Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 02:31 PM JST

PDB ID	:	7ELD
EMDB ID	:	EMD-31181
Title	:	Cryo-EM structure of Arabidopsis DCL1 in complex with pri-miRNA 166f
Authors	:	Wei, X.; Ke, H.; Feng, Y.
Deposited on	:	2021-04-09
Resolution	:	4.60 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:

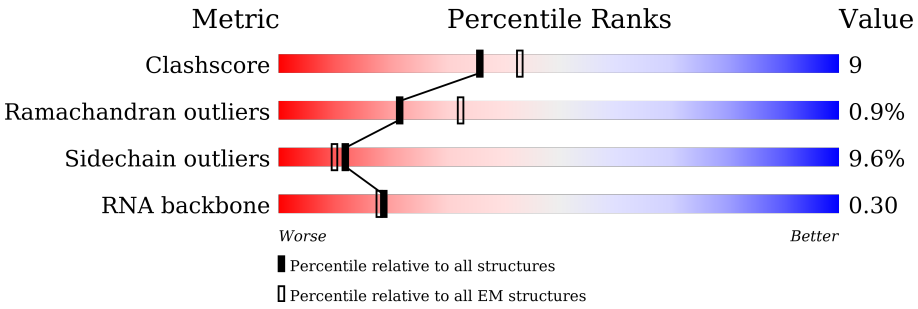
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.60 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
RNA backbone	4643	859

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	1909	43% 15% 40%
2	B	148	32% 37% 5% 26%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11282 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 Endoribonuclease Dicer homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1137	8976	5726	1548	1642	60	0	0

- Molecule 2 is a RNA chain called pri-miRNA 166f.

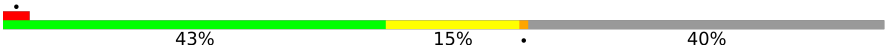
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	109	2306	1032	398	767	109	0	0

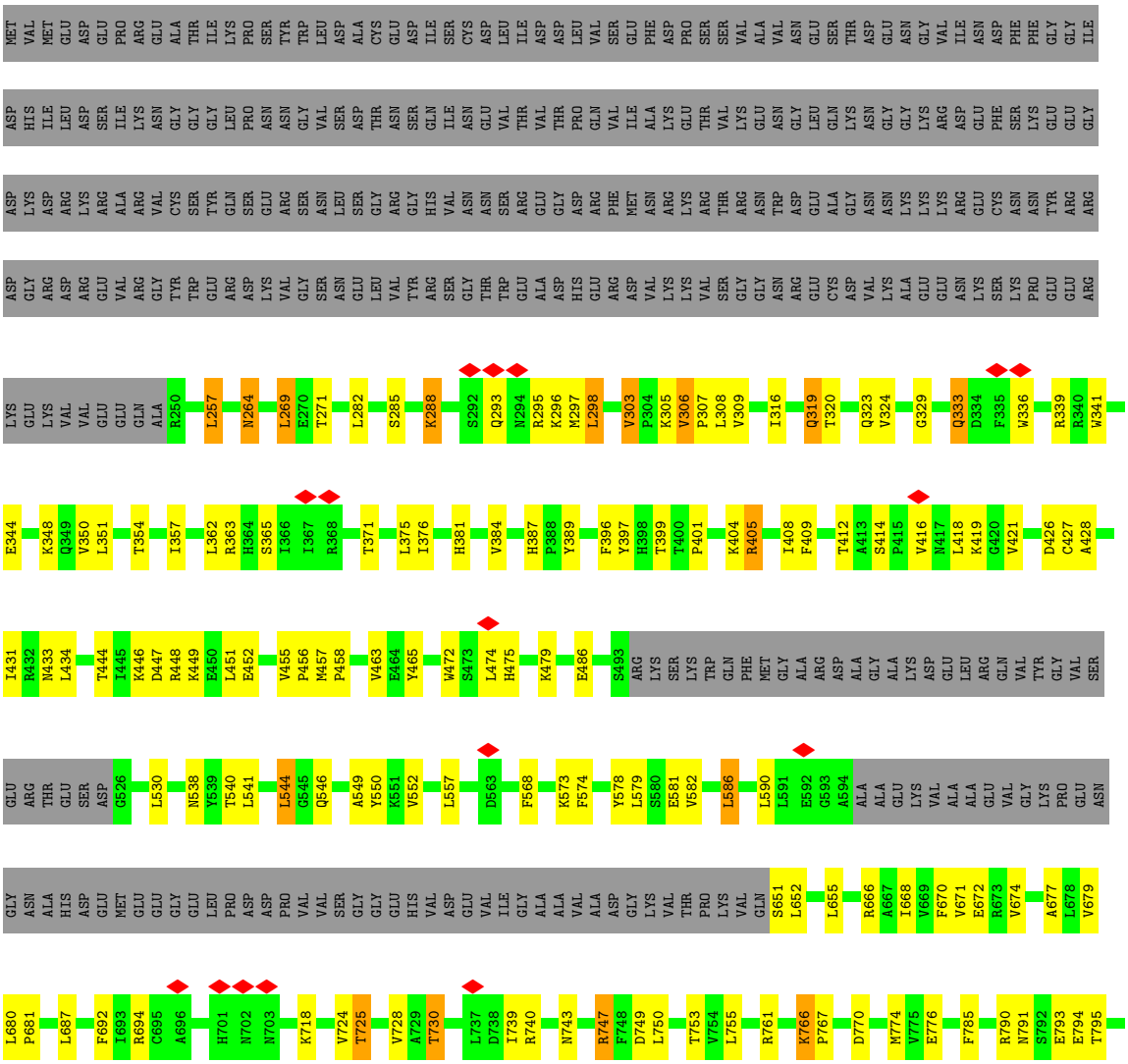
3 Residue-property plots (i)

