



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 04:59 PM EST

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

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

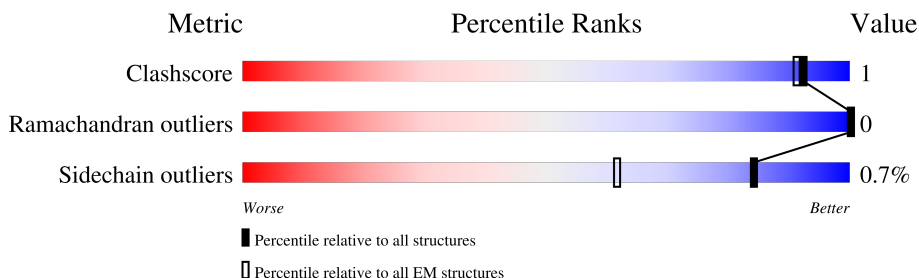
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

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

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

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

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

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



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

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

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

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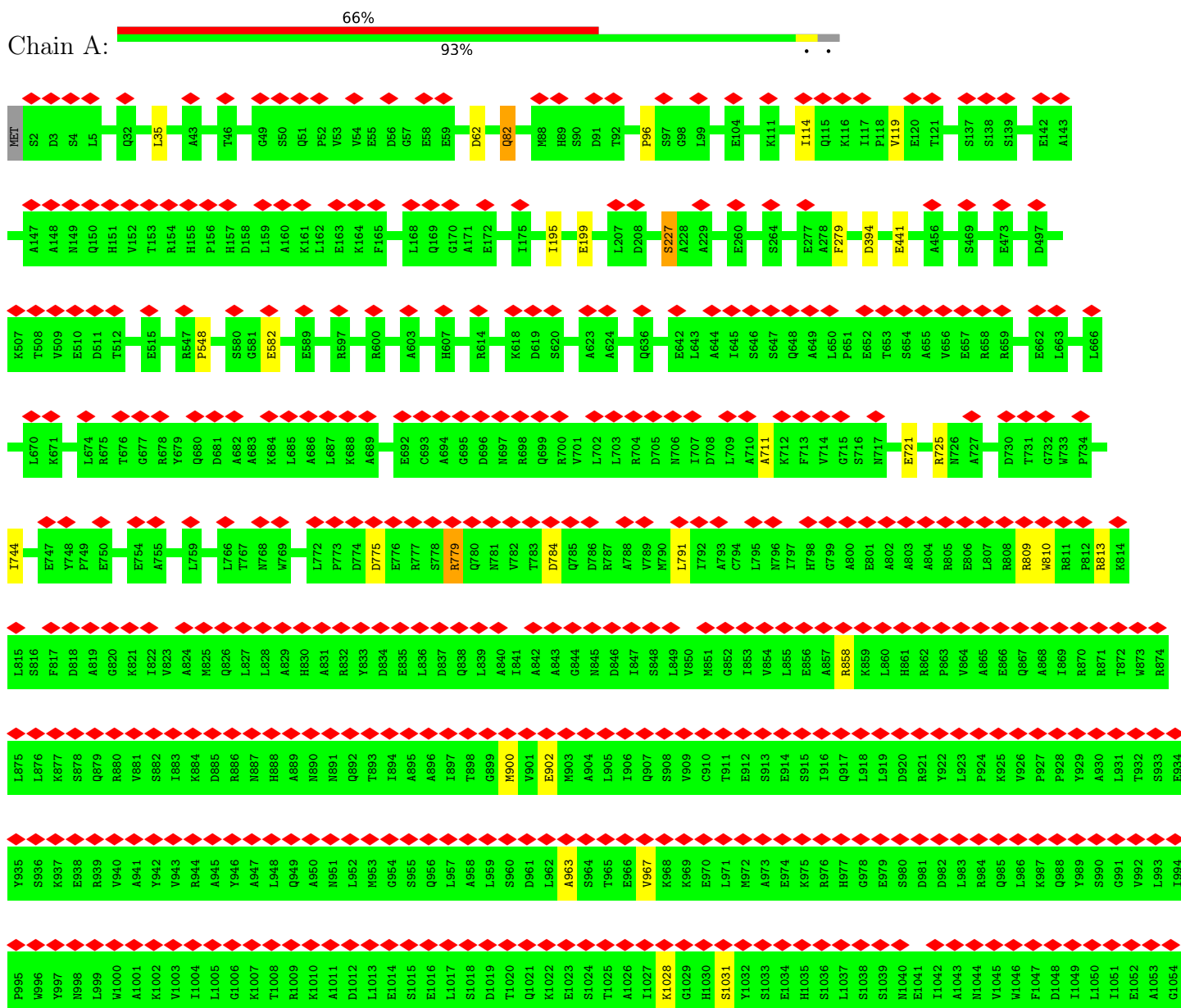
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Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0
4	G	1	Total 1	Mg 1	0
4	H	1	Total 1	Mg 1	0

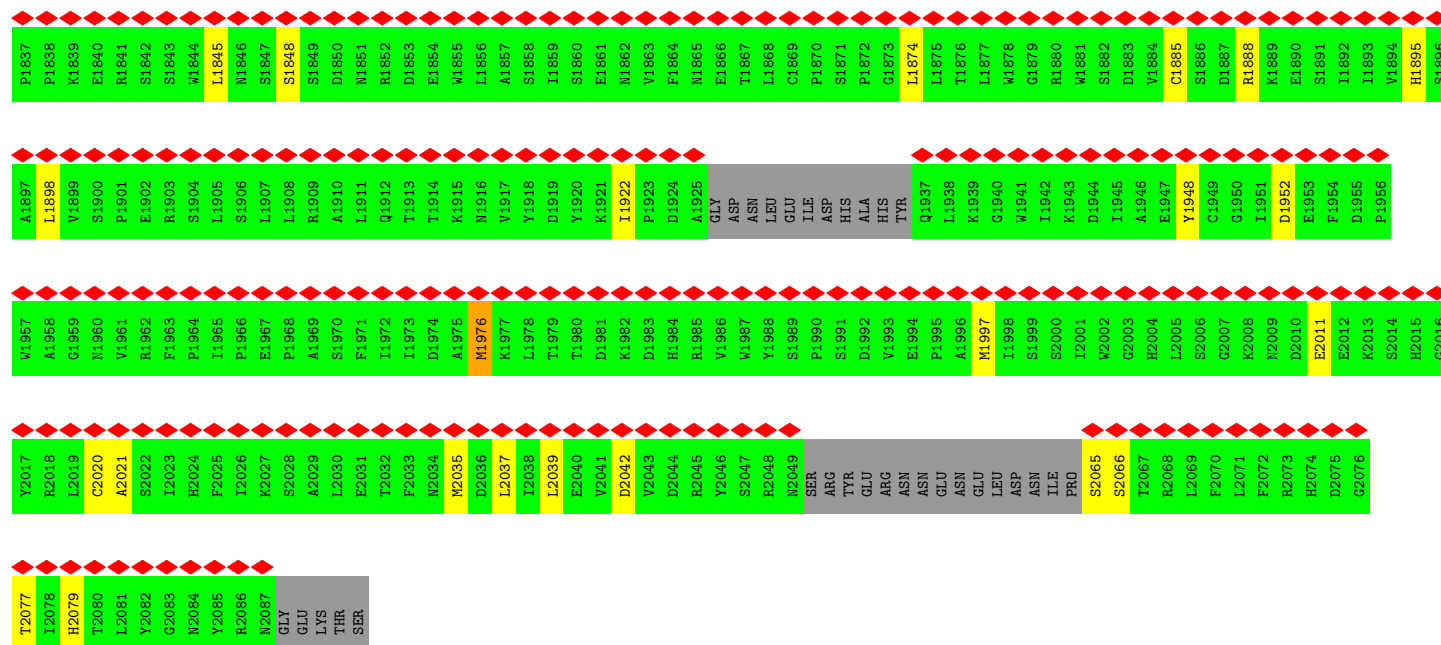
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

