Full wwPDB EM Validation Report

May 27, 2024 – 01:45 PM JST

PDB ID	:	7ELE
EMDB ID	:	EMD-31182
Title	:	Cryo-EM structure of Arabidopsis DCL1 in complex with pre-miRNA 166f
Authors	:	Wei, X.; Ke, H.; Feng, Y.
Deposited on	:	2021-04-09
Resolution	:	4.90 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:

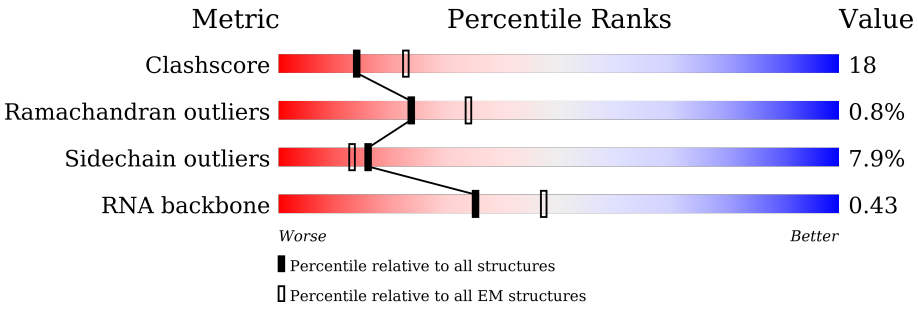
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.90 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	34% 24% 40%
2	G	89	17% 57% 19% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10733 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 pre-miRNA 166f.

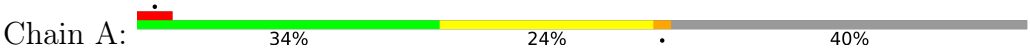
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	G	83	1757	786	303	585	83	0	0

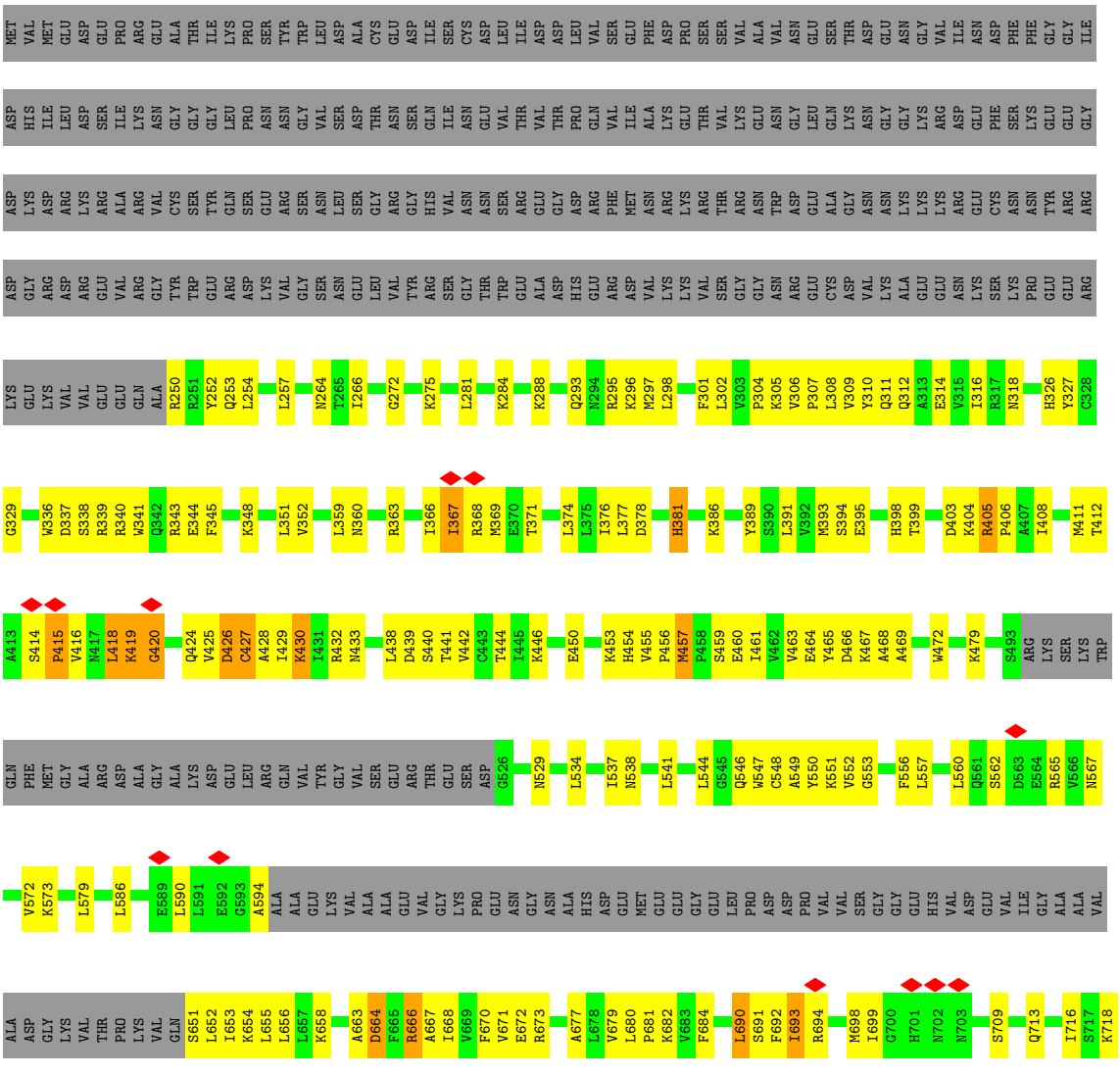
3 Residue-property plots (i)

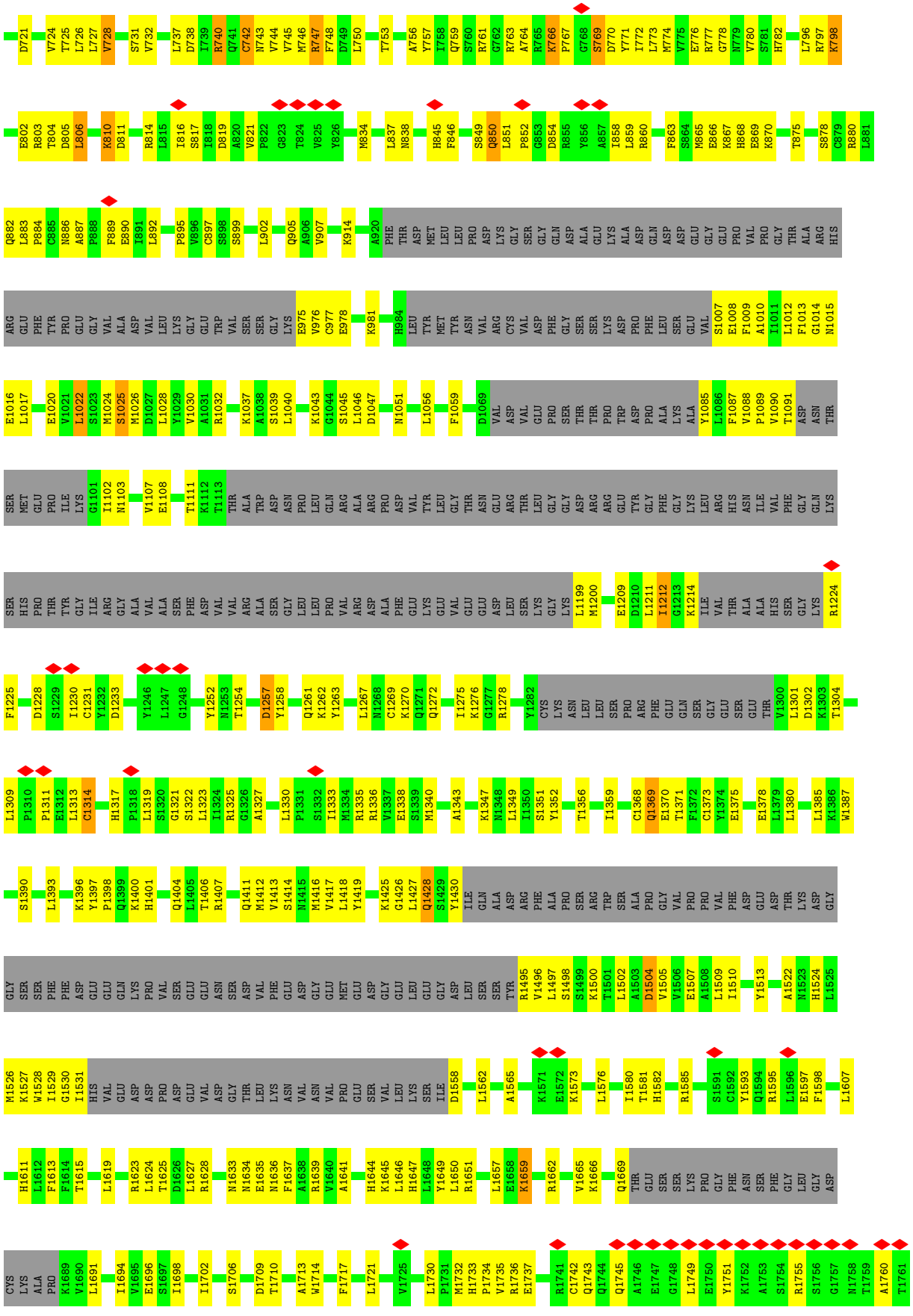
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

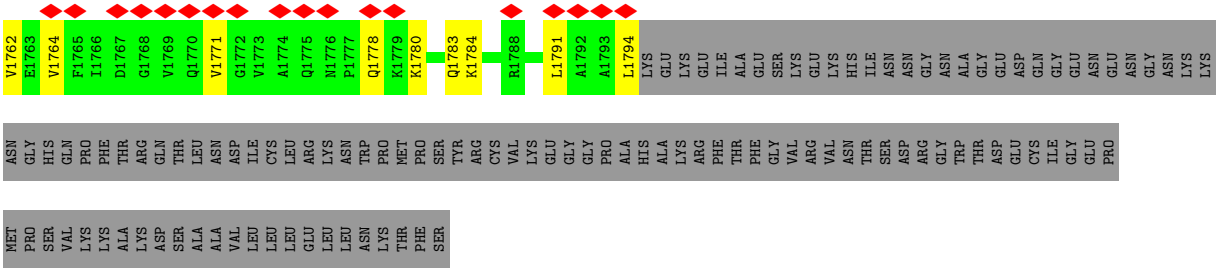
- Molecule 1: Endoribonuclease Dicer homolog 1

Chain A:



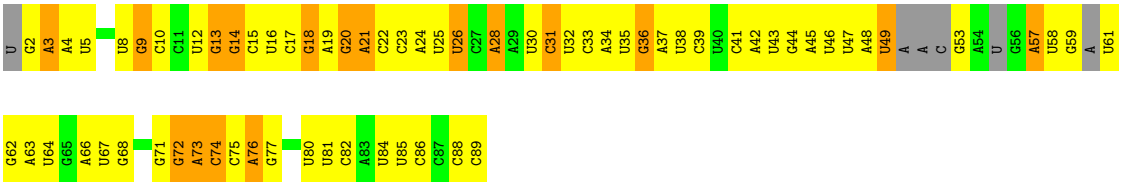






• Molecule 2: pre-miRNA 166f

Chain G: 17% 57% 19% 7%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	300148	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	0.028	Depositor
Minimum map value	-0.012	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	0.40	0/9133	0.59	0/12319
2	G	0.57	0/1958	1.13	0/3039
All	All	0.44	0/11091	0.73	0/15358

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	315	0
2	G	1757	0	893	57	0
All	All	10733	0	10042	361	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 (361) 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:670:PHE:HB2	1:A:747:ARG:HA	1.53	0.91
2:G:28:A:H62	2:G:59:G:N2	1.70	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:PHE:HA	1:A:1088:VAL:O	1.72	0.88
1:A:424:GLN:HG2	1:A:429:ILE:HB	1.63	0.81
2:G:28:A:H62	2:G:59:G:H21	1.24	0.81
2:G:36:G:H1	2:G:47:U:H3	1.27	0.80
2:G:26:U:H3	2:G:62:G:H1	1.27	0.79
2:G:26:U:O2	2:G:62:G:N2	2.23	0.72
1:A:869:GLU:HA	1:A:875:THR:HA	1.72	0.71
1:A:250:ARG:HH11	1:A:453:LYS:HZ3	1.38	0.71
2:G:61:U:H4'	2:G:61:U:OP2	1.86	0.70
1:A:1736:ARG:NH2	2:G:18:G:N3	2.39	0.70
1:A:767:PRO:HD2	1:A:769:SER:HB3	1.74	0.69
