



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 02:57 PM UTC

PDB ID : 6U5T / pdb_00006u5t
EMDB ID : EMD-20655
Title : Electron cryomicroscopy Structure of *S. cerevisiae* FAS in the Apo state
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2019-08-28
Resolution : 2.90 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.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 EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

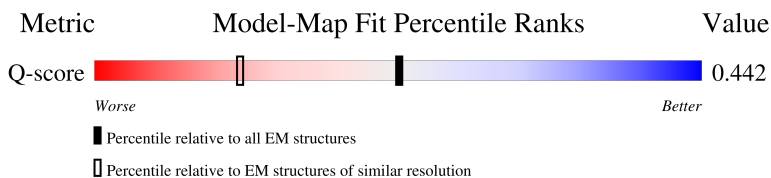
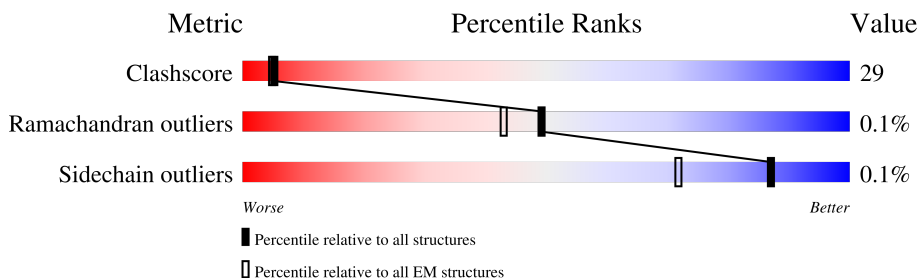
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	1887	26% 45% 40% 14%
2	G	2073	46% 48% 50% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28233 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	1616	Total	C	N	O	S	0	0
			12202	7703	2086	2368	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2033	Total	C	N	O	S	0	0
			15995	10253	2660	3026	56		

There are 22 discrepancies between the modelled and reference sequences:

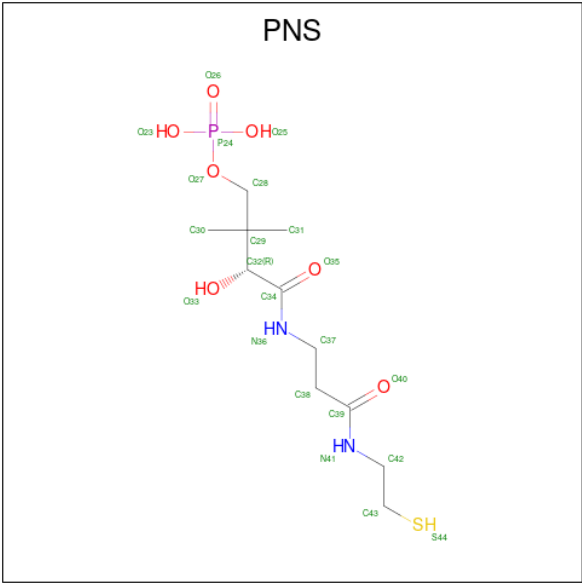
Chain	Residue	Modelled	Actual	Comment	Reference
G	2052	ASP	-	expression tag	UNP P07149
G	2053	TYR	-	expression tag	UNP P07149
G	2054	LYS	-	expression tag	UNP P07149
G	2055	ASP	-	expression tag	UNP P07149
G	2056	HIS	-	expression tag	UNP P07149
G	2057	ASP	-	expression tag	UNP P07149
G	2058	GLY	-	expression tag	UNP P07149
G	2059	ASP	-	expression tag	UNP P07149
G	2060	TYR	-	expression tag	UNP P07149
G	2061	LYS	-	expression tag	UNP P07149
G	2062	ASP	-	expression tag	UNP P07149
G	2063	HIS	-	expression tag	UNP P07149
G	2064	ASP	-	expression tag	UNP P07149
G	2065	ILE	-	expression tag	UNP P07149
G	2066	ASP	-	expression tag	UNP P07149
G	2067	TYR	-	expression tag	UNP P07149
G	2068	LYS	-	expression tag	UNP P07149
G	2069	ASP	-	expression tag	UNP P07149
G	2070	ASP	-	expression tag	UNP P07149
G	2071	ASP	-	expression tag	UNP P07149
G	2072	ASP	-	expression tag	UNP P07149

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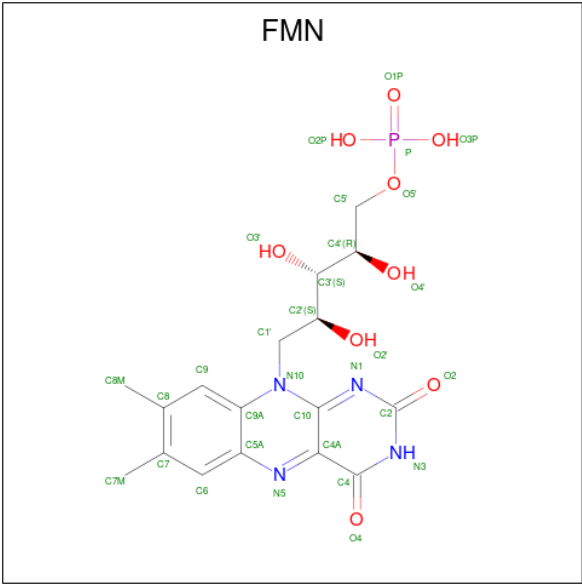
Chain	Residue	Modelled	Actual	Comment	Reference
G	2073	LYS	-	expression tag	UNP P07149

- Molecule 3 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).

