



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 04:15 PM UTC

PDB ID : 6U5U / pdb_00006u5u
EMDB ID : EMD-20656
Title : Electron cryomicroscopy Structure of *S. cerevisiae* FAS in the KS-stalled state
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2019-08-28
Resolution : 2.80 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 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

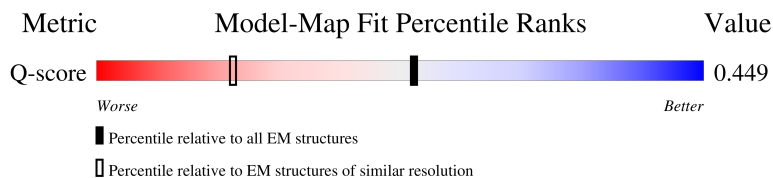
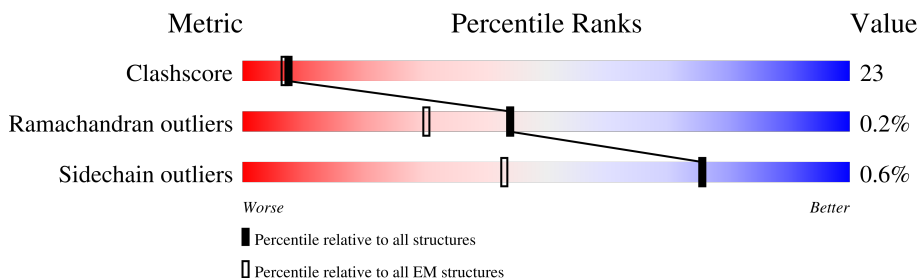
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	25% 53% 32% 15%
2	G	2073	47% 52% 46% .

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	G	2102	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28298 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	1611	Total	C	N	O	S	0	0
			12171	7684	2081	2362	44		

- 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:

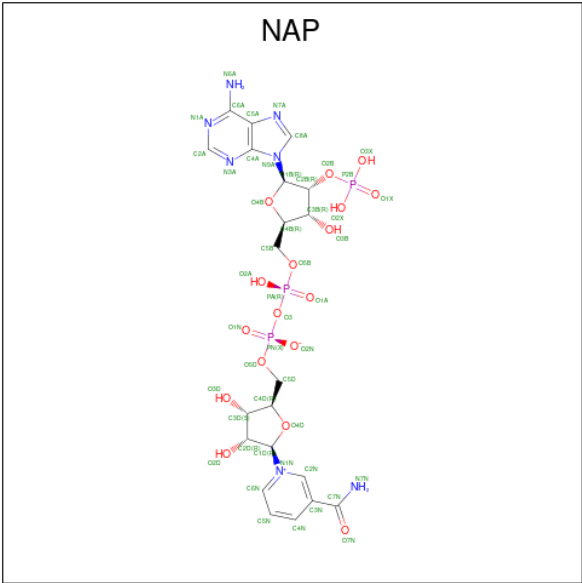
Chain	Residue	Modelled	Actual	Comment	Reference
G	2052	ASP	-	expression tag	UNP P07149
G	2053	TYR	-	expression tag	UNP P07149
G	2054	LYS	-	expression tag	UNP P07149
G	2055	ASP	-	expression tag	UNP P07149
G	2056	HIS	-	expression tag	UNP P07149
G	2057	ASP	-	expression tag	UNP P07149
G	2058	GLY	-	expression 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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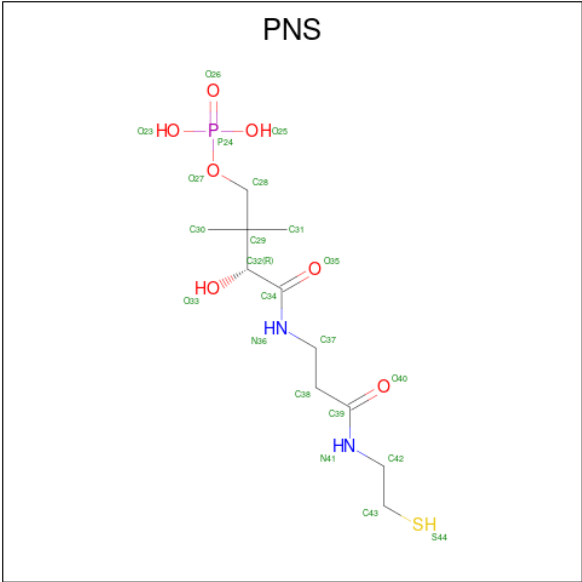
Chain	Residue	Modelled	Actual	Comment	Reference
G	2073	LYS	-	expression tag	UNP P07149

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



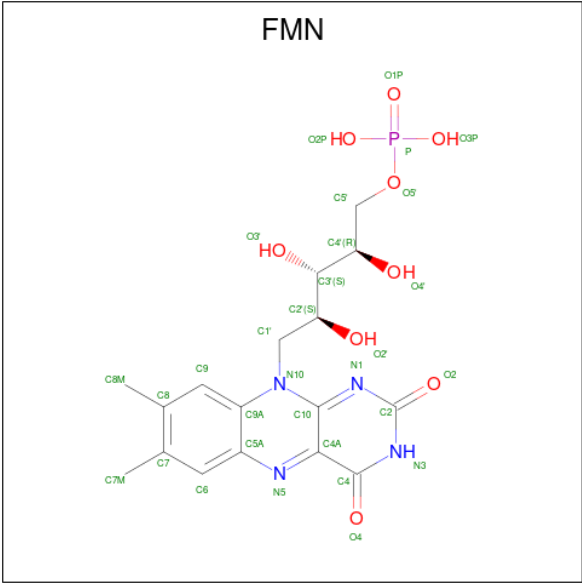
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	G	1	Total	C	N	O	P	0
			48	21	7	17	3	

