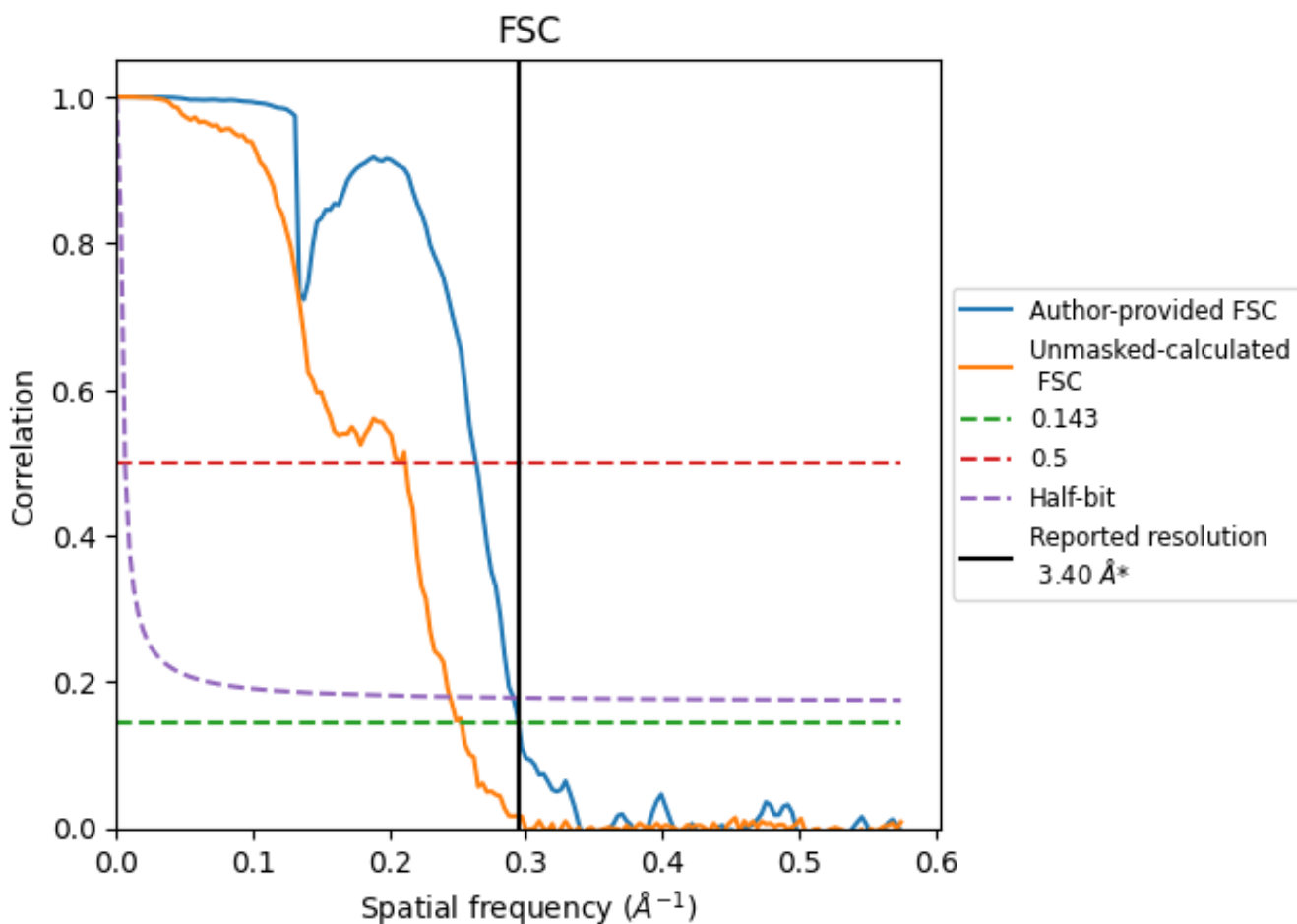


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

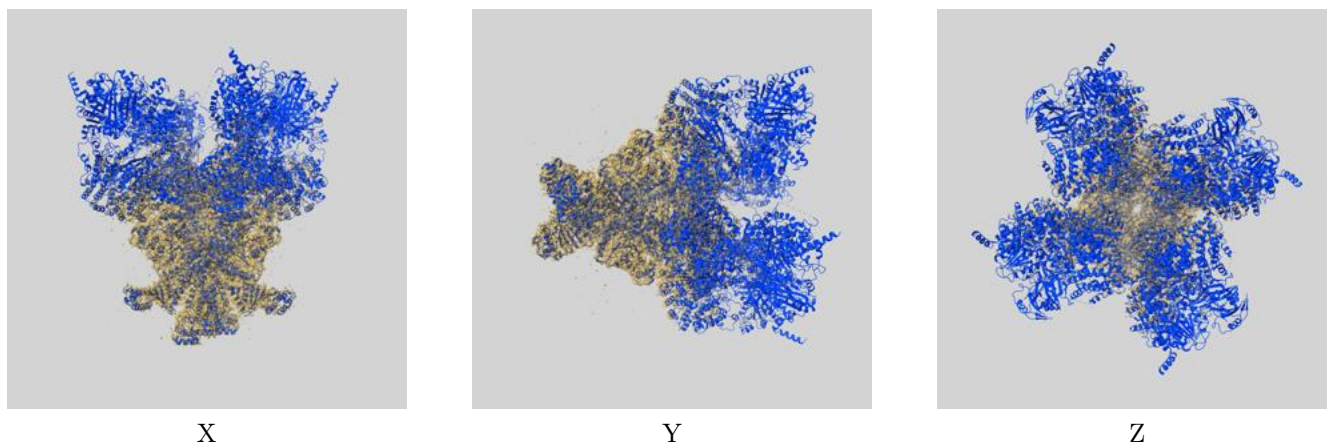
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.80	3.44
Unmasked-calculated*	3.95	4.83	4.09

\*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](#)

