Full wwPDB EM Validation Report ⓘ

Jun 20, 2024 – 03:10 AM JST

PDB ID	:	7WO9
EMDB ID	:	EMD-32643
Title	:	Cryo-EM structure of full-length Nup188
Authors	:	Zhao, L.; Li, Z.Q.; Sui, S.F.
Deposited on	:	2022-01-20
Resolution	:	2.81 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:

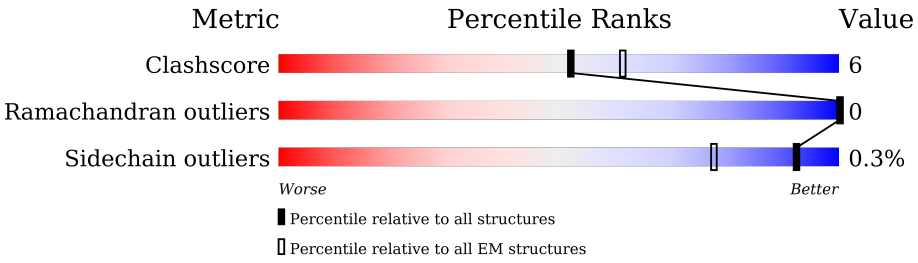
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.81 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1655	12% 81% 15% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12743 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 Nucleoporin NUP188.

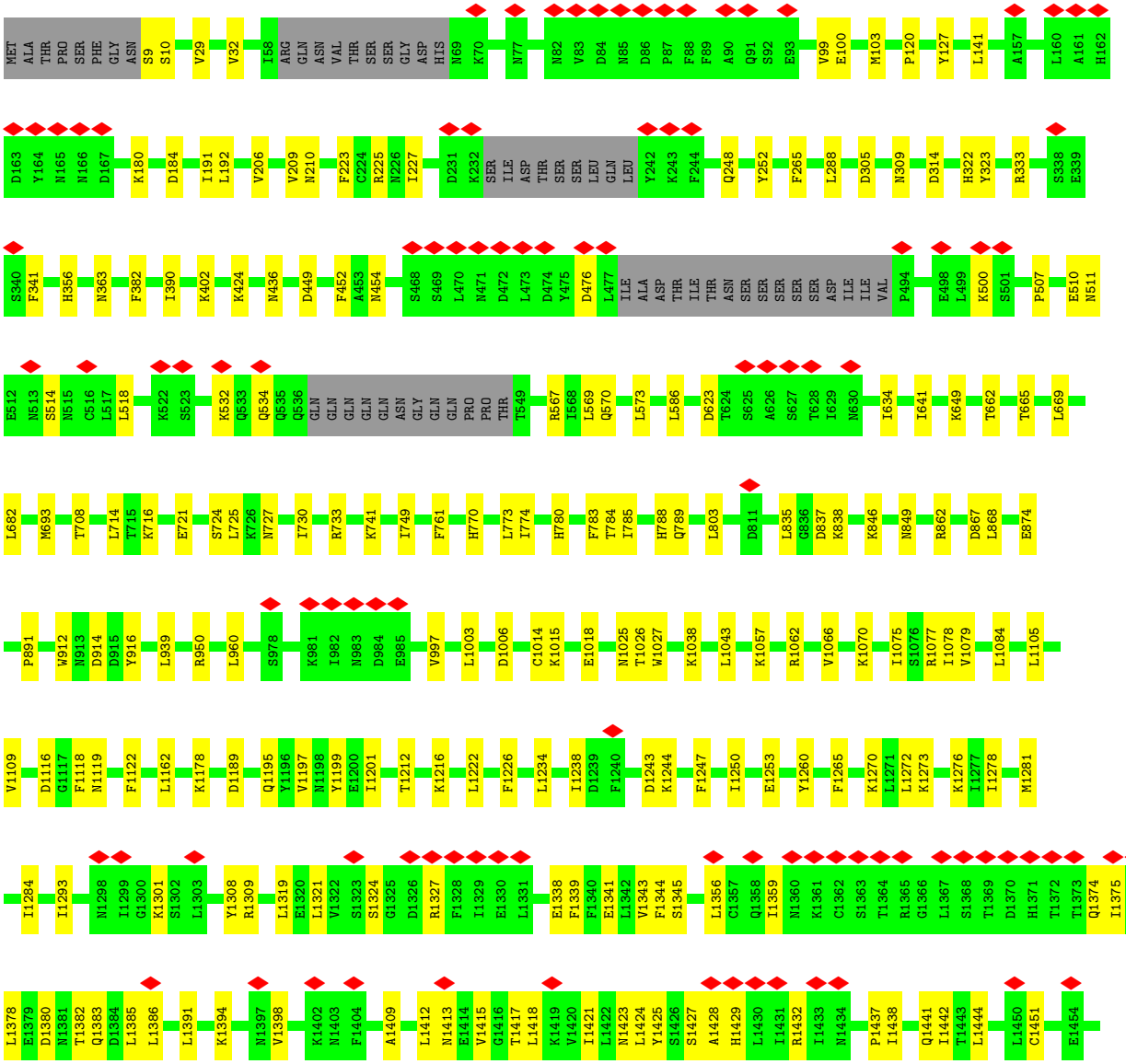
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1581	12743	8262	2036	2416	29	0	0

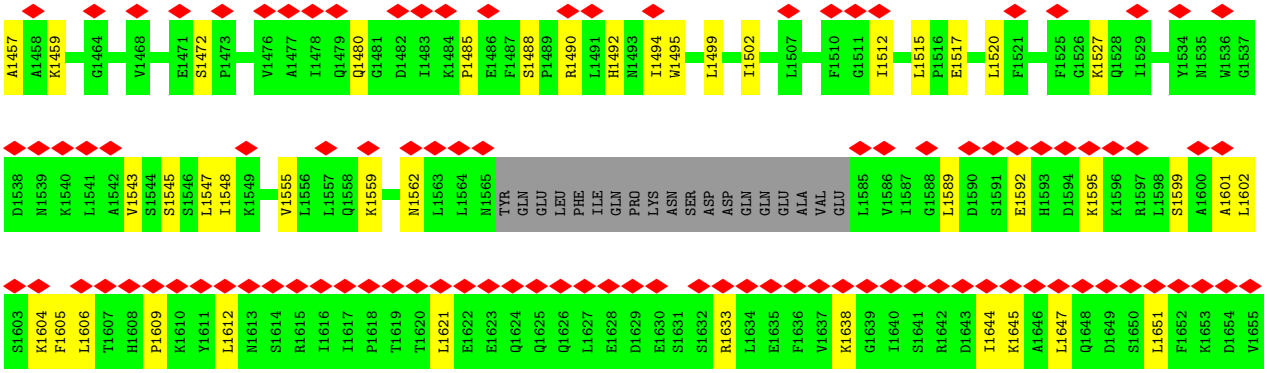
3 Residue-property plots (i)

