



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 06:06 AM UTC

PDB ID : 9WZX / pdb_00009wzx
EMDB ID : EMD-66411
Title : Cryo-EM structure of Fks1 in open state
Authors : Bai, L.; You, Z.L.
Deposited on : 2025-09-29
Resolution : 3.72 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.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

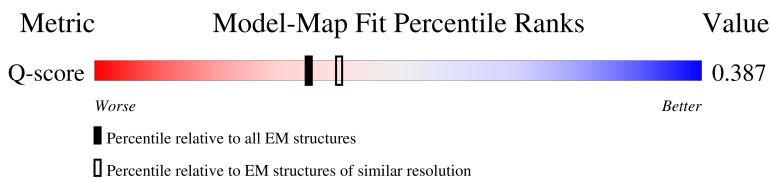
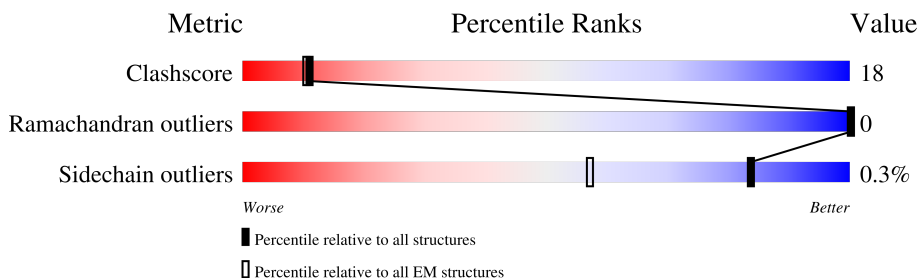
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 3.72 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	10474 (3.22 - 4.22)

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	F	1876	 52% 27% 21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12117 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.

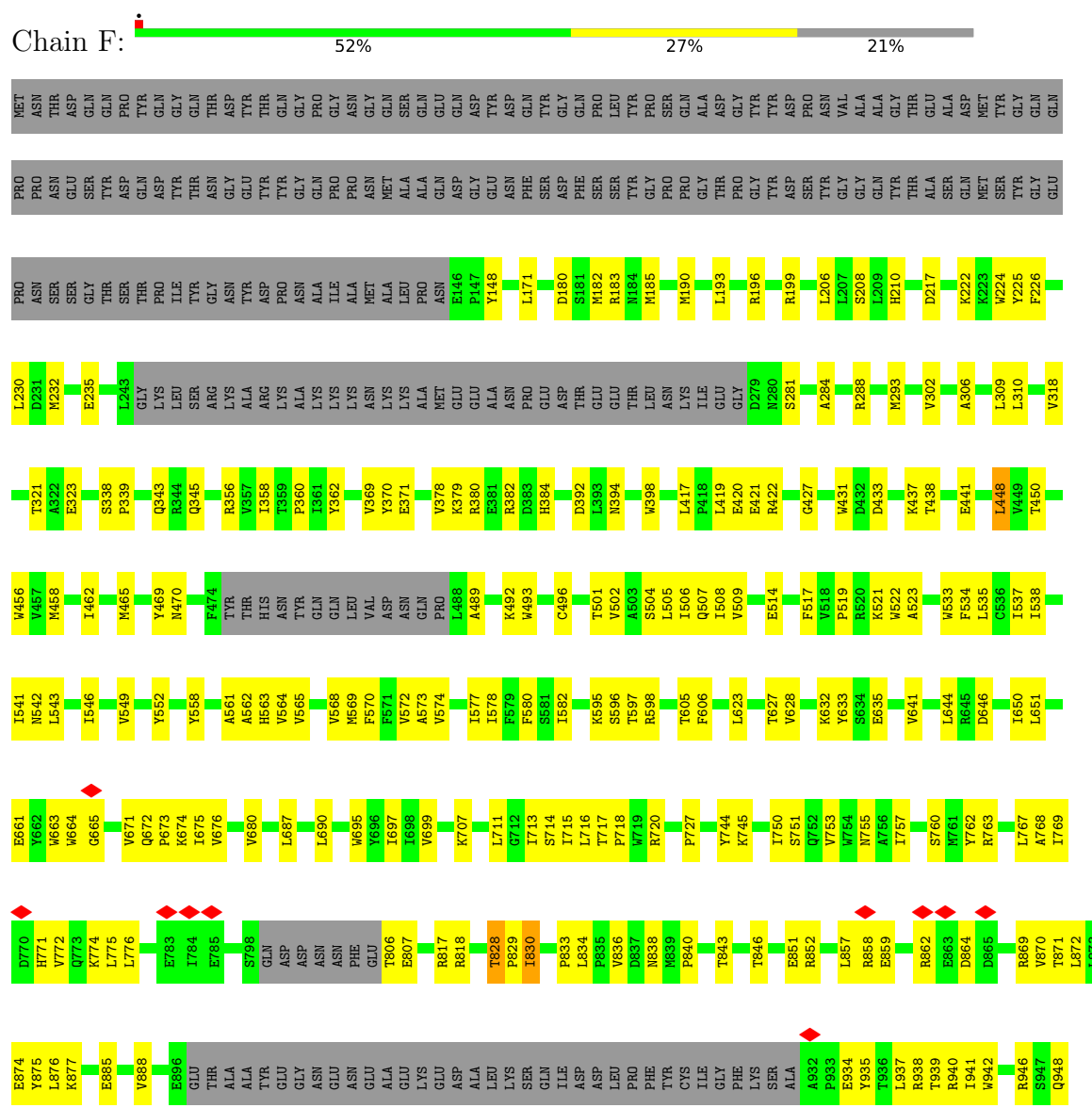
- Molecule 1 is a protein called 1,3-beta-glucan synthase component FKS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	1485	12117	7919	2023	2103	72	0	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: 1,3-beta-glucan synthase component FKS1



M1848	P1761	F1887	M1457	V1355	GLY	GLN	P1066	R952
T1851	K1762	M1690	L1488	T1359	THR	THR	K1067	T953
G1852	D1764	I1610	M1459	F1462	LEU	PHE	L1072	Y954
Q1853	H1767	N1613	F1462	F1370	ASN	THR	M1075	F957
Q1854	M1770	L1617	Q1469	V1374	THR	LEU	P1076	L966
Q1859	L1771	M1621	A1470	V1375	THR	F1180	D1080	L967
SER	F1772	S1624	P1471	L1378	LYS	A1181	M1085	Y968
HIS	W1773	CYS	L1472	I1379	ILE	T1182	F1092	R969
THR	L1774	CYS	L1473	I1379	GLY	T1183	Q1186	Y976
THR	K1775	ASP	W1474	E1402	ALA	Q1186	F1092	E984
HIS	P1776	SER	W1475	A1405	GLY	G1189	I1101	Q985
THR	S1777	GLY	W1476	G1406	MET	K1190	D1102	L986
THR	R1778	SER	A1477	T1408	GLY	L1191	A1103	E987
PRO	Q1779	GLY	S1478	L1397	LYS	M1270	N1104	M993
SER	Q1779	LEU	L1479	S1398	LYS	L1271	Q1105	K999
LEU	I1780	ALA	S1480	E1402	LYS	G1194	D1106	V1002
LYS	R1781	GLY	S1481	A1405	LYS	H1195	E1110	S1003
THR	I1784	ASP	L1482	G1406	LYS	P1196	E1111	M1004
TRP	K1788	THR	I1483	T1408	ALA	I1199	R1116	Q1005
SER	Q1789	ALA	F1484	G1407	ALA	N1200	E1124	R1006
THR	K1789	LYS	P1486	T1408	ALA	A1201	L1125	K1009
ILE	Q1789	ARG	F1487	L1408	ALA	M1204	Q1129	F1010
LYS	L1792	HIS	V1488	S1410	ARG	T1205	Y1133	N1017
R1795	R1795	ARG	F1489	L1414	THR	G1214	R1138	L1021
M1796	M1796	ARG	L1490	L1414	ILE	K1215	E1141	P1026
K1799	K1799	LYS	P1491	A1418	GLY	G1216	A1149	I1030
Y1800	Y1800	GLY	H1492	ILE	GLY	L1217	I1150	E1036
L1803	L1803	ALA	Q1493	ALA	ALA	H1218	R1154	P1037
Y1804	Y1804	ALA	F1494	ARG	ARG	L1219	E1156	P1038
V1807	V1807	Y1571	F1499	ILE	GLY	N1220	P1045	P1045
L1808	L1808	I1565	L1500	GLY	PHE	M1227	R1046	R1046
I1810	I1810	P1567	L1501	GLY	ALA	M1228	I1047	I1047
G1813	G1813	Y1571	D1502	ALA	THR	A1229	Y1048	Y1048
I1816	I1816	I1571	Y1503	THR	THR	M1230	L1051	L1051
K1827	K1827	C1575	R1504	ILE	ALA	L1231	I1052	I1052
H1828	H1828	F1576	D1505	ARG	THR	R1232	D1053	D1053
S1832	S1832	I1577	Y1506	ARG	THR	Y1241	G1054	G1054
L1833	L1833	A1578	R1508	ARG	ARG	Q1243	H1055	H1055
V1836	V1836	F1579	N1515	I1436	ARG	K1246	C1056	C1056
V1837	V1837	T1590	GLN	I1440	THR	GLY	L1059	L1059
L1840	L1840	T1591	THR	F1445	THR	ARG	R1064	R1064
F1841	F1841	M1597	HIS	F1445	THR	ASP	GLY	GLY
I1844	I1844	S1598	ASN	I1450	THR	LEU	ALA	ALA
N1845	N1845	V1599	SER	Y1451	THR	ASP	GLY	GLY
		L1600	TRP	A1454	THR	LEU	LYS	LYS
		Q1681	ILE			GLY		
		C1682	GLY			ARG		
		H1748	TYR			ASP		
		Q1683	VAL			VAL		
		R1684	ARG			ALA		
		I1685	MET			ALA		
		I1685	SER			ALA		
		I1760	ARG			ALA		
			ARG			ALA		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142777	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.325	Depositor
Minimum map value	-1.679	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	F	0.23	1/12443 (0.0%)	0.47	3/16879 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	830	ILE	C-N	12.52	1.50	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	830	ILE	CA-C-N	18.24	138.27	119.85
1	F	830	ILE	C-N-CA	18.24	138.27	119.85
1	F	569	MET	CB-CG-SD	5.35	128.74	112.70

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	F	12117	0	12107	442	0
All	All	12117	0	12107	442	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 18.

