



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 03:46 PM JST

PDB ID : 7ELC
EMDB ID : EMD-31180
Title : Structure of monomeric complex of MACV L bound to Z and 3'-vRNA
Authors : Xu, X.; Peng, R.; Peng, Q.; Shi, Y.
Deposited on : 2021-04-09
Resolution : 3.10 Å (reported)
Based on initial models : 6KLD, 5I72

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.dev113
MolProbity : 4.02b-467
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) : 2.39

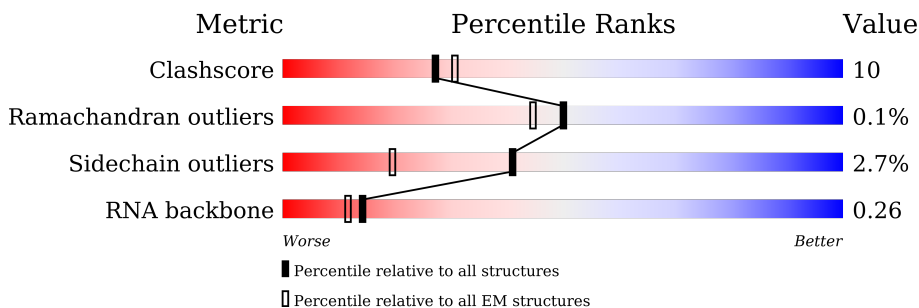
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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
RNA backbone	6643	2191

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	2209	
2	B	94	
3	C	19	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11754 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1409	Total	C	N	O	S	0	0
			11193	7135	1904	2080	74		

- Molecule 2 is a protein called RING finger protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	49	Total	C	N	O	S	0	0
			407	257	73	68	9		

- Molecule 3 is a RNA chain called 3'-vRNA promoter.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	7	Total	C	N	O	P	0	0
			149	66	25	51	7		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mn	0
			1	1	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Zn	0
			2	2	
5	B	2	Total	Zn	0
			2	2	



T81
SER
ILE
THR
VAL
PRO
VAL
GLU
PRO
SER
ALA
PRO
PRO
PRO

- Molecule 3: 3'-vRNA promoter



G	C	C	U	A	G	G	A	U	U	C	C	A	C13	U14	G15	U16	G17	C18	G19
---	---	---	---	---	---	---	---	---	---	---	---	---	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.192	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN

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	0.25	0/11386	0.42	0/15342
2	B	0.24	0/419	0.46	0/569
3	C	0.19	0/165	0.71	0/255
All	All	0.25	0/11970	0.43	0/16166

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11193	0	11253	215	0
2	B	407	0	383	13	0
3	C	149	0	76	4	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
All	All	11754	0	11712	226	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 10.

