



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:30 PM UTC

PDB ID : 8DGC / pdb_00008dgc
EMDB ID : EMD-27421
Title : Avs3 bound to phage PhiV-1 terminase
Authors : Wilkinson, M.E.; Gao, L.; Strecker, J.; Makarova, K.S.; Macrae, R.K.; Koonin, E.V.; Zhang, F.
Deposited on : 2022-06-23
Resolution : 3.40 Å(reported)

This is a 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:

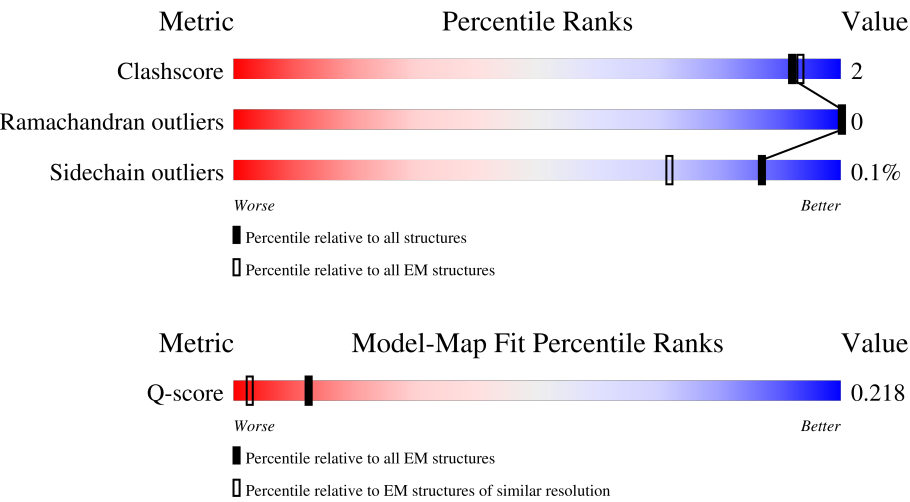
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2092	66% 94%
1	B	2092	65% 91%
1	C	2092	66% 94%
1	D	2092	65% 91%

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 81600 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SeAvs3.

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

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

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

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



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

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

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

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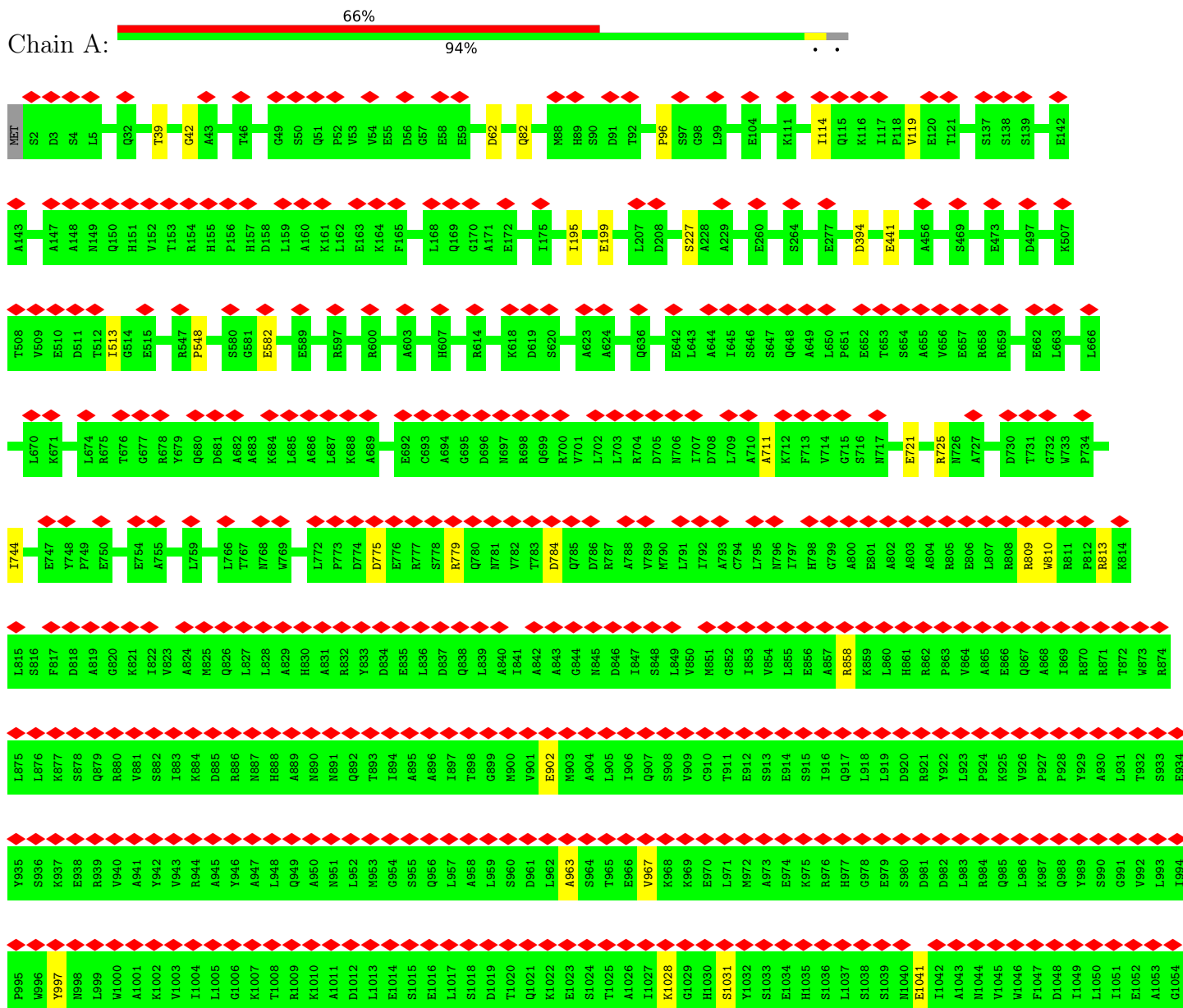
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Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0
4	G	1	Total 1	Mg 1	0
4	H	1	Total 1	Mg 1	0

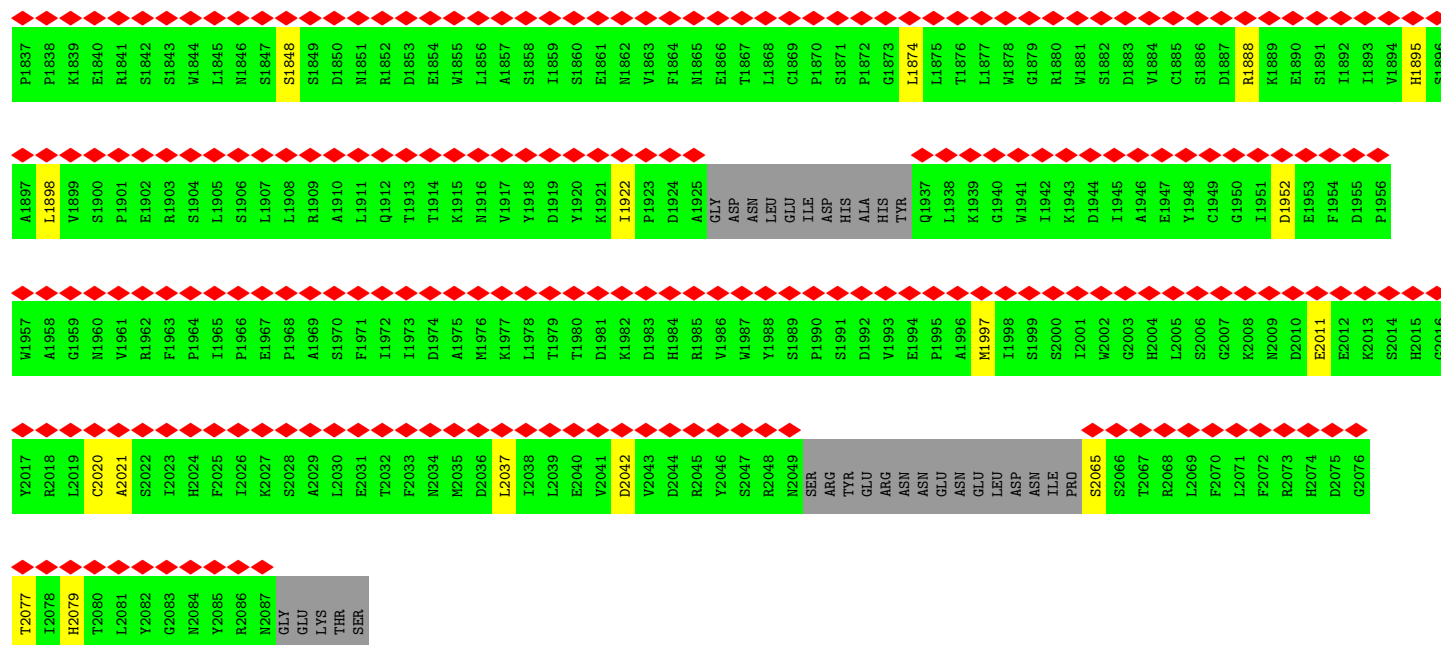
3 Residue-property plots

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

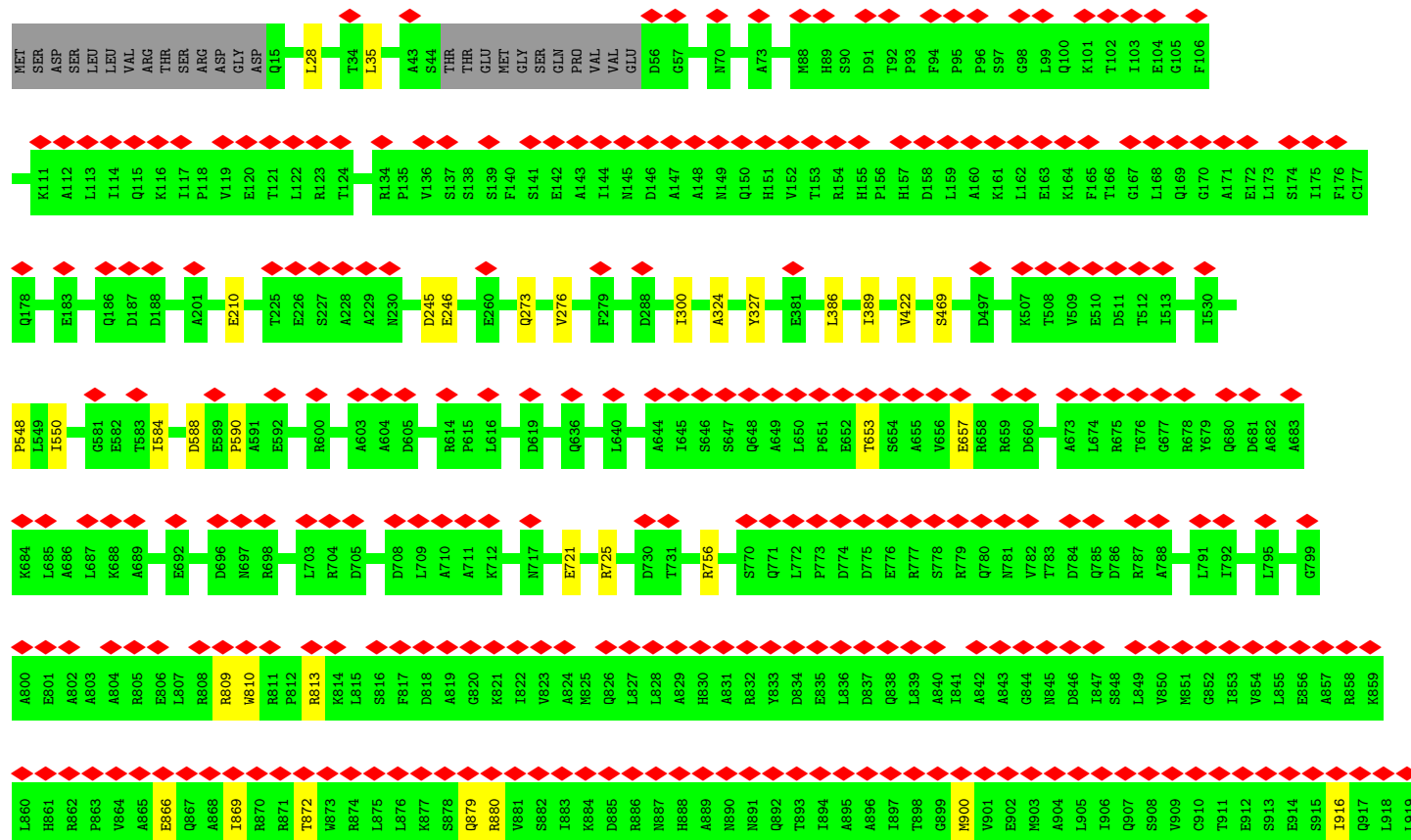
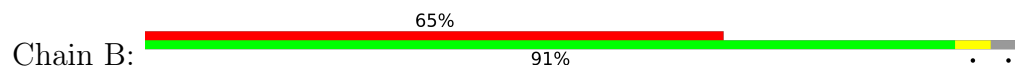
• Molecule 1: SeAvs3



D1777	K1717	F1657	M1597	G1537	K1477	Y1416	I1356	F1296	L1236	P1176	M1055
D1778	P1718	A1658	A1598	P1538	E1478	D1417	F1357	N1297	A1237	P1177	V1056
Y1779	L1719	A1659	T1599	W1539	I1479	F1418	K1358	V1298	W1238	E1178	S1057
H1780	G1720	R1660	T1600	W1540	F1480	K1419	D1359	Q1299	T1239	I1179	K1058
F1781	R1721	L1661	L1601	E1541	G1481	Y1420	C1360	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	P1544	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	K1245	R1185	I1064
Q1727	Q1727	D1667	N1607	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	R1127	W1067
L1730	F1730	L1670	F1610	E1550	S1490	W1429	S1369	A1309	L1249	L1189	S1068
E1731	E1731	I1671	Y1611	D1551	P1491	T1430	A1370	I1310	N1250	T1190	Q1069
A1732	P1732	S1672	T1612	S1552	E1492	S1431	A1371	S1311	A1251	R1191	H1070
G1733	E1733	L1673	L1613	L1553	P1493	R1432	Y1372	L1312	L1252	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	I1435	F1375	G1315	L1255	D1195	R1074
I1737	I1737	E1677	L1617	I1557	D1497	K1436	R1376	I1316	P1256	E1136	V1075
L1738	W1738	E1678	W1618	W1558	L1498		N1377	E1317	L1257	A1137	F1076
R1739	R1739	N1679	L1619	A1559	F1500	L1439	V1378	H1318	I1258	K1138	T1077
D1740	M1620	K1680	M1620	R1560	S1501	A1440	P1379	T1319	T1259	E1139	P1078
V1741	I1621	L1681	I1621	L1561	L1502	G1441	E1380	E1320	F1200	Y1140	T1079
L1742	A1622	R1682	A1622	G1562	P1503	I1442	F1381	L1321	A1201	F1141	L1080
G1743	A1623	L1683	A1623	S1563	G1504	I1443	Y1382	K1322	W1202	N1142	H1081
F1744	A1624	T1684	A1624	P1564	L1505	K1444	S1383	E1323	D1263	Q1143	F1082
K1745	R1625	N1685	R1625	A1565	L1506	E1445	E1384	R1324	W1264	A1144	S1084
G1746	V1626	Q1686	V1626	A1566	Y1507	Y1446	E1385	I1325	H1265	I1145	S1085
S1747	A1627	E1687	A1627	E1567	S1508	C1447	T1386	S1326	K1266	V1206	V1086
R1748	L1628	T1688	L1628	M1568	K1509	Q1448	F1387	G1327	G1267	E1207	C1087
M1749	D1629	L1689	D1629	R1569	L1510	R1449	I1388	L1328	D1268	I1208	A1088
W1750	D1630	T1690	D1630	W1570	E1511	F1450	K1389	Q1329	L1269	L1209	G1092
D1751	G1631	P1691	G1631	Q1571	S1512	C1451	I1390	H1330	A1210	A1210	E1089
E1752	K1632	L1692	K1632	A1572	E1514	M1452	A1391	THR	E1211	D1153	I1090
D1753	L1633	E1693	L1633	H1574	A1515	R1453	I1392	THR	S1272	E1154	S1091
E1754	L1634	A1575	A1516	A1575	L1516	I1454	S1393	VAL	V1273	G1152	G1092
R1755	I1635	V1576	D1517	R1455	R1455	K1456	R1394	SER	L1274	L1156	L1093
N1756	N1636	L1577	V1518	K1457	V1395	S1275	V1395	LYS	S1215	S1157	G1094
K1757	N1637	L1578	V1519	R1458	S1396	S1457	S1396	SER	S1216	R1158	E1095
R1758	I1638	A1578	L1519	V1459	T1397	V1459	T1397	SER	G1277	W1159	L1096
F1759	G1639	L1579	S1520	V1459	Q1398	L1460	Q1398	LEU	L1218	S1097	S1097
Y1760	Y1640	C1580	Y1521	E1461	K1399	E1461	E1400	SER	D1279	E1160	Y1098
Y1761	F1641	R1581	A1522	I1462	E1400	I1404	C1401	ASN	I1220	A1161	H1099
Q1762	F1642	M1582	L1523	I1462	C1401	T1405	S1402	ASP	I1162	L1162	F1100
D1763	H1643	S1583	D1524	P1464	S1402	A1468	S1402	ASN	L1163	D1163	E1102
R1764	Y1644	R1584	L1525	F1465	F1403	F1465	F1403	GLU	D1282	E1164	L1103
D1765	A1645	T1585	F1526	F1466	I1404	S1466	I1404	GLN	W1224	L1165	L1103
L1766	T1646	C1586	D1527	S1467	T1405	L1467	T1405		M1285	A1166	A1104
G1767	T1647	E1587	E1528	A1468	A1406	L1467	A1406		A1286	E1167	L1105
H1768	D1648	I1588	V1529	S1469	I1407	S1469	I1407		F1287	Y1168	S1106
S1769	Q1649	Q1589	K1531	R1470	G1408	R1470	G1408		T1228	L1107	L1107
L1830	P1650	G1590	D1532	L1471	A1409	E1352	E1409		A1170	A1170	W1108
A1831	H1651	I1591	E1533	S1472	I1410	W1353	I1410		G1171	G1171	R1109
D1832	V1652	L1592	D1534	G1473	F1411	E1354	F1411		K1172	K1172	D1110
R1833	L1653	Q1593	D1534	I1474	H1412	E1355	H1412		T1173	T1173	E1111
Y1773	I1654	H1594	D1536	S1475	W1413		W1413		Q1174	Q1174	H1112
R1774	R1655	A1595	I1536	E1476	G1414		G1414		R1234	R1234	S1113
R1775	H1656	I1596			L1415				I1235	I1235	D1114



