



Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 03:16 AM JST

PDB ID : 8WLA / pdb_00008wla
EMDB ID : EMD-37614
Title : Cryo-EM structure of the beta-1,3-glucan synthase FKS1-Rho1 complex
Authors : Li, J.L.; Zhu, A.Q.; Liu, J.X.; Dai, X.L.; Yan, C.Y.; Deng, D.; Wang, X.
Deposited on : 2023-09-29
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

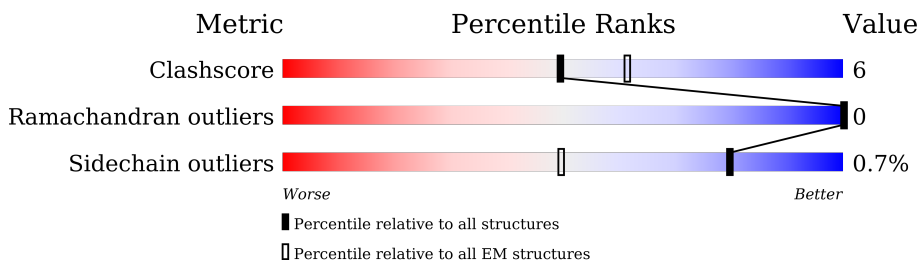
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	209	<div> <div>62%</div> <div>78% 5% • 15%</div> </div>
2	B	1876	<div> <div>51%</div> <div>72% 8% 20%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13360 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 GTP-binding protein RHO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	178	Total	C	N	O	S	0	0
			1383	873	234	269	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	HIS	GLN	engineered mutation	UNP P06780

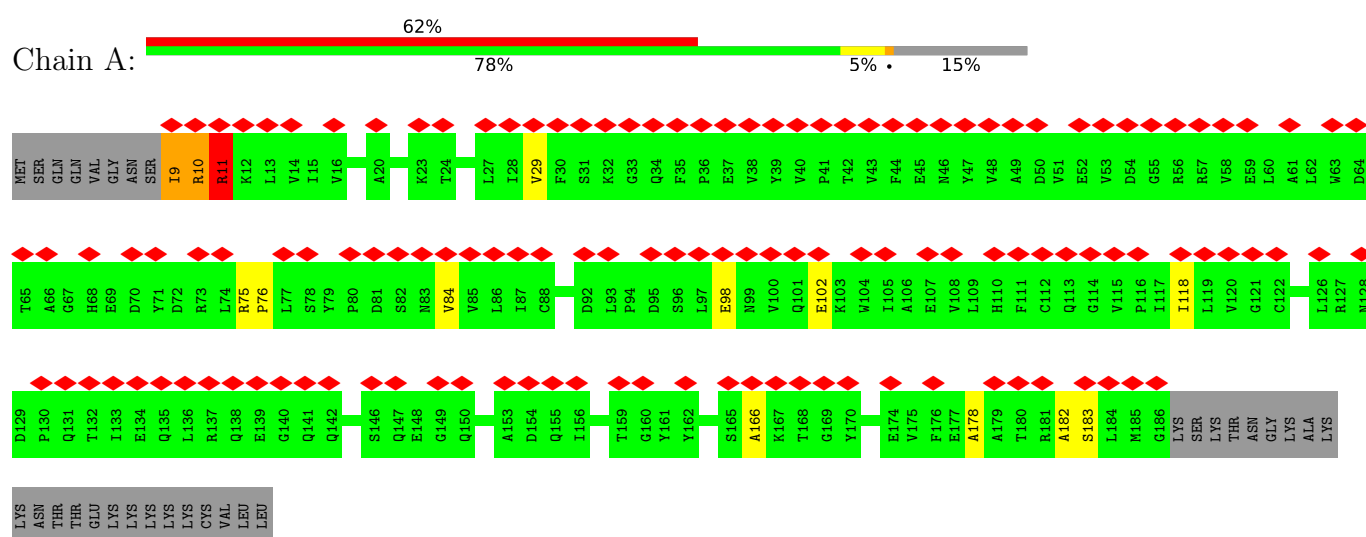
- Molecule 2 is a protein called 1,3-beta-glucan synthase component FKS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1492	Total	C	N	O	S	0	0
			11977	7799	2015	2090	73		

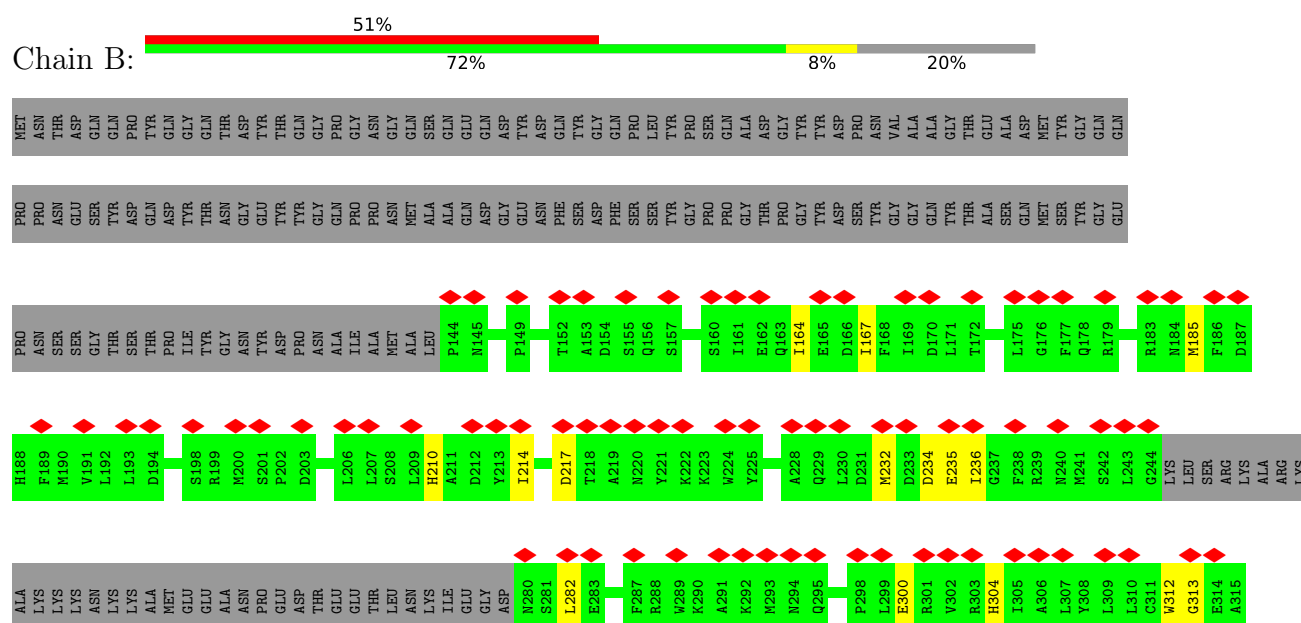
3 Residue-property plots

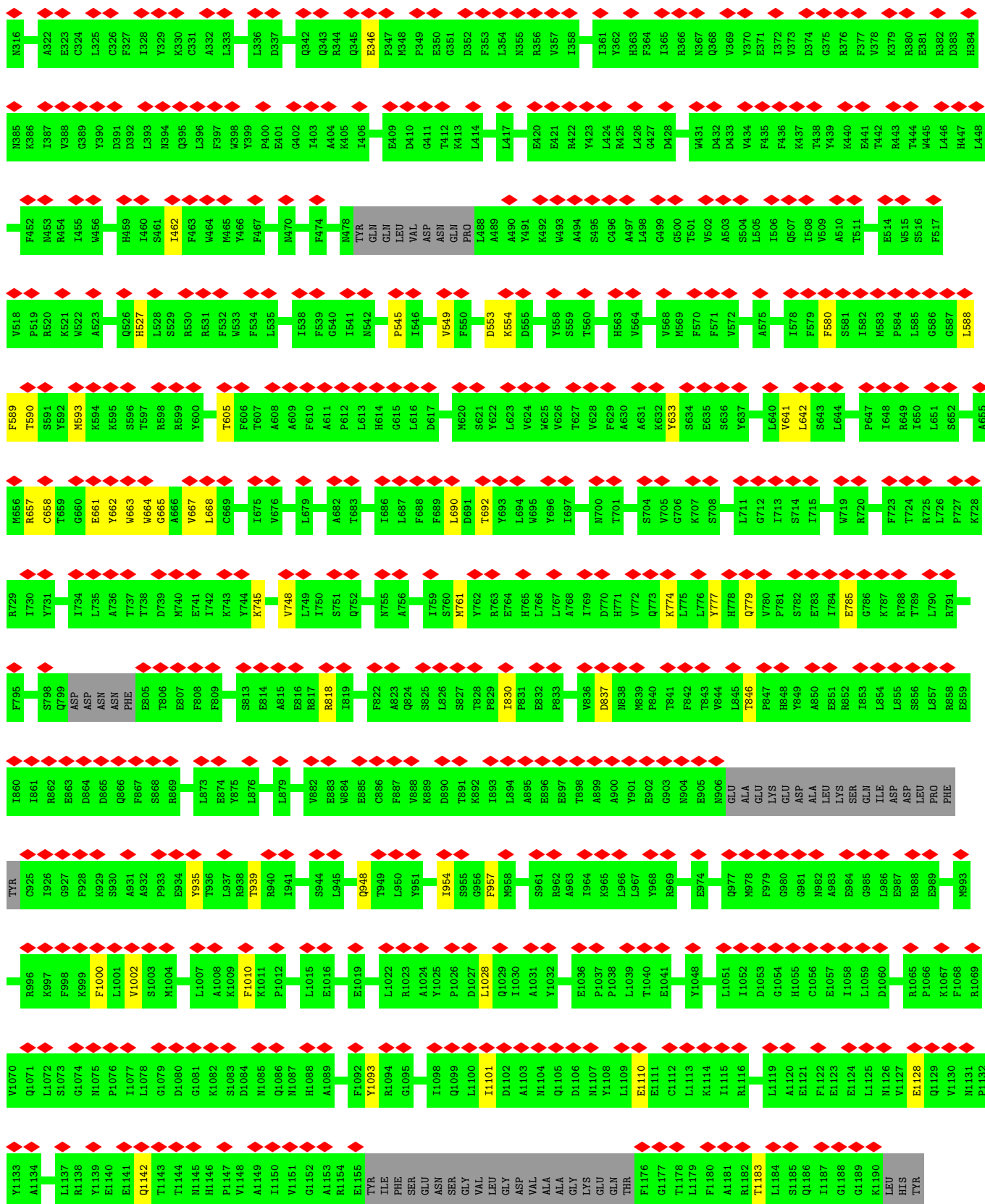
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: GTP-binding protein RHO1