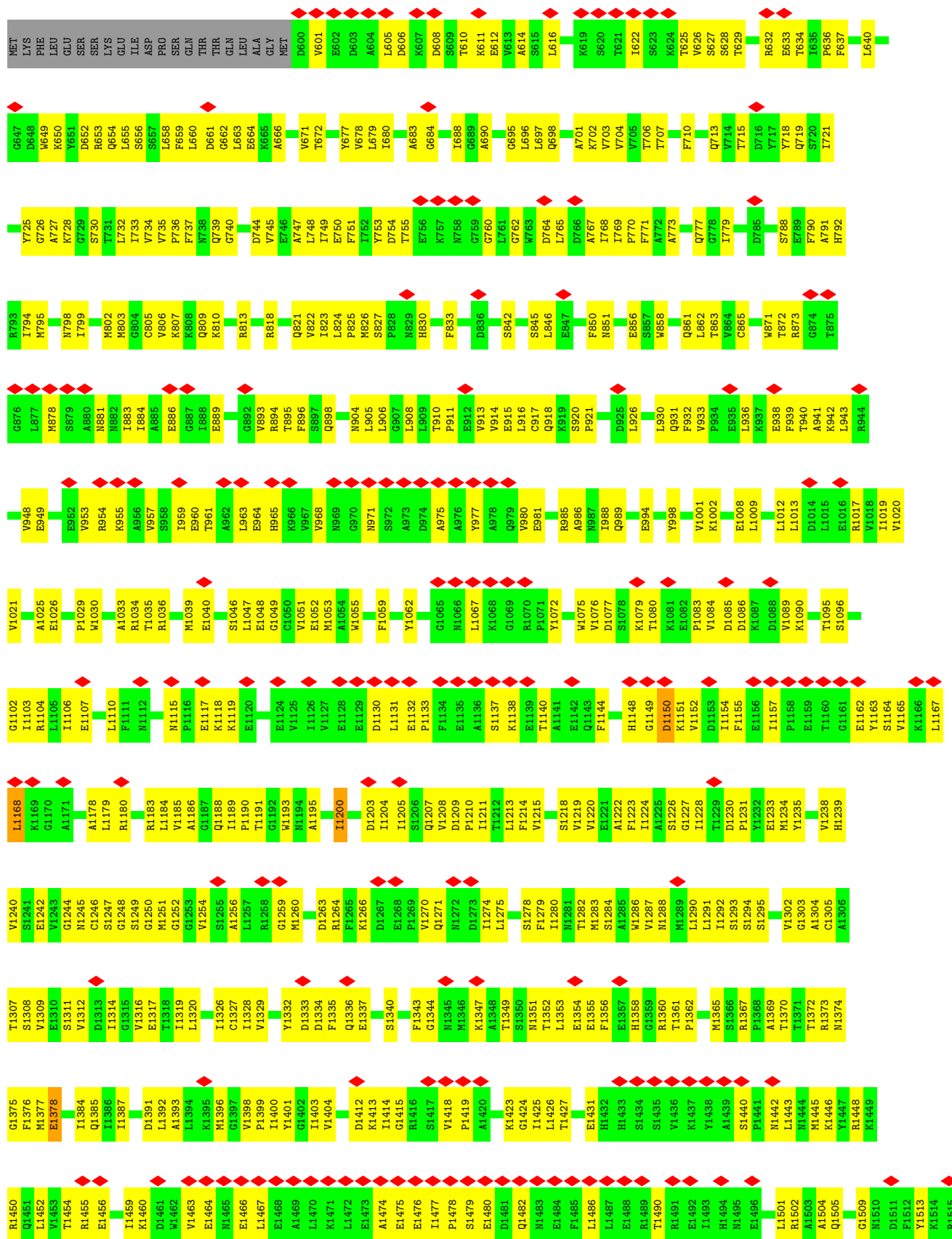


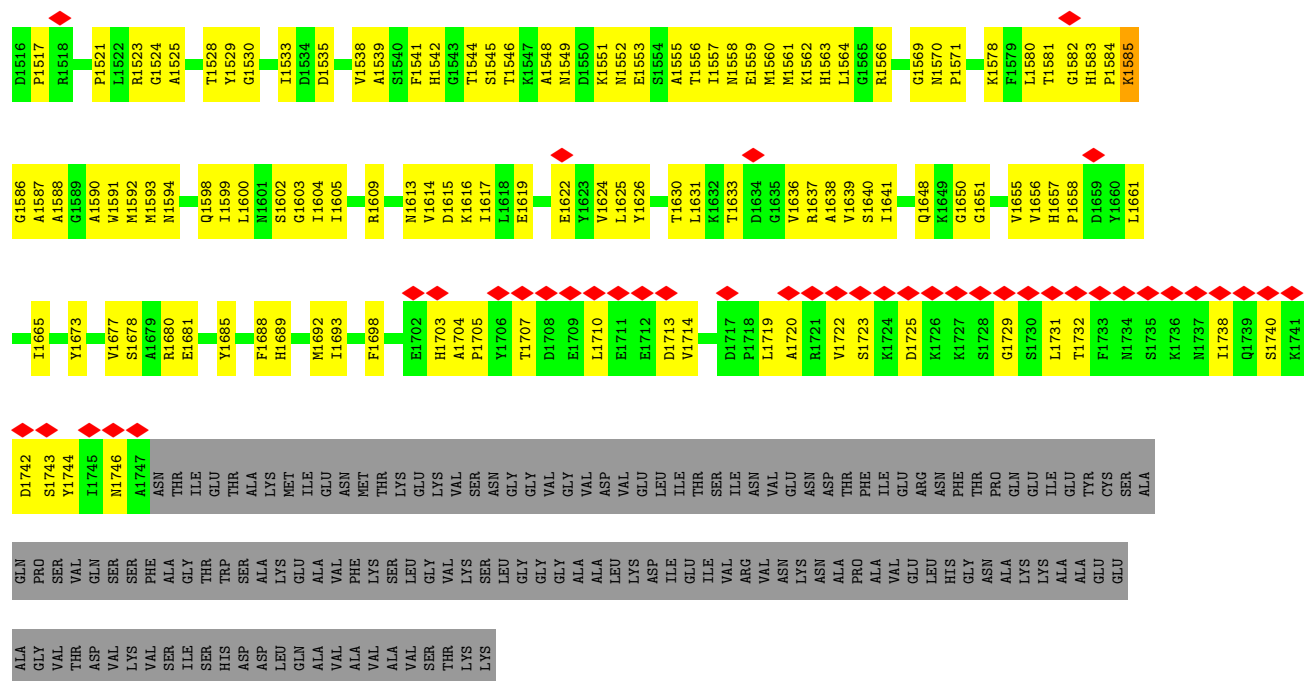
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			5	1	3	1	

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).