• Molecule 1: SeAvs3



Y1644	R1584	D1524	P1464	F1403	ASN	K1283	L1163	F1100	N1040	S980	D920
A1645	T1585	L1525	F1465	I1404	ASP	I1284	D1164	A1101	E1041	D981	R921
T1646	C1586	F1526	S1466	T1405	ASN	M1285	L1165	E1102	I1042	D982	Y922
T1647	V1587	D1527	L1467	A1406	GLN	A1286	A1166	L1103	A1043	L983	L923
D1648	I1588	E1528	A1468	I1407	G1348	F1287	E1167	A1104	N1044	R984	P924
P1649	Q1589	V1529	S1469	G1408	H1349	E1288	Y1168	L1105	V1045	Q985	K925
H1651	G1590	L1530	R1470	A1409	D1350	V1289	V1169	S1106	W1046	L986	V926
V1652	K1531	F1531	L1471	I1410	Q1351	V1290	A1170	L1107	F1047	K987	P927
L1653	D1532	E1532	S1472	F1411	E1352	Y1291	G1171	W1108	I1048	Q988	P928
L1654	G1473	G1473	G1473	H1412	W1353	Y1292	K1172	R1109	I1049	Y989	Y929
R1655	I1474	W1413	I1474	W1413	E1354	Y1293	T1173	D1110	L1050	S990	A930
R1656	S1475	G1414	S1475	G1414	S1355	T1294	Q1174	E1111	I1051	G991	L931
P1657	E1476	L1415	E1476	L1415	K1295	K1295	V1175	H1112	E1052	V992	T932
P1658	K1477	Y1416	E1478	Y1416	F1296	F1296	P1176	S1113	A1053	L993	S933
A1658	E1478	D1417	E1479	D1417	M1287	M1287	P1177	D1114	G1054	I994	E934
A1659	I1479	F1418	I1479	F1418	D1359	V1298	E1178	A1115	N1055	P995	Y935
R1660	F1480	K1419	F1480	K1419	C1360	Q1299	Q1116	V1056	V1056	W996	S936
T1661	G1481	Y1420	G1481	Y1420	D1361	W1300	I1179	I1117	S1057	Y997	K937
L1662	I1482	I1421	I1482	I1421	L1362	I1301	Y1181	K1118	K1058	R998	E938
L1663	L1483	L1422	L1483	L1422	Q1302	Q1302	K1182	A1119	D1059	L999	R939
A1664	L1484	E1423	L1484	E1423	M1303	M1303	L1183	D1060	I1060	V1000	V940
L1665	E1485	S1424	E1485	S1424	I1365	I1365	A1184	I1061	A941	A1001	A941
H1666	A1486	I1425	A1486	I1425	D1366	K1305	R1185	E1062	Y942	K1002	Y942
D1667	I1487	P1426	I1487	P1426	G1367	K1306	C1186	I1063	V943	V1003	V943
S1668	A1488	D1427	A1488	D1427	I1368	L1307	A1187	I1064	R944	I1004	R944
D1669	E1489	E1428	E1489	E1428	S1369	D1308	E1188	I1065	A945	A945	A945
L1670	S1490	W1429	S1490	W1429	A1370	A1309	L1189	K1066	Y946	G1006	Y946
I1671	P1491	Y1430	P1491	Y1430	A1371	I1310	T1190	W1067	A947	K1007	A947
S1672	E1492	T1431	E1492	T1431	Y1372	S1311	E1192	S1068	L948	T1008	L948
L1673	P1493	R1432	P1493	R1432	E1373	T1312	R1191	Q1069	R949	R1009	R949
P1674	A1494	L1433	A1494	L1433	K1374	S1313	Y1193	H1070	A950	K1010	A950
A1675	N1495	S1434	N1495	S1434	F1375	L1314	E1194	K1071	N951	N951	N951
Q1676	S1496	I1435	S1496	I1435	R1376	G1315	D1195	G1072	L952	D1012	L952
P1677	D1497	K1436	D1497	K1436	N1377	L1316	R1196	M953	M953	L1013	M953
E1678	L1498	T1437	E1678	T1437	V1378	E1317	D1197	G954	G954	E1014	G954
N1679	F1500	T1438	N1679	T1438	P1379	H1318	K1198	S955	S955	E1015	S955
K1680	S1501	L1439	K1680	L1439	A1380	T1319	H1199	Q956	Q956	E1016	Q956
L1681	L1502	A1440	L1681	A1440	F1381	E1320	F1200	L1017	L957	L1017	L957
R1682	P1503	I1443	R1682	I1443	Y1382	L1321	A1201	P1078	A958	S1018	A958
N1683	G1504	K1444	N1683	K1444	S1383	K1322	W1202	T1079	L959	D1019	L959
I1684	L1505	E1445	I1684	E1445	K1384	E1323	S1203	L1080	S960	T1020	S960
N1685	L1506	Y1446	N1685	Y1446	E1385	R1324	D1204	H1081	D961	Q1021	D961
Q1686	V1507	K1447	Q1686	K1447	T1386	I1325	T1205	K1082	L962	K1022	L962
S1687	S1508	C1447	S1687	C1447	F1387	S1326	V1206	F1083	A963	E1023	A963
T1688	K1509	Q1448	T1688	Q1448	I1388	L1327	E1207	S1085	S964	S1024	S964
L1689	L1510	R1449	L1689	R1449	K1389	G1328	I1208	V1086	T965	T1025	T965
T1689	E1511	F1450	T1689	F1450	K1390	Q1329	L1209	C1087	A1026	A1026	E966
L1690	C1451	C1451	L1690	C1451	L1330	H1330	A1210	I1027	V967	I1027	V967
P1691	M1452	M1452	P1691	M1452	I1391	THR	E1211	K1028	K968	G1029	K968
V1692	L1453	L1453	V1692	L1453	L1392	GLU	L1212	D1153	K969	H1030	K969
LEU	S1393	S1393	LEU	S1393	THR	THR	C1213	H1031	E970	L971	E970
ASP	R1394	R1394	ASP	R1394	VAL	VAL	P1214	S1091	M972	L971	M972
LVS	V1395	V1395	LVS	V1395	LYS	LYS	S1215	G1092	A973	Y1032	A973
GLU	K1396	K1396	GLU	K1396	LYS	LYS	R1158	L1093	E974	E1034	E974
ASP	S1457	S1457	ASP	S1457	THR	THR	W1159	G1095	K975	H1035	K975
HIS	R1458	R1458	HIS	R1458	ARG	ARG	L1218	L1096	R976	L1037	R976
ARG	V1459	V1459	ARG	V1459	LEU	LEU	A1161	S1097	H977	S1038	H977
GLY	Y1460	Y1460	GLY	Y1460	GLY	GLY	I1162	H1098	E978	S1039	E978
E1702	Y1640	Y1640	E1702	Y1640	C1401	C1401	S1222				
D1703	F1643	F1643	D1703	F1643	S1402	S1402					

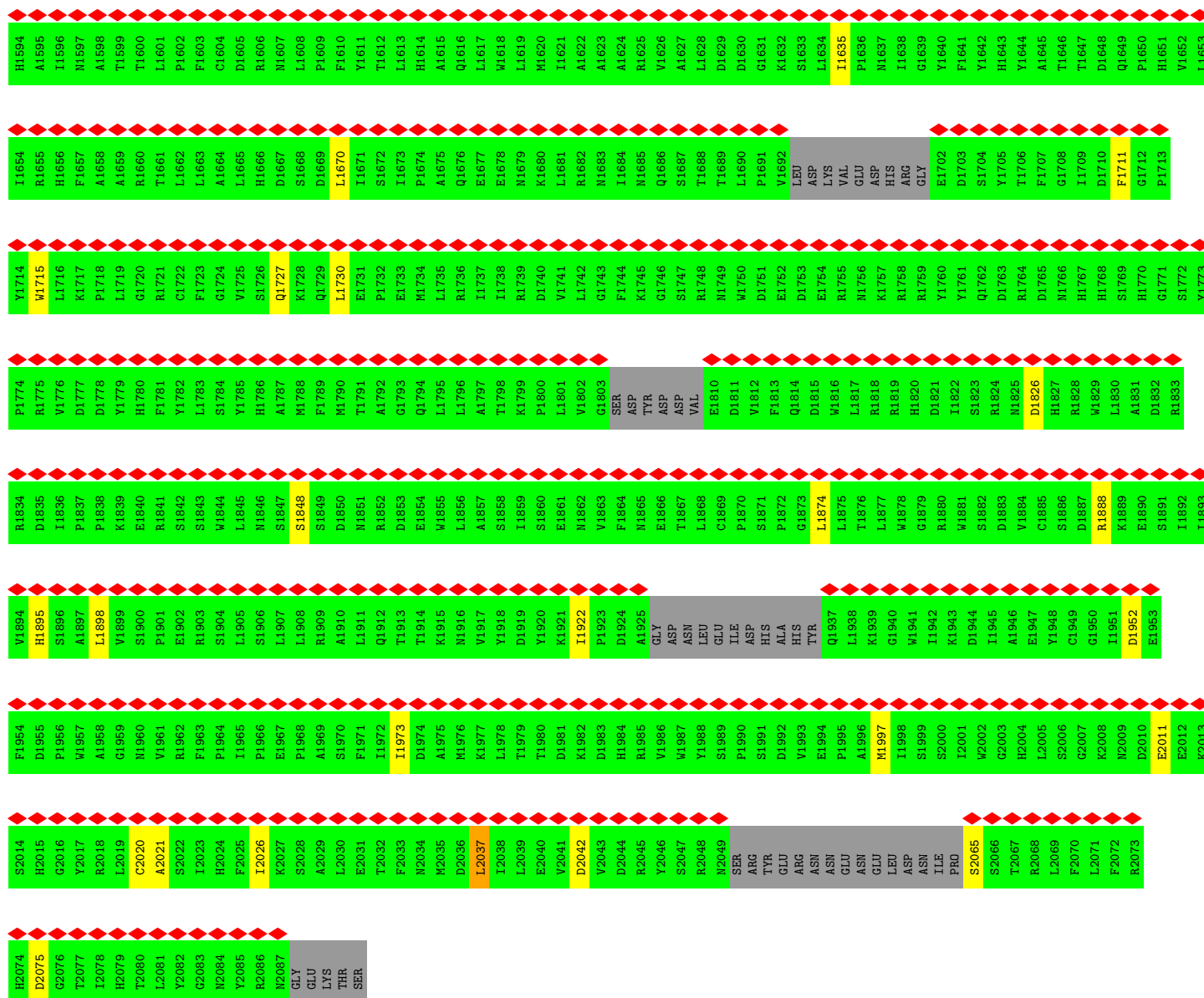
PRO	S2065	S2066	T2067	R2068	L2069	F2070	L2071	F2072	R2073	H2074	D2075	G2076	T2077	L2078	H2079	T2080	L2081	Y2082	G2083	N2084	Y2085	R2086	N2087	GLY	GLU	LYS	THR	SER																															
	L2005	S2006	G2007	K2008	N2009	D2010	E2011	E2012	K2013	S2014	H2015	G2016	Y2017	R2018	L2019	C2020	A2021	S2022	T2023	H2024	F2025	T2026	K2027	S2028	A2029	L2030	E2031	T2032	F2033	W2034	W2035	D2036	L2037	T2038	L2039	E2040	V2041	D2042	V2043	D2044	R2045	Y2046	S2047	R2048	N2049	SER	ARG	TYR	GLU	ARG	ASN	ASN	GLU	ASN	GLU	LEU	ASP	ASN	ILE
H2004	D1944	I1945	A1946	E1947	C1949	G1950	I1951	D1952	E1953	F1954	D1955	P1956	W1957	A1958	G1959	V1960	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
V1884	C1885	S1886	D1887	R1888	K1889	E1890	S1891	I1892	I1893	V1894	H1895	S1896	A1897	L1898	V1899	S1900	P1901	E1902	R1903	S1904	L1905	S1906	L1907	L1908	R1909	A1910	L1911	Q1912	T1913	T1914	K1915	M1916	V1917	Y1918	D1919	Y1920	K1921	I1922	P1923	D1924	A1925	GLY	ASN	ASP	LEU	GLU	ILE	ASP	HIS	ALA	HIS	TYR	Q1937	L1938	K1939	G1940	W1941	I1942	K1943
R1824	N1825	D1826	H1827	R1828	W1829	L1830	A1831	D1832	R1833	R1834	D1835	I1836	P1837	P1838	K1839	E1840	R1841	S1842	S1843	W1844	L1845	M1846	S1847	S1848	S1849	D1850	M1851	R1852	D1853	E1854	W1855	L1856	A1857	S1858	I1859	S1860	E1861	M1862	V1863	F1864	M1865	E1866	T1867	L1868	C1869	P1870	S1871	P1872	G1873	L1874	L1875	T1876	L1877	W1878	G1879	R1880	W1881	S1882	D1883
R1764	D1765	N1766	H1767	H1768	S1769	H1770	G1771	S1772	Y1773	P1774	R1775	V1776	D1777	D1778	Y1779	H1780	F1781	Y1782	L1783	S1784	Y1785	H1786	A1787	M1788	F1789	M1790	T1791	A1792	G1793	Q1794	L1795	L1796	A1797	T1798	K1799	P1800	L1801	V1802	G1803	SER	ASP	TYR	ASP	ASP	VAL	E1810	D1811	V1812	F1813	Q1814	D1815	W1816	L1817	R1818	R1819	H1820	D1821	I1822	S1823
S1704	Y1705	T1706	F1707	G1708	I1709	D1710	F1711	G1712	P1713	Y1714	W1715	L1716	K1717	P1718	L1719	G1720	R1721	G1722	F1723	G1724	V1725	S1726	Q1727	K1728	Q1729	L1730	E1731	P1732	E1733	M1734	L1735	R1736	I1737	I1738	R1739	D1740	V1741	L1742	G1743	F1744	K1745	G1746	S1747	R1748	N1749	W1750	D1751	E1752	D1753	E1754	R1755	M1756	K1757	R1758	R1759	Y1760	Q1762	D1763	