All (226) 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:539:LEU:HA	1:A:560:SER:O	1.73	0.88
1:A:97:THR:HA	1:A:135:VAL:HG21	1.60	0.82
2:B:58:CYS:SG	2:B:61:CYS:HB2	2.25	0.76
1:A:456:PRO:HG2	1:A:525:LEU:HB2	1.70	0.73
2:B:55:HIS:HE1	2:B:75:CYS:HB3	1.51	0.73
1:A:1420:ASP:OD1	1:A:1476:ARG:NH1	2.24	0.71
1:A:1739:SER:O	1:A:1743:ASN:ND2	2.26	0.69
1:A:274:GLY:HA3	1:A:672:VAL:HG21	1.75	0.68
2:B:55:HIS:CE1	2:B:75:CYS:HB3	2.29	0.68
1:A:287:CYS:SG	1:A:472:HIS:HE1	2.16	0.67
1:A:157:ILE:HA	1:A:160:ILE:HD12	1.76	0.67
1:A:632:LEU:HB2	1:A:703:CYS:HB3	1.76	0.67
1:A:99:ILE:HG12	1:A:138:VAL:HB	1.77	0.66
1:A:358:VAL:HG13	1:A:444:LEU:HD21	1.78	0.66
1:A:775:VAL:HG11	1:A:1200:LEU:HD13	1.79	0.65
1:A:1291:GLY:HA3	1:A:1294:ILE:HD12	1.78	0.64
1:A:697:LEU:HD23	1:A:1393:THR:HG21	1.78	0.64
1:A:1470:ASP:HB3	1:A:1722:LYS:H	1.62	0.64
1:A:412:ASN:O	1:A:416:ASN:ND2	2.30	0.64
1:A:1187:TYR:HA	1:A:1373:SER:HB2	1.80	0.63
1:A:502:LYS:HG3	1:A:1619:ILE:HG23	1.81	0.63
1:A:93:LEU:HD13	1:A:98:LEU:HB3	1.82	0.62
1:A:1409:CYS:HB3	1:A:1415:LEU:HD22	1.79	0.62
1:A:724:PHE:O	1:A:728:LYS:NZ	2.33	0.62
1:A:1560:LEU:HD13	1:A:1562:LEU:HD13	1.82	0.61
1:A:723:LYS:NZ	1:A:1128:ASN:O	2.33	0.61
1:A:331:LEU:O	1:A:335:ASN:ND2	2.34	0.61
1:A:1419:ILE:HG21	1:A:1443:VAL:HG21	1.83	0.60
1:A:549:GLY:O	1:A:553:ARG:NH2	2.35	0.60
1:A:1516:ILE:HD11	1:A:1774:ASP:HB3	1.84	0.60
1:A:1688:THR:HB	1:A:1788:ILE:HD12	1.84	0.59
1:A:587:VAL:HG11	1:A:1404:LEU:HD21	1.85	0.59
1:A:588:LEU:HD13	1:A:621:LEU:HD11	1.85	0.59
1:A:1159:THR:HB	1:A:1304:LEU:HD22	1.86	0.58
1:A:1178:VAL:O	2:B:36:ARG:NH1	2.36	0.58
1:A:456:PRO:HB2	1:A:525:LEU:HD12	1.85	0.58
1:A:68:PHE:HB2	1:A:71:VAL:HG23	1.85	0.58
1:A:186:ARG:NH2	1:A:1101:SER:OG	2.33	0.57
1:A:553:ARG:NH1	1:A:555:TYR:OH	2.35	0.57
1:A:455:ARG:HE	1:A:524:ARG:HB3	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1138:THR:O	1:A:1142:THR:HG23	2.03	0.57
1:A:1715:PHE:HB3	1:A:1805:GLN:HB2	1.85	0.57
1:A:1736:VAL:HG21	1:A:1793:LEU:HD11	1.88	0.56
1:A:395:ASP:HB3	1:A:398:GLU:HG2	1.89	0.55
1:A:1166:GLU:OE1	1:A:1169:ARG:NH2	2.39	0.55
1:A:147:TYR:HB3	1:A:157:ILE:HD13	1.87	0.55
1:A:497:LEU:HD11	1:A:571:PHE:HZ	1.70	0.55
1:A:39:LEU:HD21	1:A:168:LEU:HD13	1.89	0.55
1:A:289:ASN:HD22	1:A:292:MET:HG3	1.72	0.55
1:A:553:ARG:HH12	1:A:575:PRO:HG3	1.72	0.55
2:B:55:HIS:HE1	2:B:75:CYS:CB	2.14	0.55
1:A:539:LEU:HB3	1:A:561:ASP:HA	1.88	0.54
1:A:1177:ALA:HB1	1:A:1182:ASP:HB2	1.89	0.54
1:A:1650:CYS:HB2	1:A:1667:SER:HB2	1.89	0.54
1:A:1780:ASP:OD2	1:A:1788:ILE:N	2.41	0.53
1:A:273:LEU:HB2	1:A:656:VAL:HG12	1.90	0.53
1:A:231:ARG:HG3	1:A:789:ARG:HH12	1.73	0.53
1:A:1105:PHE:HA	1:A:1110:SER:HA	1.91	0.53
1:A:345:THR:OG1	1:A:348:ASN:ND2	2.41	0.53
1:A:502:LYS:NZ	3:C:17:G:N7	2.56	0.53
1:A:769:ASP:OD1	1:A:772:THR:OG1	2.20	0.53
2:B:39:CYS:CB	2:B:42:CYS:SG	2.96	0.53
1:A:627:ARG:NE	1:A:658:GLU:O	2.41	0.52
1:A:1417:GLU:O	1:A:1421:THR:HG23	2.09	0.52
1:A:1639:TYR:HB2	1:A:1642:GLU:HG3	1.92	0.52
1:A:236:ARG:HA	1:A:1316:LEU:HD11	1.92	0.52
1:A:1142:THR:HG22	1:A:1231:HIS:CE1	2.45	0.51
1:A:1551:ASN:HD22	1:A:1676:LYS:HD2	1.74	0.51
1:A:285:PRO:HG2	1:A:615:LEU:HD21	1.92	0.51
1:A:644:ASN:HB3	1:A:1376:GLY:HA3	1.93	0.51
1:A:536:ALA:HB3	1:A:539:LEU:HG	1.91	0.51
1:A:185:GLN:HE22	1:A:1103:THR:HG23	1.75	0.51
1:A:1425:GLN:O	1:A:1429:ASN:ND2	2.44	0.51
2:B:46:ASP:OD1	2:B:46:ASP:N	2.43	0.50
1:A:499:ASN:ND2	1:A:1449:TYR:OH	2.38	0.50
1:A:1414:GLN:O	1:A:1418:THR:HG23	2.12	0.50
1:A:1388:VAL:HG12	1:A:1389:MET:H	1.77	0.50
1:A:1582:ILE:HG13	1:A:1583:LYS:HD2	1.94	0.50
1:A:1270:PHE:O	1:A:1274:MET:HG3	2.13	0.49
1:A:1106:THR:OG1	1:A:1107:SER:N	2.45	0.49
1:A:1212:THR:OG1	1:A:1216:ARG:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:ILE:HD12	1:A:1281:PRO:HD2	1.95	0.49
1:A:710:THR:HG21	1:A:1121:TYR:CE2	2.48	0.49
1:A:1444:ASN:ND2	1:A:1461:GLU:OE1	2.46	0.49
1:A:638:PHE:HB2	1:A:655:LEU:HD13	1.94	0.49
1:A:745:THR:O	1:A:749:GLU:HG3	2.13	0.49
1:A:387:MET:HA	1:A:393:VAL:HG12	1.94	0.49
1:A:1204:LEU:HD22	1:A:1302:TYR:HD1	1.78	0.48
1:A:130:LEU:HD22	1:A:137:LEU:HD23	1.94	0.48
1:A:362:VAL:HG21	1:A:440:ASP:HB2	1.94	0.48
1:A:323:ILE:HD12	1:A:375:LEU:HD12	1.95	0.48
1:A:1490:GLU:CD	1:A:1490:GLU:H	2.16	0.48
1:A:1752:LEU:HD12	1:A:1753:THR:H	1.78	0.48
1:A:342:VAL:HG23	1:A:343:PHE:HD2	1.79	0.48
1:A:762:LYS:NZ	1:A:1363:SER:O	2.38	0.48
2:B:40:LYS:HG2	2:B:55:HIS:CG	2.49	0.47
1:A:1200:LEU:HD21	1:A:1302:TYR:CZ	2.49	0.47
1:A:1687:LEU:HD23	1:A:1779:LEU:HD11	1.94	0.47
1:A:1463:GLN:HE21	1:A:1468:TRP:HE1	1.62	0.47
1:A:1770:LEU:HD13	1:A:1773:LEU:HD12	1.96	0.47
1:A:37:PRO:HA	1:A:40:THR:HG23	1.97	0.47
1:A:289:ASN:HB3	1:A:292:MET:HB2	1.96	0.47
1:A:558:TYR:HD2	1:A:565:MET:HG2	1.80	0.47
1:A:722:GLU:HG2	1:A:1266:SER:HB3	1.97	0.47
1:A:794:VAL:HG11	1:A:1304:LEU:HD21	1.97	0.47
1:A:1463:GLN:NE2	1:A:1468:TRP:HE1	2.12	0.47
1:A:327:TYR:HB2	1:A:376:ARG:HH12	1.79	0.46
1:A:623:SER:O	1:A:623:SER:OG	2.30	0.46
1:A:735:VAL:HG13	1:A:1285:MET:HB3	1.96	0.46
1:A:364:ILE:HD13	1:A:376:ARG:HH11	1.79	0.46
1:A:802:PRO:HB3	1:A:1151:ALA:HB3	1.97	0.46
1:A:1211:ARG:HG3	1:A:1216:ARG:HA	1.97	0.46
1:A:236:ARG:HG2	1:A:1316:LEU:HD11	1.96	0.46
1:A:233:SER:O	1:A:237:GLU:HG3	2.15	0.46
1:A:46:LEU:HD11	1:A:157:ILE:HD11	1.97	0.46
