



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:12 PM UTC

PDB ID : 8QEO / pdb_00008qeo
EMDB ID : EMD-18374
Title : cryo-EM structure complex of Frizzled-7 and Clostridioides difficile toxin B
Authors : Kinsolving, J.; Bous, J.
Deposited on : 2023-09-01
Resolution : 3.26 Å (reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
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

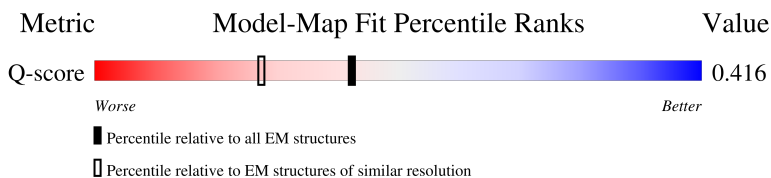
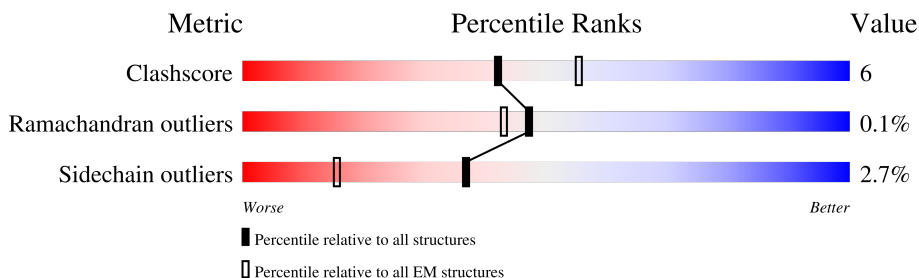
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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	217187	24013	-
Ramachandran outliers	211220	23611	-
Sidechain outliers	210688	23127	-
Q-score	-	25397	14557 (2.76 - 3.76)

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	2397	
2	B	603	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18126 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 Toxin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2146	Total	C	N	O	S	0	0
			17176	10943	2710	3477	46		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P18177
A	-12	ASP	-	expression tag	UNP P18177
A	-11	LYS	-	expression tag	UNP P18177
A	-10	LEU	-	expression tag	UNP P18177
A	-9	VAL	-	expression tag	UNP P18177
A	-8	HIS	-	expression tag	UNP P18177
A	-7	LEU	-	expression tag	UNP P18177
A	-6	ASN	-	expression tag	UNP P18177
A	-5	GLN	-	expression tag	UNP P18177
A	-4	ARG	-	expression tag	UNP P18177
A	-3	GLY	-	expression tag	UNP P18177
A	-2	LYS	-	expression tag	UNP P18177
A	-1	CYS	-	expression tag	UNP P18177
A	0	THR	-	expression tag	UNP P18177
A	2367	GLY	-	expression tag	UNP P18177
A	2368	TYR	-	expression tag	UNP P18177
A	2369	ARG	-	expression tag	UNP P18177
A	2370	PRO	-	expression tag	UNP P18177
A	2371	HIS	-	expression tag	UNP P18177
A	2372	ALA	-	expression tag	UNP P18177
A	2373	GLY	-	expression tag	UNP P18177
A	2374	LEU	-	expression tag	UNP P18177
A	2375	ARG	-	expression tag	UNP P18177
A	2376	GLY	-	expression tag	UNP P18177
A	2377	SER	-	expression tag	UNP P18177
A	2378	HIS	-	expression tag	UNP P18177
A	2379	HIS	-	expression tag	UNP P18177
A	2380	HIS	-	expression tag	UNP P18177

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2381	HIS	-	expression tag	UNP P18177
A	2382	HIS	-	expression tag	UNP P18177
A	2383	HIS	-	expression tag	UNP P18177

- Molecule 2 is a protein called Frizzled-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	121	Total	C	N	O	S	0	0
			949	600	165	172	12		

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	MET	-	initiating methionine	UNP O75084
B	11	LYS	-	expression tag	UNP O75084
B	12	THR	-	expression tag	UNP O75084
B	13	ILE	-	expression tag	UNP O75084
B	14	ILE	-	expression tag	UNP O75084
B	15	ALA	-	expression tag	UNP O75084
B	16	LEU	-	expression tag	UNP O75084
B	17	SER	-	expression tag	UNP O75084
B	18	TYR	-	expression tag	UNP O75084
B	19	ILE	-	expression tag	UNP O75084
B	20	PHE	-	expression tag	UNP O75084
B	21	CYS	-	expression tag	UNP O75084
B	22	LEU	-	expression tag	UNP O75084
B	23	VAL	-	expression tag	UNP O75084
B	24	PHE	-	expression tag	UNP O75084
B	25	ALA	-	expression tag	UNP O75084
B	26	ASP	-	expression tag	UNP O75084
B	27	TYR	-	expression tag	UNP O75084
B	28	LYS	-	expression tag	UNP O75084
B	29	ASP	-	expression tag	UNP O75084
B	30	ASP	-	expression tag	UNP O75084
B	31	ASP	-	expression tag	UNP O75084
B	32	ASP	-	expression tag	UNP O75084
B	575	SER	-	expression tag	UNP O75084
B	576	ARG	-	expression tag	UNP O75084
B	577	LEU	-	expression tag	UNP O75084
B	578	GLU	-	expression tag	UNP O75084
B	579	VAL	-	expression tag	UNP O75084
B	580	LEU	-	expression tag	UNP O75084

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	581	PHE	-	expression tag	UNP O75084
B	582	GLN	-	expression tag	UNP O75084
B	583	GLY	-	expression tag	UNP O75084
B	584	PRO	-	expression tag	UNP O75084
B	585	TRP	-	expression tag	UNP O75084
B	586	SER	-	expression tag	UNP O75084
B	587	HIS	-	expression tag	UNP O75084
B	588	PRO	-	expression tag	UNP O75084
B	589	GLN	-	expression tag	UNP O75084
B	590	PHE	-	expression tag	UNP O75084
B	591	GLU	-	expression tag	UNP O75084
B	592	LYS	-	expression tag	UNP O75084
B	593	GLY	-	expression tag	UNP O75084
B	594	GLY	-	expression tag	UNP O75084
B	595	GLY	-	expression tag	UNP O75084
B	596	SER	-	expression tag	UNP O75084
B	597	GLY	-	expression tag	UNP O75084
B	598	GLY	-	expression tag	UNP O75084
B	599	GLY	-	expression tag	UNP O75084
B	600	SER	-	expression tag	UNP O75084
B	601	GLY	-	expression tag	UNP O75084
B	602	GLY	-	expression tag	UNP O75084
B	603	GLY	-	expression tag	UNP O75084
B	604	SER	-	expression tag	UNP O75084
B	605	TRP	-	expression tag	UNP O75084
B	606	SER	-	expression tag	UNP O75084
B	607	HIS	-	expression tag	UNP O75084
B	608	PRO	-	expression tag	UNP O75084
B	609	GLN	-	expression tag	UNP O75084
B	610	PHE	-	expression tag	UNP O75084
B	611	GLU	-	expression tag	UNP O75084
B	612	LYS	-	expression tag	UNP O75084

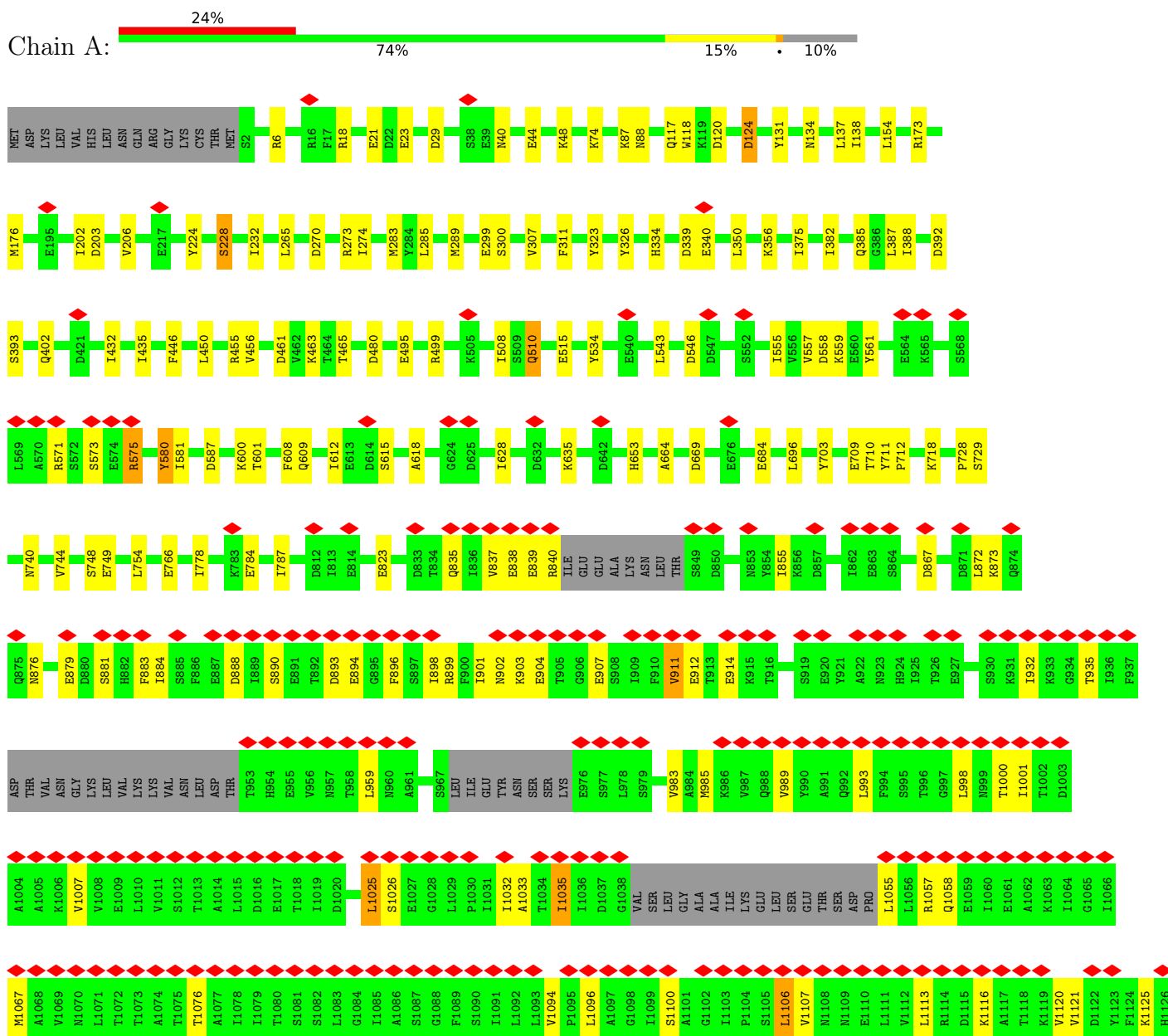
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0