• Molecule 2: 1,3-beta-glucan synthase component FKS1





K1827	H1828	I1829	G1830	D1831	K1765	F1766	H1767	S1768	L1771	F1772	W1773	L1774	K1775	P1776	S1777	I1778	Q1779	I1780	R1781	P1782	P1783	I1784	Y1785	S1786	L1787	K1788	Q1789	T1790	A1791	R1792	L1793	K1794	R1795	M1796	V1797	K1798	K1799	Y1800	C1801	S1802	L1803	Y1804	F1805	L1806	V1807	L1808	A1809	I1810	F1811	A1812	I1815	I1816	G1817	P1818	A1819	V1820		
PHE	LYS	ASN	ASP	HIS	ALA	ASN	THR	ALA	PHE	TRP	THR	GLY	LYS	TRP	GLY	MET	GLY	TYR	MET	ALA	TRP	T1724	Q1725	P1726	S1727	R1728	E1729	L1730	T1731	A1732	K1733	V1734	I1735	E1736	L1737	S1738	E1739	F1740	A1741	A1742	D1743	F1744	V1745	L1746	G1747	I1750	L1751	I1752	C1753	Q1754	L1755	P1756	L1757	I1758	I1759			
I1760	P1761	K1762	I1763	D1764	K1765	F1766	H1767	S1768	L1771	F1772	W1773	L1774	K1775	P1776	S1777	I1778	Q1779	I1780	R1781	P1782	P1783	I1784	Y1785	S1786	L1787	K1788	Q1789	T1790	A1791	R1792	L1793	K1794	R1795	M1796	V1797	K1798	K1799	Y1800	C1801	S1802	L1803	Y1804	F1805	L1806	V1807	L1808	A1809	I1810	F1811	A1812	I1815	I1816	G1817	P1818	A1819	V1820		
GLY	S1640	V1641	M1642	A1643	G1644	I1645	A1646	H1647	G1648	V1649	A1650	V1651	I1652	V1653	H1654	I1655	F1657	F1658	I1659	V1660	M1661	W1662	V1663	L1664	E1665	S1666	F1667	N1668	F1669	V1670	R1671	I1672	L1673	I1674	G1675	V1676	V1677	T1678	C1679	I1680	Q1681	C1682	Q1683	R1684	L1685	I1686	F1687	H1688	C1689	M1690	T1691	A1692	L1693	M1694	L1695	T1696	ARG	GLU
F1576	I1577	A1578	F1579	T1580	F1581	I1582	N1583	A1584	Q1585	T1586	G1587	V1588	K1589	T1590	T1591	D1592	R1595	W1596	M1597	S1598	V1599	L1600	R1601	I1602	I1603	I1604	C1605	T1606	L1607	A1608	P1609	I1610	A1611	V1612	N1613	L1614	G1615	V1616	L1617	F1618	M1621	G1622	C1625	C1626	S1627	G1628	P1629	LEU	PHE	GLY	MET	CYS	CYS	LYS	LYS	THR		
Q1516	Y1517	H1518	R1519	M1520	S1521	W1522	I1523	G1524	Y1525	Y1526	R1527	M1528	S1529	R1530	A1531	R1532	I1533	T1534	GLY	PHE	LYS	ARG	LYS	VAL	GLY	ASP	GLU	SER	GLU	LYS	ALA	ALA	GLY	ASP	ALA	SER	ARG	A1555	H1556	R1557	T1558	N1559	L1560	I1561	M1562	A1563	E1564	I1565	T1566	P1567	C1568	A1569	I1570	Y1571	A1572	G1574	C1575	
S1448	A1449	M1452	G1453	A1454	R1455	S1456	M1457	L1458	M1459	L1460	L1461	F1462	G1463	H1467	A1470	L1473	W1474	F1475	W1476	A1477	S1478	L1479	S1480	S1481	L1482	A1485	P1486	F1487	V1488	F1489	N1490	P1491	H1492	Q1493	F1494	A1495	W1496	E1497	D1498	F1499	F1500	L1501	L1502	Y1503	R1504	D1505	Y1506	I1507	R1508	W1509	R1512	N1515						
GLN	ARG	PHE	CYS	HIS	LEU	SER	LEU	SER	PRO	MET	PHE	GLU	VAL	PHE	ALA	GLY	GLN	ILE	TYR	SER	ALA	LEU	SER	ASP	LEU	LEU	LEU	ASP	GLY	GLY	ALA	ARG	TYR	ILE	SER	THR	GLY	GLY	GLY	PHE	ALA	ARG	I1436	F1437	F1438	S1439	I1440	L1441	Y1442	S1443	F1444	F1445	A1446	G1447				
L1318	A1322	H1323	E1324	S1325	I1326	M1327	C1328	I1329	Y1330	D1331	R1332	N1333	K1334	P1335	K1336	V1339	L1340	Y1341	P1342	Y1346	M1347	F1348	Q1349	P1350	A1351	V1352	R1356	R1357	L1360	I1364	V1365	F1366	W1367	I1368	A1369	F1370	V1371	P1372	I1373	V1374	V1375	Q1376	E1377	L1378	I1379	E1380	R1381	G1382	L1383	LYS	ALA	THR						
ILE	LEU	ASN	PHE	THR	THR	LYS	ILE	GLY	ALA	MET	G1267	E1268	Q1269	M1270	L1271	S1272	R1273	E1274	Y1275	Y1276	Y1277	L1278	L1282	P1283	Y1284	D1285	R1286	F1287	L1288	T1289	F1290	Y1291	Y1292	A1293	H1294	P1295	G1296	F1297	H1298	L1299	N1300	N1301	K1302	F1303	I1304	Q1305	L1306	S1307	L1308	Q1309	M1310	F1311	M1312	L1315	V1316	N1317		
GLY	H1195	P1196	D1197	F1198	I1199	N1200	A1201	T1202	F1203	M1204	T1205	T1206	R1207	G1208	G1209	V1210	S1211	K1212	A1213	Q1214	K1215	GLY	LEU	HIS	LEU	ASN	E1221	D1222	A1225	G1226	M1227	N1228	A1229	M1230	L1231	R1232	G1233	G1234	R1235	I1236	K1237	H1238	C1239	E1240	I1241	Y1242	Q1243	C1244	G1245	K1246	G1247	ARG	ASP	LEU	GLY	PHE	GLY	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93892	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.961	Depositor
Minimum map value	-1.330	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.229	Depositor
Map size (\AA)	278.272, 278.272, 278.272	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.16	0/1409	0.27	0/1916
2	B	0.15	0/12295	0.32	0/16696
All	All	0.15	0/13704	0.32	0/18612

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ARG	Sidechain
1	A	11	ARG	Sidechain