• Molecule 1: SeAvs3

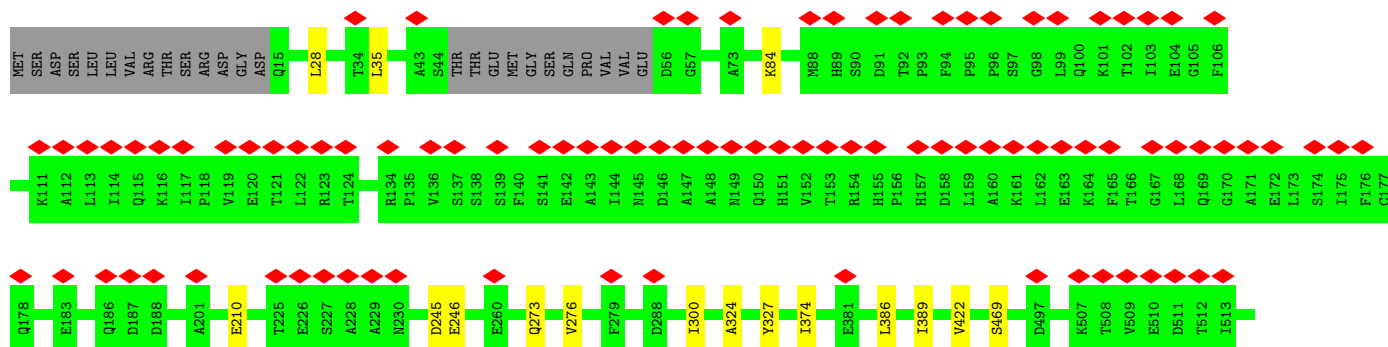
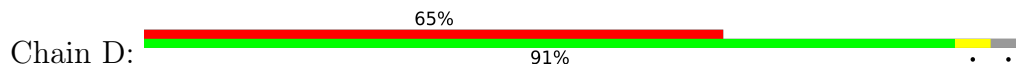


RET	S2	D3	S4	L5	Q32	A43	T46	G49	S50	Q51	P52	V53	V54	E55	D56	G57	E58	E59	D62	Q82	M88	H89	S90	D91	T92	P96	S97	G98	L99	E104	K111	I114	Q115	K116	I117	P118	V119	E120	T121	S137	S138	S139	E142	A143	A147							
A148	N149	Q150	H151	V152	T153	R154	H155	P156	D158	L159	A160	K161	L162	E163	K164	F165	L168	Q169	G170	A171	E172	L175	I195	E199	L207	D208	S227	A228	A229	E260	S264	E277	D394	E441	A456	S469	E473	D497	K507	T508	V509	E510										
D511	T512	I513	G514	E515	I530	R547	P548	L552	S580	G581	E582	T583	I584	E589	R597	R600	A603	H607	R614	K618	D619	S620	A623	A624	Q636	E642	L643	L644	L645	S646	S647	Q648	A649	L650	P651	E652	T653	S654	A655	V656	E657	R658	R659	E662								
L663	L666	L670	K671	L674	R675	T676	G677	R678	Q680	D681	A682	A683	K684	L685	A686	L687	K688	A689	E692	C693	A694	G695	D696	N697	R698	Q699	R700	V701	L702	L703	R704	D705	N706	L707	A708	A710	A711	K712	F713	V714	G715	S716	N717	E721	R725	N726	A727	D730	T731	G732		
W733	P734	I744	E747	Y748	F749	E750	E754	A755	L759	L766	T767	N768	W769	L772	P773	D774	D775	E776	R777	S778	R779	Q780	W781	V782	T783	D784	Q785	D786	R787	A788	W789	D790	L791	A792	A793	L795	W796	I797	H798	G799	E800	E801	A802	A803	A804	R805	E806	L807	R808	R809	W810	R811





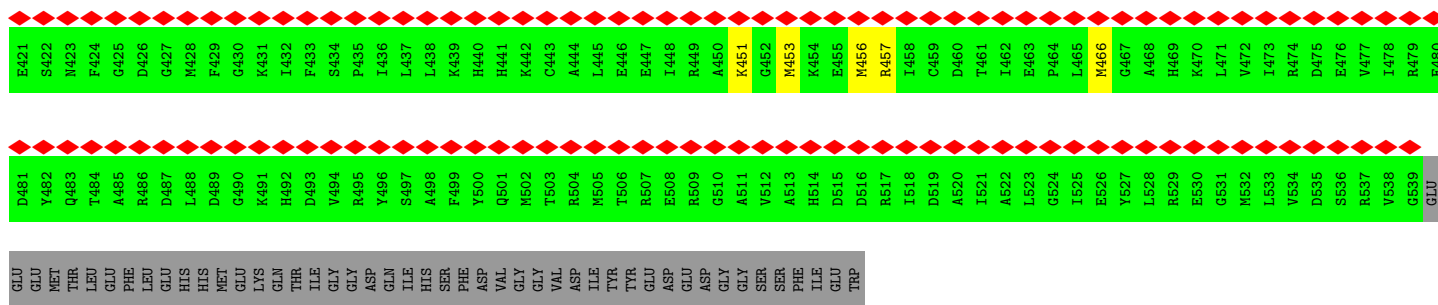
• Molecule 1: SeAvs3



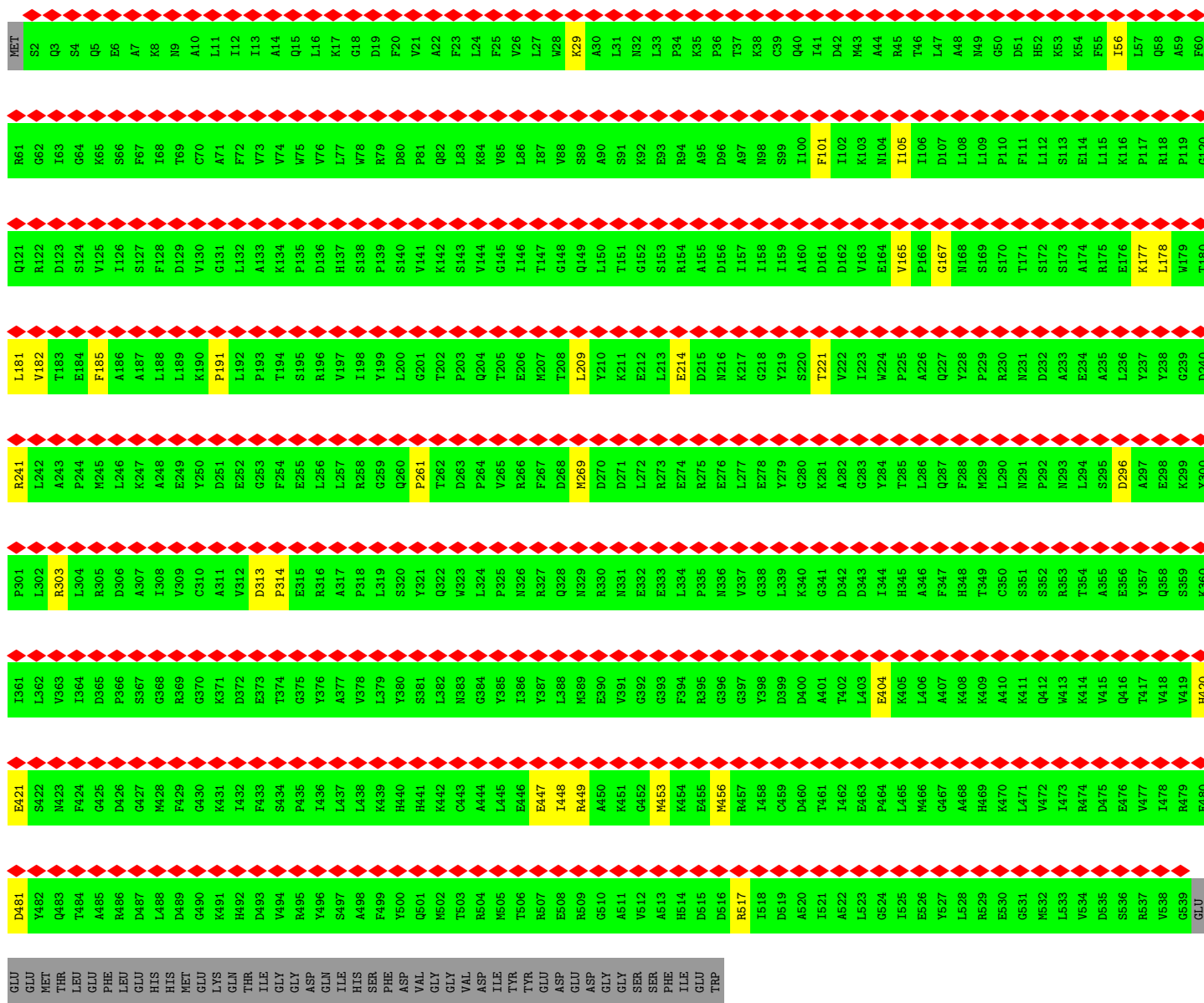
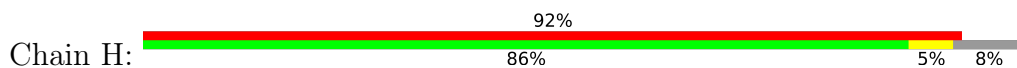
C1401	SER	I1281	A1161	Y1098	S1038	G978	L918	R858	G799	A682	I530
S1402	SER	D1282	I1162	H1099	S1039	E979	L919	K959	G799	A683	P548
F1403	ASN	K1283	L1163	F1100	N1040	S980	D920	L860	A800	K684	L549
I1404	ASN	I1284	D1164	A1101	E1041	D981	R921	H861	E801	L685	I550
T1405	GLU	M1285	L1165	A1102	A1042	D982	Y922	R862	A802	A686	G581
A1406	GLN	A1286	E1167	L1103	A1043	L983	L923	P863	A803	L687	E582
I1407		F1287	Y1168	A1104	N1045	R984	P924	V864	A804	K688	T583
G1408		V1288	V1169	L1105	V1046	Q985	K925	A865	A805	A689	I584
A1409		F1229	L1107	S1106	W1047	K987	Y926	E866	E806	E592	D588
I1410		G1230	L1108	W1108	D1048	Q988	P928	Q867	L807	E592	D588
F1411		N1231	W1109	W1109	I1049	Y989	Y929	A868	R808	D696	E589
H1412		H1232	D1110	D1110	L1050	S990	A930	I869	R809	N697	P590
W1413		S1233	E1111	E1111	L1051	G991	L931	R870	R811	N697	A591
S1414		S1234	H1112	H1112	E1052	Y992	T932	R871	P812	B698	E592
L1415		I1235	S1113	S1113	A1053	L993	S933	T872	R813	L703	R600
Y1416		L1236	D1114	D1114	G1054	I994	E934	W873	K814	R704	A603
F1417		A1237	A1115	A1115	N1055	P995	Y935	L874	L815	D705	A604
D1418		W1238	Q1116	Q1116	V1056	W996	Y936	L875	S816	D708	D605
K1419		T1239	Q1117	Q1117	S1057	Y997	K937	L876	F817	L709	R614
L1420		I1240	K1118	K1118	S1058	N998	E938	S877	D818	A710	P615
I1421		E1241	A1119	A1119	D1059	L999	R939	Q879	A819	K712	L616
L1422		K1242	L1183	L1183	D1060	W1000	Y940	R880	G820	N717	D619
E1423		L1243	A1184	A1184	V1061	A1001	A941	V881	G821	E721	Q636
S1424		V1244	R1185	R1185	E1062	K1002	Y942	S882	V823	R725	L640
I1425		K1245	C1186	C1186	N1063	V1003	V943	I883	M925	D730	A644
P1426		N1247	A1187	A1187	I1064	I1004	R944	K884	Q826	T731	I645
D1427		K1248	E1188	E1188	I1065	L1005	A945	D885	L827	R756	S846
A1428		L1249	L1189	L1189	K1066	G1006	Y946	R886	L828	A849	S847
W1429		I1250	T1190	T1190	W1067	K1007	A947	N887	A829	H830	Q848
T1430		A1251	R1191	R1191	S1068	T1008	L948	H888	H831	R832	Q849
S1431		E1252	E1192	E1192	Q1069	K1009	Q949	A889	R832	Q992	A649
R1432		L1253	Y1193	Y1193	H1070	K1010	A950	N890	R833	L772	L850
L1433		D1254	W1194	W1194	K1071	A1011	N951	N891	Y833	P773	P851
S1434		L1255	D1195	D1195	G1072	D1012	L952	Q992	D834	D774	E852
I1435		P1256	L1196	L1196	N1073	L1013	N953	T893	L836	T653	T653
K1436		L1257	D1197	D1197	R1074	E1014	G954	I894	L836	S854	S854
T1437		I1258	K1198	K1198	V1075	S1015	S955	A895	D837	A855	A855
T1438		T1259	H1199	H1199	F1076	E1016	Q956	A896	Q838	V856	V856
L1439		F1260	F1200	F1200	P1078	L1017	L957	T897	E776	E857	E857
A1440		E1261	A1201	A1201	P1078	S1018	A958	T898	R777	R779	R658
I1443		L1321	W1202	W1202	T1079	D1019	L959	G899	A840	Q780	R658
K1444		K1322	S1203	S1203	L1080	T1020	S960	I841	R778	N781	R659
E1445		E1323	D1204	D1204	H1081	Q1021	L961	A842	V783	V783	A673
Y1446		R1324	T1205	T1205	R1082	K1022	L962	N900	D784	D784	L674
A1447		L1325	W1206	W1206	F1083	E1023	A963	A904	Q785	R786	R675
Q1448		S1326	E1207	E1207	S1084	S1024	S964	A904	R877	L791	T676
T1449		G1327	I1208	I1208	V1086	T1025	T965	L905	V850	G777	G677
F1450		L1328	L1209	L1209	C1087	A1026	E966	I906	N845	A788	E677
C1451		Q1329	L1270	L1270	C1087	I1027	Y967	Q907	L849	L792	L792
M1452		THR	L1330	L1330	S1088	K1028	K968	S908	V850	L795	L795
R1453		GLU	D1271	D1271	A1088	G1029	K969	V909	N851		
I1454		THR	S1272	S1272	D1153	H1030	E970	C910	G852		
K1455		VAL	V1273	V1273	E1154	I1031	L971	T911	I853		
R1456		SER	P1214	P1214	N1155	Y1032	A973	E912	V854		
K1457		SER	S1215	S1215	L1156	S1033	E974	S913	L855		
L1458		LYS	S1275	S1275	S1157	L1093	E974	E914	E856		
L1459		SER	S1276	S1276	R1158	E1034	E974	E914	E856		
Y1460		LEU	C1277	C1277	W1159	H1035	K975	S915	A857		
E1461		LEU	D1278	D1278	E1160	S1036	R976	I916			
			D1280	D1280	S1097	L1037	H977	Q917			

- Molecule 2: Terminase, large subunit





- 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: MG, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/16499	0.54	1/22369 (0.0%)
1	B	0.25	0/16319	0.56	2/22123 (0.0%)
1	C	0.25	0/16499	0.54	1/22369 (0.0%)
1	D	0.25	0/16319	0.56	4/22123 (0.0%)
2	E	0.23	0/4363	0.57	4/5899 (0.1%)
2	F	0.24	0/4363	0.57	2/5899 (0.0%)
2	G	0.24	0/4363	0.58	4/5899 (0.1%)
2	H	0.23	0/4363	0.57	1/5899 (0.0%)
All	All	0.25	0/83088	0.56	19/112580 (0.0%)

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

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

There are no bond length outliers.