1:A:670:PHE:HB3	1:A:750:LEU:HD12	1.73	0.69
1:A:652:LEU:HD12	1:A:655:LEU:HD22	1.75	0.68
1:A:866:GLU:HB3	1:A:878:SER:HB2	1.75	0.68
1:A:1706:SER:HB2	1:A:1709:ASP:HB3	1.75	0.68
1:A:546:GLN:HB3	1:A:590:LEU:HD22	1.75	0.68
1:A:304:PRO:HG2	1:A:305:LYS:HE3	1.76	0.68
1:A:314:GLU:O	1:A:318:ASN:HB2	1.94	0.67
2:G:59:G:O3'	2:G:61:U:H5"	1.95	0.66
1:A:1565:ALA:O	1:A:1644:HIS:ND1	2.30	0.65
1:A:1319:LEU:HD11	1:A:1323:LEU:HD23	1.77	0.65
1:A:408:ILE:HB	1:A:440:SER:HB2	1.78	0.65
1:A:1507:GLU:HA	1:A:1510:ILE:HD12	1.77	0.65
1:A:852:PRO:HA	1:A:860:ARG:HH21	1.62	0.65
1:A:464:GLU:HB2	1:A:777:ARG:HB2	1.77	0.64
1:A:1526:MET:O	1:A:1530:GLY:N	2.28	0.64
1:A:892:LEU:HD23	1:A:907:VAL:HG23	1.78	0.64
1:A:747:ARG:HG3	1:A:750:LEU:HB2	1.78	0.64
2:G:28:A:N6	2:G:59:G:H21	1.95	0.64
1:A:1411:GLN:NE2	1:A:1412:MET:SD	2.71	0.64
1:A:479:LYS:HD3	1:A:541:LEU:HD11	1.80	0.63
1:A:293:GLN:HB3	1:A:296:LYS:HB3	1.79	0.63
1:A:548:CYS:SG	1:A:549:ALA:N	2.71	0.63
1:A:560:LEU:HD13	1:A:579:LEU:HD13	1.79	0.63
1:A:811:ASP:HA	1:A:814:ARG:HE	1.64	0.63
1:A:1013:PHE:HD1	1:A:1015:ASN:H	1.47	0.63
2:G:47:U:H2'	2:G:48:A:H8	1.65	0.62
1:A:266:ILE:HB	1:A:442:VAL:HA	1.80	0.62
1:A:1645:LYS:HD2	1:A:1647:HIS:HE1	1.65	0.61
1:A:393:MET:HG2	1:A:438:LEU:HA	1.81	0.61
1:A:756:ALA:O	1:A:759:GLN:HB3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:VAL:HB	1:A:774:MET:HA	1.83	0.61
1:A:466:ASP:HB3	1:A:468:ALA:H	1.65	0.61
1:A:1230:ILE:O	1:A:1276:LYS:NZ	2.34	0.61
1:A:264:ASN:ND2	1:A:439:ASP:O	2.34	0.60
1:A:1351:SER:HG	1:A:1513:TYR:HH	1.47	0.60
1:A:1736:ARG:HH22	2:G:18:G:H1'	1.66	0.60
1:A:1496:VAL:HG22	1:A:1500:LYS:HE3	1.84	0.60
1:A:1343:ALA:O	1:A:1347:LYS:HB2	2.02	0.60
2:G:43:U:H3'	2:G:44:G:H8	1.67	0.60
1:A:420:GLY:O	1:A:424:GLN:HB2	2.03	0.59
1:A:1646:LEU:HD13	1:A:1649:TYR:HB2	1.85	0.59
1:A:465:TYR:HA	1:A:776:GLU:HA	1.83	0.58
1:A:1322:SER:HA	1:A:1325:ARG:HE	1.68	0.58
1:A:1749:LEU:HB3	1:A:1762:VAL:HG22	1.85	0.58
1:A:1211:LEU:HD23	1:A:1317:HIS:HB3	1.85	0.58
1:A:469:ALA:HB3	1:A:547:TRP:HE1	1.67	0.58
1:A:671:VAL:HG22	1:A:748:PHE:HB3	1.85	0.58
1:A:1267:LEU:O	1:A:1270:LYS:NZ	2.37	0.58
1:A:1733:HIS:O	1:A:1737:GLU:HB2	2.04	0.58
1:A:1228:ASP:HB2	1:A:1278:ARG:HG3	1.85	0.58
1:A:890:GLU:HG3	1:A:914:LYS:HD3	1.84	0.58
1:A:1398:PRO:O	1:A:1595:ARG:NH2	2.35	0.57