All (442) 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:F:232:MET:CE	1:F:235:GLU:HG3	1.61	1.30
1:F:828:THR:HG22	1:F:829:PRO:CD	1.69	1.20
1:F:830:ILE:HG12	1:F:1241:TYR:CD2	1.78	1.19
1:F:1378:LEU:CD2	1:F:1383:LEU:HD13	1.71	1.18
1:F:232:MET:HE3	1:F:235:GLU:CG	1.74	1.16
1:F:828:THR:CG2	1:F:829:PRO:HD2	1.76	1.13
1:F:1378:LEU:HD22	1:F:1383:LEU:HD13	1.15	1.10
1:F:1154:ARG:NH1	1:F:1156:TYR:HD2	1.49	1.07
1:F:1378:LEU:CD2	1:F:1383:LEU:CD1	2.31	1.07
1:F:232:MET:HE1	1:F:281:SER:O	1.54	1.04
1:F:1378:LEU:HD22	1:F:1383:LEU:CD1	1.89	1.00
1:F:232:MET:CE	1:F:281:SER:O	2.14	0.94
1:F:830:ILE:HD11	1:F:1241:TYR:CB	1.99	0.93
1:F:1378:LEU:HD21	1:F:1383:LEU:HD12	1.54	0.88
1:F:1378:LEU:HD21	1:F:1383:LEU:CD1	2.04	0.86
1:F:230:LEU:HD23	1:F:230:LEU:H	1.45	0.81
1:F:1380:GLU:OE2	1:F:1775:LYS:HE2	1.82	0.78
1:F:1344:GLY:HA3	1:F:1851:THR:HG22	1.64	0.77
1:F:830:ILE:HD11	1:F:1241:TYR:HB2	1.67	0.77
1:F:1649:VAL:HA	1:F:1652:ILE:HG22	1.65	0.76
1:F:830:ILE:CD1	1:F:1241:TYR:CG	2.69	0.76
1:F:1154:ARG:NH1	1:F:1156:TYR:CD2	2.35	0.74
1:F:1182:ARG:HA	1:F:1186:GLN:HB2	1.68	0.74
1:F:830:ILE:HG12	1:F:1241:TYR:CE2	2.23	0.73
1:F:1575:CYS:HB3	1:F:1678:THR:HG22	1.68	0.73
1:F:1312:MET:HB3	1:F:1459:MET:HG2	1.68	0.73
1:F:1381:ARG:HE	1:F:1773:TRP:CD1	2.07	0.73
1:F:199:ARG:NH1	1:F:1124:GLU:O	2.23	0.72
1:F:1154:ARG:HH12	1:F:1156:TYR:HB3	1.53	0.72
1:F:371:GLU:HG2	1:F:380:ARG:HB2	1.71	0.72
1:F:1046:ARG:HG3	1:F:1071:GLN:HE22	1.55	0.72
1:F:1381:ARG:NE	1:F:1773:TRP:CD1	2.60	0.70
1:F:1690:MET:HE1	1:F:1735:ILE:HG13	1.74	0.69
1:F:675:ILE:HD13	1:F:1577:ILE:HD13	1.74	0.69
1:F:846:THR:HB	1:F:1002:VAL:HG12	1.73	0.69
1:F:1048:TYR:HB3	1:F:1071:GLN:HA	1.73	0.69
1:F:1490:ASN:HB3	1:F:1493:GLN:HB2	1.75	0.69
1:F:230:LEU:HD23	1:F:230:LEU:N	2.08	0.68
1:F:1854:GLN:HA	1:F:1854:GLN:HE21	1.57	0.68
1:F:1380:GLU:OE2	1:F:1775:LYS:CE	2.40	0.68
1:F:470:ASN:HD22	1:F:641:VAL:HG13	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:535:LEU:HD23	1:F:538:ILE:HD11	1.75	0.68
1:F:502:VAL:O	1:F:506:ILE:HD12	1.94	0.68
1:F:828:THR:HG22	1:F:829:PRO:HD2	0.81	0.68
1:F:1687:PHE:HD2	1:F:1735:ILE:HG23	1.58	0.68
1:F:1344:GLY:CA	1:F:1851:THR:HG22	2.24	0.68
1:F:830:ILE:HG12	1:F:1241:TYR:CG	2.28	0.68
1:F:392:ASP:OD1	1:F:1273:ARG:NH2	2.28	0.67
1:F:1381:ARG:NH2	1:F:1773:TRP:CD1	2.63	0.67
1:F:1381:ARG:CZ	1:F:1773:TRP:HD1	2.08	0.67
1:F:1381:ARG:HH21	1:F:1773:TRP:CD1	2.12	0.66
1:F:232:MET:CE	1:F:235:GLU:CG	2.52	0.66
1:F:857:LEU:HD13	1:F:940:ARG:HH12	1.59	0.66
1:F:1683:GLN:O	1:F:1687:PHE:HD1	1.80	0.65
1:F:232:MET:HE3	1:F:235:GLU:HG3	0.77	0.65
1:F:1504:ARG:HD2	1:F:1800:TYR:HE1	1.62	0.65
1:F:1006:ARG:HG3	1:F:1010:PHE:HE1	1.62	0.65
1:F:1220:ASN:OD1	1:F:1269:GLN:NE2	2.30	0.65
1:F:635:GLU:HG2	1:F:695:TRP:HE1	1.62	0.65
1:F:1154:ARG:NH1	1:F:1156:TYR:HB3	2.11	0.65
1:F:834:LEU:O	1:F:1116:ARG:NH1	2.30	0.64
1:F:1005:GLN:OE1	1:F:1085:ASN:ND2	2.30	0.64
1:F:384:HIS:NE2	1:F:1216:GLY:O	2.30	0.64
1:F:501:THR:HG21	1:F:546:ILE:HD13	1.80	0.64
1:F:565:VAL:HA	1:F:568:VAL:HG12	1.79	0.64
1:F:762:TYR:HB2	1:F:767:LEU:HD23	1.78	0.64
1:F:1381:ARG:NE	1:F:1773:TRP:HD1	1.96	0.64
1:F:1840:LEU:HD23	1:F:1841:PHE:HB3	1.81	0.63
1:F:869:ARG:HH22	1:F:1780:ILE:HA	1.62	0.63
1:F:1576:PHE:CZ	1:F:1602:ILE:HG21	2.34	0.63
1:F:828:THR:CG2	1:F:829:PRO:CD	2.55	0.63
1:F:830:ILE:CG1	1:F:1241:TYR:CD2	2.69	0.63
1:F:818:ARG:NE	1:F:1110:GLU:OE1	2.30	0.62
1:F:760:SER:HA	1:F:763:ARG:HD3	1.81	0.62
1:F:1469:GLN:HG3	1:F:1471:PRO:HD2	1.81	0.62
1:F:762:TYR:HD2	1:F:767:LEU:HG	1.64	0.62
1:F:623:LEU:O	1:F:627:THR:HG23	2.00	0.62
1:F:1854:GLN:HA	1:F:1854:GLN:NE2	2.13	0.62
1:F:1655:ILE:HD12	1:F:1658:PHE:HE1	1.65	0.61
1:F:771:HIS:O	1:F:774:LYS:N	2.32	0.61
1:F:1036:GLU:OE2	1:F:1046:ARG:NH1	2.33	0.61
1:F:1561:ILE:HG22	1:F:1692:ALA:HB1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1379:ILE:HD11	1:F:1383:LEU:HD22	1.82	0.61
1:F:224:TRP:HD1	1:F:323:GLU:HG3	1.66	0.60
1:F:543:LEU:HD12	1:F:546:ILE:HD11	1.83	0.60
1:F:1343:ILE:HD11	1:F:1852:GLY:O	2.00	0.60
1:F:180:ASP:OD1	1:F:183:ARG:NH1	2.34	0.60
1:F:1694:MET:HE2	1:F:1728:ARG:HG2	1.83	0.60
1:F:433:ASP:N	1:F:433:ASP:OD1	2.34	0.60
1:F:830:ILE:HD11	1:F:1241:TYR:CG	2.34	0.60
1:F:1656:ALA:O	1:F:1660:VAL:HG23	2.01	0.60
1:F:1047:ILE:HD12	1:F:1072:LEU:HB2	1.84	0.60
1:F:1154:ARG:HH11	1:F:1156:TYR:HD2	0.73	0.60
1:F:870:VAL:HG22	1:F:871:THR:H	1.65	0.60
1:F:1294:HIS:HB2	1:F:1295:PRO:HD3	1.84	0.60
1:F:573:ALA:O	1:F:577:ILE:HG13	2.02	0.59
1:F:1583:ASN:ND2	1:F:1665:GLU:OE2	2.34	0.59
1:F:1827:LYS:NZ	1:F:1828:HIS:O	2.27	0.59
1:F:1199:ILE:HD12	1:F:1204:MET:HG2	1.85	0.59
1:F:1731:THR:O	1:F:1735:ILE:HG12	2.02	0.59
1:F:538:ILE:HA	1:F:541:ILE:HG12	1.84	0.59
1:F:1685:LEU:HD23	1:F:1686:ILE:HD13	1.85	0.59
1:F:852:ARG:HA	1:F:852:ARG:CZ	2.33	0.59
1:F:1312:MET:HA	1:F:1312:MET:HE2	1.85	0.59
1:F:1471:PRO:O	1:F:1474:TRP:HB2	2.02	0.59
1:F:345:GLN:OE1	1:F:345:GLN:N	2.33	0.58
1:F:1854:GLN:O	1:F:1854:GLN:HG3	2.04	0.58
1:F:1318:LEU:HD21	1:F:1351:ALA:HB1	1.85	0.58
1:F:1380:GLU:HG3	1:F:1775:LYS:HZ2	1.68	0.58
1:F:713:ILE:HG22	1:F:715:ILE:H	1.69	0.58
1:F:771:HIS:O	1:F:775:LEU:HD23	2.04	0.58
1:F:1398:SER:HB2	1:F:1402:GLU:HG3	1.86	0.57
1:F:1609:PRO:O	1:F:1613:ASN:ND2	2.37	0.57
1:F:661:GLU:OE1	1:F:1597:ASN:N	2.34	0.57
1:F:1662:TRP:HD1	1:F:1672:MET:HG3	1.69	0.57
1:F:1493:GLN:HB3	1:F:1499:PHE:HE1	1.69	0.56
1:F:1380:GLU:HG3	1:F:1775:LYS:NZ	2.19	0.56
1:F:318:VAL:HG21	1:F:358:ILE:HD12	1.85	0.56
1:F:1193:TYR:OH	1:F:1230:MET:SD	2.59	0.56
1:F:1450:ILE:HG22	1:F:1746:LEU:HD13	1.87	0.56
1:F:1813:GLY:HA2	1:F:1816:ILE:HG22	1.88	0.56
1:F:1217:LEU:HB2	1:F:1219:LEU:HD13	1.87	0.56
1:F:1436:ILE:O	1:F:1493:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:ARG:HD2	1:F:382:ARG:HE	1.70	0.56
1:F:232:MET:HE2	1:F:281:SER:O	2.00	0.55
1:F:1489:PHE:HA	1:F:1767:HIS:CE1	2.41	0.55
1:F:1617:LEU:O	1:F:1621:MET:HG2	2.05	0.55
1:F:840:PRO:HG3	1:F:1125:LEU:HD21	1.88	0.55
1:F:935:TYR:O	1:F:939:THR:HG23	2.05	0.55
1:F:938:ARG:C	1:F:938:ARG:HH11	2.15	0.55
1:F:1492:HIS:HB3	1:F:1780:ILE:HG21	1.89	0.55
1:F:1795:ARG:HH12	1:F:1799:LYS:HB2	1.71	0.55
1:F:1344:GLY:C	1:F:1851:THR:HG22	2.32	0.55
1:F:1036:GLU:OE1	1:F:1048:TYR:OH	2.19	0.55
1:F:1440:ILE:HD12	1:F:1440:ILE:H	1.72	0.55
1:F:1489:PHE:HA	1:F:1767:HIS:NE2	2.22	0.55
1:F:1804:TYR:O	1:F:1808:LEU:HG	2.07	0.55
1:F:1150:ILE:HD11	1:F:1196:PRO:HA	1.89	0.55
1:F:597:THR:O	1:F:598:ARG:HD2	2.07	0.54
1:F:370:TYR:H	1:F:379:LYS:HA	1.72	0.54
1:F:1407:GLN:HG3	1:F:1481:SER:HB3	1.89	0.54
1:F:1687:PHE:CE2	1:F:1735:ILE:HD12	2.43	0.54
1:F:1291:TYR:O	1:F:1295:PRO:HD2	2.07	0.54
1:F:538:ILE:O	1:F:542:ASN:ND2	2.40	0.54
1:F:568:VAL:O	1:F:572:VAL:HG12	2.08	0.54
1:F:570:PHE:O	1:F:574:VAL:HG22	2.07	0.54
1:F:830:ILE:CG1	1:F:1241:TYR:CG	2.90	0.54
1:F:1489:PHE:HA	1:F:1767:HIS:HE2	1.72	0.54
1:F:864:ASP:HB3	1:F:870:VAL:HG23	1.89	0.54
