



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 04:23 AM EST

PDB ID : 6U5W
EMDB ID : EMD-20658
Title : Electron cryomicroscopy structure of C. albicans FAS in the KS-stalled state
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2019-08-28
Resolution : 3.30 Å (reported)
Based on initial model : 2UV8

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

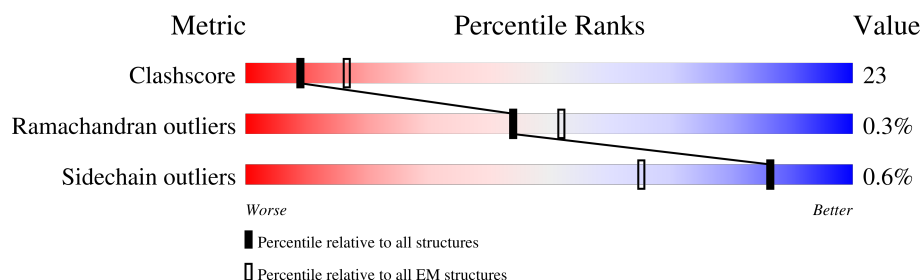
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	1722	<div> <div>21%</div> <div>51%</div> <div>32%</div> <div>17%</div> </div>
2	B	2037	<div> <div>51%</div> <div>54%</div> <div>45%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAP	A	1901	-	-	X	-
3	NAP	B	2102	-	-	X	-
4	FMN	B	2101	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27482 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 Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1435	Total	C	N	O	S	0	0
			11309	7178	1895	2190	46		

There are 173 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	HIS	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	MET	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	MET	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	TYR	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	MET	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	350	VAL	SER	conflict	UNP P43098
A	351	ASP	ARG	conflict	UNP P43098
A	353	ASN	LYS	conflict	UNP P43098
A	354	LYS	GLN	conflict	UNP P43098
A	356	ALA	LEU	conflict	UNP P43098
A	813	THR	PRO	conflict	UNP P43098
A	1066	LYS	GLN	conflict	UNP P43098
A	1123	VAL	ILE	conflict	UNP P43098
A	1444	GLU	LYS	conflict	UNP P43098
A	1742	SER	ASN	conflict	UNP P43098

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2033	Total	C	N	O	S	0	0
			16046	10286	2662	3044	54		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0

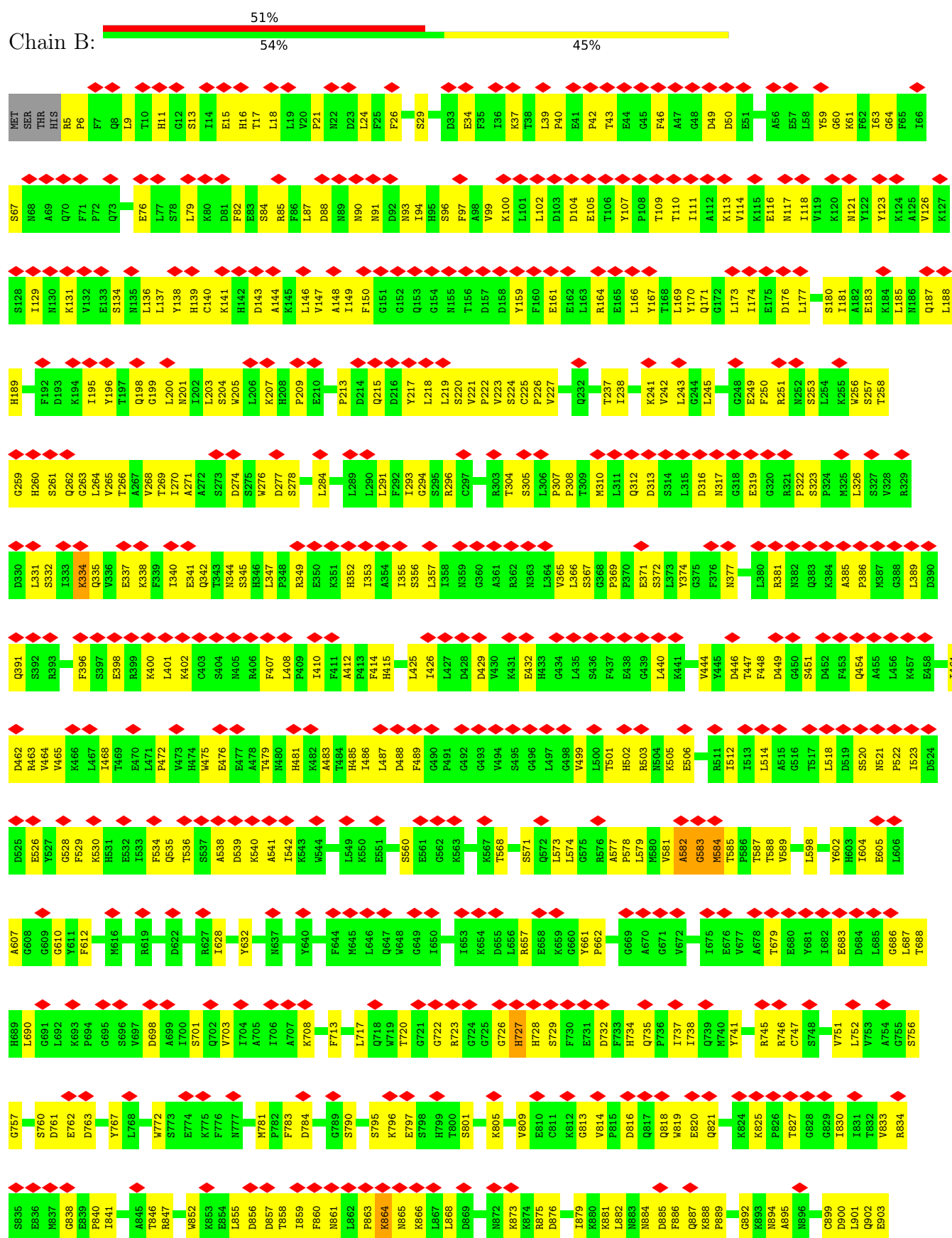
- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			31	17	4	9	1	