1:A:673:ARG:NH2	2:G:47:U:O3'	2.37	0.57
1:A:1012:LEU:O	1:A:1085:TYR:N	2.37	0.57
1:A:1527:LYS:HD3	1:A:1531:ILE:HB	1.86	0.57
1:A:679:VAL:HA	1:A:682:LYS:HE3	1.87	0.57
1:A:738:ASP:O	1:A:740:ARG:NH1	2.38	0.57
1:A:302:LEU:HB3	1:A:377:LEU:HD13	1.87	0.57
1:A:731:SER:OG	1:A:732:VAL:N	2.38	0.57
1:A:1730:LEU:O	1:A:1733:HIS:ND1	2.38	0.57
1:A:1272:GLN:HE21	1:A:1311:PRO:HD2	1.69	0.56
1:A:1200:MET:SD	1:A:1200:MET:N	2.69	0.56
1:A:567:ASN:HD21	1:A:572:VAL:HB	1.70	0.56
1:A:336:TRP:HB3	1:A:340:ARG:HE	1.69	0.56
1:A:403:ASP:HB3	1:A:406:PRO:HB3	1.88	0.56
1:A:860:ARG:HB3	1:A:884:PRO:HB3	1.88	0.56
1:A:1641:ALA:O	1:A:1645:LYS:N	2.39	0.56
1:A:537:ILE:HB	1:A:556:PHE:HE2	1.70	0.56
1:A:1751:TYR:O	1:A:1778:GLN:NE2	2.39	0.55
1:A:252:TYR:OH	1:A:444:THR:O	2.25	0.55
1:A:1199:LEU:HB2	1:A:1269:CYS:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:HIS:O	1:A:405:ARG:NH2	2.39	0.55
1:A:699:ILE:HD13	2:G:49:U:H5	1.71	0.55
1:A:1007:SER:OG	1:A:1103:ASN:ND2	2.39	0.55
1:A:1230:ILE:HG22	1:A:1275:ILE:HD13	1.87	0.55
1:A:1710:THR:O	1:A:1714:TRP:HB2	2.07	0.55
1:A:845:HIS:CD2	2:G:57:A:H1'	2.42	0.55
1:A:977:CYS:HA	1:A:1045:SER:H	1.70	0.55
1:A:1385:LEU:HD21	1:A:1413:VAL:HG13	1.88	0.55
1:A:837:LEU:HD12	1:A:905:GLN:HB2	1.89	0.54
1:A:1646:LEU:HA	1:A:1649:TYR:HD2	1.72	0.54
1:A:426:ASP:HB2	1:A:805:ASP:HB2	1.88	0.54
1:A:978:GLU:HB3	1:A:1043:LYS:HB2	1.90	0.54
2:G:31:C:H2'	2:G:32:U:C6	2.42	0.54
1:A:391:LEU:O	1:A:394:SER:OG	2.24	0.54
1:A:432:ARG:HD2	1:A:806:LEU:HA	1.90	0.54
1:A:802:GLU:HG3	1:A:803:ARG:HG3	1.90	0.54
1:A:693:ILE:HB	1:A:727:LEU:HB3	1.90	0.54
1:A:560:LEU:HD22	1:A:579:LEU:HD22	1.89	0.53
1:A:889:PHE:N	1:A:890:GLU:OE1	2.41	0.53
1:A:465:TYR:HD1	1:A:778:GLY:H	1.55	0.53
2:G:47:U:H2'	2:G:48:A:C8	2.44	0.53
2:G:74:C:H2'	2:G:75:C:C6	2.43	0.53
1:A:360:ASN:HA	1:A:363:ARG:HG3	1.90	0.53
1:A:381:HIS:CD2	1:A:418:LEU:HA	2.44	0.53
1:A:272:GLY:HA3	1:A:275:LYS:HG3	1.91	0.53
1:A:456:PRO:HB2	1:A:766:LYS:HB3	1.91	0.53
1:A:699:ILE:HD13	2:G:49:U:C5	2.42	0.53
2:G:72:G:H3'	2:G:73:A:H8	1.73	0.53
2:G:58:U:H3'	2:G:59:G:H8	1.74	0.53
1:A:468:ALA:HB2	1:A:651:SER:HB2	1.91	0.53
1:A:867:LYS:HE3	1:A:869:GLU:HB2	1.91	0.53
1:A:883:LEU:HB3	1:A:887:ALA:HB3	1.90	0.53
1:A:680:LEU:HB3	1:A:684:PHE:CE2	2.43	0.53