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



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

- Molecule 5 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



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



Q1529	G1394	F1457	G1394	V1329	W1267	T1189	ASP	Q1046	T969	K877	M906	F726	I663
K1530	S1397	D1458	S1397	G1330	K1268	T1193	SER	D1047	K962	N878	I807	P727	P664
V1531	R1398	L1459	R1398	W1331	L1269	L1197	SER	Q1049	L964	K879	A808	I728	L665
N1532	N1399	L1460	N1399	R1332	D1272	P1200	VAL	R1050	V881	V881	K809	A729	I666
L1533	G1400	K1461	G1400	L1335	P1274	P1201	SER	T1051	P882	P882	E810	L730	K667
E1534	K1401	K1462	K1401	I1336	P1275	V1201	GLU	C1052	I967	I967	V811	T733	E668
N1535	V1403	T1463	V1403	F1338	P1276	Q1202	D1123	L1053	D974	E885	K812	G734	E669
P1536	M1404	L1464	M1404	P1339	P1277	G1203	S1124	L1054	K975	A886	T813	G735	K671
L1537	E1405	T1465	E1405	P1340	N1276	G1204	A1125	H1055	P976	K887	S814	R736	S671
P1538	V1406	F1466	V1406	N1341	D1277	E1204	V1126	G1056	D977	R888	P815	G737	K672
I1539	S1409	E1467	S1409	F1343	F1279	L1205	K1128	V1058	E978	D889	D816	G738	G673
A1540	F1410	T1468	F1410	D1344	D1280	K1206	A1129	Q1061	A979	Y890	H740	H740	Y674
L1542	F1411	K1475	F1411	G1345	P1281	I1210	T1130	F1062	I980	I891	S742	H741	Q677
D1543	R1413	N1476	R1413	D1346	R1282	L1213	S1131	T1063	E981	K894	T821	F743	F678
S1544	G1414	A1477	G1414	L1347	V1284	L1214	S1132	K1064	K982	N896	A822	F743	L679
V1545	N1415	K1478	N1415	K1348	D1285	K1215	T1133	V1065	F984	N897	D829	E744	T880
T1546	Y1416	S1481	Y1416	L1350	K1286	E1216	D1134	D1067	Y887	D898	D830	D745	G682
S1548	T1417	K1484	T1417	V1351	G1287	N1217	E1135	E1068	R991	F899	K831	A746	A883
T1549	D1418	K1485	D1418	H1352	K1288	I1218	E1136	P1069	R991	Q901	W832	H747	G684
N1550	F1419	F1486	F1419	S1354	D1289	T1219	S1137	I1070	Q993	K902	E833	T748	G685
E1551	E1420	G1487	E1420	N1355	E1291	M1220	W1138	K1071	F994	P902	Q834	P749	V686
P1552	N1421	P1488	N1421	G1356	E1292	M1221	L1142	M1074	D999	T906	T835	H751	P686
Y1553	F1423	G1489	F1423	Y1357	T1293	H1223	A1143	M1074	I1000	N908	K937	Y754	S687
R1555	Q1424	V1491	Q1424	K1358	A1294	I1224	E1146	H1078	D1001	Q909	I843	Y757	L688
V1556	K1425	K1496	K1425	M1359	D1297	E1225	I1147	D1079	I1009	A911	V845	I763	E689
D1559	E1428	E1500	E1428	G1362	D1298	N1226	N1148	G1080	M1009	R912	R847	M764	Y694
L1560	P1429	I1501	P1429	A1363	D1299	E1225	W1149	H1081	P1010	D813	S848	L765	I695
N1561	V1430	G1502	V1430	L1366	T1301	N1226	R1150	I1082	G1011	L914	E849	I766	E696
P1562	Y1431	I1503	Y1431	Q1367	H1302	T1228	H1151	L1085	M1012	M917	M850	F767	T697
I1563	Q1432	V1504	Q1432	G1369	V1304	D1230	L1155	H1087	K1013	T918	G851	G768	L698
H1564	M1433	D1505	M1433	D1370	G1305	K1232	F1158	Y1090	V1018	Y919	E952	G770	G699
R1567	H1435	Y1506	H1435	V1371	N1306	P1234	D1162	G1091	D1022	R825	P853	F771	L700
H1568	K1436	E1507	K1436	V1372	N1307	V1234	K1163	D1092	R1023	L926	I854	G772	L703
F1569	T1437	A1510	T1437	T1373	E1307	S1235	M1164	D1093	R1024	I932	K856	S773	G704
A1570	S1438	S1511	S1438	T1374	C1308	L1239	N1168	S1095	F1025	R933	R860	A774	L705
N1574	K1439	H1512	K1439	T1375	E1309	Y1240	P1169	K1096	F1029	T935	G861	D775	K706
L1575	D1440	G1513	D1440	A1376	D1310	M1241	I1170	I1097	K1030	Q838	V862	D776	P707
P1576	I1441	P1515	I1441	V1377	F1311	F1242	R1171	P1098	K1031	F939	M863	W785	I710
G1577	A1442	V1516	A1442	G1379	F1312	N1243	K1172	A1099	D1032	D940	L864	K788	D711
T1578	V1443	V1517	V1443	S1380	V1312	P1250	N1176	E1101	S1033	R944	K866	F789	A712
L1579	L1444	D1518	L1444	V1381	S1313	I1251	P1177	E1101	L1034	R944	E867	M794	I713
I1579	R1445	F1519	R1445	N1382	R1314	L1251	Q1177	S1107	S1037	R952	F868	P795	T714
T1580	S1446	L1520	S1446	N1383	P1315	M1255	Q1178	P1108	E1038	R953	D869	F796	G715
H1581	K1447	K1521	K1447	Q1384	D1316	E1256	G1179	V1109	H1039	R953	E870	D797	V716
G1582	E1448	R1522	E1448	P1385	R1317	D1257	M1180	VAL	E1038	V854	T871	I717	N718
M1583	W1449	M1523	W1449	T1386	T1318	Q1260	V1181	GLN	E1041	E855	R872	S803	I719
F1584	K1388	G1524	K1388	G1387	M1319	R1261	L1182	SER	E1041	E855	F873	R804	A720
S1585	T1389	S1525	T1389	K1389	A1321	K1263	I1184	GLN	V1044	F968	N874	V805	K721
S1586	V1390	T1526	V1390	V1390	A1322	E1264	I1184	VAL	D1045				A722
V1589	D1391	L1527	D1391	D1391	M1323		G1187						H723
R1590	E1456	E1528	E1456	E1456	D1324		N1188						F724
A1591					F1325								N725
L1592					A1326								
I1593					V1327								
					V1328								

V2029	A1965	R1905	D1845	M1784	L1719	E1654	E1594
Y2030	C1966	A1906	E1846	E1785	H1720	A1655	N1595
D2031	I1967	L1907	L1847	K1786	F1721	E1656	W1596
L2032	P1968	D1908	G1848	A1787	G1722	I1657	A1597
T2033	L1969	T1909	R1849	A1788	G1726	E1658	A1598
G2034	V1970	V1910	S1850	F1789	R1730	Q1659	D1599
S2035	G1971	T1911	N1851	E1790	E1731	P1660	S1600
E2036	I1972	N1912	Y1852	K1793	N1732	V1661	V1601
P2037	S1973	V1913	G1853	S1794	Y1733	T1662	S1602
L2038	V1974	L1914	M1854	K1795	S1734	T1663	S1603
K2039	P1975	N1915	I1855	G1796	A1735	F1664	R1604
E2040	F1976	F1916	I1856	L1797	M1736	V1665	V1605
I2041	H1977	I1917	A1857	I1798	I1737	F1666	R1606
L2042	S1978	K1918	N1858	P1799	F1738	T1667	G1607
D2043	T1979	L1919	P1859	A1800	E1739	G1668	Y1608
W2045		Q1920	G1860	D1801	T1740	Q1669	T1609
E2046	M1982	K1921	R1861	A1802	I1741	G1670	C1610
K2047	N1983	I1922	V1862	T1803	V1742	S1671	F1612
Y2048	G1984	D1923	A1863	F1804	D1743	Q1672	V1613
E2049	V1985	I1924	I1864	A1805	G1744	E1673	D1614
Q2050	K1986	I1925	S1865	G1806	K1745	Q1674	M1615
SER	P1987	T1925	F1866	H1807	L1746	G1675	V1616
	F1988	E1926	S1867	S1808	K1747	G1676	L1617
ASP	K1989	L1927	Q1868	L1809	T1748	M1676	P1618
TYR	S1990	Q1928	E1869	G1810	E1749	G1677	M1619
LYS	F1991	K1929	A1870	E1811	M1750	M1678	T1620
HIS	L1992	S1930	L1871	Y1812	I1751	D1679	A1621
ASP	K1993	L1931	Q1872	A1813	F1752	L1680	L1622
GLY	K1994	S1932	Y1873	A1814	K1753	Y1681	K1623
ASP	N1995	L1933	V1874	L1815	E1754	K1682	T1624
TYR	I1996	E1934	V1875	A1816	K1755	T1683	S1625
ASP	K1997	E1935	E1876	S1817	M1756	S1684	I1626
HIS	E1998	V1936	V1877	L1818	E1757	K1685	Q1627
ASP	K1999	V1937	R1877	A1819	H1758	A1686	H1628
ILE	N2000	E1937	V1878	D1820	S1759	A1687	V1629
ASP	V2001	G1938	G1879	V1821	Y1762	Q1688	G1630
TYR	K2002	H1939	K1880	M1822	T1763	D1689	M1631
LYS		L1940	R1881	S1823	F1764	V1690	I1632
ASP	R2005	F1941	T1882	I1824	R1765	W1691	M1633
ASP		E1942	G1883	E1825	S1766	D1695	G1634
ASP	K2009	I1943	L1884	S1826	K1768	F1698	R1635
LYS	Y2010	I1944	L1885	L1827	E1767	T1701	K1636
		D1945	L1886	V1828	K1768		L1637
N2013		E1946	V1886	E1829	G1769		I1638
L2014		A1947	E1887	V1830	L1770		K1639
T2015		S1948	I1888	F1831	L1771	F1704	F1640
A2016		K1949	V1889	Y1833	S1772	S1705	E1641
K2017		K1950	N1890	R1834	A1773	I1706	T1642
P2018		S1951	Y1891	G1835	T1774	L1707	R1643
F2019		A1952	N1892	M1836	Q1775	D1708	M1644
Q2020		V1953	G1893	T1837	F1776	I1709	E1645
V2021		K1954	E1894	M1838	T1777	I1711	D1646
T2022		P1955	N1895	Q1839	Q1778	N1712	D1647
K2023		R1956	Q1896	V1840	P1779	M1713	V1648
E2024		P1957	Q1897	A1841	P1779	P1714	V1649
Y2025		V1957	Y1898	V1842	A1780	P1715	V1650
F2026		L1958	V1899	P1843	L1781	V1715	L1651
Q2027		K1959	A1900	R1844	T1782	N1716	T1652
D2028		L1960	A1901		L1783	L1717	G1653
		E1961	G1902			T1718	
		R1962	D1903				
		G1963	L1904				
		F1964					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	594818	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	2.727	Depositor
Minimum map value	-1.412	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.706	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: NAP, 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	1/12392 (0.0%)	0.72	12/16775 (0.1%)
2	G	0.40	0/16360	0.56	1/22198 (0.0%)
All	All	0.50	1/28752 (0.0%)	0.63	13/38973 (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	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1033	ALA	CA-C	-5.79	1.44	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	LYS	N-CA-C	7.98	120.44	109.11
1	A	1280	ILE	N-CA-C	-6.97	105.26	113.42
2	G	1278	ASP	N-CA-C	-6.21	106.39	112.97
1	A	1174	TYR	N-CA-C	5.90	117.49	109.11
1	A	142	ASP	CA-C-N	-5.86	111.63	122.06