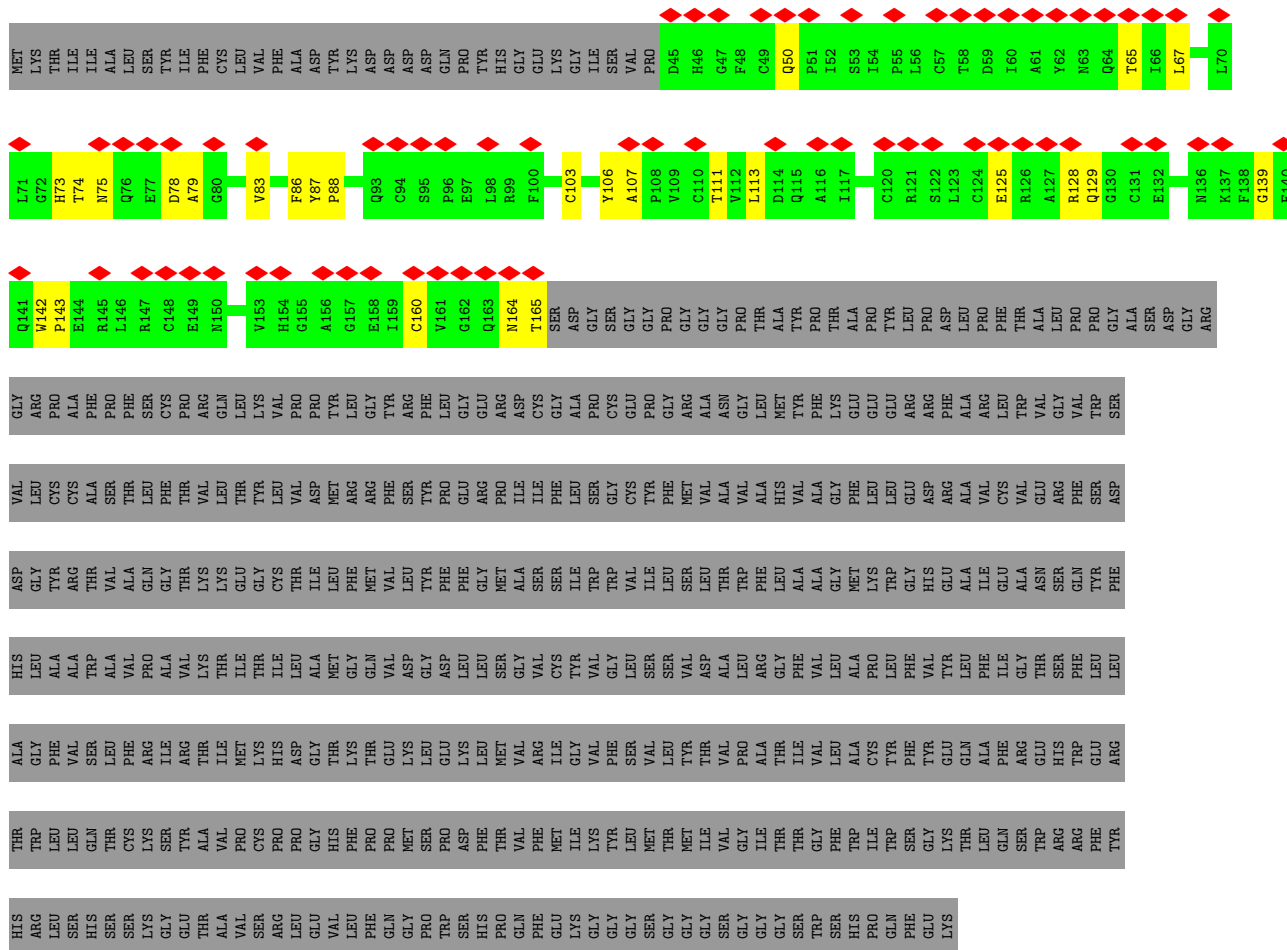
3 Residue-property plots

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

• Molecule 1: Toxin B



TRP	Y2148	N2063	S1981	F1899	I1795	R1652	D1546	K1446	E1358	A1268	R1196	L1219	ILE
TYR	F2149	N2064	D1982	S1900	Y1804	Q1653	E1547	I1447	S1359	F1269	E1197	V1130	TYR
ASP	Y2150	K2065	D1983	T1901	Y1805	P1659	K1548	N1453	D1360	I1270	P1198	E1131	ASP
MET	I2151	I2066	V1984	D1903	E1805	L1663	L1552	N1454	K1361	A1271	H1199	T1132	MET
GLU	D2152	D2071	M1985	F1905	D1806	L1663	D1558	E1455	I1362	D1272	S1201	E1133	GLU
ASN	D2153	K1986	Q1986	K1906	G1907	G1667	E1559	E1456	K1363	A1273	L1202	G1134	ASN
GLY	N2154	A2075	K1987	Y1907	L1808	G1667	I1565	Q1457	K1364	L1274	Y1203	V1135	GLY
SER	D2155	V2076	I1992	F1908	I1809	T1672	I1565	K1458	G1365	T1275	F1136	F1137	SER
ASP	G2156	V2077	V1673	G1810	I1809	T1672	I1565	K1458	G1365	T1275	K1210	T1137	ASP
LYS	T2157	E2083	M1993	L1912	Y1811	I1674	G1573	N1459	D1366	T1277	E1211	T1138	LYS
THR	Q2158	D2084	D1994	T1913	S1817	S1677	N1574	I1460	I1368	L1278	L1212	L1139	THR
PHE	T2159	G2085	M1995	L1914	L1818	C1687	T1576	I1460	E1369	E1283	L1213	D1140	PHE
ASN	G2160	K1996	K1996	Y1819	Y1819	V1688	N1577	D1466	G1370	D1284	D1214	D1141	ASN
PRO	V2161	Y2089	D2000	E1916	N1820	K1690	S1578	S1467	I1371	E1284	L1215	K1142	PRO
THR	F2162	E2092	D2001	N1917	L1835	T1699	D1579	E1468	L1375	I1287	K1216	T1143	THR
LYS	D2163	E2092	S2002	L1918	D1840	D1700	S1583	K1470	E1379	N1288	D1218	M1144	LYS
ALA	T2164	D2093	T2002	E1919	D1840	N1703	F1584	E1471	M1380	N1290	L1219	M1145	ALA
CYS	S2165	T2094	G2003	E1919	K1846	I1704	L1585	N1476	H1387	L1291	L1222	D1148	CYS
LYS	D2166	A2095	V2004	A1922	N1850	T1705	F1584	N1476	F1391	D1292	N1227	L1150	LYS
GLY	G2167	E2096	K2005	I1923	K1846	I1704	L1585	N1476	F1391	S1293	R1228	Y1151	GLY
ILE	Y2168	E2096	K2006	I1923	N1850	T1705	L1585	N1476	F1391	M1294	E1232	E1154	ILE
ASN	K2169	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	ASN
LEU	D2170	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	LEU
ILE	S2171	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	ILE
ASP	A2172	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	ASP
ILE	L2173	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	ILE
LYS	D2174	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	LYS
TYR	A2175	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	TYR
PHE	N2176	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	PHE
ASP	G2177	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	ASP
GLU	N2178	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	GLU
LYS	Y2182	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	LYS
GLY	F2182	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	GLY
ILE	A2185	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	ILE
ARG	V2186	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	ARG
THR	E2187	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
GLY	Y2188	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	GLY
LEU	S2189	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	LEU
ILE	G2190	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	ILE
PHE	L2191	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	PHE
GLU	V2192	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	GLU
ASN	R2193	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	ASN
ASN	V2194	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	ASN
TYR	GLY	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	TYR
THR	GLU	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
ASN	VAL	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	ASN
GLU	T2136	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	GLU
ASN	T2137	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	ASN
GLY	T2138	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	GLY
PHE	GLY	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	PHE
GLU	GLU	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	GLU
THR	GLU	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	D2001	L1918	D1840	N1703	F1584	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092	S2002	E1919	K1846	I1704	L1585	N1476	F1391	E1232	E1232	E1154	THR
THR	TYR	E2092											



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151385	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.453	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.875	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	579.6, 579.6, 579.6	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1592, 1.1592, 1.1592	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: ZN

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	0.18	0/17497	0.31	0/23686
2	B	0.14	0/974	0.34	0/1325
All	All	0.17	0/18471	0.31	0/25011

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	17176	0	16623	215	0
2	B	949	0	910	16	0
3	A	1	0	0	0	0
All	All	18126	0	17533	230	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 6.