1:A:327:TYR:HB3	1:A:329:GLY:H	1.75	0.52
1:A:850:GLN:HE21	1:A:1401:HIS:HE2	1.57	0.52
1:A:1336:ARG:NH1	1:A:1340:MET:SD	2.75	0.52
1:A:1380:LEU:HD13	1:A:1613:PHE:HD2	1.72	0.52
2:G:14:G:H2'	2:G:15:C:C6	2.44	0.52
1:A:1611:HIS:O	1:A:1615:THR:N	2.41	0.52
1:A:266:ILE:HD11	1:A:438:LEU:HD11	1.91	0.52
1:A:308:LEU:O	1:A:312:GLN:NE2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:SER:HA	1:A:1037:LYS:O	2.10	0.52
1:A:264:ASN:HB3	1:A:408:ILE:H	1.75	0.52
1:A:1030:VAL:HG23	1:A:1032:ARG:H	1.74	0.52
1:A:1056:LEU:HD21	1:A:1108:GLU:HG3	1.92	0.52
2:G:43:U:H3'	2:G:44:G:C8	2.44	0.52
1:A:1406:THR:HG23	1:A:1598:PHE:HE1	1.75	0.51
1:A:883:LEU:HG	1:A:890:GLU:HB2	1.90	0.51
1:A:534:LEU:HD23	1:A:538:ASN:HD21	1.76	0.51
1:A:667:ALA:HB3	1:A:728:VAL:HG22	1.92	0.51
1:A:899:SER:HB3	1:A:902:LEU:HB2	1.92	0.51
1:A:1496:VAL:HG12	1:A:1498:SER:H	1.76	0.51
1:A:399:THR:HB	1:A:405:ARG:HG2	1.93	0.51
1:A:428:ALA:H	1:A:805:ASP:HB3	1.76	0.51
1:A:1026:MET:HG2	1:A:1336:ARG:HG2	1.92	0.51
1:A:266:ILE:N	1:A:441:THR:O	2.39	0.51
1:A:1634:ASN:HA	1:A:1637:PHE:CD2	2.46	0.51
2:G:41:C:H3'	2:G:42:A:H8	1.76	0.51
1:A:1760:ALA:HB3	1:A:1771:VAL:HG13	1.93	0.50
2:G:28:A:H61	2:G:59:G:H2'	1.76	0.50
1:A:1573:LYS:HG3	1:A:1576:LEU:HD13	1.94	0.50
1:A:360:ASN:OD1	1:A:363:ARG:NH1	2.44	0.50
1:A:1059:PHE:HB2	1:A:1111:THR:HG23	1.94	0.50
2:G:26:U:N3	2:G:62:G:N1	2.35	0.50
1:A:1356:THR:HB	1:A:1359:ILE:HB	1.92	0.50
2:G:26:U:O4	2:G:62:G:O6	2.28	0.50
1:A:250:ARG:HH22	1:A:454:HIS:HB2	1.77	0.50
1:A:666:ARG:HB2	1:A:742:CYS:HA	1.93	0.50
1:A:386:LYS:HB2	2:G:36:G:OP2	2.12	0.50
1:A:1619:LEU:HD22	1:A:1623:ARG:HH12	1.76	0.50
1:A:348:LYS:HD2	1:A:351:LEU:HD13	1.94	0.49
1:A:672:GLU:OE2	1:A:673:ARG:NH2	2.40	0.49
1:A:1375:GLU:HA	1:A:1378:GLU:HB3	1.94	0.49
2:G:38:U:H2'	2:G:39:C:C6	2.47	0.49
1:A:378:ASP:HA	1:A:411:MET:HB2	1.94	0.49
1:A:1275:ILE:HB	1:A:1309:LEU:HB2	1.94	0.49
1:A:467:LYS:HD2	1:A:653:ILE:N	2.27	0.49
1:A:753:THR:HB	1:A:756:ALA:HB3	1.93	0.49
1:A:567:ASN:O	1:A:573:LYS:NZ	2.33	0.49
1:A:976:VAL:O	1:A:1046:LEU:N	2.45	0.49
1:A:306:VAL:HB	2:G:53:G:OP1	2.13	0.49
1:A:882:GLN:NE2	1:A:883:LEU:O	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:GLU:HB3	1:A:1045:SER:HB2	1.95	0.49
1:A:472:TRP:HB2	1:A:546:GLN:HG3	1.95	0.49