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	1383	0	1351	9	0
2	B	11977	0	11777	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13360	0	13128	146	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 (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:662:TYR:CD2	2:B:663:TRP:CD1	2.34	1.14
2:B:1590:THR:CB	2:B:1858:TYR:OH	1.95	1.13
2:B:662:TYR:CD2	2:B:663:TRP:HD1	1.67	1.12
2:B:662:TYR:CE2	2:B:663:TRP:CD1	2.44	1.04
2:B:957:PHE:CE2	2:B:1101:ILE:HD13	1.92	1.04
2:B:957:PHE:CE2	2:B:1101:ILE:CD1	2.43	1.01
2:B:1000:PHE:HE1	2:B:1002:VAL:CG2	1.73	1.00
2:B:662:TYR:CE2	2:B:663:TRP:HD1	1.82	0.92
2:B:1000:PHE:CE1	2:B:1002:VAL:HG23	2.07	0.89
2:B:1000:PHE:CE1	2:B:1002:VAL:CG2	2.55	0.89
2:B:1668:ASN:HD22	2:B:1671:ARG:HG3	1.39	0.88
2:B:1657:PHE:HA	2:B:1660:VAL:HG12	1.54	0.86
2:B:1590:THR:CB	2:B:1858:TYR:HH	1.90	0.85
2:B:1653:VAL:CG1	2:B:1657:PHE:CE2	2.63	0.81
1:A:98:GLU:O	1:A:102:GLU:HG3	1.83	0.79
2:B:1668:ASN:ND2	2:B:1671:ARG:HG3	1.97	0.77
2:B:1657:PHE:O	2:B:1660:VAL:HG12	1.86	0.76
2:B:662:TYR:HD2	2:B:663:TRP:CD1	1.97	0.76
2:B:1641:VAL:O	2:B:1645:ILE:HG13	1.87	0.74
2:B:1499:PHE:CZ	2:B:1751:LEU:HD22	2.26	0.71
2:B:1653:VAL:HG12	2:B:1657:PHE:CE2	2.26	0.71
2:B:1657:PHE:CA	2:B:1660:VAL:HG12	2.21	0.70
2:B:948:GLN:N	2:B:948:GLN:OE1	2.25	0.70
2:B:957:PHE:CZ	2:B:1101:ILE:HD13	2.27	0.69
2:B:1596:VAL:CG1	2:B:1601:ARG:HH22	2.07	0.68
2:B:957:PHE:HE2	2:B:1101:ILE:CD1	2.07	0.66
2:B:1183:THR:HB	2:B:1375:VAL:HG21	1.78	0.66
2:B:1653:VAL:CG1	2:B:1657:PHE:HE2	2.06	0.66
2:B:1657:PHE:HA	2:B:1660:VAL:CG1	2.23	0.65
2:B:1596:VAL:CG1	2:B:1601:ARG:NH2	2.59	0.65
2:B:1000:PHE:HE1	2:B:1002:VAL:HG23	1.44	0.64
2:B:1657:PHE:C	2:B:1660:VAL:HG12	2.22	0.63
2:B:1367:TRP:O	2:B:1371:VAL:HG13	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:588:LEU:HD23	2:B:589:PHE:CE2	2.35	0.61
2:B:957:PHE:HE2	2:B:1101:ILE:HD12	1.63	0.61
2:B:957:PHE:CE2	2:B:1101:ILE:HD12	2.31	0.61
2:B:935:TYR:O	2:B:939:THR:HG23	2.01	0.61
2:B:1653:VAL:HG13	2:B:1657:PHE:CE2	2.35	0.61
2:B:346:GLU:N	2:B:346:GLU:OE1	2.35	0.60
2:B:777:TYR:O	2:B:779:GLN:NE2	2.34	0.60
2:B:1612:VAL:HG11	2:B:1653:VAL:HG21	1.84	0.60
2:B:1608:ALA:HB1	2:B:1657:PHE:CZ	2.38	0.58
2:B:210:HIS:CE1	2:B:214:ILE:HD11	2.40	0.57
2:B:664:TRP:HE1	2:B:668:LEU:HD12	1.70	0.57
2:B:846:THR:HB	2:B:1002:VAL:HG22	1.85	0.57
2:B:1651:VAL:HG22	2:B:1741:ALA:HA	1.85	0.56
2:B:837:ASP:N	2:B:837:ASP:OD1	2.38	0.56
2:B:1664:LEU:HD22	2:B:1840:LEU:HD23	1.87	0.56
2:B:1855:MET:SD	2:B:1855:MET:N	2.79	0.56
2:B:1843:PRO:HB2	2:B:1846:THR:CG2	2.36	0.55
2:B:234:ASP:OD1	2:B:235:GLU:N	2.39	0.55
2:B:662:TYR:CE2	2:B:663:TRP:NE1	2.73	0.55
2:B:662:TYR:HE2	2:B:663:TRP:CD1	2.17	0.54
2:B:1668:ASN:HD22	2:B:1671:ARG:CG	2.15	0.54
1:A:98:GLU:HG2	1:A:102:GLU:OE2	2.08	0.54
2:B:1657:PHE:O	2:B:1660:VAL:CG1	2.53	0.54
2:B:1294:HIS:HB2	2:B:1295:PRO:HD3	1.90	0.54
2:B:300:GLU:O	2:B:304:HIS:ND1	2.41	0.54
2:B:1858:TYR:O	2:B:1858:TYR:CG	2.60	0.54
2:B:1128:GLU:N	2:B:1128:GLU:OE1	2.38	0.54
2:B:1843:PRO:HB2	2:B:1846:THR:HG23	1.90	0.53
2:B:761:MET:HE1	2:B:818:ARG:HE	1.72	0.53
2:B:1495:ALA:HB3	2:B:1498:ASP:HB3	1.91	0.52
2:B:1503:TYR:CD1	2:B:1751:LEU:HD13	2.44	0.52
2:B:663:TRP:HB2	2:B:664:TRP:CE3	2.45	0.52
2:B:1341:VAL:HB	2:B:1342:PRO:HD3	1.92	0.52
2:B:657:ARG:O	2:B:1586:THR:HA	2.12	0.50
2:B:664:TRP:HB2	2:B:667:VAL:HG22	1.94	0.49
2:B:1596:VAL:HG11	2:B:1601:ARG:HH22	1.78	0.49
2:B:662:TYR:HE2	2:B:663:TRP:NE1	2.10	0.49
2:B:657:ARG:O	2:B:1586:THR:O	2.29	0.49
2:B:1590:THR:N	2:B:1858:TYR:OH	2.46	0.49
2:B:745:LYS:O	2:B:748:VAL:HG12	2.13	0.49
2:B:1503:TYR:CD1	2:B:1751:LEU:CD1	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1448:SER:O	2:B:1449:ALA:HB3	2.12	0.49
2:B:1727:SER:O	2:B:1731:THR:HG23	2.12	0.49
2:B:1649:VAL:O	2:B:1653:VAL:HG23	2.13	0.48
2:B:545:PRO:O	2:B:549:VAL:HG23	2.14	0.48
2:B:553:ASP:OD1	2:B:554:LYS:N	2.47	0.48
2:B:1664:LEU:CD2	2:B:1840:LEU:HD23	2.45	0.47
2:B:1733:LYS:O	2:B:1737:LEU:HG	2.14	0.47
2:B:236:ILE:HD13	2:B:605:THR:HG22	1.96	0.47
2:B:185:MET:HE3	2:B:313:GLY:HA3	1.97	0.47
2:B:527:HIS:CD2	2:B:593:MET:HE1	2.50	0.47
2:B:232:MET:HE3	2:B:282:LEU:HA	1.97	0.47
2:B:1673:LEU:O	2:B:1676:VAL:HG12	2.16	0.46
2:B:1000:PHE:HE1	2:B:1002:VAL:HG21	1.68	0.46
2:B:664:TRP:HB2	2:B:667:VAL:CG2	2.45	0.46
2:B:1371:VAL:O	2:B:1375:VAL:HG23	2.16	0.46
2:B:1845:ASN:C	2:B:1846:THR:HG23	2.41	0.46
1:A:29:VAL:HG11	1:A:166:ALA:O	2.16	0.46
2:B:692:THR:HG21	2:B:1292:TYR:OH	2.15	0.46
2:B:1665:GLU:HG3	2:B:1672:MET:CA	2.46	0.45
1:A:75:ARG:N	1:A:76:PRO:HD2	2.32	0.45
2:B:1595:ARG:O	2:B:1837:VAL:HG23	2.16	0.45
2:B:1371:VAL:N	2:B:1372:PRO:HD2	2.32	0.45
2:B:1659:ILE:O	2:B:1663:VAL:HG23	2.17	0.45
1:A:9:ILE:HB	1:A:11:ARG:HH11	1.81	0.44
2:B:830:ILE:HG22	2:B:1241:TYR:CD1	2.53	0.44
2:B:185:MET:HE1	2:B:312:TRP:CZ3	2.52	0.44
2:B:185:MET:HE1	2:B:312:TRP:HZ3	1.82	0.44
2:B:1858:TYR:O	2:B:1858:TYR:CD2	2.70	0.44
1:A:178:ALA:O	1:A:182:ALA:N	2.50	0.44
2:B:462:ILE:HG21	2:B:633:TYR:CE1	2.53	0.43
2:B:664:TRP:CD1	2:B:664:TRP:O	2.71	0.43
1:A:84:VAL:HG23	1:A:118:ILE:HB	2.00	0.43
2:B:1371:VAL:HG22	2:B:1372:PRO:HD3	2.00	0.43
2:B:1641:VAL:O	2:B:1645:ILE:CG1	2.64	0.43
2:B:690:LEU:HD23	2:B:1365:VAL:HG11	2.01	0.43
2:B:217:ASP:OD2	2:B:1142:GLN:NE2	2.49	0.43
2:B:1653:VAL:HG12	2:B:1657:PHE:CD2	2.54	0.43
2:B:185:MET:HE3	2:B:313:GLY:CA	2.49	0.43
2:B:590:THR:HA	2:B:593:MET:HE3	2.00	0.43
2:B:1522:TRP:CZ2	2:B:1526:VAL:HG11	2.54	0.42
2:B:527:HIS:HD2	2:B:593:MET:HE1	1.85	0.42