All (230) 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:907:GLU:N	1:A:907:GLU:OE1	2.14	0.80
1:A:299:GLU:O	1:A:300:SER:OG	2.02	0.74
1:A:40:ASN:ND2	1:A:44:GLU:OE1	2.20	0.74
1:A:876:ASN:ND2	1:A:912:GLU:OE1	2.20	0.73
1:A:669:ASP:OD1	1:A:718:LYS:NZ	2.22	0.73
1:A:837:VAL:O	1:A:840:ARG:NH1	2.22	0.73
1:A:1149:ASP:OD1	1:A:1228:ARG:NH2	2.24	0.71
1:A:1184:ILE:HD12	1:A:1185:ASP:N	2.08	0.68
2:B:125:GLU:OE1	2:B:128:ARG:NH2	2.26	0.68
1:A:1653:GLN:OE1	1:A:1689:ASN:ND2	2.25	0.68
2:B:67:LEU:HD12	2:B:107:ALA:O	1.93	0.68
1:A:74:LYS:NZ	1:A:867:ASP:OD1	2.26	0.67
1:A:587:ASP:OD2	1:A:653:HIS:NE2	2.26	0.67
1:A:1625:CYS:SG	1:A:1626:ASP:N	2.68	0.67
1:A:455:ARG:NE	1:A:823:GLU:OE2	2.29	0.66
1:A:1349:ASP:OD2	1:A:1364:LYS:NZ	2.22	0.66
1:A:872:LEU:HD11	1:A:911:VAL:HG12	1.77	0.66
1:A:748:SER:OG	1:A:749:GLU:OE1	2.13	0.64
1:A:1558:ASP:OD1	1:A:1559:GLU:N	2.29	0.64
1:A:1184:ILE:HD13	1:A:1266:TYR:CD1	2.33	0.63
1:A:1711:ASN:OD1	1:A:1711:ASN:N	2.32	0.62
2:B:78:ASP:OD1	2:B:79:ALA:N	2.31	0.62
1:A:1366:ASP:OD1	1:A:1367:LEU:N	2.32	0.62
1:A:1106:LEU:HD13	1:A:1107:VAL:H	1.65	0.62
1:A:385:GLN:NE2	1:A:515:GLU:OE2	2.32	0.61
1:A:1912:ASN:N	1:A:1917:ASN:O	2.28	0.61
1:A:1429:ILE:HD11	1:A:1447:ILE:HD11	1.83	0.61
1:A:1353:ARG:NH1	1:A:1407:SER:O	2.34	0.60
1:A:1433:LEU:N	1:A:1471:GLU:OE1	2.35	0.60
1:A:1184:ILE:HD13	1:A:1266:TYR:CE1	2.36	0.59
1:A:1129:LEU:O	1:A:1133:GLU:N	2.35	0.59
1:A:87:LYS:NZ	1:A:88:ASN:OD1	2.36	0.59
1:A:1548:LYS:O	1:A:1603:LYS:N	2.34	0.59
1:A:283:MET:CB	1:A:388:ILE:HG22	2.33	0.59
1:A:120:ASP:OD2	1:A:356:LYS:NZ	2.36	0.59
1:A:339:ASP:OD1	1:A:340:GLU:N	2.35	0.59
1:A:6:ARG:NH1	1:A:29:ASP:OD1	2.36	0.58
1:A:1121:VAL:O	1:A:1125:LYS:N	2.26	0.57
1:A:1025:LEU:HD11	1:A:1035:ILE:HG23	1.86	0.57
1:A:873:LYS:NZ	1:A:879:GLU:O	2.38	0.57
1:A:855:ILE:HD11	1:A:1651:ASN:HD21	1.70	0.57
2:B:83:VAL:O	2:B:86:PHE:N	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:LEU:HD13	1:A:1203:TYR:HE2	1.69	0.56
2:B:83:VAL:HG13	2:B:106:TYR:CE2	2.40	0.56
1:A:728:PRO:O	1:A:729:SER:OG	2.21	0.56
2:B:111:THR:O	2:B:113:LEU:N	2.39	0.56
1:A:1984:VAL:O	1:A:1986:GLN:NE2	2.38	0.56
1:A:138:ILE:HG21	1:A:265:LEU:HD21	1.88	0.55
1:A:1498:TYR:O	1:A:1500:ASP:N	2.39	0.55
1:A:1625:CYS:HA	1:A:1631:ILE:HA	1.88	0.55
1:A:23:GLU:OE1	1:A:23:GLU:N	2.34	0.55
1:A:1766:ARG:NH2	1:A:1804:TYR:OH	2.40	0.55
1:A:884:ILE:HD12	1:A:884:ILE:H	1.72	0.54
2:B:164:ASN:O	2:B:165:THR:OG1	2.19	0.54
2:B:50:GLN:O	2:B:65:THR:N	2.41	0.54
1:A:323:TYR:HB2	1:A:350:LEU:HD13	1.90	0.53
1:A:1252:ASP:OD1	1:A:1264:TRP:NE1	2.39	0.53
1:A:1100:SER:N	1:A:1148:ASP:OD2	2.42	0.52
1:A:1275:ILE:HD11	1:A:1278:LEU:HD21	1.90	0.52
1:A:1113:LEU:HD13	1:A:1120:VAL:HG13	1.92	0.52
1:A:2151:ILE:HD11	1:A:2155:GLY:HA2	1.92	0.52
1:A:893:ASP:OD1	1:A:894:GLU:N	2.43	0.52
1:A:1144:MET:HE1	1:A:1215:LEU:HD23	1.92	0.52
1:A:1171:ARG:NH1	1:A:1197:GLU:O	2.43	0.52
1:A:784:GLU:OE1	1:A:784:GLU:N	2.43	0.51
1:A:2141:VAL:HG23	1:A:2143:ASN:O	2.09	0.51
1:A:959:LEU:HB2	1:A:1650:GLY:HA3	1.90	0.51
1:A:1749:PHE:HZ	1:A:1795:ILE:HG21	1.75	0.51
1:A:558:ASP:O	1:A:561:TYR:N	2.42	0.51
1:A:1164:LEU:HD12	1:A:1210:LYS:HE2	1.92	0.51
1:A:1291:LEU:HB2	1:A:1323:TYR:CZ	2.46	0.51
1:A:749:GLU:OE1	1:A:749:GLU:N	2.44	0.51
1:A:1552:LEU:HD23	1:A:1585:LEU:HD13	1.92	0.51
1:A:575:ARG:NE	1:A:601:THR:OG1	2.42	0.51
1:A:1483:LEU:HG	1:A:1527:LEU:HD21	1.93	0.51
1:A:1492:VAL:HG11	1:A:1516:VAL:HG21	1.93	0.50
1:A:835:GLN:O	1:A:839:GLU:N	2.44	0.50
1:A:1731:VAL:N	1:A:1781:SER:O	2.37	0.50
1:A:600:LYS:NZ	1:A:744:VAL:O	2.38	0.50
1:A:1483:LEU:HD21	1:A:1527:LEU:HG	1.94	0.50
1:A:1659:PRO:HD3	1:A:1674:ILE:HD11	1.93	0.50
1:A:1483:LEU:HD11	1:A:1527:LEU:HD11	1.93	0.50
1:A:1154:GLU:HB3	1:A:1163:VAL:HG12	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:NE	1:A:766:GLU:OE2	2.42	0.50
1:A:1184:ILE:HG12	1:A:1267:PHE:H	1.76	0.50
1:A:2036:PHE:HB2	1:A:2075:ALA:HB3	1.94	0.50
1:A:1583:SER:HA	1:A:1631:ILE:HD11	1.94	0.49
1:A:883:PHE:HB2	1:A:901:ILE:HB	1.94	0.49
1:A:1881:ILE:HG22	1:A:1884:LYS:H	1.77	0.49
1:A:1624:ILE:HB	1:A:1634:TYR:HB2	1.95	0.49
1:A:375:ILE:HD13	1:A:382:ILE:HG23	1.94	0.49
1:A:653:HIS:O	1:A:664:ALA:N	2.43	0.49
1:A:1184:ILE:HG21	1:A:1265:ARG:O	2.12	0.49
1:A:1672:THR:O	1:A:1672:THR:OG1	2.29	0.49
1:A:1907:TYR:CE2	1:A:1909:ALA:HB2	2.47	0.49
1:A:778:ILE:HG23	1:A:787:ILE:HG23	1.94	0.49
1:A:1634:TYR:HA	1:A:1649:VAL:HG13	1.94	0.49
1:A:881:SER:HA	1:A:902:ASN:HA	1.95	0.48
1:A:1000:THR:HG22	1:A:1001:ILE:N	2.28	0.48
1:A:581:ILE:HD12	1:A:581:ILE:H	1.77	0.48
1:A:1113:LEU:HD13	1:A:1120:VAL:HG22	1.95	0.48
1:A:1336:ILE:HD11	1:A:1391:PHE:CE2	2.48	0.48
1:A:1634:TYR:HA	1:A:1649:VAL:CG1	2.43	0.48
1:A:2170:TYR:O	1:A:2188:TYR:OH	2.30	0.48
1:A:612:ILE:O	1:A:615:SER:OG	2.25	0.48
1:A:1703:ASN:OD1	1:A:1732:ASN:ND2	2.39	0.48
1:A:154:LEU:HD11	1:A:534:TYR:HB3	1.95	0.48
1:A:1935:ILE:HB	1:A:1965:ALA:HB3	1.96	0.48
2:B:103:CYS:O	2:B:107:ALA:N	2.47	0.48
2:B:142:TRP:O	2:B:143:PRO:C	2.57	0.47
1:A:1219:LEU:HD11	1:A:1299:ILE:HG12	1.96	0.47
1:A:461:ASP:OD1	1:A:463:LYS:NZ	2.47	0.47
1:A:21:GLU:OE1	1:A:21:GLU:N	2.39	0.47
1:A:608:PHE:CD2	1:A:618:ALA:HB2	2.49	0.47
1:A:1168:GLU:HG3	1:A:1201:SER:HA	1.95	0.47
1:A:989:VAL:HG13	1:A:993:LEU:HD12	1.95	0.47
1:A:1672:THR:OG1	1:A:1700:ASP:OD1	2.31	0.47
1:A:1901:THR:OG1	1:A:1902:GLU:N	2.46	0.47
1:A:1787:LYS:NZ	1:A:1840:ASP:OD2	2.37	0.47
1:A:1970:ASN:OD1	1:A:1971:GLN:N	2.48	0.47
1:A:1375:LEU:HD23	1:A:1425:TYR:CG	2.50	0.47
1:A:1485:VAL:HG11	1:A:1516:VAL:HB	1.97	0.47
1:A:899:ARG:CZ	1:A:901:ILE:HD11	2.45	0.46
1:A:1357:ILE:HG12	1:A:1362:ILE:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1120:VAL:HG21	1:A:1276:THR:O	2.15	0.46
1:A:1175:GLY:O	1:A:1261:GLU:N	2.43	0.46
1:A:1184:ILE:HD12	1:A:1184:ILE:C	2.40	0.46
1:A:1717:VAL:HB	1:A:1765:ILE:HG23	1.96	0.46
1:A:18:ARG:HG2	1:A:1667:GLY:HA3	1.98	0.46
1:A:1355:VAL:HG13	1:A:1362:ILE:HB	1.97	0.46
1:A:2089:TYR:CG	1:A:2104:ILE:HD13	2.50	0.46
1:A:124:ASP:OD1	1:A:124:ASP:N	2.47	0.46
1:A:176:MET:HE3	1:A:176:MET:O	2.16	0.46
1:A:1598:LEU:HD11	2:B:139:GLY:HA3	1.98	0.46
1:A:224:TYR:O	1:A:228:SER:OG	2.29	0.45
1:A:1237:THR:N	1:A:1238:PRO:HD3	2.32	0.45
2:B:73:HIS:CG	2:B:79:ALA:HB2	2.51	0.45
1:A:1151:VAL:HG11	1:A:1227:ASN:HA	1.98	0.45
1:A:1565:ILE:HD12	1:A:1612:ILE:CD1	2.47	0.45
1:A:283:MET:CG	1:A:388:ILE:HG22	2.47	0.45
1:A:1222:LEU:HD21	1:A:1298:PHE:HE2	1.82	0.45
1:A:1349:ASP:OD1	1:A:1407:SER:N	2.48	0.45
1:A:1548:LYS:HB2	1:A:1602:ILE:HA	1.98	0.45
1:A:283:MET:HB2	1:A:388:ILE:HG22	1.98	0.44
1:A:1737:SER:OG	1:A:1786:ASP:OD2	2.27	0.44
1:A:557:VAL:HG23	1:A:609:GLN:OE1	2.17	0.44
1:A:1437:MET:HG2	1:A:1497:VAL:HG11	1.98	0.44
2:B:83:VAL:HG13	2:B:106:TYR:HE2	1.81	0.44
1:A:1185:ASP:OD1	1:A:1186:HIS:N	2.41	0.44
1:A:696:LEU:HD12	1:A:740:ASN:HB2	2.00	0.44
1:A:1958:PHE:HA	1:A:1965:ALA:HA	2.00	0.44
1:A:855:ILE:HD11	1:A:1651:ASN:ND2	2.30	0.44
1:A:711:TYR:HB3	1:A:712:PRO:HD3	2.00	0.44
1:A:1025:LEU:HD12	1:A:1033:ALA:HB1	1.99	0.44
1:A:1699:THR:O	1:A:1729:ILE:HD12	2.18	0.44
1:A:1878:GLU:OE2	1:A:1901:THR:OG1	2.27	0.44
1:A:1880:ILE:HG22	1:A:1882:ASP:H	1.83	0.44
1:A:270:ASP:O	1:A:273:ARG:HG2	2.18	0.44
1:A:446:PHE:CZ	1:A:450:LEU:HD11	2.52	0.44
1:A:546:ASP:N	1:A:546:ASP:OD1	2.50	0.44
1:A:134:ASN:O	1:A:203:ASP:N	2.51	0.43
1:A:456:VAL:HG11	1:A:465:THR:HG23	2.00	0.43
1:A:1360:ASP:OD1	1:A:1361:LYS:N	2.48	0.43
1:A:1677:SER:HA	1:A:1705:THR:HB	2.00	0.43
1:A:1412:ILE:HD13	1:A:1443:ILE:HD11	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:GLU:OE1	1:A:904:GLU:N	2.52	0.43
1:A:703:TYR:CD1	1:A:710:THR:HG21	2.53	0.43
1:A:1346:ILE:O	1:A:1404:LEU:HA	2.18	0.43
1:A:573:SER:OG	1:A:575:ARG:NE	2.51	0.43
1:A:1094:VAL:O	1:A:1096:LEU:N	2.50	0.43
1:A:1366:ASP:OD1	1:A:1446:LYS:NZ	2.52	0.43
1:A:580:TYR:CZ	1:A:608:PHE:HZ	2.37	0.43
1:A:932:ILE:O	1:A:935:THR:OG1	2.32	0.43
1:A:1636:ILE:HG23	1:A:1638:PHE:CE1	2.54	0.43
1:A:137:LEU:O	1:A:206:VAL:HG11	2.18	0.43
1:A:1189:SER:O	1:A:1266:TYR:OH	2.31	0.43
1:A:1622:GLU:O	1:A:1634:TYR:N	2.52	0.43
1:A:1195:TYR:O	1:A:1196:ARG:NH1	2.38	0.43
1:A:1412:ILE:CD1	1:A:1443:ILE:HD11	2.48	0.43
1:A:1504:PRO:O	1:A:1505:SER:C	2.62	0.43
1:A:1689:ASN:OD1	1:A:1690:LYS:N	2.52	0.43
1:A:289:MET:HE3	1:A:510:GLN:HB3	2.00	0.42
1:A:1846:LYS:O	1:A:1850:ASN:N	2.50	0.42
1:A:2048:ASN:HB2	1:A:2052:GLU:HG2	2.00	0.42
1:A:432:ILE:HA	1:A:435:ILE:HG12	2.01	0.42
1:A:495:GLU:O	1:A:499:ARG:HG2	2.20	0.42
1:A:754:LEU:HD12	1:A:754:LEU:O	2.20	0.42
1:A:1160:ASN:HA	1:A:1215:LEU:HD12	2.00	0.42
1:A:1649:VAL:HG23	1:A:1650:GLY:N	2.34	0.42
1:A:117:GLN:NE2	1:A:326:TYR:HB3	2.34	0.42
1:A:118:TRP:CE2	1:A:285:LEU:HD13	2.54	0.42
1:A:1180:VAL:HG12	1:A:1181:THR:HG23	2.01	0.42
1:A:872:LEU:CD2	1:A:898:ILE:HG21	2.49	0.42
1:A:2142:GLN:NE2	1:A:2149:PHE:O	2.49	0.42
1:A:202:ILE:O	1:A:206:VAL:HG23	2.20	0.42
1:A:635:LYS:NZ	1:A:684:GLU:OE1	2.52	0.42
1:A:307:VAL:HG13	1:A:311:PHE:HD2	1.83	0.42
1:A:902:ASN:OD1	1:A:903:LYS:N	2.50	0.42
1:A:299:GLU:C	1:A:300:SER:HG	2.12	0.42
1:A:1025:LEU:HB3	1:A:1026:SER:H	1.76	0.42
1:A:1164:LEU:HD13	1:A:1203:TYR:CE2	2.53	0.42
1:A:1181:THR:OG1	1:A:1185:ASP:OD2	2.37	0.42
1:A:1578:SER:O	1:A:1579:ASP:HB2	2.19	0.42
1:A:559:LYS:HB2	1:A:628:ILE:HB	2.01	0.42
1:A:1996:LYS:NZ	1:A:2049:GLU:OE1	2.53	0.42
2:B:74:THR:OG1	2:B:75:ASN:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2060:LEU:O	1:A:2066:ILE:HA	2.20	0.41
1:A:835:GLN:NE2	1:A:838:GLU:OE1	2.53	0.41
2:B:164:ASN:C	2:B:165:THR:HG1	2.23	0.41
1:A:1251:LEU:HA	1:A:1254:ILE:HD12	2.03	0.41
1:A:872:LEU:HD13	1:A:914:GLU:HG3	2.02	0.41
1:A:1323:TYR:O	1:A:1324:ALA:HB3	2.21	0.41
2:B:87:TYR:N	2:B:88:PRO:HD2	2.35	0.41
1:A:131:TYR:CD1	1:A:232:ILE:HG21	2.56	0.41
1:A:283:MET:HA	1:A:388:ILE:HG22	2.03	0.41
1:A:1291:LEU:HD21	1:A:1298:PHE:HE1	1.84	0.41
1:A:1287:ILE:HG22	1:A:1289:ILE:HG13	2.03	0.41
1:A:1329:GLN:NE2	1:A:1357:ILE:HD11	2.35	0.41
1:A:1621:PHE:CZ	1:A:1638:PHE:CE1	3.09	0.41
1:A:2045:ASP:OD1	1:A:2045:ASP:N	2.53	0.41
1:A:888:ASP:OD2	1:A:899:ARG:NH1	2.53	0.41
1:A:985:MET:HE2	1:A:985:MET:HA	2.02	0.41
1:A:1289:ILE:HG22	1:A:1291:LEU:CD1	2.50	0.41
1:A:1721:ASP:OD1	1:A:1721:ASP:N	2.51	0.41
1:A:1584:PHE:O	1:A:1584:PHE:CG	2.74	0.40
1:A:334:HIS:NE2	1:A:709:GLU:OE2	2.46	0.40
1:A:1287:ILE:HD12	1:A:1287:ILE:N	2.37	0.40
1:A:1428:LEU:HG	1:A:1461:PRO:HG2	2.03	0.40
1:A:402:GLN:NE2	1:A:480:ASP:OD2	2.55	0.40
1:A:890:SER:O	1:A:896:PHE:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2136/2397 (89%)	1959 (92%)	174 (8%)	3 (0%)	48 76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	119/603 (20%)	99 (83%)	20 (17%)	0	100	100
All	All	2255/3000 (75%)	2058 (91%)	194 (9%)	3 (0%)	47	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1499	MET
1	A	1631	ILE
1	A	1193	ILE