All (19) bond angle outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	191	PRO	CA-N-CD	-8.61	99.94	112.00
2	E	191	PRO	CA-N-CD	-8.59	99.98	112.00
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
1	D	993	LEU	CA-C-N	6.20	124.14	120.24
1	D	993	LEU	C-N-CA	6.20	124.14	120.24
2	E	165	VAL	N-CA-C	-5.67	104.54	109.19
2	G	165	VAL	N-CA-C	-5.61	104.59	109.19
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
2	G	389	MET	CG-SD-CE	-5.34	89.15	100.90
2	E	389	MET	CG-SD-CE	-5.32	89.20	100.90
2	F	389	MET	CG-SD-CE	-5.32	89.21	100.90
2	E	191	PRO	N-CD-CG	-5.05	95.63	103.20
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
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	37	0
1	B	15974	0	15804	52	0
1	C	16152	0	15975	37	0
1	D	15974	0	15804	51	0
2	E	4273	0	4283	15	0
2	F	4273	0	4283	19	0
2	G	4273	0	4283	18	0
2	H	4273	0	4283	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	244	0

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

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:E:43:MET:HE1	2:E:63:ILE:HD13	1.85	0.57
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
2:G:43:MET:HE1	2:G:63:ILE:HD13	1.85	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
2:G:380:TYR:CG	2:G:389:MET:HE1	2.44	0.53
2:F:261:PRO:HD3	2:F:269:MET:HE3	1.91	0.53
1:D:810:TRP:O	1:D:813:ARG:NH1	2.42	0.53
1:B:1388:ILE:O	1:B:1392:ILE:HG13	2.09	0.53
2:E:380:TYR:CG	2:E:389:MET:HE1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:261:PRO:HD3	2:H:269:MET:HE3	1.95	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
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
1:D:869:ILE:HG13	1:D:900:MET:HE1	1.95	0.48
1:B:869:ILE:HG13	1:B:900:MET:HE1	1.95	0.48
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:B:1854:GLU:CD	1:B:1854:GLU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1284:ILE:HD13	1:D:1314:LEU:HD23	1.95	0.48
1:D:1854:GLU:H	1:D:1854:GLU:CD	2.21	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:C:997:TYR:OH	1:C:1041:GLU:OE2	2.32	0.47
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:A:227:SER:O	1:A:227:SER:OG	2.28	0.46
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:OE2	1:B:938:GLU:N	2.49	0.46
1:B:1997:MET:HE3	1:B:1997:MET:HB2	1.79	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:E:214:GLU:CD	2:E:241:ARG:HH12	2.24	0.46
2:F:453:MET:HG2	2:F:456:MET:H	1.80	0.46
2:F:466:MET:HE3	2:F:466:MET:HB2	1.83	0.46
2:H:214:GLU:CD	2:H:241:ARG:HH12	2.24	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:F:380:TYR:CG	2:F:389:MET:HE1	2.50	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
2:F:380:TYR:CD2	2:F:389:MET:HE1	2.52	0.45
1:A:1711:PHE:O	1:A:1715:TRP:HB2	2.17	0.45
1:C:1711:PHE:O	1:C:1715:TRP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:938:GLU:OE2	1:D:938:GLU:N	2.50	0.45
2:F:214:GLU:CD	2:F:241:ARG:HH12	2.24	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:A:1997:MET:HE3	1:A:1997:MET:HB2	1.81	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:E:175:ARG:HD2	2:E:207:MET:HE2	2.00	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
2:G:214:GLU:CD	2:G:241:ARG:HH12	2.25	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:1855:TRP:HE3	1:B:1856:LEU:HD23	1.83	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
2:E:380:TYR:CD2	2:E:389:MET:HE1	2.54	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
2:G:466:MET:HE3	2:G:466:MET:HB2	1.85	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:1300:ASN:HD22	1:D:1302:GLN:CD	2.28	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:1300:ASN:HD22	1:B:1302:GLN:CD	2.27	0.42
1:B:1973:ILE:H	1:B:1973:ILE:HG13	1.58	0.42
2:E:466:MET:HE3	2:E:466:MET:HB2	1.86	0.42
1:A:784:ASP:OD1	1:A:784:ASP:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1855:TRP:HE3	1:D:1856:LEU:HD23	1.83	0.42
1:A:997:TYR:OH	1:A:1041:GLU:OE2	2.32	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:A:39:THR:OG1	1:A:42:GLY:O	2.32	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
2:G:380:TYR:CD2	2:G:389:MET:HE1	2.53	0.42
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
2:F:269:MET:HE2	2:F:272:LEU:HD12	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:175:ARG:HD2	2:G:207:MET:HE2	2.03	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
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

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

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

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

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	513	ILE
1	B	972	MET
1	B	1365	ILE
1	B	1973	ILE
1	C	513	ILE

Continued on next page...

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Mol	Chain	Res	Type
1	C	2037	LEU
1	D	972	MET
1	D	1005	LEU
1	D	1365	ILE
2	F	372	ASP
2	F	488	LEU
2	H	404	GLU
2	H	448	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	481	ASN
1	A	492	ASN
1	A	907	GLN
1	A	956	GLN
1	A	1070	HIS
1	A	1155	ASN
1	A	1199	HIS
1	A	1589	GLN
1	A	1637	ASN
1	A	1683	ASN
1	A	1827	HIS
1	A	1895	HIS
1	A	2004	HIS
1	B	82	GLN
1	B	149	ASN
1	B	907	GLN
1	B	956	GLN
1	B	1155	ASN
1	B	1292	HIS
1	B	1666	HIS
1	B	1683	ASN
1	B	1770	HIS
1	B	1827	HIS
1	B	2004	HIS
1	C	181	HIS
1	C	481	ASN
1	C	492	ASN
1	C	608	GLN
1	C	907	GLN
1	C	956	GLN

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Mol	Chain	Res	Type
1	C	1155	ASN
1	C	1199	HIS
1	C	1589	GLN
1	C	1637	ASN
1	C	1683	ASN
1	C	1827	HIS
1	C	1895	HIS
1	C	2004	HIS
1	D	82	GLN
1	D	149	ASN
1	D	372	GLN
1	D	879	GLN
1	D	887	ASN
1	D	907	GLN
1	D	1155	ASN
1	D	1232	HIS
1	D	1292	HIS
1	D	1666	HIS
1	D	1683	ASN
1	D	1770	HIS
1	D	1827	HIS
1	D	2004	HIS
2	E	5	GLN
2	E	49	ASN
2	E	423	ASN
2	F	5	GLN
2	F	49	ASN
2	F	58	GLN
2	F	227	GLN
2	F	291	ASN
2	G	49	ASN
2	G	58	GLN
2	G	423	ASN
2	H	5	GLN
2	H	15	GLN
2	H	49	ASN
2	H	58	GLN
2	H	227	GLN
2	H	291	ASN
2	H	441	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ATP	D	2101	4	32,33,33	0.70	1 (3%)	48,52,52	0.39	0
3	ATP	G	601	4	32,33,33	0.46	0	48,52,52	0.32	0
3	ATP	C	2101	4	32,33,33	0.56	1 (3%)	48,52,52	0.32	0
3	ATP	H	601	4	32,33,33	0.44	0	48,52,52	0.32	0
3	ATP	E	601	4	32,33,33	0.44	0	48,52,52	0.32	0
3	ATP	B	2101	4	32,33,33	0.69	1 (3%)	48,52,52	0.39	0
3	ATP	A	2101	4	32,33,33	0.56	1 (3%)	48,52,52	0.31	0
3	ATP	F	601	4	32,33,33	0.46	0	48,52,52	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	D	2101	4	-	4/22/38/38	0/3/3/3

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

All (4) bond length outliers are listed below:

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

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

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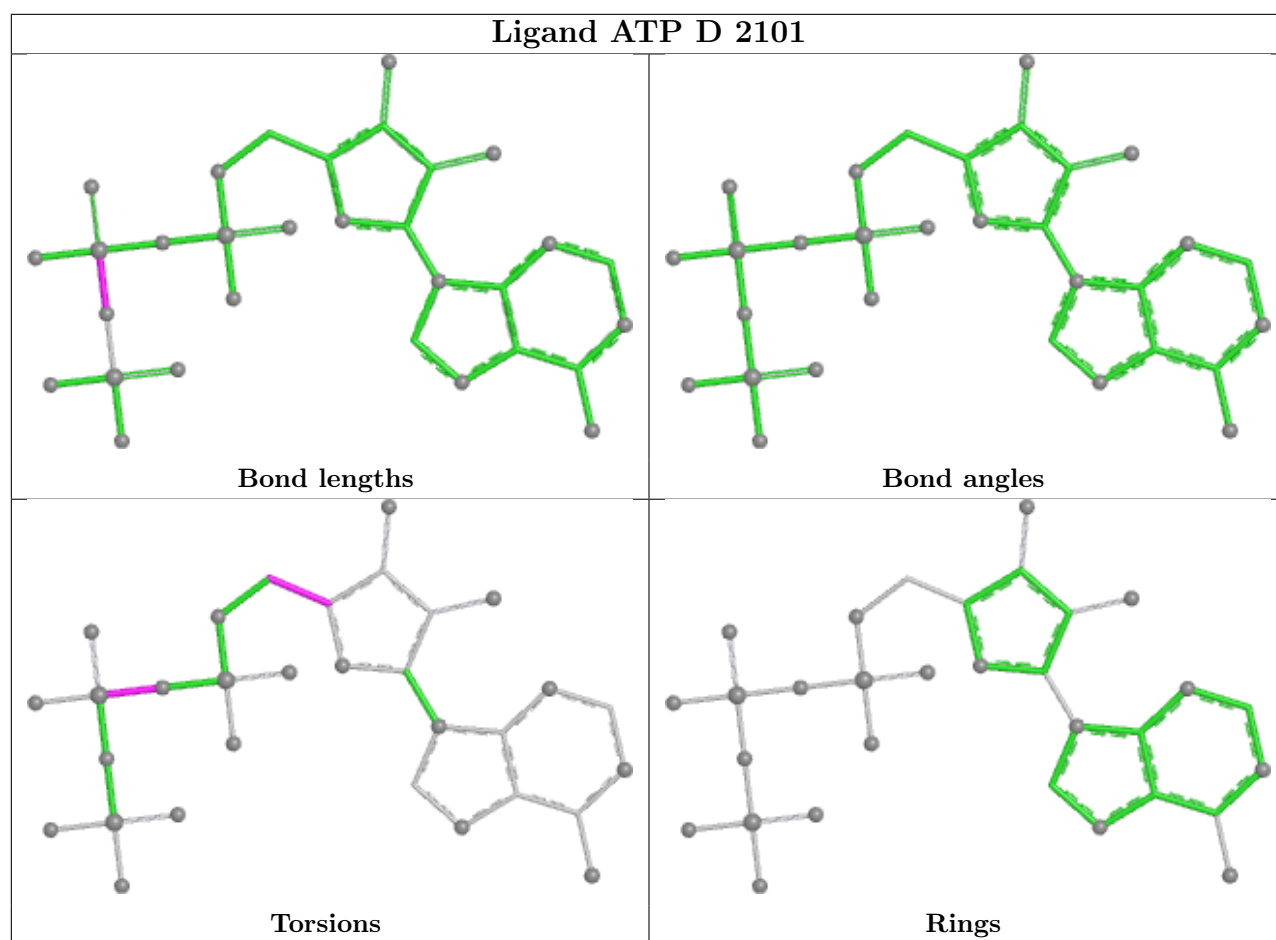
Continued from previous page...

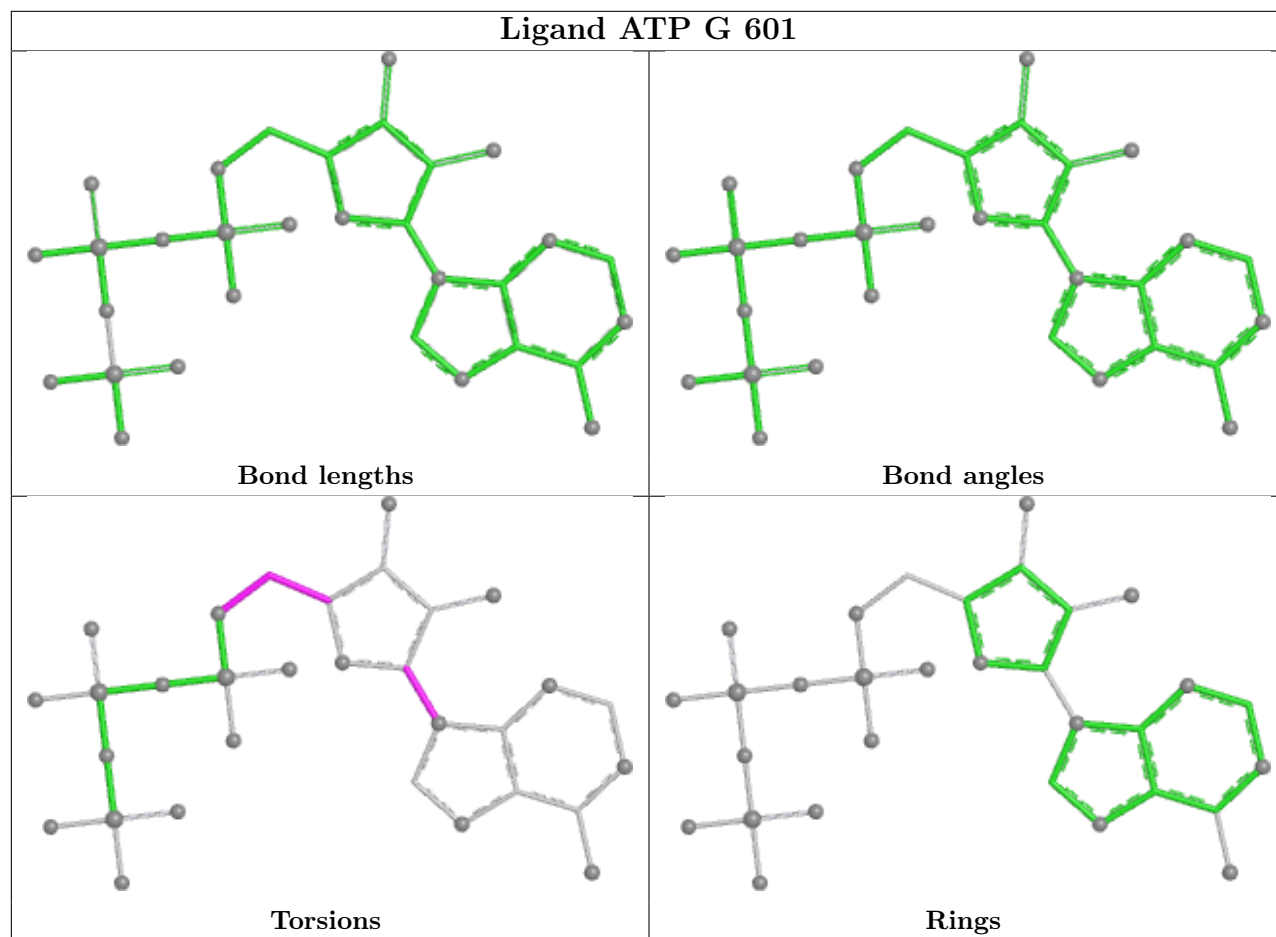
Mol	Chain	Res	Type	Atoms
3	A	2101	ATP	PA-O3A-PB-O2B
3	C	2101	ATP	PA-O3A-PB-O2B
3	E	601	ATP	C2'-C1'-N9-C8
3	G	601	ATP	C2'-C1'-N9-C8
3	B	2101	ATP	PA-O3A-PB-O1B
3	D	2101	ATP	PA-O3A-PB-O1B