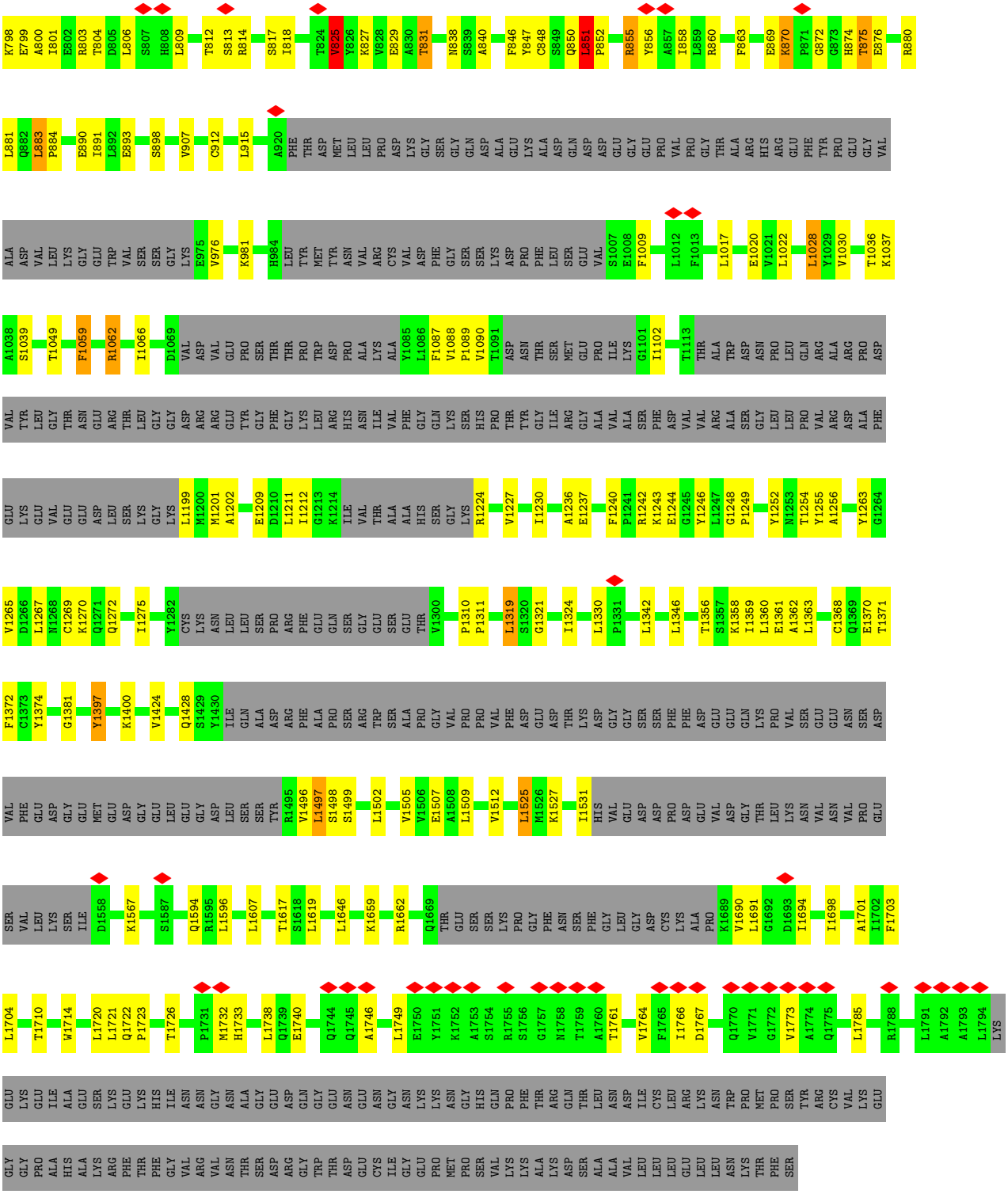
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Endoribonuclease Dicer homolog 1

Chain A:

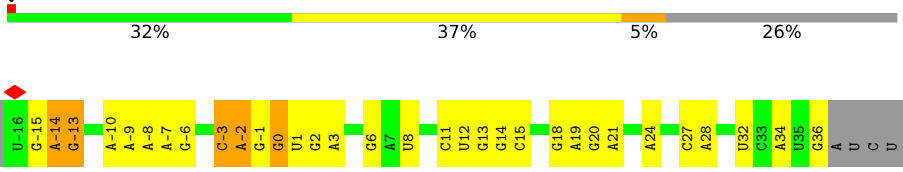


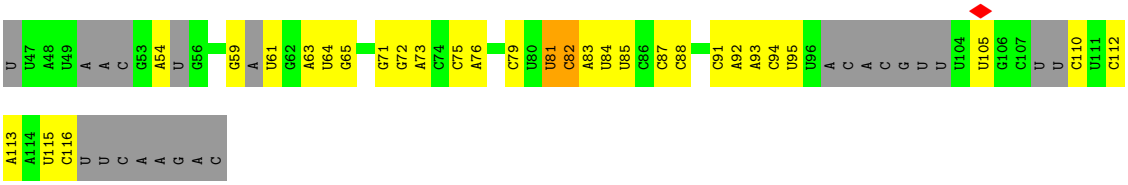




• Molecule 2: pri-miRNA 166f

Chain B:




U U47 A48 U49 A A C G53 A54 U G56 G59 A U61 G62 A63 U64 G65 G71 G72 A73 C74 C75 A76 C79 U80 U81 C82 A83 U84 U85 C86 C87 C88 C91 A92 A93 C94 U95 U96 A C A C G U U U104 U105 G106 C107 U U C110 U111 C112
A113 A114 U115 C116 U U C A A G A C

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	653929	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64	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	0.026	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	202.80002, 202.80002, 202.80002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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	0.66	0/9133	0.65	0/12319
2	B	0.21	0/2568	0.65	0/3981
All	All	0.59	0/11701	0.65	0/16300

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	8976	0	9149	165	0
2	B	2306	0	1175	24	0
All	All	11282	0	10324	184	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 9.