1:A:112:PHE:HE1	1:A:143:GLY:HA3	1.80	0.46
1:A:495:LEU:HD23	3:C:18:C:C2	2.51	0.46
1:A:744:LEU:HG	1:A:1108:ILE:HD13	1.98	0.46
1:A:1171:ILE:HA	1:A:1174:MET:HE3	1.98	0.46
1:A:1527:LEU:HB2	1:A:1680:TRP:HB2	1.96	0.46
1:A:1537:SER:O	1:A:1541:VAL:HG23	2.16	0.46
1:A:1518:LEU:HD11	1:A:1529:GLY:HA3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HA	1:A:167:ILE:HG12	1.98	0.46
1:A:359:ASN:HA	1:A:362:VAL:HG12	1.97	0.45
1:A:480:SER:O	1:A:484:MET:HG2	2.16	0.45
1:A:1512:GLU:OE2	1:A:1769:ARG:NH2	2.48	0.45
2:B:39:CYS:C	2:B:41:CYS:H	2.20	0.45
1:A:104:PHE:HD2	1:A:106:ARG:HG2	1.81	0.45
1:A:1197:SER:HB2	1:A:1288:LEU:HA	1.97	0.45
1:A:343:PHE:CE1	1:A:417:CYS:HB2	2.51	0.45
1:A:1388:VAL:HG12	1:A:1389:MET:N	2.31	0.45
1:A:743:LYS:HE2	1:A:743:LYS:HB2	1.77	0.45
1:A:501:MET:SD	1:A:576:LYS:HB3	2.57	0.45
1:A:501:MET:HG3	1:A:550:GLU:HA	1.98	0.45
1:A:1364:LYS:HA	1:A:1364:LYS:HD3	1.67	0.45
1:A:1486:HIS:CD2	1:A:1487:ASP:H	2.34	0.45
1:A:89:ASP:N	1:A:102:GLU:OE1	2.39	0.45
1:A:270:LEU:HD22	1:A:638:PHE:CE2	2.51	0.45
1:A:1754:PRO:HG2	1:A:1755:PHE:CD1	2.52	0.45
1:A:541:GLY:HA2	1:A:559:LEU:HD23	1.99	0.45
1:A:43:PHE:HE2	1:A:191:LEU:HD11	1.82	0.44
1:A:206:HIS:O	1:A:206:HIS:ND1	2.50	0.44
1:A:1167:PHE:CE1	1:A:1383:LYS:HD2	2.52	0.44
1:A:382:VAL:HB	1:A:565:MET:SD	2.56	0.44
1:A:801:ASN:HA	1:A:802:PRO:HD3	1.90	0.44
1:A:1152:VAL:O	1:A:1156:MET:HG2	2.17	0.44
1:A:1471:GLY:O	1:A:1476:ARG:NH2	2.48	0.44
1:A:534:TYR:HA	1:A:540:VAL:HG23	1.99	0.44
1:A:713:ARG:NH2	1:A:1121:TYR:OH	2.50	0.44
1:A:1195:THR:O	1:A:1366:ASN:ND2	2.49	0.44
1:A:1528:THR:HG23	1:A:1541:VAL:HG11	2.00	0.44
1:A:1702:LYS:HG3	1:A:1813:ILE:HB	1.99	0.44
1:A:1232:LEU:HD11	1:A:1287:VAL:HG13	2.00	0.44
1:A:51:GLU:HA	1:A:103:THR:HG21	2.00	0.44
1:A:380:LEU:H	1:A:380:LEU:HD23	1.81	0.44
1:A:458:MET:HB3	1:A:523:VAL:HG23	1.99	0.44
1:A:1187:TYR:CE1	1:A:1375:ILE:HD11	2.53	0.44
1:A:285:PRO:HG2	1:A:615:LEU:HD11	2.00	0.44
1:A:1655:CYS:SG	1:A:1664:CYS:N	2.91	0.44
1:A:327:TYR:HB2	1:A:376:ARG:NH1	2.33	0.44
1:A:1115:LEU:HA	1:A:1138:THR:HB	2.00	0.44
1:A:1142:THR:HG22	1:A:1231:HIS:HE1	1.82	0.44
1:A:193:ASN:OD1	1:A:194:VAL:N	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:CYS:HB3	1:A:1166:GLU:HG3	2.01	0.43
1:A:654:LYS:HE2	1:A:1371:PRO:HG2	2.01	0.43
1:A:728:LYS:NZ	1:A:1289:ASP:OD2	2.51	0.43
1:A:238:GLU:HG2	1:A:782:TYR:CE2	2.54	0.43
1:A:414:VAL:HA	1:A:417:CYS:SG	2.58	0.43
1:A:1246:TYR:CD1	1:A:1267:GLU:HG3	2.53	0.43
1:A:1578:VAL:HB	1:A:1582:ILE:HD11	1.99	0.43
1:A:553:ARG:NH1	1:A:575:PRO:HG3	2.33	0.43
1:A:559:LEU:HD23	1:A:559:LEU:HA	1.86	0.43
1:A:400:VAL:HG11	1:A:444:LEU:HB3	2.01	0.42
1:A:164:LEU:HD12	1:A:167:ILE:HD11	2.00	0.42
1:A:1482:GLU:OE1	1:A:1814:ARG:NH2	2.52	0.42
1:A:1693:LEU:O	1:A:1696:TRP:NE1	2.52	0.42
1:A:1742:ARG:HD2	1:A:1769:ARG:NH1	2.33	0.42
2:B:58:CYS:SG	2:B:61:CYS:N	2.77	0.42
1:A:1272:GLN:O	1:A:1276:LEU:HB2	2.18	0.42
1:A:1527:LEU:HD23	1:A:1680:TRP:HE3	1.84	0.42
1:A:474:LEU:O	1:A:477:GLU:N	2.41	0.42
1:A:634:GLY:O	1:A:655:LEU:HD22	2.19	0.42
1:A:756:LEU:HD21	1:A:1232:LEU:HD21	2.02	0.42
1:A:1194:PRO:HD3	1:A:1292:GLN:HE21	1.85	0.42
1:A:1440:SER:HB3	1:A:1459:ALA:HB1	2.02	0.42
2:B:58:CYS:SG	2:B:61:CYS:CB	2.99	0.42
1:A:1743:ASN:O	1:A:1745:PRO:HD3	2.18	0.42
1:A:636:ARG:HB2	1:A:700:SER:OG	2.20	0.42
1:A:693:PHE:CZ	1:A:1379:VAL:HG21	2.55	0.42
1:A:1209:GLU:HG3	1:A:1211:ARG:HH21	1.85	0.42
1:A:73:LEU:HD21	1:A:98:LEU:HD22	2.02	0.42
1:A:687:LEU:HD21	2:B:64:THR:HG21	2.02	0.42
1:A:60:CYS:SG	1:A:90:GLY:HA3	2.60	0.42
1:A:508:ARG:HH11	1:A:512:ASN:HB2	1.85	0.42
1:A:637:TYR:CE2	1:A:1372:LYS:HD2	2.55	0.42
1:A:502:LYS:HE2	3:C:15:G:H1'	2.02	0.42
1:A:498:ILE:HG22	1:A:1619:ILE:HD11	2.02	0.41
1:A:1327:SER:O	1:A:1327:SER:OG	2.34	0.41
1:A:773:PRO:HA	1:A:1368:PHE:CZ	2.55	0.41
1:A:1270:PHE:CZ	1:A:1281:PRO:HG2	2.55	0.41
1:A:1427:ILE:CG1	1:A:1436:VAL:HG21	2.49	0.41
1:A:580:LEU:O	1:A:584:SER:OG	2.36	0.41
1:A:1619:ILE:HD13	1:A:1619:ILE:HA	1.84	0.41
2:B:54:ASP:OD1	2:B:54:ASP:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:HG22	1:A:376:ARG:NH1	2.35	0.41
1:A:574:ASP:OD1	1:A:575:PRO:HD2	2.20	0.41
1:A:1223:SER:O	1:A:1227:ILE:HG13	2.20	0.41
1:A:222:LEU:HD21	1:A:1202:LEU:HD13	2.03	0.41
1:A:544:PHE:HE2	1:A:558:TYR:HB2	1.85	0.41
1:A:681:GLY:HA3	1:A:685:ALA:HB2	2.02	0.41
1:A:209:ARG:HA	1:A:209:ARG:HD2	1.72	0.41
1:A:1157:LYS:HE3	1:A:1158:TYR:CE2	2.56	0.41
1:A:1402:ALA:O	1:A:1406:ASN:ND2	2.54	0.41
1:A:1473:ARG:HB3	1:A:1791:HIS:HE1	1.85	0.41
1:A:1684:SER:O	1:A:1688:THR:HG23	2.20	0.41
1:A:1191:LYS:O	1:A:1195:THR:OG1	2.25	0.41
1:A:289:ASN:ND2	1:A:292:MET:HG3	2.33	0.40
1:A:705:LEU:HD23	1:A:1401:ALA:HB2	2.04	0.40
1:A:1655:CYS:SG	1:A:1664:CYS:HB2	2.60	0.40
1:A:1736:VAL:O	1:A:1740:ILE:HG13	2.21	0.40
1:A:299:THR:HG23	1:A:485:ARG:HB3	2.03	0.40
1:A:456:PRO:HA	1:A:558:TYR:CZ	2.56	0.40
1:A:1361:LEU:HD23	1:A:1361:LEU:HA	1.92	0.40
1:A:504:SER:N	3:C:15:G:O6	2.51	0.40
1:A:67:ARG:H	1:A:67:ARG:HG2	1.67	0.40
1:A:719:LYS:HE3	1:A:719:LYS:HB2	1.85	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	1377/2209 (62%)	1254 (91%)	122 (9%)	1 (0%)	48	79
2	B	47/94 (50%)	37 (79%)	10 (21%)	0	100	100
All	All	1424/2303 (62%)	1291 (91%)	132 (9%)	1 (0%)	50	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	738	PRO