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: Nucleoporin NUP188

Chain A:




A1457 A1458 K1459 G1464 V1468 E1471 S1472 P1473 V1476 A1477 I1478 Q1479 Q1480 G1481 D1482 I1483 K1484 P1485 E1486 F1487 S1488 P1489 R1490 L1491 H1492 N1493 I1494 W1495 L1499 I1502 L1507 F1510 G1511 I1512 L1515 P1516 E1517 L1520 F1521 F1525 G1526 K1527 Q1528 I1529 Y1534 N1535 W1536 G1537
D1538 N1539 K1540 L1541 A1542 V1543 S1544 S1545 S1546 L1547 I1548 K1549 V1555 L1556 L1557 Q1558 K1559 N1562 L1563 L1564 N1565 TYR GLN GLU LEU PHE ILE GLN PRO LYS ASN SER ASP ASP GLN GLN GLU ALA VAL GLU L1585 V1586 I1587 G1588 L1589 D1590 S1591 E1592 H1593 D1594 K1595 K1596 R1597 L1598 S1599 A1600 A1601 L1602
S1603 K1604 F1605 L1606 T1607 H1608 P1609 K1610 Y1611 L1612 N1613 S1614 R1615 I1616 I1617 P1618 T1619 T1620 L1621 E1622 E1623 Q1624 Q1625 Q1626 L1627 E1628 D1629 E1630 S1631 S1632 R1633 L1634 E1635 F1636 V1637 K1638 G1639 I1640 S1641 R1642 D1643 I1644 K1645 A1646 L1647 Q1648 D1649 S1650 L1651 F1652 K1653 D1654 V1655

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	607216	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.066	Depositor
Minimum map value	-2.175	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	320.63998, 320.63998, 320.63998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.668, 0.668, 0.668	Depositor