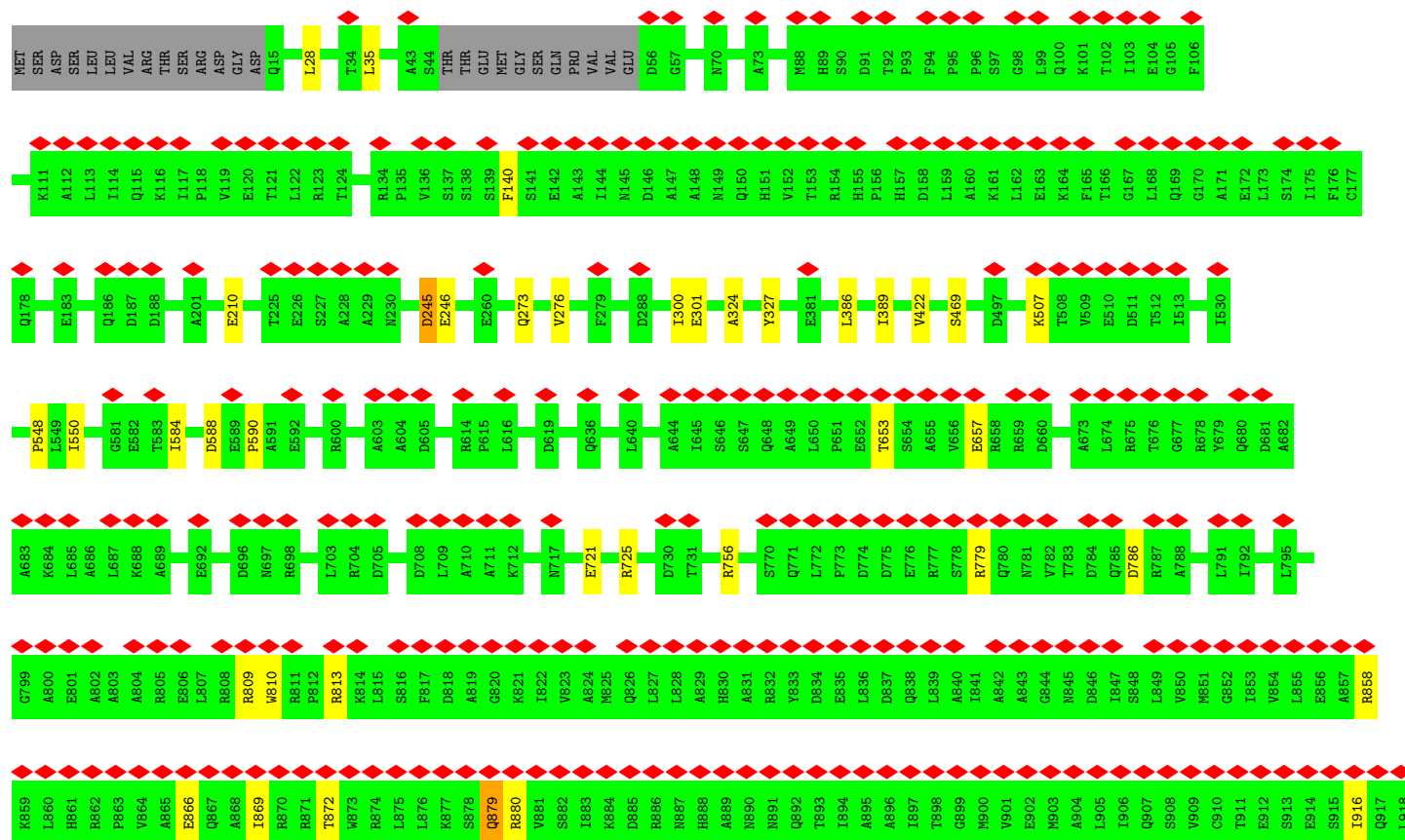
• Molecule 1: SeAvs3



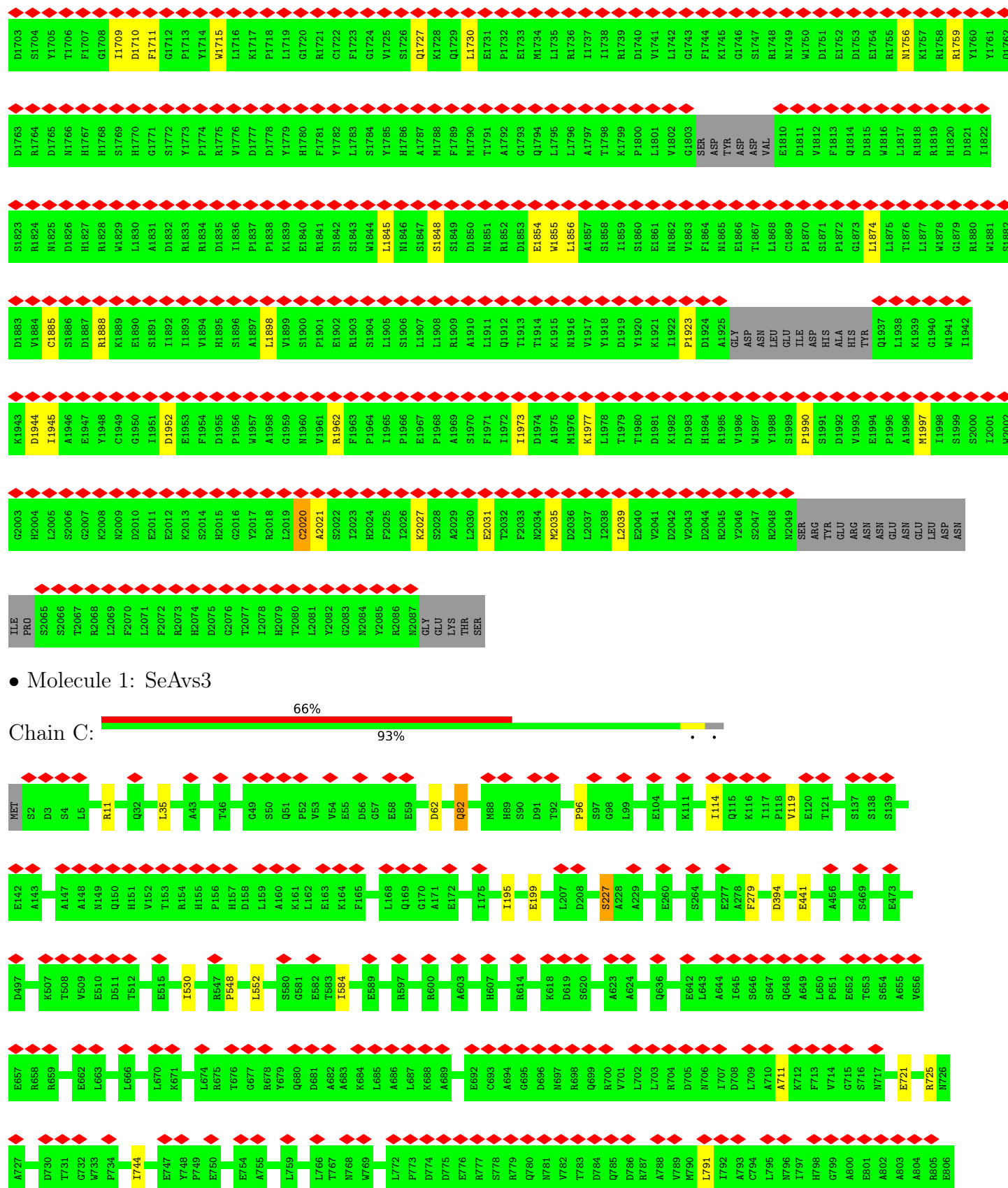
D1777	K1717	F1657	M1597	G1537	K1477	Y1416	I1356	F1296	L1236	P1176	M1055
D1778	P1718	A1658	A1598	P1538	E1478	D1417	F1357	N1297	A1237	P1177	V1056
Y1779	L1719	A1659	T1599	W1539	I1479	F1418	K1358	V1298	W1238	E1178	S1057
H1780	G1720	R1660	T1600	F1540	F1480	K1419	D1359	Q1299	T1239	I1179	K1058
F1781	R1721	L1661	L1601	E1541	G1481	Y1420	C1360	N1300	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	N1303	L1243	L1183	E1062
Y1785	V1725	L1665	P1605	P1545	E1485	S1424	S1364	L1304	V1244	A1184	M1063
H1786	S1726	H1666	R1606	P1546	A1486	I1425	L1365	K1305	R1245	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	P1729	D1669	P1609	E1549	E1489	E1428	L1368	D1308	E1248	K1067	W1067
L1730	L1730	L1670	F1610	E1550	S1490	W1429	S1369	A1309	L1249	L1188	S1068
E1731	E1731	I1671	Y1611	D1551	P1491	T1430	A1370	I1310	N1250	T1190	Q1069
P1732	P1732	S1672	T1612	S1552	E1492	S1431	A1371	S1311	A1251	R1191	H1070
E1733	E1733	L1673	L1613	L1553	P1493	R1432	Y1372	L1252	L1192	E1192	K1071
M1734	M1734	P1674	H1614	A1554	A1494	L1433	E1373	S1313	D1253	Y1193	G1072
L1735	L1735	A1675	A1615	G1555	M1495	S1434	K1374	L1314	A1254	V1194	M1073
R1736	R1736	Q1676	Q1616	Y1556	S1496	S1435	F1375	G1315	L1255	D1195	R1074
I1737	I1737	E1677	L1617	I1557	D1497	K1436	R1376	I1316	P1256	P1136	F1075
L1738	L1738	W1678	W1618	W1558	R1498		N1377	E1317	L1257	E1136	F1076
R1739	R1739	N1679	L1619	A1559	F1500	L1439	V1378	H1318	I1258	K1138	T1077
D1740	D1740	K1680	M1620	R1560	S1501	A1440	P1379	T1319	T1259	H1139	P1078
V1741	V1741	L1681	I1621	L1561	L1502	G1441	E1380	E1320	F1260	Y1140	T1079
L1742	L1742	R1682	A1622	G1562	P1503	I1442	F1381	L1321	E1261	F1141	L1080
G1743	G1743	A1683	A1623	S1563	G1504	I1443	Y1382	K1322	N1262	N1142	H1081
F1744	F1744	T1684	A1624	P1564	L1506	E1445	S1383	E1323	D1263	Q1143	F1082
K1745	K1745	N1685	R1625	E1565	Y1507	Y1446	K1384	R1324	W1264	A1144	S1084
G1746	G1746	A1686	V1626	A1566	S1508	C1447	E1385	I1325	H1265	I1145	S1085
S1747	S1747	S1687	A1627	E1567	K1509	Q1448	T1386	S1326	K1266	V1206	V1086
R1748	R1748	T1688	L1628	M1568	K1509	Q1448	F1387	G1327	C1267	E1207	C1087
M1749	M1749	D1629	D1629	R1569	L1510	R1449	I1388	L1328	D1268	I1208	A1088
W1750	W1750	L1690	D1630	W1570	E1511	F1450	K1389	Q1329	L1269	L1209	G1152
D1751	D1751	P1691	G1631	Q1571	S1512	C1451	I1390	H1330	A1210	A1210	E1089
E1752	E1752	L1692	K1632	A1572	E1514	R1452	A1391	THR	E1211	E1211	I1090
D1753	D1753	L1693	S1633	H1574	A1515	I1454	L1392	THR	S1272	D1153	S1091
E1754	E1754	A1575	L1634	A1575	L1516	R1455	S1393	VAL	V1273	E1154	G1092
R1755	R1755	V1576	I1635	V1576	D1517	K1456	R1394	SER	L1274	L1156	L1093
L1817	L1817	N1637	P1636	L1577	V1518	S1457	V1395	LYS	S1275	S1157	G1094
R1818	R1818	I1638	N1637	L1577	V1519	R1458	K1396	SER	S1276	R1158	E1095
R1819	R1819	H1638	I1638	A1578	S1520	V1459	T1397	SER	C1277	W1159	L1096
H1820	H1820	ARG	G1639	L1579	Y1521	V1460	Q1398	LEU	T1278	L1218	S1097
D1821	D1821	GLY	Y1640	C1580	A1522	E1461	K1399	SER	D1279	A1219	Y1098
I1822	I1822	E1702	F1641	R1581	L1523	I1462	E1400	SER	I1280	I1220	H1099
S1823	S1823	D1703	F1642	M1582	L1524	I1463	C1401	ASN	K1281	I1162	F1100
R1824	R1824	Y1705	H1643	S1583	D1524	P1464	S1402	ASN	D1282	L1163	E1102
N1825	N1825	T1706	R1584	R1584	F1526	F1465	F1403	GLU	D1283	D1164	L1103
D1826	D1826	F1707	T1585	T1585	F1527	S1466	I1404	GLN	K1284	W1224	L1104
H1827	H1827	G1708	E1528	C1586	D1527	S1466	T1405		M1285	R1225	A1104
R1828	R1828	F1709	V1529	E1529	E1529	L1467	A1406		A1286	D1226	L1105
W1829	W1829	I1709	V1529	V1529	V1529	S1469	I1407		F1287	R1227	S1106
L1830	L1830	D1710	L1530	K1531	L1530	R1470	Q1408		E1288	T1228	L1107
A1831	A1831	F1711	Q1589	Q1589	Q1589	L1471	G1408		V1289	A1170	W1108
D1832	D1832	G1712	E1590	I1591	D1532	S1472	I1410		V1290	G1171	R1109
R1833	R1833	P1713	H1651	I1591	E1533	G1473	F1411		Y1291	K1172	D1110
R1834	R1834	Y1714	V1652	F1592	D1534	I1474	H1412		H1292	T1173	E1111
D1835	D1835	W1715	L1653	Q1593	D1534	I1474	H1412		Y1293	Q1174	H1112
I1836	I1836	L1716	I1654	H1594	D1536	S1475	G1414		T1294	V1175	S1113
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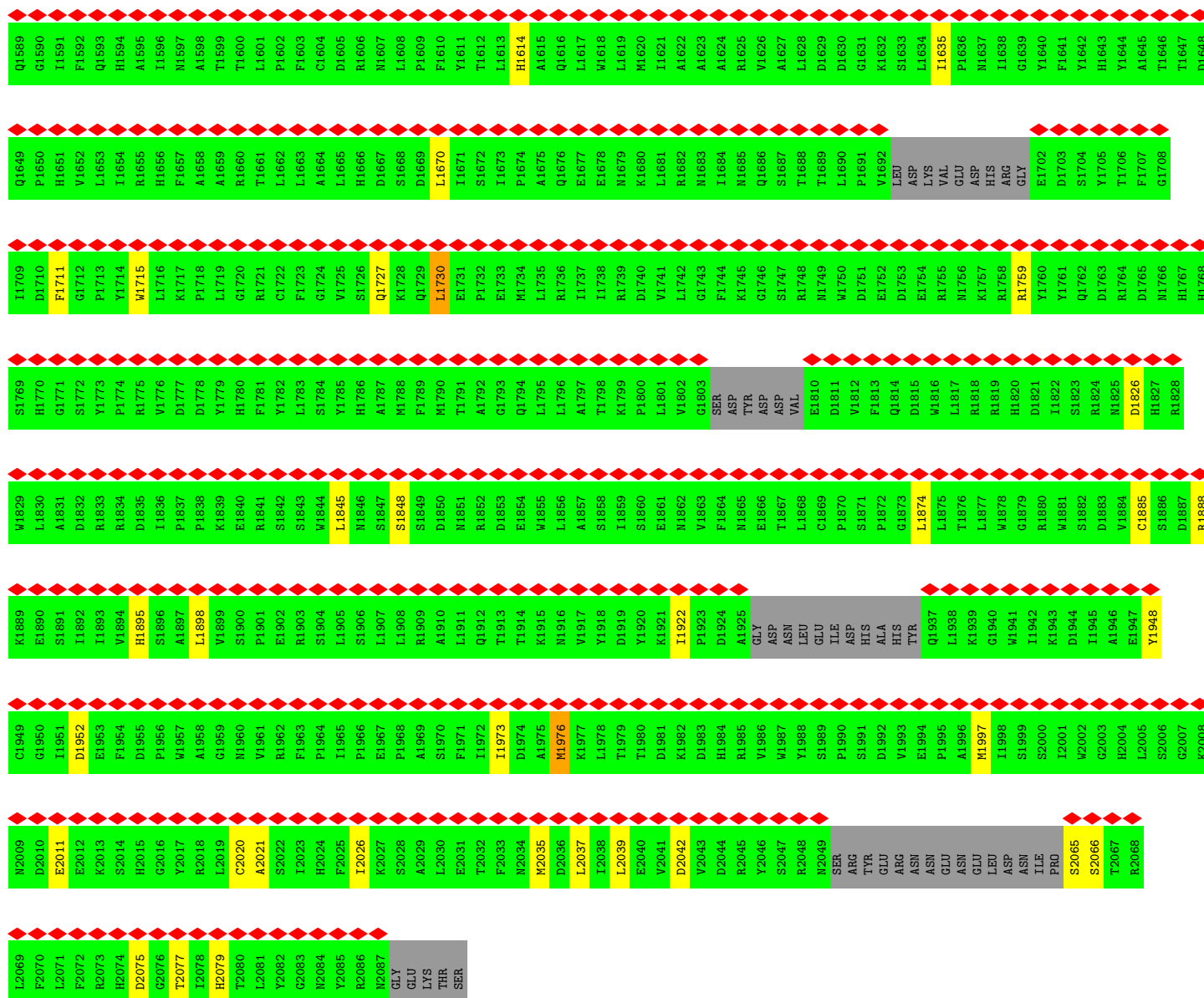
• Molecule 1: SeAvs3



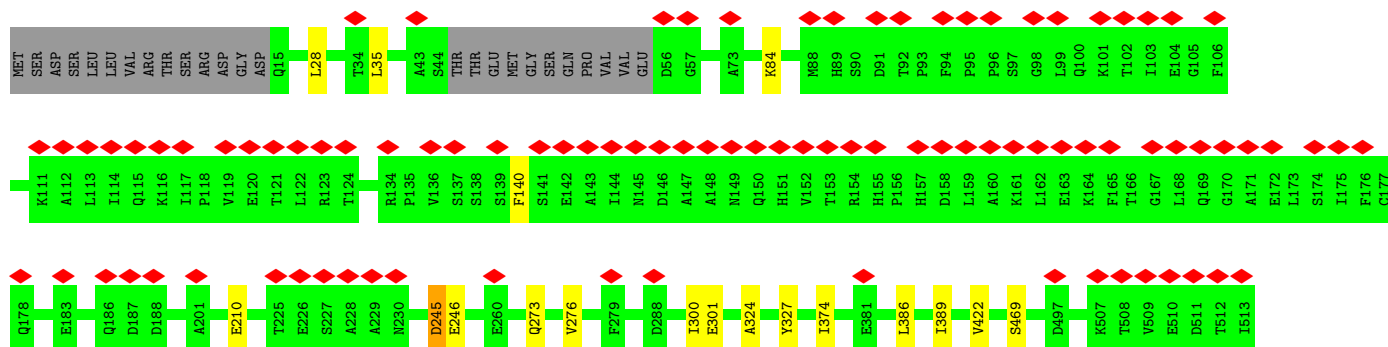
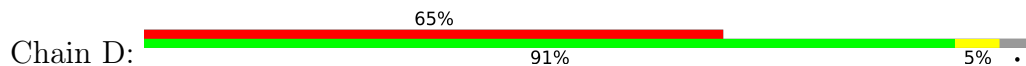
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A1645	T1585	L1525	F1465	I1404	ASP	I1284	W1224	D1164	A1101	E1041	D981	R921
T1646	C1586	F1526	S1466	T1405	ASN	M1285	R1225	L1165	E1102	I1042	D982	Y922
T1647	L1587	D1527	S1467	A1406	GLU	A1286	R1226	A1166	L1103	A1043	L983	L923
L1648	T1588	E1528	A1468	I1407		F1287	R1227	E1167	A1104	N1044	R984	P924
Q1649	Q1589	V1529	S1469	G1408	G1348	E1288	T1228	Y1168	L1105	V1045	Q985	K925
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V1652	F1592	D1532	S1472	F1411	E1352	Y1291	G1231	G1171	W1108	I1048	Q988	P928
L1653	Q1593	E1533	G1473	H1412	W1353	H1292	H1232	K1172	R1109	I1049	Y989	Y929
I1654	H1594	D1534	I1474	W1413	E1354	Y1293	R1233	T1173	D1110	L1050	S990	A930
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A1659	T1599	W1539	I1479	F1418	D1359	V1298	W1238	E1178	A1115	N1055	P995	Y935
R1660	T1600	M1540	F1480	K1419	C1360	Q1299	T1239	I1179	Q1116	V1056	W996	S936
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L1665	D1605	P1545	E1485	S1424	I1365	L1304	V1244	A1184	D1124	V1061	A1001	A941
H1666	P1606	P1546	A1486	I1425	K1366	K1305	K1245	R1185	L1125	E1062	K1002	Y942
D1667	L1607	T1547	I1487	P1426	G1367	K1306	K1246	C1186	S1126	N1063	V1003	V943
S1668	H1608	H1548	A1488	D1427	I1368	L1307	N1247	A1187	R1127	I1064	I1004	R944
D1669	P1609	V1549	E1489	E1428	S1369	D1308	K1248	E1188	S1128	I1065	L1005	A945
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L1673	L1613	L1553	A1494	R1432	E1373	T1312	L1252	E1192	L1132	Q1069	R1009	Q949
P1674	H1614	A1554	N1495	L1433	L1374	S1313	D1253	Y1193	D1133	H1070	K1010	A950
A1675	A1615	G1555	S1496	S1434	F1375	L1314	A1254	V1194	E1134	K1071	A1011	N951
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H1678	W1618	W1558	T1437	T1437	V1378	E1317	D1257	D1197	A1137	R1074	G1014	G954
N1679	L1619	A1559	L1438	T1438	P1379	H1318	L1258	K1198	K1138	V1075	S1015	S955
K1680	M1620	R1560	S1501	L1439	E1380	T1319	T1259	H1199	E1139	E1076	E1016	Q956
L1681	L1621	L1561	L1502	A1440	F1381	E1320	F1260	F1200	Y1140	T1077	L1017	L957
R1682	A1622	G1562	P1503	T1443	Y1382	L1321	E1261	A1201	F1141	P1078	S1018	A958
N1683	A1623	S1563	G1504	K1444	S1383	E1322	N1262	W1202	N1142	T1079	D1019	L959
I1684	A1624	P1564	L1505	L1445	K1384	E1323	D1263	S1203	Q1143	L1080	T1020	S960
N1685	R1625	E1565	L1506	E1445	K1385	R1324	W1264	D1204	A1144	H1081	Q1021	D961
Q1686	V1626	V1507	S1507	Y1446	T1386	L1325	H1265	T1205	I1145	K1082	K1022	L962
S1687	A1627	A1566	F1387	C1447	F1387	S1326	K1266	V1206	E1146	F1083	E1023	A963
T1688	L1628	E1567	I1388	Q1448	I1388	G1327	C1267	E1207	S1084	S1024	S1024	S964
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GLU	P1636	V1576	D1517	K1456	K1396	SER	S1275	S1215	L1156	G1092	Y1032	M972
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HS	T1638	A1578	L1519	R1458	G1398	LYS	C1277	A1217	R1158	G1094	E1034	E974
ARG	G1639	L1579	V1459	V1459	G1398	SER	S1277	W1159	W1159	E1095	H1035	K975
GLY	Y1640	C1580	Y1521	F1460	K1399	LEU	D1278	A1219	A1161	L1096	S1036	R976
E1702	F1641	R1581	E1461	T1462	E1400	SER	D1280	I1220		S1097	L1037	H977
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G1555	S1496	S1434	K1374	G1315	L1255	D1195	I1136	V1075	S955	S955	E835	E835
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H1574	L1516	R1455	R1394	SER	L1274	P1214	S1157	E1095	E1034	E974	L855	L855
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V1576	V1518	S1457	V1396	LYS	S1276	S1216	W1159	L1097	S1036	R976	S915	S915
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M1582	D1524	F1463	ASN	ASN	D1282	S1222	D1165	E1102	I1042	D981	R862	R862
S1583	L1525	P1464	GLU	GLN	D1283	R1223	L1166	L1103	A1043	D982	P863	P863
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C1586	E1528	L1467	A1406		A1286	D1226				Q985	V926	V926
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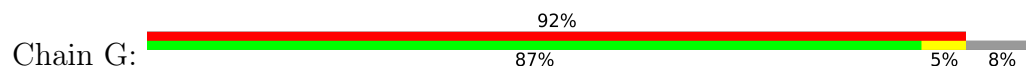
● Molecule 1: SeAvs3