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	1930/2163 (89%)	1878 (97%)	52 (3%)	39	61
2	B	106/505 (21%)	104 (98%)	2 (2%)	50	67
All	All	2036/2668 (76%)	1982 (97%)	54 (3%)	37	61

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	124	ASP
1	A	228	SER
1	A	274	ILE
1	A	387	LEU
1	A	392	ASP
1	A	393	SER
1	A	508	ILE
1	A	510	GLN
1	A	543	LEU
1	A	555	ILE
1	A	571	ARG
1	A	575	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	580	TYR
1	A	911	VAL
1	A	983	VAL
1	A	998	LEU
1	A	1007	VAL
1	A	1025	LEU
1	A	1032	ILE
1	A	1035	ILE
1	A	1055	LEU
1	A	1057	ARG
1	A	1058	GLN
1	A	1067	MET
1	A	1076	THR
1	A	1106	LEU
1	A	1116	LYS
1	A	1137	THR
1	A	1138	LEU
1	A	1163	VAL
1	A	1183	ASP
1	A	1184	ILE
1	A	1194	THR
1	A	1244	GLU
1	A	1336	ILE
1	A	1387	HIS
1	A	1476	ASN
1	A	1490	ASP
1	A	1494	ILE
1	A	1542	LEU
1	A	1625	CYS
1	A	1672	THR
1	A	1687	CYS
1	A	1711	ASN
1	A	1765	ILE
1	A	1770	VAL
1	A	1835	LEU
1	A	1864	TYR
1	A	1884	LYS
1	A	1962	THR
1	A	1972	ILE
2	B	129	GLN
2	B	160	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	553	GLN
1	A	924	HIS
1	A	992	GLN
1	A	1329	GLN
1	A	1511	ASN
1	A	2042	HIS
1	A	2048	ASN
1	A	2147	ASN
1	A	2184	GLN
2	B	46	HIS

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

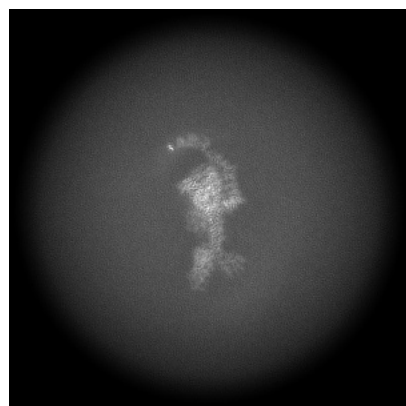
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18374. These allow visual inspection of the internal detail of the map and identification of artifacts.