● Molecule 2: Fatty acid synthase subunit beta



M904	M905	Y906	K907	E908	L916	K920	K921	S922	H923	I926	D927	V928	L930	R931	M932	M933	Y934	R939	R940	E943	R944	F945	S948	A949	G950	T951	L954	L955	Q956	N957	F958	N959	Q960	L961	N962	E963	P964	E965	Q966	F967	T968	A969	D970	F971	F972	E973	K974	Q977	K980									
Q981	L982	I983	S984	E985	E986	D987	C988	D989	Y990	F991	L992	M993	L994	R997	P998	G999	Q1000	K1001	P1002	V1003	P1004	F1005	V1006	P1007	V1008	L1009	D1010	E1011	F1012	F1013	F1014	F1015	F1016	F1017	K1018	K1019	D1020	S1021	L1022	W1023	Q1024	S1025	E1026	D1027	L1028	E1029	S1030	W1031	V1032	D1033	E1034	D1035	W1036	Q1037	R1038	I1041	L1042	
H1043	G1044	P1045	V1046	A1047	S1048	Q1049	Y1050	K1053	K1122	V1054	D1055	E1056	P1057	I1058	G1059	D1060	I1061	L1062	S1063	S1064	I1065	H1066	E1067	K1075	P1200	E1076	A1079	G1080	D1081	E1082	S1083	K1084	V1087	V1088	E1089	Y1090	G1093	K1094	K1095	P1096	A1097	S1098	V1099	S1100	A1101	T1102	S1103	V1104	N1105	I1106	I1107	D1108	G1109	N1110	Q1111	V1112		
E1115	I1116	D1117	S1118	E1119	L1120	P1121	K1122	K1123	Q1124	E1125	W1126	L1127	D1128	L1129	L1130	A1131	G1132	T1133	E1134	L1135	W1136	W1137	W1138	Q1139	A1140	F1141	I1142	S1143	T1144	D1145	R1146	I1147	V1148	G1149	G1150	S1151	K1152	H1153	M1156	P1157	L1158	H1159	D1160	I1161	T1162	V1163	P1164	A1165	K1166	H1167	S1168	K1169	V1170	I1171	I1172	D1173	K1174	
K1175	T1176	K1177	L1178	T1180	A1181	F1182	E1183	I1184	N1185	K1186	G1187	D1188	L1189	L1190	P1191	V1192	V1193	E1194	I1195	E1196	L1197	V1198	K1199	N1201	T1202	I1203	S1206	E1209	H1210	R1211	T1212	A1213	D1214	T1215	N1216	P1217	V1218	A1219	L1220	P1221	F1222	L1223	Y1224	K1225	T1226	N1227	P1228	A1229	D1230	G1231	F1232	A1233	T1234	I1235	L1236			
E1237	I1238	M1239	E1240	D1241	R1242	R1245	I1246	K1247	E1248	F1249	Y1250	W1251	G1256	S1257	S1258	V1259	P1260	Y1261	S1262	N1263	D1264	I1265	N1266	V1267	E1268	K1269	I1270	I1271	L1272	G1273	D1274	E1275	I1276	I1277	I1278	S1279	F1286	T1287	H1288	A1289	I1290	G1291	N1292	C1294	D1295	D1296	F1297	V1298	D1299	P1300	G1302	K1303	A1304	T1305				
L1306	A1307	P1308	M1309	D1310	F1311	A1312	I1313	V1314	T1315	G1316	W1317	K1318	T1321	K1322	A1323	F1324	P1325	P1326	K1327	S1328	V1329	D1330	G1331	D1332	L1333	K1335	L1336	V1337	H1338	L1339	S1340	N1341	G1342	Y1343	G1344	M1345	I1346	T1347	G1348	A1349	P1351	L1352	K1353	K1354	G1355	D1356	V1357	P1358	S1359	T1360	E1363	A1366	V1367	L1368				
M1369	Q1370	P1371	K1374	L1375	V1376	E1377	I1382	Y1383	R1384	E1385	G1386	M1390	Q1395	F1396	R1399	G1400	E1401	Y1402	N1403	D1404	Y1405	C1406	N1407	T1408	E1414	T1415	P1416	P1417	Q1418	V1419	A1420	F1421	G1422	S1423	A1424	K1425	D1426	L1427	A1428	V1429	L1430	R1431	S1432	K1433	E1434	W1435	F1436	H1437	L1438	E1439	K1440	D1441	V1442					
Q1443	F1444	D1445	V1446	L1447	T1448	F1449	R1450	C1451	E1452	S1453	K1456	F1457	K1458	S1459	A1460	N1461	Y1462	Y1463	S1464	K1467	T1468	T1469	G1470	Q1471	E1475	L1476	P1477	T1478	K1479	E1480	Y1481	L1482	Q1483	V1484	G1485	S1486	V1487	Y1489	E1490	A1491	G1492	H1497	P1498	D1501	Y1502	L1503	S1504	H1505	G1506	M1507	K1508	T1509	F1510					
E1511	E1512	S1513	E1517	M1518	A1519	I1520	P1521	L1522	S1523	S1524	G1525	E1526	E1527	L1528	T1529	S1530	K1531	A1532	P1533	G1534	T1535	M1536	E1537	P1538	I1541	V1542	S1543	G1544	D1545	Y1546	M1547	P1548	I1549	H1550	V1551	S1552	R1553	V1554	F1555	A1556	A1557	K1560	G1563	T1564	I1565	T1566	H1567	G1568	M1569	Y1570	S1571	S1572	A1573	S1574				
I1575	R1576	A1577	L1578	V1579	E1580	E1581	W1582	A1583	A1584	M1585	M1586	V1587	A1588	A1589	R1590	V1591	R1592	A1593	F1594	K1595	C1596	D1597	F1598	V1599	G1600	M1601	V1602	L1603	P1604	M1605	D1606	T1607	L1608	Q1609	T1610	T1611	M1612	E1613	H1614	M1617	I1618	N1619	G1620	R1621	K1622	I1623	I1624	K1625	V1626	E1627	T1628	R1629	M1630	V1631	E1632	T1633	E1634	L1635
P1636	V1637	L1638	T1639	G1640	E1641	A1642	E1643	I1644	E1645	Q1646	P1647	T1648	T1649	T1650	Y1651	V1652	T1654	G1655	Q1656	G1657	S1658	Q1659	E1660	Q1661	G1662	M1663	G1664	M1665	E1666	L1667	Y1668	N1669	S1670	S1671	E1672	V1673	A1674	R1675	E1676	V1677	V1678	D1679	K1680	L1683	H1684	F1685	V1686	N1687	M1688	Y1689	G1690	F1691	L1694	D1695	Q1698			
M1699	N1702	E1703	L1704	T1705	I1706	H1707	F1708	G1709	K1712	G1713	R1714	A1715	I1716	R1717	D1718	M1719	Y1720	I1721	G1722	M1723	M1724	F1725	E1726	T1727	I1728	G1729	E1730	D1731	G1732	A1733	L1734	K1735	S1736	E1737	K1738	I1739	F1740	K1741	D1742	I1743	D1744	E1745	S1749	Y1750	T1751	F1752	V1753	S1754	P1755	T1756	G1757	L1758	S1760	A1761	T1762			

L2009	L1948	A1888	V1828	Q1763
T2010	E1949	A1889	A1829	F1764
K2011	R1950	G1890	V1830	T1765
E2012	G1951	D1891	P1831	Q1766
Y2013	F1952	L1892	R1832	P1767
F2014	A1953	R1893	D1833	A1768
Q2015	V1954	A1894	E1834	L1769
S2016	I1955	L1895	L1835	T1770
V2017	P1956	D1896	G1836	L1771
Y2018	L1957	T1897	R1837	M1772
D2019	K1958	L1898	S1838	L1773
T2021	G1959	T1899	N1839	
K2022	I1960	N1900	Y1840	Y1777
S2023	S1961	V1901	G1841	E1778
E2024	V1962	L1902	M1842	D1779
K2025	P1963	N1903	V1843	I1780
T2026	F1964	V1904	A1844	
K2027	H1965	L1905	V1845	K1783
S2028	S1966	K1906	N1846	G1784
I2029	S1967	I1907	P1847	L1785
L2030	Y1968	N1908	S1848	I1786
D2031	L1969	K1909	R1849	P1787
N2032	M1970	I1910	V1850	S1788
W2033		D1911	S1851	D1789
E2034	Y1973	I1912	A1852	I1790
Q2035	K1974	V1913	T1853	M1791
Y2036	P1975	K1914	F1854	F1792
E2037	Q1977	L1915	D1855	A1793
	R1978	Q1916	D1856	G1794
	F1979	E1917	S1857	H1795
	L1980	Q1918	A1858	S1796
	C1981	M1919	L1859	L1797
	K1982	S1920	R1860	G1798
	I1984	I1921	F1861	E1799
	P1985	E1922	V1862	Y1800
	K1986	K1923	V1863	
	S1987	V1924	D1864	L1803
	S1988	K1925	E1865	S1804
	V1989	E1926	V1866	S1805
	K1990	H1927	A1867	L1806
	P1991	L1928	N1868	A1807
	Q1992	Y1929	K1869	N1808
	L1993	E1930	T1870	V1809
	D1994	I1931	K1871	M1810
	I1995	V1932	L1872	P1811
	G1996	D1933	L1873	I1812
	K1997	E1934	L1874	E1813
	Y1998	V1935	E1875	S1814
	I1999	A1936	I1876	L1815
	P2000	A1937	V1877	V1816
	N2001	K1938	P1877	D1817
	L2002	T2003	N1878	V1818
	T2003	S1939	Y1879	V1819
	A2004	L1940	N1880	
	K2005	A1941	V1881	R1822
	P2006	K1942	E1882	G1823
	F2007	P1943	N1883	M1824
	E2008	Q1944	Q1884	T1825
		P1945	Q1885	M1826
		I1946	Y1886	Q1827
		D1947	V1887	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	24417	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTFFIND4 within cryoSPARC2	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.942	Depositor
Minimum map value	-0.817	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.133	Depositor
Recommended contour level	0.704	Depositor
Map size (\AA)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.54	0/11536	0.52	0/15595
2	B	0.42	0/16415	0.49	1/22269 (0.0%)
All	All	0.47	0/27951	0.50	1/37864 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	2004	ALA	C-N-CA	-5.59	107.73	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1301	GLY	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	11309	0	11219	475	0
2	B	16046	0	16024	829	0
3	A	48	0	25	34	0
3	B	48	0	25	50	0
4	B	31	0	17	51	0
All	All	27482	0	27310	1265	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 23.