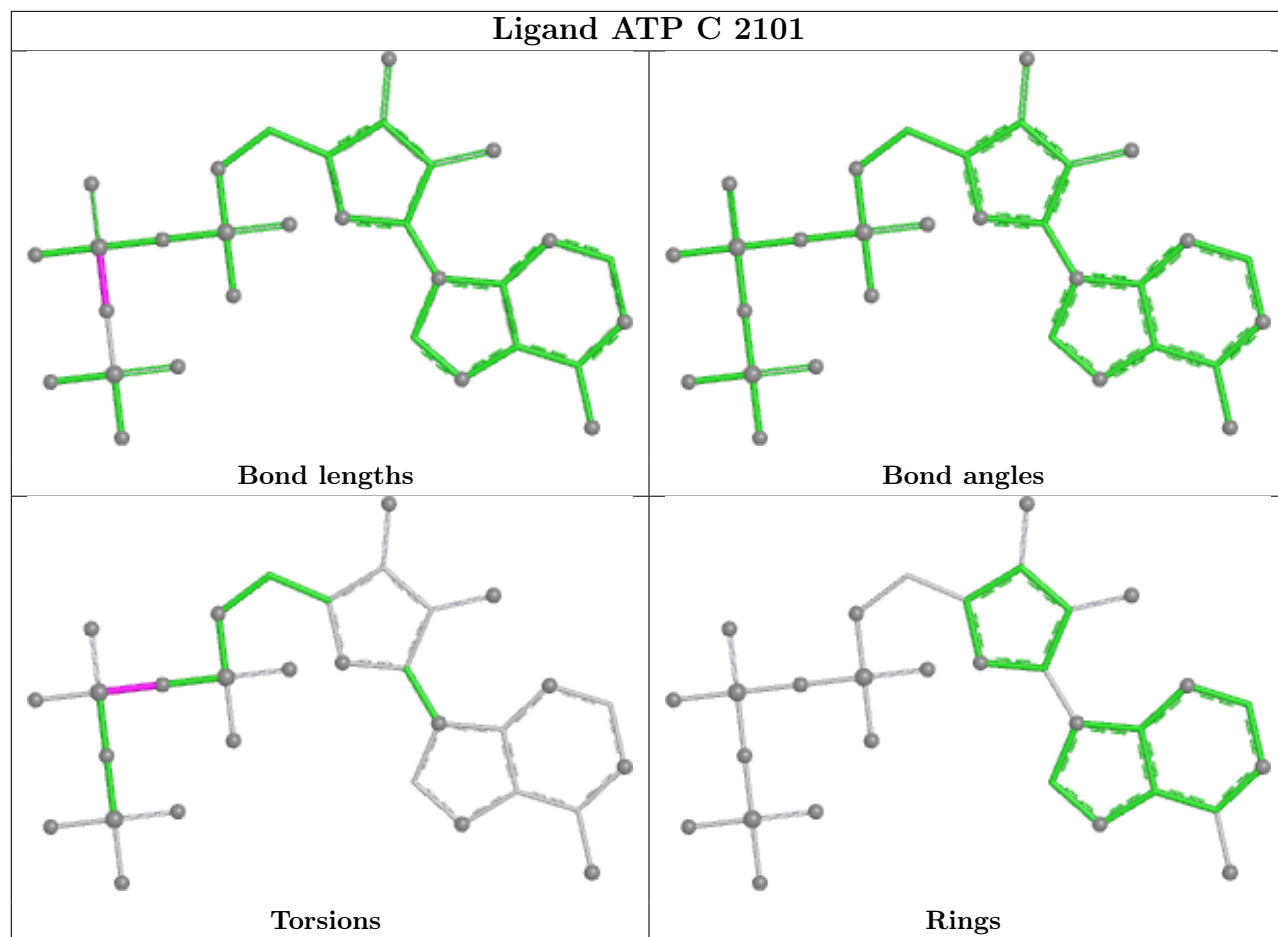
There are no ring outliers.

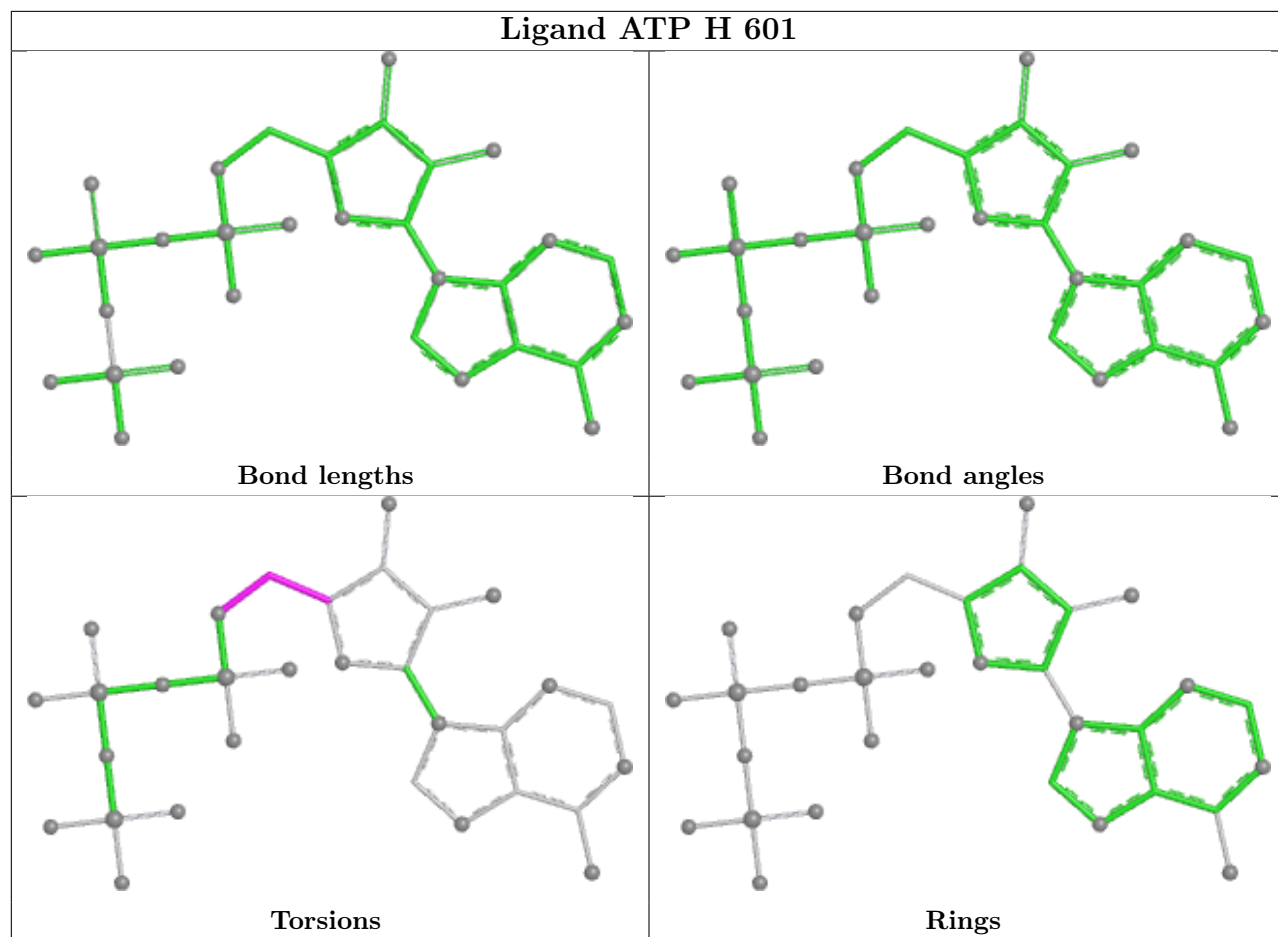
No monomer is involved in short contacts.

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.