1:F:1381:ARG:CZ	1:F:1773:TRP:CD1	2.89	0.54
1:F:1571:TYR:HB3	1:F:1681:GLN:NE2	2.23	0.54
1:F:596:SER:OG	1:F:597:THR:N	2.39	0.54
1:F:869:ARG:NH2	1:F:1779:GLN:O	2.41	0.54
1:F:651:LEU:HD21	1:F:673:PRO:HB2	1.90	0.53
1:F:858:ARG:O	1:F:858:ARG:NH1	2.40	0.53
1:F:1772:PHE:HA	1:F:1776:PRO:HD3	1.89	0.53
1:F:1414:LEU:HD21	1:F:1482:LEU:C	2.33	0.53
1:F:1342:PRO:HB2	1:F:1345:CYS:SG	2.49	0.53
1:F:338:SER:HB2	1:F:420:GLU:HG3	1.90	0.53
1:F:371:GLU:N	1:F:378:VAL:O	2.41	0.53
1:F:369:VAL:HG23	1:F:370:TYR:HD1	1.73	0.53
1:F:650:ILE:HD11	1:F:1347:ASN:O	2.08	0.53
1:F:830:ILE:HD11	1:F:1241:TYR:HB3	1.87	0.53
1:F:217:ASP:N	1:F:217:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1038:PRO:HD3	1:F:1045:PRO:HB3	1.91	0.53
1:F:1486:PRO:HA	1:F:1489:PHE:CZ	2.44	0.53
1:F:651:LEU:O	1:F:674:LYS:NZ	2.37	0.52
1:F:502:VAL:HG12	1:F:506:ILE:HD11	1.90	0.52
1:F:1056:CYS:SG	1:F:1064:ARG:NH1	2.82	0.52
1:F:458:MET:O	1:F:633:TYR:OH	2.26	0.52
1:F:751:SER:O	1:F:755:ASN:HB2	2.10	0.52
1:F:1220:ASN:H	1:F:1224:TYR:HD2	1.58	0.52
1:F:1687:PHE:CD2	1:F:1735:ILE:HG23	2.43	0.52
1:F:1841:PHE:CZ	1:F:1844:ILE:HA	2.45	0.52
1:F:1725:GLN:OE1	1:F:1729:GLU:HG2	2.10	0.52
1:F:206:LEU:HD21	1:F:302:VAL:HG23	1.90	0.52
1:F:1748:HIS:O	1:F:1752:ILE:HG23	2.09	0.52
1:F:462:ILE:HA	1:F:465:MET:HB2	1.90	0.52
1:F:1183:THR:HB	1:F:1375:VAL:HG11	1.90	0.52
1:F:226:PHE:HA	1:F:230:LEU:HD21	1.91	0.51
1:F:595:LYS:NZ	1:F:596:SER:O	2.32	0.51
1:F:1381:ARG:HE	1:F:1773:TRP:NE1	2.06	0.51
1:F:1397:LEU:HB3	1:F:1402:GLU:OE2	2.11	0.51
1:F:714:SER:O	1:F:714:SER:OG	2.25	0.51
1:F:1004:MET:HB2	1:F:1030:ILE:HG23	1.91	0.51
1:F:230:LEU:N	1:F:230:LEU:CD2	2.74	0.51
1:F:687:LEU:HD12	1:F:690:LEU:HD12	1.92	0.51
1:F:1479:LEU:HA	1:F:1482:LEU:HB2	1.91	0.51
1:F:966:LEU:HA	1:F:969:ARG:HG2	1.91	0.51
1:F:199:ARG:HB3	1:F:838:ASN:HB2	1.93	0.51
1:F:1194:GLY:O	1:F:1196:PRO:HD2	2.10	0.51
1:F:1380:GLU:CD	1:F:1775:LYS:HZ3	2.19	0.51
1:F:441:GLU:HG3	1:F:1271:LEU:HD21	1.93	0.51
1:F:753:VAL:O	1:F:757:ILE:HG23	2.10	0.51
1:F:851:GLU:OE1	1:F:851:GLU:N	2.44	0.51
1:F:1605:CYS:HA	1:F:1657:PHE:CE1	2.46	0.50
1:F:836:VAL:HG11	1:F:968:TYR:HA	1.94	0.50
1:F:954:ILE:HD12	1:F:1021:LEU:HD21	1.93	0.50
1:F:1841:PHE:HZ	1:F:1844:ILE:HA	1.76	0.50
1:F:1473:LEU:HA	1:F:1476:TRP:HB2	1.93	0.50
1:F:1733:LYS:O	1:F:1736:GLU:HG3	2.12	0.50
1:F:646:ASP:O	1:F:650:ILE:HG22	2.12	0.50
1:F:534:PHE:O	1:F:537:ILE:HG13	2.11	0.50
1:F:937:LEU:O	1:F:941:ILE:HG22	2.12	0.50
1:F:1450:ILE:HD13	1:F:1483:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:874:GLU:HA	1:F:877:LYS:HG2	1.93	0.49
1:F:1381:ARG:NH2	1:F:1773:TRP:HD1	2.04	0.49
1:F:1341:VAL:HG13	1:F:1342:PRO:HD3	1.94	0.49
1:F:818:ARG:NH2	1:F:1110:GLU:OE2	2.44	0.49
1:F:1102:ASP:OD2	1:F:1105:GLN:NE2	2.44	0.49
1:F:470:ASN:ND2	1:F:641:VAL:HG13	2.24	0.49
1:F:1380:GLU:OE2	1:F:1775:LYS:NZ	2.46	0.49
1:F:1807:VAL:HA	1:F:1810:ILE:HG12	1.94	0.49
1:F:661:GLU:HB3	1:F:665:GLY:HA3	1.95	0.49
1:F:1649:VAL:O	1:F:1653:VAL:HG12	2.12	0.49
1:F:1505:ASP:HA	1:F:1508:ARG:HG2	1.94	0.49
1:F:1101:ILE:HB	1:F:1105:GLN:HG3	1.95	0.48
1:F:1129:GLN:CD	1:F:1129:GLN:N	2.71	0.48
1:F:938:ARG:NH1	1:F:939:THR:HA	2.28	0.48
1:F:1559:ASN:HA	1:F:1562:MET:HE2	1.96	0.48
1:F:323:GLU:HG2	1:F:398:TRP:CD1	2.48	0.48
1:F:967:LEU:CD2	1:F:1116:ARG:HE	2.26	0.48
1:F:1662:TRP:CD1	1:F:1672:MET:HG3	2.48	0.48
1:F:450:THR:HG21	1:F:517:PHE:HE2	1.79	0.48
1:F:872:LEU:H	1:F:872:LEU:HD23	1.79	0.48
1:F:1598:SER:HA	1:F:1601:ARG:HH11	1.79	0.48
1:F:1854:GLN:HE21	1:F:1854:GLN:CA	2.21	0.48
1:F:852:ARG:HA	1:F:852:ARG:NH1	2.29	0.48
1:F:1832:SER:OG	1:F:1836:VAL:O	2.30	0.48
1:F:565:VAL:HA	1:F:568:VAL:CG1	2.44	0.47
1:F:356:ARG:HG3	1:F:427:GLY:HA3	1.96	0.47
1:F:360:PRO:HB2	1:F:431:TRP:HD1	1.79	0.47
1:F:859:GLU:CD	1:F:862:ARG:HB2	2.39	0.47
1:F:869:ARG:HH12	1:F:1781:ARG:H	1.61	0.47
1:F:1410:SER:O	1:F:1414:LEU:HD13	2.14	0.47
1:F:1582:ILE:HG21	1:F:1674:ILE:HD13	1.96	0.47
1:F:1799:LYS:HE3	1:F:1803:LEU:HD11	1.95	0.47
1:F:306:ALA:O	1:F:310:LEU:HD12	2.15	0.47
1:F:1600:LEU:HA	1:F:1603:ILE:HG12	1.96	0.47
1:F:651:LEU:O	1:F:651:LEU:HD23	2.14	0.47
1:F:1006:ARG:HH11	1:F:1009:LYS:NZ	2.11	0.47
1:F:493:TRP:HA	1:F:496:CYS:SG	2.54	0.47
1:F:1141:GLU:OE1	1:F:1141:GLU:N	2.48	0.47
1:F:1224:TYR:CD1	1:F:1227:MET:HE3	2.50	0.47
1:F:339:PRO:O	1:F:343:GLN:HG2	2.15	0.47
1:F:505:LEU:O	1:F:509:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:HIS:HE1	1:F:293:MET:SD	2.37	0.47
1:F:597:THR:HG23	1:F:598:ARG:H	1.79	0.47
1:F:942:TRP:O	1:F:946:ARG:HG2	2.14	0.47
1:F:1105:GLN:HE22	1:F:1246:LYS:HA	1.79	0.47
1:F:1601:ARG:NH2	1:F:1840:LEU:O	2.39	0.47
1:F:1111:GLU:HG3	1:F:1243:GLN:HB3	1.96	0.47
1:F:768:ALA:HB3	1:F:771:HIS:CE1	2.50	0.46
1:F:1414:LEU:HB2	1:F:1485:ALA:HB3	1.97	0.46
1:F:1682:CYS:O	1:F:1686:ILE:HG12	2.14	0.46
1:F:369:VAL:HG23	1:F:370:TYR:CD1	2.50	0.46
1:F:504:SER:O	1:F:508:ILE:HG13	2.15	0.46
1:F:1610:ILE:HA	1:F:1613:ASN:HD21	1.79	0.46
1:F:952:ARG:NH2	1:F:1106:ASP:OD1	2.47	0.46
1:F:885:GLU:O	1:F:888:VAL:HG22	2.14	0.46
1:F:1378:LEU:HD21	1:F:1383:LEU:HA	1.97	0.46
1:F:321:THR:HG22	1:F:394:ASN:HB3	1.98	0.46
1:F:507:GLN:HE21	1:F:580:PHE:HB3	1.81	0.46
1:F:1828:HIS:CD2	1:F:1844:ILE:HD11	2.51	0.46
1:F:1845:ASN:OD1	1:F:1845:ASN:N	2.47	0.46
1:F:1189:GLY:HA3	1:F:1193:TYR:HB2	1.97	0.46
1:F:1347:ASN:O	1:F:1348:PHE:HD1	1.98	0.46
1:F:1217:LEU:HD12	1:F:1219:LEU:HD22	1.98	0.46
1:F:744:TYR:HD2	1:F:745:LYS:HZ3	1.63	0.46
1:F:1359:THR:HG22	1:F:1475:PHE:HE2	1.81	0.46
1:F:185:MET:HE2	1:F:309:LEU:O	2.16	0.46
1:F:171:LEU:HD23	1:F:171:LEU:HA	1.79	0.46
1:F:967:LEU:HD23	1:F:1116:ARG:HE	1.81	0.46
1:F:1272:SER:OG	1:F:1273:ARG:N	2.48	0.46
1:F:1690:MET:C	1:F:1690:MET:SD	2.99	0.46
1:F:1327:MET:SD	1:F:1327:MET:N	2.90	0.45
1:F:437:LYS:O	1:F:438:THR:HG22	2.16	0.45
1:F:976:VAL:HG22	1:F:986:LEU:HD11	1.98	0.45
1:F:1006:ARG:HG3	1:F:1010:PHE:CE1	2.45	0.45
1:F:1026:PRO:HA	1:F:1054:GLY:HA3	1.98	0.45
1:F:1687:PHE:CD2	1:F:1735:ILE:HD12	2.52	0.45
1:F:362:TYR:OH	1:F:1075:ASN:O	2.20	0.45
1:F:533:TRP:O	1:F:537:ILE:HG12	2.15	0.45
1:F:1579:PHE:HA	1:F:1582:ILE:HG22	1.98	0.45
1:F:1761:PRO:O	1:F:1764:ASP:HB3	2.16	0.45
1:F:806:THR:O	1:F:807:GLU:HG3	2.16	0.45
1:F:1379:ILE:C	1:F:1381:ARG:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1445:PHE:CE2	1:F:1450:ILE:HD11	2.51	0.45
1:F:1827:LYS:HG3	1:F:1828:HIS:H	1.82	0.45
1:F:217:ASP:HA	1:F:222:LYS:HD3	1.97	0.45
1:F:537:ILE:O	1:F:541:ILE:HG23	2.16	0.45
1:F:767:LEU:CD1	1:F:771:HIS:HB2	2.46	0.45
1:F:767:LEU:HD11	1:F:772:VAL:HB	1.99	0.45
1:F:1336:LYS:HE2	1:F:1336:LYS:HA	1.99	0.45
1:F:1383:LEU:O	1:F:1383:LEU:HG	2.16	0.45
1:F:549:VAL:HA	1:F:552:TYR:HE1	1.82	0.45
1:F:644:LEU:HD11	1:F:680:VAL:HG12	1.97	0.45
1:F:1359:THR:HG22	1:F:1475:PHE:CE2	2.52	0.45
1:F:1149:ALA:HB1	1:F:1204:MET:HE1	1.99	0.45
1:F:210:HIS:CE1	1:F:1133:TYR:HH	2.25	0.45
1:F:417:LEU:HB3	1:F:421:GLU:OE2	2.16	0.45