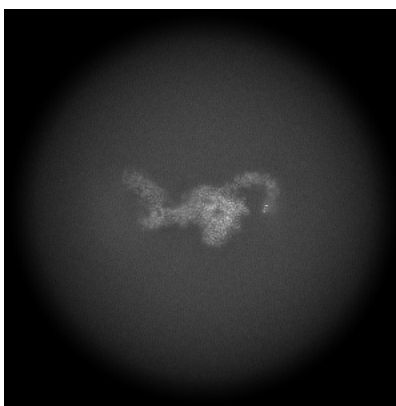
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

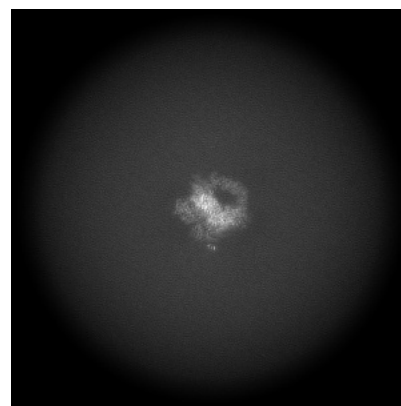
6.1.1 Primary map



X

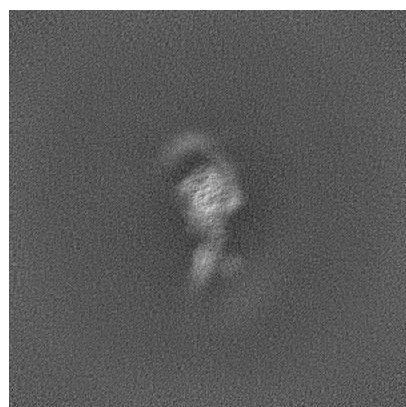


Y

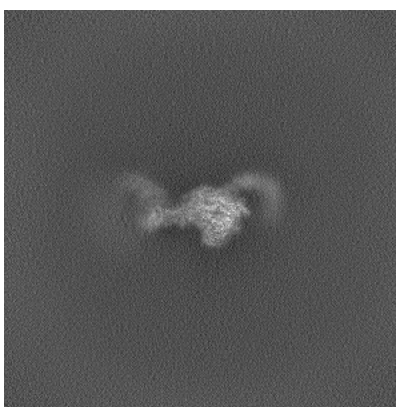


Z

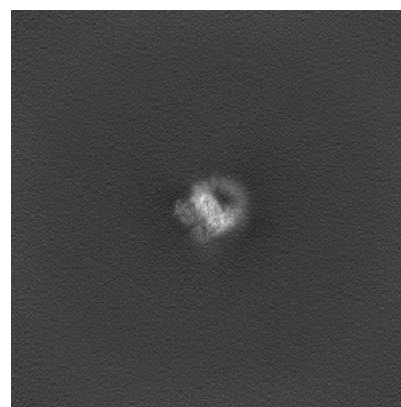
6.1.2 Raw map



X



Y



Z

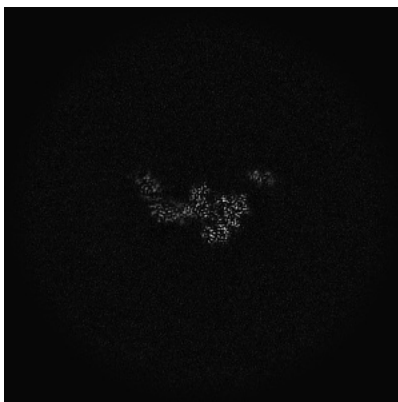
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

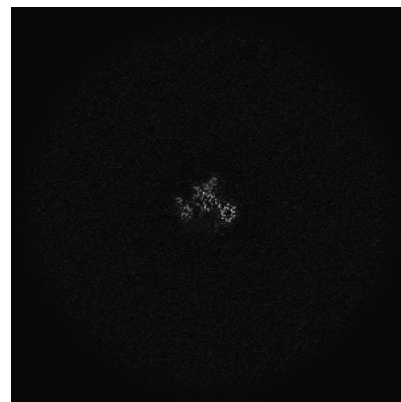
6.2.1 Primary map



X Index: 250



Y Index: 250

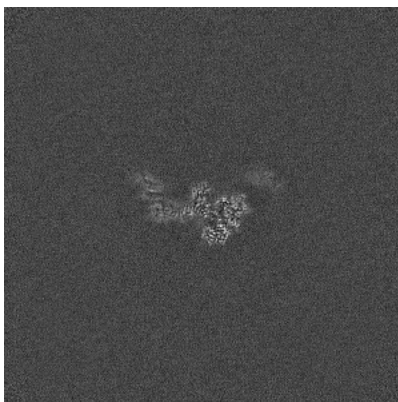


Z Index: 250

6.2.2 Raw map



X Index: 250



Y Index: 250

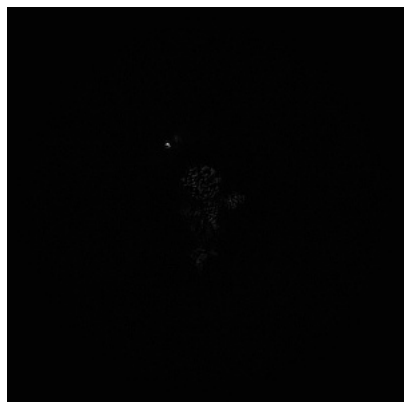


Z Index: 250

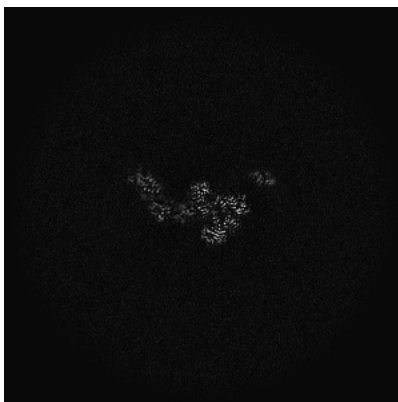
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

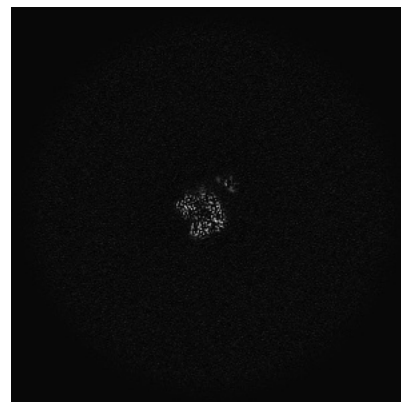
6.3.1 Primary map



X Index: 254

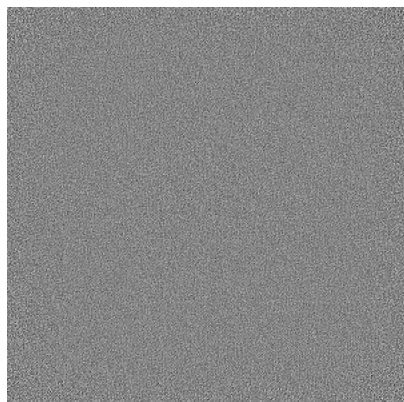


Y Index: 248

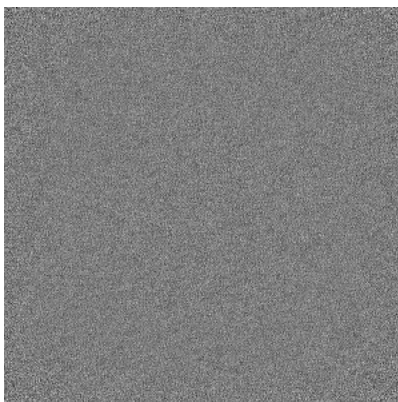


Z Index: 275

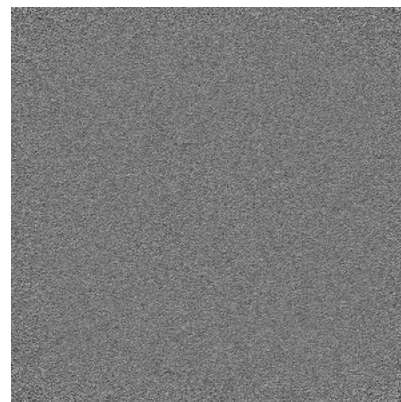
6.3.2 Raw map



X Index: 0



Y Index: 0

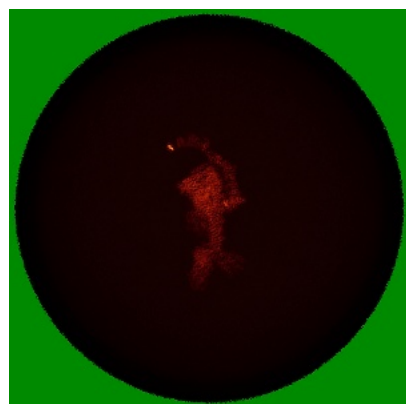


Z Index: 0

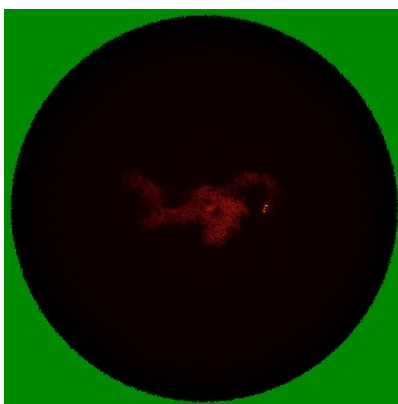
The images above show the largest variance slices of the map in three orthogonal directions.