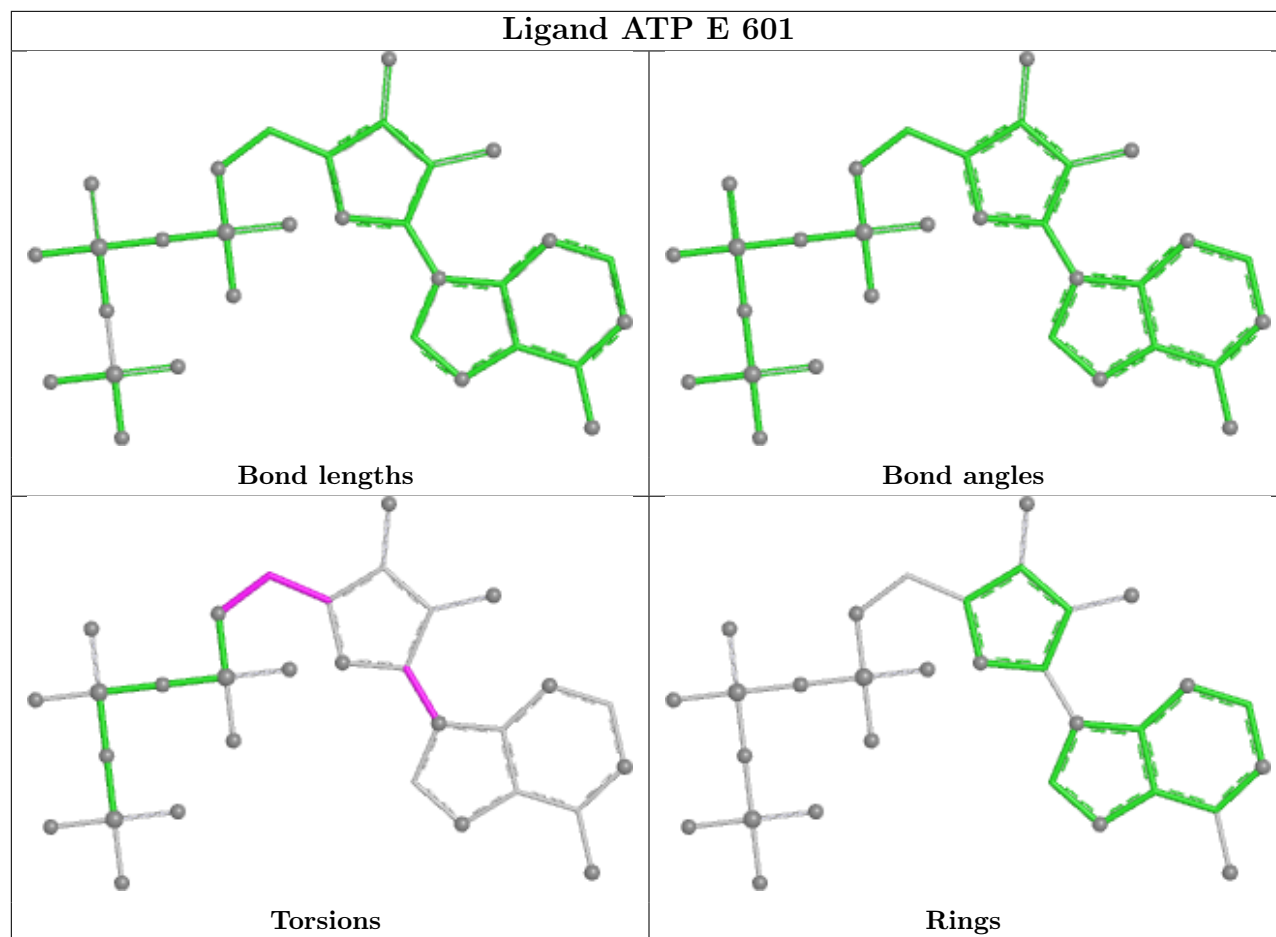


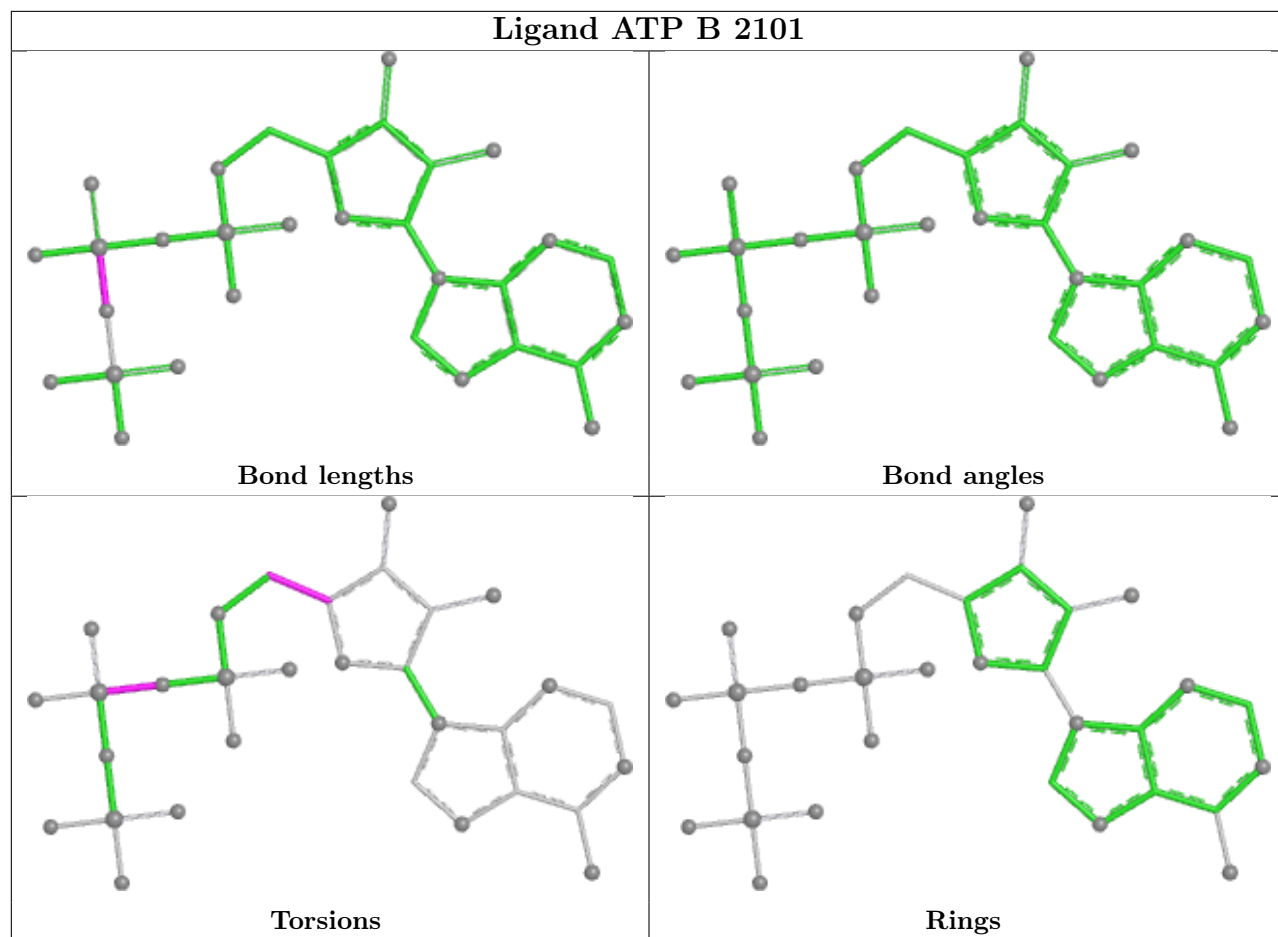


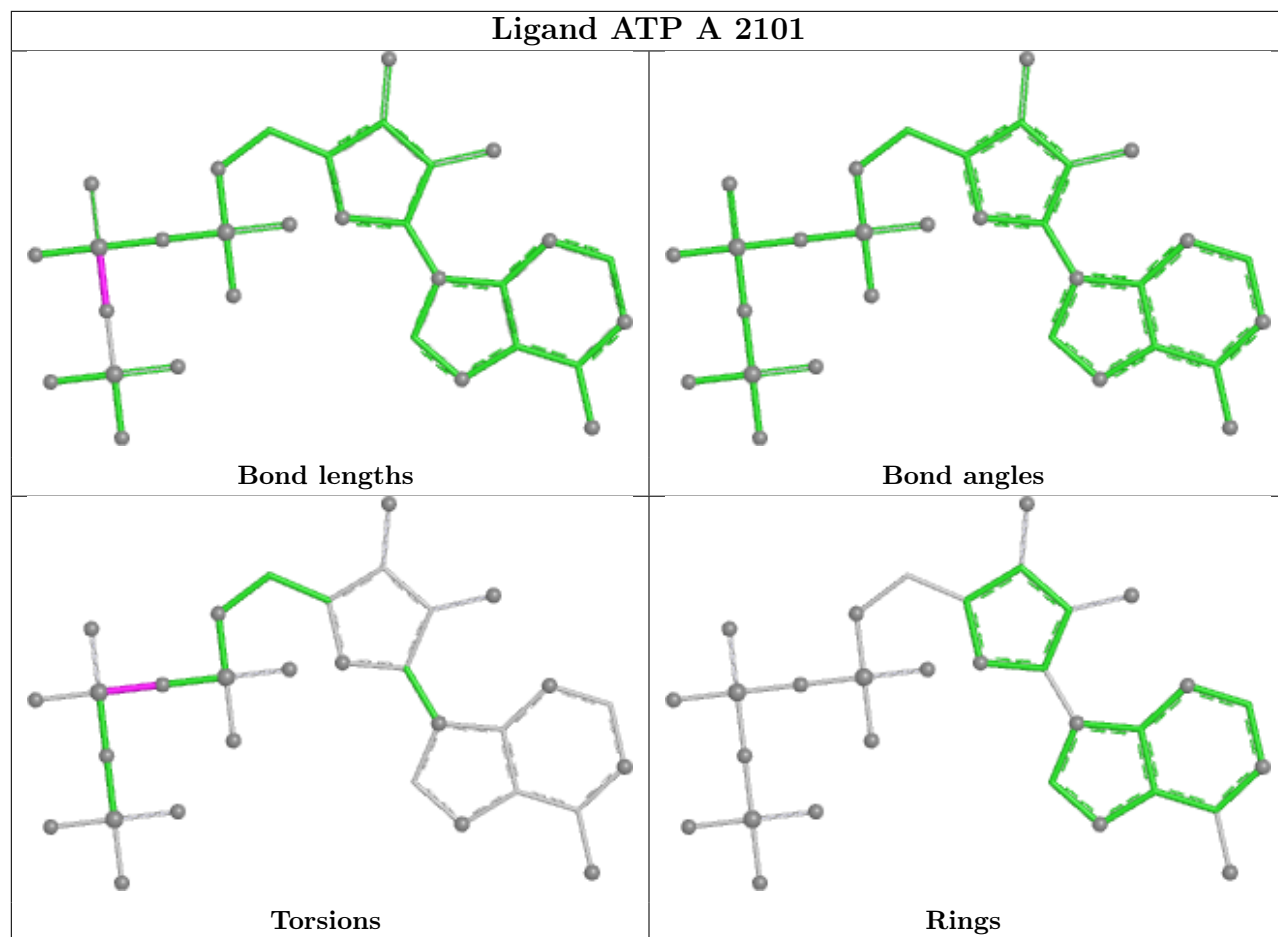


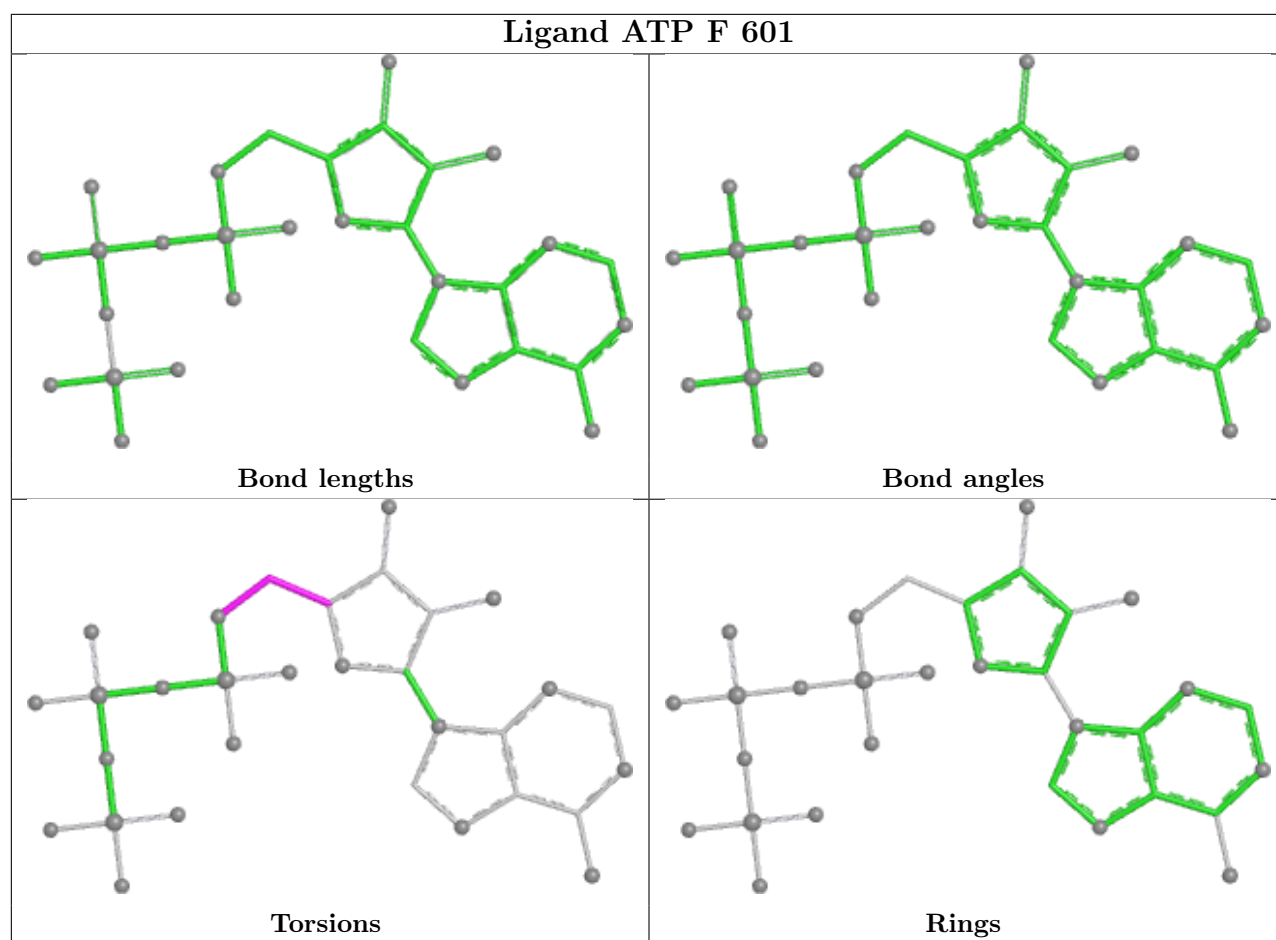


Ligand ATP E 601









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

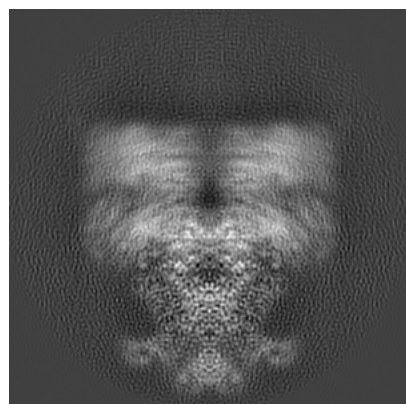
6 Map visualisation [i](#)

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

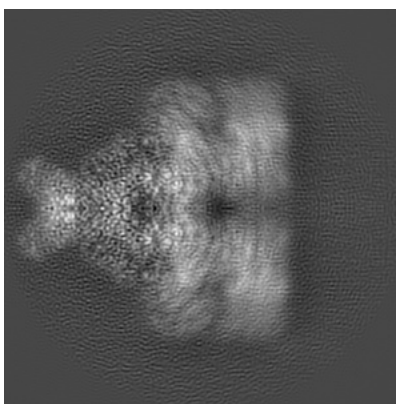
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

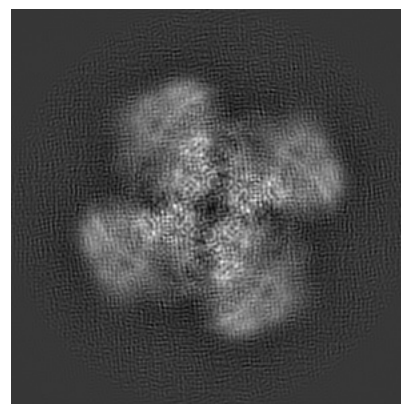
6.1.1 Primary map



X

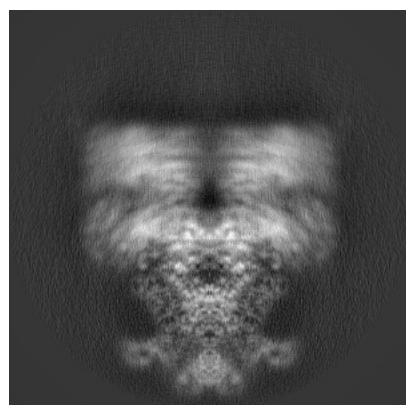


Y

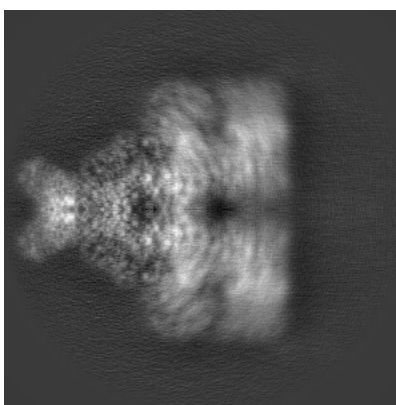


Z

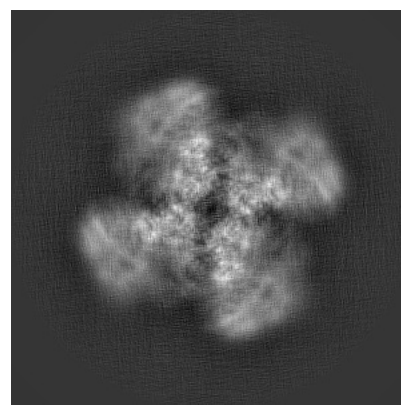
6.1.2 Raw map



X



Y

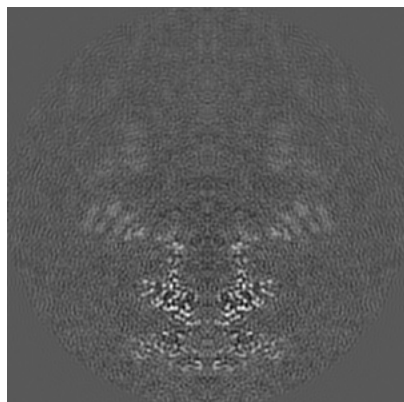


Z

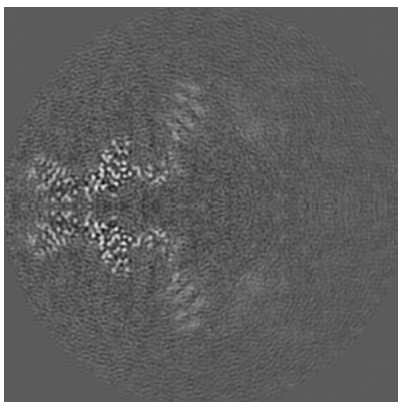
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

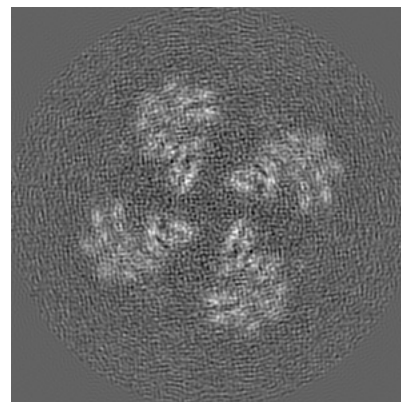
6.2.1 Primary map



X Index: 180

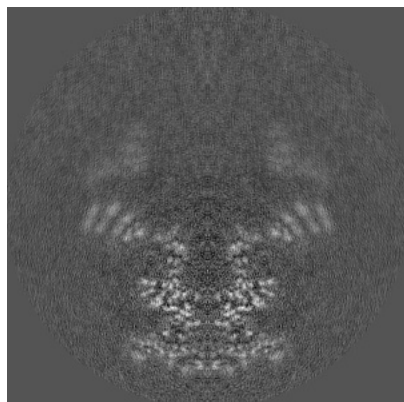


Y Index: 180

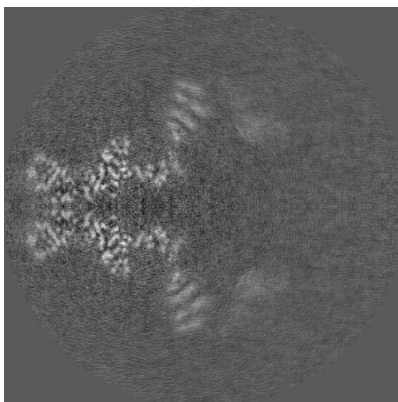


Z Index: 180

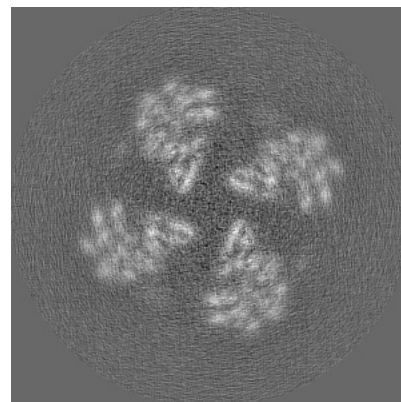
6.2.2 Raw map



X Index: 180



Y Index: 180

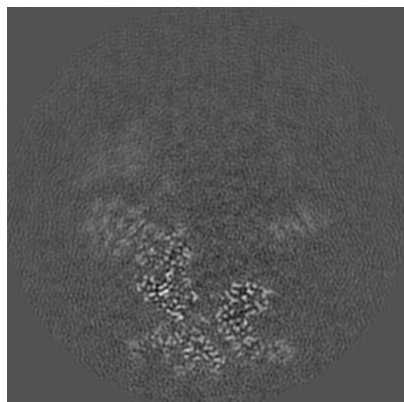


Z Index: 180

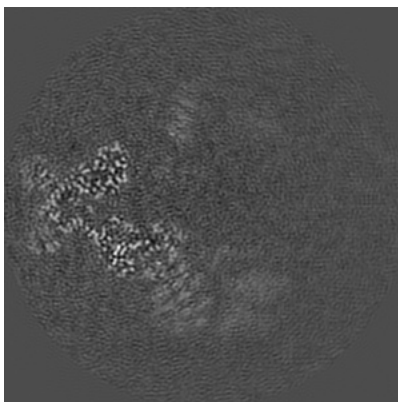
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