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E1160	A1161	I1162	L1163	D1164	L1165	A1166	E1167	V1168	V1169	A1170	G1171	K1172	T1173	Q1174	W1175	P1176	P1177	E1178	I1179	S1180	Y1181	K1182	L1183	A1184	R1185	C1186	A1187	E1188	L1189	T1190	R1191	E1192	Y1193	V1194	D1195	R1196	D1197	K1198	H1199	F1200	A1201	W1202	S1203	D1204	T1205	E1206	E1207	I1208	L1209	A1210	E1211	L1212	C1213	P1214	S1215	S1216	A1217	L1218	A1219		
S1097	Y1098	H1099	F1100	E1101	E1102	L1103	A1104	L1105	S1106	L1107	W1108	R1109	D1110	E1111	H1112	S1113	D1114	A1115	Q1116	I1117	K1118	A1119	I1123	D1124	L1125	S1126	R1127	S1128	L1129	I1130	S1131	L1132	D1133	E1134	P1135	E1136	A1137	K1138	E1139	Y1140	F1141	N1142	Q1143	A1144	I1145	E1146	W1147	K1150	L1151	D1153	E1154	N1155	L1156	S1157	L1158	W1159					
E1160	A1161	I1162	L1163	D1164	L1165	A1166	E1167	V1168	V1169	A1170	G1171	K1172	T1173	Q1174	W1175	P1176	P1177	E1178	I1179	S1180	Y1181	K1182	L1183	A1184	R1185	C1186	A1187	E1188	L1189	T1190	R1191	E1192	Y1193	V1194	D1195	R1196	D1197	K1198	H1199	F1200	A1201	W1202	S1203	D1204	T1205	E1206	E1207	I1208	L1209	A1210	E1211	L1212	C1213	P1214	S1215	S1216	A1217	L1218	A1219		
S1097	Y1098	H1099	F1100	E1101	E1102	L1103	A1104	L1105	S1106	L1107	W1108	R1109	D1110	E1111	H1112	S1113	D1114	A1115	Q1116	I1117	K1118	A1119	I1123	D1124	L1125	S1126	R1127	S1128	L1129	I1130	S1131	L1132	D1133	E1134	P1135	E1136	A1137	K1138	E1139	Y1140	F1141	N1142	Q1143	A1144	I1145	E1146	W1147	K1150	L1151	D1153	E1154	N1155	L1156	S1157	L1158	W1159					
E1160	A1161	I1162	L1163	D1164	L1165	A1166	E1167	V1168	V1169	A1170	G1171	K1172	T1173	Q1174	W1175	P1176	P1177	E1178	I1179	S1180	Y1181	K1182	L1183	A1184	R1185	C1186	A1187	E1188	L1189	T1190	R1191	E1192	Y1193	V1194	D1195	R1196	D1197	K1198	H1199	F1200	A1201	W1202	S1203	D1204	T1205	E1206	E1207	I1208	L1209	A1210	E1211	L1212	C1213	P1214	S1215	S1216	A1217	L1218	A1219		
S1097	Y1098	H1099	F1100	E1101	E1102	L1103	A1104	L1105	S1106	L1107	W1108	R1109	D1110	E1111	H1112	S1113	D1114	A1115	Q1116	I1117	K1118	A1119	I1123	D1124	L1125	S1126	R1127	S1128	L1129	I1130	S1131	L1132	D1133	E1134	P1135	E1136	A1137	K1138	E1139	Y1140	F1141	N1142	Q1143	A1144	I1145	E1146	W1147	K1150	L1151	D1153	E1154	N1155	L1156	S1157	L1158	W1159					
E1160	A1161	I1162	L1163	D1164	L1165	A1166	E1167	V1168	V1169	A1170	G1171	K1172	T1173	Q1174	W1175	P1176	P1177	E1178	I1179	S1180	Y1181	K1182	L1183	A1184	R1185	C1186	A1187	E1188	L1189	T1190	R1191	E1192	Y1193	V1194	D1195	R1196	D1197	K1198	H1199	F1200	A1201	W1202	S1203	D1204	T1205	E1206	E1207	I1208	L1209	A1210	E1211	L1212	C1213	P1214							

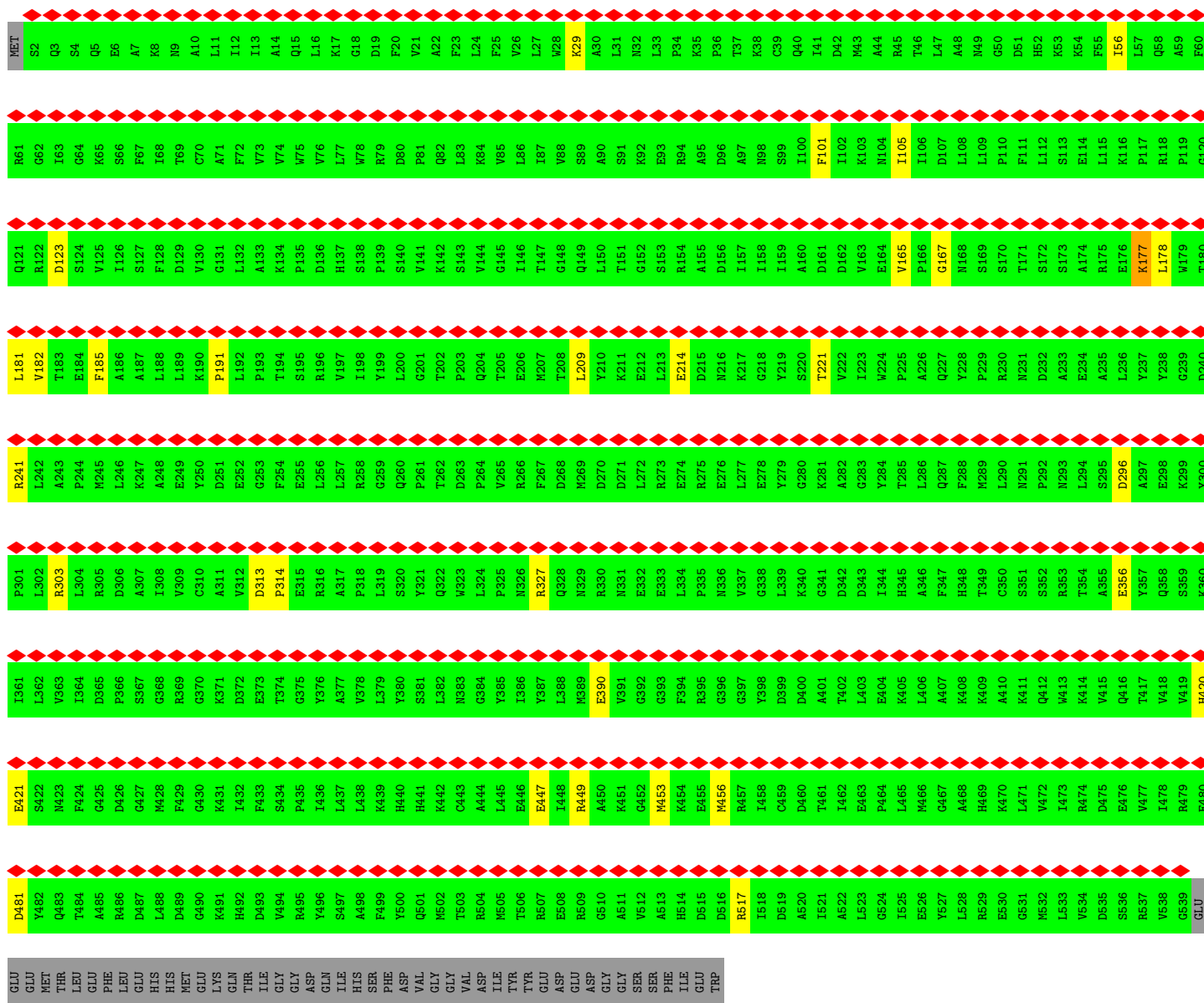
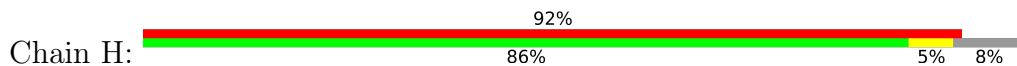
R241	P301	I361	E421	D481	GLU
L242	L302	L362	S422	Y482	GLU
A243	R303	V363	M423	Q483	MET
P244	L304	I364	F424	T484	THR
M245	R305	D365	G425	A485	LEU
L246	D306	P366	G426	R486	PHE
K247	A307	S367	G427	D487	LEU
A248	I308	G368	M428	L488	HIS
E249	V309	R369	F429	D489	HIS
Y250	C310	G370	G430	G490	MET
D251	A311	K371	K431	K491	GLU
E252	V312	D372	I432	H492	LYS
G253	D313	E373	F433	D493	GLN
F254	P314	T374	S434	V494	THR
E255	E315	G375	P435	R495	ILE
L256	R316	Y376	I436	Y496	GLY
L257	A317	A377	S497	S497	ASP
R258	P318	V378	L438	A498	GLN
G259	L319	L379	K439	F499	HIS
Q260	S320	Y380	H440	Y500	SER
P261	Y321	S381	H441	Q501	PHE
T262	Q322	L382	K442	M502	ASP
D263	W323	N383	C443	T503	VAL
P264	L324	G384	A444	R504	VAL
V265	P325	Y385	L445	M505	ASP
R266	N326	I386	L446	T506	ILE
F267	R327	Y387	E447	R507	TYR
D268	Q328	L388	I448	E508	GLU
M269	N329	M389	R449	R509	ASP
D270	R330	E390	A450	G510	ASP
D271	N331	V391	K451	A511	GLY
L272	E332	G392	G452	V512	SER
R273	E333	G393	M453	A513	SER
E274	L334	F394	K454	H514	PHE
R275	P335	R395	E455	D515	ILE
E276	N336	G396	M456	D516	GLU
L277	V337	G397	R457	R517	TRP
E278	G338	Y398	I458	I518	
Y279	L339	D399	C459	D519	
G280	K340	D400	D460	A520	
K281	G341	A401	T461	I521	
A282	D342	T402	I462	A522	
G283	D343	L403	E463	L523	
Y284	I344	E404	P464	G524	
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	E530	
N291	S351	K411	L471	G531	
P292	S352	Q412	V472	M532	
N293	R353	W413	I473	L533	
L294	T354	K414	R474	V534	
S295	A355	V415	D475	D535	
D296	E356	Q416	E476	S536	
A297	Y357	T417	V477	R537	
E298	Q358	V418	I478	V538	
K299	S359	V419	R479	G539	
Y300	K360	H420	E480	GLU	

• Molecule 2: Terminase, large subunit



MET	R61	Q121	L181	R241	P301	I361	E421	D481	GLU
S2	G62	R122	V182	L242	L302	L362	S422	Y482	GLU
Q3	I63	D123	T183	A243	R303	V363	M423	Q483	MET
S4	G64	S124	E184	P244	L304	I364	F424	T484	THR
Q5	K65	I125	F185	M245	D306	D365	G425	A485	LEU
E6	S66	I126	A186	L246	A307	P366	G426	R486	PHE
A7	F67	S127	A187	K247	I308	S367	G427	D487	LEU
K8	T68	F128	L188	A248	V309	G368	M428	L488	HIS
N9	T69	D129	L189	E249	C310	R369	F429	D489	HIS
A10	C70	V130	K190	Y250	A311	G370	G430	G490	MET
L11	A71	G131	P191	D251	V312	K371	K431	K491	GLU
I12	F72	L132	L192	E252	D313	D372	I432	H492	GLN
I13	V73	A133	P193	G253	P314	E373	F433	D493	THR
A14	V74	K134	T194	F254	E315	T374	S434	V494	ILE
Q15	W75	P135	S195	E255	R316	G375	P435	R495	GLY
L16	V76	D136	R196	L256	A317	Y376	I436	Y496	ASP
K17	L77	H137	V197	L257	P318	A377	S497	S497	GLN
G18	W78	I138	I198	R258	L319	V378	L438	A498	HIS
D19	R79	P139	Y199	G259	S320	L379	K439	F499	SER
F20	D80	S140	L200	Q260	Y321	Y380	H440	Y500	PHE
V21	P81	V141	G201	P261	Q322	S381	H441	Q501	ASP
A22	K82	K142	T202	T262	W323	L382	K442	M502	VAL
F23	L83	S143	P203	D263	L324	N383	C443	T503	VAL
L24	K84	V144	Q204	P264	P325	G384	A444	R504	ASP
F25	V85	G145	T205	V265	N326	Y385	L445	M505	ILE
V26	L86	I146	E206	R266	R327	I386	L446	T506	TYR
L27	I87	T147	M207	F267	Q328	Y387	E447	R507	GLU
W28	V88	G148	T208	D268	N329	L388	I448	E508	ASP
K29	S89	L149	L209	M269	R330	M389	R449	R509	ASP
A30	A90	L150	Y210	D270	N331	E390	A450	G510	GLY
L31	S91	T151	K211	D271	E332	V391	K451	A511	SER
N32	K92	G152	E212	L272	E333	G392	G452	V512	SER
L33	E93	S153	L213	R273	L334	G393	M453	A513	PHE
P34	R94	R154	E214	E274	P335	F394	K454	H514	ILE
K35	A95	A155	D215	R275	N336	R395	E455	D515	GLU
P36	D96	D156	N216	E276	V337	G396	M456	D516	TRP
T37	A97	I157	K217	E277	G338	G397	R457	R517	
K38	N98	I158	G218	L277	E278	Y398	I458	I518	
C39	S99	I159	Y219	Y279	L339	D399	C459	D519	
Q40	I100	A160	S220	G280	K340	D400	D460	A520	
I41	F101	D161	T221	K281	G341	A401	T461	I521	
D42	I102	D162	V222	A282	D342	T402	I462	A522	
M43	K103	V163	I223	G283	D343	L403	E463	L523	
A44	N104	E164	W224	Y284	I344	E404	P464	G524	
R45	I105	V165	P225	T285	H345	K405	L465	I525	
T46	I106	P166	A226	L286	A346	L406	M466	E526	
L47	D107	G167	Q227	Q287	F347	A407	G467	Y527	
A48	L108	N168	Y228	F288	H348	K408	A468	L528	
N49	P109	S169	P229	M289	T349	K409	H469	R529	
G50	P110	S170	R230	L290	C350	A410	K470	E530	
D51	F111	T171	N231	N291	S351	K411	L471	G531	
K53	L112	S172	D232	P292	S352	Q412	V472	M532	
K54	E114	A174	E234	L294	R353	W413	I473	L533	
F55	L115	R175	A235	S295	T354	K414	R474	V534	
I56	K116	E176	L236	D296	A355	V415	D475	D535	
L57	P117	K177	Y237	A297	E356	Q416	E476	S536	
Q58	L118	L178	Y238	E298	Y357	T417	V477	R537	
A59	P119	W179	G239	K299	Q358	V418	I478	V538	
F60	G120	T180	D240	Y300	S359	V419	R479	G539	

- Molecule 2: Terminase, large subunit



4 Experimental information

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/16499	0.62	6/22369 (0.0%)
1	B	0.31	0/16319	0.62	5/22123 (0.0%)
1	C	0.31	0/16499	0.61	6/22369 (0.0%)
1	D	0.31	0/16319	0.62	5/22123 (0.0%)
2	E	0.30	0/4363	0.66	6/5899 (0.1%)
2	F	0.31	0/4363	0.65	3/5899 (0.1%)
2	G	0.30	0/4363	0.66	5/5899 (0.1%)
2	H	0.30	0/4363	0.64	2/5899 (0.0%)
All	All	0.31	0/83088	0.63	38/112580 (0.0%)

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

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

There are no bond length outliers.