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:785:GLU:N	2:B:785:GLU:OE1	2.52	0.42
2:B:657:ARG:HD2	2:B:1858:TYR:CD1	2.54	0.42
2:B:1725:GLN:N	2:B:1726:PRO:HD2	2.34	0.42
1:A:75:ARG:N	1:A:76:PRO:CD	2.83	0.42
2:B:1329:ILE:HG22	2:B:1330:TYR:N	2.34	0.42
2:B:1349:GLN:O	2:B:1352:VAL:HG22	2.20	0.42
2:B:1495:ALA:HB3	2:B:1498:ASP:CB	2.49	0.42
2:B:1608:ALA:HB1	2:B:1657:PHE:CE1	2.55	0.42
2:B:774:LYS:N	2:B:774:LYS:HD2	2.35	0.42
2:B:1093:TYR:CD1	2:B:1093:TYR:C	2.98	0.42
2:B:1499:PHE:CG	2:B:1758:ILE:HD11	2.54	0.42
2:B:1817:GLY:N	2:B:1818:PRO:HD2	2.35	0.42
1:A:9:ILE:HD11	1:A:183:SER:HB2	2.02	0.41
2:B:954:ILE:HD12	2:B:1028:LEU:HD11	2.02	0.41
2:B:1596:VAL:HG13	2:B:1601:ARG:NH2	2.35	0.41
2:B:1757:LEU:HD23	2:B:1757:LEU:C	2.45	0.41
2:B:1560:LEU:O	2:B:1563:ALA:HB3	2.20	0.41
2:B:1340:LEU:HD22	2:B:1340:LEU:H	1.85	0.41
2:B:164:ILE:O	2:B:167:ILE:HG22	2.20	0.41
2:B:1294:HIS:HB2	2:B:1295:PRO:CD	2.50	0.41
2:B:1662:TRP:CD1	2:B:1667:PHE:HA	2.55	0.41
2:B:641:VAL:HG13	2:B:642:LEU:N	2.35	0.41
2:B:661:GLU:O	2:B:665:GLY:CA	2.69	0.41
2:B:1334:LYS:HG2	2:B:1335:PRO:HD2	2.02	0.41
2:B:1516:GLN:O	2:B:1518:HIS:CD2	2.74	0.41
2:B:1438:PHE:CD1	2:B:1438:PHE:C	2.99	0.41
2:B:1669:PHE:CE2	2:B:1673:LEU:HD11	2.55	0.41
2:B:1503:TYR:HD1	2:B:1751:LEU:CD1	2.34	0.40
2:B:1672:MET:C	2:B:1672:MET:SD	3.05	0.40
2:B:580:PHE:HE1	2:B:588:LEU:HD21	1.86	0.40
2:B:1690:MET:O	2:B:1694:MET:HG2	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	176/209 (84%)	171 (97%)	5 (3%)	0	100	100
2	B	1466/1876 (78%)	1437 (98%)	29 (2%)	0	100	100
All	All	1642/2085 (79%)	1608 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	151/180 (84%)	148 (98%)	3 (2%)	50	70
2	B	1264/1620 (78%)	1257 (99%)	7 (1%)	84	90
All	All	1415/1800 (79%)	1405 (99%)	10 (1%)	80	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	10	ARG
1	A	11	ARG
2	B	658	CYS
2	B	1010	PHE
2	B	1110	GLU
2	B	1328	CYS
2	B	1346	TYR
2	B	1467	HIS
2	B	1658	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	385	ASN
2	B	604	GLN
2	B	1013	HIS
2	B	1347	ASN
2	B	1518	HIS
2	B	1668	ASN
2	B	1748	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](#)

There are no ligands in this entry.

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.

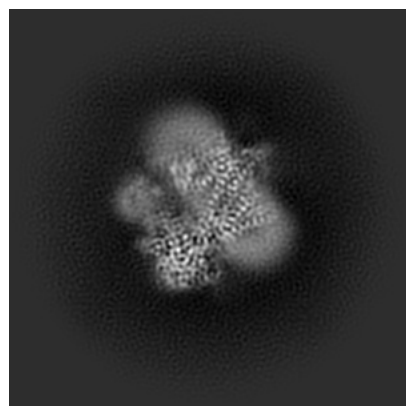
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37614. These allow visual inspection of the internal detail of the map and identification of artifacts.

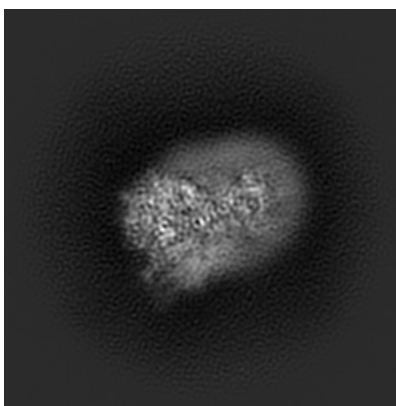
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

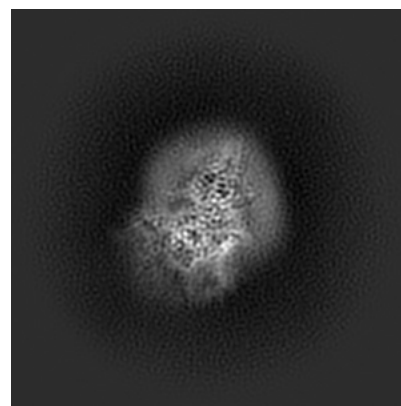
6.1.1 Primary map



X

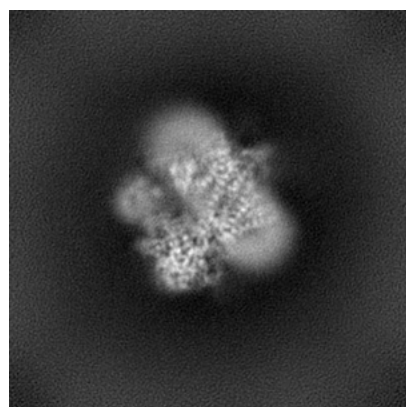


Y

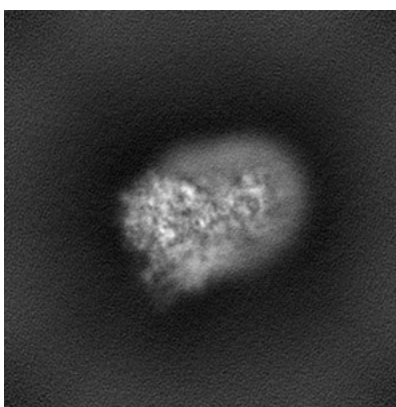


Z

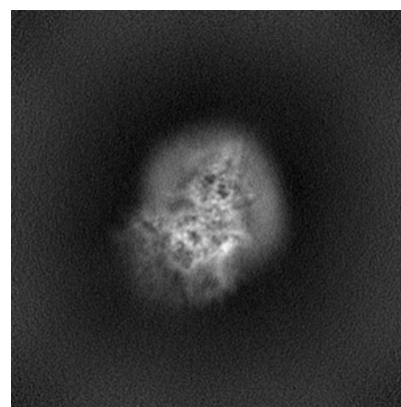
6.1.2 Raw map



X



Y

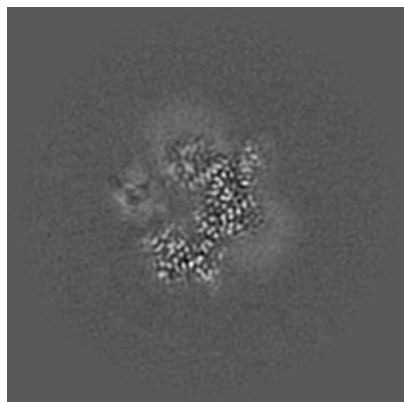


Z

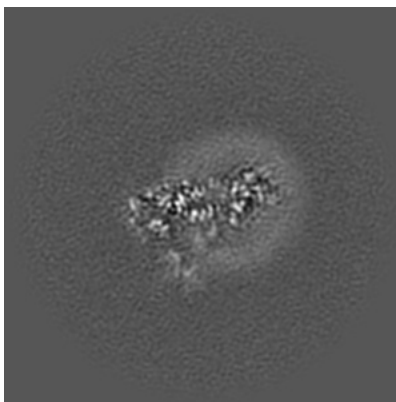
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