5 Model quality

5.1 Standard geometry

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	0.24	0/12977	0.42	0/17577

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

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	12743	0	13037	148	0
All	All	12743	0	13037	148	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 (148) 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:1394:LYS:O	1:A:1398:VAL:HG23	1.44	1.15
1:A:1398:VAL:HG12	1:A:1398:VAL:O	1.73	0.85
1:A:773:LEU:HD12	1:A:773:LEU:O	1.83	0.78
1:A:1382:THR:HA	1:A:1386:LEU:HD23	1.73	0.69
1:A:1428:ALA:O	1:A:1432:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:NH1	1:A:341:PHE:O	2.24	0.69
1:A:1398:VAL:O	1:A:1398:VAL:CG1	2.42	0.67
1:A:1319:LEU:HD21	1:A:1398:VAL:HG21	1.77	0.67
1:A:1543:VAL:HA	1:A:1547:LEU:HD22	1.77	0.66
1:A:1512:ILE:HA	1:A:1515:LEU:HD23	1.78	0.66
1:A:1490:ARG:HH22	1:A:1621:LEU:HB2	1.61	0.64
1:A:1589:LEU:O	1:A:1595:LYS:NZ	2.27	0.64
1:A:1356:LEU:HD11	1:A:1423:ASN:HB3	1.79	0.64
1:A:649:LYS:NZ	1:A:693:MET:SD	2.70	0.63
1:A:1062:ARG:NH2	1:A:1189:ASP:OD1	2.31	0.63
1:A:721:GLU:O	1:A:727:ASN:ND2	2.33	0.62
1:A:1018:GLU:HG2	1:A:1077:ARG:HE	1.65	0.61
1:A:1293:ILE:HD11	1:A:1308:TYR:HB3	1.82	0.61
1:A:1599:SER:HA	1:A:1602:LEU:HD12	1.83	0.60
1:A:1644:ILE:HD13	1:A:1647:LEU:HD21	1.83	0.60
1:A:100:GLU:HG2	1:A:891:PRO:HD2	1.82	0.60
1:A:390:ILE:O	1:A:424:LYS:NZ	2.32	0.60
1:A:1605:PHE:HD1	1:A:1612:LEU:HD11	1.67	0.60
1:A:1309:ARG:NH1	1:A:1383:GLN:OE1	2.33	0.59
1:A:1319:LEU:HD21	1:A:1398:VAL:CG2	2.32	0.59
1:A:939:LEU:HB3	1:A:997:VAL:HG11	1.85	0.59
1:A:1234:LEU:O	1:A:1238:ILE:HG12	2.03	0.58
1:A:1592:GLU:HA	1:A:1595:LYS:HE2	1.85	0.57
1:A:180:LYS:NZ	1:A:184:ASP:OD1	2.37	0.56
1:A:206:VAL:O	1:A:210:ASN:ND2	2.38	0.56
1:A:780:HIS:O	1:A:784:THR:OG1	2.23	0.56
1:A:716:LYS:HG3	1:A:774:ILE:HG12	1.88	0.56
1:A:1216:LYS:HD3	1:A:1260:TYR:CZ	2.41	0.56
1:A:1601:ALA:HA	1:A:1604:LYS:HD2	1.87	0.55
1:A:1356:LEU:HA	1:A:1359:ILE:HG12	1.89	0.55
1:A:569:LEU:HD23	1:A:634:ILE:HD11	1.88	0.55
1:A:1003:LEU:HD22	1:A:1038:LYS:HG3	1.88	0.54
1:A:532:LYS:O	1:A:534:GLN:NE2	2.41	0.53
1:A:1043:LEU:HD22	1:A:1078:ILE:HG12	1.91	0.53
1:A:209:VAL:HG11	1:A:288:LEU:HD13	1.90	0.53
1:A:1066:VAL:HG12	1:A:1070:LYS:HE3	1.90	0.52
1:A:141:LEU:HD22	1:A:191:ILE:HG23	1.92	0.52
1:A:305:ASP:OD2	1:A:322:HIS:NE2	2.36	0.51
1:A:436:ASN:OD1	1:A:586:LEU:HD11	2.10	0.51
1:A:1609:PRO:HB2	1:A:1633:ARG:HD2	1.91	0.51
1:A:1385:LEU:HD22	1:A:1442:ILE:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:PHE:HD1	1:A:1197:VAL:HG21	1.76	0.51
1:A:225:ARG:NH2	1:A:314:ASP:O	2.45	0.50
1:A:1025:ASN:OD1	1:A:1026:THR:N	2.45	0.50
1:A:1057:LYS:NZ	1:A:1116:ASP:O	2.44	0.50
1:A:1222:LEU:HD13	1:A:1226:PHE:HD2	1.75	0.50
1:A:1409:ALA:HB1	1:A:1459:LYS:HE3	1.92	0.50
1:A:476:ASP:OD1	1:A:500:LYS:NZ	2.36	0.50
1:A:1278:ILE:HD11	1:A:1324:SER:HB3	1.92	0.49
1:A:1339:PHE:O	1:A:1343:VAL:HG12	2.10	0.49
1:A:507:PRO:HG2	1:A:510:GLU:HB2	1.94	0.49
1:A:1418:LEU:HA	1:A:1421:ILE:HB	1.94	0.49
1:A:1444:LEU:HD22	1:A:1495:TRP:HA	1.95	0.49
1:A:1555:VAL:HG11	1:A:1647:LEU:HD22	1.94	0.49
1:A:1201:ILE:HD13	1:A:1247:PHE:CD2	2.48	0.49
1:A:1014:CYS:O	1:A:1018:GLU:HG3	2.12	0.48
1:A:1492:HIS:HA	1:A:1495:TRP:CE2	2.48	0.48
1:A:1602:LEU:HA	1:A:1605:PHE:CE2	2.48	0.48
1:A:1412:LEU:HD13	1:A:1417:THR:HG21	1.96	0.48
1:A:1425:TYR:CE2	1:A:1429:HIS:HE1	2.31	0.48
1:A:1272:LEU:HD21	1:A:1321:LEU:HD13	1.95	0.48
1:A:1273:LYS:HB2	1:A:1276:LYS:HZ3	1.78	0.47
1:A:1374:GLN:OE1	1:A:1378:LEU:N	2.43	0.47
1:A:570:GLN:HE22	1:A:623:ASP:HB2	1.78	0.47
1:A:449:ASP:HB3	1:A:452:PHE:HB3	1.96	0.47
1:A:785:ILE:HD13	1:A:1162:LEU:HD22	1.96	0.47
1:A:567:ARG:NH1	1:A:623:ASP:OD1	2.42	0.47
1:A:1432:ARG:HH21	1:A:1437:PRO:HB3	1.80	0.47
1:A:1413:ASN:HD21	1:A:1459:LYS:HD3	1.80	0.47
1:A:1212:THR:O	1:A:1216:LYS:HG2	2.15	0.47
1:A:1480:GLN:O	1:A:1527:LYS:NZ	2.36	0.47
1:A:1559:LYS:HA	1:A:1562:ASN:HB2	1.97	0.47
1:A:1025:ASN:HB3	1:A:1084:LEU:HD21	1.96	0.46
1:A:1559:LYS:HD2	1:A:1651:LEU:HD13	1.97	0.46
1:A:727:ASN:HB3	1:A:730:ILE:HD12	1.98	0.46
1:A:1344:PHE:CZ	1:A:1391:LEU:HD22	2.51	0.46
1:A:1377:ASN:ND2	1:A:1380:ASP:OD2	2.48	0.46
1:A:1485:PRO:HG3	1:A:1547:LEU:HD11	1.98	0.46
1:A:120:PRO:HB3	1:A:127:TYR:CG	2.51	0.46
1:A:950:ARG:HG3	1:A:1015:LYS:HD2	1.98	0.46
1:A:1421:ILE:O	1:A:1424:LEU:HG	2.16	0.46
1:A:1119:ASN:HB3	1:A:1122:PHE:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ASN:O	1:A:514:SER:OG	2.32	0.45
1:A:708:THR:HG23	1:A:749:ILE:HD13	1.98	0.45
1:A:1281:MET:O	1:A:1284:ILE:HG22	2.16	0.45
1:A:1385:LEU:HD12	1:A:1386:LEU:HD22	1.97	0.45
1:A:248:GLN:O	1:A:252:TYR:HB3	2.16	0.45
1:A:1195:GLN:HG2	1:A:1199:TYR:CE2	2.51	0.45
1:A:837:ASP:OD1	1:A:838:LYS:N	2.50	0.45
1:A:1605:PHE:CD1	1:A:1612:LEU:HD11	2.50	0.45
1:A:1451:CYS:HA	1:A:1457:ALA:HB2	2.00	0.44
1:A:9:SER:OG	1:A:10:SER:N	2.50	0.44
1:A:1545:SER:HA	1:A:1548:ILE:HD12	1.99	0.44
1:A:1645:LYS:HD3	1:A:1645:LYS:HA	1.77	0.44
1:A:99:VAL:O	1:A:103:MET:HG2	2.17	0.44
1:A:1018:GLU:HG2	1:A:1077:ARG:NE	2.31	0.44
1:A:309:ASN:OD1	1:A:356:HIS:NE2	2.44	0.44
1:A:573:LEU:HD13	1:A:641:ILE:HG13	2.00	0.44
1:A:914:ASP:OD1	1:A:914:ASP:N	2.51	0.44
1:A:1432:ARG:NH2	1:A:1437:PRO:HB3	2.33	0.44
1:A:662:THR:HA	1:A:714:LEU:HD13	2.00	0.44
1:A:912:TRP:HB2	1:A:916:TYR:HD1	1.83	0.44
1:A:682:LEU:HB3	1:A:741:LYS:HD2	1.98	0.43
1:A:223:PHE:O	1:A:227:ILE:HG12	2.18	0.43
1:A:1638:LYS:HA	1:A:1638:LYS:HD3	1.71	0.43
1:A:1438:ILE:O	1:A:1441:GLN:NE2	2.43	0.43
1:A:1444:LEU:HD21	1:A:1494:ILE:HG22	2.01	0.43
1:A:783:PHE:CZ	1:A:803:LEU:HD22	2.54	0.43
1:A:1216:LYS:HD3	1:A:1260:TYR:CE2	2.54	0.43
1:A:518:LEU:HD12	1:A:518:LEU:HA	1.89	0.43
1:A:665:THR:HG23	1:A:669:LEU:HD13	2.00	0.43
1:A:716:LYS:NZ	1:A:770:HIS:CD2	2.87	0.43
1:A:724:SER:OG	1:A:725:LEU:N	2.52	0.42
1:A:761:PHE:CE2	1:A:835:LEU:HD22	2.54	0.42
1:A:788:HIS:CD2	1:A:789:GLN:HG2	2.55	0.42
1:A:1359:ILE:HD13	1:A:1427:SER:OG	2.19	0.42
1:A:1075:ILE:O	1:A:1079:VAL:HG22	2.20	0.42
1:A:846:LYS:HA	1:A:849:ASN:ND2	2.34	0.42
1:A:1488:SER:O	1:A:1492:HIS:HB3	2.20	0.41
1:A:29:VAL:O	1:A:32:VAL:HG12	2.20	0.41
1:A:323:TYR:HD2	1:A:382:PHE:HZ	1.68	0.41
1:A:862:ARG:HD2	1:A:874:GLU:OE2	2.20	0.41
1:A:867:ASP:OD1	1:A:868:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:PHE:CD1	1:A:1270:LYS:HG2	2.54	0.41
1:A:1309:ARG:HD3	1:A:1383:GLN:OE1	2.20	0.41
1:A:1006:ASP:N	1:A:1006:ASP:OD1	2.54	0.41
1:A:1105:LEU:O	1:A:1109:VAL:HG22	2.19	0.41
1:A:1418:LEU:HA	1:A:1421:ILE:HD12	2.03	0.41
1:A:1250:ILE:HA	1:A:1253:GLU:HG2	2.02	0.41
1:A:1243:ASP:OD1	1:A:1244:LYS:N	2.52	0.41
1:A:960:LEU:HD22	1:A:1027:TRP:CD1	2.56	0.41
1:A:1343:VAL:HG13	1:A:1344:PHE:N	2.36	0.41
1:A:192:LEU:HD11	1:A:265:PHE:CE1	2.56	0.40
1:A:363:ASN:HD21	1:A:402:LYS:HD2	1.87	0.40
1:A:1338:GLU:O	1:A:1341:GLU:HG3	2.21	0.40
1:A:1273:LYS:H	1:A:1276:LYS:HE2	1.85	0.40
1:A:1327:ARG:HA	1:A:1327:ARG:HD2	1.82	0.40
1:A:1345:SER:HB3	1:A:1415:VAL:HG11	2.03	0.40
1:A:1499:LEU:HA	1:A:1502:ILE:HG12	2.04	0.40
1:A:1517:GLU:O	1:A:1520:LEU:HG	2.21	0.40
1:A:1374:GLN:OE1	1:A:1375:ILE:N	2.55	0.40
1:A:1429:HIS:CE1	1:A:1472:SER:HB3	2.57	0.40
1:A:1602:LEU:O	1:A:1606:LEU: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	1569/1655 (95%)	1503 (96%)	66 (4%)	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	1489/1557 (96%)	1485 (100%)	4 (0%)	92 97