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1132	GLU	Peptide
1	A	1173	LEU	Peptide
1	A	1584	PRO	Peptide
1	A	1716	LEU	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	12171	0	11679	520	0
2	G	15995	0	15978	792	0
3	A	48	0	22	19	0
3	G	48	0	25	27	0
4	A	5	0	0	0	0
5	G	31	0	19	4	0
All	All	28298	0	27723	1290	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 1290 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:G:740:HIS:HB2	3:G:2102:NAP:C7N	1.22	1.59
1:A:147:ALA:CB	1:A:214:GLN:HA	1.50	1.41
2:G:740:HIS:HD2	3:G:2102:NAP:C2N	1.33	1.39
2:G:740:HIS:HD2	3:G:2102:NAP:C3N	1.40	1.34
2:G:740:HIS:CB	3:G:2102:NAP:C7N	2.06	1.32

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	1601/1887 (85%)	1433 (90%)	161 (10%)	7 (0%)	30	60
2	G	2029/2073 (98%)	1883 (93%)	146 (7%)	0	100	100
All	All	3630/3960 (92%)	3316 (91%)	307 (8%)	7 (0%)	44	72

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	LYS
1	A	179	LYS
1	A	195	GLY
1	A	1609	ARG
1	A	180	SER

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	1230/1566 (78%)	1220 (99%)	10 (1%)	73	90
2	G	1772/1810 (98%)	1765 (100%)	7 (0%)	84	94
All	All	3002/3376 (89%)	2985 (99%)	17 (1%)	76	92

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	993	GLN
2	G	1680	LEU
1	A	1298	ILE
1	A	1307	THR
1	A	1384	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69

such sidechains are listed below:

Mol	Chain	Res	Type
2	G	1696	ASN
2	G	1807	HIS
2	G	1928	GLN
2	G	142	ASN
2	G	99	ASN

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](#)

4 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	$\# Z > 2$
3	NAP	G	2102	-	50,52,52	1.17	5 (10%)	71,80,80	1.55	9 (12%)
5	FMN	G	2101	-	33,33,33	1.23	5 (15%)	48,50,50	1.28	8 (16%)
4	PNS	A	1902	1	1,4,21	0.65	0	0,4,29	-	-
3	NAP	A	1901	-	50,52,52	2.66	27 (54%)	71,80,80	2.43	24 (33%)

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	NAP	G	2102	-	-	6/35/67/67	0/5/5/5
5	FMN	G	2101	-	-	3/18/18/18	0/3/3/3
4	PNS	A	1902	1	-	0/0/2/27	-
3	NAP	A	1901	-	-	6/35/67/67	0/5/5/5

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1901	NAP	C3N-C7N	-5.46	1.42	1.50
3	A	1901	NAP	C5A-N7A	-5.29	1.29	1.39
3	A	1901	NAP	PN-O3	-4.93	1.54	1.59
3	A	1901	NAP	O4D-C4D	-4.91	1.34	1.45
3	G	2102	NAP	C5A-C4A	4.76	1.47	1.39

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1901	NAP	C4D-O4D-C1D	-9.30	101.40	109.92
3	G	2102	NAP	C5A-C4A-N3A	-5.86	118.65	126.72
3	A	1901	NAP	C5A-C4A-N3A	-5.78	118.76	126.72
3	A	1901	NAP	O3D-C3D-C4D	-5.30	95.86	111.08
3	A	1901	NAP	C6N-N1N-C2N	-5.22	117.44	121.88

There are no chirality outliers.

5 of 15 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-O3
3	A	1901	NAP	C5D-O5D-PN-O2N
3	A	1901	NAP	C4D-C5D-O5D-PN
3	G	2102	NAP	C5D-O5D-PN-O1N

There are no ring outliers.

3 monomers are involved in 50 short contacts:

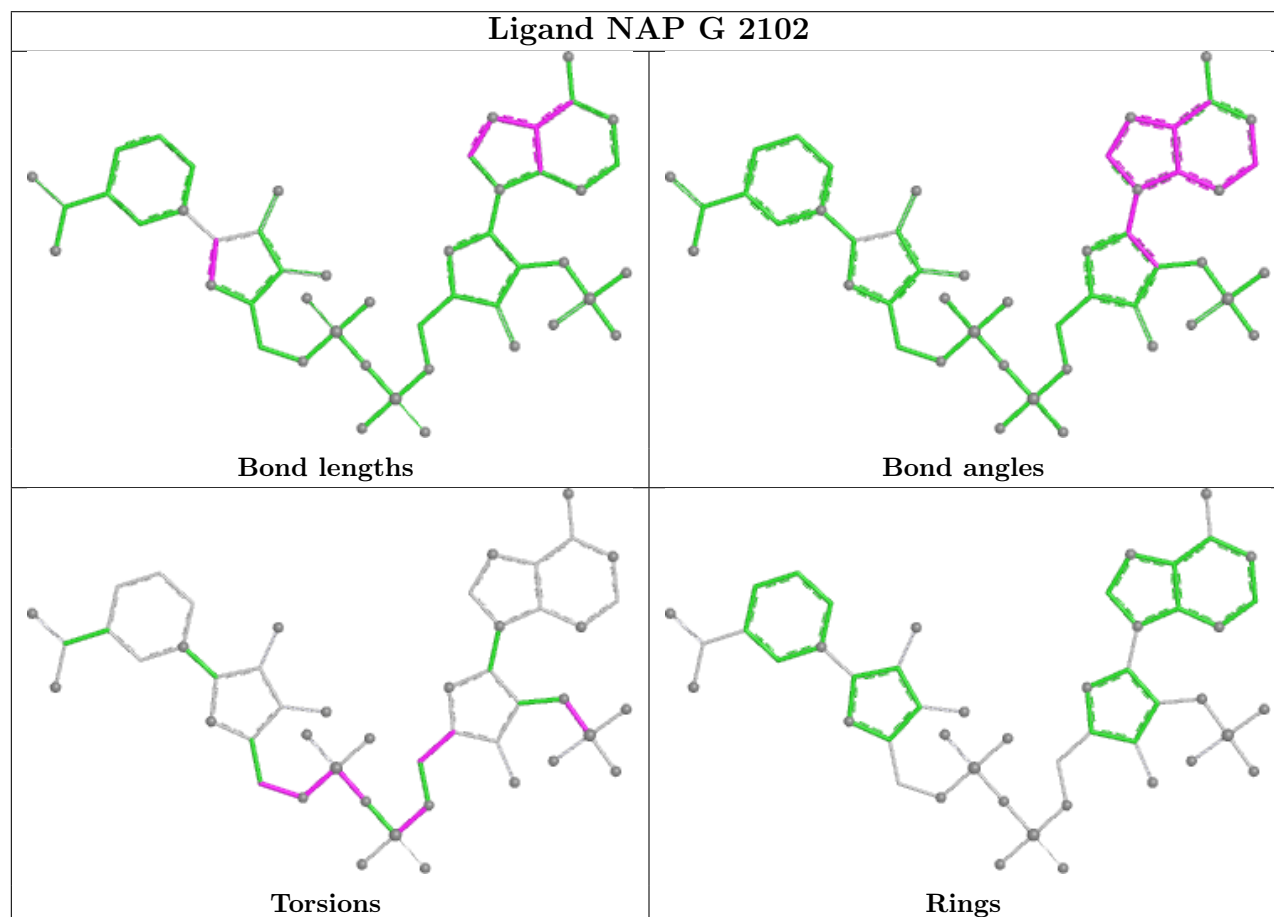
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2102	NAP	27	0
5	G	2101	FMN	4	0