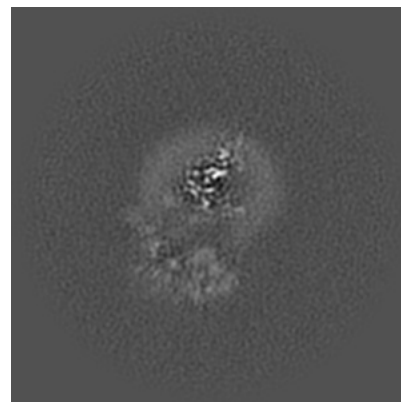
6.2.1 Primary map



X Index: 128

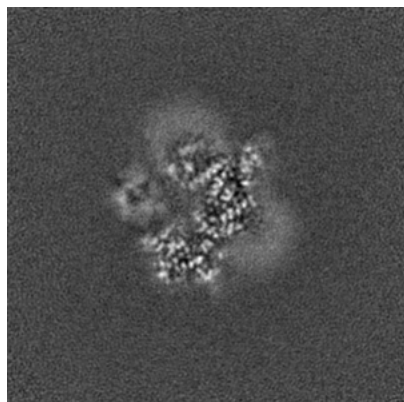


Y Index: 128

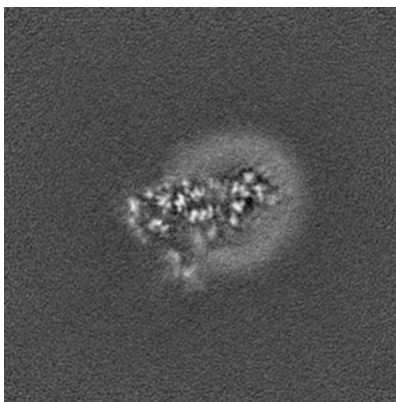


Z Index: 128

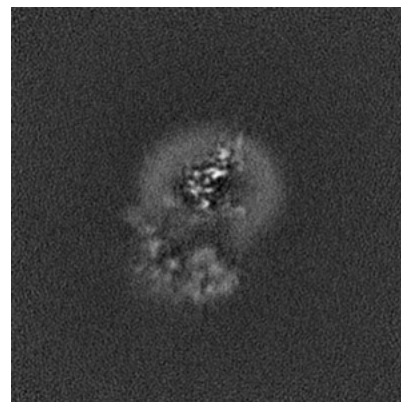
6.2.2 Raw map



X Index: 128



Y Index: 128

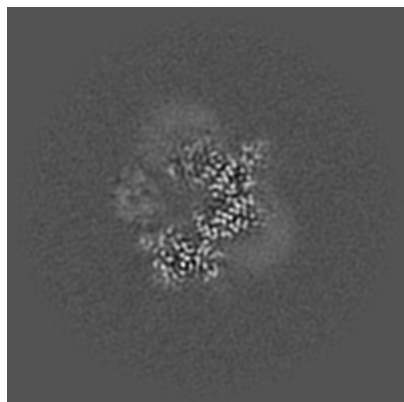


Z Index: 128

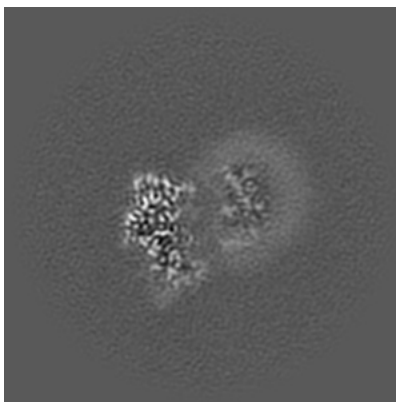
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

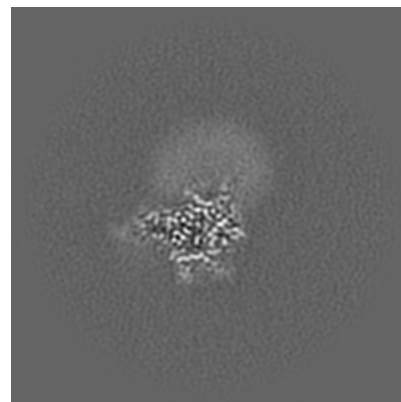
6.3.1 Primary map



X Index: 130

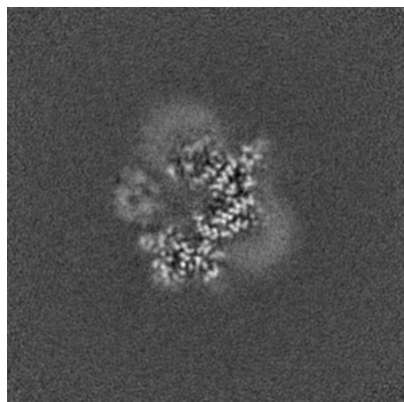


Y Index: 113

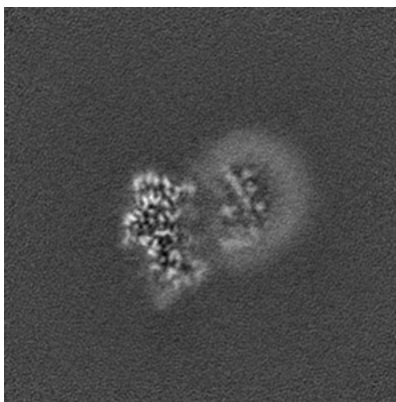


Z Index: 103

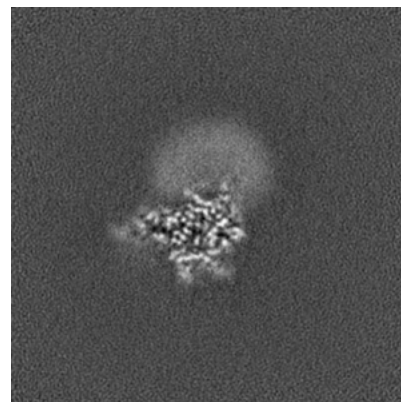
6.3.2 Raw map



X Index: 130



Y Index: 113

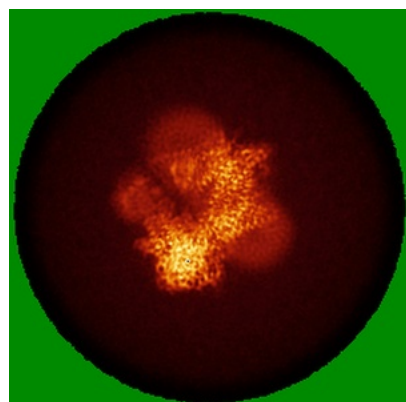


Z Index: 103

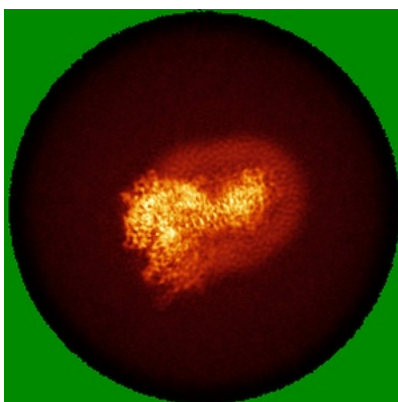
The images above show the largest variance slices of the map in three orthogonal directions.

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

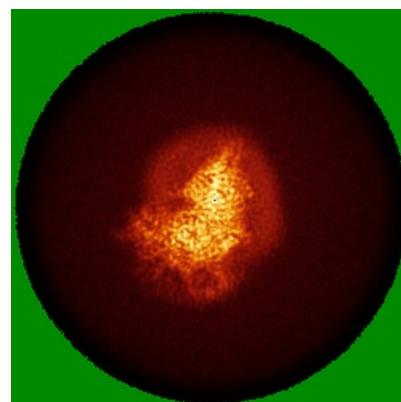
6.4.1 Primary map



X

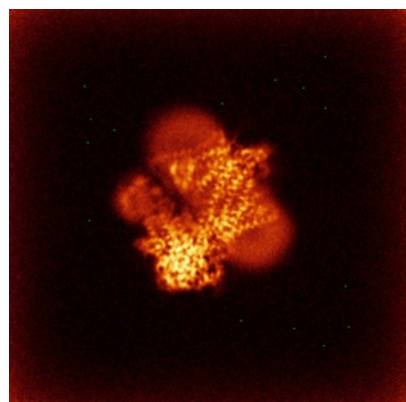


Y



Z

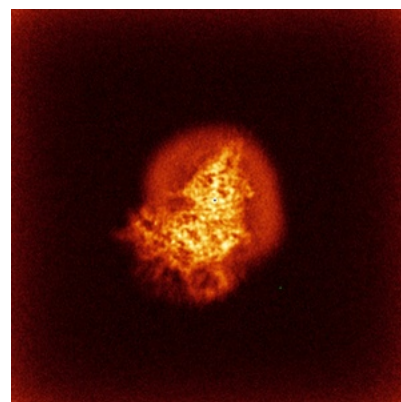
6.4.2 Raw map



X



Y

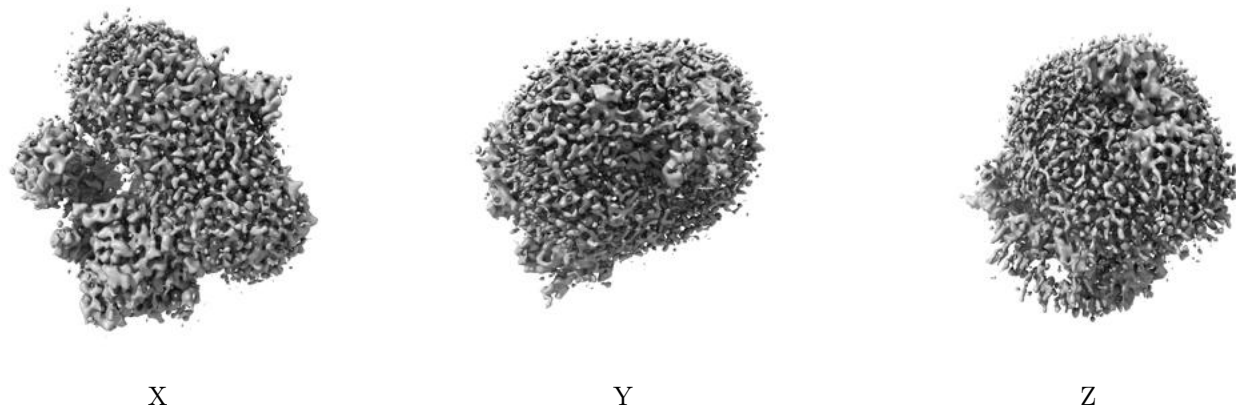


Z

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.