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

Mol	Chain	Res	Type
1	A	454	ASN
1	A	733	ARG
1	A	1178	LYS
1	A	1301	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

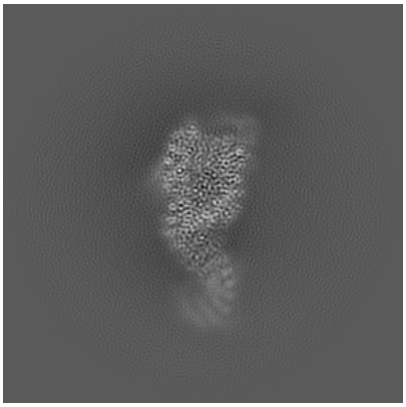
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32643. These allow visual inspection of the internal detail of the map and identification of artifacts.

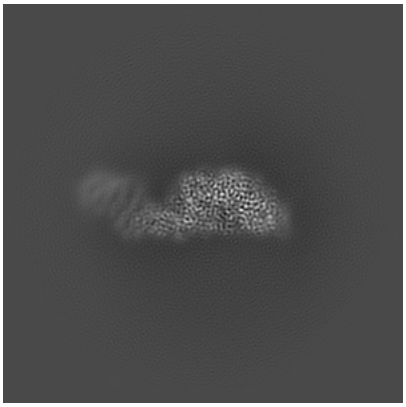
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

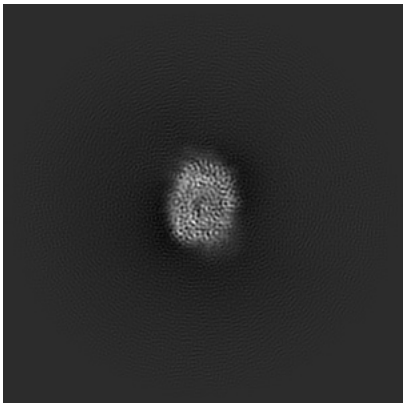
6.1.1 Primary map



X



Y

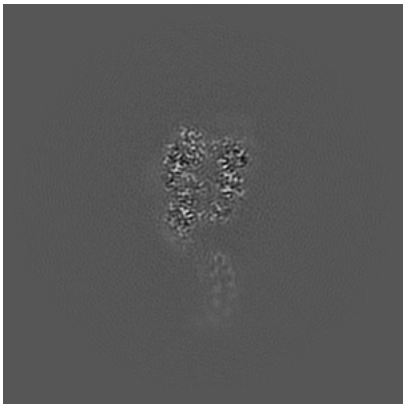


Z

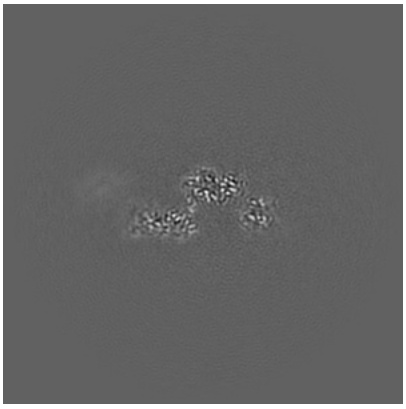
The images above show the map projected in three orthogonal directions.

6.2 Central slices

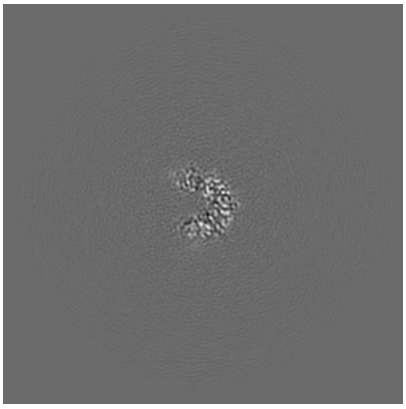
6.2.1 Primary map



X Index: 240



Y Index: 240

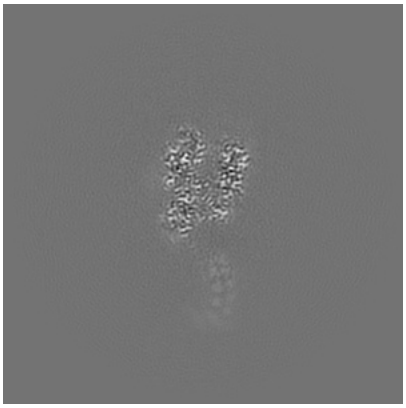


Z Index: 240

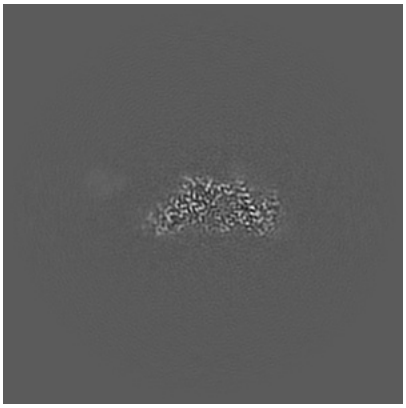
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