The worst 5 of 1265 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:B:584:MET:HE2	4:B:2101:FMN:C7	1.26	1.61
2:B:584:MET:HB3	4:B:2101:FMN:C5A	1.29	1.61
1:A:712:PHE:CE1	1:A:717:THR:HG22	1.35	1.58
2:B:727:HIS:ND1	3:B:2102:NAP:C4N	1.79	1.45
2:B:727:HIS:ND1	3:B:2102:NAP:C3N	1.73	1.44

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	1427/1722 (83%)	1306 (92%)	115 (8%)	6 (0%)	34 66
2	B	2031/2037 (100%)	1860 (92%)	168 (8%)	3 (0%)	51 81
All	All	3458/3759 (92%)	3166 (92%)	283 (8%)	9 (0%)	44 71

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	879	ALA
2	B	582	ALA
1	A	623	THR
1	A	876	LEU
2	B	727	HIS

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	1222/1445 (85%)	1211 (99%)	11 (1%)	78	87
2	B	1780/1784 (100%)	1772 (100%)	8 (0%)	91	95
All	All	3002/3229 (93%)	2983 (99%)	19 (1%)	86	91

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	873	LYS
2	B	1714	ARG
2	B	1837	ARG
2	B	1667	LEU
1	A	1501	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	818	GLN
2	B	1965	HIS
2	B	884	ASN
2	B	2035	GLN
2	B	1688	ASN

5.3.3 RNA ⓘ

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](#)

3 ligands are modelled in this entry.

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
4	FMN	B	2101	-	33,33,33	6.33	21 (63%)	48,50,50	1.29	5 (10%)
3	NAP	B	2102	-	45,52,52	0.81	1 (2%)	56,80,80	1.23	4 (7%)
3	NAP	A	1901	-	45,52,52	0.81	1 (2%)	56,80,80	1.22	4 (7%)

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
4	FMN	B	2101	-	-	5/18/18/18	0/3/3/3
3	NAP	B	2102	-	-	6/31/67/67	0/5/5/5
3	NAP	A	1901	-	-	11/31/67/67	0/5/5/5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2101	FMN	C6-C7	12.63	1.58	1.39
4	B	2101	FMN	C9-C9A	12.27	1.59	1.39
4	B	2101	FMN	C6-C5A	11.98	1.58	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2101	FMN	C9-C8	11.14	1.55	1.39
4	B	2101	FMN	C4A-N5	10.59	1.51	1.30

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2102	NAP	PN-O3-PA	-3.57	120.58	132.83
3	A	1901	NAP	PN-O3-PA	-3.52	120.76	132.83
3	B	2102	NAP	C3D-C2D-C1D	3.39	106.08	100.98
3	A	1901	NAP	C3D-C2D-C1D	3.38	106.06	100.98
3	B	2102	NAP	N3A-C2A-N1A	-3.19	123.69	128.68

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1901	NAP	C5B-O5B-PA-O1A
3	A	1901	NAP	C5D-O5D-PN-O1N
3	A	1901	NAP	C5D-O5D-PN-O2N
3	B	2102	NAP	C5D-O5D-PN-O1N
4	B	2101	FMN	C2'-C3'-C4'-C5'

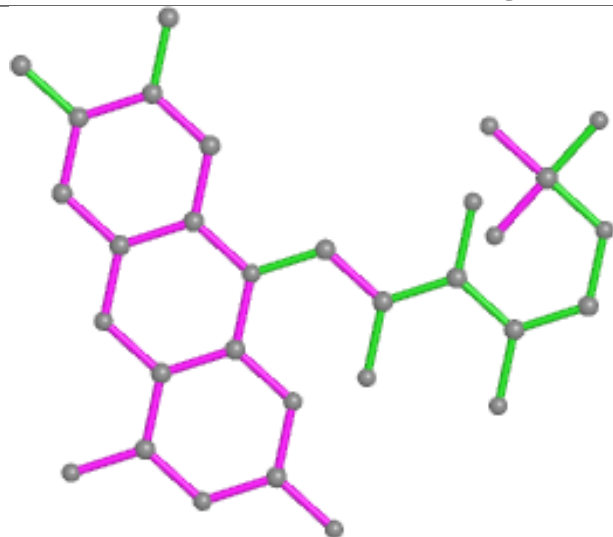
There are no ring outliers.

3 monomers are involved in 135 short contacts:

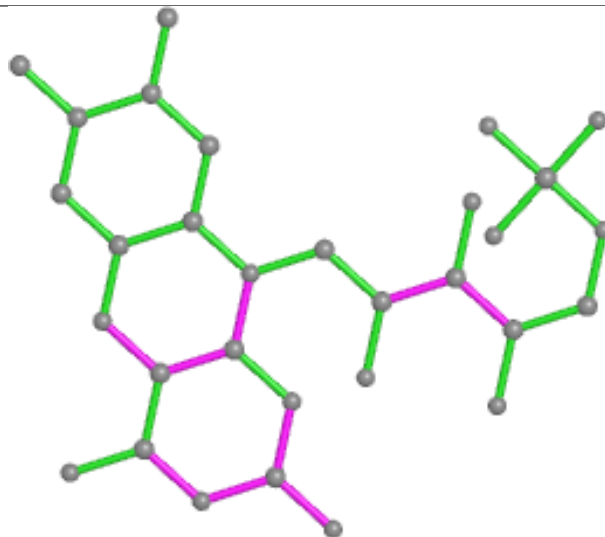
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2101	FMN	51	0
3	B	2102	NAP	50	0
3	A	1901	NAP	34	0

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.