1:A:776:GLU:O	1:A:782:HIS:NE2	2.46	0.49
1:A:1007:SER:HB3	1:A:1089:PRO:HB2	1.95	0.49
1:A:1496:VAL:HA	1:A:1500:LYS:HE3	1.95	0.49
2:G:20:G:H3'	2:G:21:A:H8	1.78	0.49
1:A:1528:TRP:HD1	1:A:1529:ILE:HG23	1.78	0.48
1:A:718:LYS:O	1:A:724:VAL:HB	2.12	0.48
1:A:742:CYS:SG	1:A:764:ALA:HB2	2.53	0.48
1:A:1528:TRP:CD1	1:A:1529:ILE:HG23	2.49	0.48
2:G:67:U:H2'	2:G:68:G:C8	2.48	0.48
1:A:295:ARG:NH1	1:A:344:GLU:O	2.47	0.48
1:A:433:ASN:HB3	1:A:821:VAL:HG11	1.94	0.48
1:A:1008:GLU:O	1:A:1090:VAL:N	2.38	0.48
1:A:394:SER:OG	1:A:395:GLU:OE2	2.32	0.48
1:A:981:LYS:HG2	1:A:1010:ALA:HA	1.94	0.48
1:A:1252:TYR:CD1	1:A:1258:TYR:HA	2.48	0.48
1:A:541:LEU:HD13	1:A:546:GLN:HE22	1.79	0.48
1:A:699:ILE:HG21	2:G:49:U:C5	2.49	0.48
1:A:1504:ASP:N	1:A:1504:ASP:OD1	2.45	0.48
2:G:67:U:H2'	2:G:68:G:H8	1.78	0.48
1:A:1702:ILE:HG21	1:A:1713:ALA:HB2	1.96	0.48
1:A:1212:ILE:HB	1:A:1314:CYS:SG	2.54	0.47
1:A:418:LEU:O	1:A:419:LYS:HB3	2.15	0.47
1:A:553:GLY:O	1:A:557:LEU:HG	2.15	0.47
1:A:305:LYS:HB2	1:A:308:LEU:HB2	1.97	0.47
1:A:326:HIS:CE1	1:A:352:VAL:HG21	2.50	0.47
1:A:337:ASP:HA	1:A:340:ARG:HD2	1.95	0.47
1:A:1607:LEU:HD22	1:A:1714:TRP:CD2	2.50	0.47
1:A:586:LEU:O	1:A:590:LEU:HG	2.14	0.47
1:A:837:LEU:HB2	1:A:905:GLN:HG3	1.96	0.47
1:A:666:ARG:HH11	1:A:740:ARG:H	1.62	0.47
1:A:1028:LEU:HD11	1:A:1333:ILE:HD11	1.95	0.47
1:A:337:ASP:HA	1:A:340:ARG:HB2	1.97	0.47
1:A:1624:LEU:HD23	1:A:1627:LEU:HD21	1.96	0.47
1:A:1047:ASP:OD1	1:A:1047:ASP:N	2.43	0.46
1:A:1425:LYS:HE2	1:A:1528:TRP:HE1	1.80	0.46
2:G:12:U:H2'	2:G:13:G:C8	2.50	0.46
1:A:713:GLN:HA	1:A:716:ILE:HD12	1.98	0.46
1:A:1335:ARG:O	1:A:1338:GLU:HG2	2.15	0.46
1:A:1597:GLU:HG2	1:A:1696:GLU:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1636:ASN:HA	1:A:1639:ARG:HG3	1.97	0.46
1:A:677:ALA:HA	1:A:680:LEU:HG	1.97	0.46
1:A:281:LEU:HD23	1:A:284:LYS:HZ1	1.79	0.46
1:A:339:ARG:HG3	1:A:343:ARG:NH2	2.30	0.46
1:A:418:LEU:H	1:A:418:LEU:HG	1.57	0.46
1:A:424:GLN:HG3	1:A:430:LYS:HZ2	1.81	0.46
1:A:1562:LEU:HB3	1:A:1649:TYR:CG	2.50	0.46
1:A:547:TRP:HB3	1:A:594:ALA:HA	1.98	0.46
1:A:1791:LEU:HA	1:A:1794:LEU:HG	1.97	0.46
2:G:75:C:H2'	2:G:76:A:H8	1.81	0.46
1:A:467:LYS:HD3	1:A:654:LYS:HG2	1.97	0.46
1:A:1694:ILE:O	1:A:1698:ILE:HG12	2.16	0.46
1:A:780:VAL:HG12	1:A:782:HIS:CE1	2.50	0.45