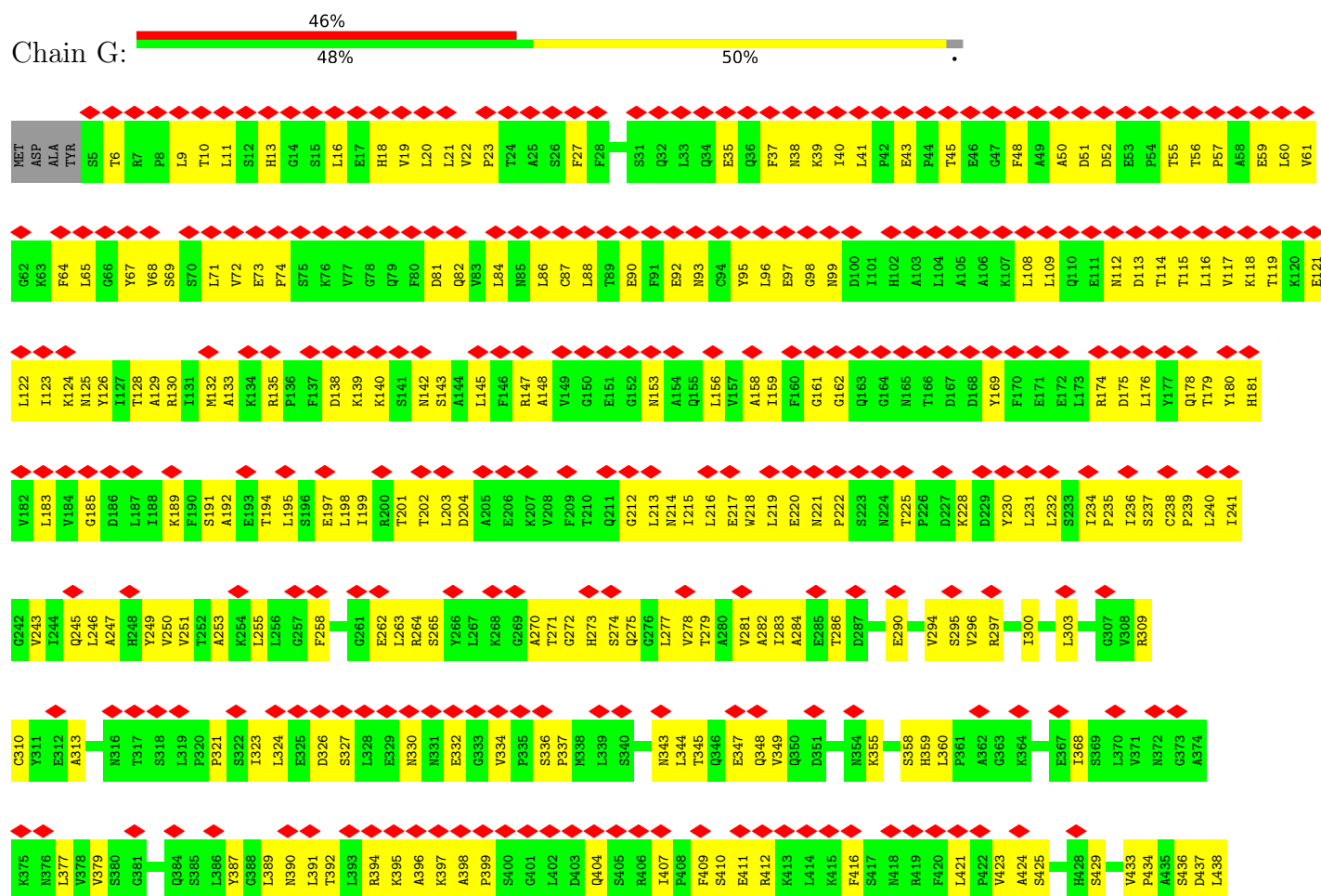


Mol	Chain	Residues	Atoms					AltConf
4	G	1	Total	C	N	O	P	0
			31	17	4	9	1	





• Molecule 2: Fatty acid synthase subunit beta



A1303	I439	G508	G575	I649	A722	F501	R874	L951	E1026	I1097	V1166	N1243	A1303
V1304	M440	A509	E580	I652	H723	R804	L875	R952	K1030	P1098	S1167	N1244	G1305
G1305	K441	S510	T581	Y653	P724	V605	P876	R953	K1031	A1099	P1168	D1245	G1306
N1306	D442	G511	K582	V654	N725	M806	K877	E956	D1032	V1100	R1170	N1246	C1308
C1308	L443	L512	L586	F657	A729	A808	K878	R957	L1033	E1101	R1171	A1249	N1307
E1309	V444	G513	L587	M658	K731	K809	L880	K960	L1034	P1108	K1172	I1250	C1309
D1310	K445	V514	L515	E657	Q730	E810	V881	K960	W1035	V1109	V1173	I1251	D1310
F1311	M446	L516	G588	M658	L731	E910	P882	T963	W1036	V1109	K1174	S1252	F1311
V1312	M447	T516	P590	W661	G735	V811	P883	L966	S1037	ASP	K1175	E1253	F1311
S1313	W451	H517	L593	G662	R736	K812	L884	L967	E1038	VAL	P1176	E1254	V1312
R1314	A452	R518	V594	I663	G739	D816	L884	Q968	H1039	GLN	S1177	M1255	S1313
R1315	K453	N519	P595	L665	H740	A817	E885	I967	L1040	SER	Q1178	R1256	R1314
P1315	K454	K520	G596	L666	H741	K818	K887	A886	E1041	GLN	G1179	D1257	P1315
D1316	I455	G524	M597	K657	S742	K819	R888	D974	A1042	VAL	M1180	D1258	D1316
R1317	Q456	G525	T598	E668	F743	C520	D889	K975	V1043	ASP	E1183	R1259	R1317
C1317	Q456	R526	T599	E669	S744	R821	Y890	P976	V1044	SER	E1184	Q1260	T1318
T1318	V459	R526	C600	R670	D745	G626	L891	D977	W1045	SER	M1186	R1261	M1319
M1319	Y460	V529	T601	K672	A746	V627	L892	E978	D1046	VAL	G1187	I1262	L1320
A1321	D461	A530	V602	G673	L751	D830	R894	R894	D1047	SER	T1188	K1263	A1321
P1322	G465	G531	D605	G673	Q752	K831	L895	E981	R1050	GLU	M1188	E1264	P1322
M1323	S466	T532	F506	Y674	H750	E832	R896	K982	T1051		T1189	M1265	M1323
D1324	D467	L533	V607	Q677	F759	E833	D898	A986	C1052		T1193	Y1266	D1324
I1327	L468	D534	T610	F678	H760	E834	P902	A989	I1053	F1127	L1197	K1268	I1327
V1328	R469	I535	N612	L619	H761	Q834	F904	A990	H1055	K1128	S1198	W1270	V1328
G1330	V470	N536	G814	L619	N762	K837	P907	R991	G1056	A1129	L1199	I1271	G1330
W1331	L471	P537	Y615	L619	I763	V844	Y907	R991	P1057	T1130	P1200	D1272	W1331
A1333	S472	D538	T616	E689	M764	T845	N908	E992	V1058	S1131	Q1202	E1273	A1333
I1334	G473	D540	I617	E689	L765	V846	Y908	E992	V1059	S1132	L1197	P1274	I1334
K1336	S474	D549	E618	E689	I766	R847	G909	Q998	K1064	T1133	E1204	N1276	K1336
A1337	E477	F547	L619	E689	F767	S848	Q910	Q998	V1065	A1135	L1205	I1277	A1337
I1338	R478	I548	L619	E689	G768	E849	R912	Q999	V1066	E1136	K1206	D1278	I1338
F1339	D481	F548	L619	E689	G769	E850	D913	D999	D1067	L1142	L1213	F1279	F1339
P1340	C482	D549	L619	E689	G770	G851	L914	I1000	E1068	A1143	L1214	D1280	P1340
N1341	I483	E546	Y624	E689	D775	E852	L915	D1001	P1069	G1144	K1215	P1281	N1341
V1342	I484	E546	F625	E689	D776	P853	T916	H1002	I1070	S1145	E1216	R1282	V1342
V1343	R485	I547	S626	E689	I777	P855	T916	H1002	K1071	G1146	E1217	D1283	V1343
D1344	L486	F548	A628	E689	T778	H856	Y922	N996	S1072	E1147	I1218	V1284	D1344
G1345	F487	D549	G629	E689	P779	R857	V922	N996	K1072	I1148	I1219	I1285	G1345
L1347	V488	D549	M630	E689	E784	A858	L926	I1009	I1073	N1148	Q1220	K1286	L1347
L1348	K489	V550	T631	E689	W785	A858	L926	P1010	M1074	W1149	E1225	G1287	L1348
K1349	W490	T551	G630	E689	S786	R859	V927	M1009	D1075	H1151	E1226	K1288	K1349
L1350	E491	S552	D635	E689	T787	R860	E928	M1011	H1078	A1152	M1226	D1289	L1350
V1351	K491	N553	S636	E689	I787	G861	E928	M1011	D1079	S1153	R1227	F1290	V1351
H1352	T494	G554	V637	E689	D790	V862	E928	K1013	H1080	F1154	T1228	E1291	H1352
L1353	Q495	L555	V638	E689	Y791	L864	R933	V1018	H1081	L1155	M1229	I1292	L1353
S1354	Q496	K556	E643	E689	M794	R866	R934	P1019	L1085	C1156	D1230	T1293	S1354
Y1357	F496	K557	K643	E689	P795	E867	T935	V1020	L1086	S1157	G1231	K1294	Y1357
I1360	H500	N558	T646	E689	F796	F668	R936	V1021	L1086	F1158	D1232	E1296	I1360
P1361	L501	L562	F647	E689	D797	E869	Y943	D1022	Y1090	I1159	L1236	V1297	P1361
G1362	L502	Y565	G648	E689	G798	E870	F946	R1023	G1091	D1162	L1237	D1299	G1362
A1363	D503	K568		E689	F799	T871	F950	R1024	D1092	K1163	L1238	F1300	A1363
L1366	F504	L569		E689	L800	L872		F1025	D1093	M1164	Y1240	H1302	L1366
	G505	I570		E689					E1094	F1165			
	P506	K571		E689									
	G507	K573		E689									
		S574		E689									