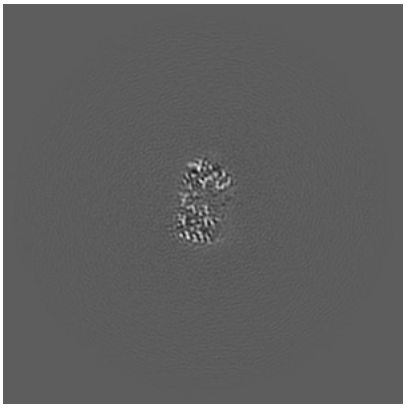
6.3.1 Primary map



X Index: 243



Y Index: 217

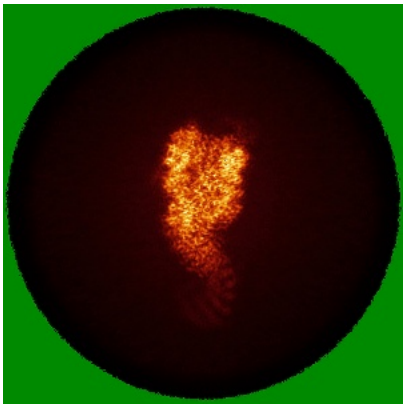


Z Index: 292

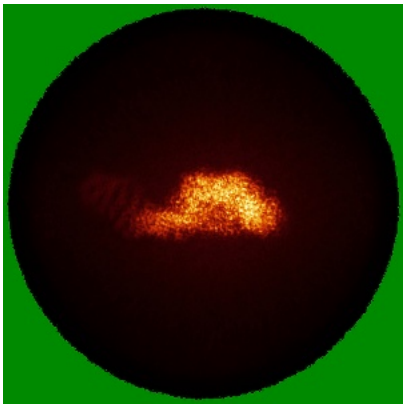
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

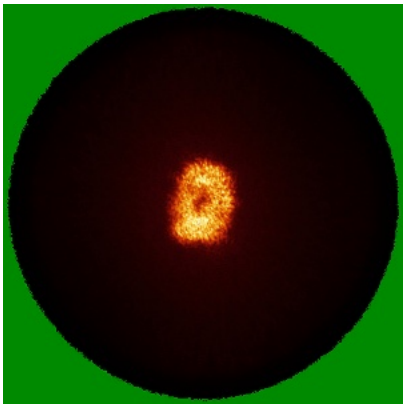
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

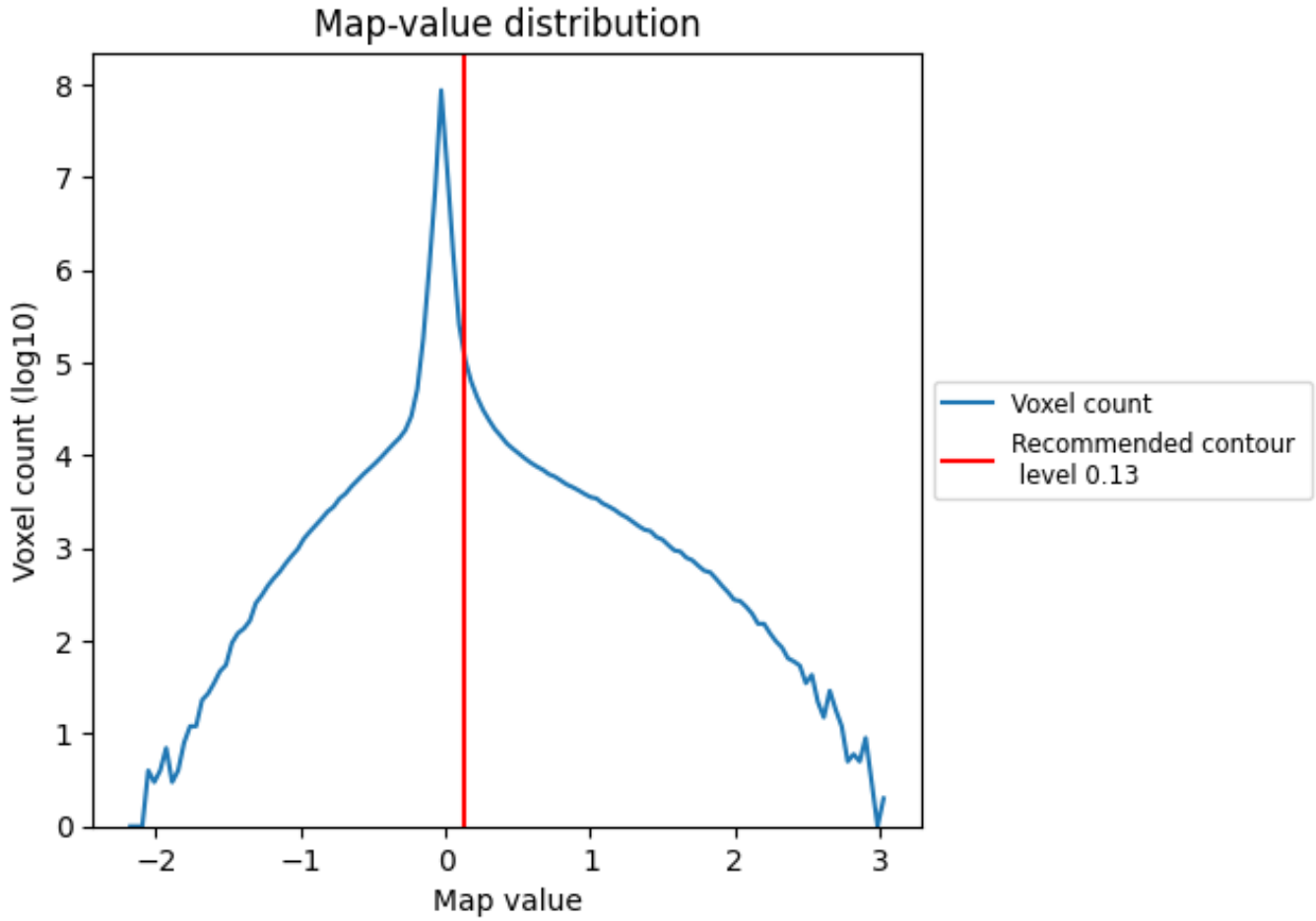
6.6 Mask visualisation (i)