All (38) bond angle outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	191	PRO	CA-N-CD	-8.29	99.89	111.50
2	H	191	PRO	CA-N-CD	-8.27	99.93	111.50
2	G	191	PRO	CA-N-CD	-8.26	99.94	111.50
2	E	191	PRO	CA-N-CD	-8.23	99.98	111.50
2	F	123	ASP	CB-CG-OD2	8.07	125.56	118.30
2	H	123	ASP	CB-CG-OD2	8.04	125.54	118.30
1	A	96	PRO	N-CD-CG	-7.22	92.38	103.20
1	C	96	PRO	N-CD-CG	-7.20	92.41	103.20
2	E	123	ASP	CB-CG-OD2	6.98	124.58	118.30
2	E	162	ASP	CB-CG-OD1	6.94	124.55	118.30
2	G	389	MET	CG-SD-CE	-6.91	89.15	100.20
2	G	162	ASP	CB-CG-OD1	6.89	124.50	118.30
2	E	389	MET	CG-SD-CE	-6.87	89.20	100.20
2	F	389	MET	CG-SD-CE	-6.87	89.21	100.20
1	D	1845	LEU	CA-CB-CG	6.62	130.53	115.30
1	B	1845	LEU	CA-CB-CG	6.61	130.49	115.30
1	D	245	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	245	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	1845	LEU	CA-CB-CG	5.37	127.64	115.30
1	D	1923	PRO	N-CD-CG	-5.35	95.17	103.20
1	B	1923	PRO	N-CD-CG	-5.34	95.19	103.20
1	C	35	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	35	LEU	CA-CB-CG	5.34	127.57	115.30
1	C	1730	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	1845	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	1730	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	791	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	791	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	1976	MET	CB-CG-SD	5.09	127.67	112.40
1	C	1976	MET	CB-CG-SD	5.08	127.64	112.40
2	E	319	LEU	CA-CB-CG	5.05	126.92	115.30
2	E	191	PRO	N-CD-CG	-5.05	95.63	103.20
2	G	319	LEU	CA-CB-CG	5.04	126.89	115.30
2	G	191	PRO	N-CD-CG	-5.02	95.67	103.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
1	D	548	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16152	0	15975	34	0
1	B	15974	0	15804	49	0
1	C	16152	0	15975	37	0
1	D	15974	0	15804	49	0
2	E	4273	0	4283	11	0
2	F	4273	0	4283	14	0
2	G	4273	0	4283	13	0
2	H	4273	0	4283	16	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
3	E	31	0	12	0	0
3	F	31	0	12	0	0
3	G	31	0	12	0	0
3	H	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
All	All	81600	0	80786	221	0

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

All (221) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:165:VAL:HG12	2:F:167:GLY:H	1.55	0.72
2:H:165:VAL:HG12	2:H:167:GLY:H	1.55	0.70
2:G:165:VAL:HG12	2:G:167:GLY:H	1.61	0.65
1:B:1944:ASP:OD2	1:B:1945:ILE:N	2.30	0.65
2:E:165:VAL:HG12	2:E:167:GLY:H	1.61	0.64
1:D:1944:ASP:OD2	1:D:1945:ILE:N	2.30	0.64
1:B:245:ASP:OD2	1:B:246:GLU:N	2.32	0.63
1:D:245:ASP:OD2	1:D:246:GLU:N	2.32	0.63
1:B:1898:LEU:HB3	1:B:2035:MET:HG2	1.81	0.63
1:D:1898:LEU:HB3	1:D:2035:MET:HG2	1.81	0.62
1:A:1028:LYS:HE3	1:A:1031:SER:HB2	1.81	0.62
1:C:1028:LYS:HE3	1:C:1031:SER:HB2	1.82	0.62
1:C:62:ASP:OD2	1:C:82:GLN:NE2	2.33	0.61
1:B:469:SER:OG	1:B:756:ARG:NH1	2.33	0.61
1:C:1635:ILE:HD11	1:C:1670:LEU:HD12	1.82	0.61
1:D:1635:ILE:HD11	1:D:1670:LEU:HD12	1.83	0.61
1:D:469:SER:OG	1:D:756:ARG:NH1	2.33	0.61
1:A:62:ASP:OD2	1:A:82:GLN:NE2	2.33	0.60
1:B:1635:ILE:HD11	1:B:1670:LEU:HD12	1.83	0.60
1:A:1635:ILE:HD11	1:A:1670:LEU:HD12	1.83	0.60
1:D:963:ALA:HB1	1:D:967:VAL:HG23	1.83	0.60
2:G:43:MET:HE1	2:G:63:ILE:HD13	1.83	0.59
1:C:1848:SER:O	1:C:1888:ARG:NH2	2.35	0.59
1:B:963:ALA:HB1	1:B:967:VAL:HG23	1.83	0.59
2:E:43:MET:HE1	2:E:63:ILE:HD13	1.83	0.59
1:A:1490:SER:OG	1:A:1492:GLU:OE1	2.21	0.58
1:A:1848:SER:O	1:A:1888:ARG:NH2	2.35	0.58
1:C:1490:SER:OG	1:C:1492:GLU:OE1	2.21	0.58
1:D:1490:SER:OG	1:D:1492:GLU:OE1	2.22	0.56
1:B:1490:SER:OG	1:B:1492:GLU:OE1	2.22	0.56
1:B:1388:ILE:HD12	1:B:1407:ILE:HD11	1.88	0.56
1:A:809:ARG:NH2	2:E:539:GLY:O	2.38	0.56
1:D:1388:ILE:HD12	1:D:1407:ILE:HD11	1.87	0.55
1:B:879:GLN:NE2	1:B:880:ARG:O	2.40	0.55
1:D:1388:ILE:O	1:D:1392:ILE:HG13	2.07	0.55
1:D:210:GLU:N	1:D:210:GLU:OE2	2.39	0.54
1:B:210:GLU:N	1:B:210:GLU:OE2	2.39	0.54
1:B:1227:ARG:NH1	1:B:1536:ASP:OD1	2.36	0.54
1:A:2077:THR:OG1	1:A:2079:HIS:NE2	2.41	0.54
1:C:1302:GLN:HA	1:C:1305:LYS:HE3	1.90	0.53
1:D:928:PRO:HD2	1:D:931:LEU:HD23	1.90	0.53
1:D:810:TRP:O	1:D:813:ARG:NH1	2.42	0.53

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

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

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

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

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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

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

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

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

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

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	G	601	4	26,33,33	0.67	0	31,52,52	0.74	2 (6%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	G	601	4	-	3/18/38/38	0/3/3/3
3	ATP	D	2101	4	-	4/18/38/38	0/3/3/3
3	ATP	A	2101	4	-	2/18/38/38	0/3/3/3
3	ATP	B	2101	4	-	4/18/38/38	0/3/3/3
3	ATP	E	601	4	-	2/18/38/38	0/3/3/3
3	ATP	F	601	4	-	3/18/38/38	0/3/3/3
3	ATP	H	601	4	-	2/18/38/38	0/3/3/3
3	ATP	C	2101	4	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2101	ATP	C5-C6-N6	2.28	123.82	120.35
3	C	2101	ATP	C5-C6-N6	2.27	123.80	120.35
3	B	2101	ATP	C5-C6-N6	2.19	123.67	120.35
3	D	2101	ATP	C5-C6-N6	2.18	123.66	120.35
3	F	601	ATP	C5-C6-N6	2.13	123.59	120.35
3	H	601	ATP	C5-C6-N6	2.11	123.56	120.35
3	E	601	ATP	C5-C6-N6	2.11	123.55	120.35
3	G	601	ATP	C5-C6-N6	2.07	123.49	120.35
3	H	601	ATP	PB-O3B-PG	2.05	139.87	132.83
3	E	601	ATP	PB-O3B-PG	2.04	139.84	132.83
3	F	601	ATP	PB-O3B-PG	2.02	139.76	132.83

Continued on next page...

Continued from previous page...

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

There are no chirality outliers.

All (22) torsion outliers are listed below:

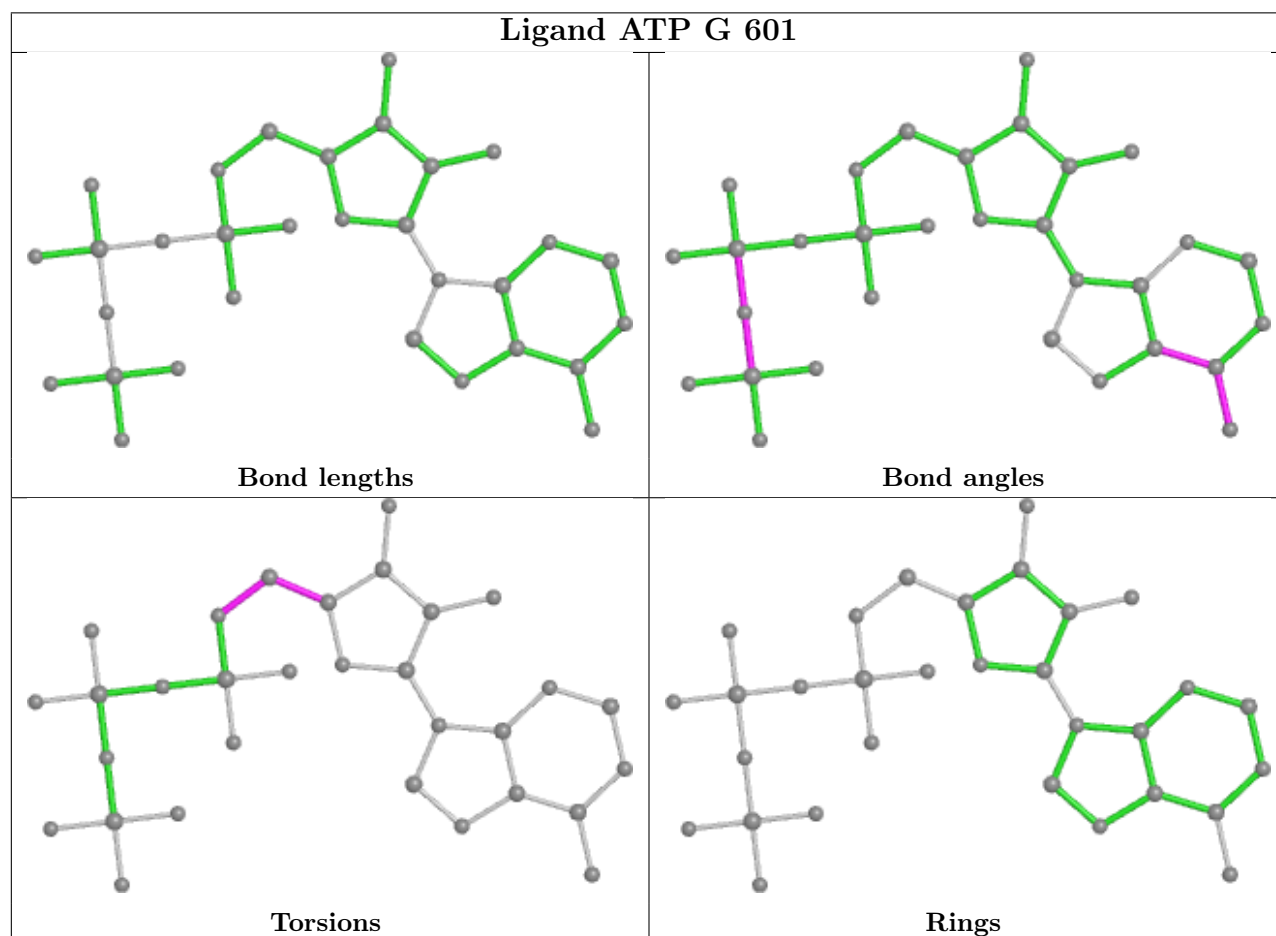
Mol	Chain	Res	Type	Atoms
3	E	601	ATP	O4'-C4'-C5'-O5'
3	H	601	ATP	O4'-C4'-C5'-O5'
3	B	2101	ATP	O4'-C4'-C5'-O5'
3	B	2101	ATP	C3'-C4'-C5'-O5'
3	D	2101	ATP	O4'-C4'-C5'-O5'
3	D	2101	ATP	C3'-C4'-C5'-O5'
3	F	601	ATP	O4'-C4'-C5'-O5'
3	G	601	ATP	O4'-C4'-C5'-O5'
3	A	2101	ATP	PA-O3A-PB-O1B
3	C	2101	ATP	PA-O3A-PB-O1B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

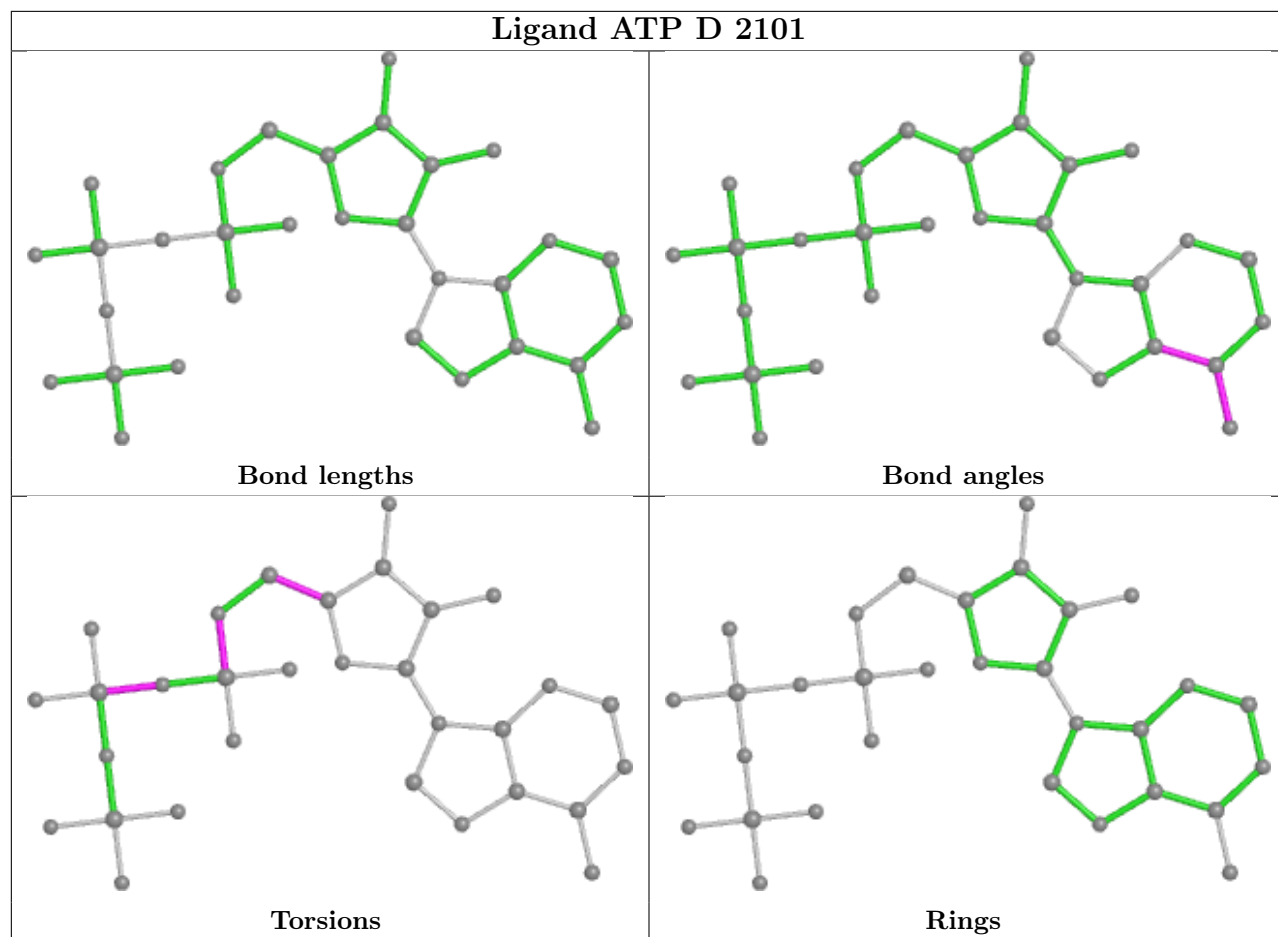
There are no ring outliers.