F2026	A1965	R1905	M1784	T1718	L1651	H1581	M1514	A1442	Q1367
Q2027	C1966	A1906	A1787	T1719	T1652	G1582	D1518	V1443	D1370
D2028	T1967	L1907	A1788	H1720	E1656	M1583	F1519	R1444	
V2029	P1968	D1908	F1789	F1721	E1657	F1584	L1520	S1446	T1378
V2030	L1969	T1909	E1790	R1728	E1658	R1590	K1521	K1447	E1379
D2031	V1970	V1910	D1791	T1729	E1659	A1591	R1522	K1448	S1380
L2032	G1971	T1911	L1792	R1730	P1660	L1592	M1523	V1449	V1381
T2033	I1972	N1912	K1793	E1731	V1661	L1593	G1524	F1450	V1382
G2034	I1973	N1913	S1794		T1662	E1594	S1525	Q1451	N1383
S2035	V1974	V1914	K1795	S1734	T1663	M1595	D1453	L1452	Q1384
E2036	P1975	N1915	G1796	A1735	V1665	V1596	D1454	T1386	F1385
P2037	F1976	F1916	L1797	M1736	V1666	A1597	E1455	T1387	T1387
L2038	H1977	I1917	I1798	I1737	T1667	A1598	E1456	K1388	
K2039	S1978	K1918	P1799	E1738	T1668	D1599	K1530	I1389	
E2040	T1979	L1919	A1800	F1739	G1668	S1600	V1531	V1390	
L2041	Y1980	Q1920	D1801	T1740	Q1669	V1601	M1532	D1458	
D2042	L1981	K1921	T1802	I1741	Q1670		L1533	L1459	
D2043	M1982	I1922	F1804	V1742	S1671	R1604	E1534	L1460	
N2044	N1983	D1923	A1805	D1743	Q1672	V1605	M1535	N1461	
V2045	G1984	I1924	G1806	G1744	E1673	R1606	P1536	F1466	
E2046	V1985	I1925	H1807	K1745	E1674	G1607	I1537	E1467	
K2047	K1986	I1926	S1808	L1746	G1675	Y1608	T1468	T1468	
Y2048	P1987	I1927	L1809	K1747	M1676		E1469	T1470	
F1988	S1867	L1927	L1809	T1748	M1677		F1471	V1472	
E2049	Q1868	Q1928	G1810	E1749	M1678		A1540		
Q2050	E1869	K1929	E1811	K1750	M1679		V1541		
SER	F1991	S1930	Y1812	I1751	D1679		L1542		
ASP	L1871	L1931	A1813	F1752	M1680		D1543		
LYS	Q1872	S1932	L1814	K1753	Y1681		S1544		
THR	Y1873	L1933	L1815	E1754	K1682		T1545		
ASP	V1874	L1934	A1816	H1755	T1683		T1546		
GLY	V1875	E1934	S1817	H1756	S1684		P1547		
ASP	E1876	E1935	L1818	E1757	K1685		S1548		
LYS	R1877	V1936	A1819	H1758	A1686		T1549		
LYS	V1878	E1937	D1820	S1759	A1687		M1550		
ASP	K1879	G1938	V1821	Q1688	D1688		E1551		
HIS	R1880	L1940	M1822	Y1762	D1689		P1552		
ASP	I1881	F1941	S1823	T1763	V1690				
ASP	T1882	E1942	E1824	F1764	W1691		R1555		
LYS	G1883	I1943	E1825	R1765	N1692		D1559		
ASP	W1884	I1944	S1826	S1766	A1694		L1560		
ASP	L1885	D1945	V1828	E1767	W1695				
ASP	V1886	E1946	E1829	K1768	W1696				
ASP	E1887	I1947	V1830	G1769	H1697		I1563		
ASP	L1888	S1948	V1831	L1770	F1698		H1564		
ASP	V1889	K1949	F1832	L1771	T1701		S1566		
ASP	N1890	L2014	R1834	S1772	S1705		H1567		
ASP	Y1891	T2015	G1835	T1774	I1706		V1568		
LYS	N1892	A2016	T1836	A1773	L1707		F1569		
ASP	V1893	K2017	T1837	Q1775	D1708		Y1572		
ASP	E1894	P2018	M1838	F1776	I1573		A1510		
ASP	N1895	F2019	Q1839	T1777	N1574		S1511		
ASP	P1955	Q2020	V1840	Q1778	E1645		L1575		
ASP	R1956	V2021	A1841	P1779	D1646		P1576		
ASP	Y1898	T2022	V1842	T1782	D1647		G1577		
ASP	F1957	K2023	P1843	L1783	V1648		T1578		
ASP	L1958	E2024	R1844		V1649		I1579		
LYS	K1959						T1580		
	L1960								
	E1961								
	I1962								
	G1963								
	F1964								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	637823	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	2.591	Depositor
Minimum map value	-1.261	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.696	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	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: PNS, 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	0.61	0/12424	0.53	1/16819 (0.0%)
2	G	0.42	1/16360 (0.0%)	0.44	1/22198 (0.0%)
All	All	0.51	1/28784 (0.0%)	0.48	2/39017 (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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1721	PHE	CA-CB	-5.74	1.44	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1971	GLY	N-CA-C	-5.81	108.17	115.08
1	A	1150	ASP	N-CA-C	-5.51	105.85	112.58

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1294	SER	Peptide
1	A	702	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12202	0	11715	713	0
2	G	15995	0	15978	928	0
3	A	5	0	0	0	0
4	G	31	0	19	1	0
All	All	28233	0	27712	1601	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 29.

The worst 5 of 1601 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)
1:A:1335:PHE:HD1	1:A:1378:GLU:HG3	1.07	1.12
1:A:1343:PHE:CE2	1:A:1585:LYS:NZ	2.18	1.10
1:A:1333:ASP:OD2	1:A:1585:LYS:HB2	1.52	1.09
1:A:1584:PRO:HB2	1:A:1587:ALA:HB3	1.34	1.04
1:A:1335:PHE:HD1	1:A:1378:GLU:CG	1.71	1.02

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1608/1887 (85%)	1329 (83%)	275 (17%)	4 (0%)	43	72
2	G	2029/2073 (98%)	1771 (87%)	258 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3637/3960 (92%)	3100 (85%)	533 (15%)	4 (0%)	49	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1585	LYS
1	A	179	LYS
1	A	1168	LEU
1	A	58	GLN

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	1233/1566 (79%)	1231 (100%)	2 (0%)	87	96
2	G	1772/1810 (98%)	1772 (100%)	0	100	100
All	All	3005/3376 (89%)	3003 (100%)	2 (0%)	87	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1200	ILE
1	A	1378	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	390	ASN
2	G	1061	GLN
2	G	451	ASN
2	G	1002	HIS
2	G	1088	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	G	3051	-	33,33,33	1.15	2 (6%)	48,50,50	1.28	8 (16%)
3	PNS	A	1888	1	1,4,21	0.62	0	0,4,29	-	-

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	G	3051	-	-	3/18/18/18	0/3/3/3
3	PNS	A	1888	1	-	0/0/2/27	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3051	FMN	C4A-N5	3.05	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3051	FMN	C10-N1	2.21	1.37	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3051	FMN	C4-N3-C2	-3.52	119.38	125.64
4	G	3051	FMN	C4A-C4-N3	2.74	120.23	113.25
4	G	3051	FMN	C5A-C9A-N10	2.69	120.40	117.97
4	G	3051	FMN	C4A-C10-N10	2.65	120.28	116.48
4	G	3051	FMN	O4-C4-C4A	-2.61	119.65	126.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