Continued on next page...

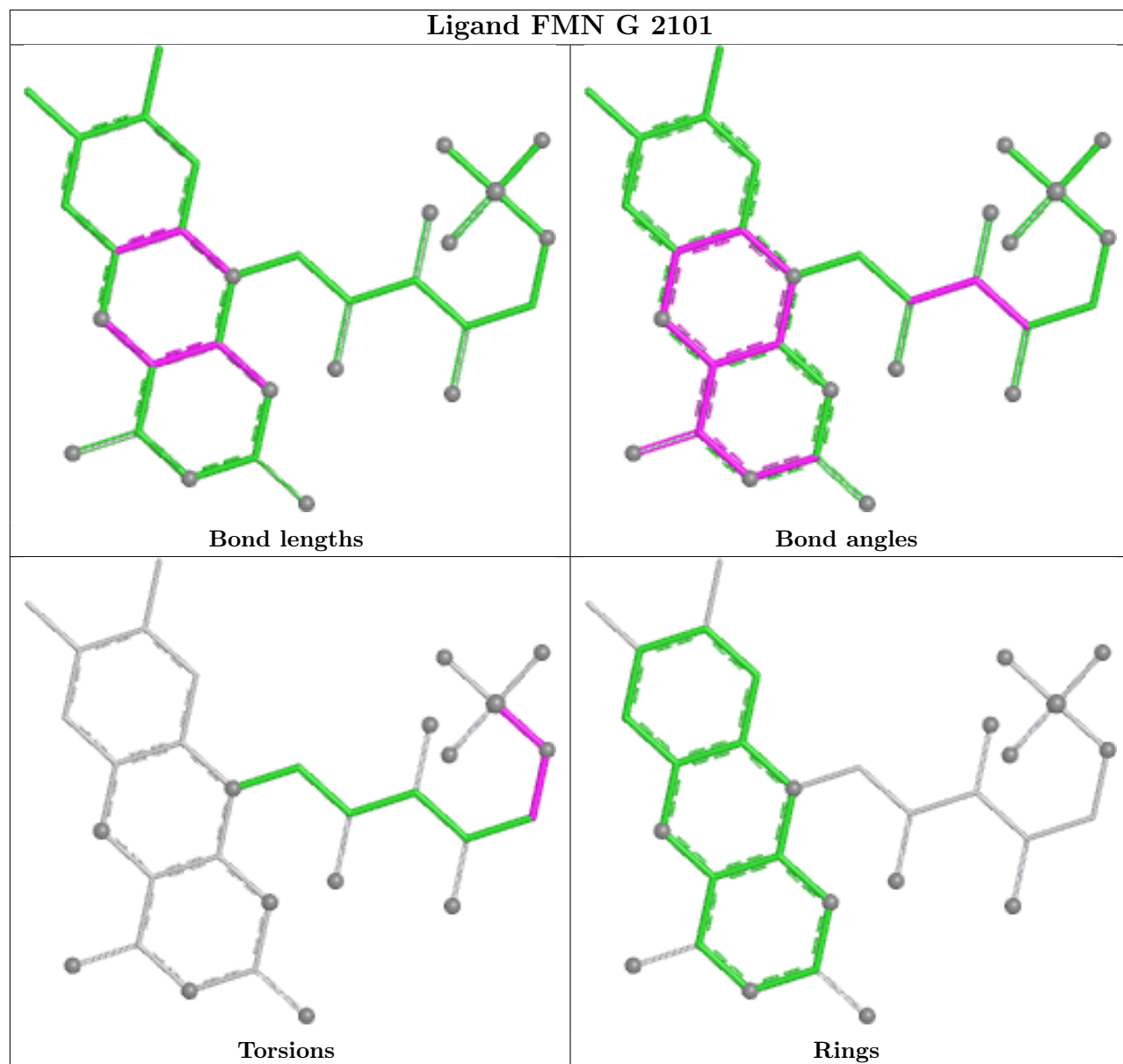
Continued from previous page...

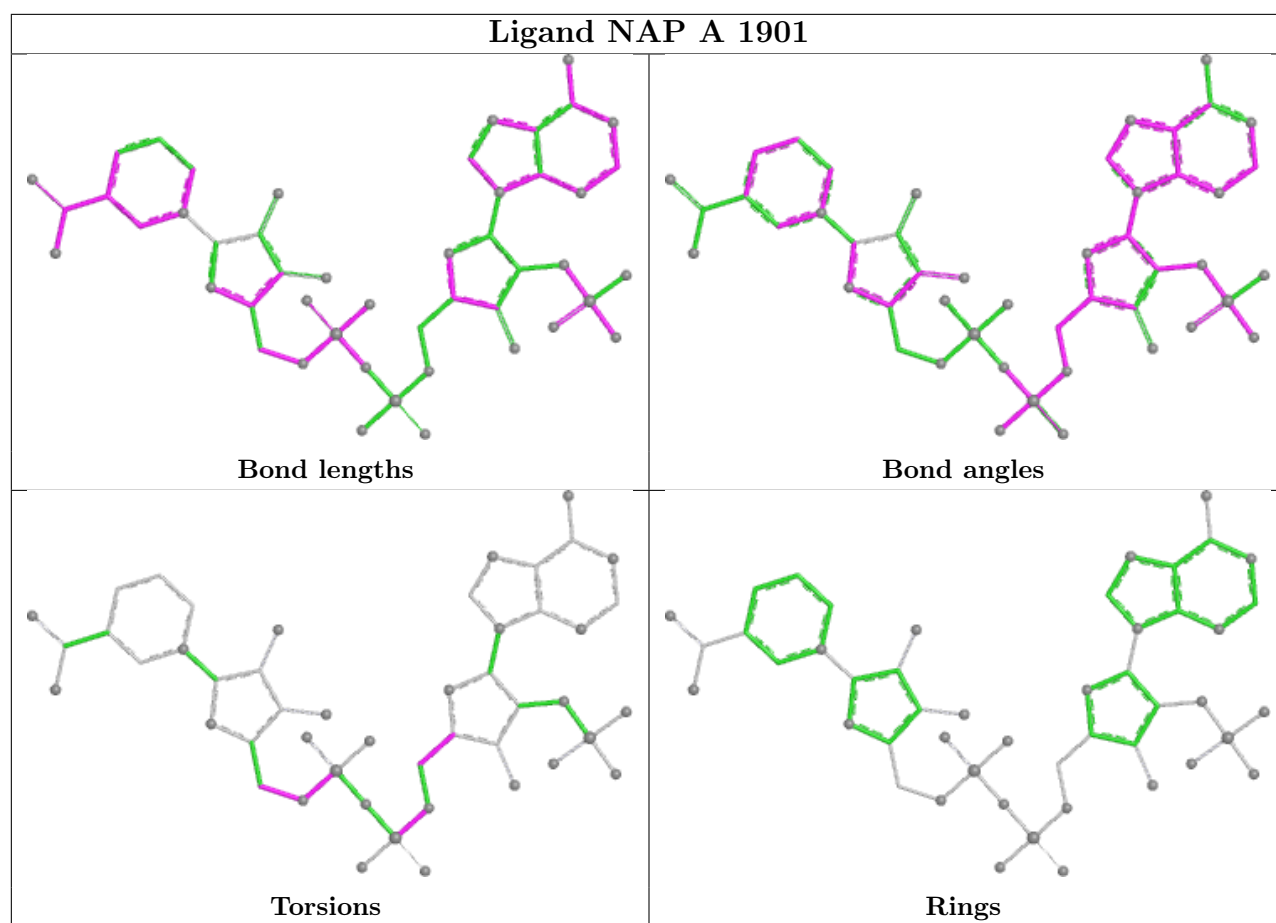
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1901	NAP	19	0