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	1271/2007 (63%)	1241 (98%)	30 (2%)	44	70
2	B	47/88 (53%)	42 (89%)	5 (11%)	5	21
All	All	1318/2095 (63%)	1283 (97%)	35 (3%)	41	67

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	114	LYS
1	A	185	GLN
1	A	189	HIS
1	A	231	ARG
1	A	234	THR
1	A	261	THR
1	A	435	LEU
1	A	449	GLN
1	A	451	LEU
1	A	513	GLU
1	A	523	VAL
1	A	740	LEU
1	A	743	LYS
1	A	750	ASP
1	A	799	LYS
1	A	1174	MET
1	A	1290	MET
1	A	1317	LEU
1	A	1409	CYS
1	A	1426	CYS
1	A	1463	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1473	ARG
1	A	1511	PHE
1	A	1625	MET
1	A	1634	LYS
1	A	1693	LEU
1	A	1715	PHE
1	A	1717	TRP
1	A	1747	LEU
2	B	36	ARG
2	B	43	TRP
2	B	51	THR
2	B	66	LEU
2	B	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	125	ASN
1	A	148	ASN
1	A	149	ASN
1	A	185	GLN
1	A	189	HIS
1	A	289	ASN
1	A	442	ASN
1	A	449	GLN
1	A	472	HIS
1	A	522	ASN
1	A	546	GLN
1	A	647	HIS
1	A	741	ASN
1	A	771	GLN
1	A	788	ASN
1	A	1128	ASN
1	A	1206	GLN
1	A	1231	HIS
1	A	1275	GLN
1	A	1279	GLN
1	A	1331	GLN
1	A	1463	GLN
1	A	1486	HIS
1	A	1496	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1551	ASN
1	A	1712	ASN
1	A	1726	GLN
1	A	1734	ASN
1	A	1738	GLN
1	A	1743	ASN
1	A	1783	ASN
1	A	1791	HIS
1	A	1812	HIS
2	B	53	ASN
2	B	55	HIS
2	B	62	HIS
2	B	63	GLN
2	B	68	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	6/19 (31%)	4 (66%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	14	U
3	C	15	G
3	C	16	U
3	C	19	G

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

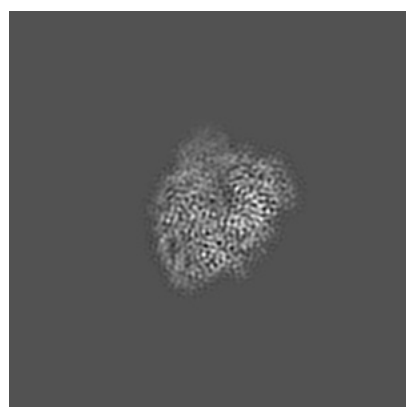
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31180. These allow visual inspection of the internal detail of the map and identification of artifacts.

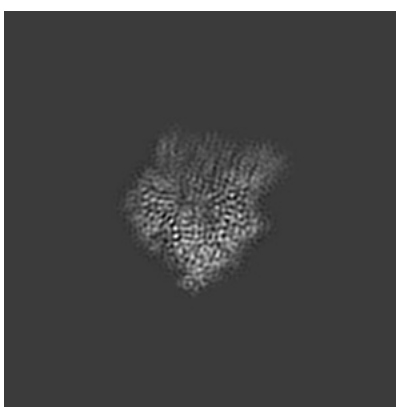
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

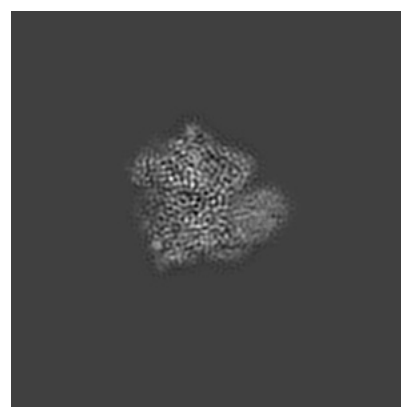
6.1.1 Primary map



X



Y

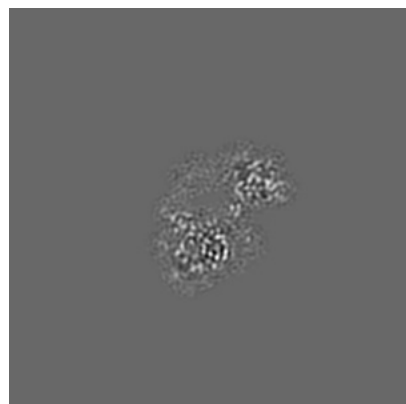


Z

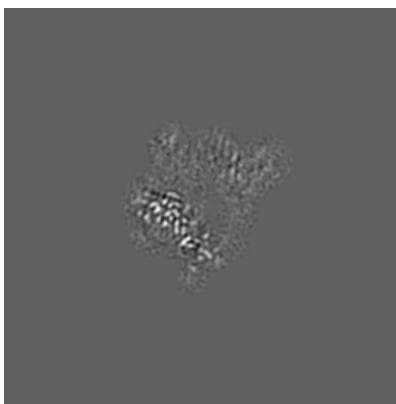
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

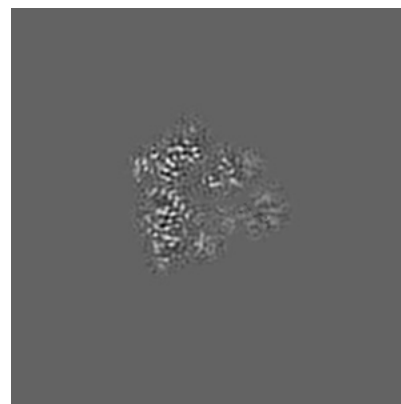
6.2.1 Primary map



X Index: 128



Y Index: 128

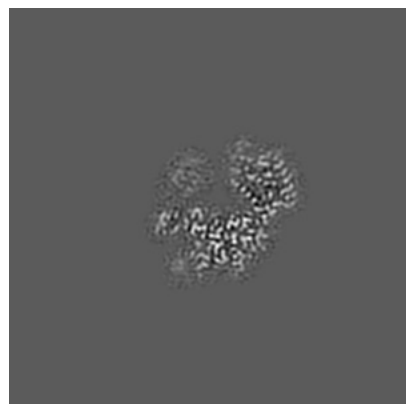


Z Index: 128

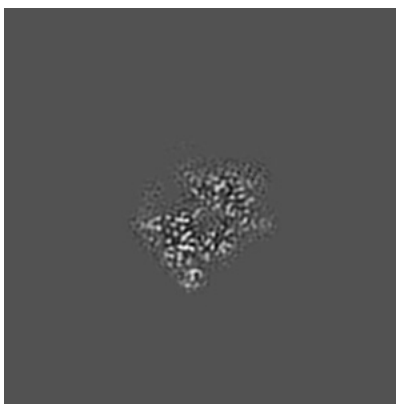
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