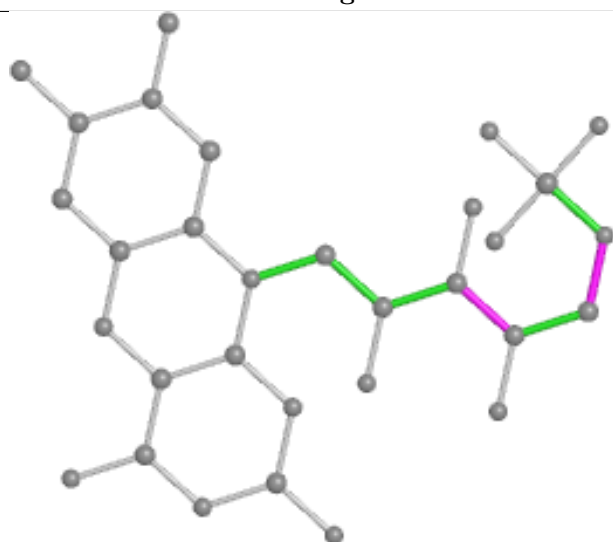
Ligand FMN B 2101



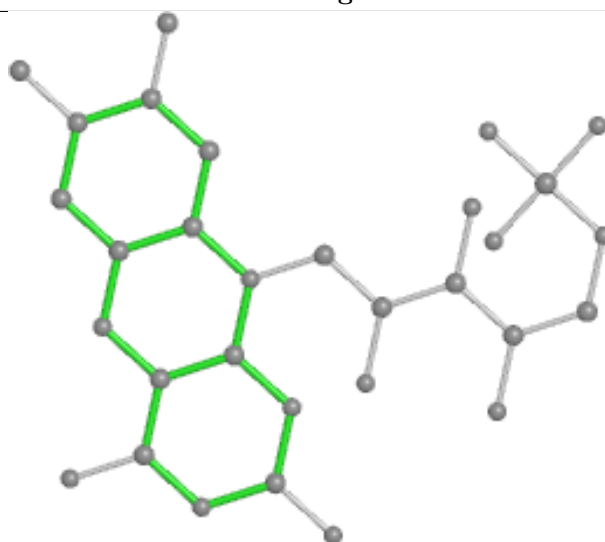
Bond lengths



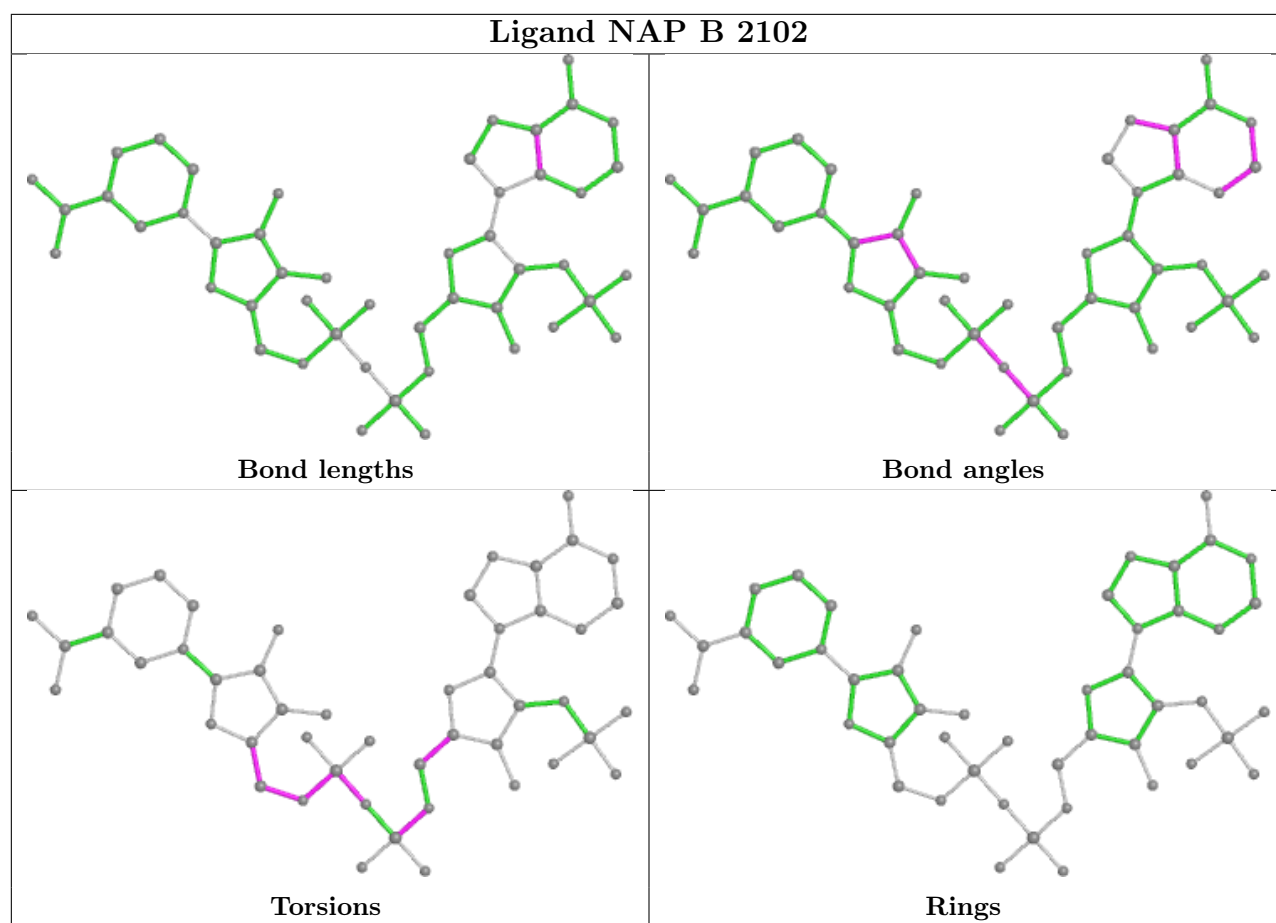
Bond angles

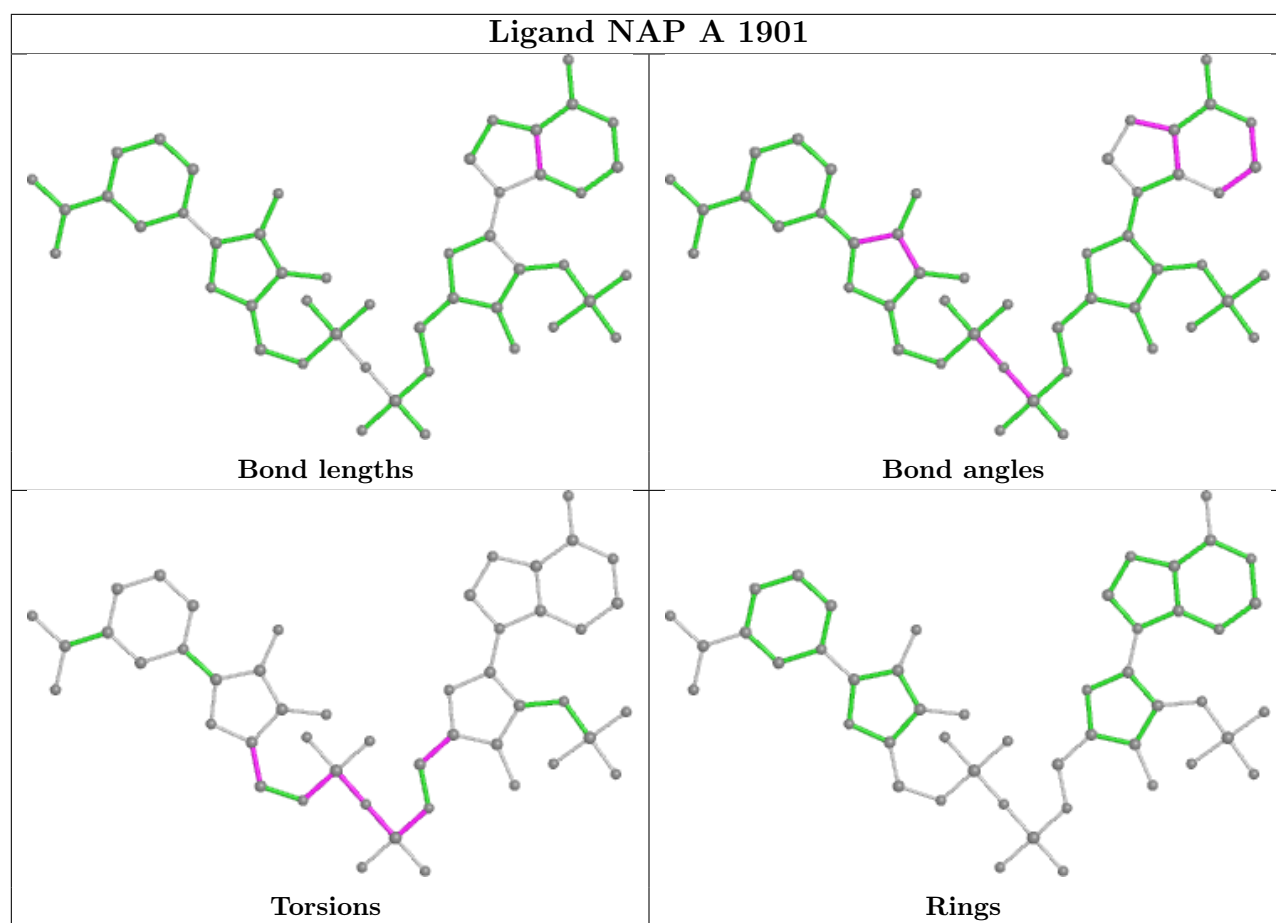


Torsions



Rings





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.

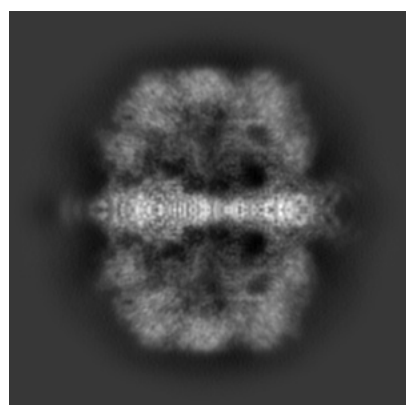
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20658. These allow visual inspection of the internal detail of the map and identification of artifacts.

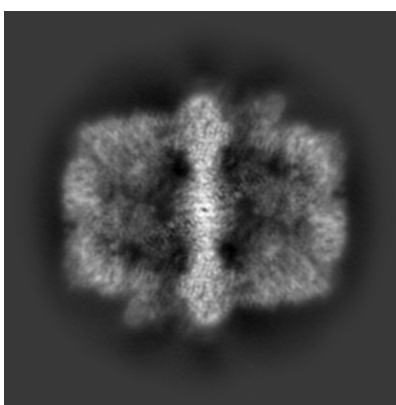
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

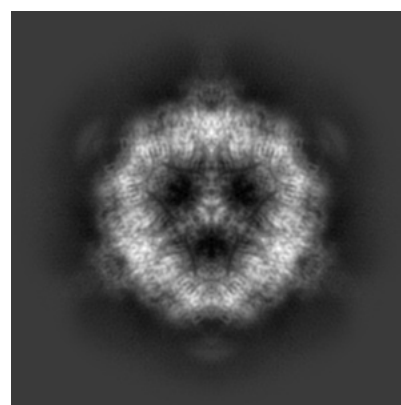
6.1.1 Primary map



X



Y

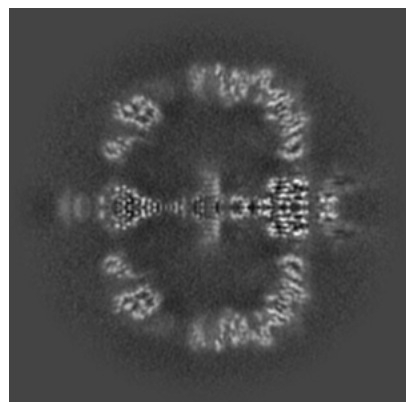