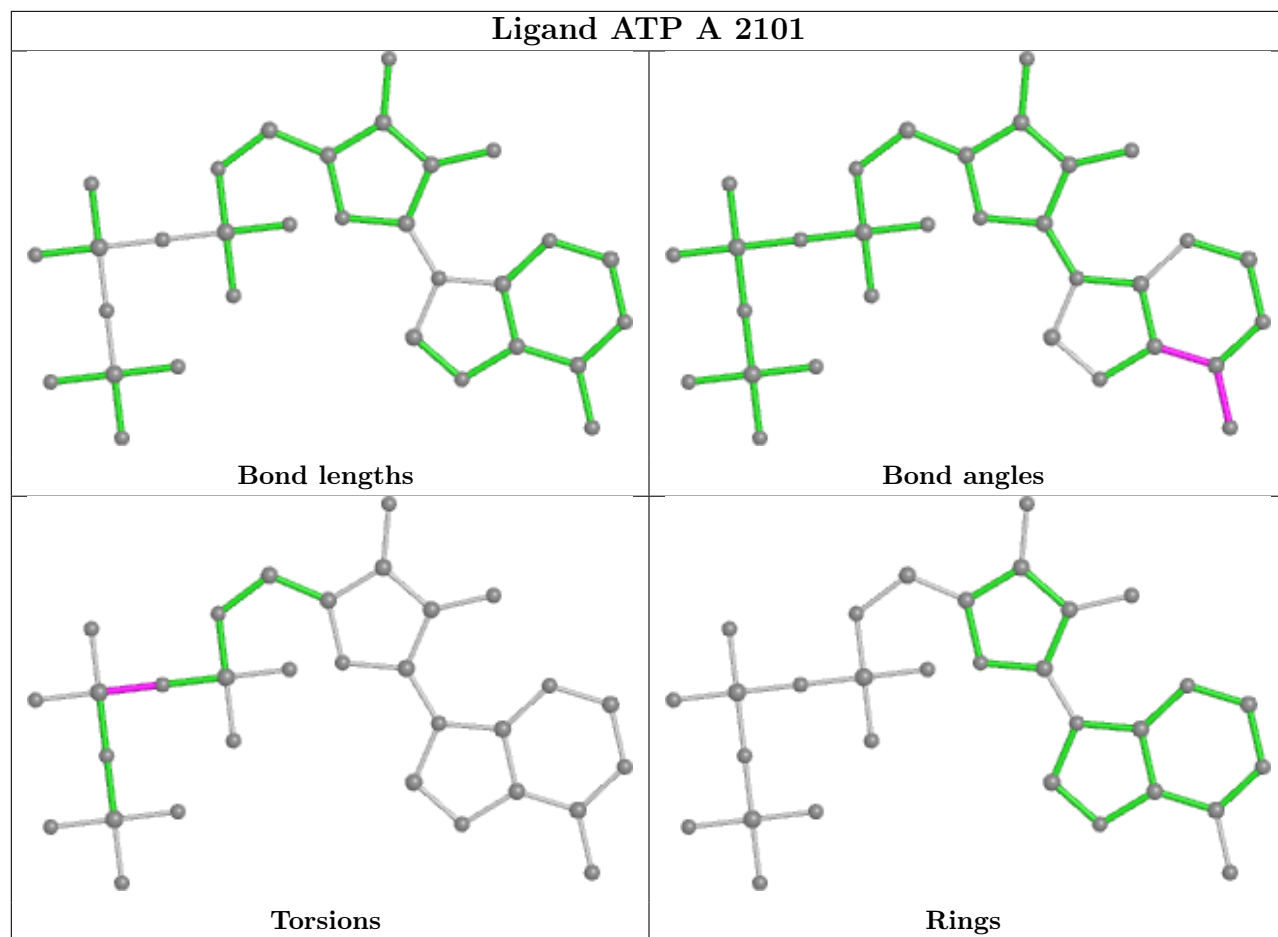
No monomer is involved in short contacts.

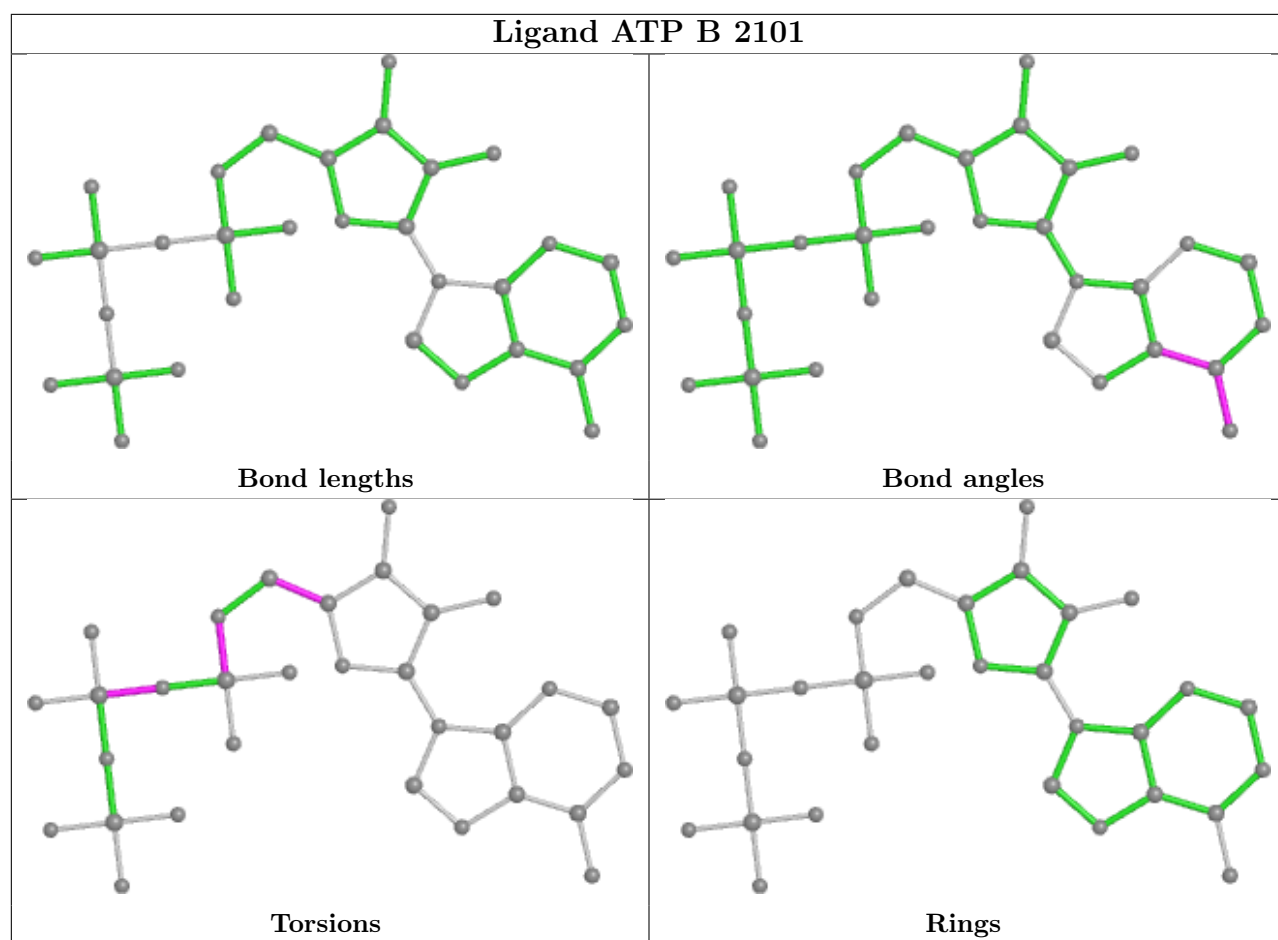
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

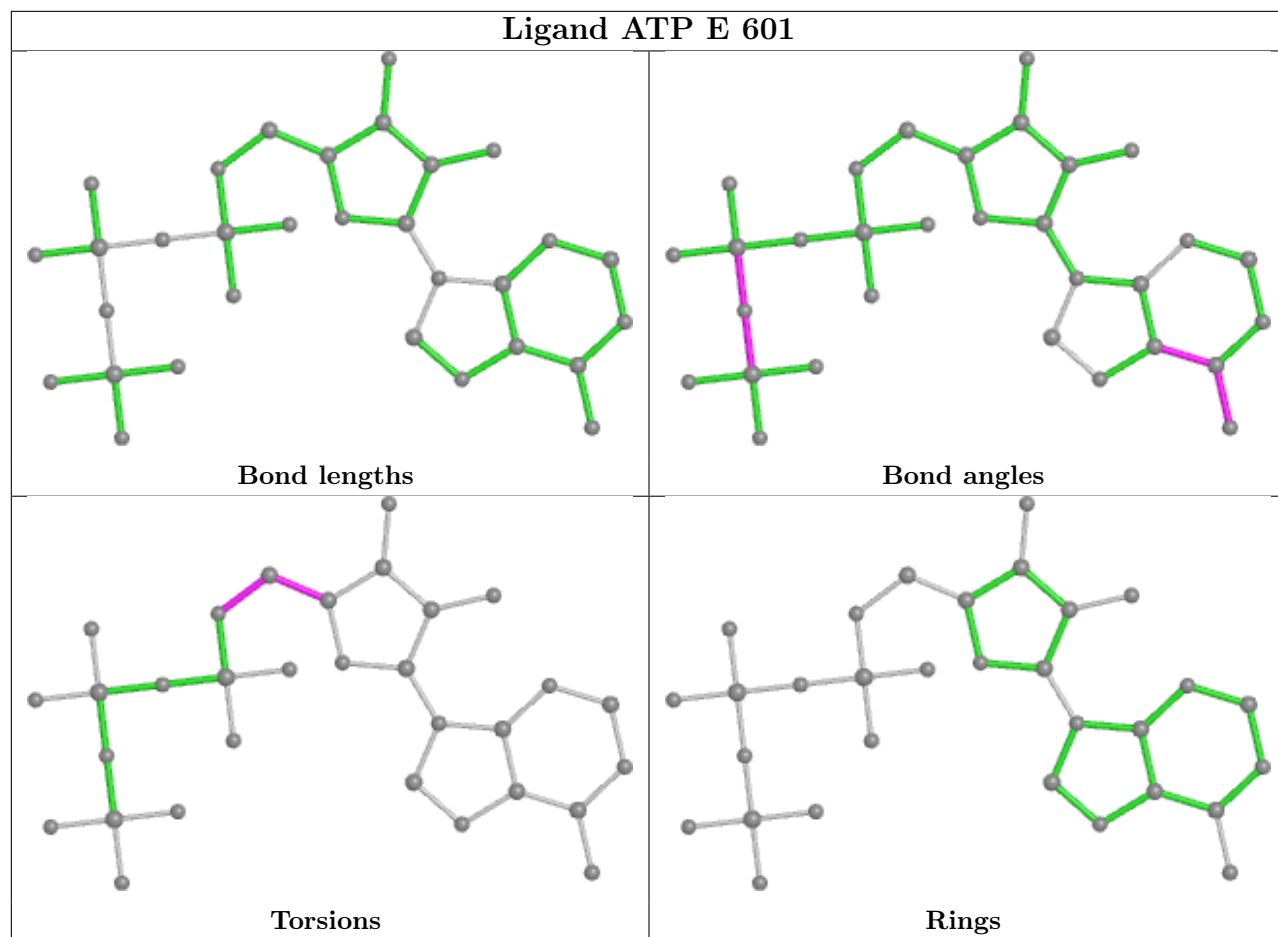
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