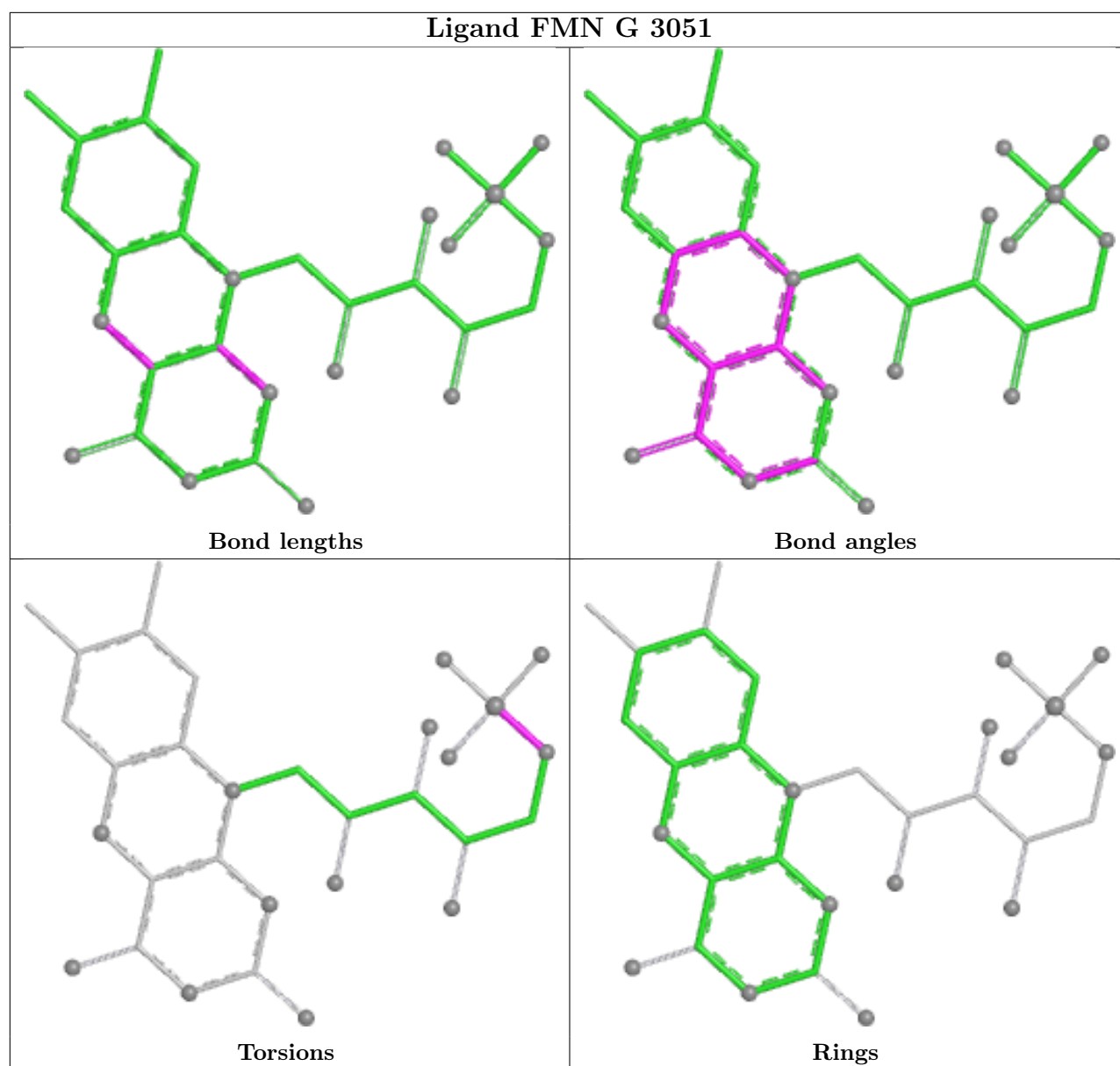
Mol	Chain	Res	Type	Atoms
4	G	3051	FMN	C5'-O5'-P-O1P
4	G	3051	FMN	C5'-O5'-P-O2P
4	G	3051	FMN	C5'-O5'-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3051	FMN	1	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.



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.

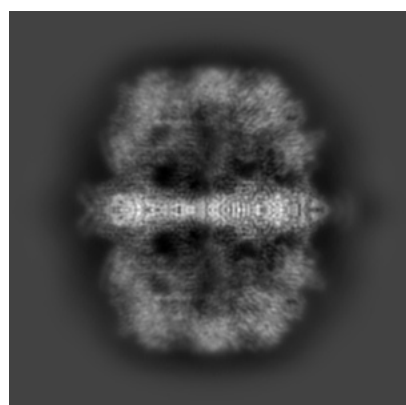
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20655. These allow visual inspection of the internal detail of the map and identification of artifacts.

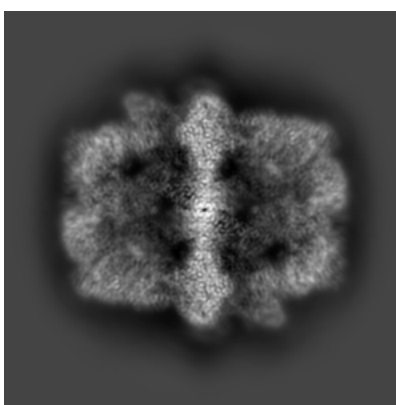
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

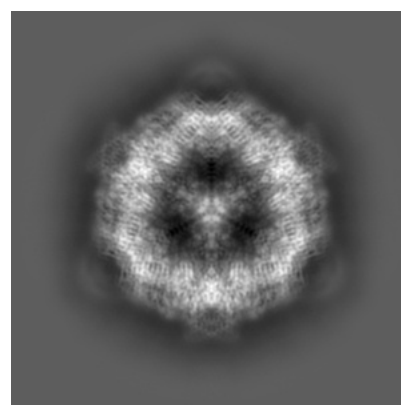
6.1.1 Primary map



X



Y

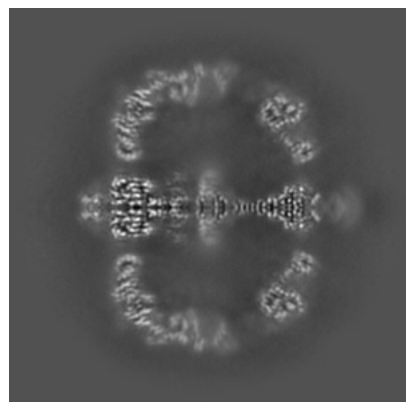


Z

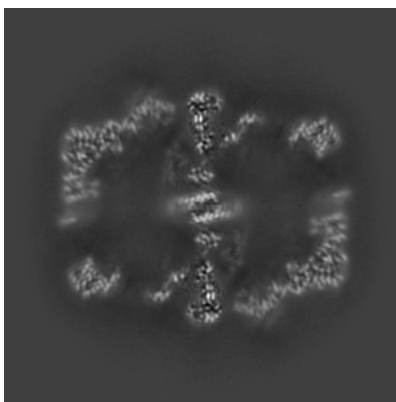
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

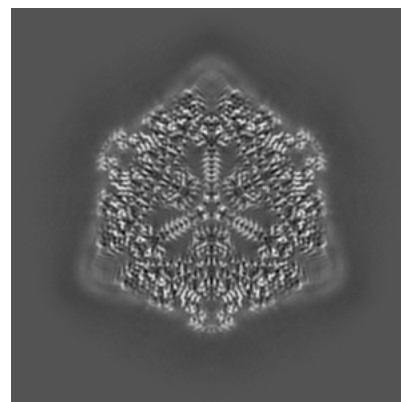
6.2.1 Primary map



X Index: 176



Y Index: 176

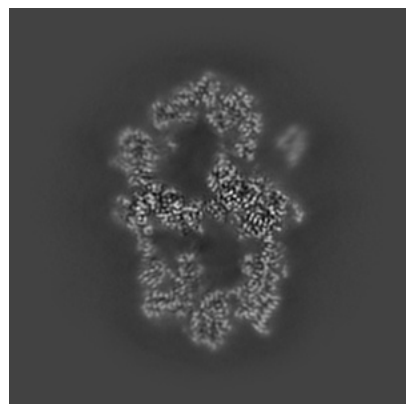


Z Index: 176

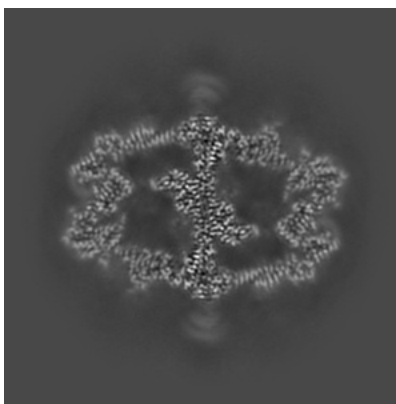
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

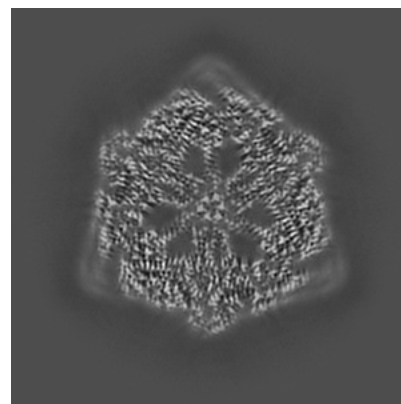
6.3.1 Primary map



X Index: 237



Y Index: 121

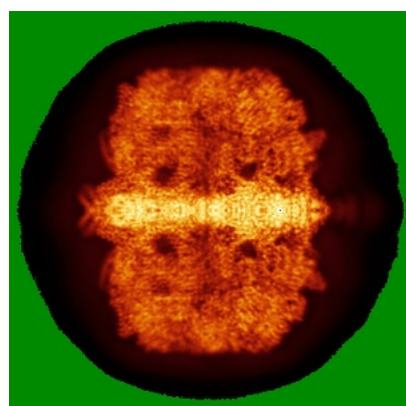


Z Index: 172

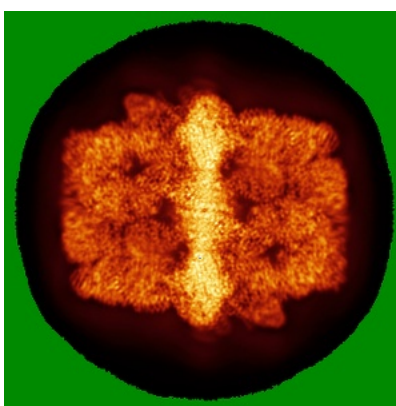
The images above show the largest variance slices of the map in three orthogonal directions.