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 G 2101





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.

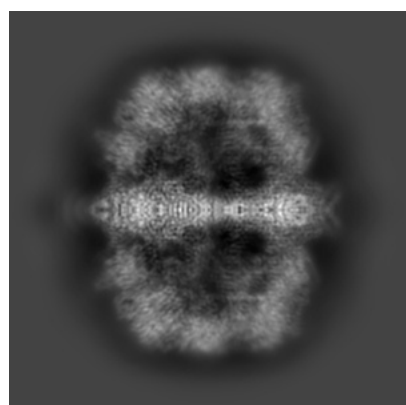
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20656. These allow visual inspection of the internal detail of the map and identification of artifacts.

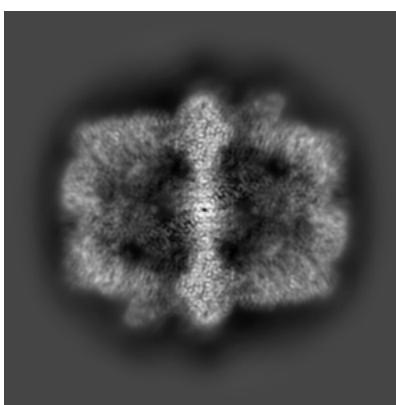
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

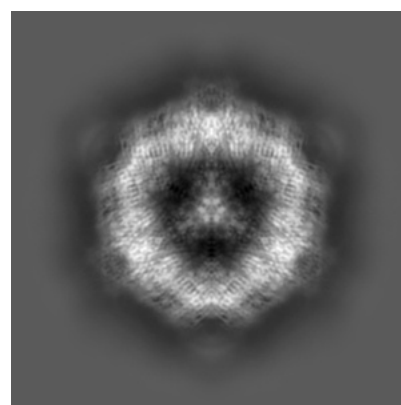
6.1.1 Primary map



X



Y

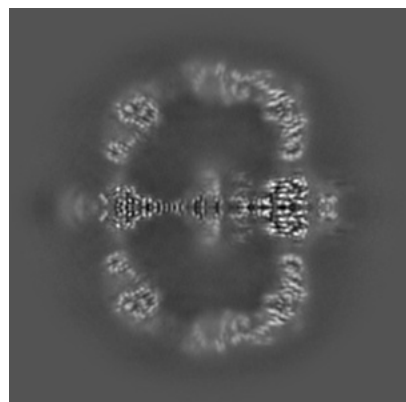


Z

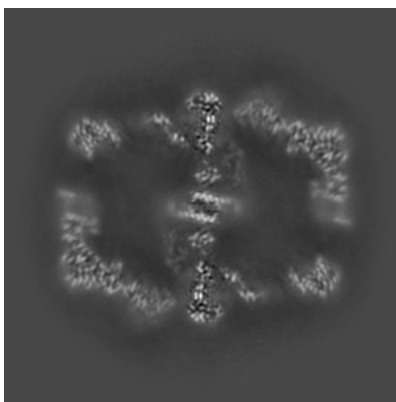
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

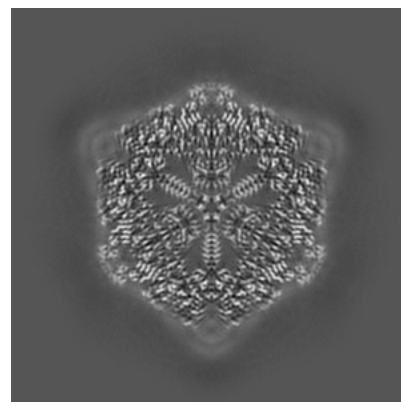
6.2.1 Primary map



X Index: 176



Y Index: 176

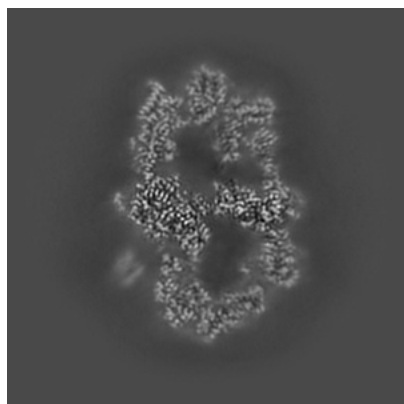


Z Index: 176

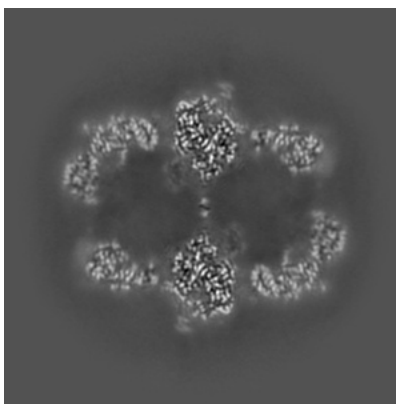
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

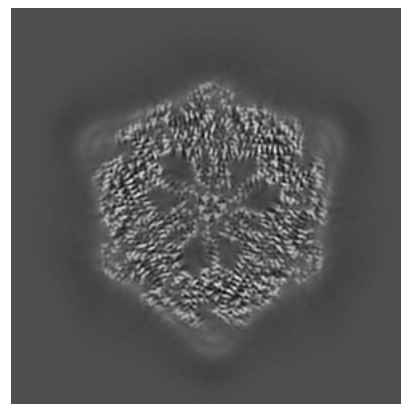
6.3.1 Primary map



X Index: 237



Y Index: 140

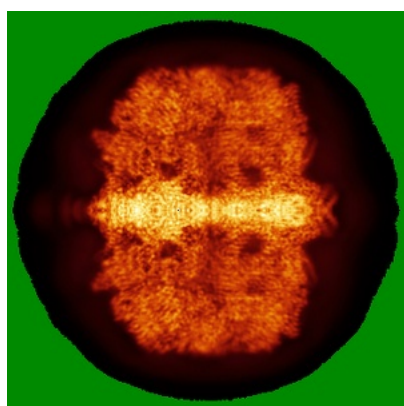


Z Index: 172

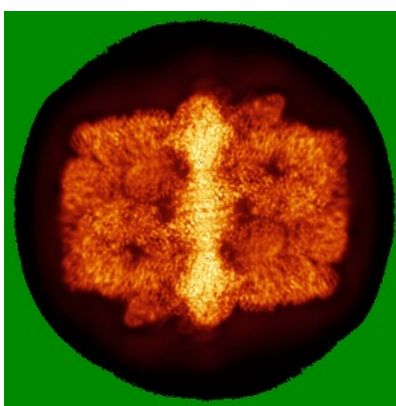
The images above show the largest variance slices of the map in three orthogonal directions.