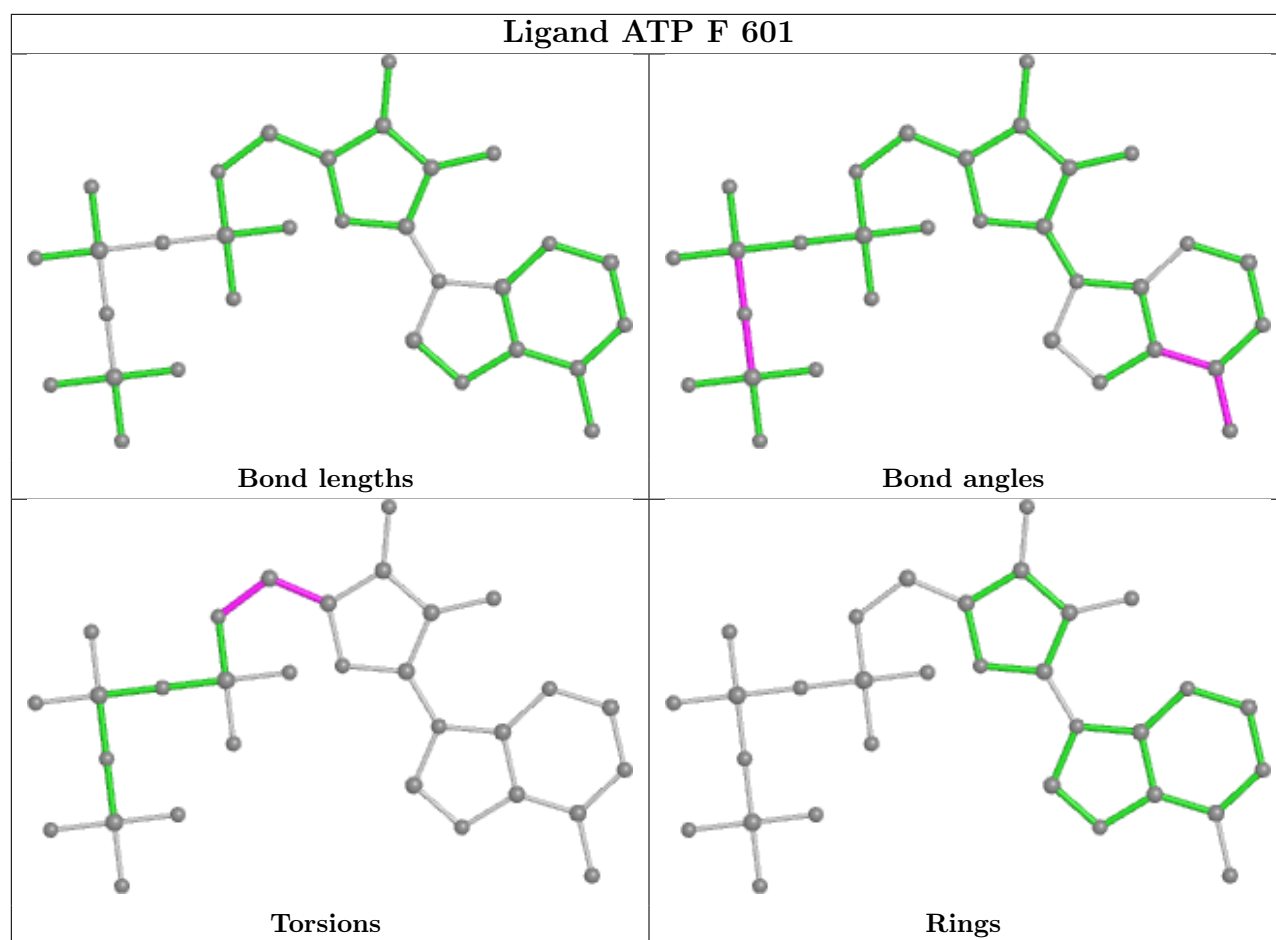


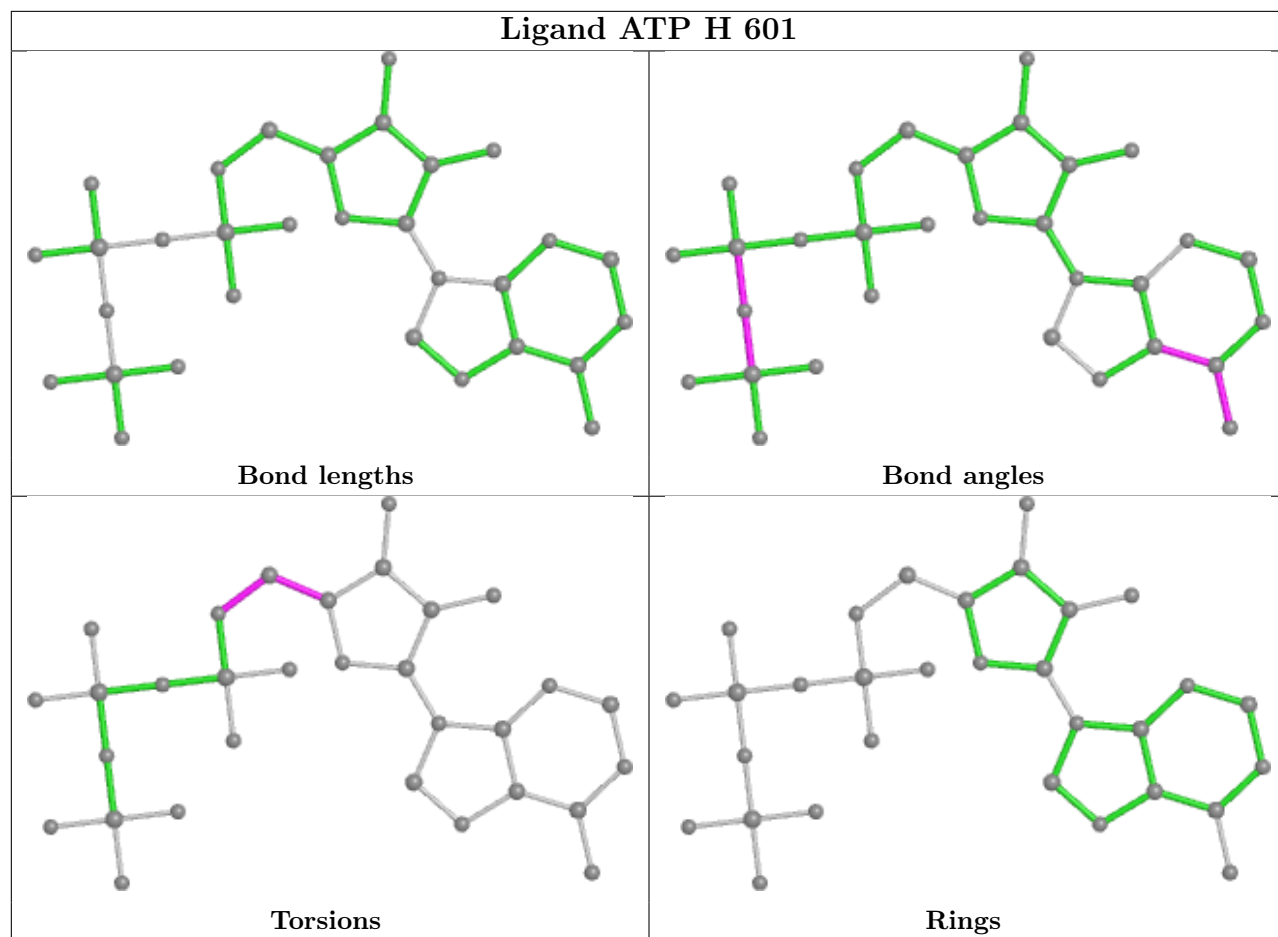


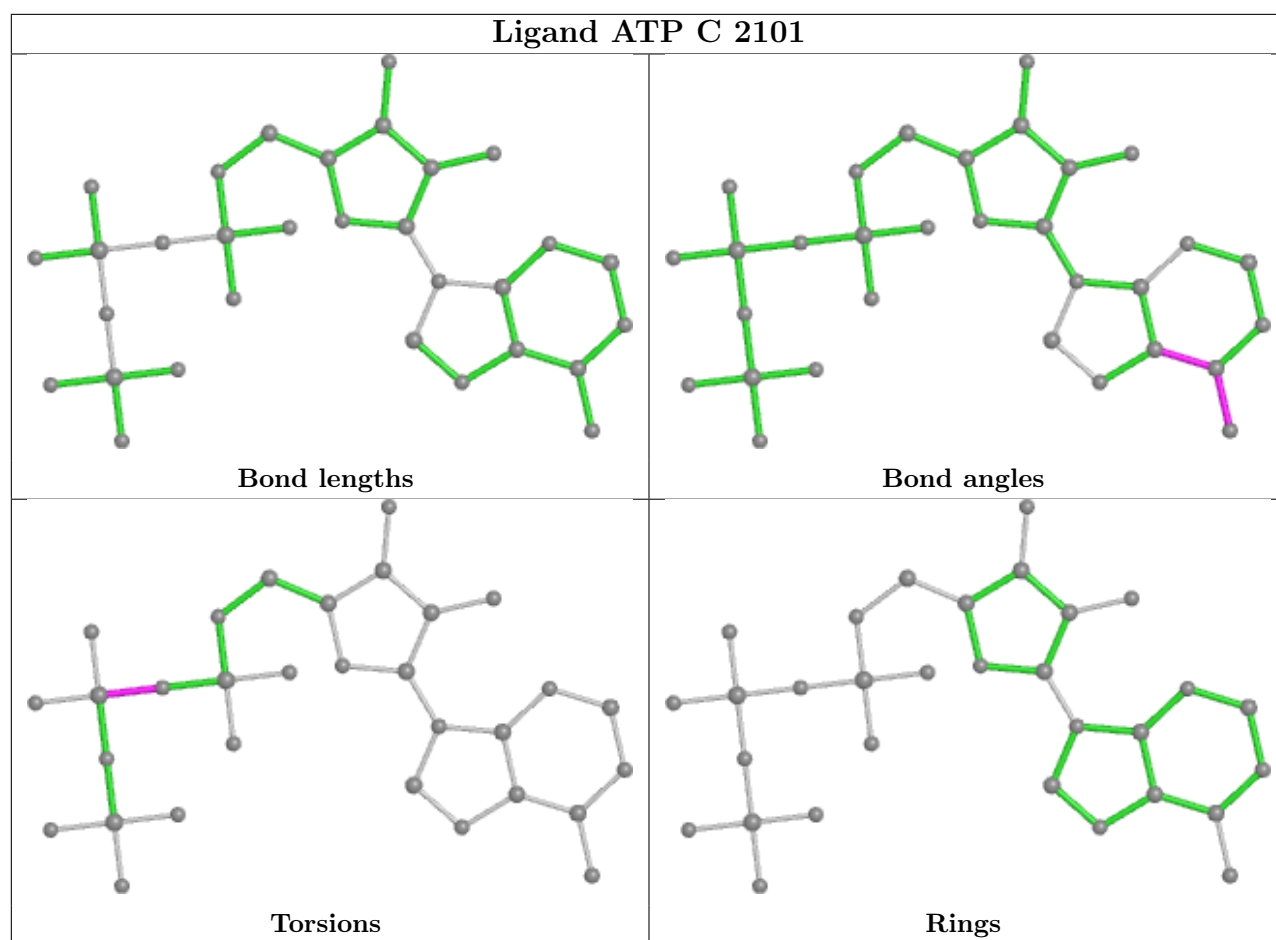












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

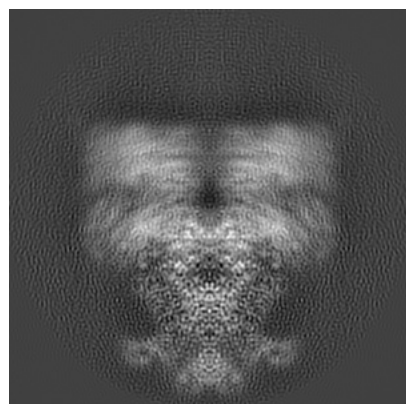
6 Map visualisation [i](#)

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

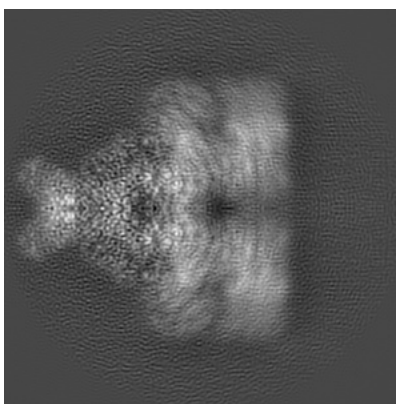
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

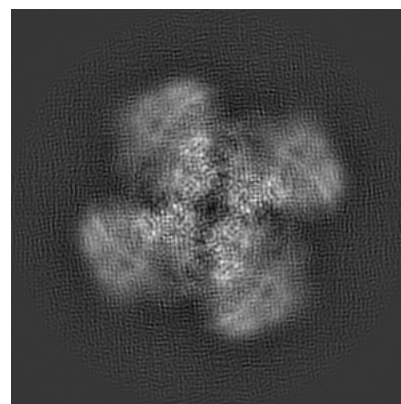
6.1.1 Primary map



X

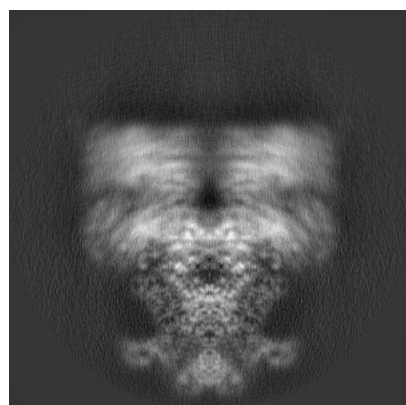


Y

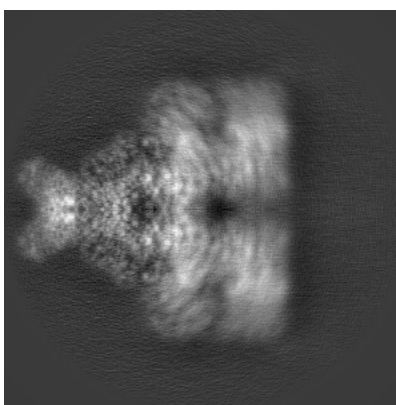


Z

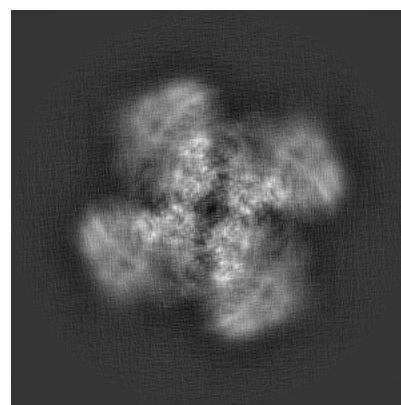
6.1.2 Raw map



X



Y

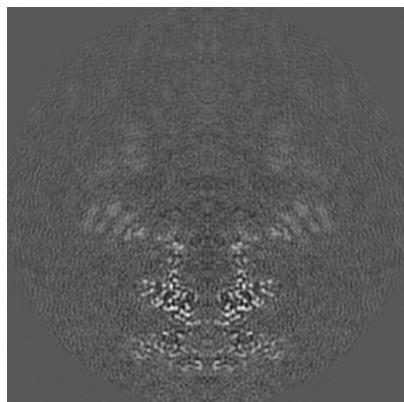


Z

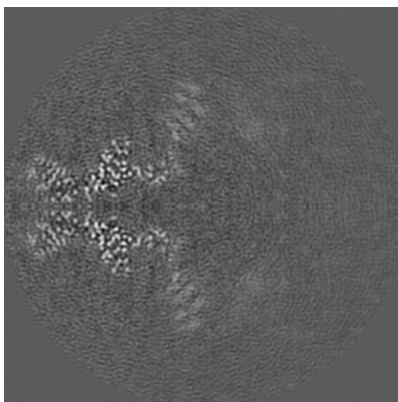
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