All (184) 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:840:ALA:HB2	1:A:912:CYS:HB2	1.41	1.02
1:A:264:ASN:HB3	1:A:408:ILE:H	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1346:LEU:HD22	1:A:1359:ILE:CG2	2.10	0.80
1:A:1346:LEU:HD22	1:A:1359:ILE:HG21	1.67	0.77
1:A:456:PRO:HG3	1:A:766:LYS:HA	1.66	0.76
1:A:578:TYR:O	1:A:581:GLU:HG3	1.86	0.76
1:A:860:ARG:HE	1:A:884:PRO:HG3	1.51	0.75
1:A:475:HIS:HB3	1:A:546:GLN:HE21	1.53	0.74
1:A:333:GLN:HB2	1:A:336:TRP:HB2	1.68	0.73
1:A:1017:LEU:HB3	1:A:1022:LEU:HD11	1.71	0.72
1:A:472:TRP:HB3	1:A:475:HIS:HB2	1.69	0.72
1:A:293:GLN:HB3	1:A:296:LYS:HB2	1.70	0.72
1:A:363:ARG:NE	1:A:838:ASN:HB3	2.06	0.71
1:A:427:CYS:HA	1:A:795:THR:HG22	1.73	0.70
1:A:671:VAL:HG21	1:A:677:ALA:HB2	1.73	0.70
2:B:59:G:O3'	2:B:61:U:H5"	1.93	0.69
1:A:428:ALA:HB1	1:A:431:ILE:HB	1.76	0.67
1:A:1428:GLN:HB3	1:A:1502:LEU:HD21	1.76	0.66
1:A:876:GLU:HG3	1:A:898:SER:HA	1.79	0.65
1:A:880:ARG:HA	1:A:893:GLU:HG3	1.80	0.64
1:A:1397:TYR:HB2	1:A:1400:LYS:HB2	1.78	0.64
1:A:463:VAL:HG11	1:A:655:LEU:HD21	1.79	0.63
1:A:1236:ALA:HB2	1:A:1267:LEU:HD23	1.80	0.63
1:A:306:VAL:HG13	1:A:307:PRO:HD3	1.81	0.62
1:A:1346:LEU:HD22	1:A:1359:ILE:HG22	1.83	0.61
1:A:1740:GLU:HG2	2:B:93:A:H4'	1.82	0.61
1:A:323:GLN:HB2	1:A:348:LYS:HA	1.83	0.60
1:A:1236:ALA:HB1	1:A:1256:ALA:HB2	1.83	0.60
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.32	0.60
1:A:381:HIS:HA	1:A:418:LEU:HD23	1.83	0.59
1:A:1646:LEU:HD21	1:A:1698:ILE:HG13	1.84	0.59
1:A:840:ALA:HB2	1:A:912:CYS:CB	2.25	0.59
1:A:568:PHE:HA	1:A:573:LYS:HE2	1.85	0.58
2:B:82:C:H2'	2:B:83:A:C8	2.39	0.58
1:A:418:LEU:HD21	1:A:434:LEU:HD22	1.85	0.58
1:A:1269:CYS:HB3	1:A:1272:GLN:HB2	1.86	0.58
1:A:672:GLU:HB2	1:A:749:ASP:HB2	1.85	0.57
1:A:452:GLU:HA	1:A:455:VAL:HB	1.85	0.57
1:A:825:VAL:HG22	1:A:831:THR:HG22	1.86	0.57
1:A:456:PRO:HG3	1:A:766:LYS:CA	2.34	0.57
1:A:666:ARG:HD3	1:A:725:THR:HG21	1.87	0.56
1:A:851:LEU:HB3	1:A:852:PRO:HD3	1.86	0.56
1:A:344:GLU:HG3	1:A:351:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:C:H4'	2:B:110:C:OP2	2.03	0.56
1:A:1346:LEU:HD13	1:A:1359:ILE:HG22	1.88	0.56
1:A:652:LEU:HB3	1:A:655:LEU:HD23	1.88	0.56
1:A:550:TYR:HB2	1:A:590:LEU:HB3	1.87	0.56
1:A:405:ARG:HB3	1:A:408:ILE:HD11	1.88	0.56
1:A:747:ARG:HG2	1:A:750:LEU:HB2	1.89	0.55
1:A:546:GLN:HB3	1:A:590:LEU:HD22	1.89	0.54
1:A:1497:LEU:HD12	1:A:1499:SER:HB2	1.89	0.54
1:A:578:TYR:O	1:A:582:VAL:HG23	2.08	0.54
2:B:91:C:H2'	2:B:92:A:C8	2.44	0.53
1:A:285:SER:HA	1:A:288:LYS:HE2	1.89	0.53
2:B:-3:C:H2'	2:B:-2:A:C8	2.44	0.53
1:A:1211:LEU:HB3	1:A:1224:ARG:HB3	1.89	0.53
1:A:869:GLU:HA	1:A:876:GLU:H	1.74	0.53
1:A:1062:ARG:HG2	1:A:1066:ILE:HD12	1.91	0.52
1:A:305:LYS:HD3	2:B:76:A:H5'	1.92	0.52
1:A:344:GLU:HG2	1:A:348:LYS:HD2	1.92	0.52
1:A:530:LEU:HD22	1:A:579:LEU:HD22	1.91	0.52
1:A:1009:PHE:HA	1:A:1089:PRO:HA	1.90	0.52
1:A:465:TYR:HA	1:A:774:MET:HB3	1.92	0.52
1:A:530:LEU:HB3	1:A:579:LEU:HD13	1.92	0.51
2:B:82:C:H2'	2:B:83:A:H8	1.74	0.51
1:A:305:LYS:HA	2:B:76:A:H5"	1.93	0.51
1:A:1202:ALA:HB2	1:A:1311:PRO:HG2	1.93	0.50
1:A:376:ILE:HG12	1:A:409:PHE:HB2	1.93	0.50
1:A:1263:TYR:HB2	1:A:1265:VAL:HG12	1.94	0.50
1:A:479:LYS:HE3	1:A:538:ASN:HB3	1.94	0.49
1:A:1059:PHE:HZ	1:A:1089:PRO:HD2	1.78	0.49
1:A:1248:GLY:N	1:A:1249:PRO:HD3	2.28	0.49
1:A:718:LYS:HB3	1:A:724:VAL:HG21	1.95	0.49
1:A:324:VAL:HG12	1:A:350:VAL:HB	1.93	0.48
1:A:799:GLU:C	1:A:801:ILE:H	2.15	0.48
1:A:855:ARG:HB3	1:A:858:ILE:HG12	1.94	0.48
2:B:-9:A:H2'	2:B:-8:A:C8	2.48	0.48
1:A:458:PRO:HG2	1:A:761:ARG:HG2	1.94	0.48
1:A:1227:VAL:HG13	1:A:1275:ILE:HG23	1.96	0.48
1:A:1659:LYS:O	1:A:1662:ARG:HG2	2.14	0.48
1:A:1607:LEU:HD21	1:A:1710:THR:HB	1.96	0.48
1:A:433:ASN:HD21	1:A:817:SER:HB3	1.79	0.47
1:A:544:LEU:HD21	1:A:651:SER:HB2	1.95	0.47
2:B:0:G:H2'	2:B:1:U:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:VAL:HB	1:A:774:MET:HG3	1.96	0.47
1:A:1691:LEU:O	1:A:1694:ILE:HG12	2.15	0.47
2:B:27:C:H3'	2:B:28:A:H8	1.79	0.47
1:A:475:HIS:HB3	1:A:546:GLN:NE2	2.28	0.47
1:A:586:LEU:O	1:A:590:LEU:HG	2.15	0.47
1:A:809:LEU:HB2	1:A:813:SER:HB3	1.95	0.47
1:A:1346:LEU:CD2	1:A:1359:ILE:HG22	2.45	0.47
1:A:870:LYS:HE3	1:A:870:LYS:HB2	1.42	0.46
1:A:1496:VAL:HG22	1:A:1498:SER:H	1.79	0.46
1:A:269:LEU:HD11	1:A:451:LEU:HD22	1.96	0.46
1:A:479:LYS:HB2	1:A:541:LEU:HD21	1.97	0.46
1:A:1236:ALA:HB3	1:A:1270:LYS:HA	1.97	0.46
1:A:319:GLN:HE21	1:A:319:GLN:HB2	1.56	0.46
1:A:427:CYS:HB3	1:A:798:LYS:HB2	1.96	0.46
1:A:856:TYR:HE2	2:B:81:U:H1'	1.80	0.46
1:A:447:ASP:HA	1:A:451:LEU:HD12	1.96	0.46
1:A:552:VAL:HA	1:A:679:VAL:HG11	1.97	0.46
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.76	0.46
1:A:883:LEU:HG	1:A:890:GLU:HB3	1.97	0.46
1:A:1244:GLU:HG3	1:A:1246:TYR:HD2	1.81	0.46
1:A:881:LEU:HD22	1:A:907:VAL:HG12	1.98	0.46
1:A:1746:ALA:HA	1:A:1764:VAL:HG13	1.98	0.46
2:B:11:C:H2'	2:B:12:U:C6	2.51	0.46
1:A:668:ILE:HB	1:A:739:ILE:HG21	1.96	0.45
1:A:1607:LEU:HD22	1:A:1714:TRP:HB2	1.98	0.45
1:A:329:GLY:HA2	1:A:357:ILE:HD11	1.99	0.45
1:A:1319:LEU:HD13	1:A:1324:ILE:HD11	1.98	0.45
2:B:14:G:H2'	2:B:15:C:C6	2.51	0.45
1:A:303:VAL:HG13	1:A:309:VAL:HG22	1.97	0.45
2:B:12:U:H2'	2:B:13:G:C8	2.51	0.45
1:A:799:GLU:O	1:A:801:ILE:N	2.50	0.45
1:A:803:ARG:HG2	1:A:806:LEU:HD12	1.99	0.45
1:A:1237:GLU:HB2	1:A:1270:LYS:HB3	1.97	0.45
1:A:421:VAL:HG23	1:A:795:THR:HG21	1.98	0.45
1:A:791:ASN:O	1:A:795:THR:HG23	2.17	0.44
1:A:981:LYS:HD3	1:A:1037:LYS:HD2	1.98	0.44
1:A:1505:VAL:O	1:A:1509:LEU:HG	2.18	0.44
1:A:1209:GLU:HG3	1:A:1321:GLY:H	1.83	0.44
1:A:1773:VAL:H	1:A:1785:LEU:HD23	1.83	0.44
1:A:680:LEU:N	1:A:681:PRO:HD2	2.32	0.44
1:A:1527:LYS:HD3	1:A:1531:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1362:ALA:HA	1:A:1374:TYR:HB3	2.00	0.44
2:B:-8:A:H2'	2:B:-7:A:C8	2.53	0.44
1:A:540:THR:HG21	1:A:552:VAL:HG11	2.00	0.44
1:A:1525:LEU:HD22	1:A:1525:LEU:HA	1.80	0.44
2:B:83:A:H2'	2:B:84:U:C6	2.53	0.43
1:A:404:LYS:HA	1:A:404:LYS:HD2	1.84	0.43
1:A:670:PHE:HB2	1:A:747:ARG:HA	2.01	0.43
1:A:1346:LEU:CD1	1:A:1359:ILE:HG22	2.49	0.43
1:A:680:LEU:HA	1:A:680:LEU:HD23	1.78	0.43
1:A:295:ARG:HA	1:A:295:ARG:HD3	1.79	0.43
1:A:1201:MET:HA	1:A:1272:GLN:HE22	1.84	0.43
1:A:371:THR:HA	1:A:404:LYS:HE3	2.01	0.43
1:A:396:PHE:HA	1:A:405:ARG:HH21	1.83	0.43
1:A:362:LEU:O	1:A:365:SER:HB2	2.18	0.43
1:A:465:TYR:HB3	1:A:776:GLU:HA	2.01	0.43
1:A:1567:LYS:HB2	1:A:1567:LYS:HE2	1.84	0.43
1:A:446:LYS:HB3	1:A:449:LYS:HB3	2.01	0.42
1:A:814:ARG:HA	1:A:818:ILE:HB	2.01	0.42
1:A:1594:GLN:H	1:A:1594:GLN:HG3	1.61	0.42
1:A:1690:VAL:O	1:A:1694:ILE:HG23	2.19	0.42
1:A:1722:GLN:N	1:A:1723:PRO:HD2	2.34	0.42
1:A:883:LEU:HB2	1:A:891:ILE:HG13	2.00	0.42
1:A:447:ASP:O	1:A:451:LEU:HB2	2.19	0.42
1:A:474:LEU:HD13	1:A:474:LEU:HA	1.88	0.42
1:A:743:ASN:HB3	1:A:767:PRO:O	2.19	0.42
2:B:84:U:H2'	2:B:85:U:C6	2.54	0.42
1:A:384:VAL:H	1:A:387:HIS:HB3	1.84	0.42
1:A:456:PRO:HG3	1:A:766:LYS:N	2.35	0.42
1:A:981:LYS:HE2	1:A:1039:SER:HB2	2.02	0.42
1:A:1356:THR:HB	1:A:1359:ILE:HB	2.02	0.42
2:B:94:C:H2'	2:B:95:U:C6	2.55	0.42
1:A:419:LYS:HA	1:A:419:LYS:HD2	1.66	0.42
1:A:1358:LYS:HB2	1:A:1512:VAL:HG13	2.02	0.42
1:A:1381:GLY:HA3	1:A:1507:GLU:O	2.19	0.42
2:B:-14:A:H2'	2:B:-13:G:C8	2.55	0.42
1:A:1749:LEU:HD22	1:A:1761:THR:H	1.85	0.42
1:A:1310:PRO:HA	1:A:1311:PRO:HD3	1.97	0.41
1:A:1212:ILE:H	1:A:1212:ILE:HG13	1.81	0.41
1:A:1596:LEU:HD13	1:A:1701:ALA:HB2	2.02	0.41
2:B:75:C:H2'	2:B:76:A:C8	2.55	0.41
1:A:1240:PHE:HB3	1:A:1252:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:PHE:HZ	1:A:730:THR:HG23	1.85	0.41
1:A:1236:ALA:O	1:A:1254:THR:HB	2.20	0.41
1:A:1240:PHE:HB2	1:A:1255:TYR:HA	2.02	0.41
1:A:1703:PHE:HE1	1:A:1710:THR:HA	1.85	0.41
1:A:448:ARG:HA	1:A:448:ARG:HD2	1.62	0.41
1:A:1090:VAL:HG12	1:A:1102:ILE:HA	2.02	0.41
1:A:257:LEU:HD12	1:A:282:LEU:HG	2.03	0.41
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.91	0.41
1:A:827:LYS:NZ	1:A:829:GLU:HB3	2.35	0.41
1:A:1028:LEU:HA	1:A:1028:LEU:HD13	1.82	0.41
1:A:269:LEU:HD13	1:A:269:LEU:HA	1.77	0.41
1:A:384:VAL:H	1:A:387:HIS:CB	2.34	0.41
1:A:336:TRP:HZ2	2:B:3:A:H5"	1.86	0.40
1:A:541:LEU:HB3	1:A:549:ALA:HB2	2.04	0.40
1:A:1617:THR:HB	1:A:1619:LEU:HG	2.03	0.40
1:A:869:GLU:HG3	1:A:875:THR:HA	2.04	0.40
1:A:1368:CYS:HB3	1:A:1370:GLU:HG2	2.02	0.40
2:B:87:C:H2'	2:B:88:C:C6	2.56	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	1111/1909 (58%)	1069 (96%)	32 (3%)	10 (1%)	17 56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	728	VAL
1	A	800	ALA
1	A	825	VAL