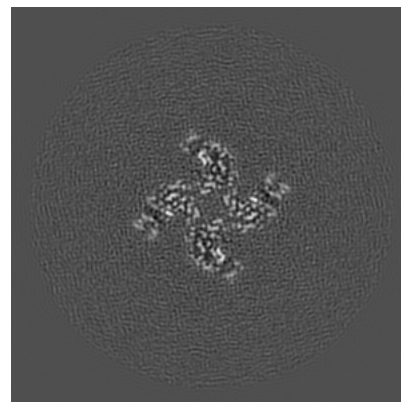
6.3.1 Primary map



X Index: 187

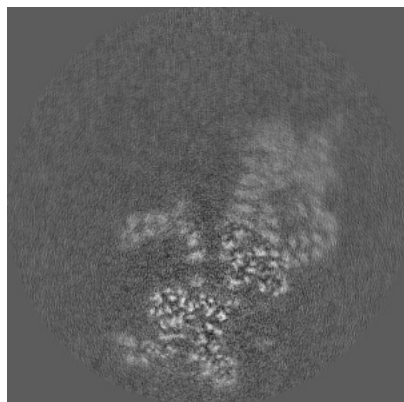


Y Index: 173

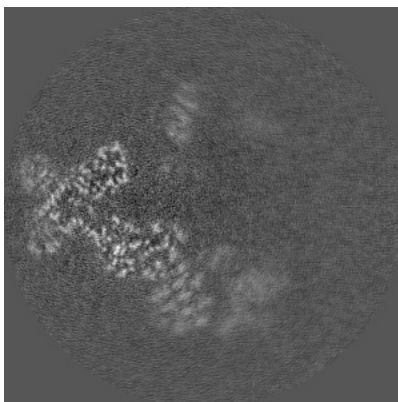


Z Index: 102

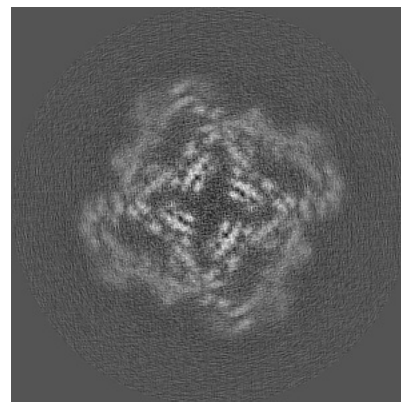
6.3.2 Raw map



X Index: 163



Y Index: 173

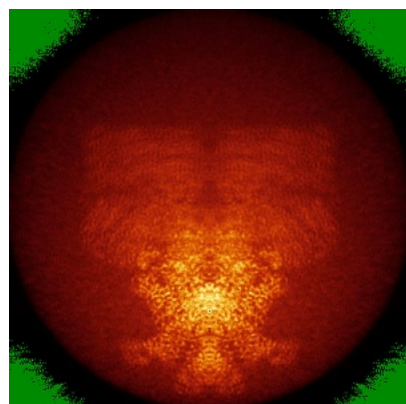


Z Index: 155

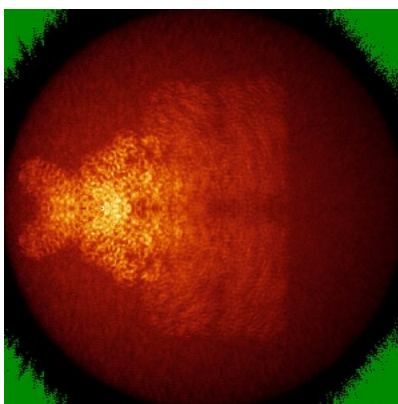
The images above show the largest variance slices of the map in three orthogonal directions.

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

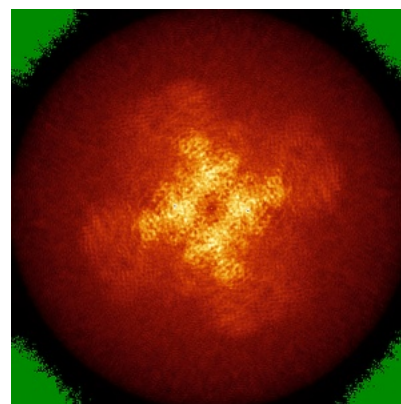
6.4.1 Primary map



X

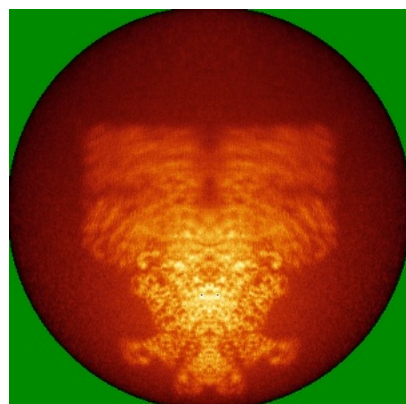


Y

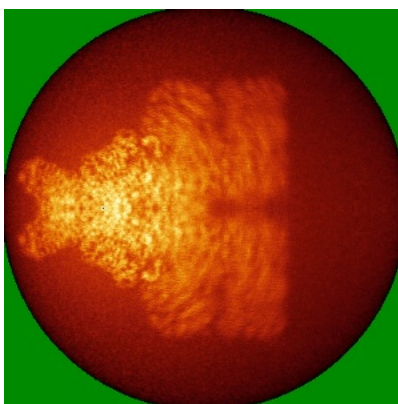


Z

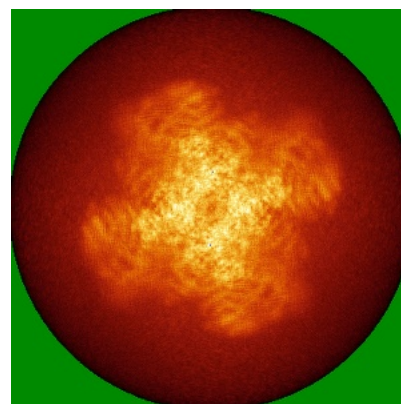
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



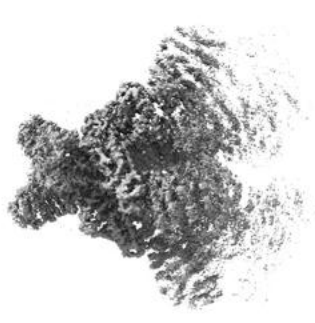
Z

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

6.5.2 Raw map



X



Y



Z

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

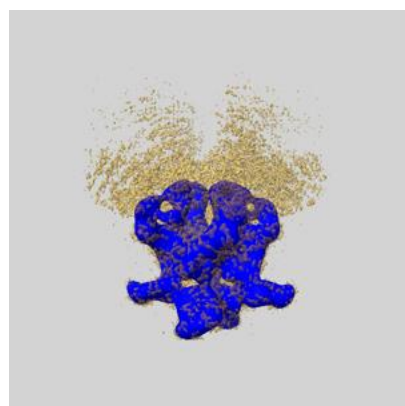
6.6 Mask visualisation [i](#)

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

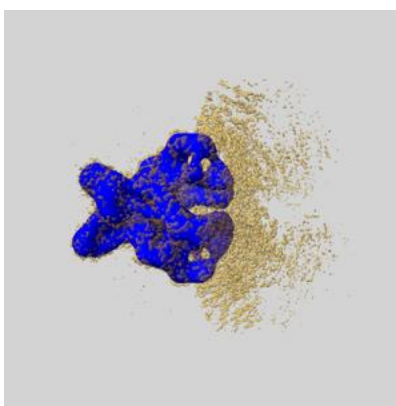
A mask typically either:

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

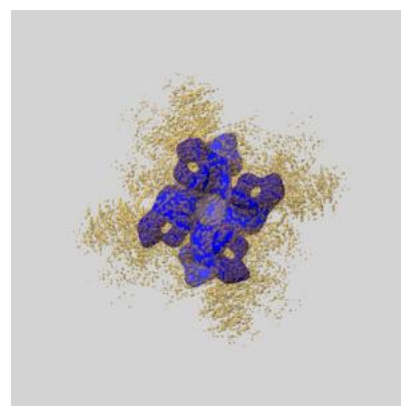
6.6.1 emd_27421_msk_1.map [i](#)



X



Y

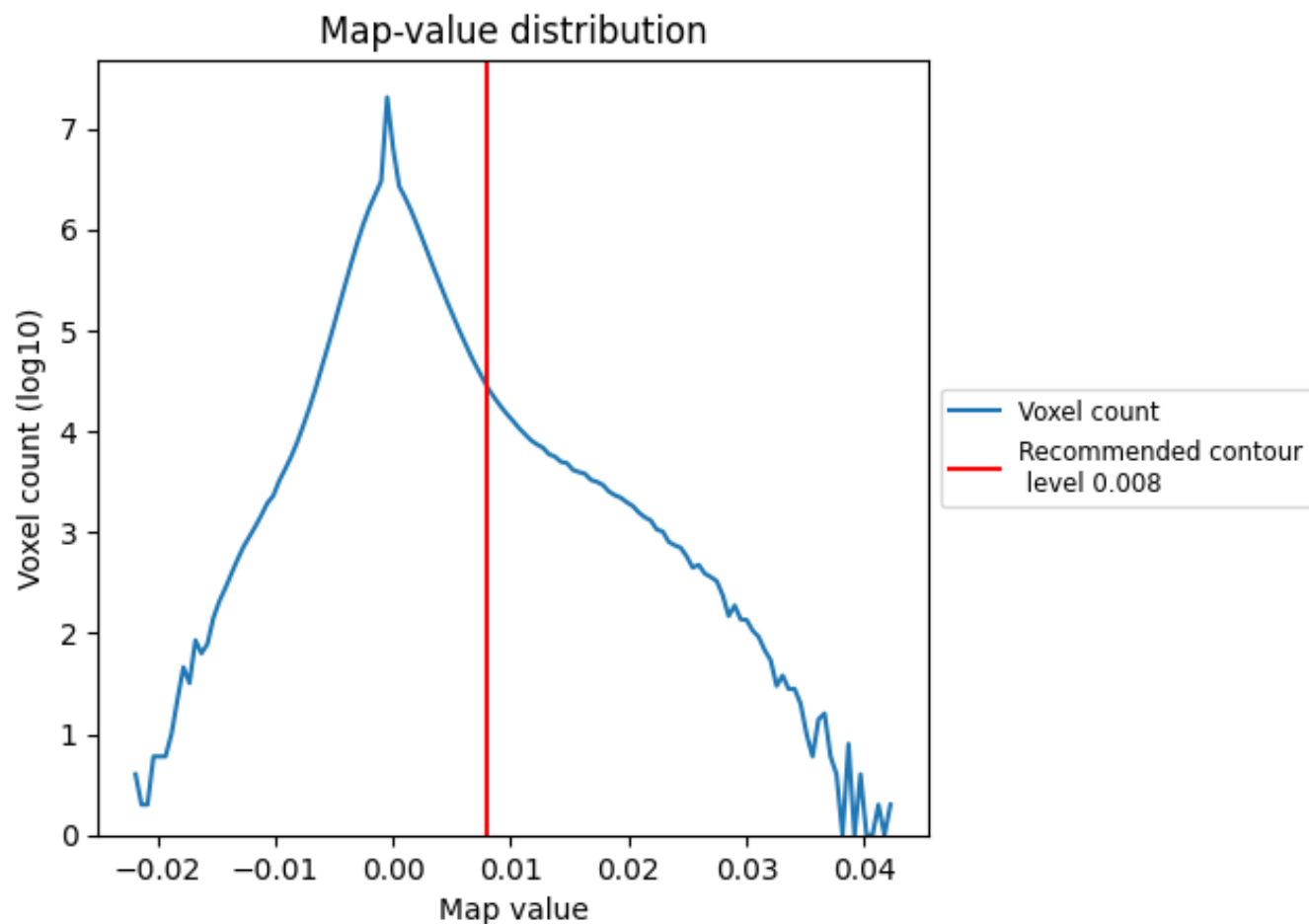


Z

7 Map analysis [i](#)

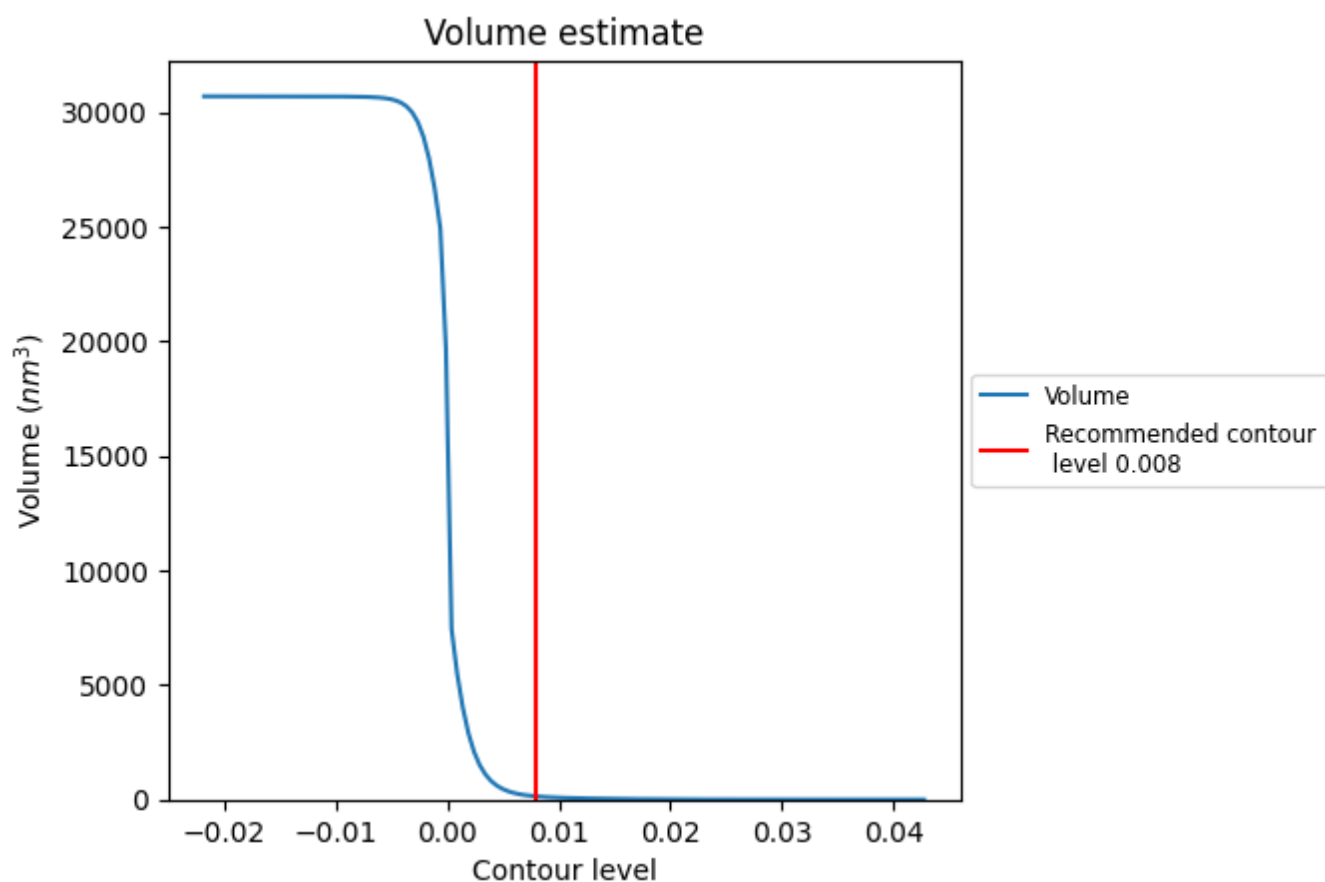
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