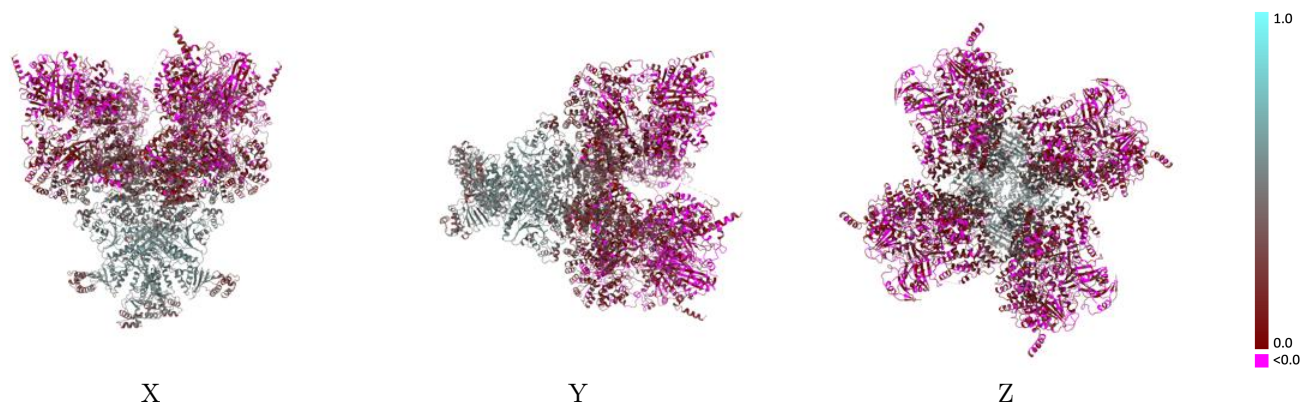
This section contains information regarding the fit between EMDB map EMD-27421 and PDB model 8DGC. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



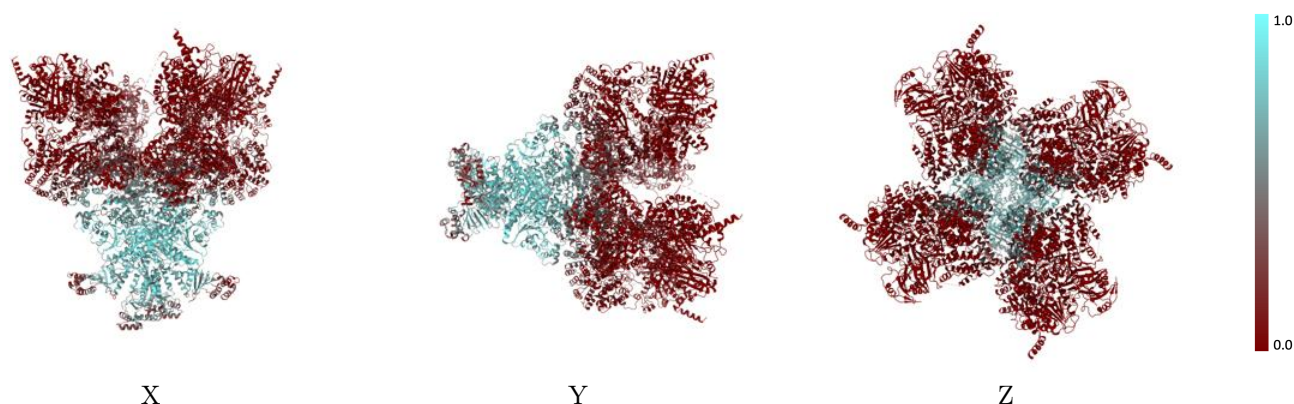
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