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

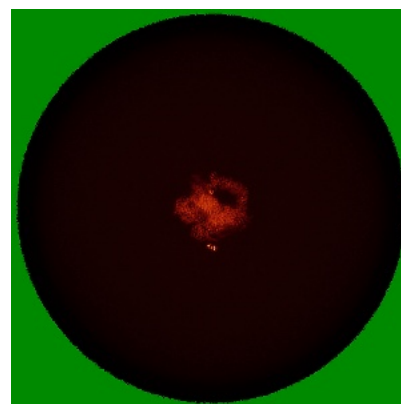
6.4.1 Primary map



X

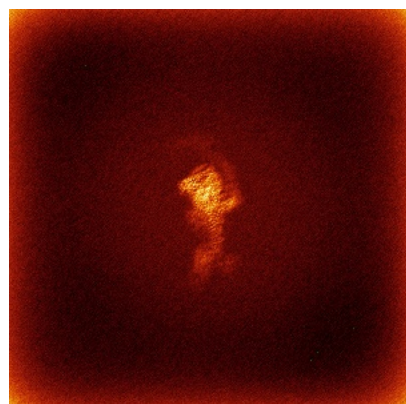


Y

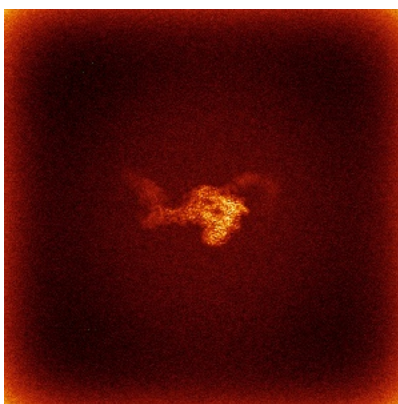


Z

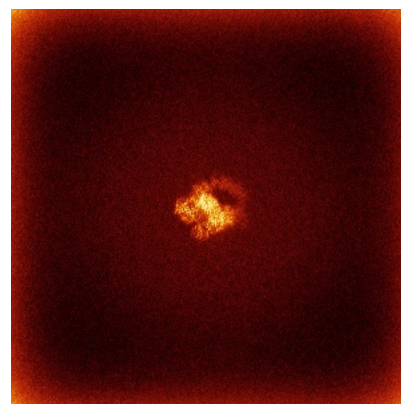
6.4.2 Raw map



X



Y

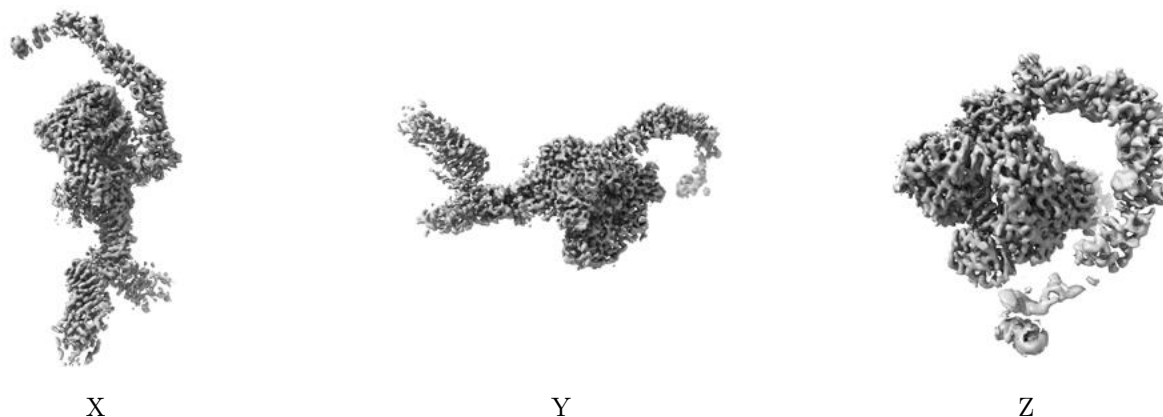


Z

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

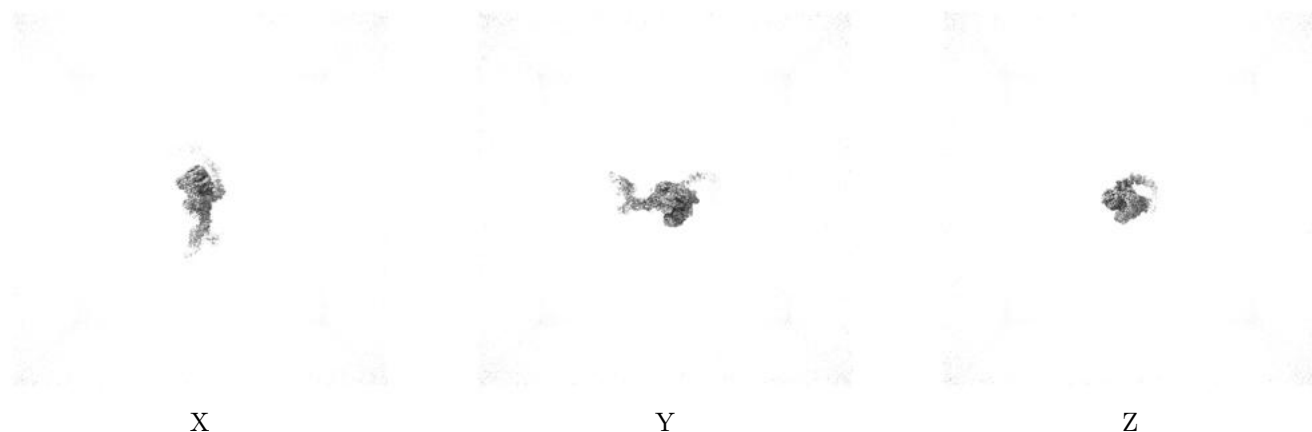
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

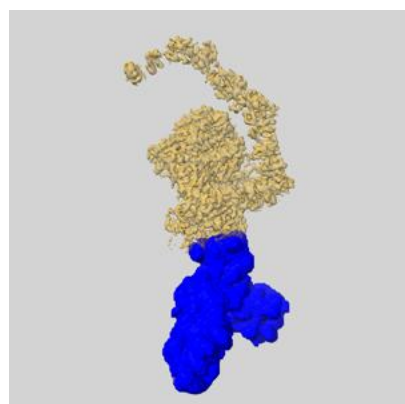
6.6 Mask visualisation [i](#)

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

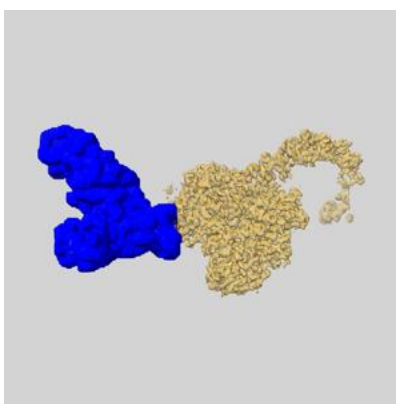
A mask typically either:

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

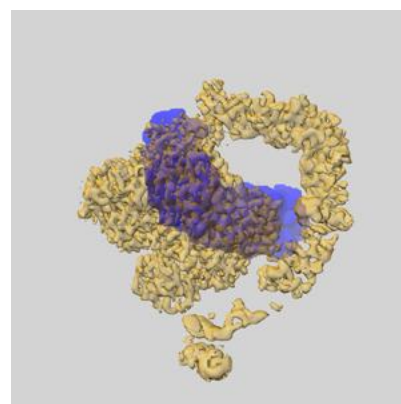
6.6.1 emd_18374_msk_1.map [i](#)



X

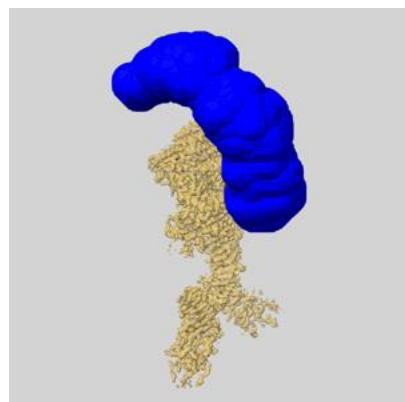


Y

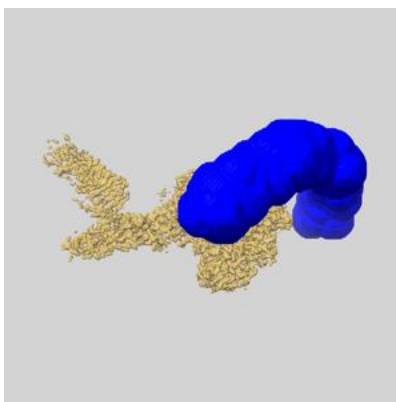


Z

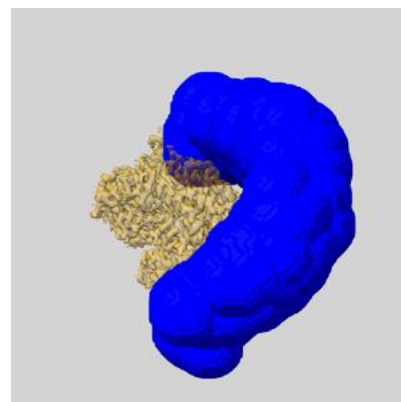
6.6.2 emd_18374_msk_2.map [i](#)



X

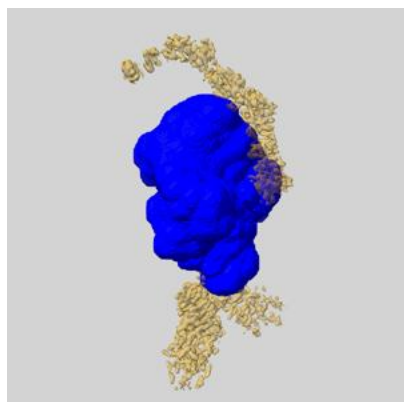


Y

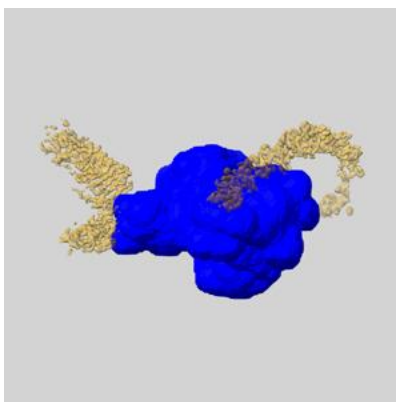


Z

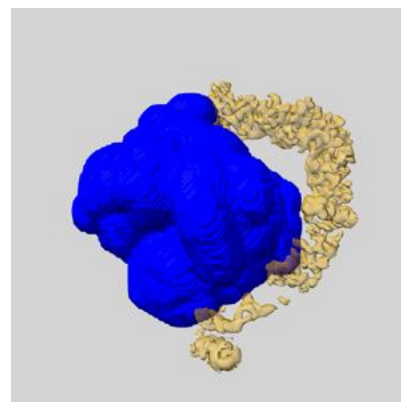
6.6.3 emd_18374_msk_3.map [i](#)