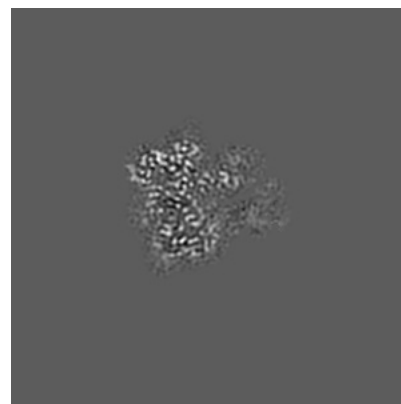
6.3.1 Primary map



X Index: 116



Y Index: 148

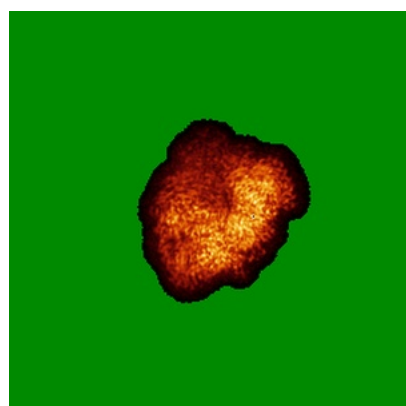


Z Index: 123

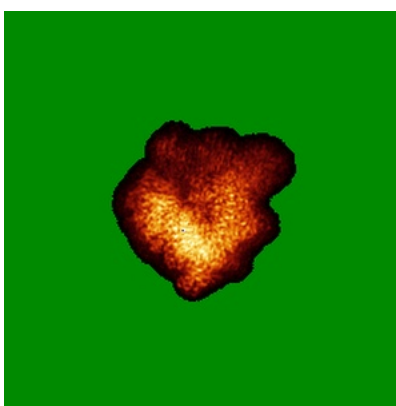
The images above show the largest variance slices of the map in three orthogonal directions.

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

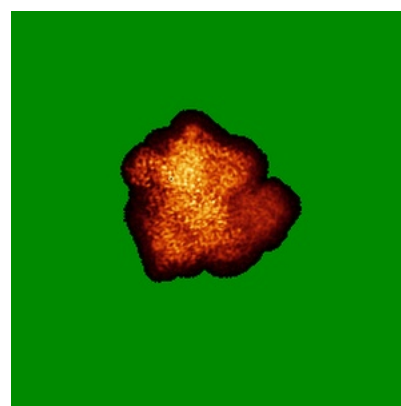
6.4.1 Primary map



X



Y

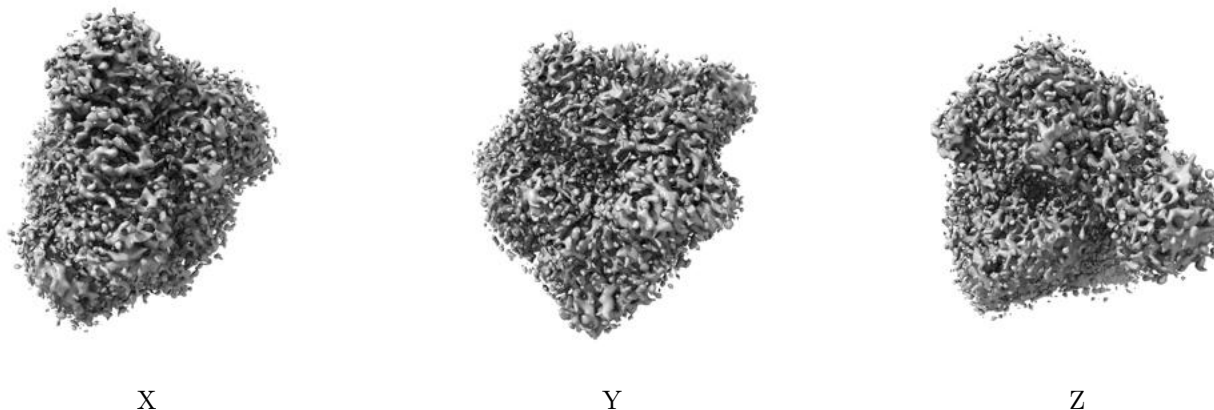


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

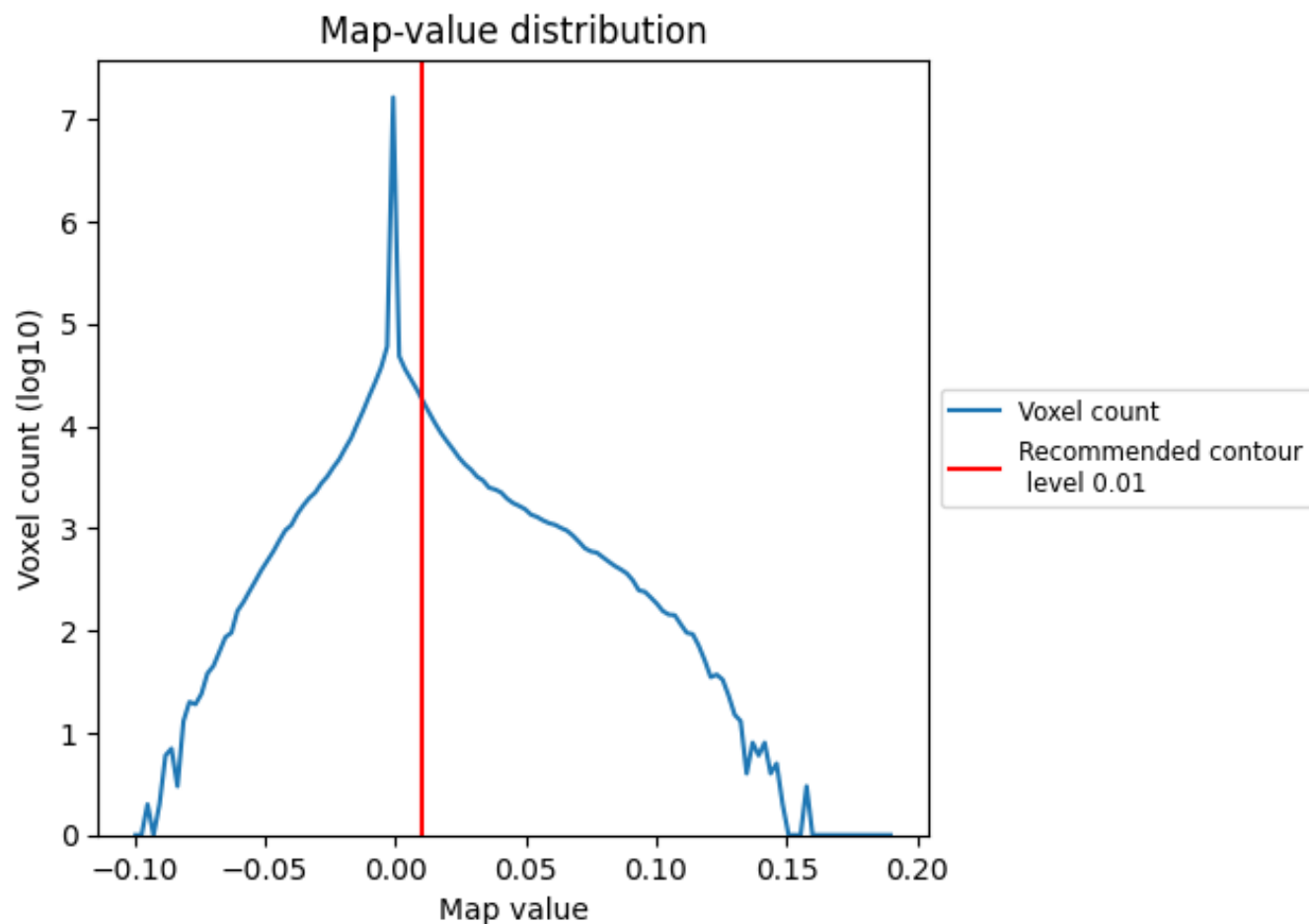
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