1:A:1633:ASN:HD21	1:A:1635:GLU:HB3	1.81	0.45
1:A:562:SER:HA	1:A:565:ARG:HD2	1.98	0.45
1:A:1397:TYR:HB2	1:A:1400:LYS:HB3	1.98	0.45
2:G:12:U:H2'	2:G:13:G:H8	1.80	0.45
1:A:301:PHE:HA	1:A:376:ILE:O	2.16	0.45
1:A:1233:ASP:OD1	1:A:1233:ASP:N	2.50	0.45
1:A:1581:THR:HA	1:A:1585:ARG:HH11	1.80	0.45
1:A:1665:VAL:O	1:A:1669:GLN:NE2	2.50	0.45
1:A:747:ARG:CG	1:A:750:LEU:HB2	2.46	0.45
2:G:3:A:H2'	2:G:4:A:C8	2.52	0.45
2:G:63:A:H2'	2:G:64:U:C6	2.52	0.45
1:A:745:VAL:HB	1:A:771:TYR:HD1	1.82	0.45
1:A:1267:LEU:HD23	1:A:1270:LYS:HA	1.99	0.45
1:A:727:LEU:O	1:A:728:VAL:HB	2.16	0.45
1:A:1505:VAL:O	1:A:1509:LEU:HG	2.17	0.45
1:A:1659:LYS:HG2	1:A:1662:ARG:HH22	1.81	0.45
1:A:1734:PRO:HB3	1:A:1784:LYS:N	2.32	0.45
1:A:868:HIS:CG	1:A:895:PRO:HB3	2.52	0.45
2:G:4:A:H2'	2:G:5:U:C6	2.52	0.45
1:A:1717:PHE:CD2	1:A:1721:LEU:HB2	2.51	0.44
2:G:41:C:H3'	2:G:42:A:C8	2.52	0.44
1:A:297:MET:HA	1:A:374:LEU:HD13	2.00	0.44
1:A:427:CYS:HB2	1:A:798:LYS:O	2.17	0.44
1:A:747:ARG:HD3	1:A:757:TYR:HB2	1.99	0.44
1:A:846:PHE:O	1:A:849:SER:OG	2.22	0.44
1:A:254:LEU:HA	1:A:257:LEU:HD12	1.99	0.44
1:A:457:MET:HE3	1:A:457:MET:HB3	1.78	0.44
2:G:23:C:H2'	2:G:24:A:C8	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1582:HIS:HA	1:A:1593:TYR:CE1	2.52	0.44
1:A:1607:LEU:HD11	1:A:1710:THR:HB	1.99	0.44
2:G:17:C:H2'	2:G:18:G:C8	2.52	0.44
1:A:652:LEU:O	1:A:656:LEU:HG	2.18	0.44
1:A:681:PRO:HB3	1:A:692:PHE:HB3	2.00	0.44
1:A:690:LEU:HD13	1:A:690:LEU:HA	1.74	0.44
1:A:1209:GLU:OE2	1:A:1322:SER:N	2.50	0.44
1:A:1734:PRO:HB2	1:A:1783:GLN:HB2	1.99	0.44
1:A:366:ILE:O	1:A:367:ILE:C	2.56	0.44
1:A:547:TRP:O	1:A:551:LYS:HG2	2.18	0.44
1:A:652:LEU:O	1:A:655:LEU:HB3	2.18	0.44
1:A:1717:PHE:HE2	1:A:1721:LEU:HD13	1.83	0.44
1:A:976:VAL:HG12	1:A:1014:GLY:HA2	2.00	0.43
1:A:810:LYS:HE3	1:A:810:LYS:HB3	1.43	0.43
1:A:863:PHE:HA	1:A:880:ARG:O	2.17	0.43
1:A:886:ASN:HD21	1:A:1401:HIS:CD2	2.36	0.43
1:A:1302:ASP:OD1	1:A:1302:ASP:N	2.51	0.43
1:A:304:PRO:O	2:G:53:G:H4'	2.18	0.43
1:A:814:ARG:HB3	1:A:819:ASP:HB2	2.00	0.43
1:A:1009:PHE:CE2	1:A:1087:PHE:HB3	2.53	0.43
1:A:845:HIS:NE2	2:G:57:A:H1'	2.34	0.43
1:A:1321:GLY:O	1:A:1325:ARG:HG3	2.18	0.43
1:A:1369:GLN:O	1:A:1370:GLU:HG2	2.17	0.43
1:A:1558:ASP:HB3	1:A:1562:LEU:HD23	2.01	0.43