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

7 Map analysis

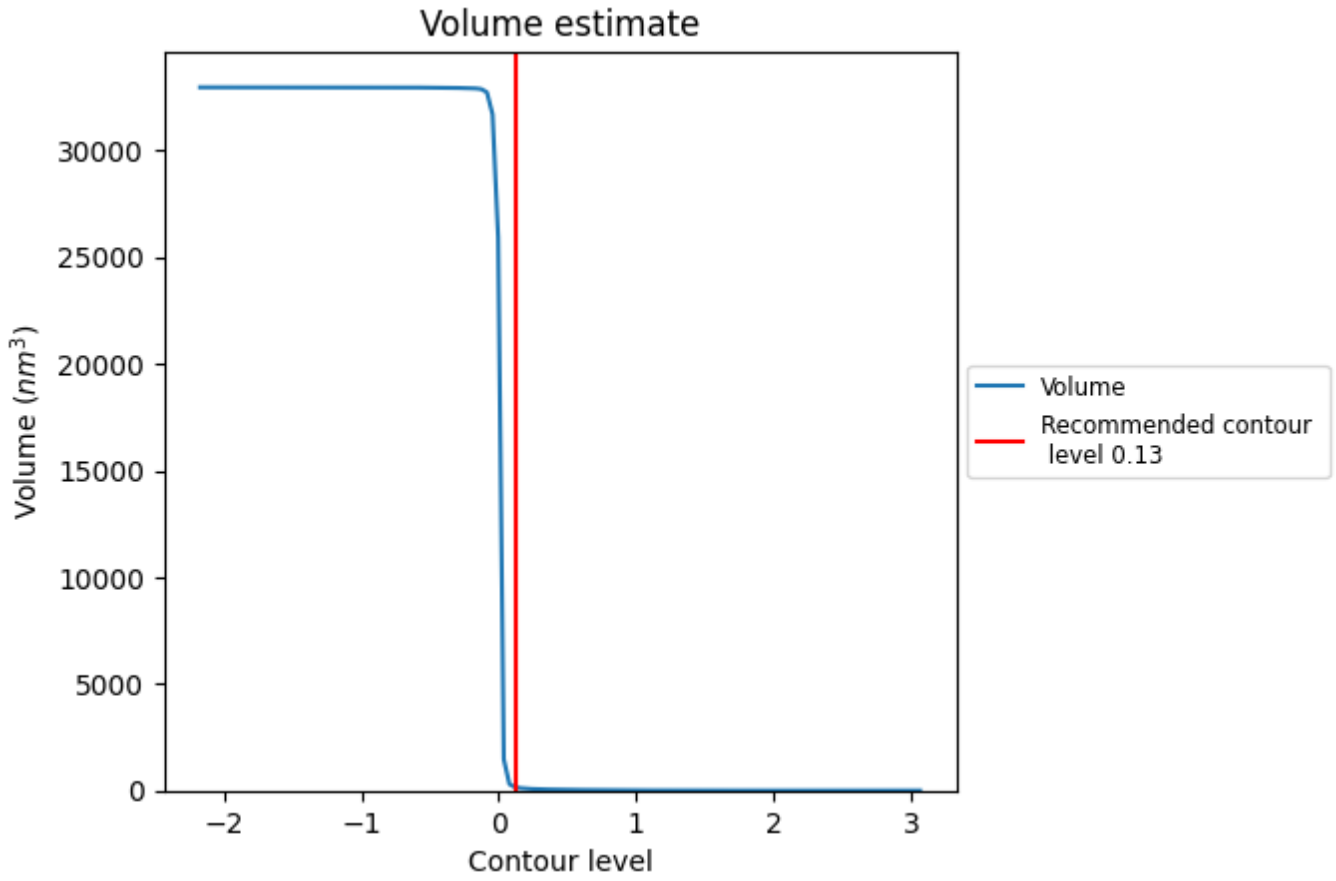
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