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

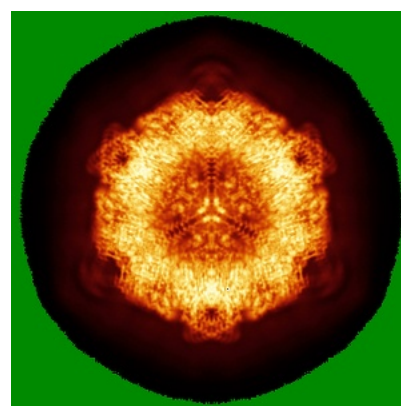
6.4.1 Primary map



X



Y

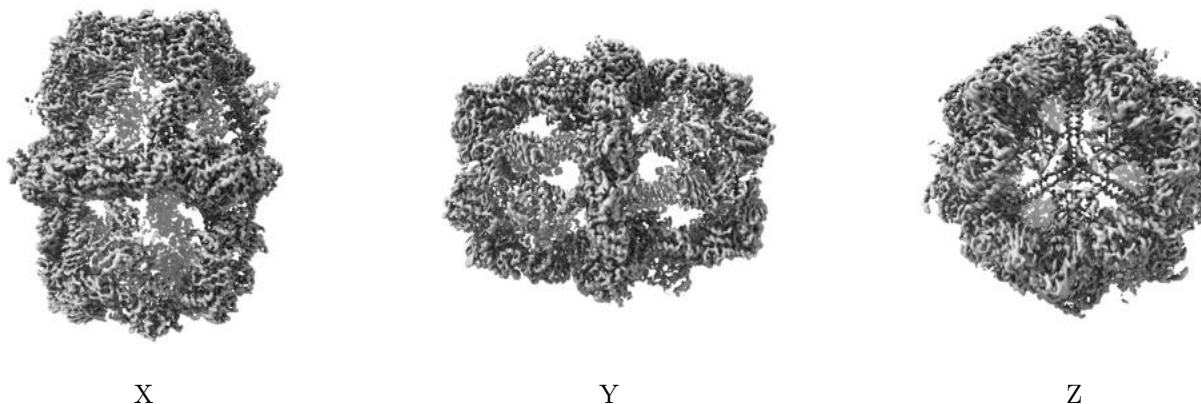


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.696. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

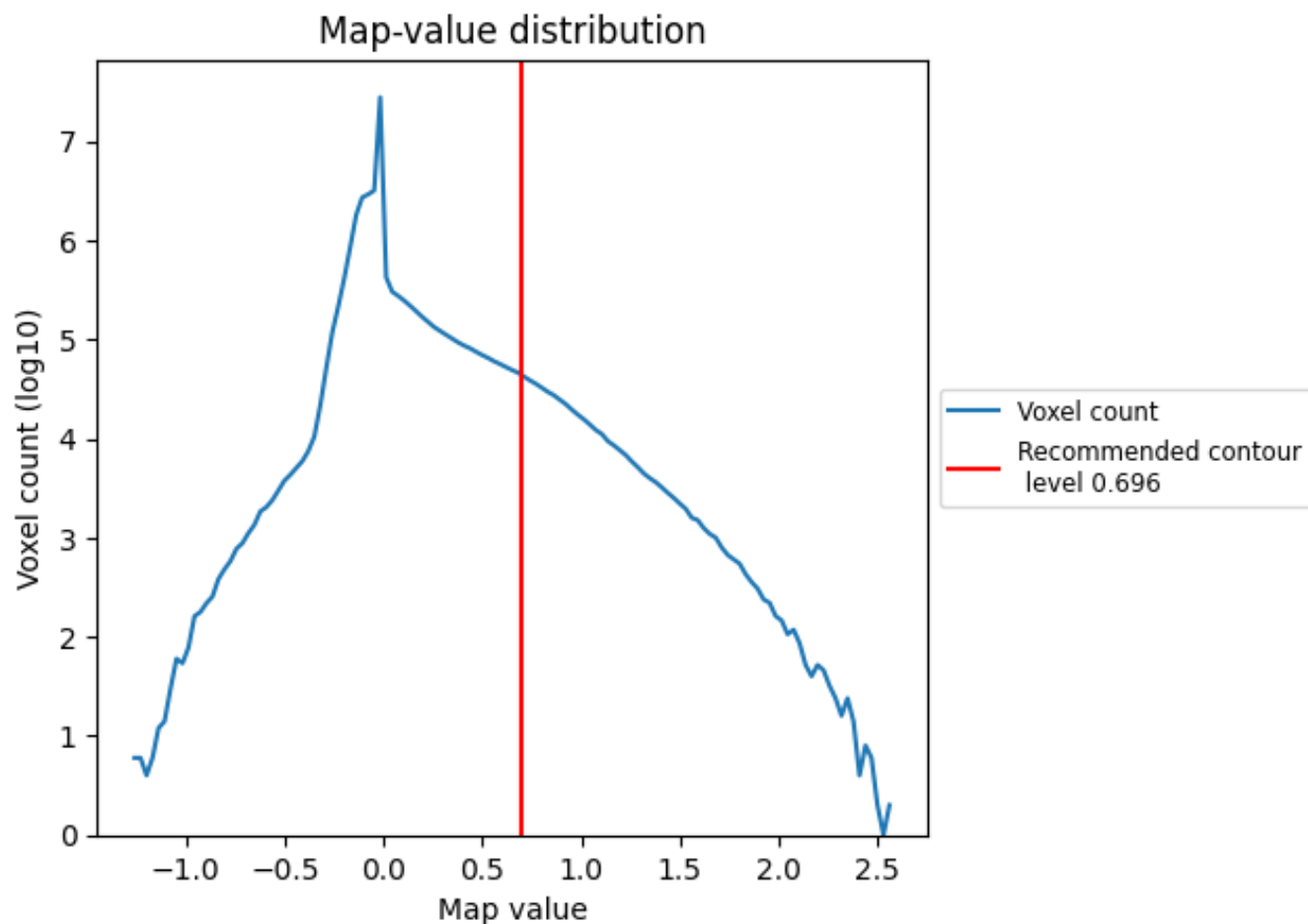
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