1:F:830:ILE:HD13	1:F:1241:TYR:CD1	2.52	0.45
1:F:1582:ILE:HG21	1:F:1674:ILE:HG21	1.99	0.45
1:F:549:VAL:HA	1:F:552:TYR:CE1	2.51	0.45
1:F:671:VAL:HG13	1:F:671:VAL:O	2.17	0.45
1:F:1351:ALA:O	1:F:1355:VAL:HG23	2.17	0.45
1:F:1571:TYR:HB3	1:F:1681:GLN:HE22	1.81	0.45
1:F:1795:ARG:HA	1:F:1795:ARG:HD2	1.77	0.45
1:F:1480:SER:O	1:F:1483:ILE:HG22	2.17	0.44
1:F:1051:LEU:HD23	1:F:1092:PHE:CG	2.52	0.44
1:F:1504:ARG:HD2	1:F:1800:TYR:CE1	2.47	0.44
1:F:469:TYR:HD1	1:F:492:LYS:HD2	1.82	0.44
1:F:558:TYR:HB3	1:F:561:ALA:HB3	2.00	0.44
1:F:635:GLU:HG2	1:F:695:TRP:NE1	2.30	0.44
1:F:875:TYR:HE1	1:F:1778:ARG:HG2	1.83	0.44
1:F:1647:HIS:HB3	1:F:1740:PHE:CE2	2.52	0.44
1:F:697:ILE:HD13	1:F:697:ILE:HA	1.91	0.44
1:F:1472:LEU:HD12	1:F:1472:LEU:HA	1.69	0.44
1:F:1642:MET:HE2	1:F:1642:MET:HA	1.99	0.44
1:F:1833:LEU:HD12	1:F:1837:VAL:HB	2.00	0.44
1:F:1155:GLU:HA	1:F:1155:GLU:OE1	2.17	0.44
1:F:1767:HIS:HA	1:F:1770:MET:HB2	2.00	0.44
1:F:148:TYR:CE2	1:F:190:MET:HB3	2.53	0.44
1:F:1334:LYS:HD2	1:F:1334:LYS:HA	1.84	0.44
1:F:1379:ILE:C	1:F:1381:ARG:N	2.75	0.44
1:F:224:TRP:HA	1:F:606:PHE:HZ	1.83	0.44
1:F:769:ILE:HA	1:F:772:VAL:HG12	1.99	0.44
1:F:1228:ASN:O	1:F:1232:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1488:VAL:O	1:F:1767:HIS:NE2	2.51	0.44
1:F:1621:MET:HE1	1:F:1730:LEU:HD21	1.98	0.44
1:F:1072:LEU:HD13	1:F:1076:PRO:HG3	1.99	0.44
1:F:872:LEU:O	1:F:876:LEU:HD22	2.18	0.43
1:F:1224:TYR:CE1	1:F:1227:MET:HE3	2.53	0.43
1:F:1788:LYS:O	1:F:1792:LEU:HG	2.18	0.43
1:F:224:TRP:CD1	1:F:323:GLU:HG3	2.51	0.43
1:F:1232:ARG:HE	1:F:1232:ARG:HB3	1.58	0.43
1:F:1506:TYR:OH	1:F:1747:GLY:HA3	2.18	0.43
1:F:1017:ASN:OD1	1:F:1017:ASN:N	2.51	0.43
1:F:323:GLU:CD	1:F:398:TRP:HE1	2.27	0.43
1:F:521:LYS:HD3	1:F:521:LYS:HA	1.83	0.43
1:F:582:ILE:HA	1:F:1284:VAL:HG11	2.01	0.43
1:F:632:LYS:HE3	1:F:633:TYR:CD1	2.53	0.43
1:F:718:PRO:HD2	1:F:720:ARG:HH11	1.83	0.43
1:F:707:LYS:HD2	1:F:711:LEU:HD23	1.99	0.43
1:F:1317:ASN:OD1	1:F:1578:ALA:HB2	2.19	0.43
1:F:1462:PHE:CD2	1:F:1462:PHE:C	2.97	0.43
1:F:857:LEU:HD23	1:F:1017:ASN:HD21	1.84	0.43
1:F:1321:LEU:HD21	1:F:1348:PHE:CE2	2.54	0.43
1:F:1760:ILE:HD11	1:F:1762:LYS:HE2	1.99	0.43
1:F:628:VAL:HG23	1:F:699:VAL:HG11	2.01	0.43
1:F:984:GLU:O	1:F:987:GLU:HG3	2.18	0.43
1:F:1493:GLN:HB3	1:F:1499:PHE:CE1	2.52	0.43
1:F:1566:ILE:HG22	1:F:1567:PRO:HD3	2.01	0.43
1:F:1602:ILE:HA	1:F:1605:CYS:SG	2.59	0.43
1:F:672:GLN:N	1:F:673:PRO:HD2	2.34	0.42
1:F:1566:ILE:N	1:F:1567:PRO:HD2	2.34	0.42
1:F:1195:HIS:CE1	1:F:1246:LYS:HE3	2.54	0.42
1:F:1201:ALA:O	1:F:1205:THR:OG1	2.15	0.42
1:F:1737:LEU:O	1:F:1740:PHE:HB3	2.19	0.42
1:F:1803:LEU:O	1:F:1807:VAL:HG22	2.19	0.42
1:F:833:PRO:HB2	1:F:1116:ARG:NH1	2.34	0.42
1:F:843:THR:HA	1:F:999:LYS:O	2.19	0.42
1:F:182:MET:SD	1:F:183:ARG:HG3	2.59	0.42
1:F:562:ALA:HA	1:F:565:VAL:HG22	2.00	0.42
1:F:578:ILE:O	1:F:582:ILE:HG23	2.20	0.42
1:F:1501:LEU:HA	1:F:1504:ARG:HD3	2.01	0.42
1:F:1502:ASP:HA	1:F:1505:ASP:OD2	2.20	0.42
1:F:1646:ALA:HA	1:F:1649:VAL:HG22	2.00	0.42
1:F:561:ALA:HA	1:F:564:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1046:ARG:HD3	1:F:1071:GLN:OE1	2.20	0.42
1:F:1138:ARG:HB3	1:F:1141:GLU:OE1	2.19	0.42
1:F:1690:MET:CE	1:F:1735:ILE:HG13	2.48	0.42
1:F:489:ALA:HB3	1:F:563:HIS:HE1	1.85	0.42
1:F:538:ILE:HD12	1:F:580:PHE:HZ	1.83	0.42
1:F:1475:PHE:O	1:F:1478:SER:OG	2.29	0.42
1:F:1638:THR:HB	1:F:1641:VAL:HB	2.02	0.42
1:F:767:LEU:HD21	1:F:772:VAL:HG23	2.02	0.42
1:F:1494:PHE:H	1:F:1499:PHE:HE1	1.67	0.42
1:F:687:LEU:HA	1:F:690:LEU:HD12	2.02	0.42
1:F:1219:LEU:HB3	1:F:1220:ASN:H	1.60	0.42
1:F:1270:MET:SD	1:F:1270:MET:N	2.92	0.42
1:F:1833:LEU:HD12	1:F:1833:LEU:HA	1.92	0.42
1:F:1006:ARG:HH11	1:F:1009:LYS:HZ2	1.67	0.42
1:F:1375:VAL:O	1:F:1379:ILE:HG12	2.20	0.42
1:F:206:LEU:HD12	1:F:206:LEU:HA	1.89	0.41
1:F:605:THR:HG23	1:F:606:PHE:CD1	2.55	0.41
1:F:934:GLU:O	1:F:937:LEU:HG	2.20	0.41
1:F:1621:MET:HG2	1:F:1621:MET:H	1.64	0.41
1:F:514:GLU:HA	1:F:517:PHE:CD2	2.55	0.41
1:F:948:GLN:HG2	1:F:1104:ASN:ND2	2.35	0.41
1:F:1056:CYS:O	1:F:1064:ARG:NH1	2.53	0.41
1:F:1059:LEU:HD21	1:F:1065:ARG:HB2	2.02	0.41
1:F:1414:LEU:HD23	1:F:1486:PRO:HD3	2.03	0.41
1:F:193:LEU:HD12	1:F:193:LEU:HA	1.94	0.41
1:F:767:LEU:HD11	1:F:772:VAL:N	2.35	0.41
1:F:771:HIS:HA	1:F:774:LYS:HG2	2.01	0.41
1:F:836:VAL:HG22	1:F:993:MET:HE1	2.02	0.41
1:F:1451:TYR:OH	1:F:1743:ASP:OD1	2.28	0.41
1:F:1326:ILE:HD11	1:F:1848:ASN:O	2.20	0.41
1:F:284:ALA:HB1	1:F:288:ARG:HH12	1.85	0.41
1:F:727:PRO:HB2	1:F:750:ILE:HD13	2.01	0.41
1:F:196:ARG:NH1	1:F:208:SER:OG	2.53	0.41
1:F:1647:HIS:CE1	1:F:1737:LEU:HD11	2.56	0.41
1:F:676:VAL:HG11	1:F:1318:LEU:HD13	2.02	0.41
1:F:769:ILE:O	1:F:772:VAL:HG12	2.21	0.41
1:F:1056:CYS:SG	1:F:1064:ARG:HD3	2.60	0.41
1:F:1191:LEU:O	1:F:1195:HIS:HB2	2.20	0.41
1:F:370:TYR:N	1:F:379:LYS:HA	2.35	0.41
1:F:1204:MET:HE2	1:F:1204:MET:HB2	1.87	0.41
1:F:1330:TYR:CZ	1:F:1335:PRO:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1414:LEU:HD11	1:F:1482:LEU:HD23	2.02	0.41
1:F:1454:ALA:HA	1:F:1457:MET:HB2	2.01	0.41
1:F:1673:LEU:HD23	1:F:1673:LEU:HA	1.82	0.41
1:F:225:TYR:O	1:F:230:LEU:CD2	2.69	0.41
1:F:419:LEU:HA	1:F:422:ARG:HG3	2.03	0.41
1:F:448:LEU:O	1:F:456:TRP:NE1	2.42	0.41
1:F:663:TRP:HD1	1:F:664:TRP:N	2.19	0.41
1:F:1462:PHE:CE1	1:F:1674:ILE:HB	2.55	0.41
1:F:1576:PHE:HE1	1:F:1682:CYS:HG	1.69	0.41
1:F:1590:THR:OG1	1:F:1591:THR:N	2.54	0.41
1:F:1789:GLN:O	1:F:1792:LEU:HD12	2.20	0.41
1:F:438:THR:HA	1:F:519:PRO:HG3	2.02	0.41
1:F:817:ARG:HE	1:F:1157:ILE:HG21	1.86	0.41
1:F:858:ARG:HA	1:F:858:ARG:HD2	1.92	0.41
1:F:953:THR:O	1:F:957:PHE:HB2	2.21	0.41
1:F:1038:PRO:HB3	1:F:1045:PRO:HA	2.03	0.41
1:F:1321:LEU:C	1:F:1321:LEU:HD23	2.46	0.41
1:F:1565:ILE:HD13	1:F:1565:ILE:HA	1.89	0.41
1:F:1370:PHE:O	1:F:1374:VAL:HG12	2.20	0.40
1:F:379:LYS:HE3	1:F:379:LYS:HB3	1.95	0.40
1:F:1652:ILE:HD12	1:F:1655:ILE:HG23	2.04	0.40
1:F:522:TRP:CG	1:F:523:ALA:N	2.89	0.40
1:F:1310:MET:HE3	1:F:1310:MET:HB2	1.87	0.40
1:F:1381:ARG:CZ	1:F:1773:TRP:O	2.69	0.40
1:F:1030:ILE:O	1:F:1051:LEU:HA	2.21	0.40
1:F:1053:ASP:O	1:F:1064:ARG:NH1	2.53	0.40
1:F:1325:SER:OG	1:F:1326:ILE:N	2.50	0.40
1:F:1405:ALA:HB1	1:F:1409:TYR:CZ	2.57	0.40
1:F:716:LEU:HB3	1:F:717:THR:H	1.73	0.40
1:F:776:LEU:HD23	1:F:776:LEU:HA	1.88	0.40
1:F:1051:LEU:HD11	1:F:1067:LYS:HE3	2.02	0.40
1:F:1796:MET:HA	1:F:1796:MET:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	1463/1876 (78%)	1352 (92%)	111 (8%)	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	F	1307/1620 (81%)	1303 (100%)	4 (0%)	86	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	448	LEU
1	F	828	THR
1	F	1310	MET
1	F	1328	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	156	GLN
1	F	173	ASN
1	F	355	ASN
1	F	526	GLN
1	F	542	ASN
1	F	778	HIS
1	F	1087	ASN
1	F	1146	HIS
1	F	1748	HIS
1	F	1779	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