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Mol	Chain	Res	Type
1	A	851	LEU
1	A	875	THR
1	A	401	PRO
1	A	414	SER
1	A	687	LEU
1	A	872	GLY
1	A	1733	HIS

5.3.2 Protein sidechains (i)

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	983/1639 (60%)	889 (90%)	94 (10%)	8 29

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	LEU
1	A	264	ASN
1	A	269	LEU
1	A	271	THR
1	A	288	LYS
1	A	297	MET
1	A	298	LEU
1	A	303	VAL
1	A	306	VAL
1	A	316	ILE
1	A	319	GLN
1	A	320	THR
1	A	333	GLN
1	A	339	ARG
1	A	341	TRP
1	A	354	THR
1	A	375	LEU
1	A	389	TYR
1	A	397	TYR

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Mol	Chain	Res	Type
1	A	399	THR
1	A	405	ARG
1	A	412	THR
1	A	416	VAL
1	A	426	ASP
1	A	444	THR
1	A	457	MET
1	A	486	GLU
1	A	544	LEU
1	A	557	LEU
1	A	574	PHE
1	A	586	LEU
1	A	674	VAL
1	A	694	ARG
1	A	725	THR
1	A	730	THR
1	A	740	ARG
1	A	747	ARG
1	A	753	THR
1	A	755	LEU
1	A	766	LYS
1	A	770	ASP
1	A	785	PHE
1	A	790	ARG
1	A	793	GLU
1	A	794	GLU
1	A	804	THR
1	A	812	THR
1	A	825	VAL
1	A	831	THR
1	A	846	PHE
1	A	847	TYR
1	A	848	CYS
1	A	850	GLN
1	A	851	LEU
1	A	855	ARG
1	A	863	PHE
1	A	870	LYS
1	A	874	HIS
1	A	883	LEU
1	A	915	LEU
1	A	976	VAL