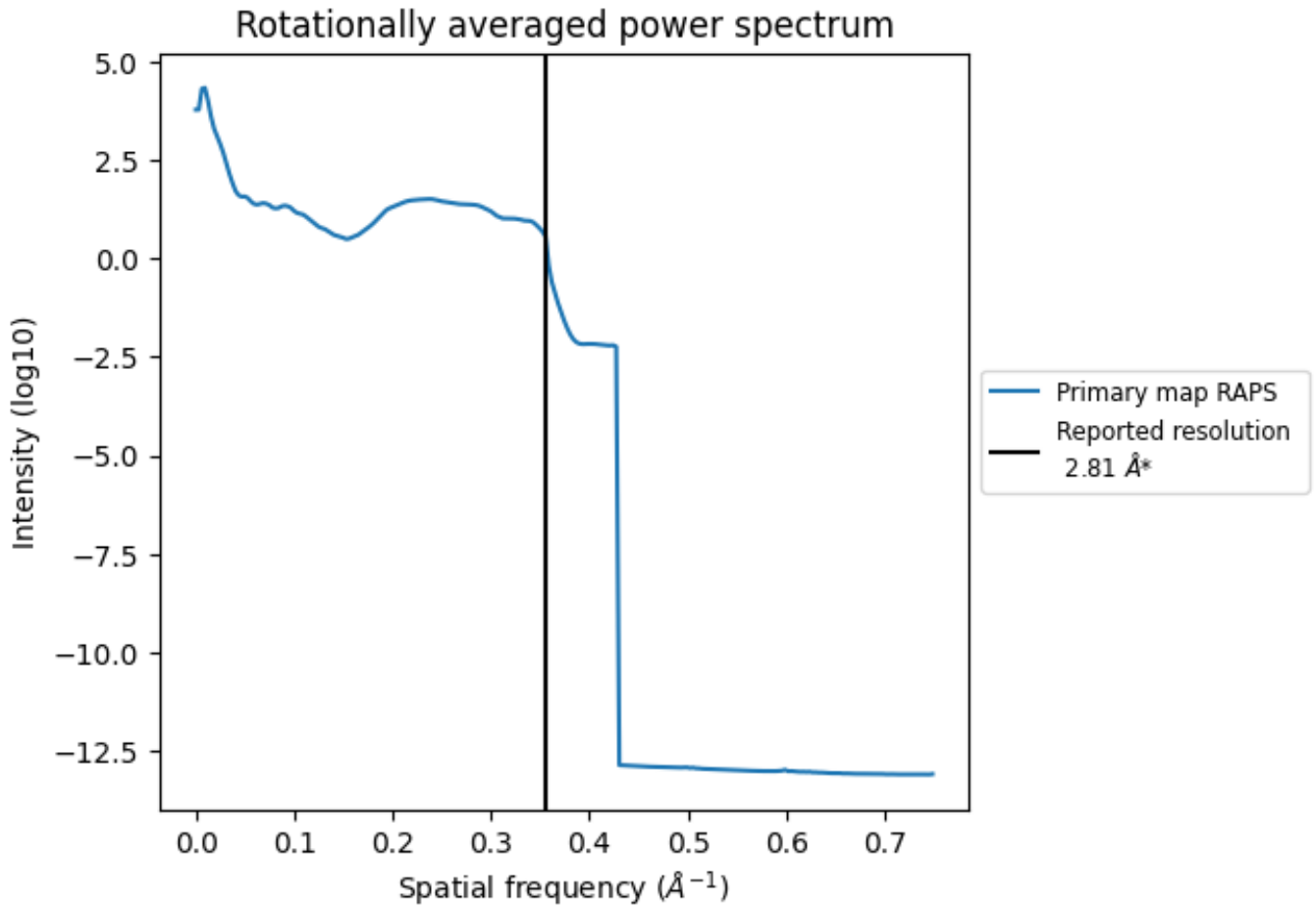
7.2 Volume estimate



The volume at the recommended contour level is 144 nm^3; this corresponds to an approximate mass of 130 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 (i)

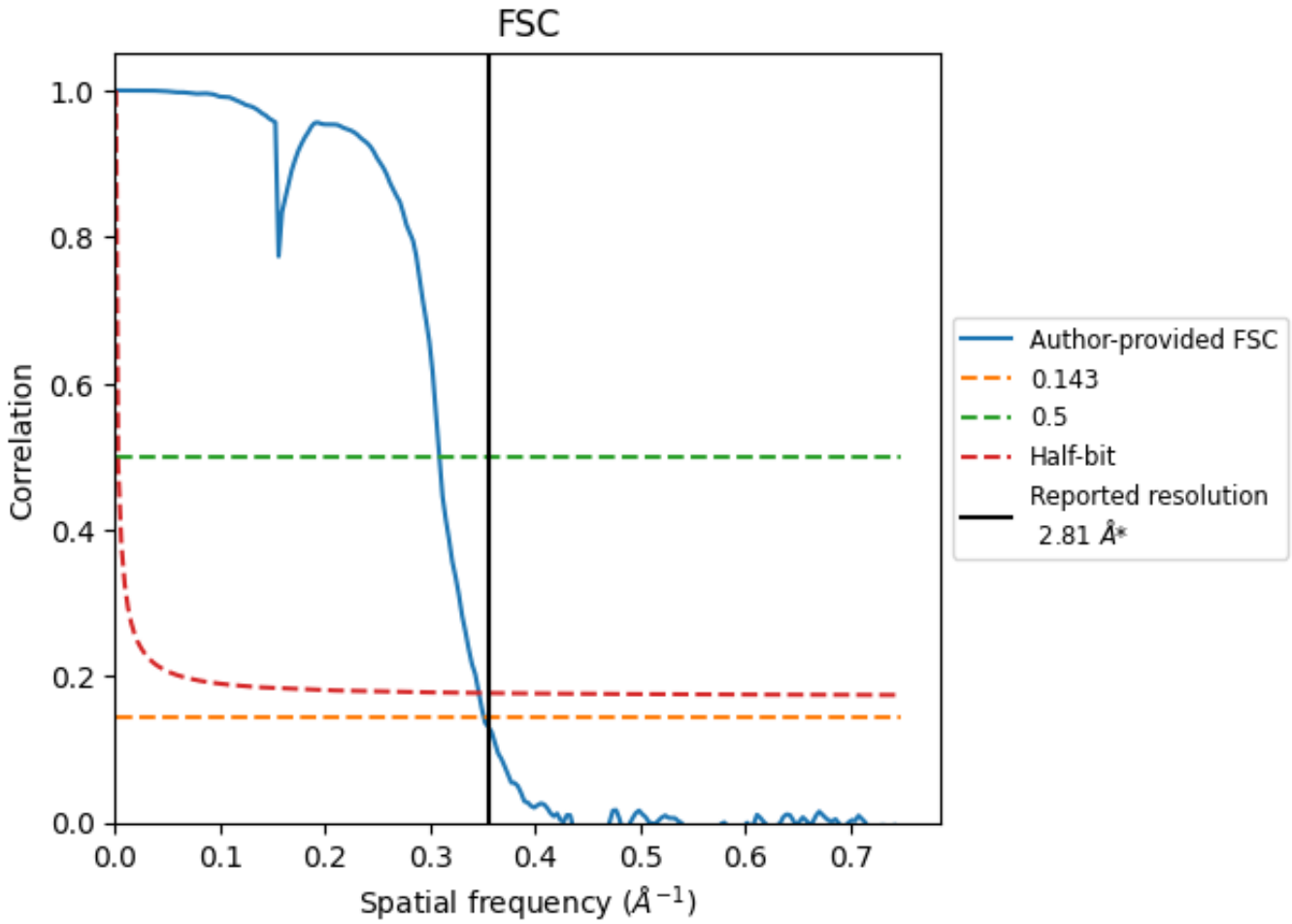


*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

8.2 Resolution estimates (i)

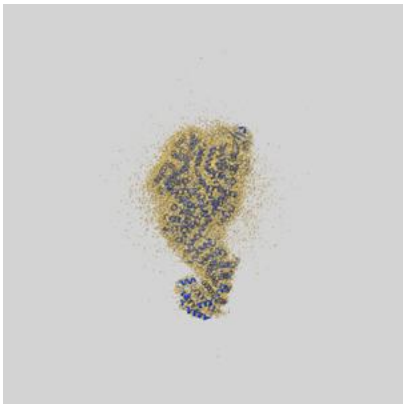
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.85	3.24	2.89
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

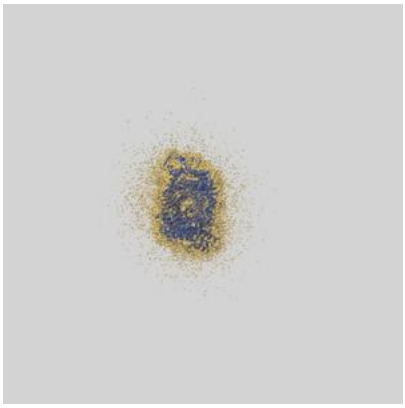
This section contains information regarding the fit between EMDB map EMD-32643 and PDB model 7WO9. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay