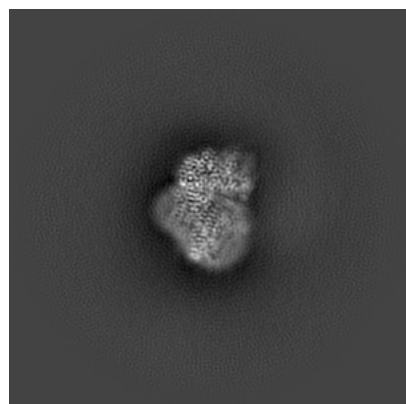
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66411. These allow visual inspection of the internal detail of the map and identification of artifacts.

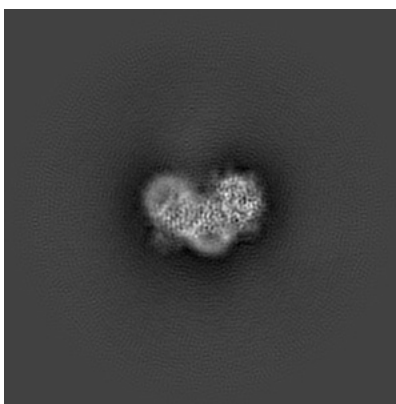
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

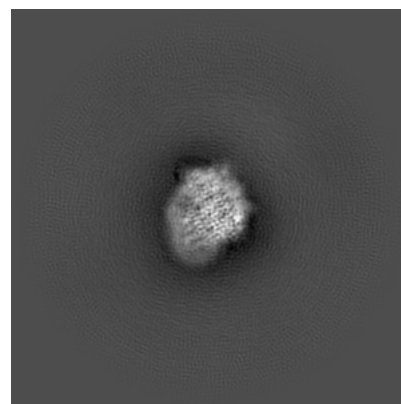
6.1.1 Primary map



X

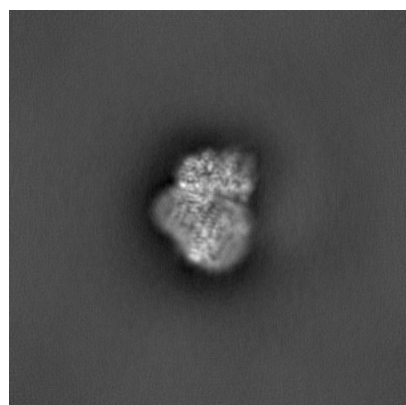


Y

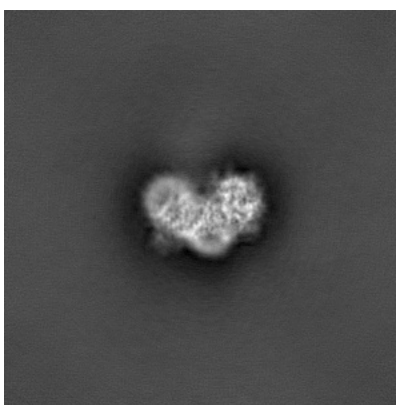


Z

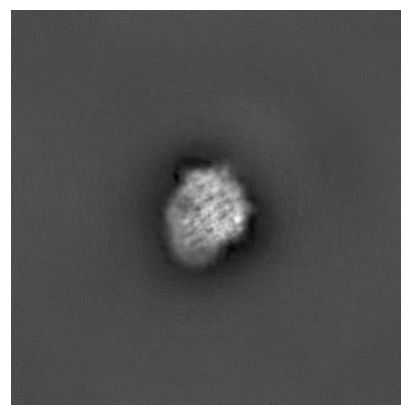
6.1.2 Raw map



X



Y

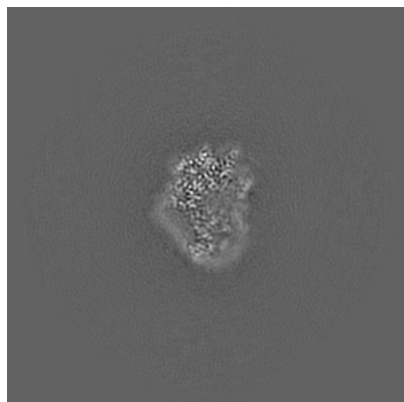


Z

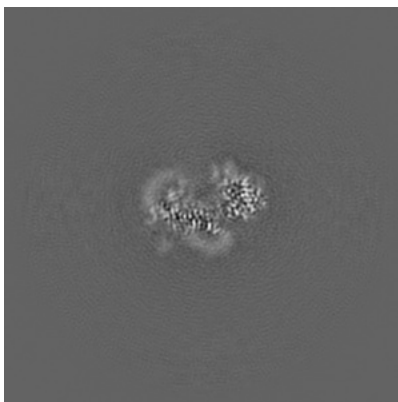
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

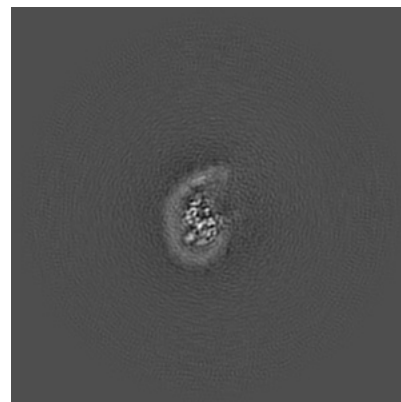
6.2.1 Primary map



X Index: 192

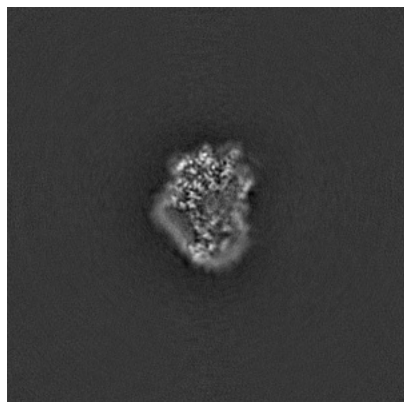


Y Index: 192

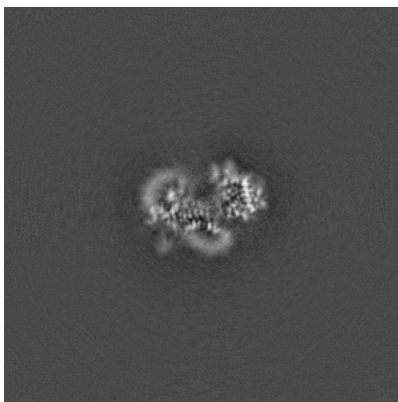


Z Index: 192

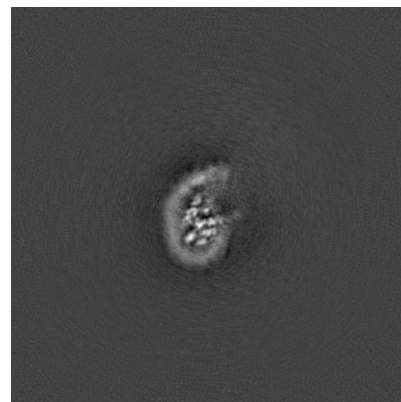
6.2.2 Raw map



X Index: 192



Y Index: 192

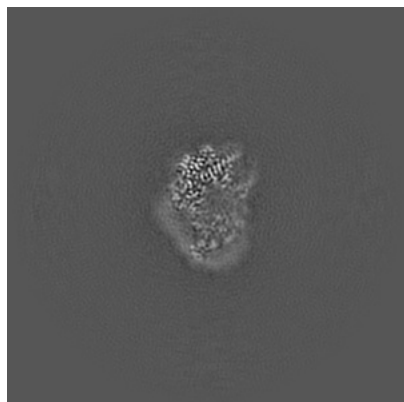


Z Index: 192

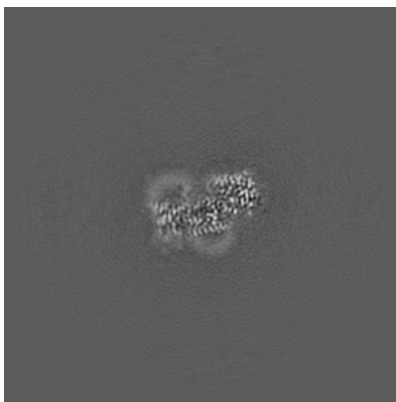
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