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Mol	Chain	Res	Type
1	A	1020	GLU
1	A	1028	LEU
1	A	1030	VAL
1	A	1036	THR
1	A	1049	THR
1	A	1059	PHE
1	A	1062	ARG
1	A	1087	PHE
1	A	1088	VAL
1	A	1199	LEU
1	A	1230	ILE
1	A	1242	ARG
1	A	1243	LYS
1	A	1319	LEU
1	A	1330	LEU
1	A	1342	LEU
1	A	1360	LEU
1	A	1361	GLU
1	A	1363	LEU
1	A	1371	THR
1	A	1372	PHE
1	A	1397	TYR
1	A	1424	VAL
1	A	1497	LEU
1	A	1525	LEU
1	A	1704	LEU
1	A	1720	LEU
1	A	1721	LEU
1	A	1726	THR
1	A	1732	MET
1	A	1738	LEU
1	A	1766	ILE
1	A	1767	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	GLN
1	A	546	GLN
1	A	1272	GLN
1	A	1328	GLN
1	A	1652	HIS

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Mol	Chain	Res	Type
1	A	1739	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	102/148 (68%)	35 (34%)	1 (0%)

All (35) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-15	G
2	B	-14	A
2	B	-13	G
2	B	-10	A
2	B	-6	G
2	B	-3	C
2	B	-2	A
2	B	-1	G
2	B	0	G
2	B	2	G
2	B	6	G
2	B	8	U
2	B	18	G
2	B	19	A
2	B	20	G
2	B	21	A
2	B	24	A
2	B	32	U
2	B	34	A
2	B	36	G
2	B	54	A
2	B	63	A
2	B	64	U
2	B	65	G
2	B	71	G
2	B	72	G
2	B	73	A
2	B	79	C
2	B	81	U
2	B	82	C
2	B	105	U

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Mol	Chain	Res	Type
2	B	112	C
2	B	113	A
2	B	115	U
2	B	116	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	115	U

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 monosaccharides 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.

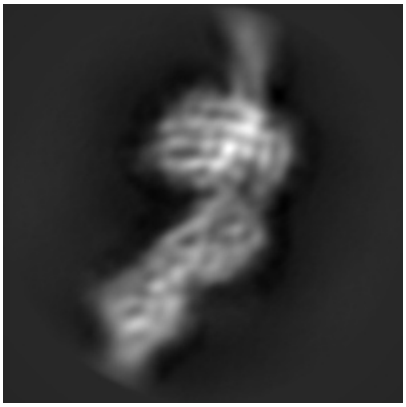
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31181. These allow visual inspection of the internal detail of the map and identification of artifacts.

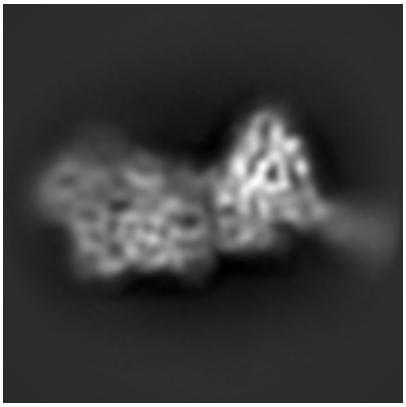
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

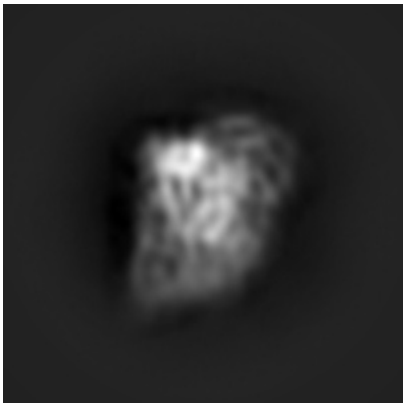
6.1.1 Primary map



X



Y

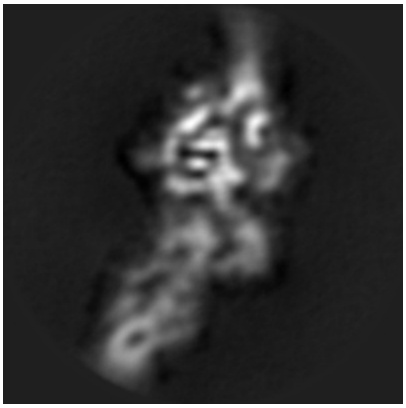


Z

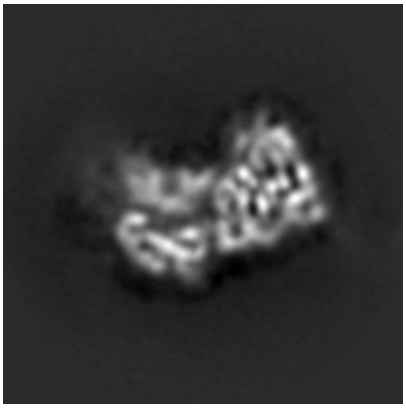
The images above show the map projected in three orthogonal directions.

6.2 Central slices

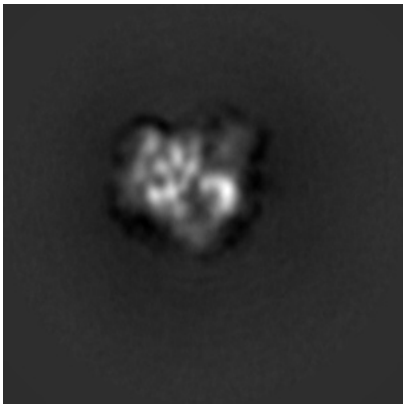
6.2.1 Primary map



X Index: 100



Y Index: 100

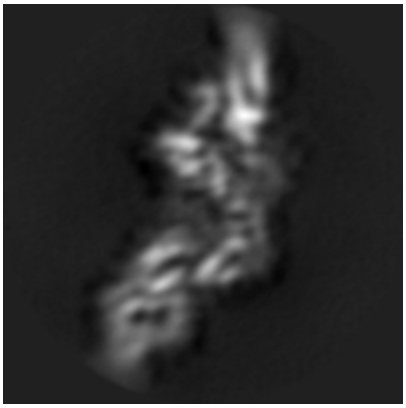


Z Index: 100

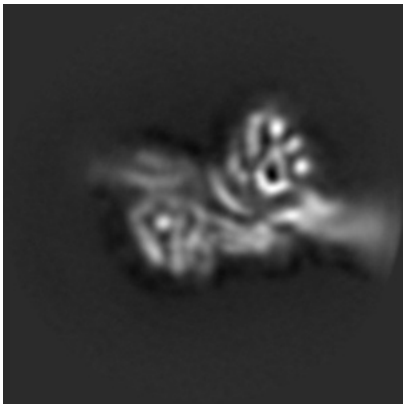
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