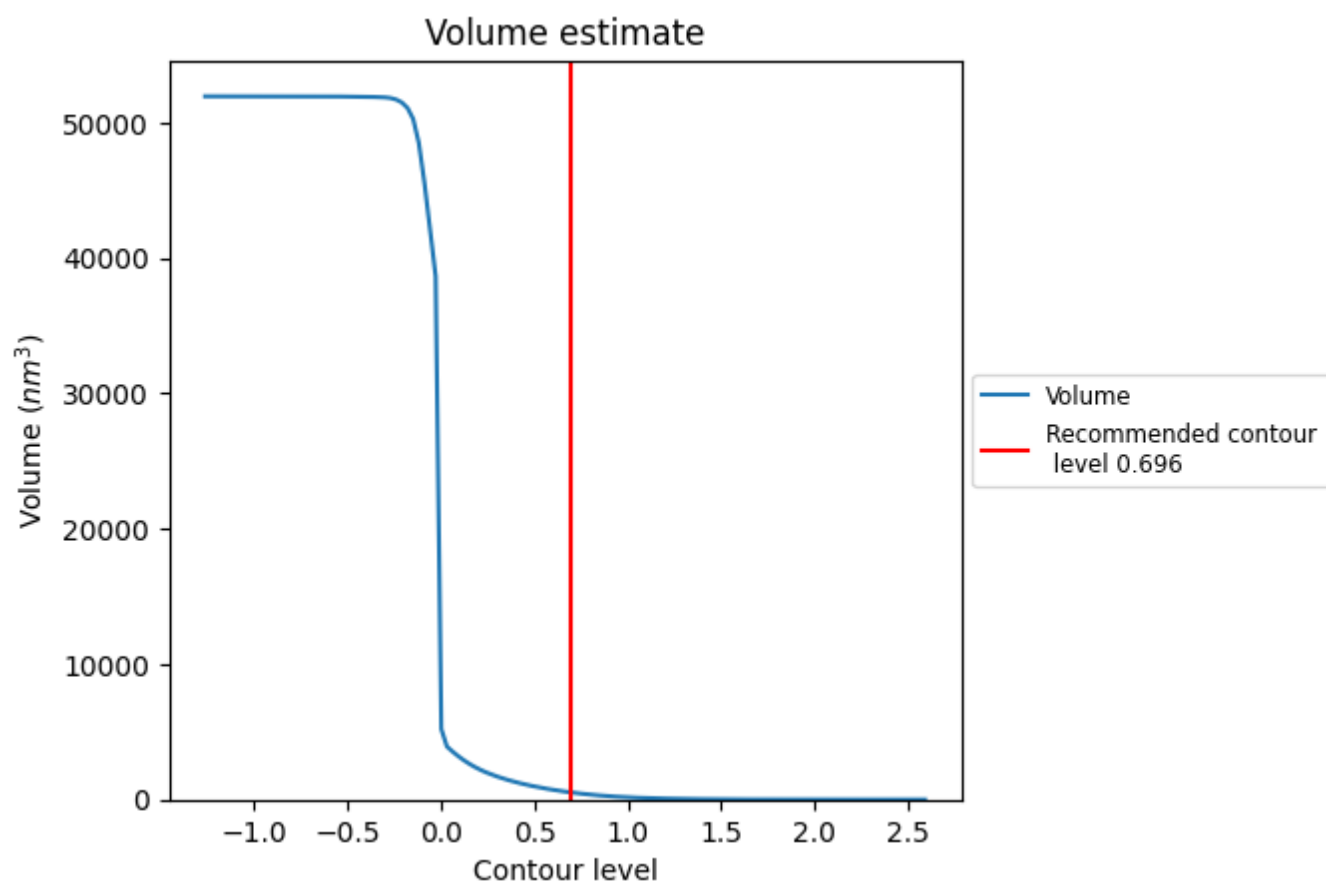
This section contains the results of statistical analysis of the map.

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.

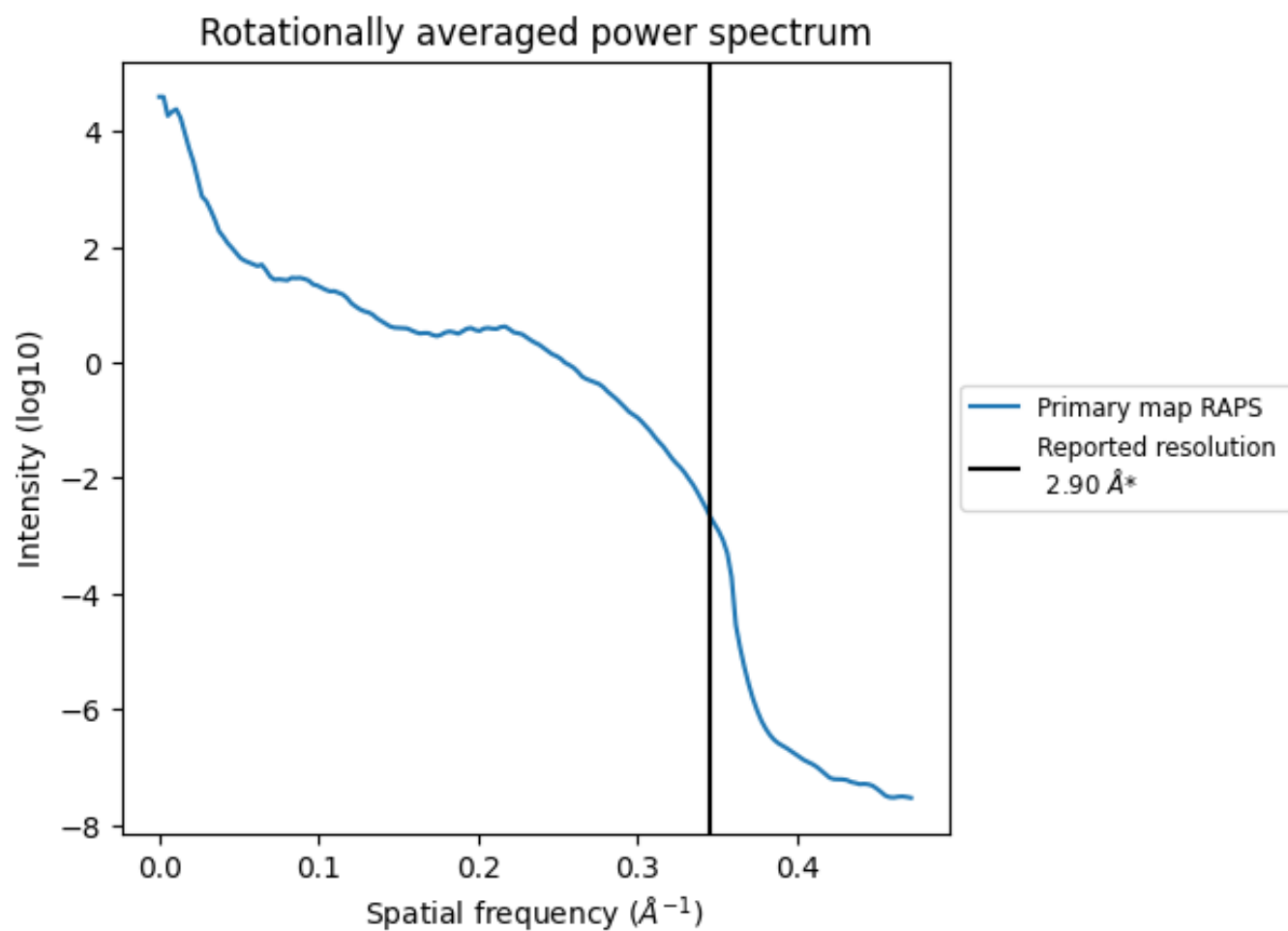
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 528 nm³; this corresponds to an approximate mass of 477 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 0.345 Å⁻¹

8 Fourier-Shell correlation

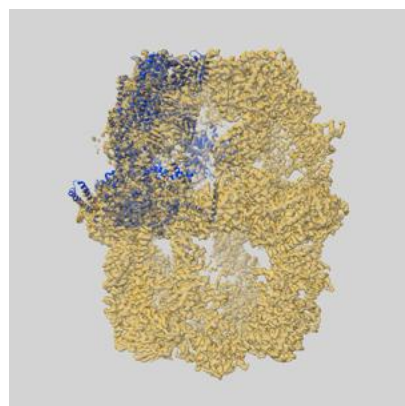
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

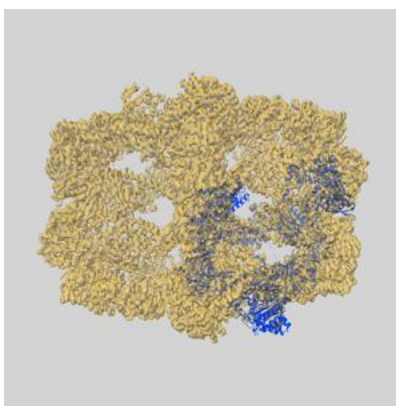
This section contains information regarding the fit between EMDB map EMD-20655 and PDB model 6U5T. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