Z

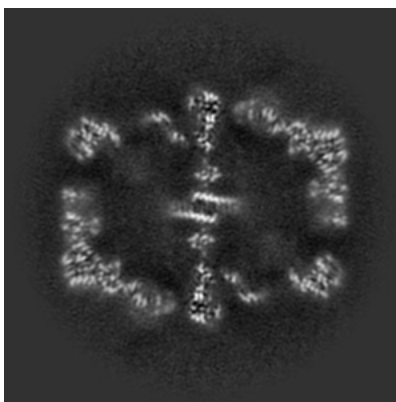
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

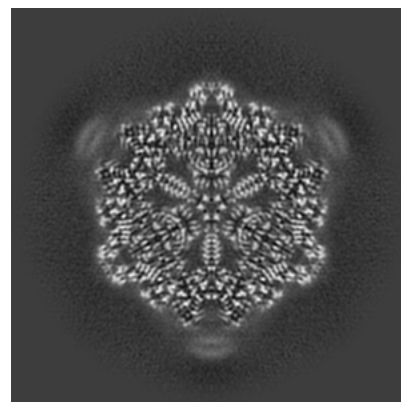
6.2.1 Primary map



X Index: 176



Y Index: 176

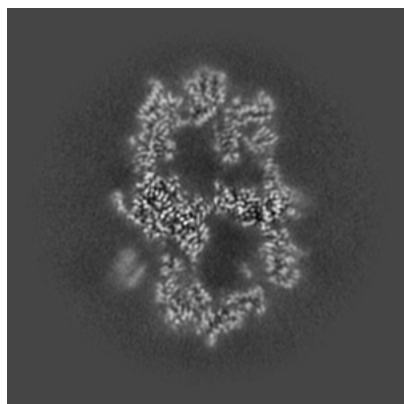


Z Index: 176

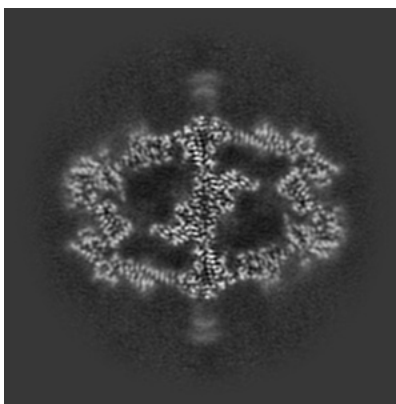
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

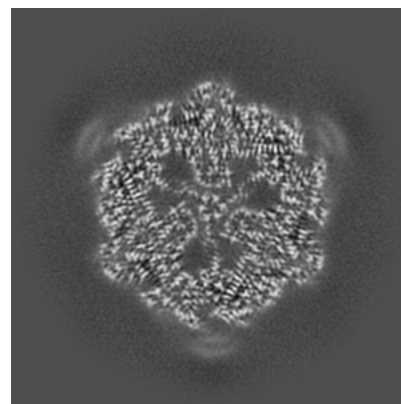
6.3.1 Primary map



X Index: 237



Y Index: 231



Z Index: 172

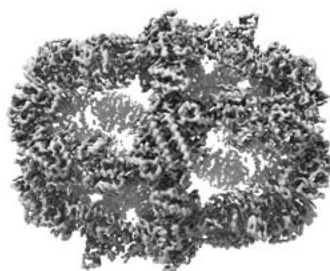
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

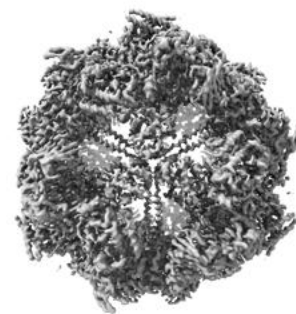
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.704. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