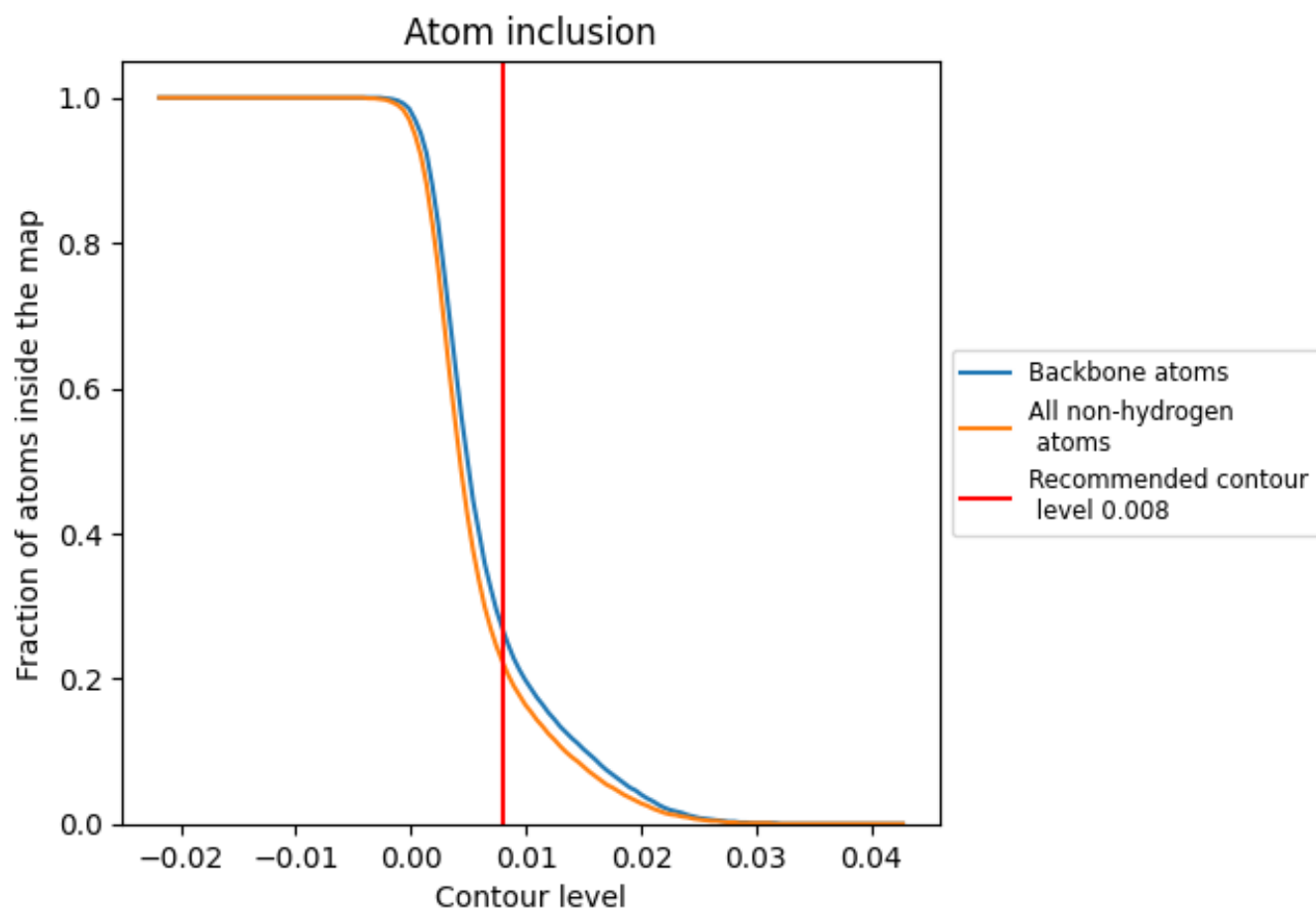
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