1:A:1755:ARG:HD3	1:A:1755:ARG:HA	1.80	0.43
1:A:371:THR:HG22	1:A:404:LYS:HZ2	1.83	0.43
2:G:80:U:H2'	2:G:81:U:C6	2.53	0.43
1:A:404:LYS:HA	1:A:404:LYS:HD3	1.70	0.43
1:A:866:GLU:HB2	1:A:880:ARG:CZ	2.49	0.43
1:A:1056:LEU:HD22	1:A:1107:VAL:HG12	2.00	0.43
1:A:1498:SER:O	1:A:1498:SER:OG	2.34	0.43
2:G:17:C:H2'	2:G:18:G:H8	1.83	0.43
2:G:23:C:H2'	2:G:24:A:H8	1.84	0.43
1:A:461:ILE:O	1:A:773:LEU:N	2.43	0.43
1:A:1378:GLU:HG3	1:A:1504:ASP:HB3	2.00	0.43
1:A:1416:MET:HA	1:A:1419:TYR:HB3	2.01	0.43
1:A:377:LEU:HD11	1:A:389:TYR:CZ	2.54	0.43
1:A:457:MET:HG3	1:A:761:ARG:HD3	2.00	0.43
1:A:858:ILE:HG22	1:A:860:ARG:HG3	2.01	0.43
2:G:22:C:H2'	2:G:23:C:C6	2.54	0.42
2:G:22:C:H2'	2:G:23:C:H6	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LYS:O	1:A:309:VAL:HG23	2.19	0.42
1:A:709:SER:O	1:A:713:GLN:NE2	2.47	0.42
1:A:865:MET:SD	1:A:865:MET:N	2.92	0.42
1:A:1393:LEU:HD23	1:A:1396:LYS:HD2	2.01	0.42
1:A:1580:ILE:HG21	1:A:1651:ARG:CZ	2.49	0.42
1:A:977:CYS:SG	1:A:1016:GLU:HB2	2.59	0.42
1:A:1028:LEU:HG	1:A:1037:LYS:HZ2	1.84	0.42
1:A:1414:SER:HB2	1:A:1417:VAL:HG23	2.00	0.42
1:A:444:THR:O	1:A:446:LYS:NZ	2.40	0.42
1:A:1426:GLY:C	1:A:1428:GLN:N	2.73	0.42
1:A:1735:VAL:HG22	1:A:1736:ARG:HH12	1.84	0.42
2:G:4:A:H2'	2:G:5:U:H6	1.84	0.42
1:A:1301:LEU:O	1:A:1304:THR:OG1	2.24	0.42
1:A:811:ASP:OD1	1:A:811:ASP:N	2.48	0.42
1:A:1327:ALA:HA	1:A:1330:LEU:HG	2.02	0.42
1:A:1343:ALA:HB1	1:A:1347:LYS:HE2	2.02	0.42
1:A:359:LEU:HD21	1:A:363:ARG:HH22	1.84	0.42
1:A:738:ASP:OD1	1:A:738:ASP:N	2.42	0.42
1:A:1022:LEU:HD22	1:A:1022:LEU:HA	1.76	0.41
1:A:1580:ILE:HG23	1:A:1650:LEU:HD12	2.01	0.41
1:A:1662:ARG:HE	1:A:1666:LYS:HE2	1.85	0.41
2:G:44:G:H2'	2:G:45:A:C8	2.55	0.41
1:A:295:ARG:HH21	1:A:298:LEU:HD11	1.85	0.41
1:A:465:TYR:N	1:A:777:ARG:H	2.18	0.41
1:A:897:CYS:SG	1:A:902:LEU:HB3	2.60	0.41
1:A:1427:LEU:HA	1:A:1430:TYR:HD2	1.85	0.41
1:A:1641:ALA:HB1	1:A:1691:LEU:HD22	2.02	0.41
1:A:1791:LEU:HD13	1:A:1794:LEU:HD11	2.01	0.41
1:A:1378:GLU:O	1:A:1507:GLU:HB3	2.20	0.41
2:G:44:G:H2'	2:G:45:A:H8	1.85	0.41
1:A:461:ILE:HD13	1:A:461:ILE:HA	1.82	0.41
2:G:2:G:H3'	2:G:3:A:H5"	2.02	0.41
1:A:338:SER:HA	1:A:341:TRP:CD1	2.56	0.41
1:A:369:MET:HB2	1:A:404:LYS:HG3	2.02	0.41
1:A:548:CYS:O	1:A:552:VAL:HG23	2.20	0.41