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

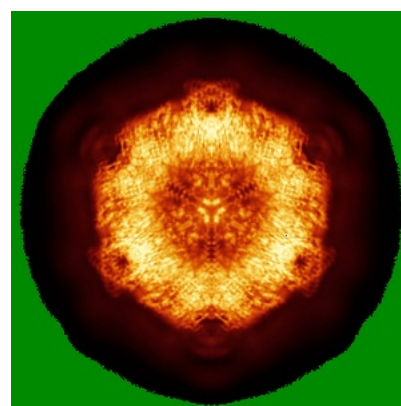
6.4.1 Primary map



X



Y

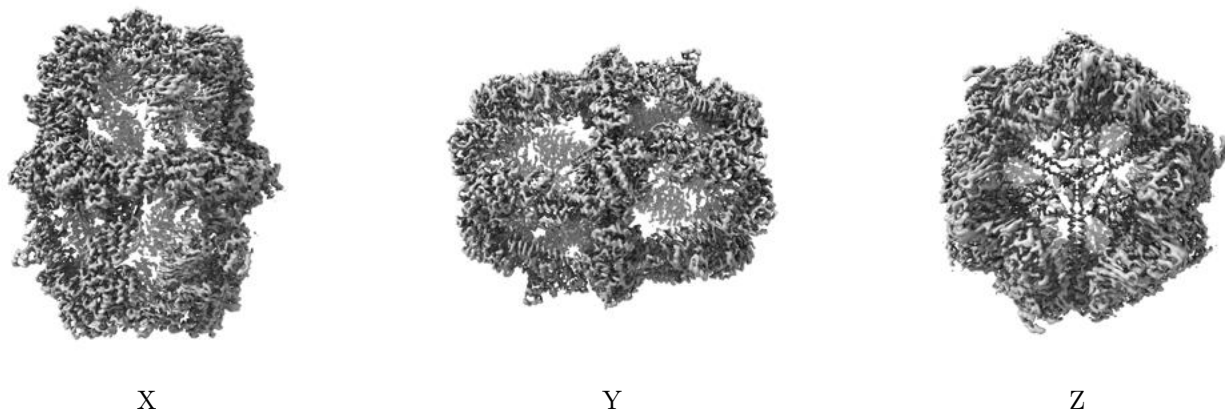


Z

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 0.706. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

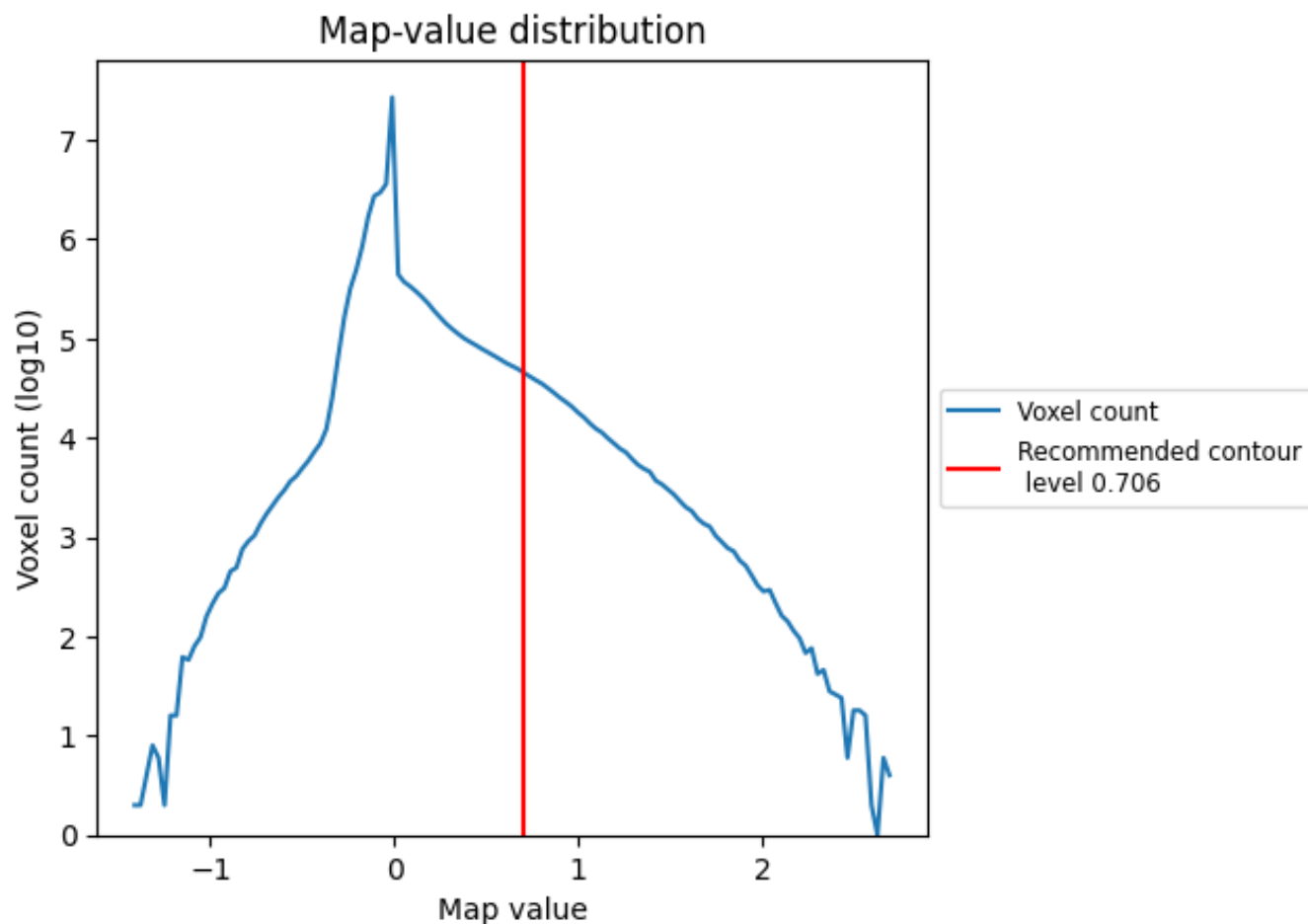
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