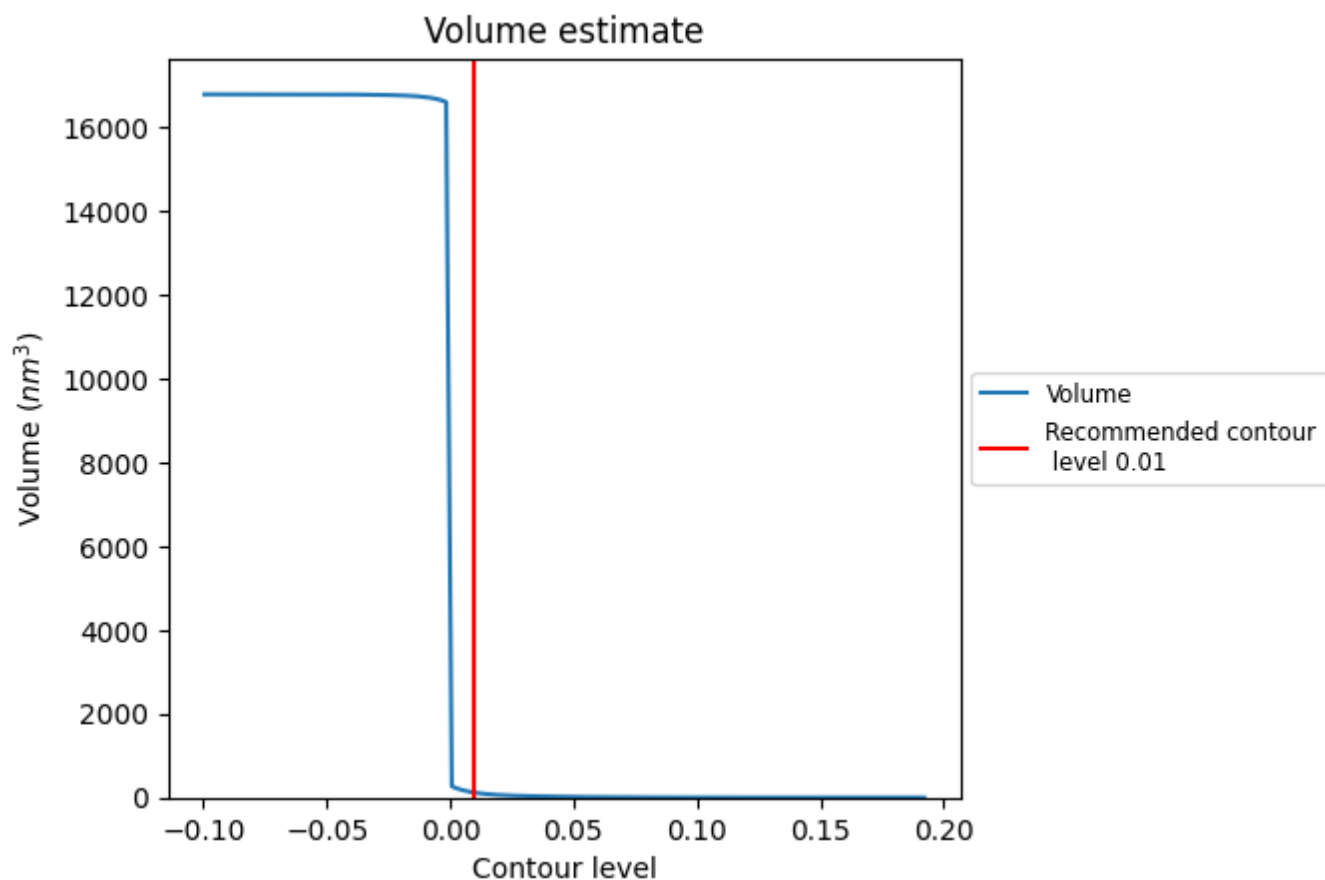
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

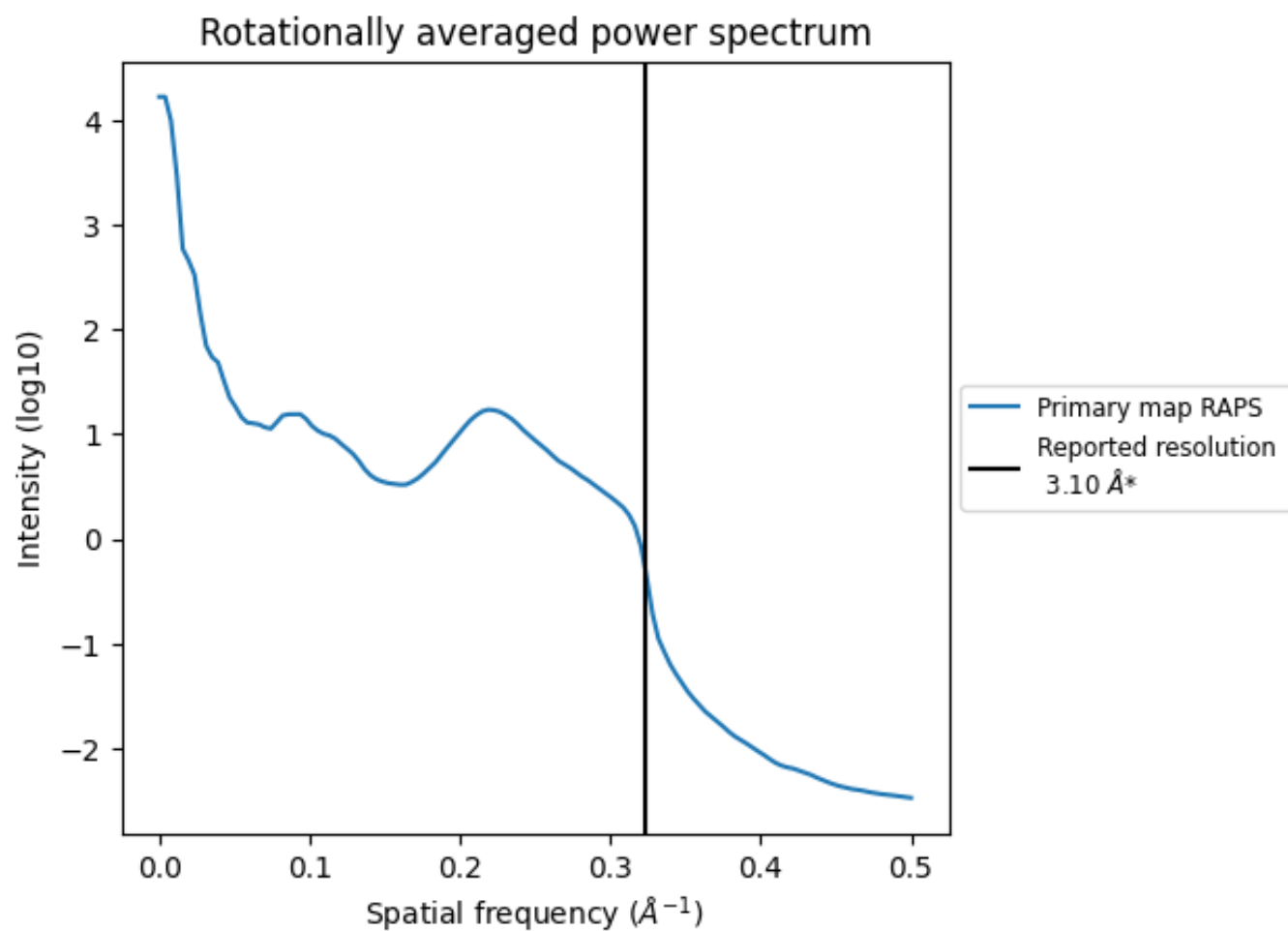
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm³; this corresponds to an approximate mass of 107 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 ⓘ