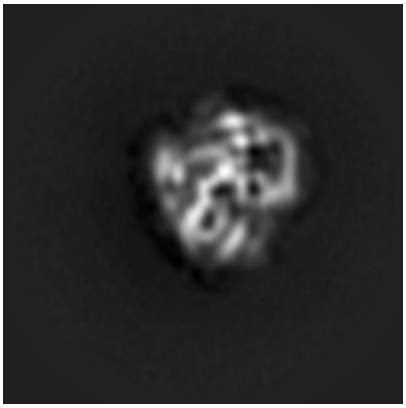
6.3.1 Primary map



X Index: 93



Y Index: 117

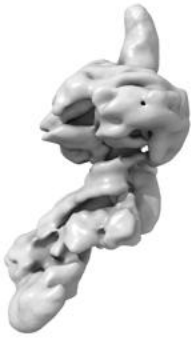


Z Index: 129

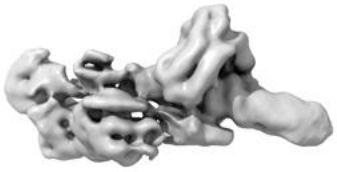
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

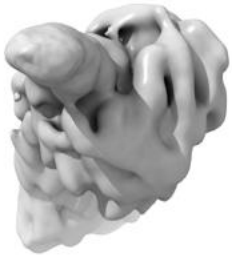
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

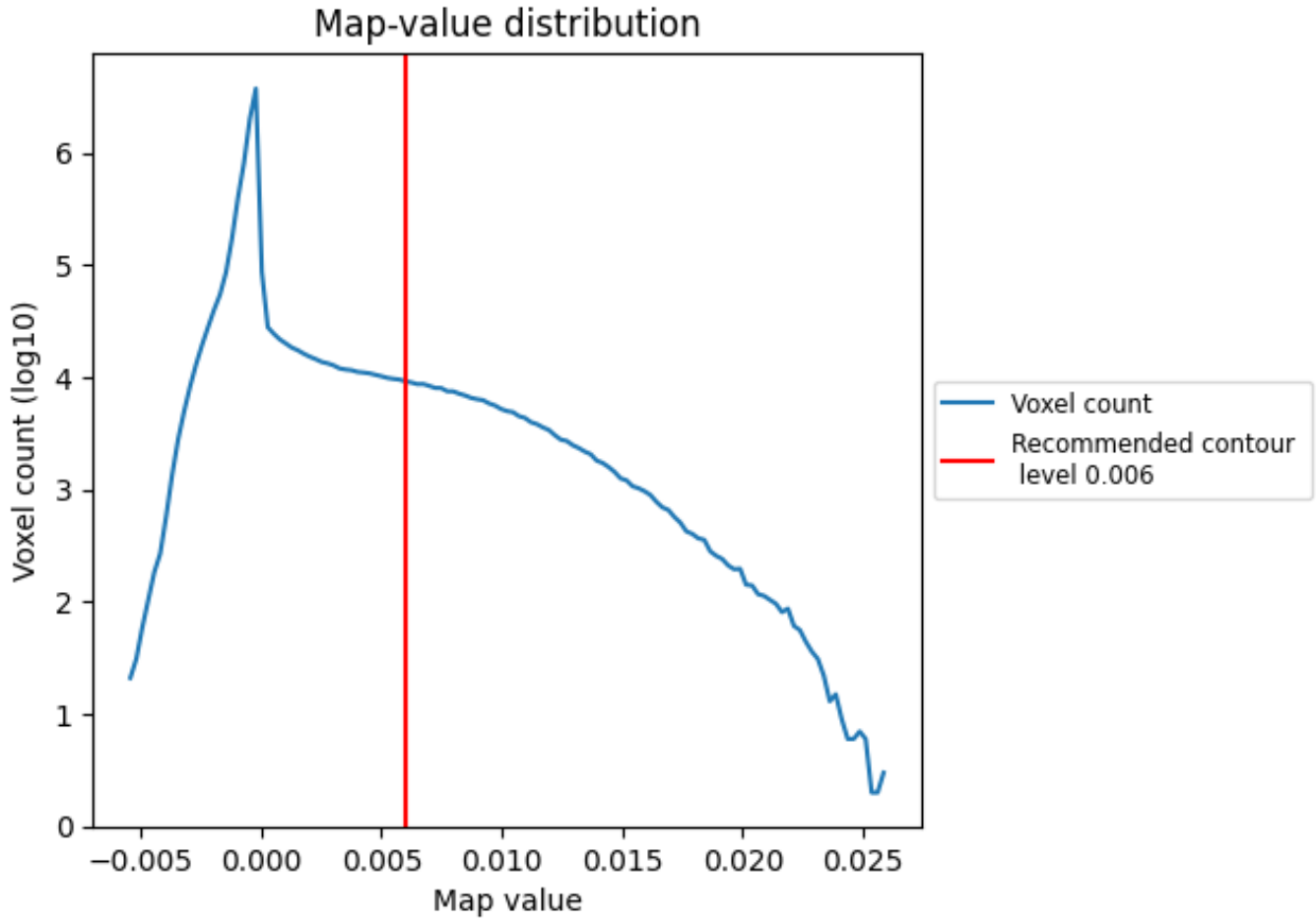
6.5 Mask visualisation (i)

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

7 Map analysis

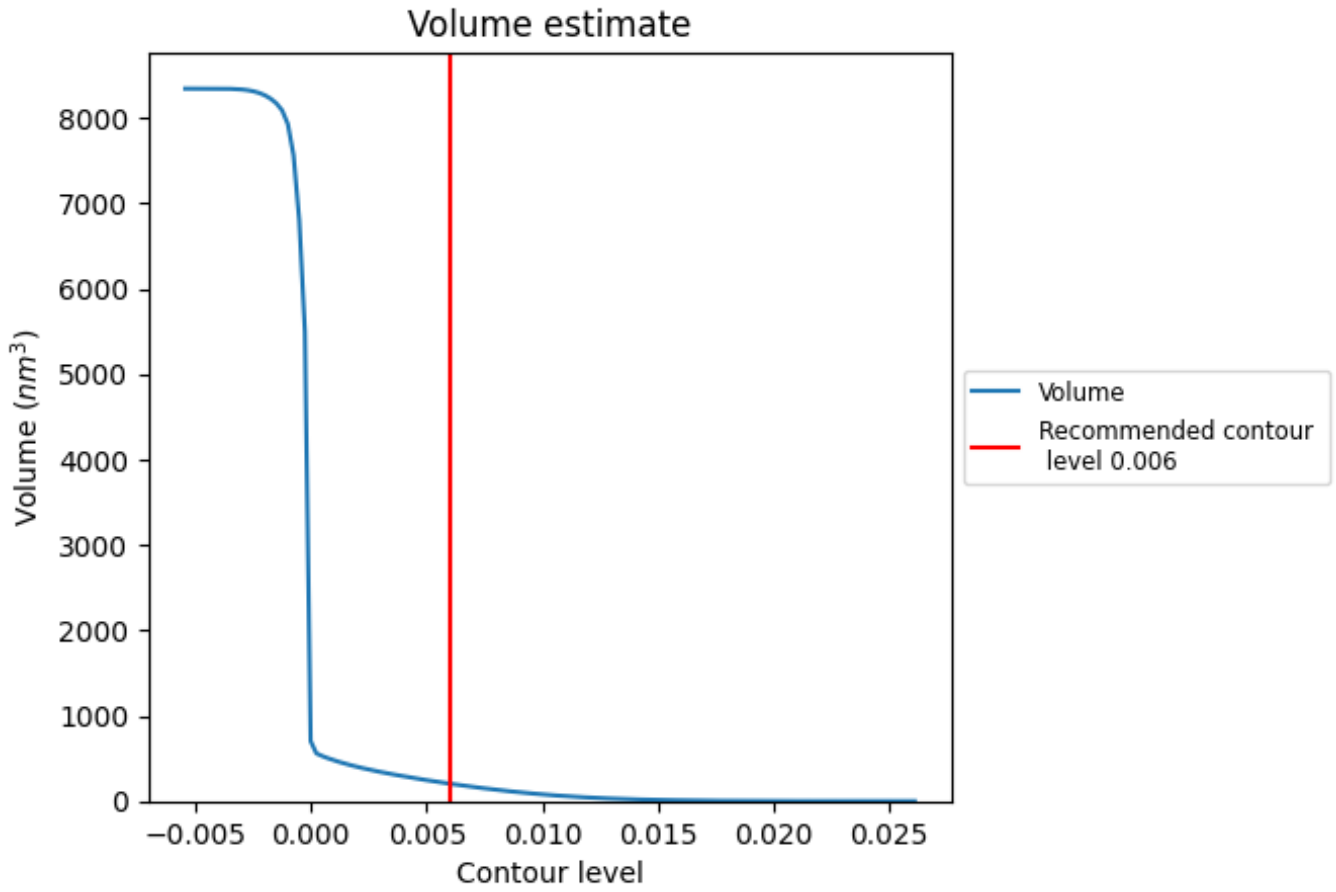
This section contains the results of statistical analysis of the map.