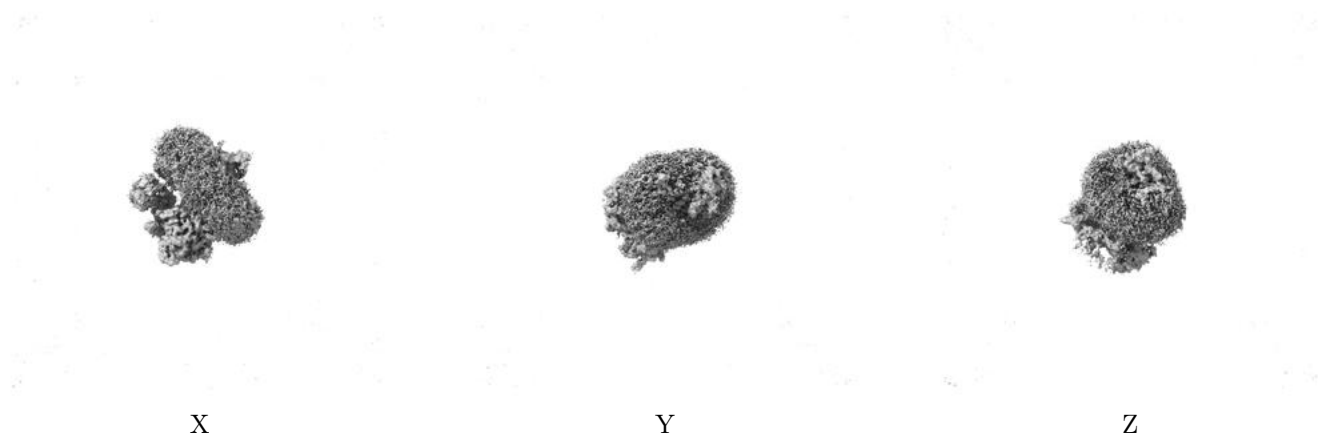
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.229. 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.

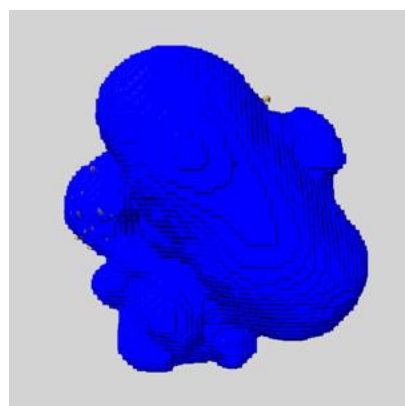
6.6 Mask visualisation [i](#)

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

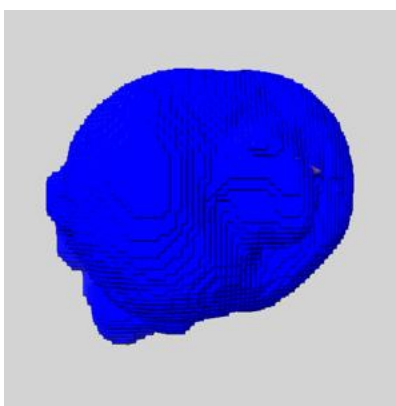
A mask typically either:

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

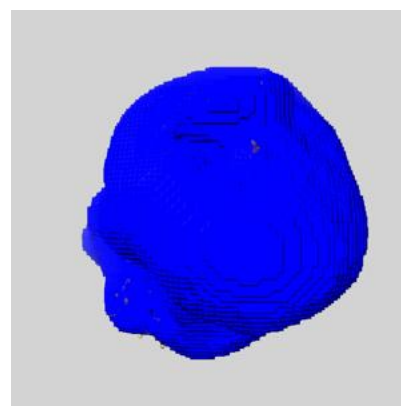
6.6.1 emd_37614_msk_1.map [i](#)



X



Y

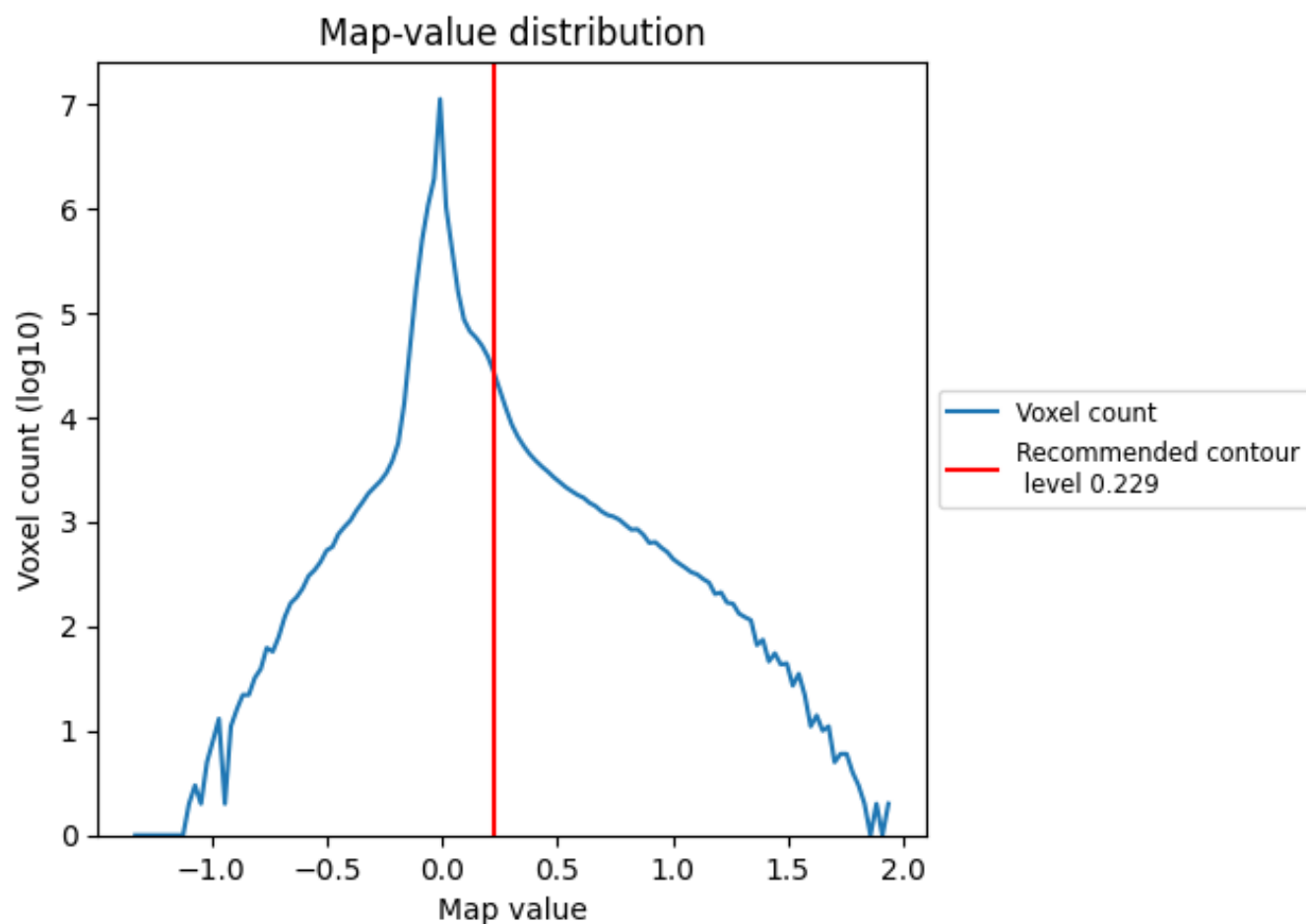


Z

7 Map analysis [i](#)

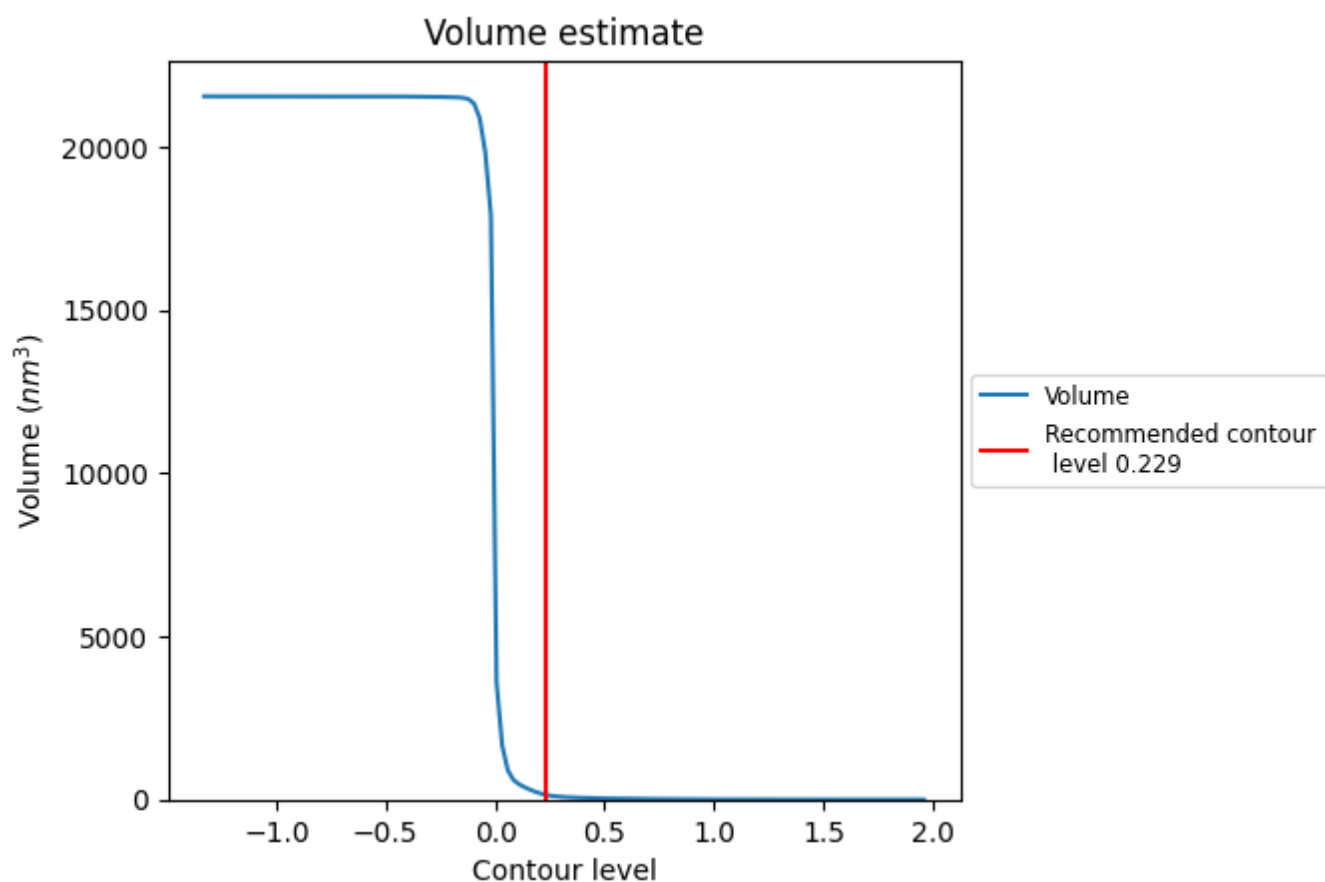
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