X



Y

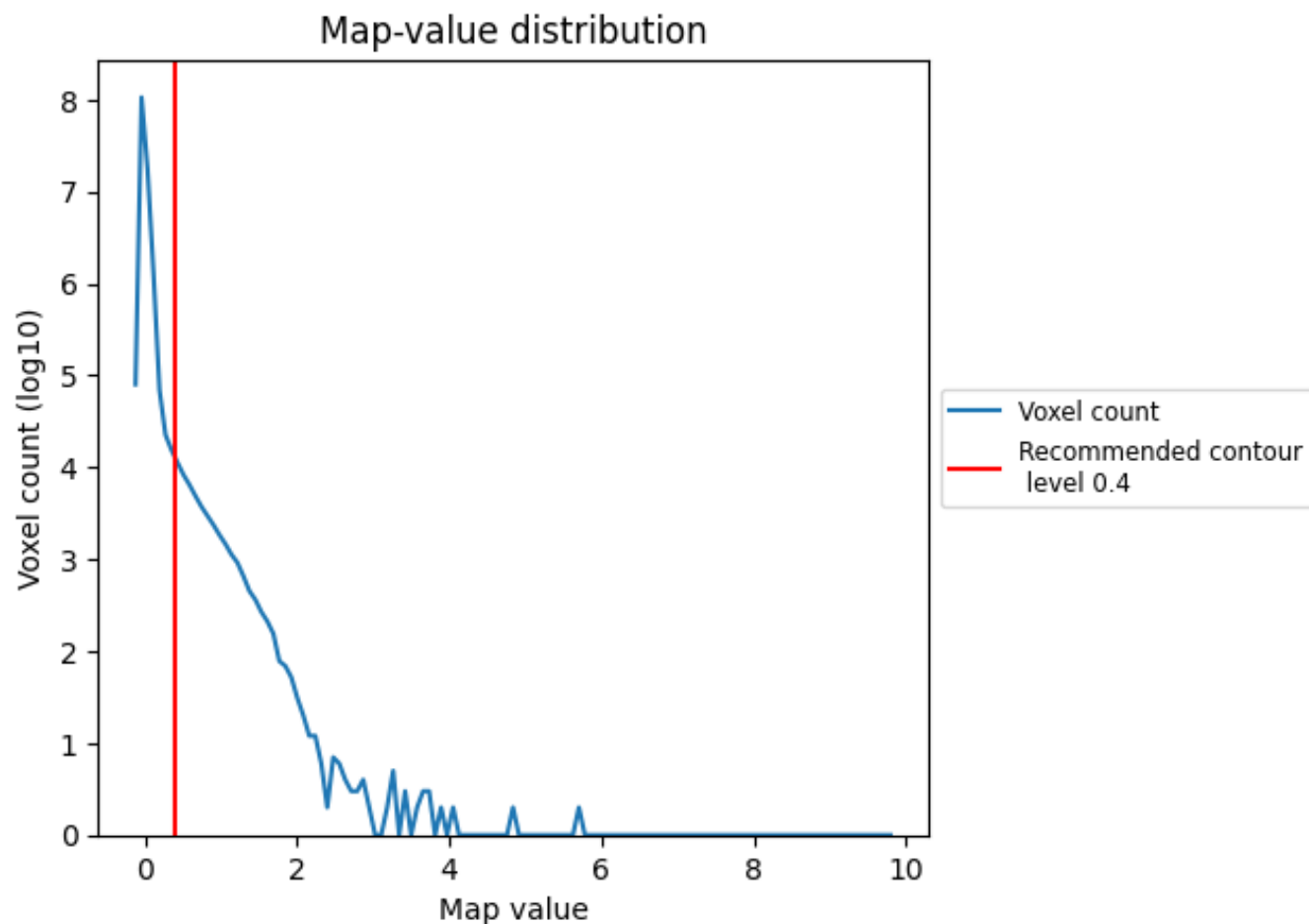


Z

7 Map analysis [i](#)

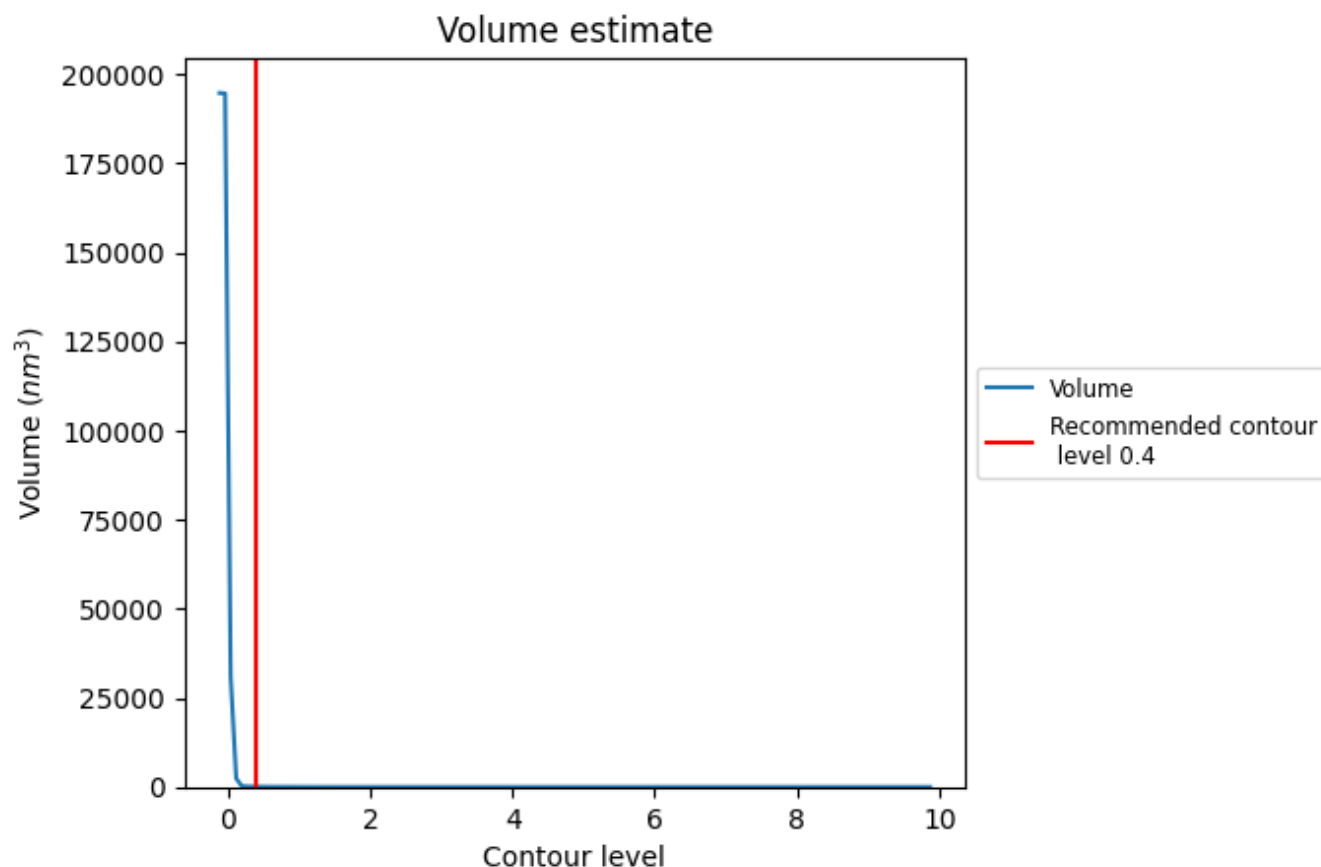
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

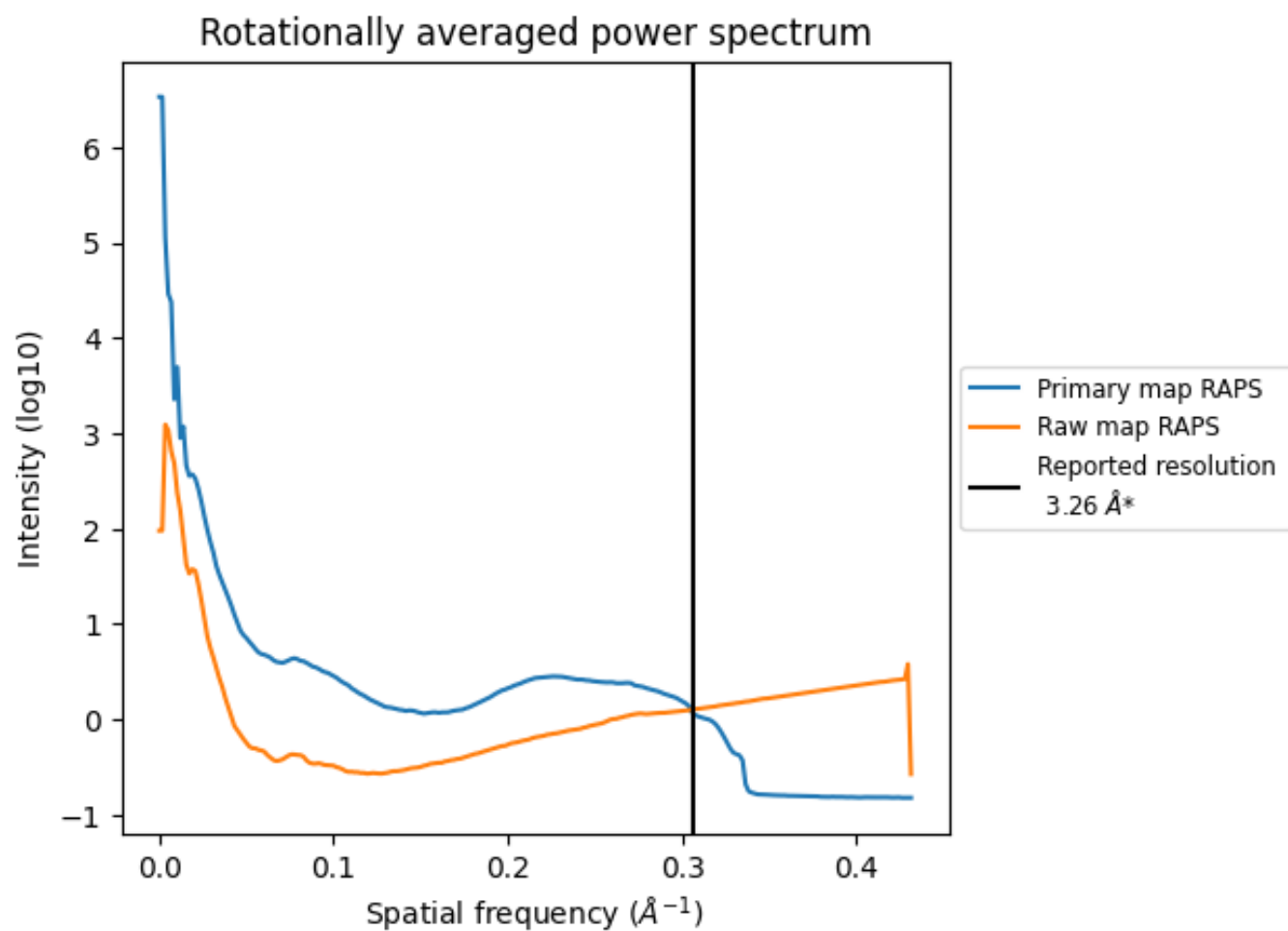
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm^3 ; this corresponds to an approximate mass of 75 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 ⓘ

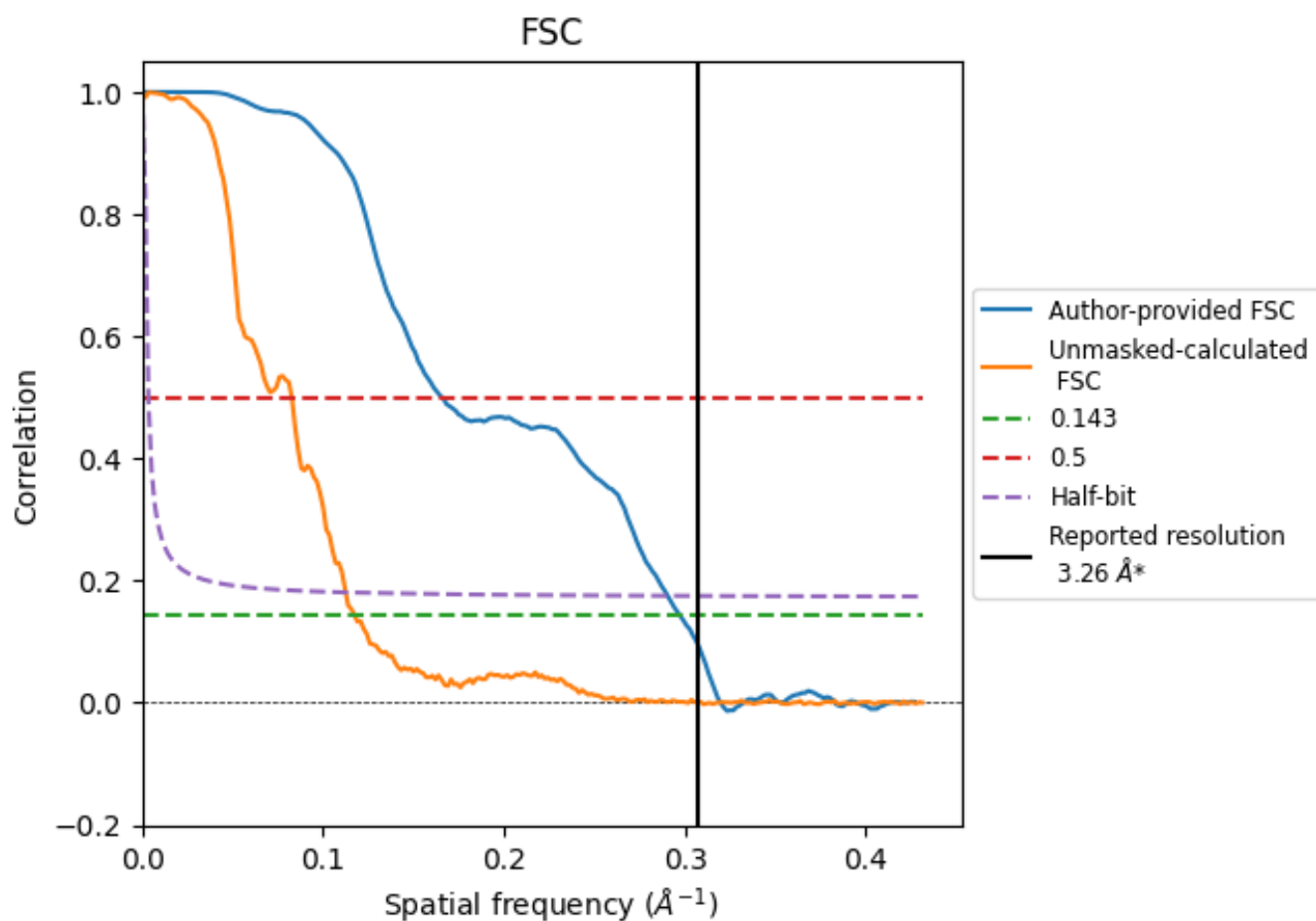


*Reported resolution corresponds to spatial frequency of 0.307 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.307 Å⁻¹