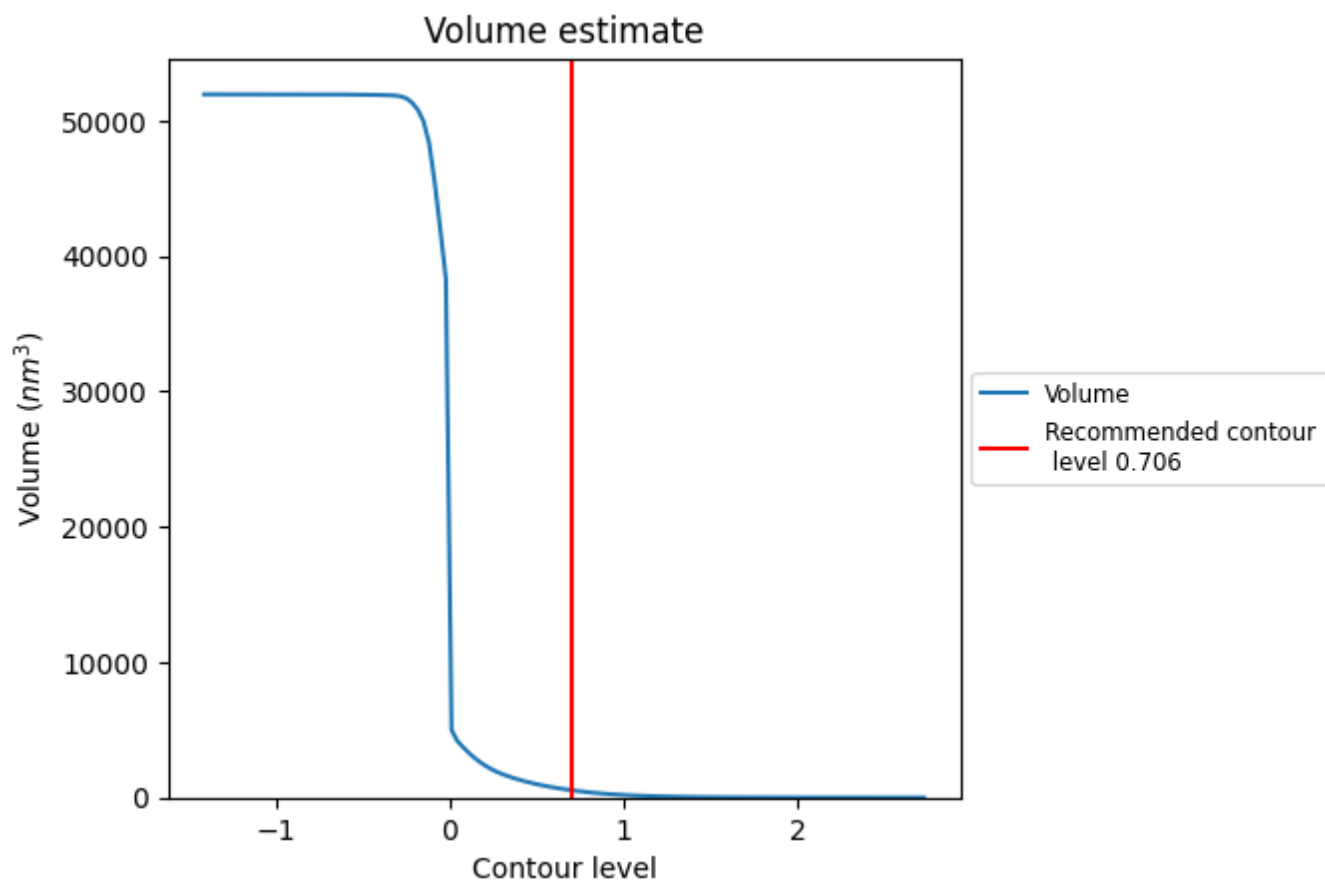
This section contains the results of statistical analysis of the map.

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.

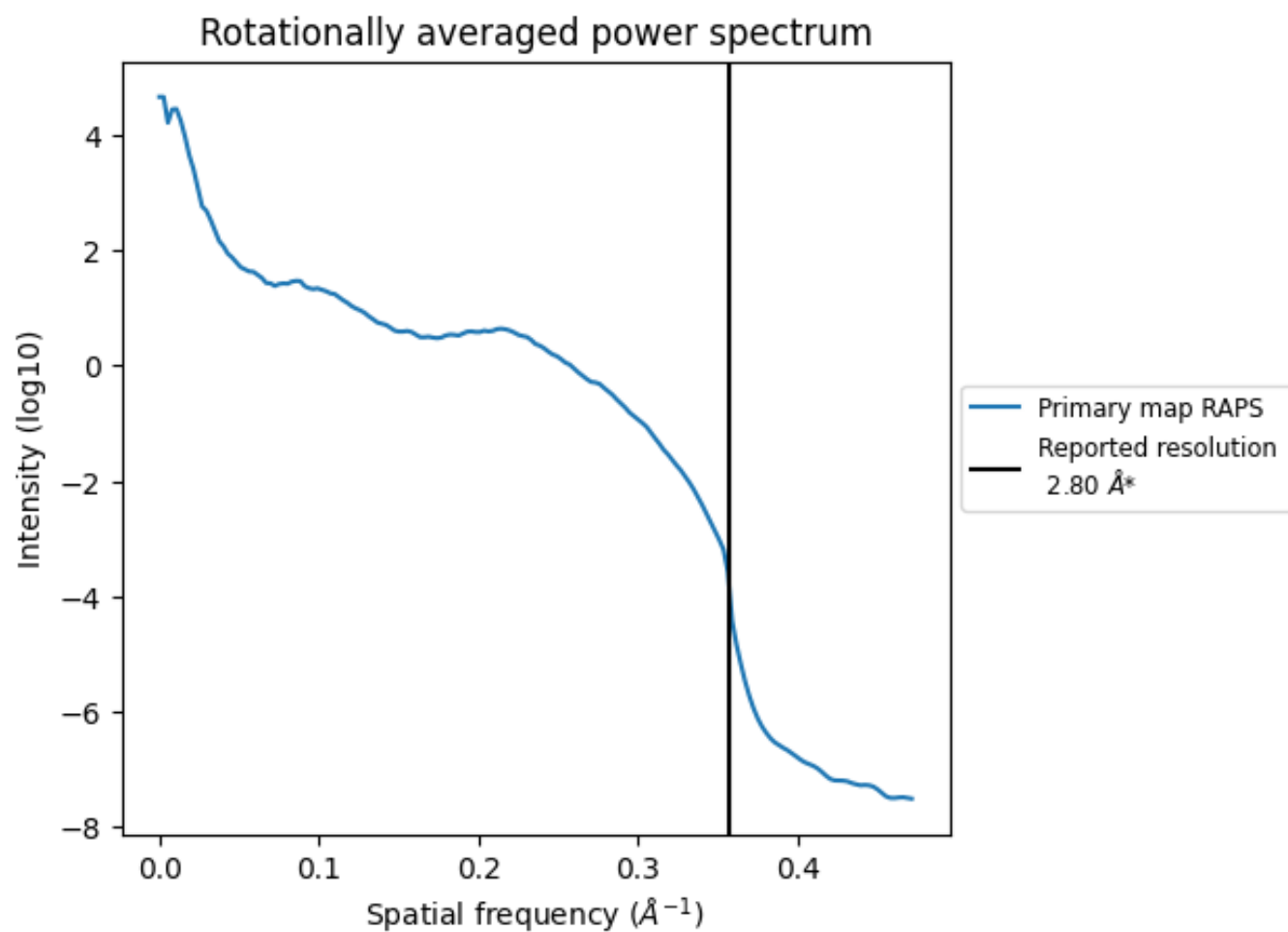
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 531 nm³; this corresponds to an approximate mass of 480 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 0.357 Å⁻¹

8 Fourier-Shell correlation

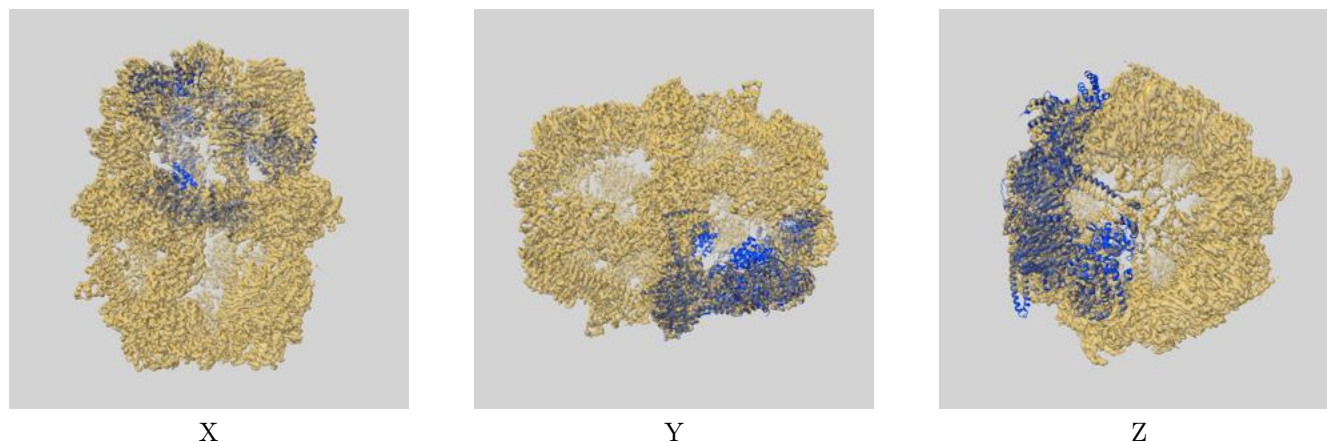
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20656 and PDB model 6U5U. Per-residue inclusion information can be found in section [3](#) on page [7](#).