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.

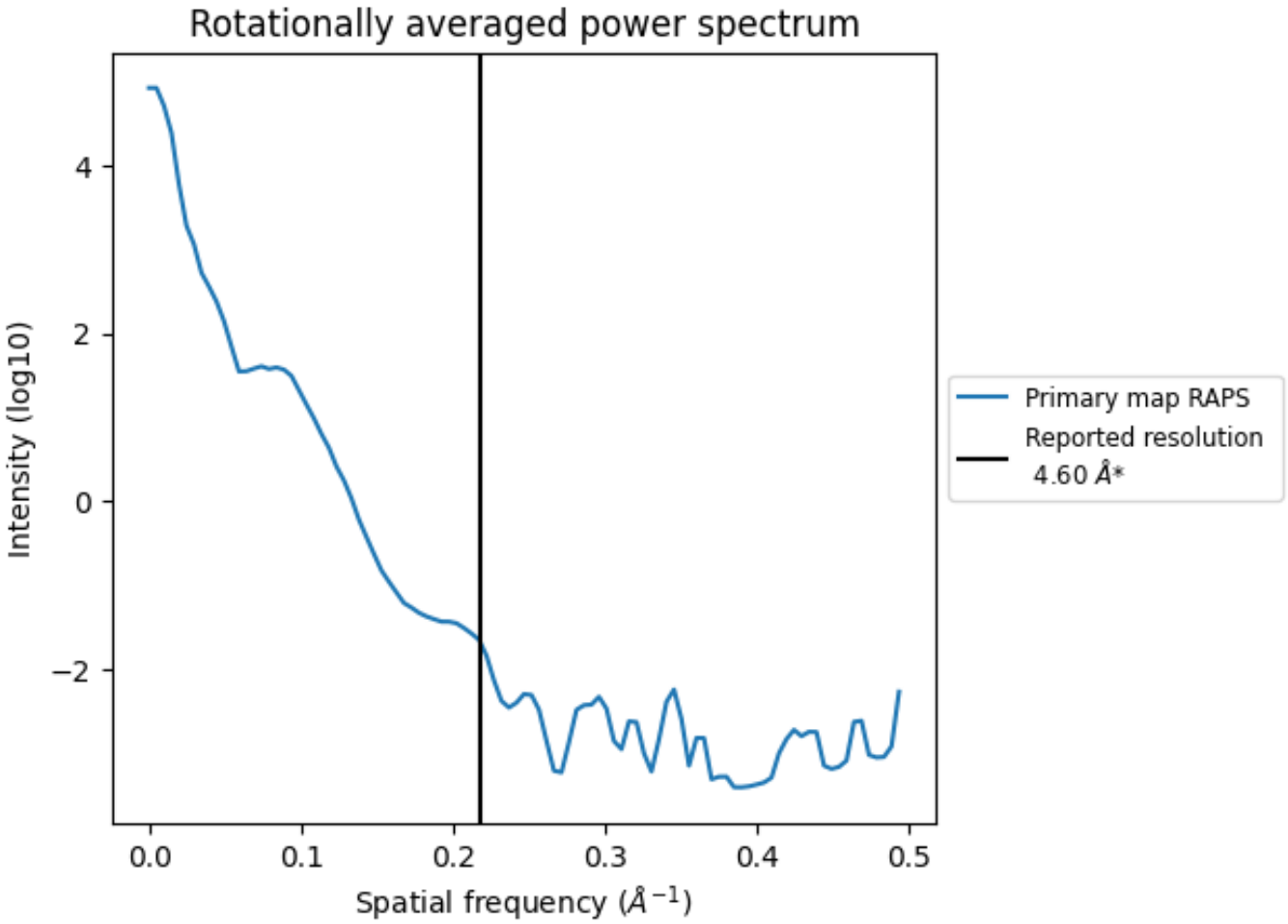
7.2 Volume estimate



The volume at the recommended contour level is 205 nm^3; this corresponds to an approximate mass of 185 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 0.217 $Å^{-1}$

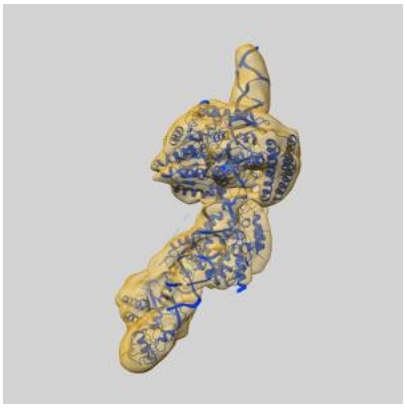
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

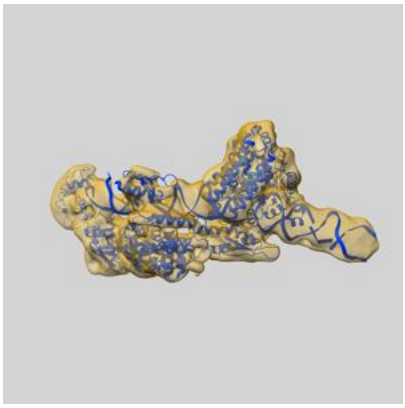
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31181 and PDB model 7ELD. Per-residue inclusion information can be found in section 3 on page 4.