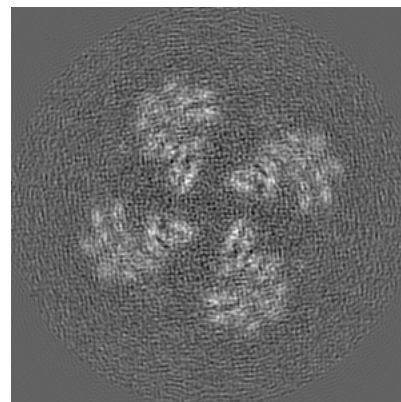
6.2.1 Primary map



X Index: 180

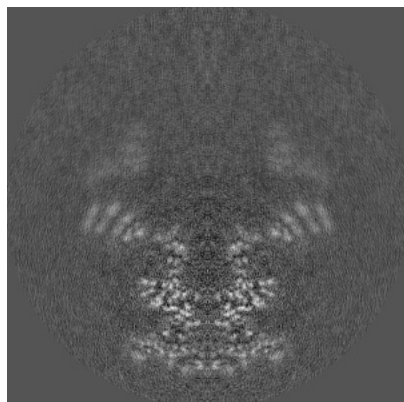


Y Index: 180

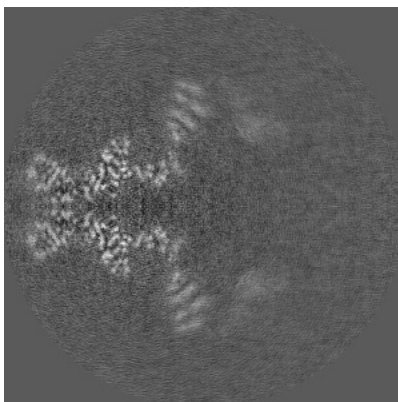


Z Index: 180

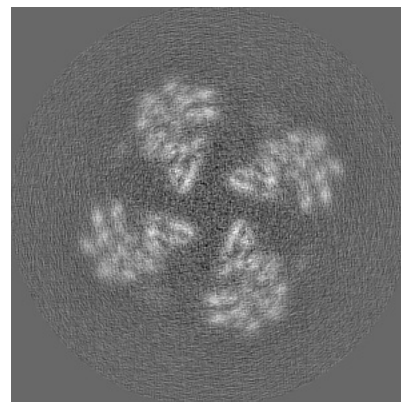
6.2.2 Raw map



X Index: 180



Y Index: 180

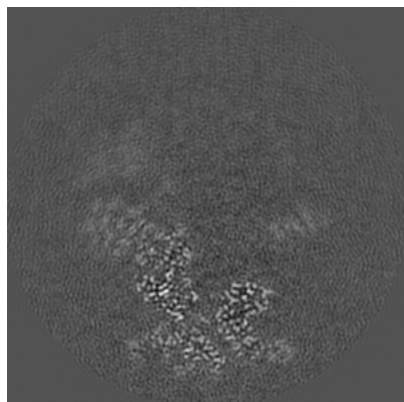


Z Index: 180

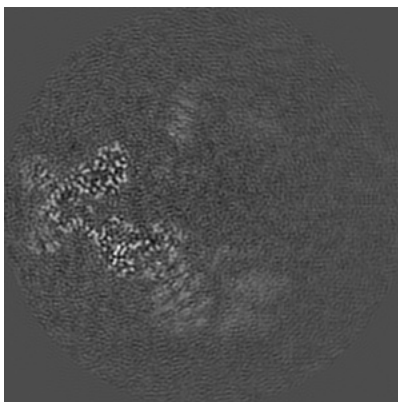
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

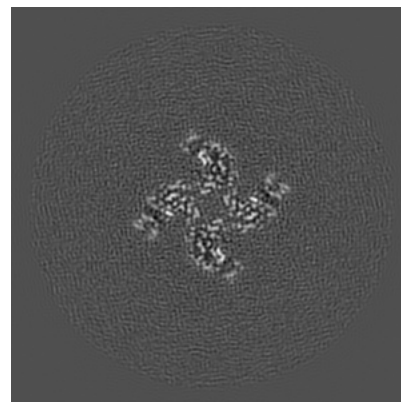
6.3.1 Primary map



X Index: 187

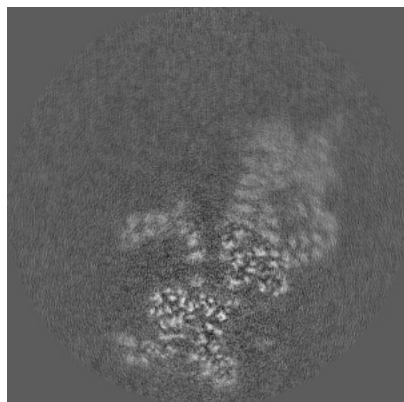


Y Index: 173

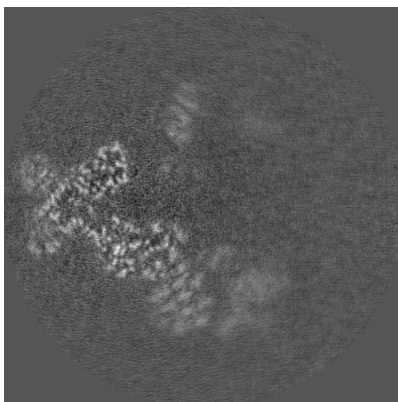


Z Index: 102

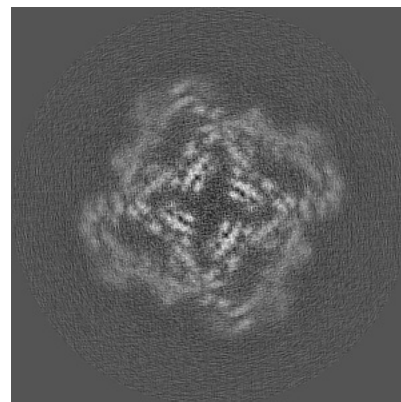
6.3.2 Raw map



X Index: 163



Y Index: 173



Z Index: 155

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



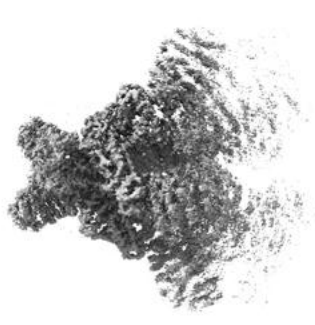
Z

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

6.4.2 Raw map



X



Y



Z

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

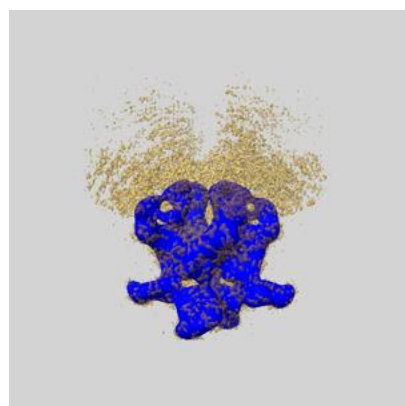
6.5 Mask visualisation [i](#)

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

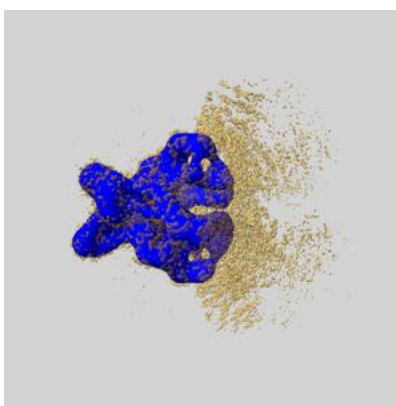
A mask typically either:

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

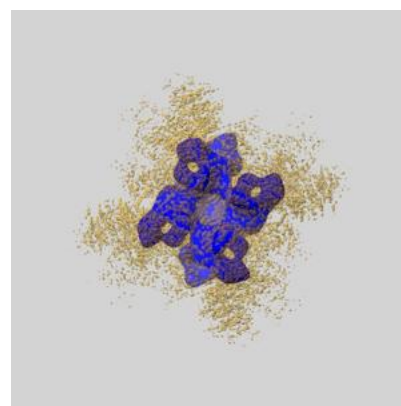
6.5.1 emd_27421_msk_1.map [i](#)



X



Y

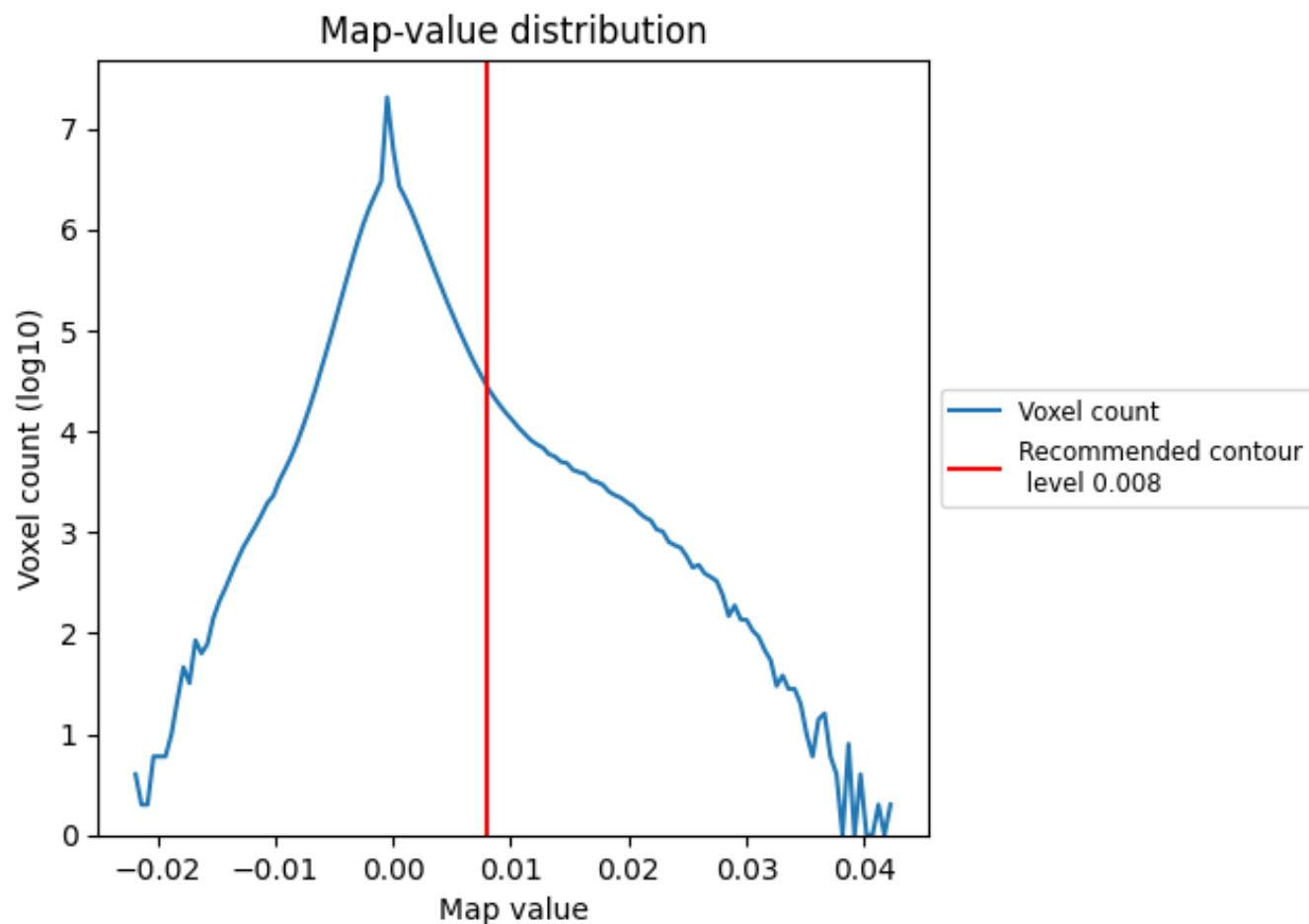


Z

7 Map analysis [i](#)

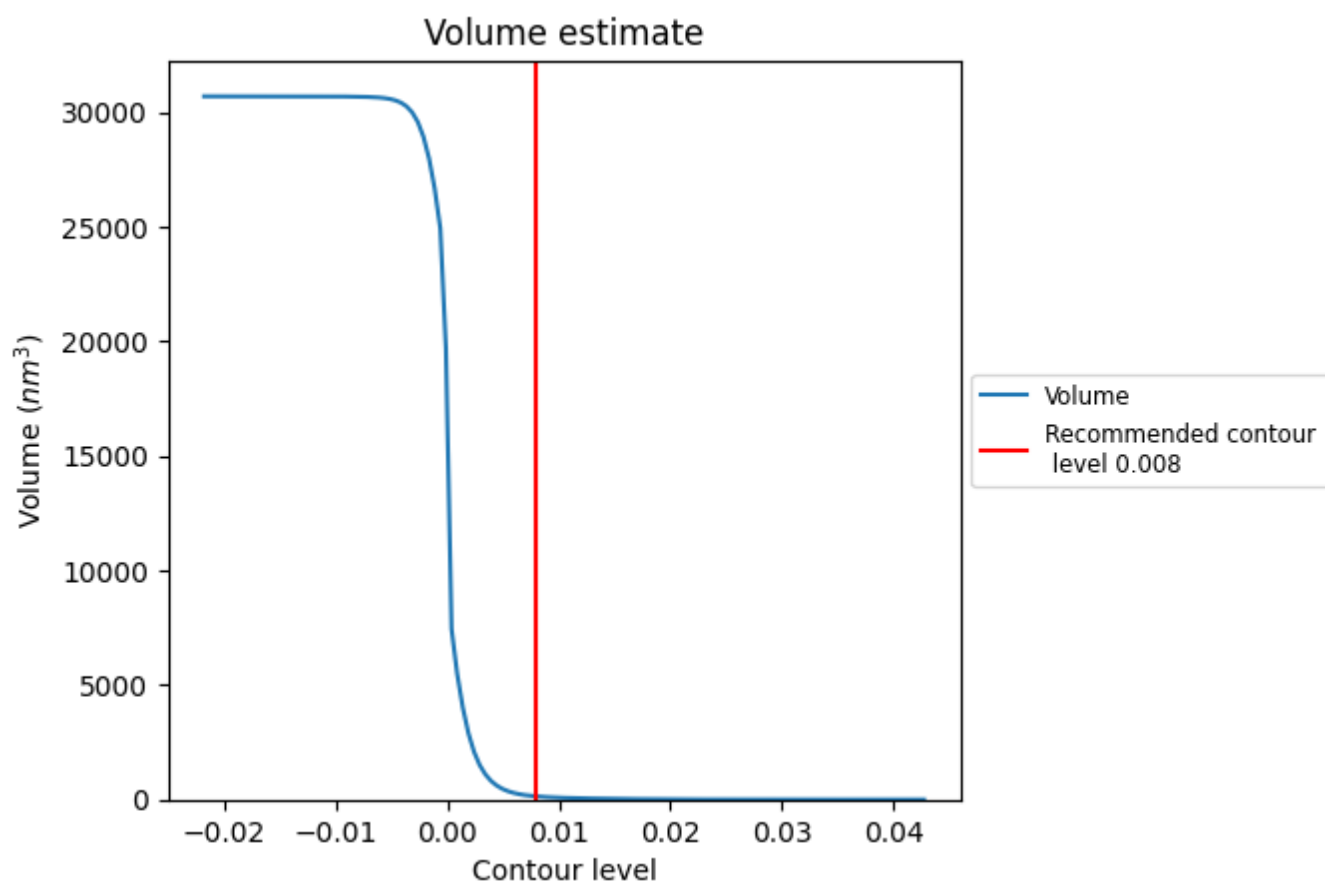
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