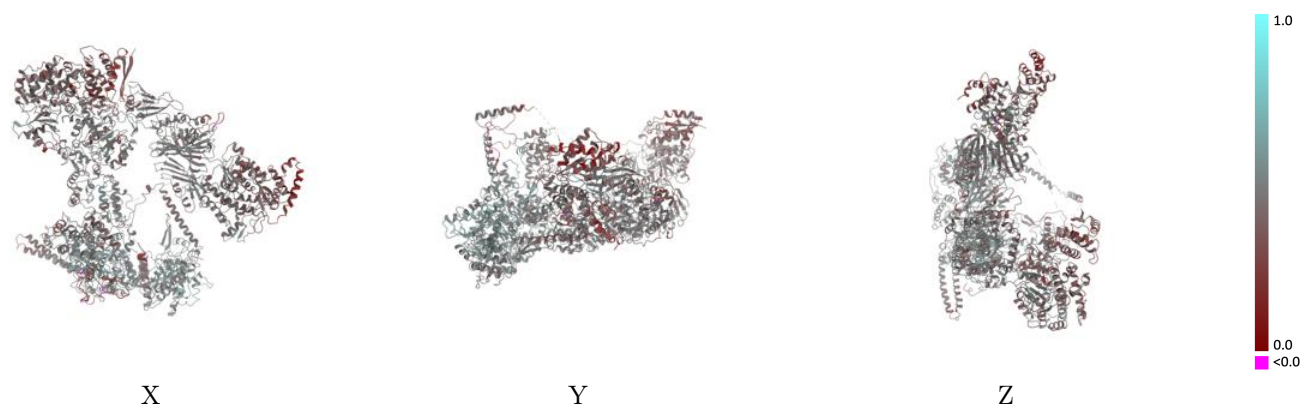
9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



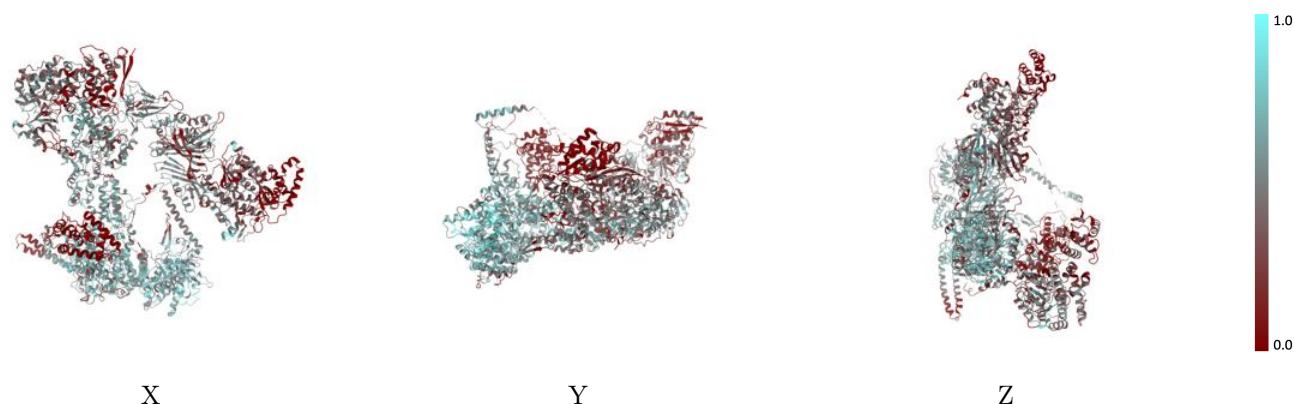
The images above show the 3D surface view of the map at the recommended contour level 0.706 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



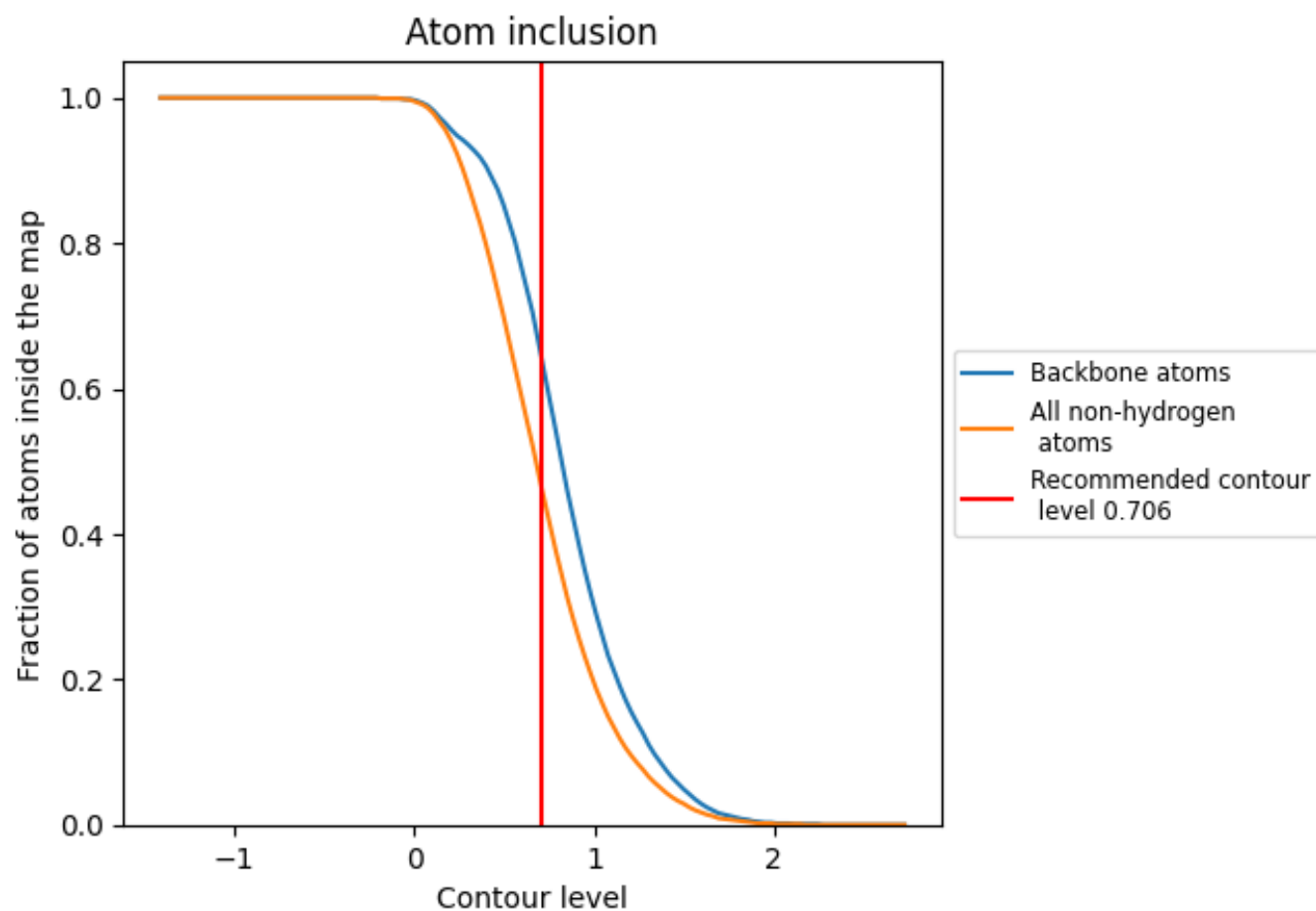
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.706).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% 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 (0.706) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4650	0.4490
A	0.5460	0.4800
G	0.4030	0.4260