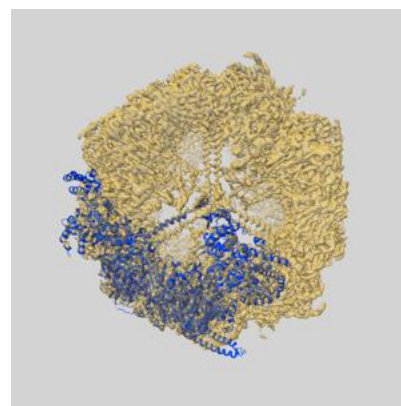
9.1.1 Map-model overlay [i](#)



X

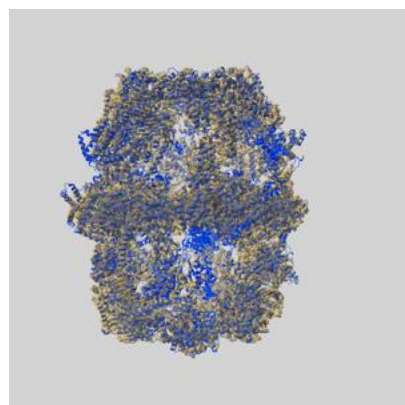


Y

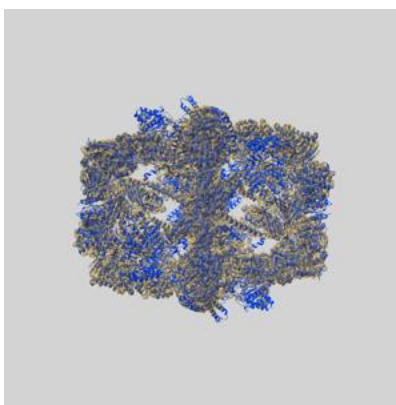


Z

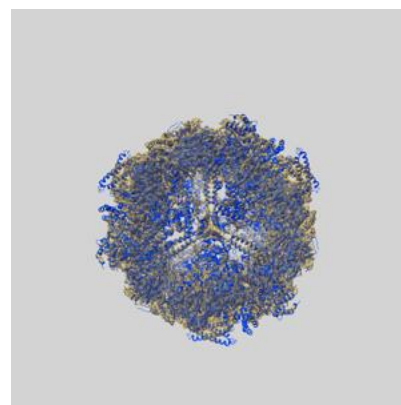
9.1.2 Map-model assembly overlay [i](#)



X



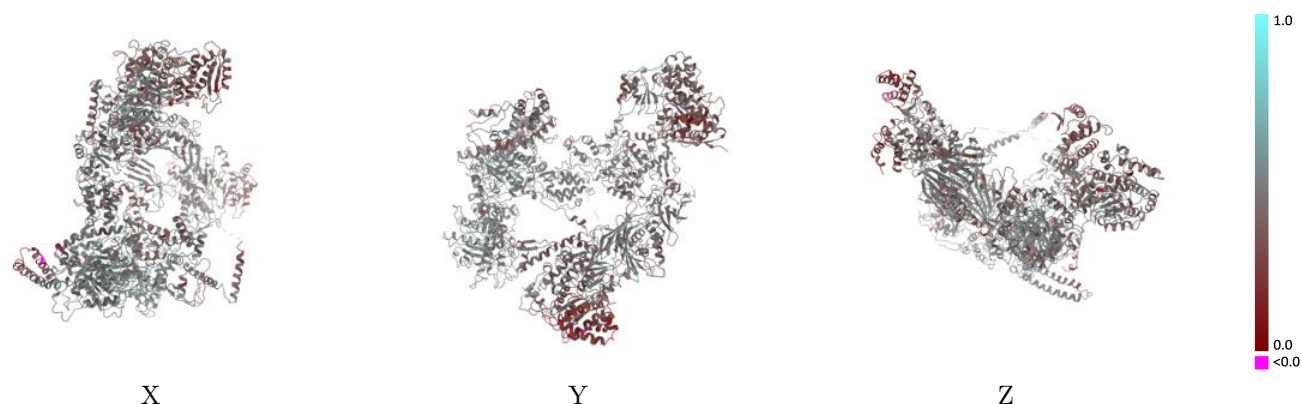
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.696 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](#)

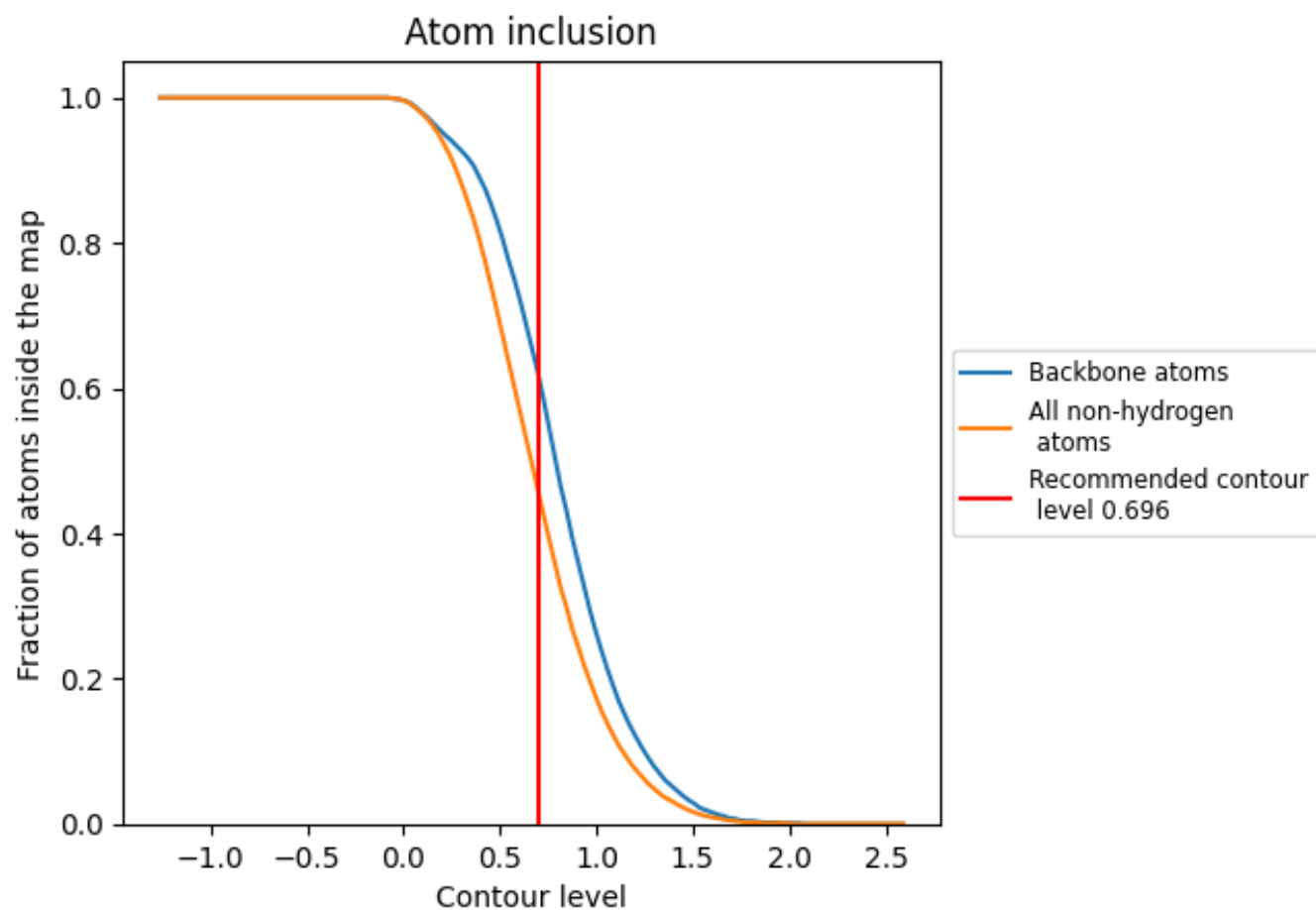


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 46% 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 (0.696) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4620	0.4420
A	0.5340	0.4690
G	0.4070	0.4210