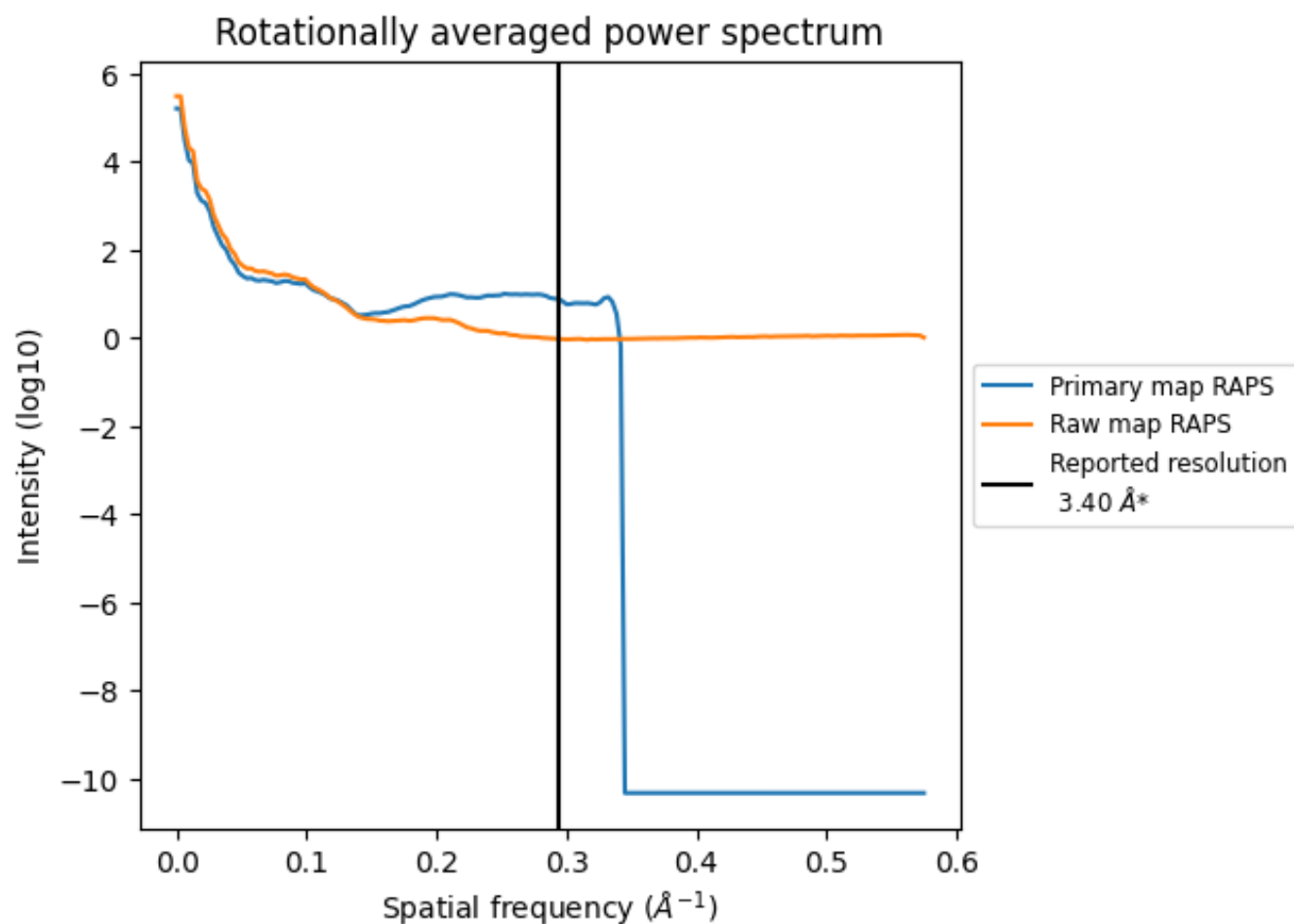
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

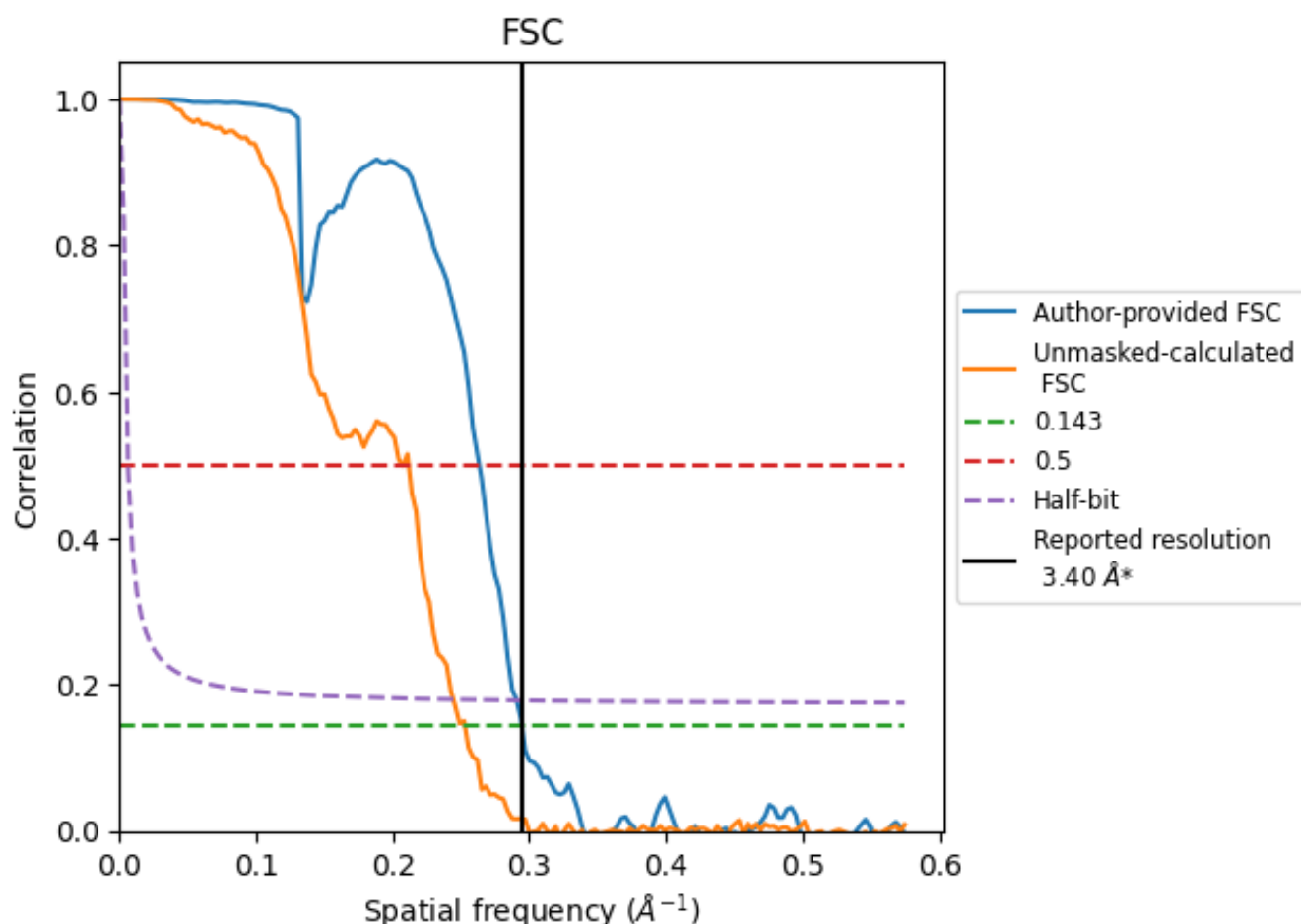


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

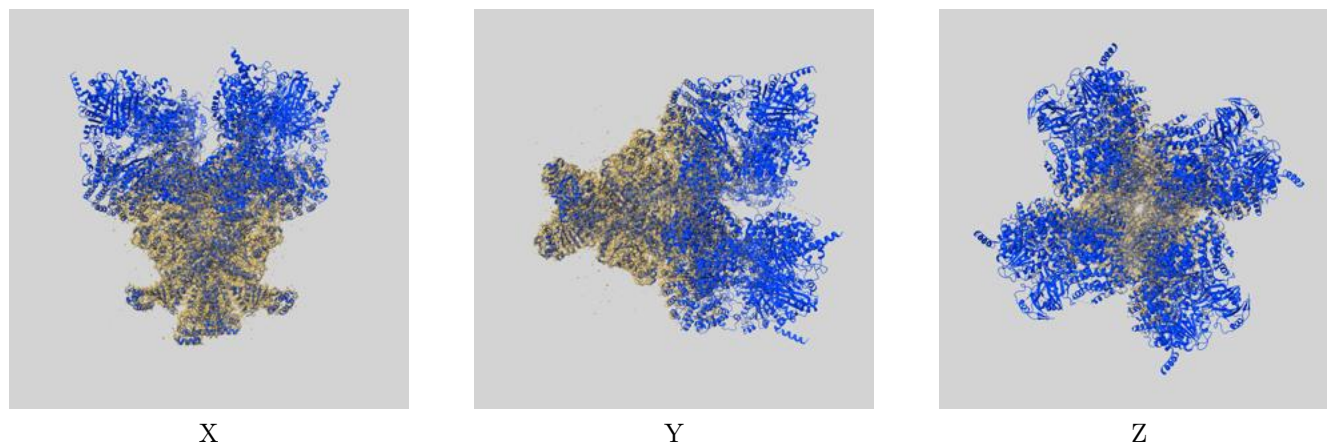
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.80	3.44
Unmasked-calculated*	3.95	4.83	4.09

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

9 Map-model fit [i](#)

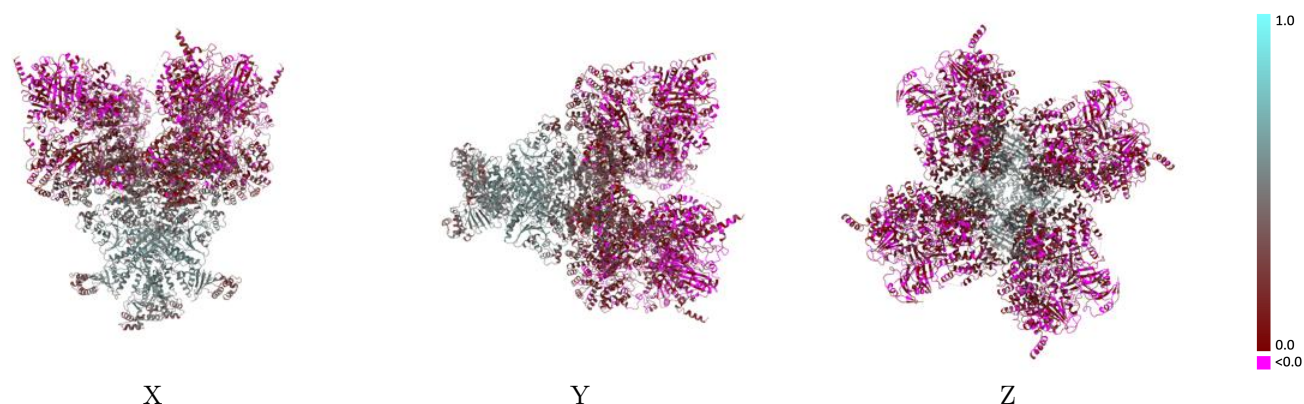
This section contains information regarding the fit between EMDB map EMD-27421 and PDB model 8DGC. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



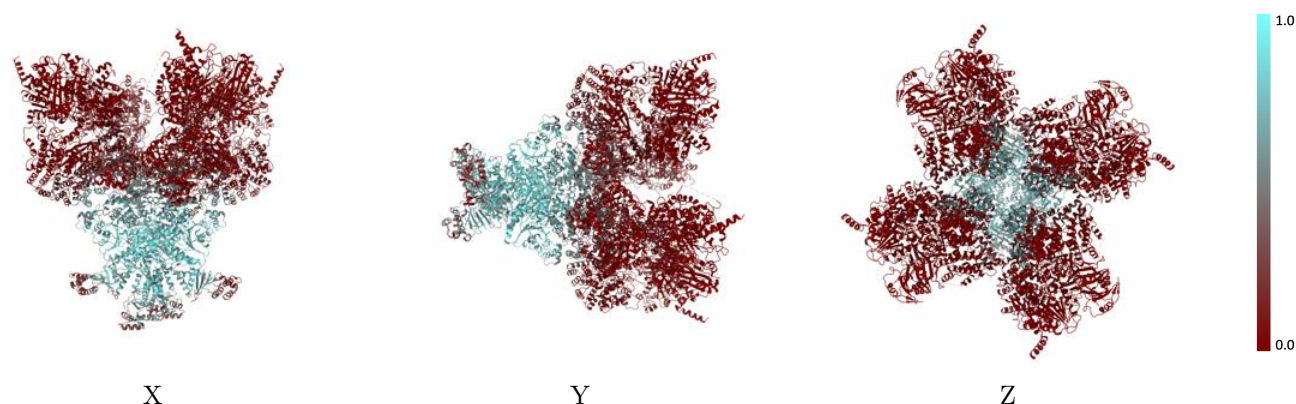
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



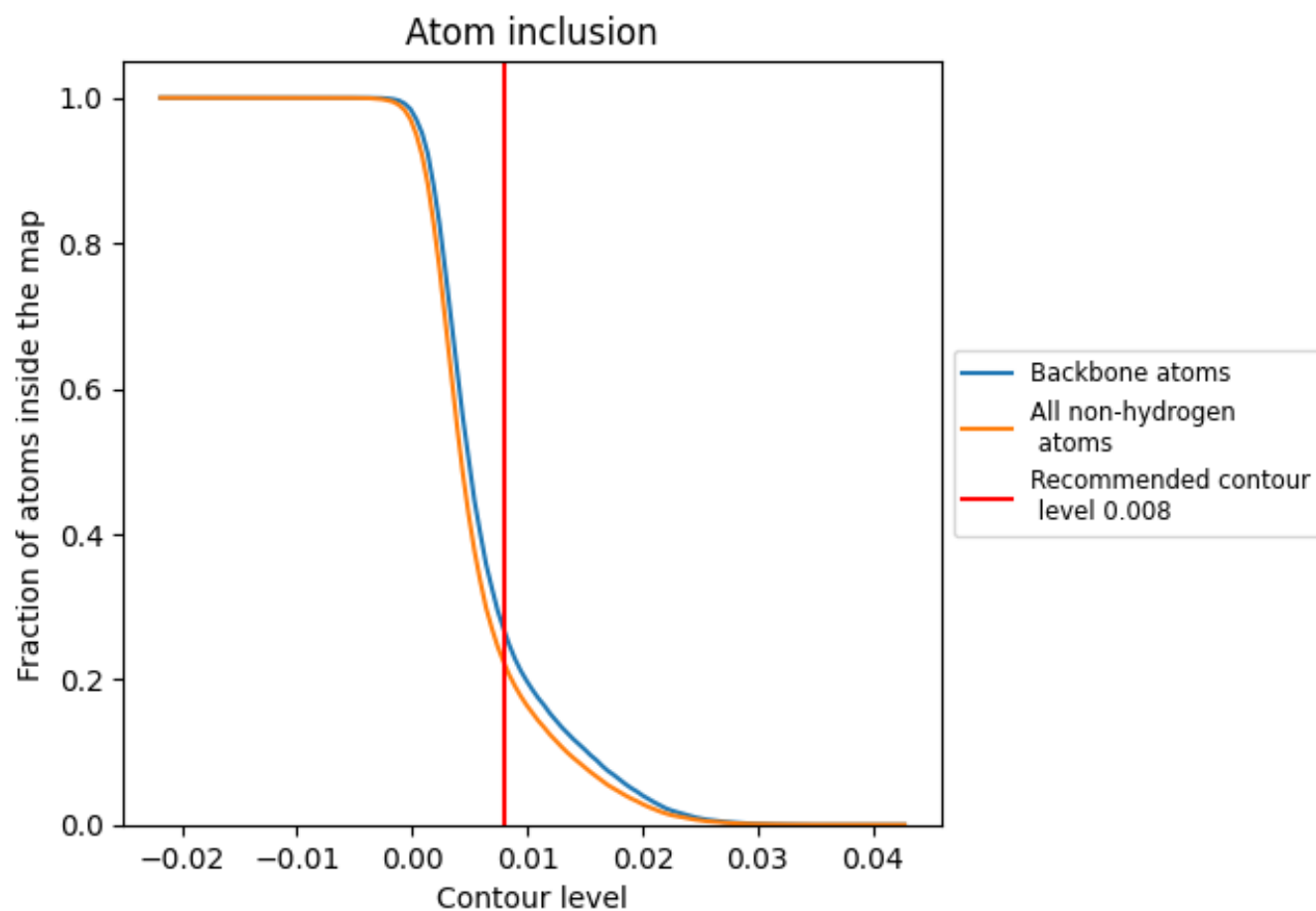
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

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

1.0

0.0

<0.0