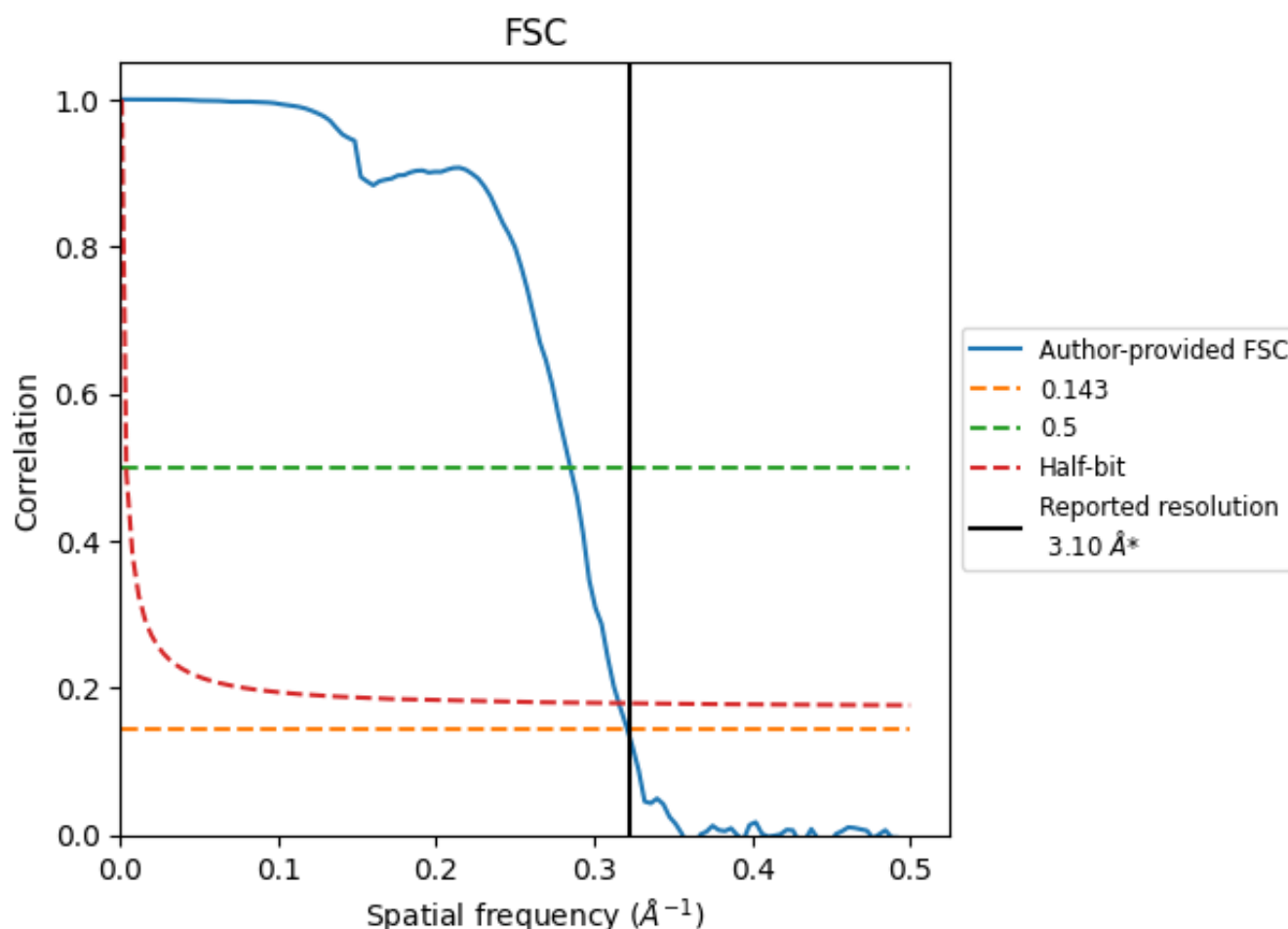


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

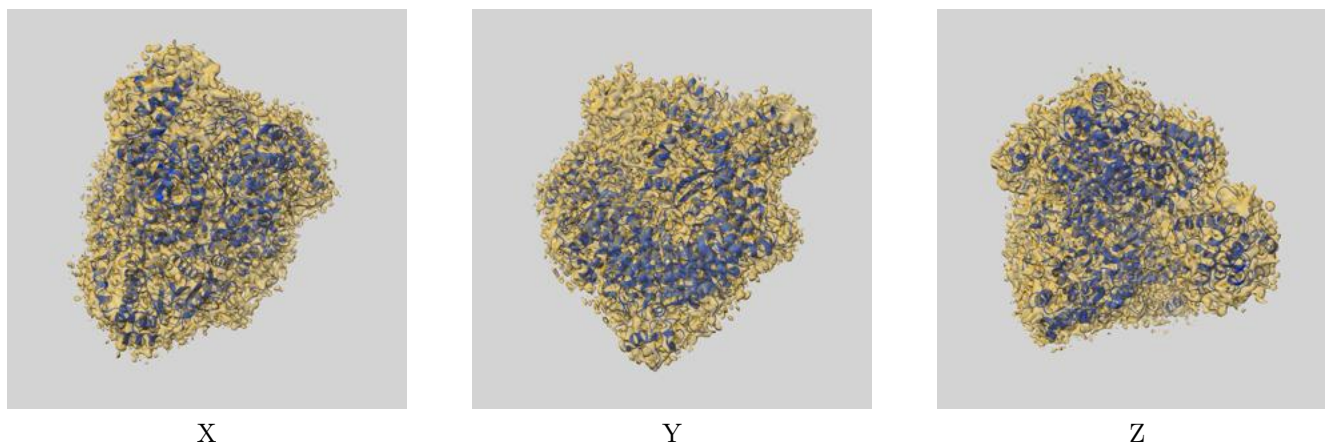
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.51	3.17
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