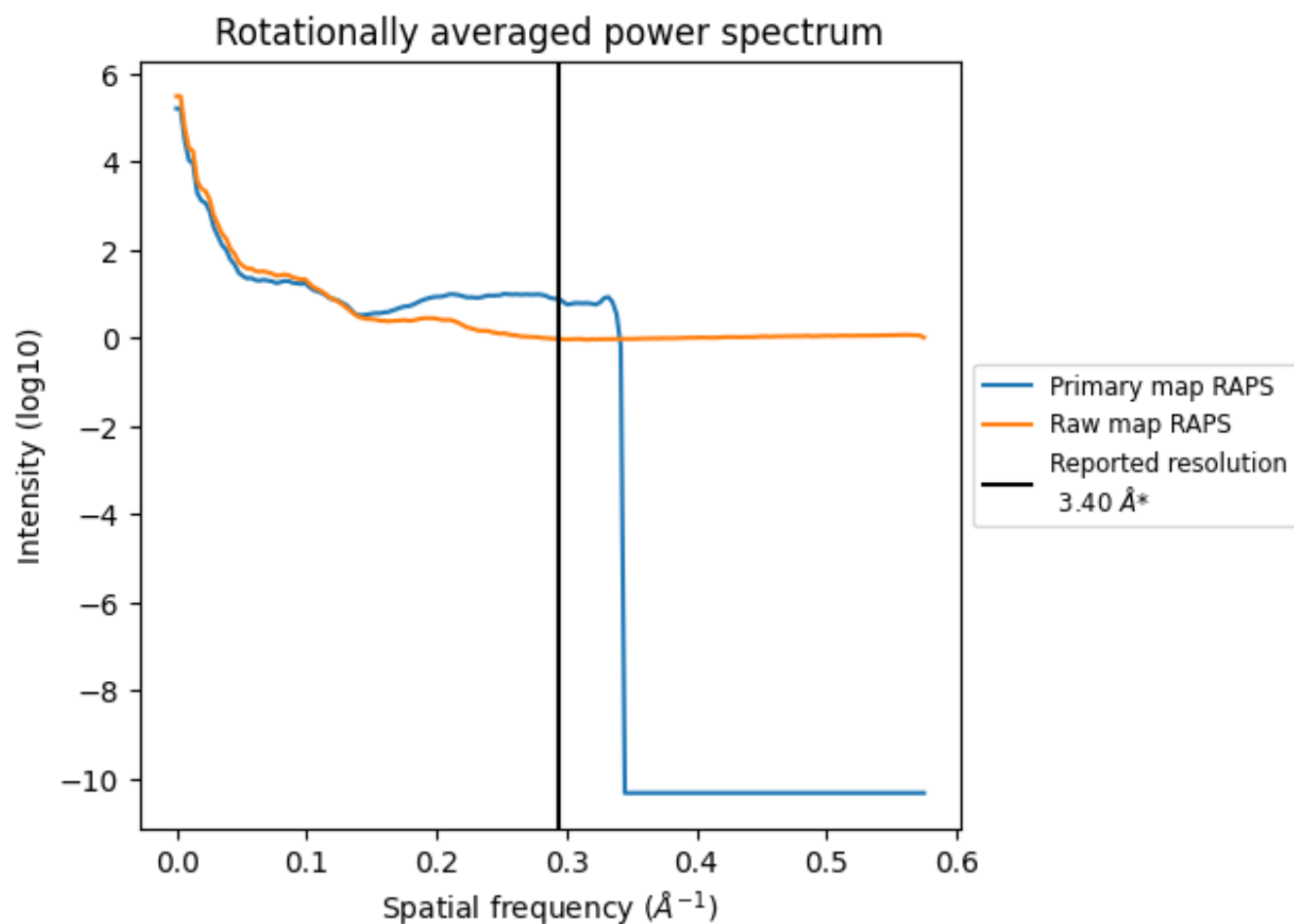
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

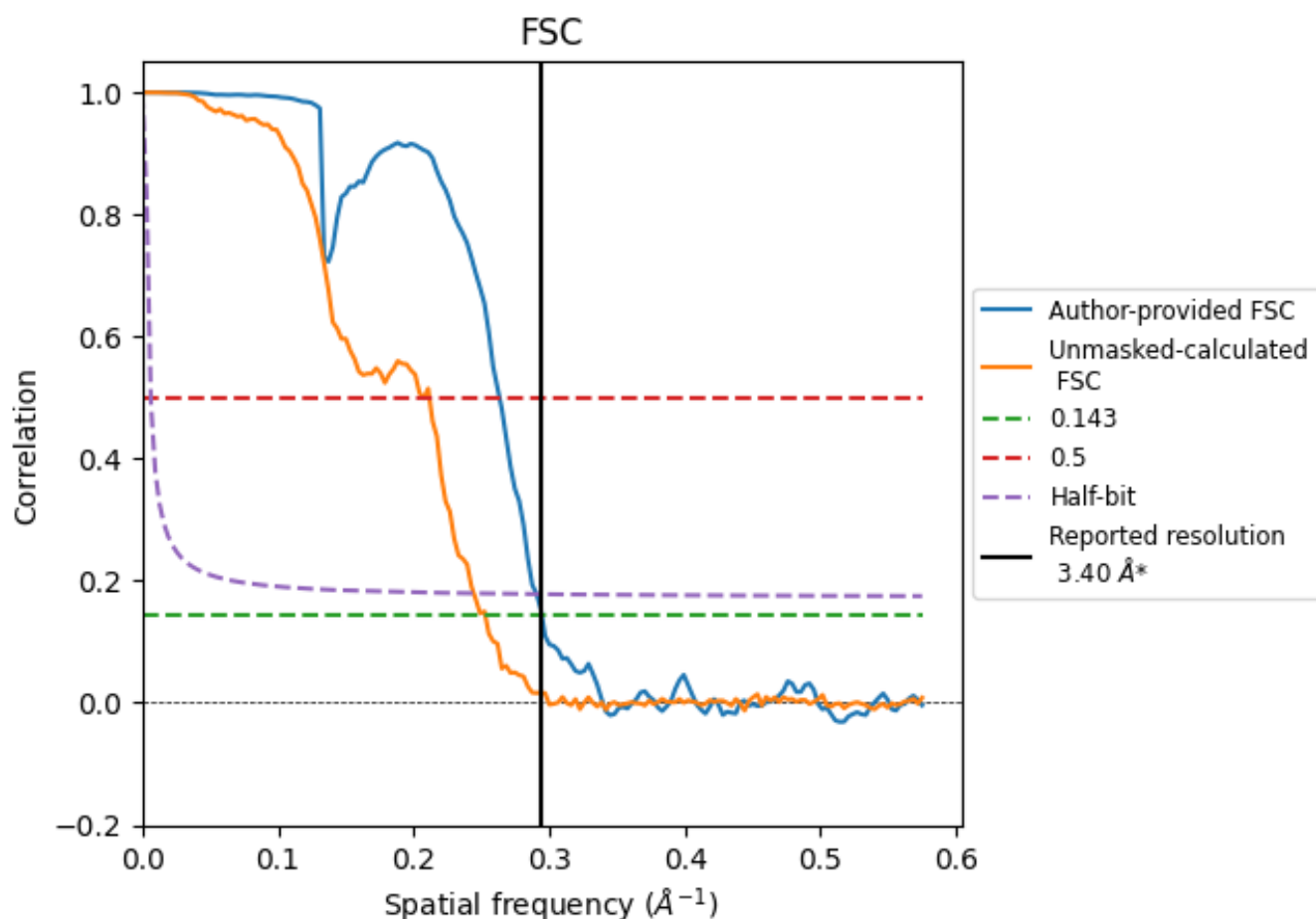


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

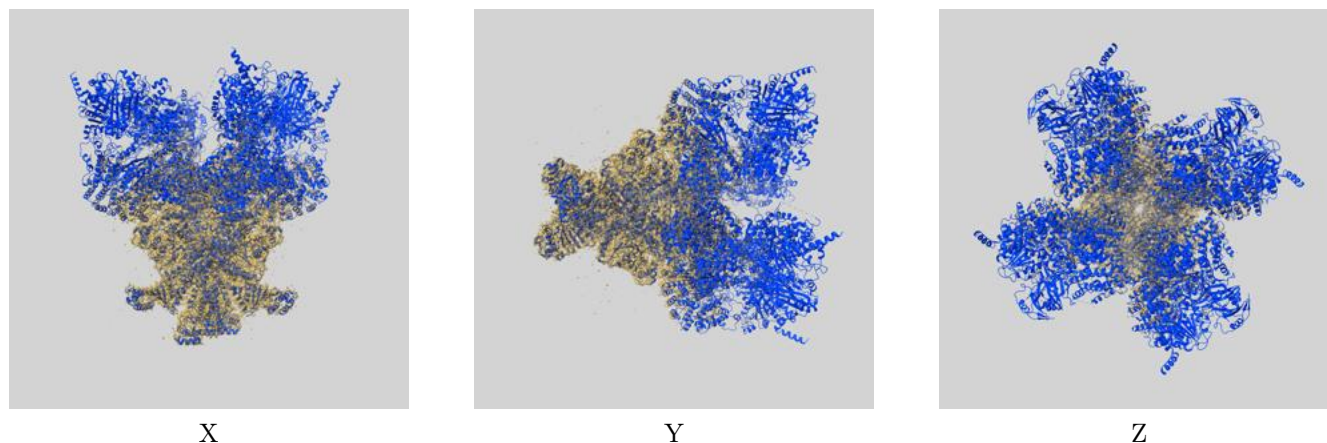
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.80	3.44
Unmasked-calculated*	3.95	4.83	4.09

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

9 Map-model fit [i](#)

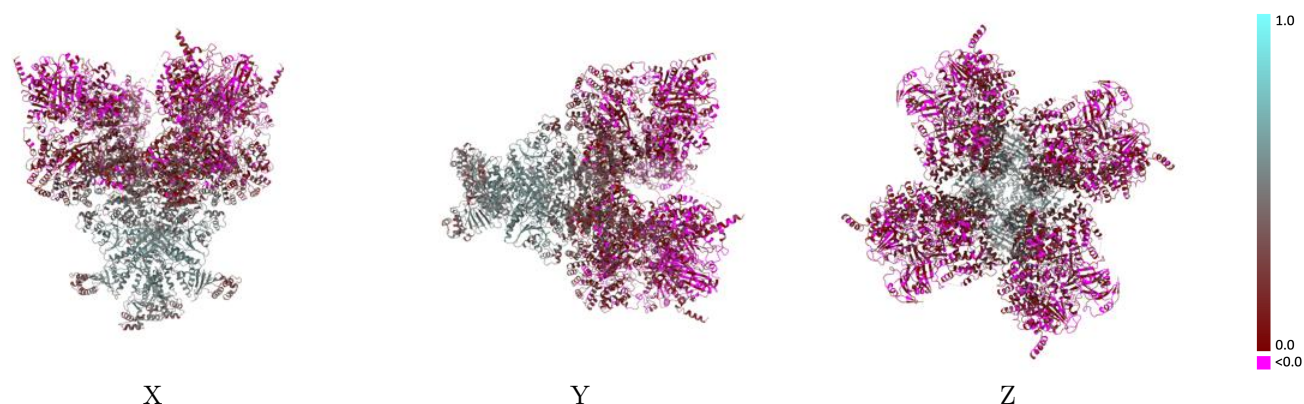
This section contains information regarding the fit between EMDB map EMD-27421 and PDB model 8DGC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



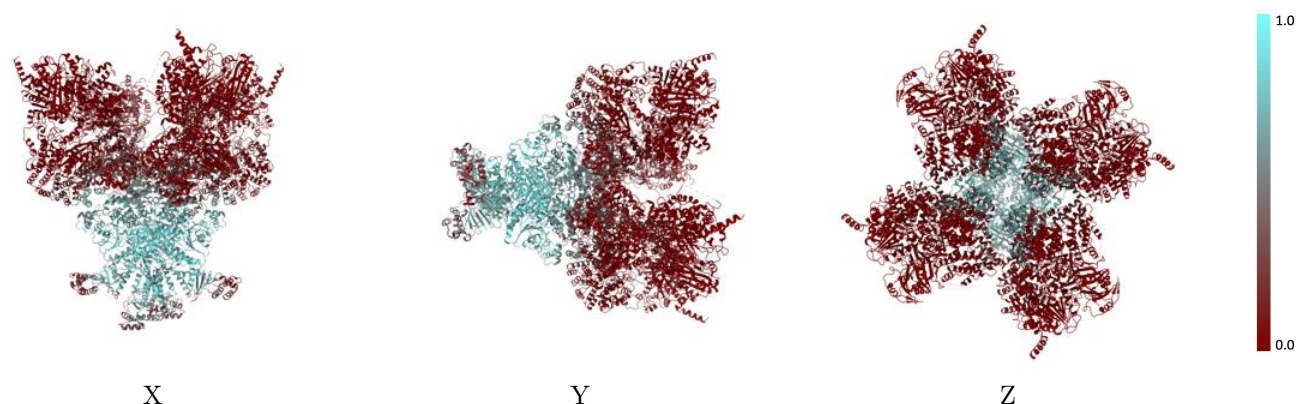
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



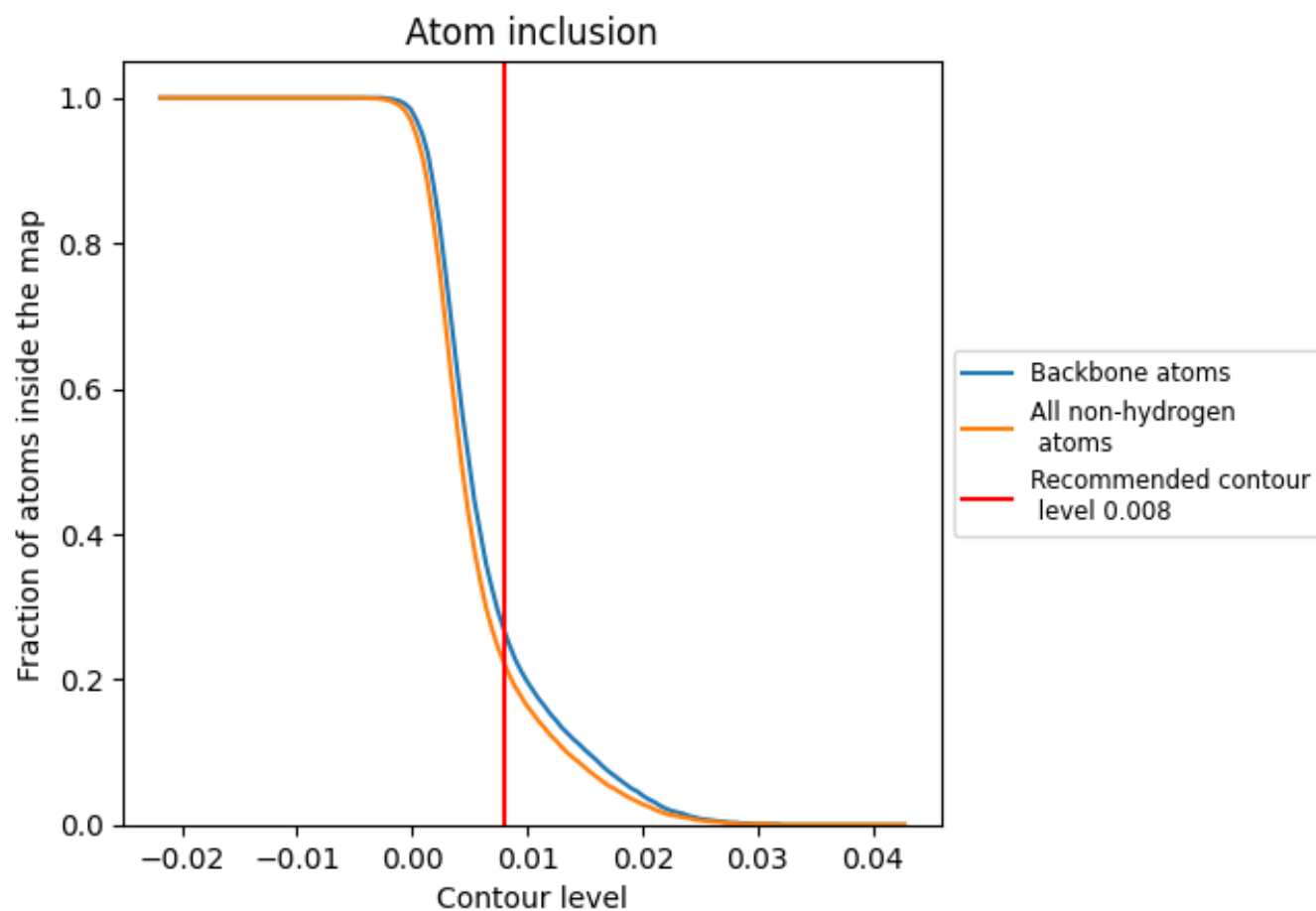
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	0.2220	0.2180
A	0.2790	0.2510
B	0.2790	0.2580
C	0.2800	0.2470
D	0.2790	0.2600
E	0.0070	0.0760
F	0.0090	0.0900
G	0.0070	0.0720
H	0.0090	0.0900

1.0

0.0

<0.0