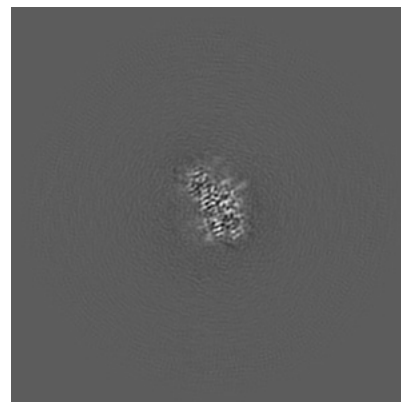
6.3.1 Primary map



X Index: 195

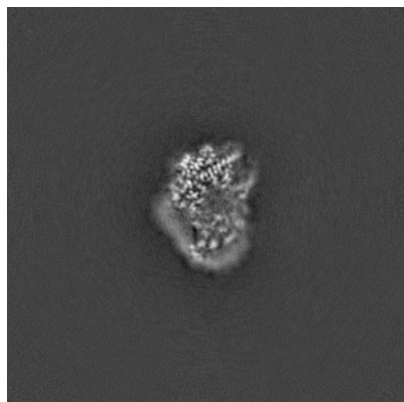


Y Index: 183

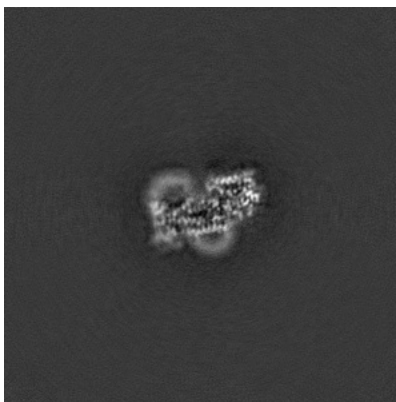


Z Index: 224

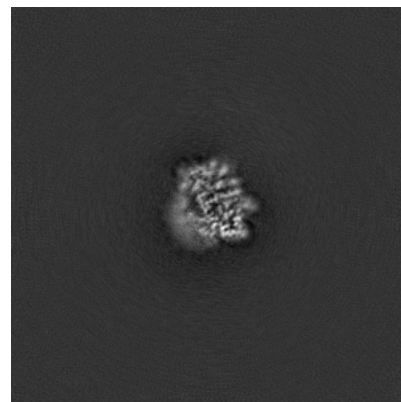
6.3.2 Raw map



X Index: 195



Y Index: 181

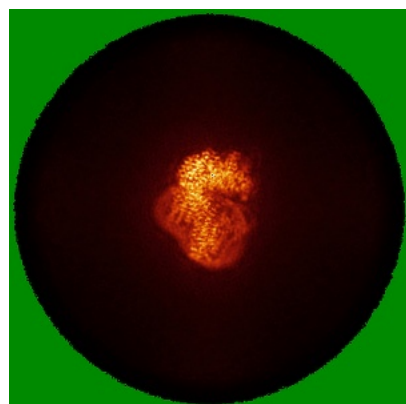


Z Index: 215

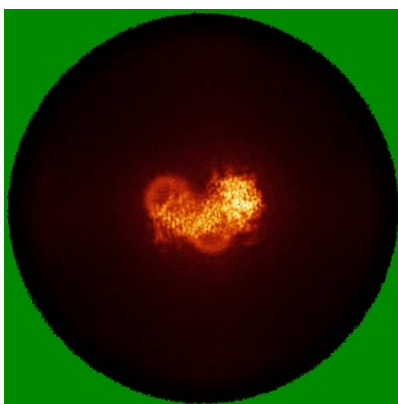
The images above show the largest variance slices of the map in three orthogonal directions.

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

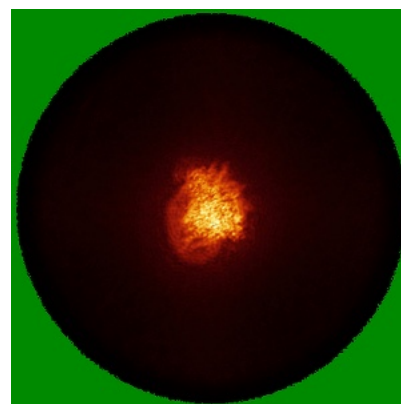
6.4.1 Primary map



X

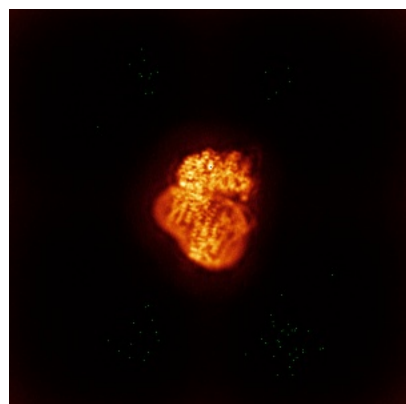


Y

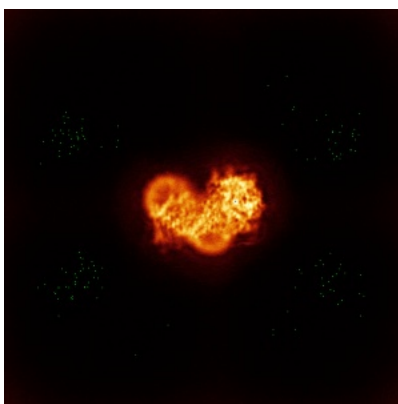


Z

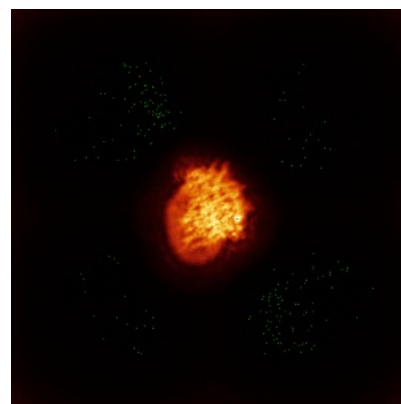
6.4.2 Raw map



X



Y

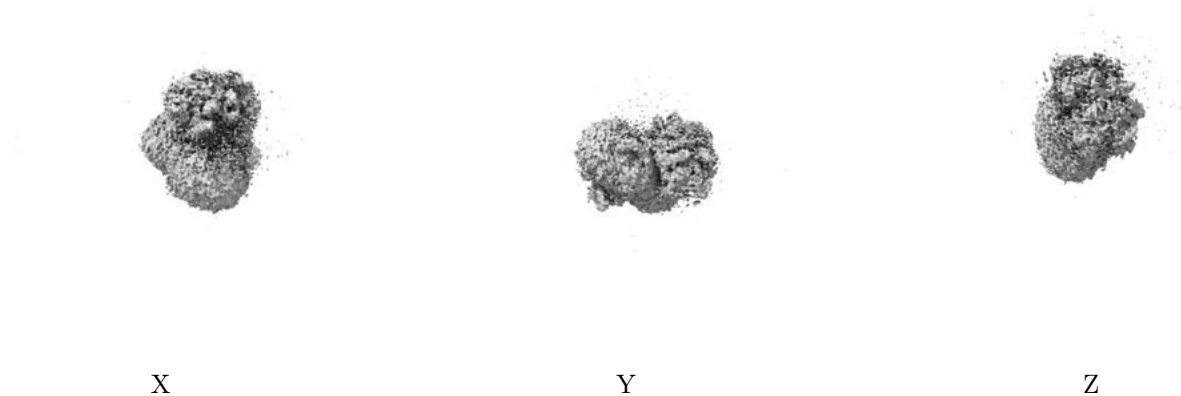


Z

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.

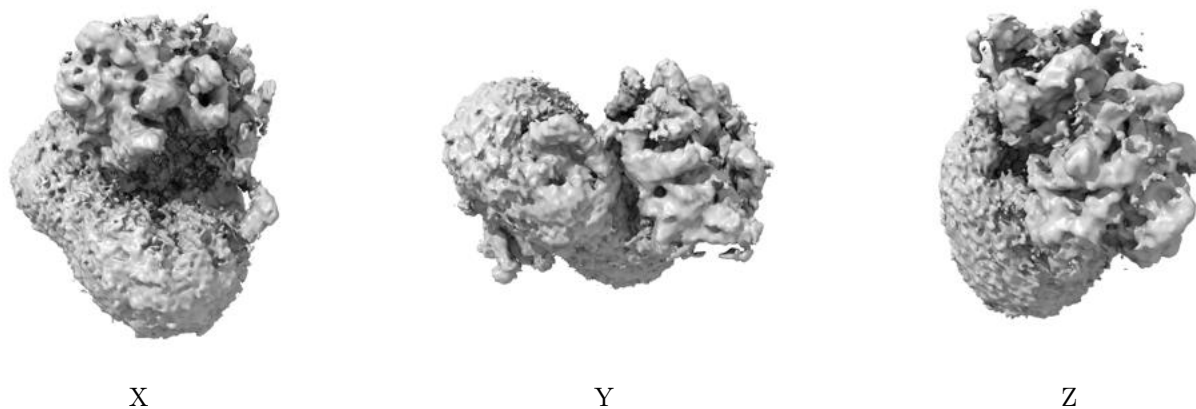
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

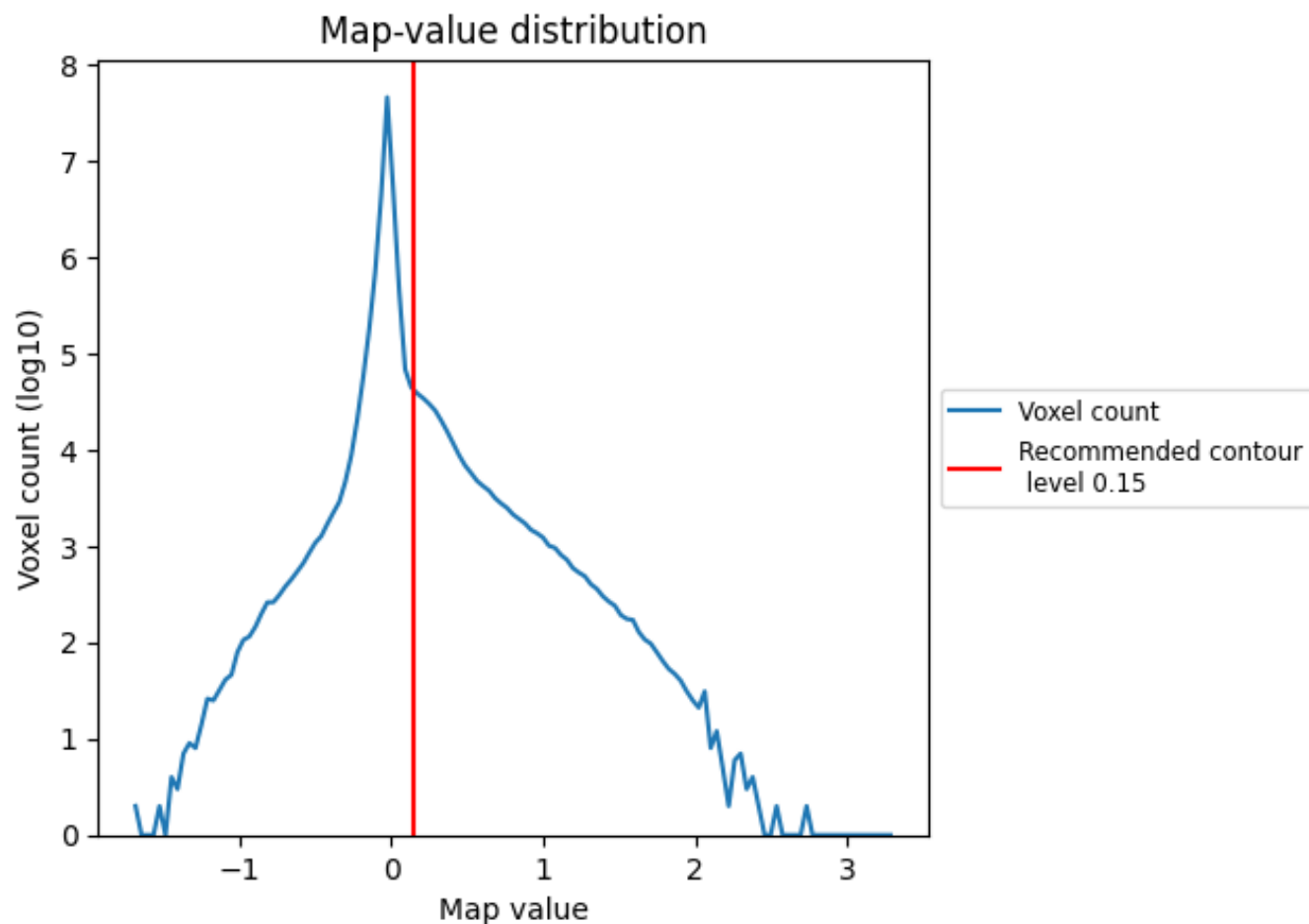
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