X

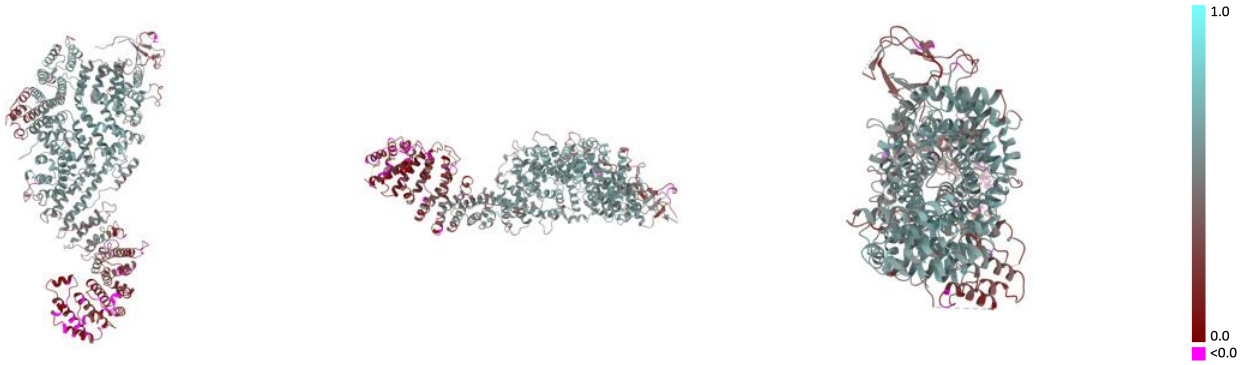
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

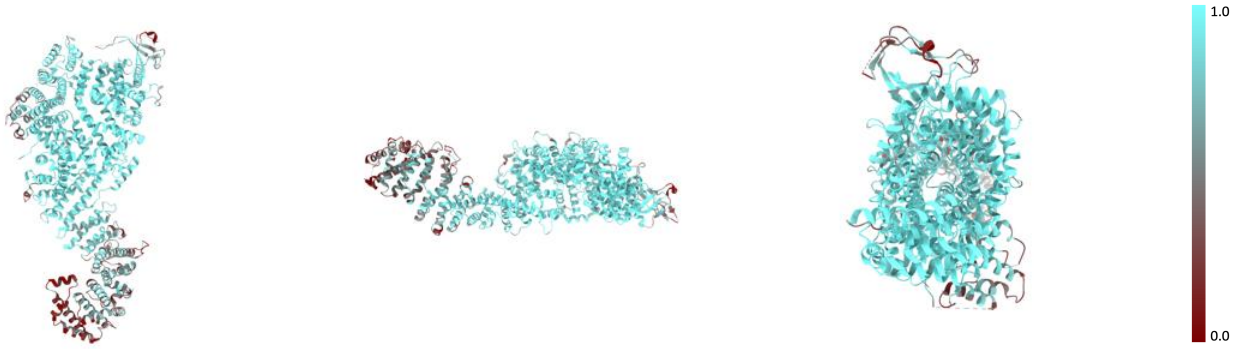
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

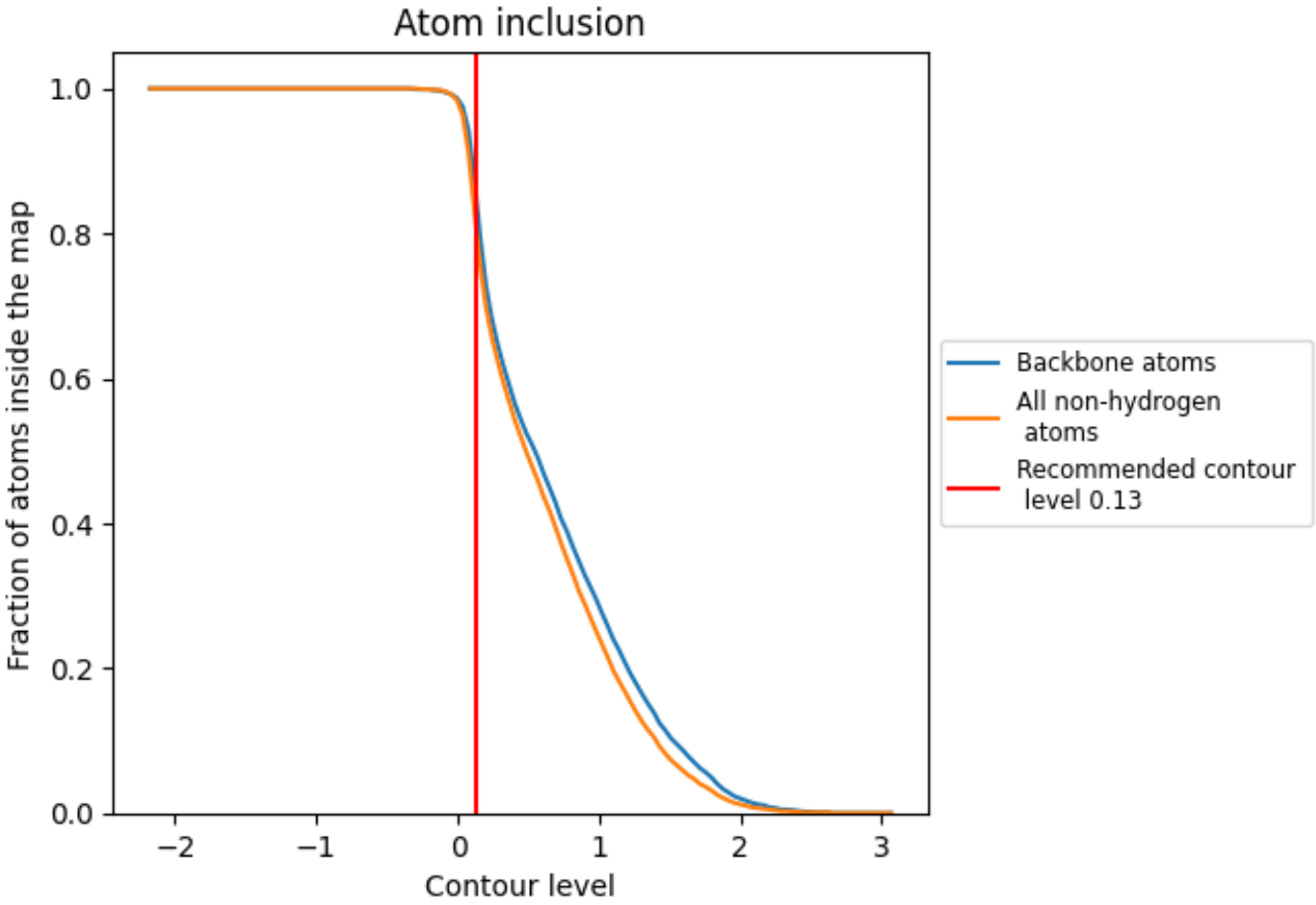
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.4460
A	0.8090	0.4460