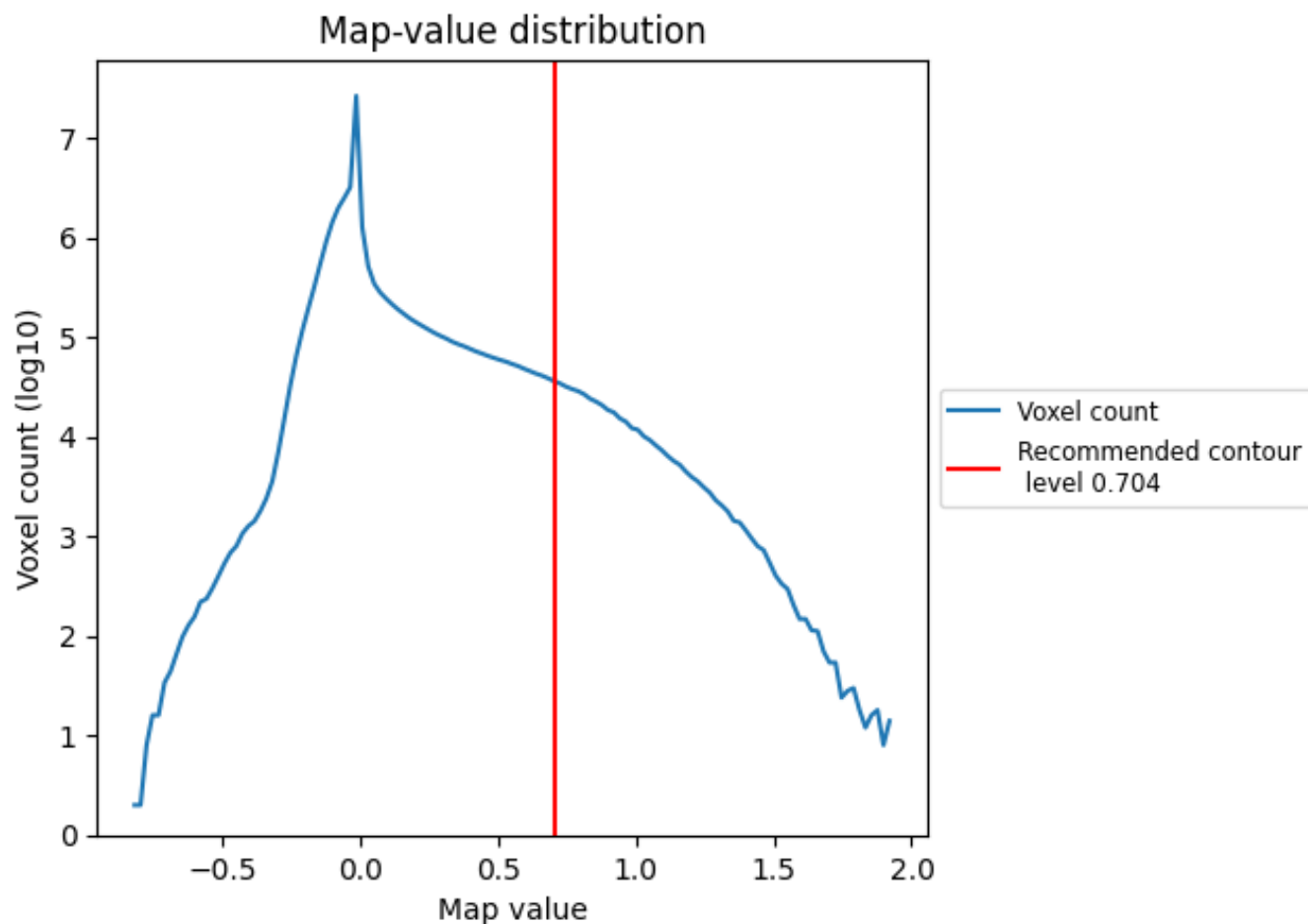
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

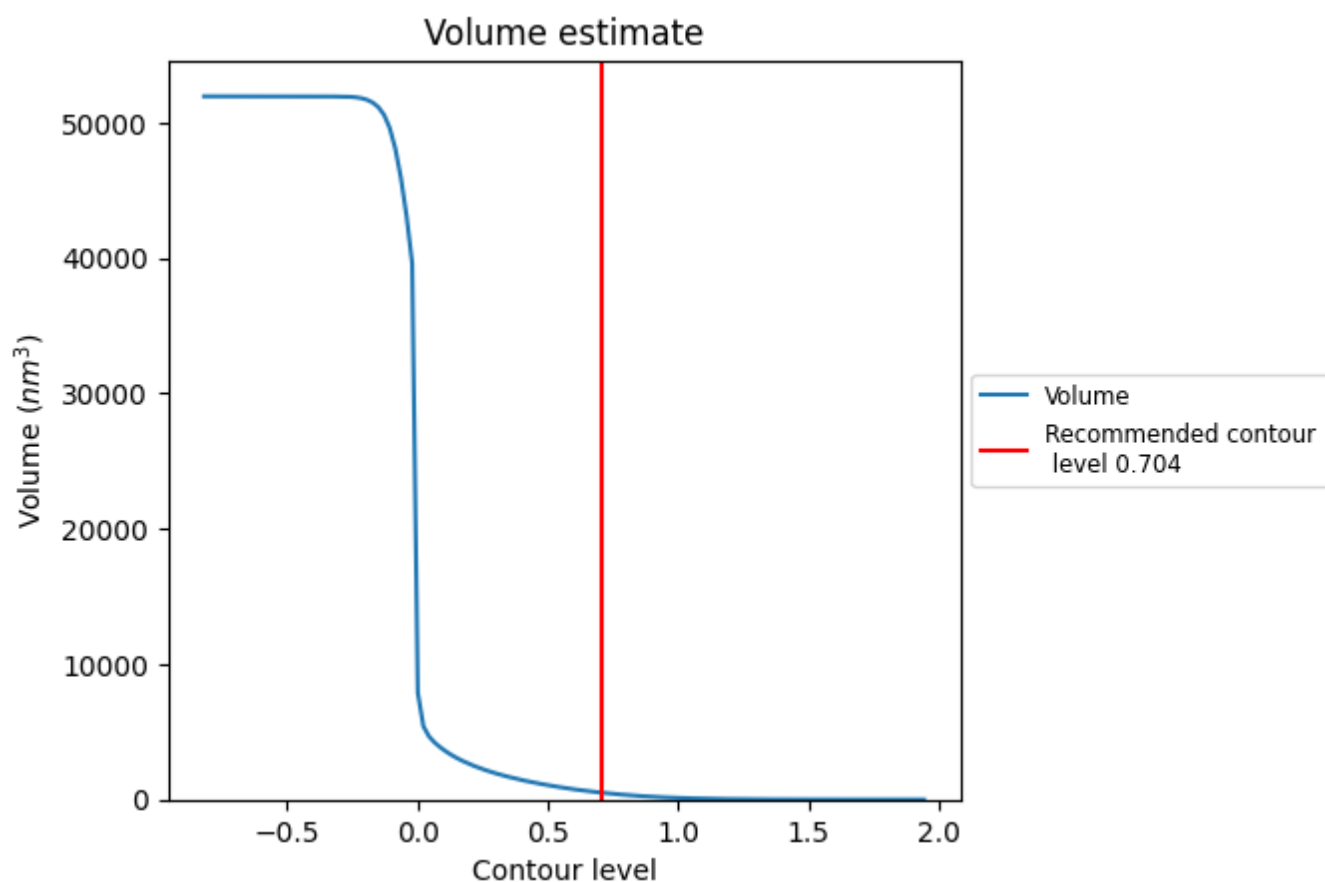
This section contains the results of statistical analysis of the map.