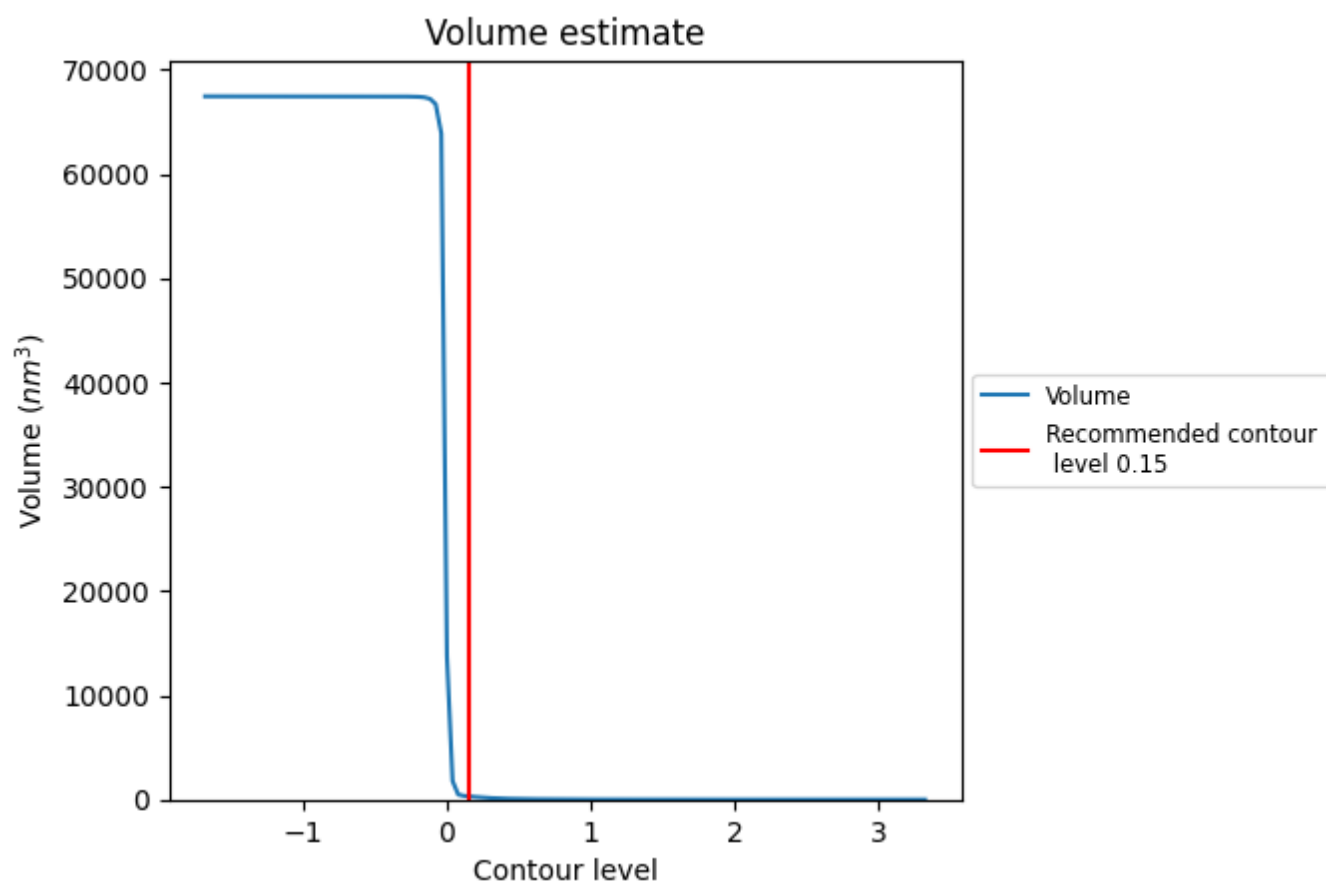
This section contains the results of statistical analysis of the map.

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.

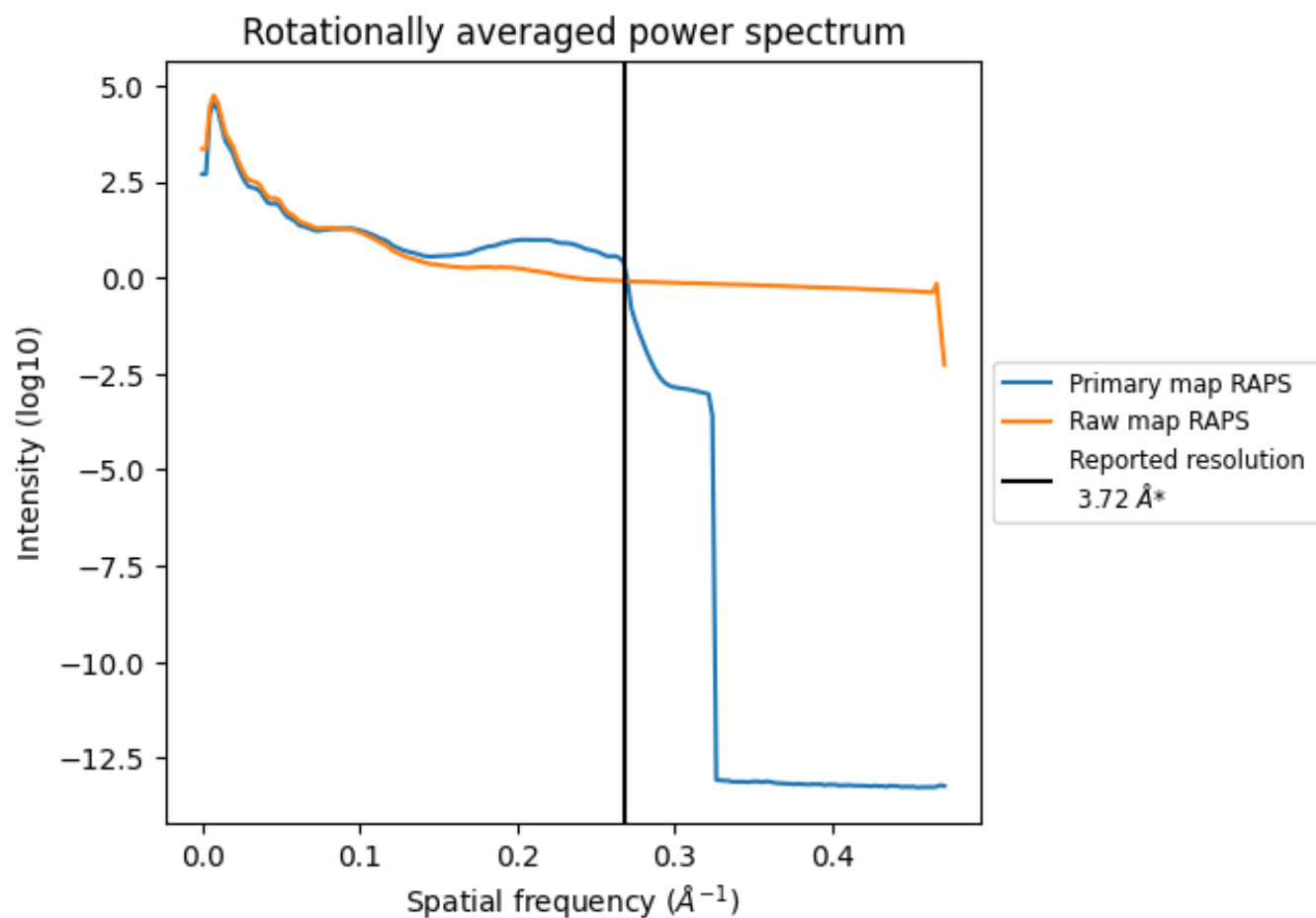
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 312 nm³; this corresponds to an approximate mass of 282 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 ⓘ