8.2 Resolution estimates [i](#)

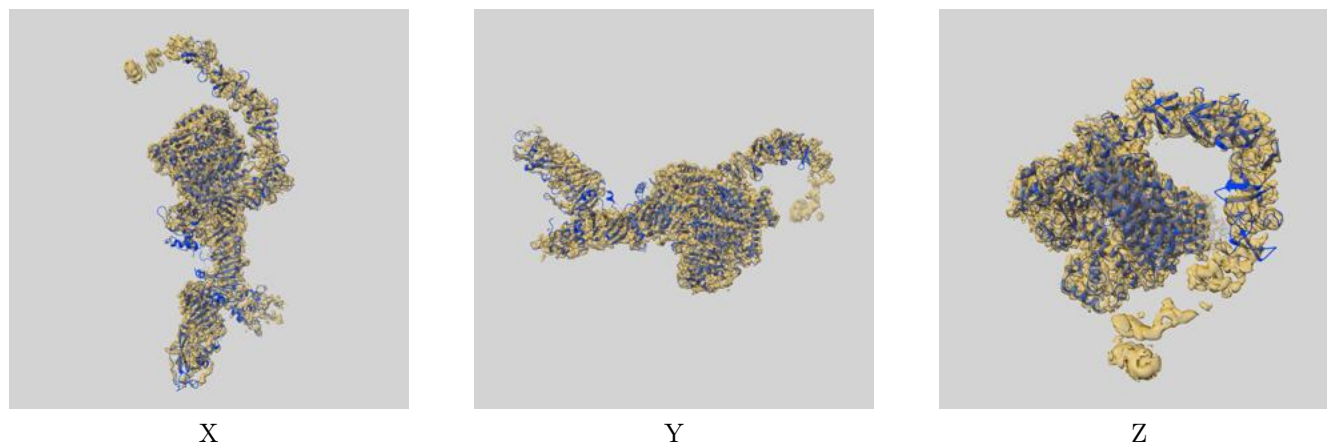
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.36	6.03	3.44
Unmasked-calculated*	8.51	12.09	8.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.51 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

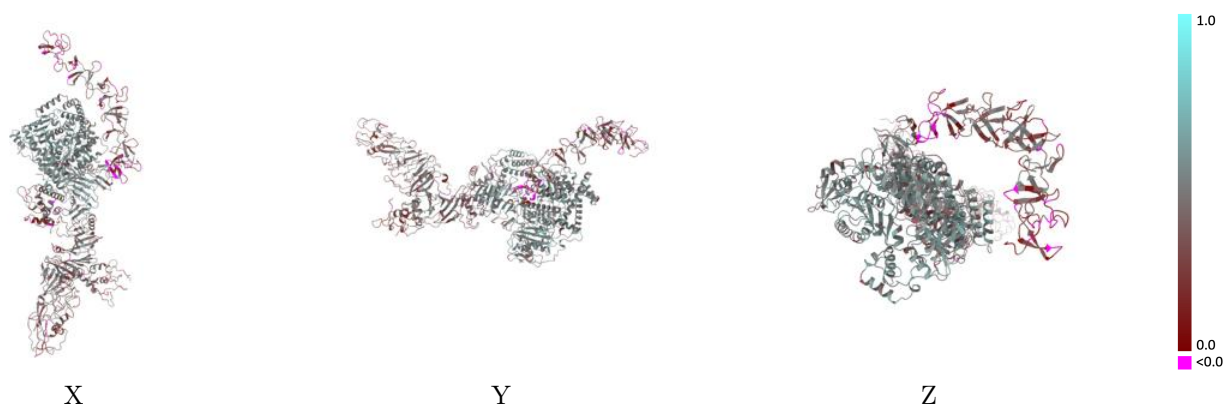
This section contains information regarding the fit between EMDB map EMD-18374 and PDB model 8QEO. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



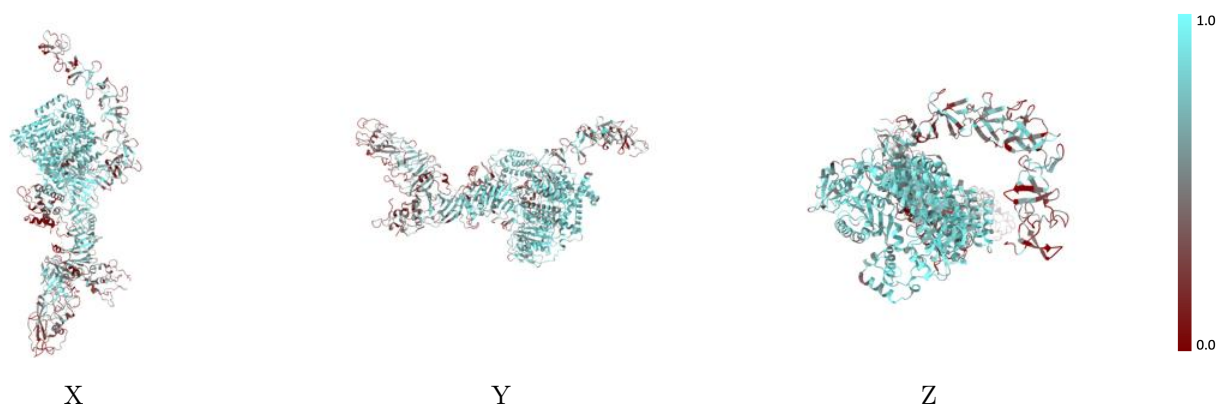
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



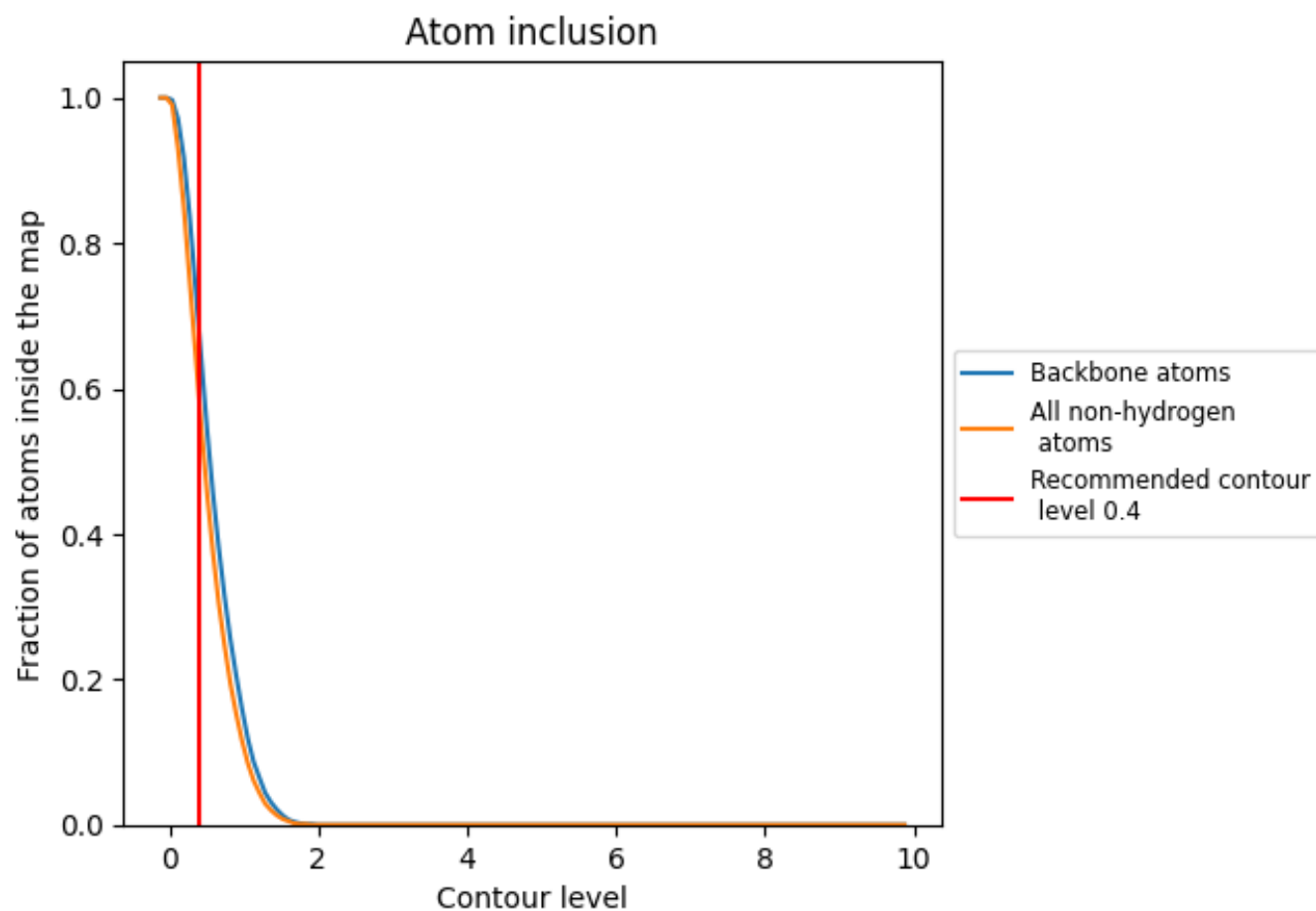
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 58% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5810	0.4160
A	0.5920	0.4200
B	0.3760	0.3350