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.

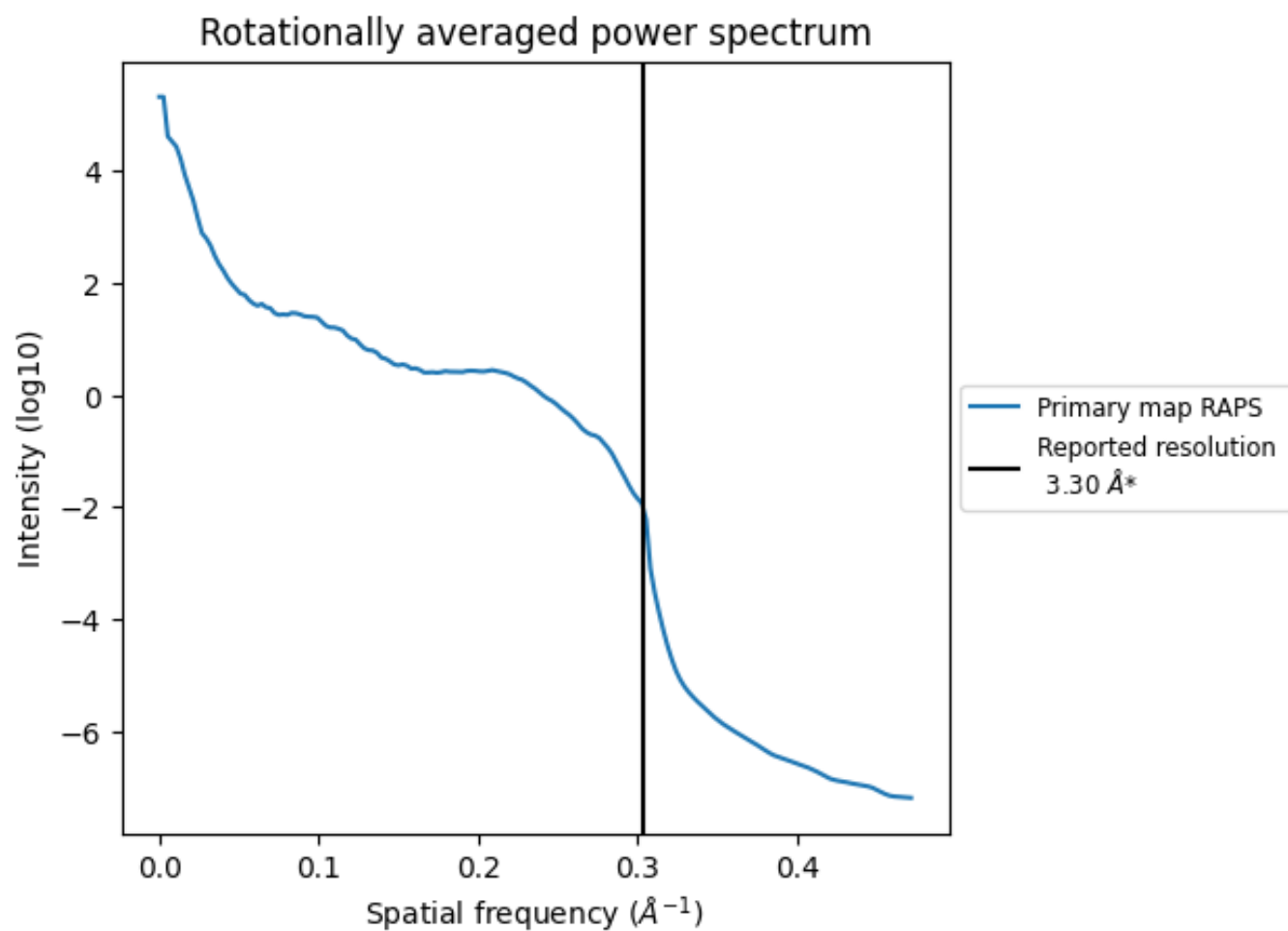
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 513 nm³; this corresponds to an approximate mass of 464 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 0.303 Å⁻¹

8 Fourier-Shell correlation

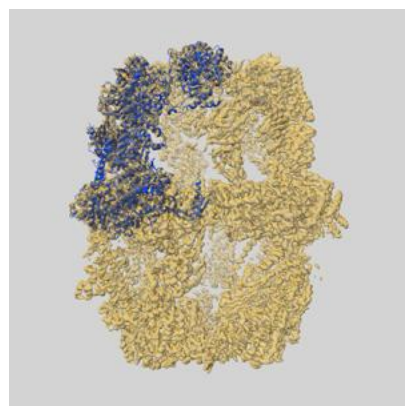
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

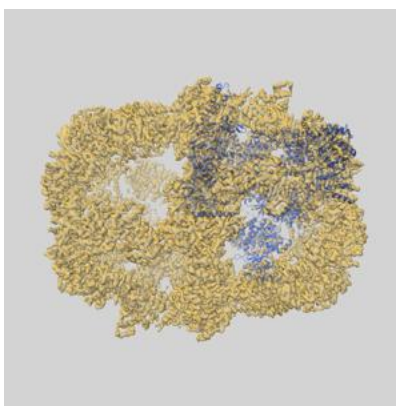
This section contains information regarding the fit between EMDB map EMD-20658 and PDB model 6U5W. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlays

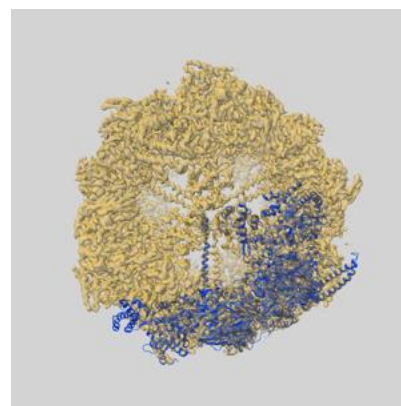
9.1.1 Map-model overlay [i](#)



X

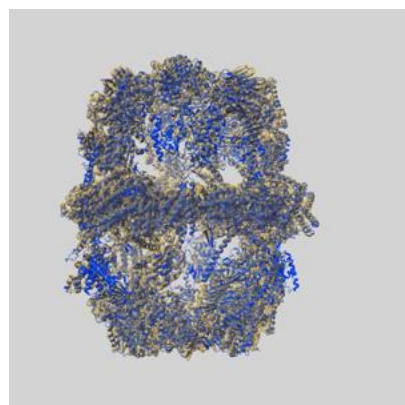


Y

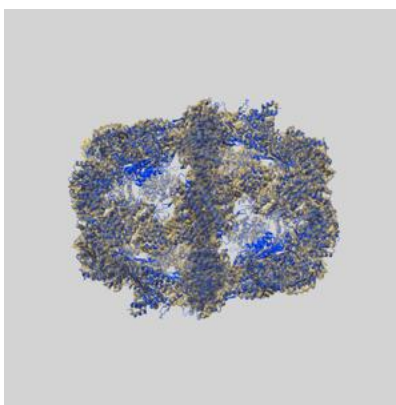


Z

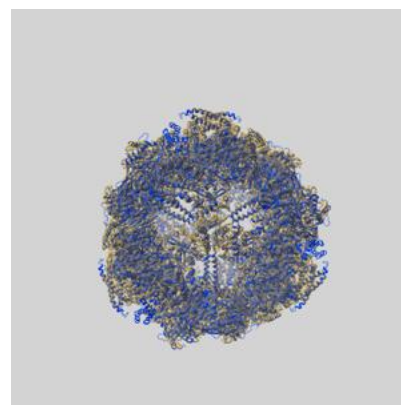
9.1.2 Map-model assembly overlay [i](#)