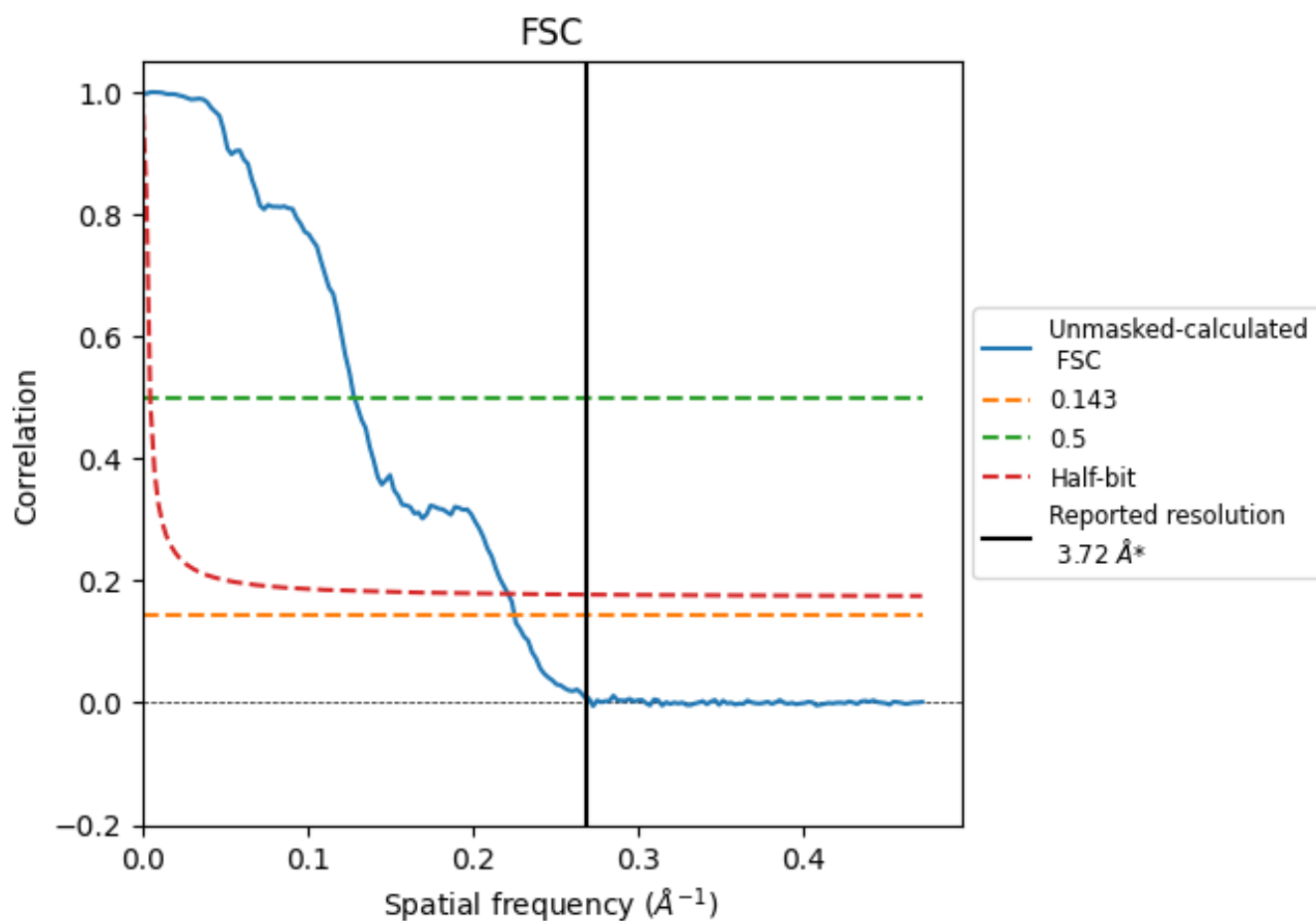


*Reported resolution corresponds to spatial frequency of 0.269 Å⁻¹

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 0.269 \AA^{-1}

8.2 Resolution estimates [i](#)

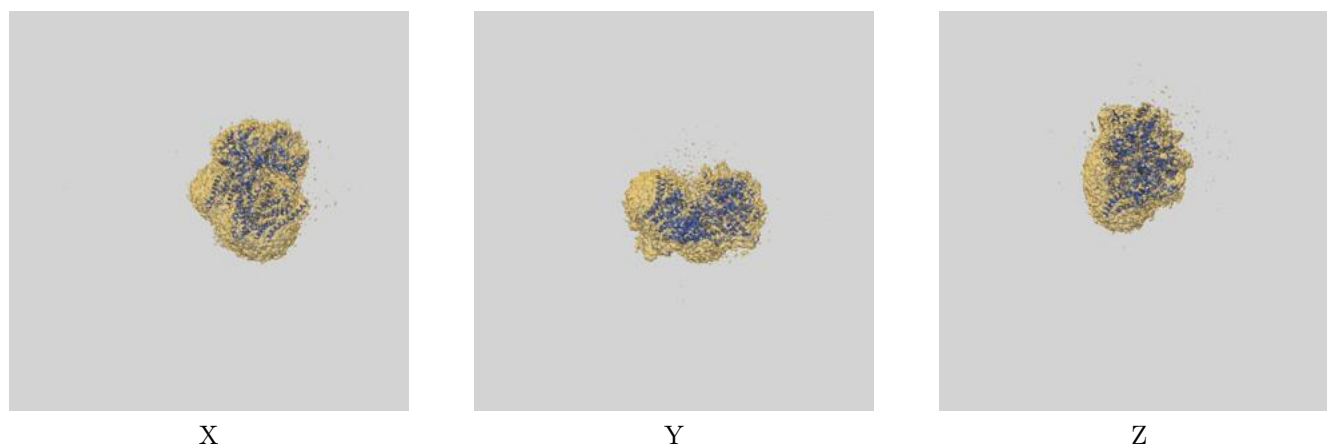
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.44	7.80	4.52

*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 4.44 differs from the reported value 3.72 by more than 10 %

9 Map-model fit [i](#)

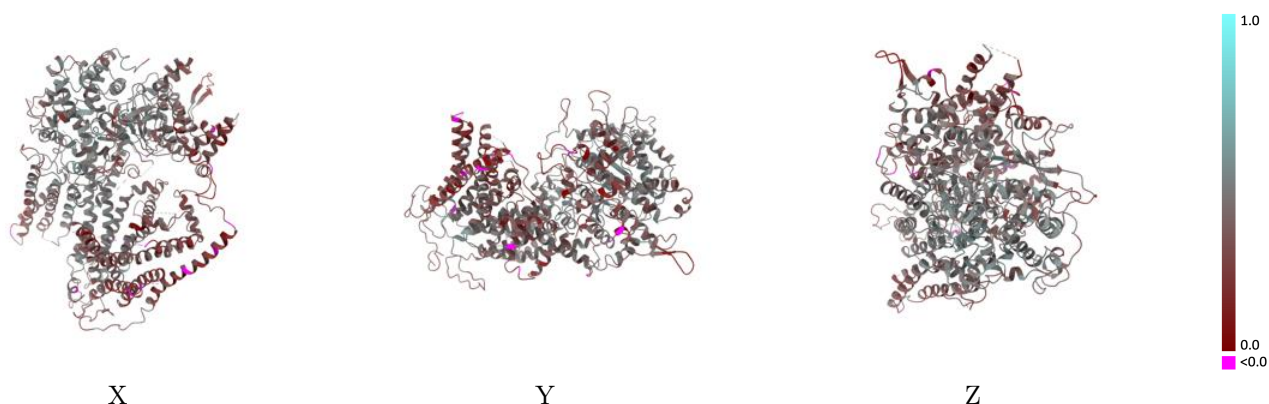
This section contains information regarding the fit between EMDB map EMD-66411 and PDB model 9WZX. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



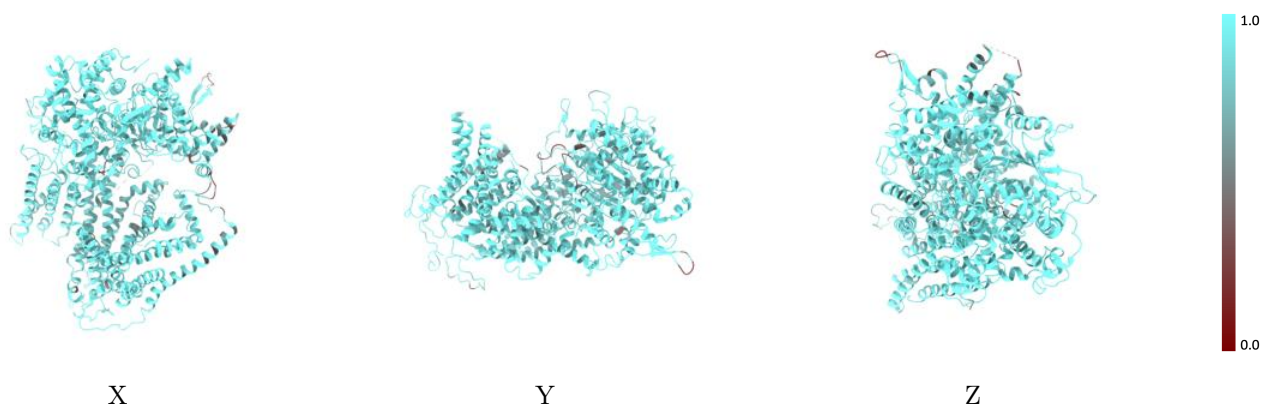
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



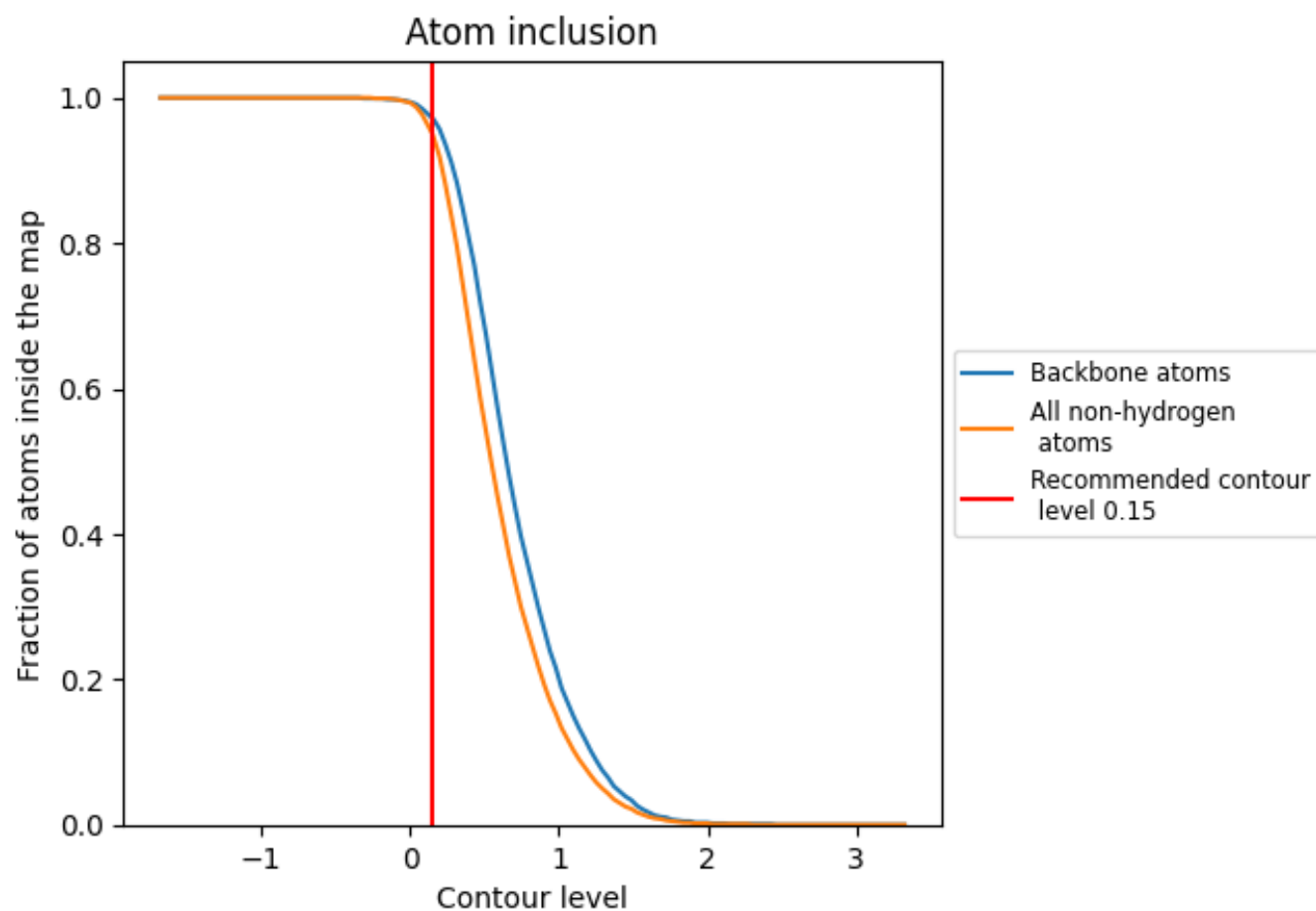
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9500	<div><div></div></div> 0.3870
F	<div><div></div></div> 0.9500	<div><div></div></div> 0.3870