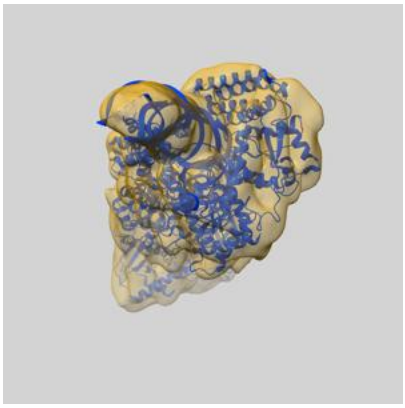
9.1 Map-model overlay



X



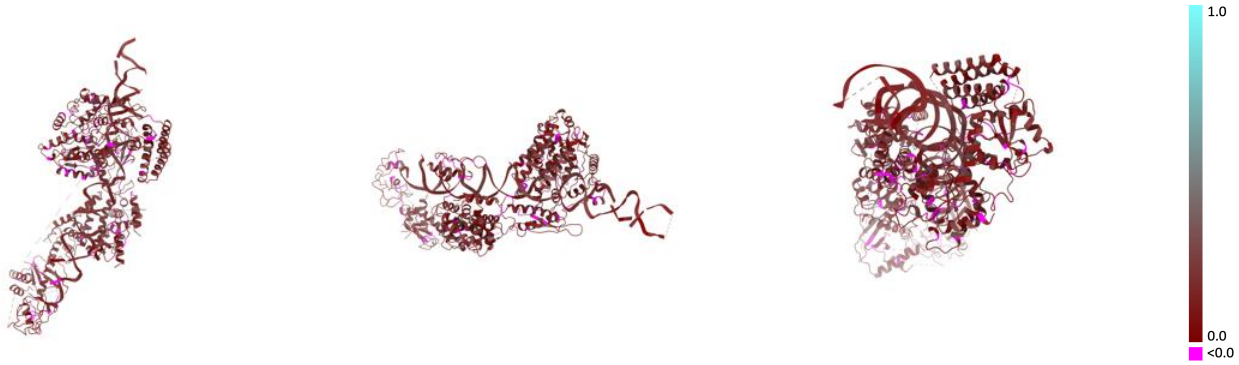
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

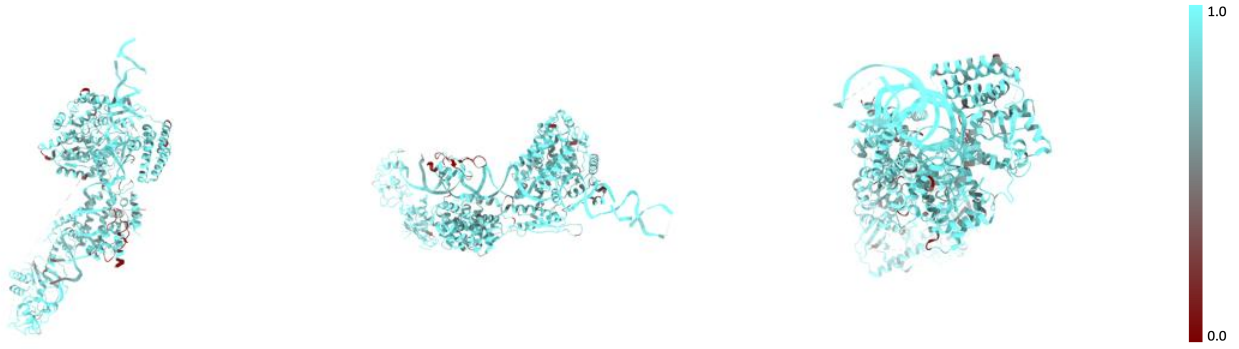
9.2 Q-score mapped to coordinate model (i)



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.

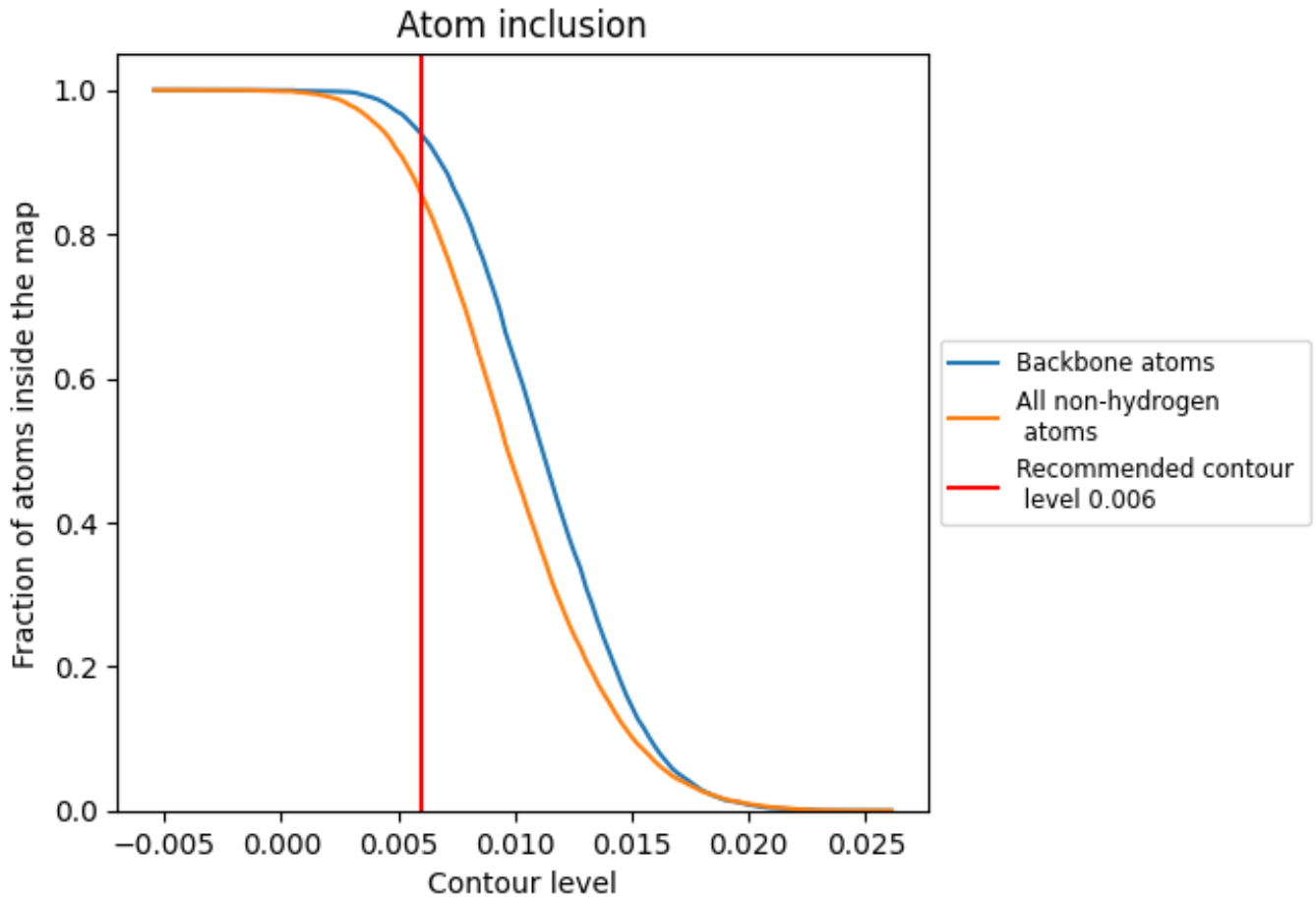
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8548	0.1570
A	0.8390	0.1500
B	0.9154	0.1860