X



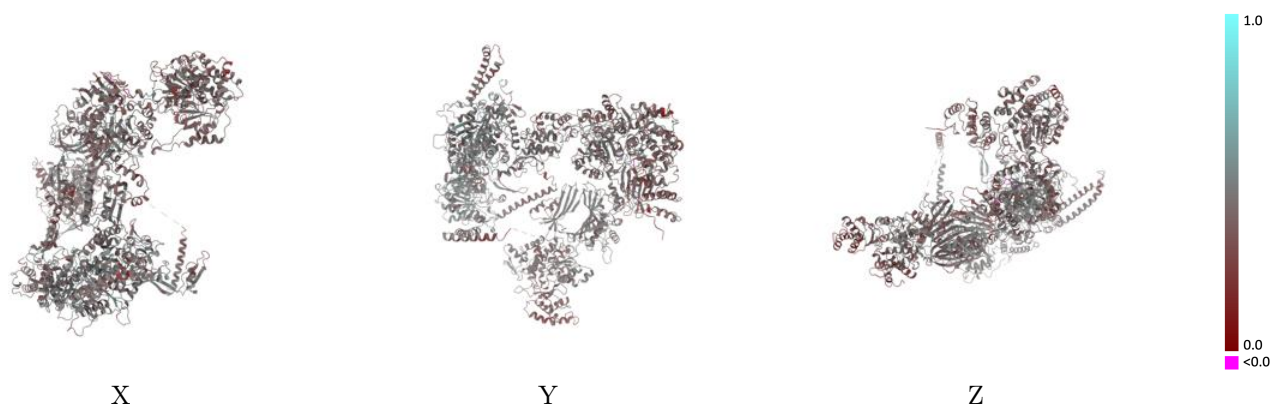
Y



Z

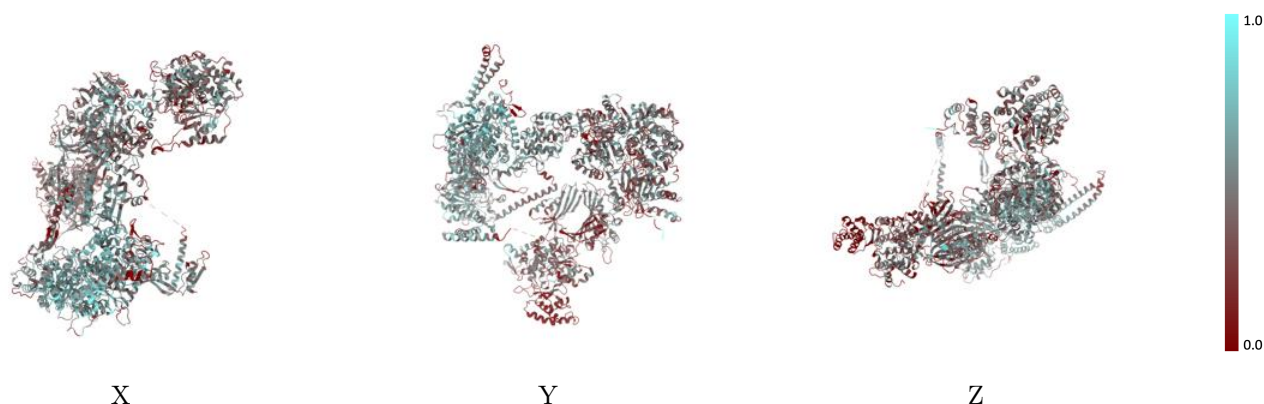
The images above show the 3D surface view of the map at the recommended contour level 0.704 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



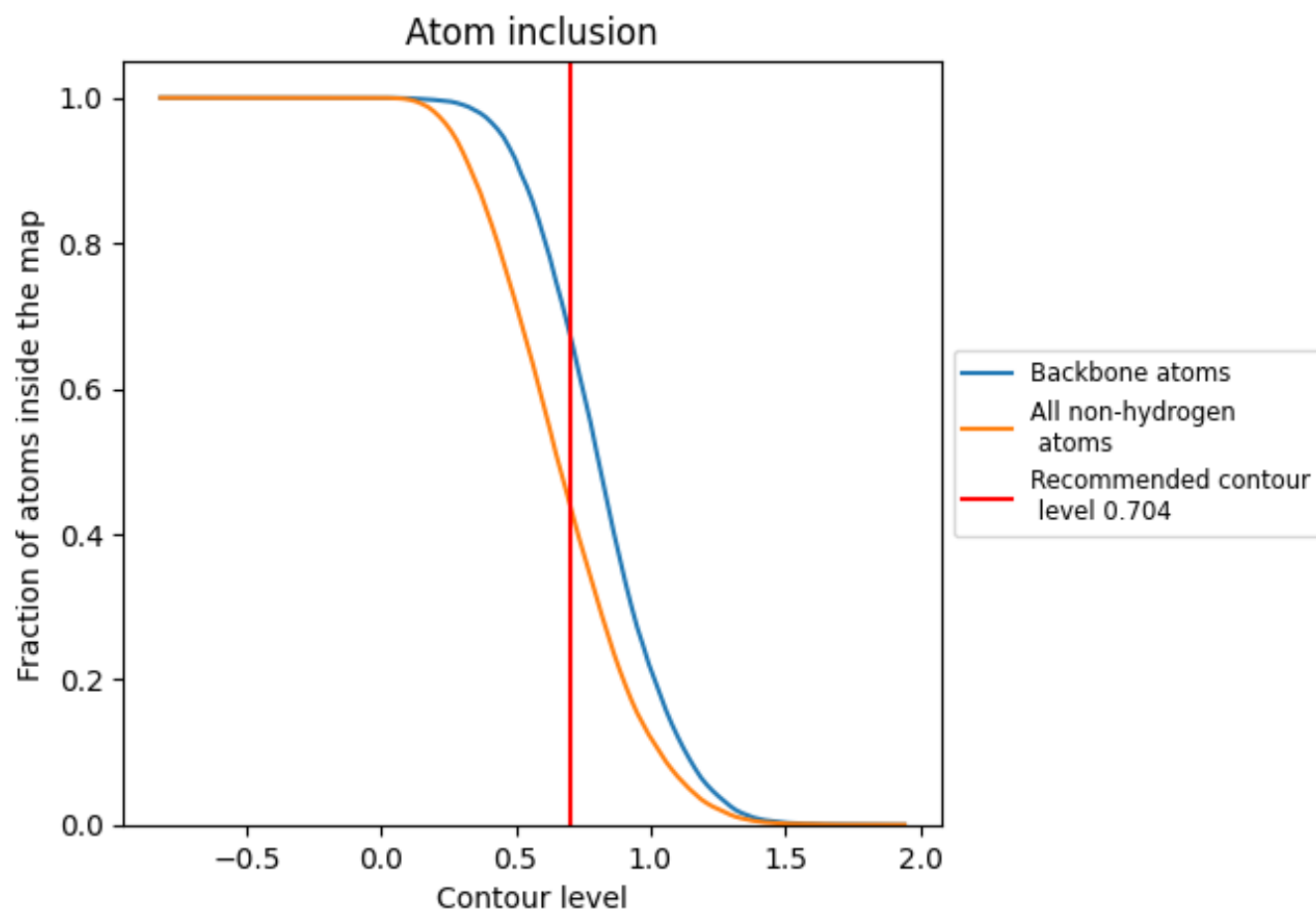
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.704).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 44% 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 (0.704) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4364	<div></div> 0.4280
A	<div></div> 0.5226	<div></div> 0.4560
B	<div></div> 0.3758	<div></div> 0.4080