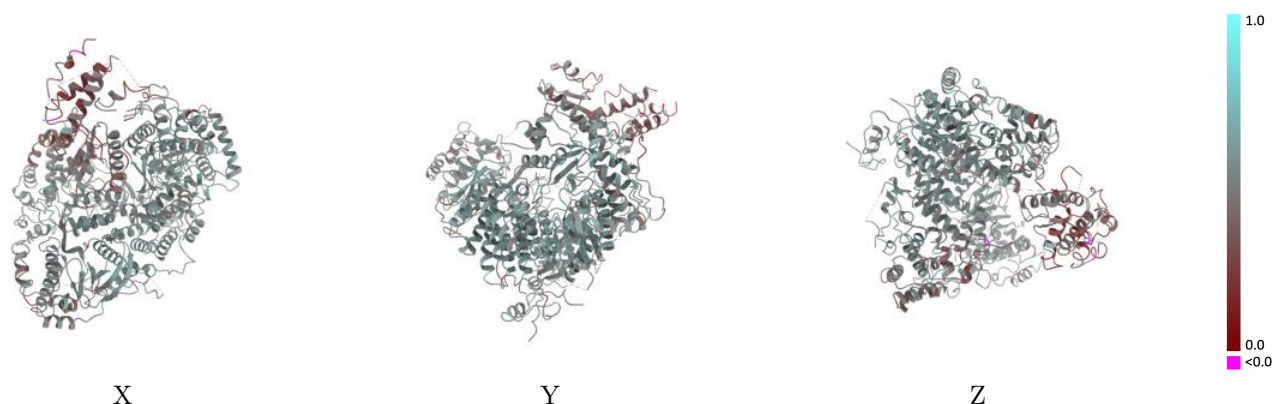
This section contains information regarding the fit between EMDB map EMD-31180 and PDB model 7ELC. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



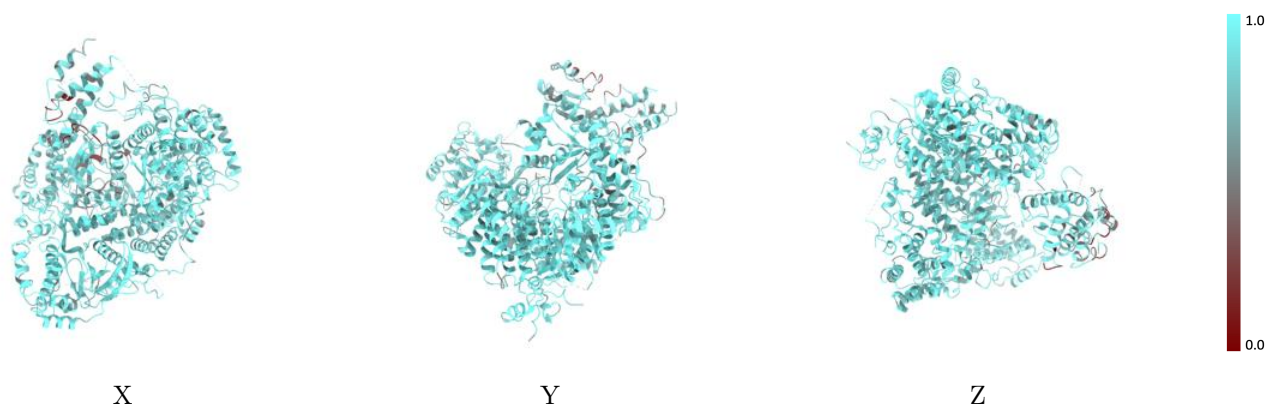
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



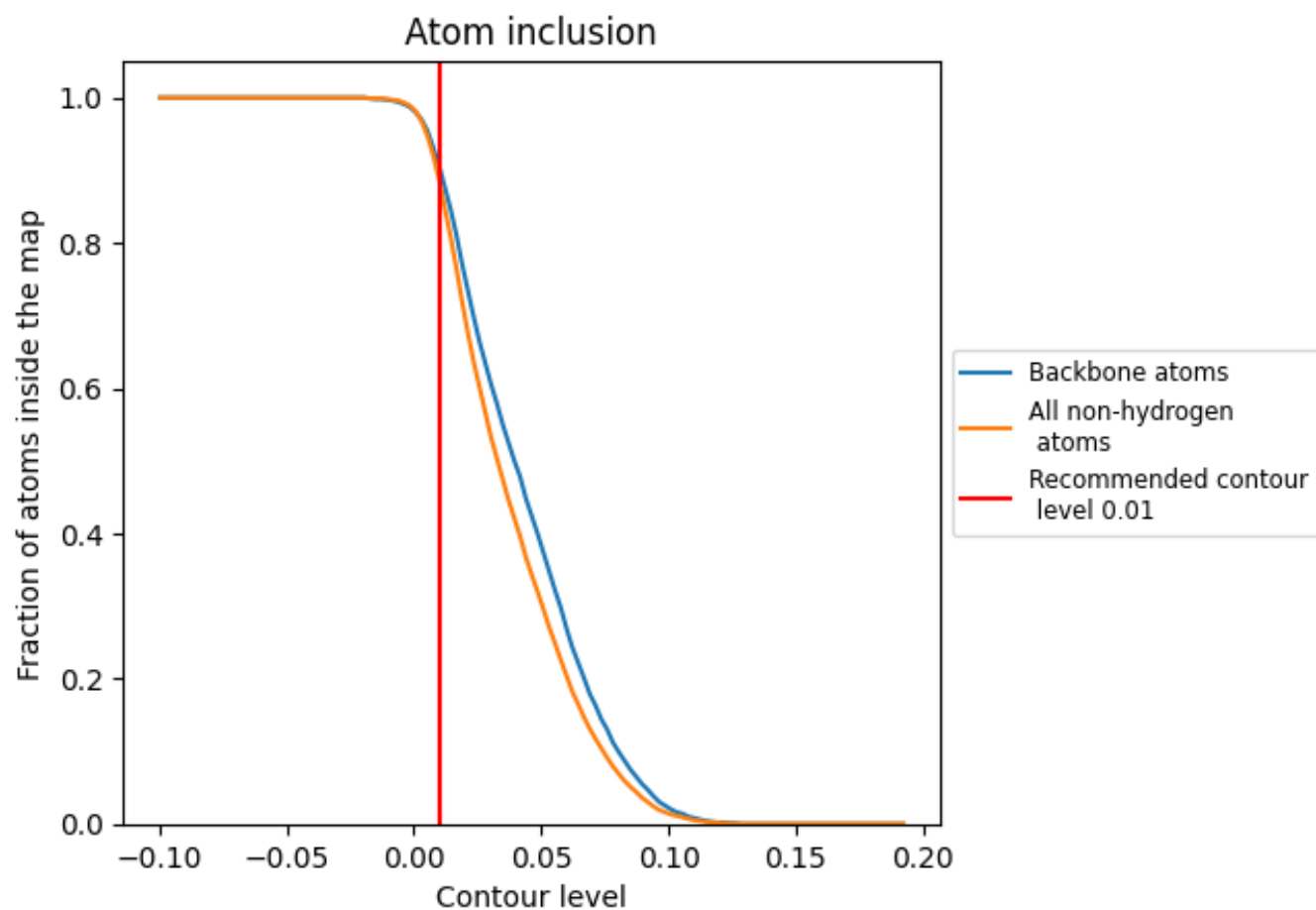
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8860	<div><div></div></div> 0.5010
A	<div><div></div></div> 0.8850	<div><div></div></div> 0.5010
B	<div><div></div></div> 0.9170	<div><div></div></div> 0.4970
C	<div><div></div></div> 0.8860	<div><div></div></div> 0.4880