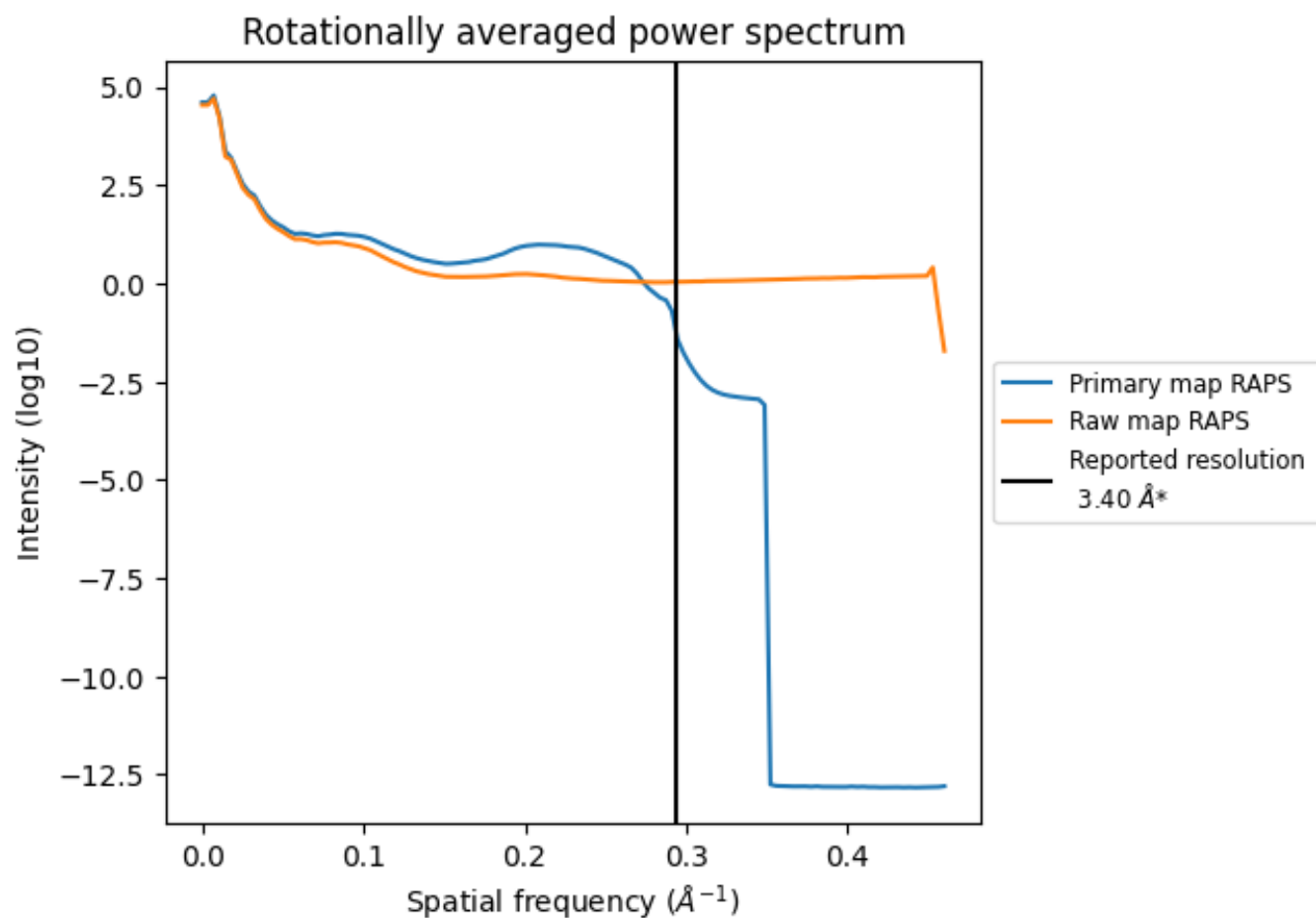
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 137 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

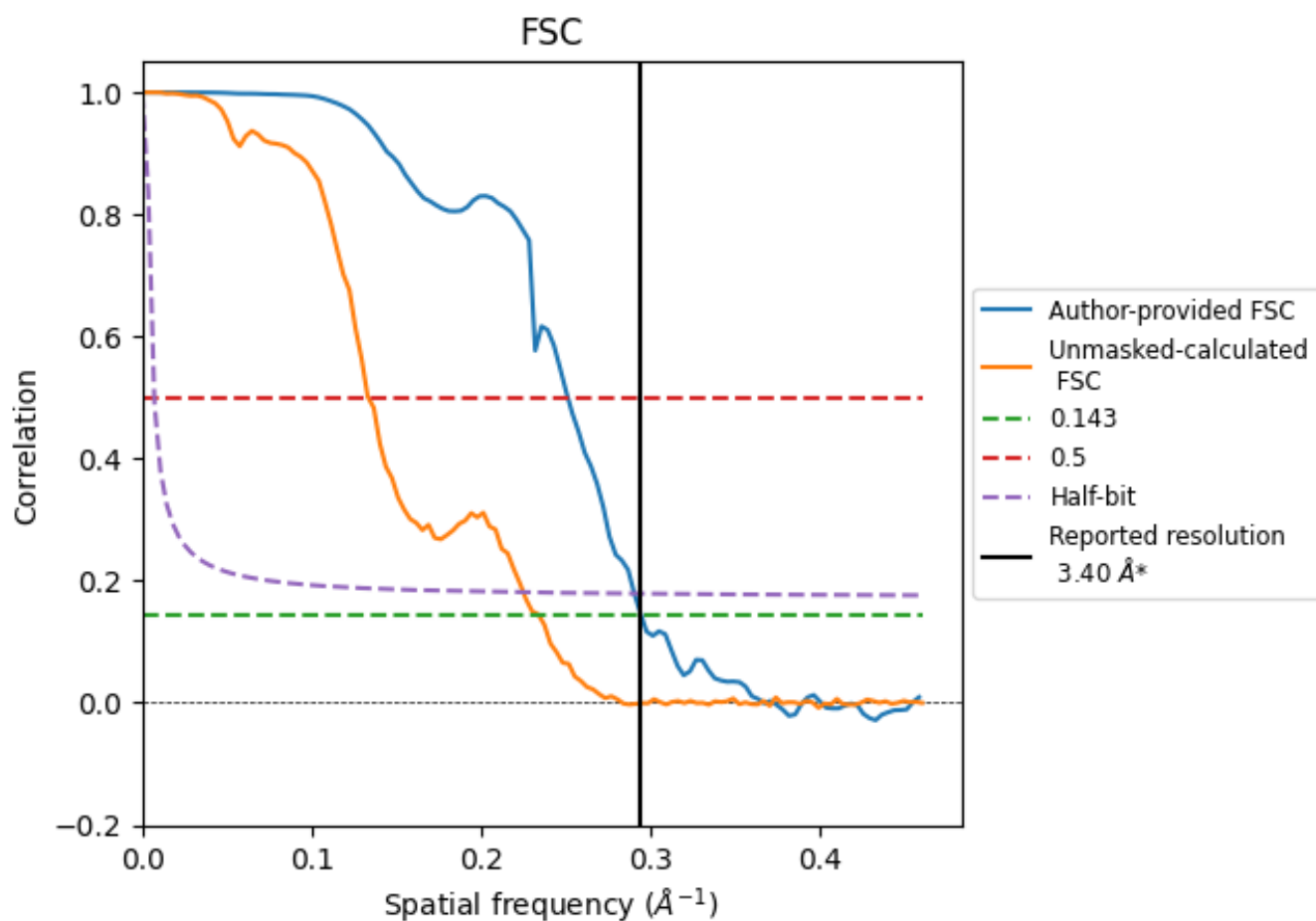


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

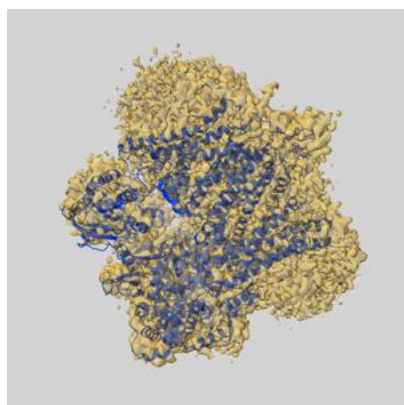
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.98	3.44
Unmasked-calculated*	4.27	7.50	4.45

*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 4.27 differs from the reported value 3.4 by more than 10 %

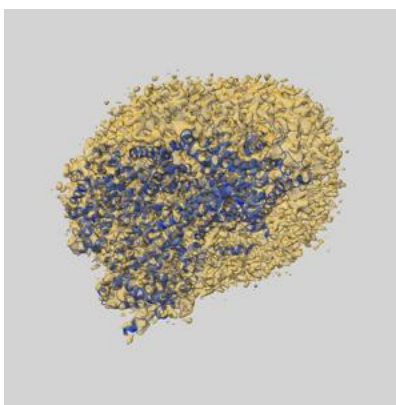
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37614 and PDB model 8WLA. Per-residue inclusion information can be found in section [3](#) on page [4](#).

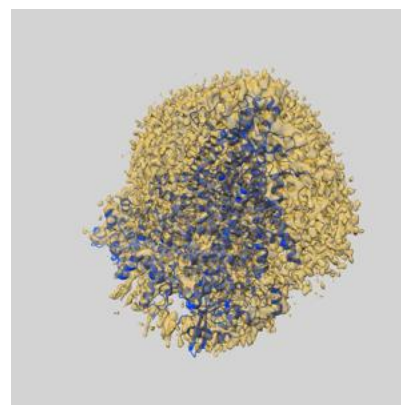
9.1 Map-model overlay [i](#)



X



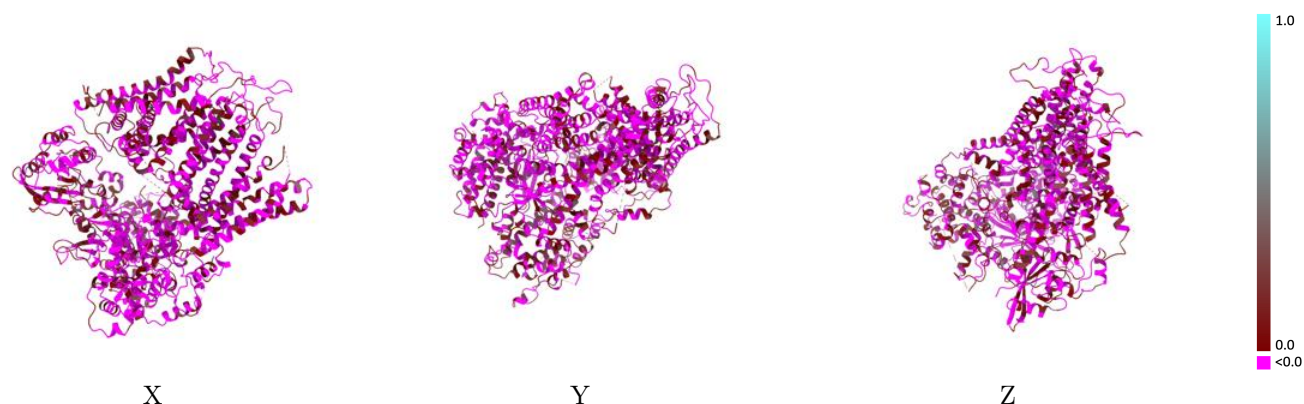
Y



Z

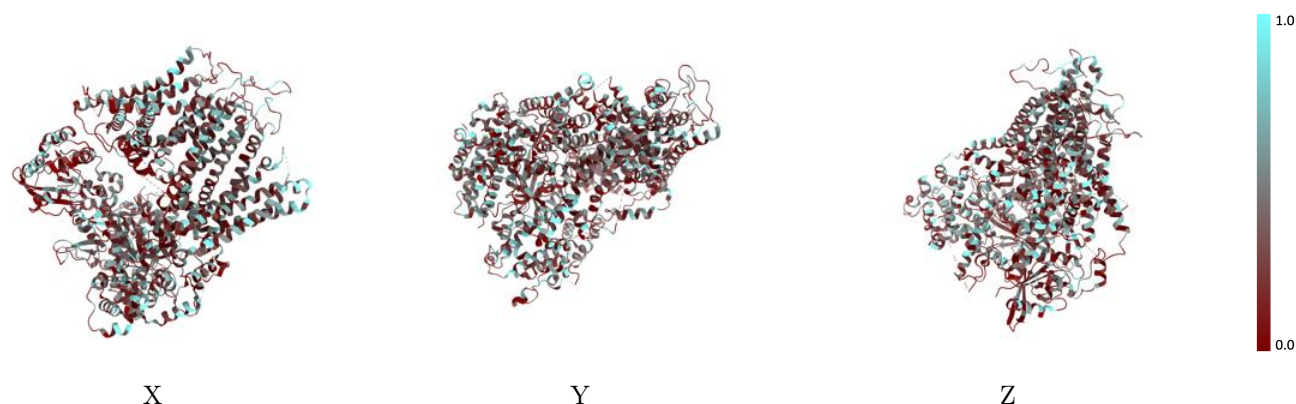
The images above show the 3D surface view of the map at the recommended contour level 0.229 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



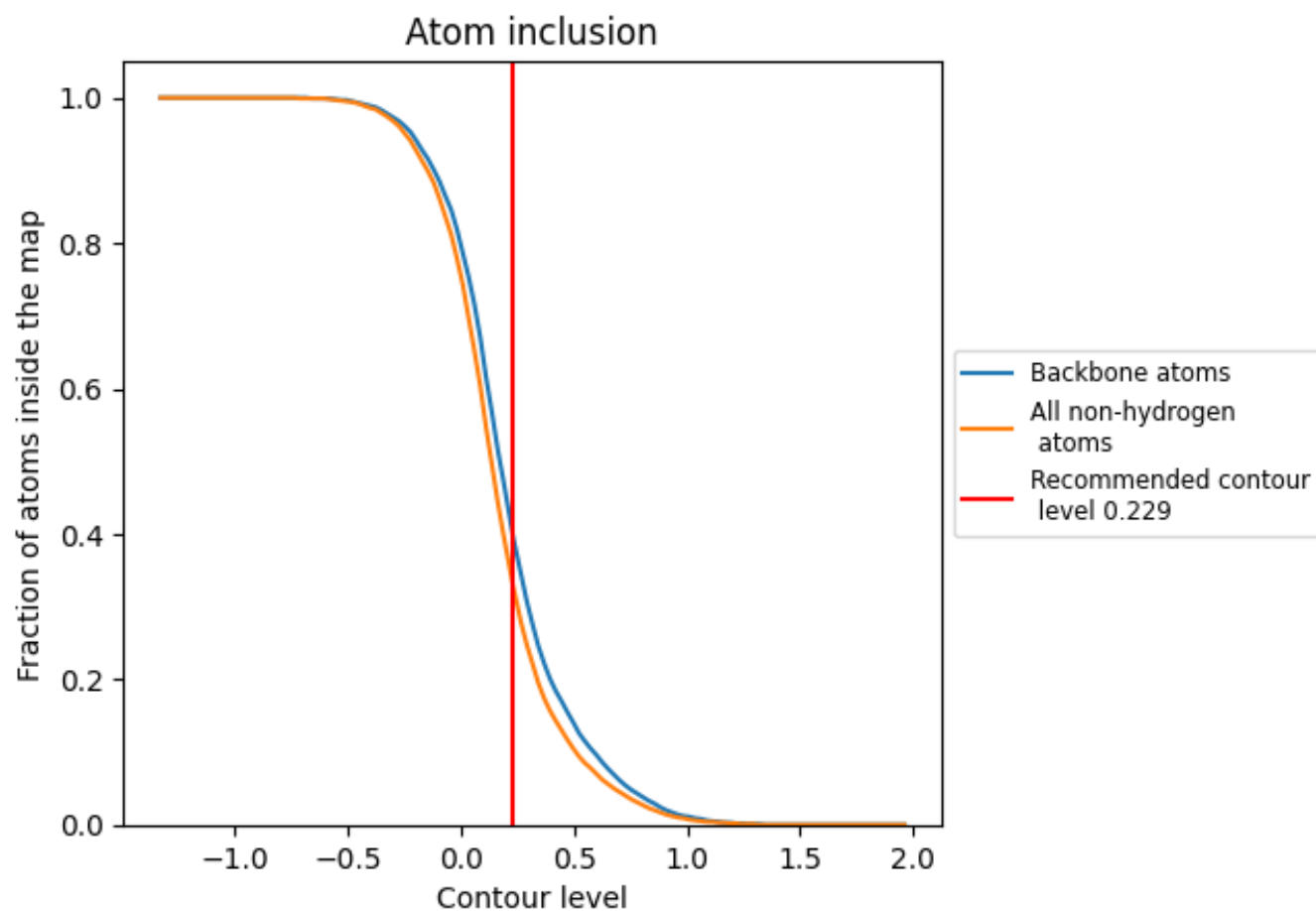
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.229).

9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 33% 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 (0.229) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3290	<div></div> -0.0500
A	<div></div> 0.2520	<div></div> -0.0100
B	<div></div> 0.3380	<div></div> -0.0540