1:A:1254:THR:OG1	1:A:1257:ASP:N	2.48	0.41
1:A:1426:GLY:C	1:A:1428:GLN:H	2.24	0.41
1:A:426:ASP:HB2	1:A:805:ASP:CB	2.50	0.41
1:A:1513:TYR:HD2	1:A:1522:ALA:HA	1.86	0.41
1:A:1732:MET:HG3	1:A:1780:LYS:NZ	2.36	0.41
1:A:327:TYR:HB3	1:A:329:GLY:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLU:O	1:A:398:HIS:NE2	2.54	0.41
1:A:834:MET:O	1:A:838:ASN:ND2	2.54	0.41
1:A:367:ILE:HB	1:A:368:ARG:H	1.73	0.41
1:A:414:SER:HB3	1:A:415:PRO:HD3	2.03	0.41
1:A:803:ARG:HA	1:A:806:LEU:HB2	2.01	0.41
1:A:1091:THR:OG1	1:A:1103:ASN:ND2	2.38	0.41
1:A:1387:TRP:O	1:A:1390:SER:OG	2.35	0.41
1:A:1418:LEU:H	1:A:1418:LEU:HG	1.78	0.41
2:G:72:G:O6	2:G:73:A:N6	2.53	0.41
1:A:716:ILE:HG12	1:A:737:LEU:HD21	2.03	0.41
1:A:1349:LEU:HB3	1:A:1352:TYR:HD1	1.86	0.41
1:A:1368:CYS:O	1:A:1371:THR:HG22	2.21	0.41
1:A:1051:ASN:OD1	1:A:1051:ASN:N	2.53	0.40
1:A:1090:VAL:HG13	1:A:1102:ILE:HA	2.02	0.40
1:A:253:GLN:OE1	1:A:253:GLN:N	2.44	0.40
1:A:1607:LEU:HD23	1:A:1607:LEU:HA	1.92	0.40
1:A:307:PRO:HA	1:A:310:TYR:CD2	2.56	0.40
2:G:46:U:H2'	2:G:47:U:C6	2.57	0.40
1:A:288:LYS:HE3	1:A:288:LYS:HB3	1.95	0.40
1:A:307:PRO:O	1:A:311:GLN:HG2	2.21	0.40
1:A:664:ASP:HB3	1:A:743:ASN:OD1	2.20	0.40
1:A:698:MET:SD	1:A:698:MET:N	2.94	0.40
1:A:1404:GLN:HA	1:A:1407:ARG:HD3	2.02	0.40
1:A:1496:VAL:C	1:A:1498:SER:H	2.24	0.40
1:A:1625:THR:O	1:A:1628:ARG:HG3	2.22	0.40
1:A:252:TYR:HB2	1:A:450:GLU:HB2	2.03	0.40
1:A:295:ARG:CZ	1:A:345:PHE:HA	2.51	0.40
1:A:316:ILE:HD12	1:A:316:ILE:HA	1.96	0.40
1:A:1231:CYS:HB3	1:A:1276:LYS:HZ1	1.86	0.40
1:A:1319:LEU:HD12	1:A:1319:LEU:HA	1.78	0.40
2:G:8:U:H2'	2:G:9:G:C8	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%)	1001 (90%)	101 (9%)	9 (1%)	19 60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ILE
1	A	663	ALA
1	A	728	VAL
1	A	817	SER
1	A	419	LYS
1	A	415	PRO
1	A	850	GLN
1	A	1497	LEU
1	A	420	GLY

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%)	905 (92%)	78 (8%)	12 38

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	HIS
1	A	405	ARG
1	A	412	THR
1	A	416	VAL
1	A	418	LEU
1	A	425	VAL
1	A	426	ASP
1	A	427	CYS
1	A	430	LYS
1	A	455	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	457	MET
1	A	459	SER
1	A	460	GLU
1	A	529	ASN
1	A	544	LEU
1	A	550	TYR
1	A	658	LYS
1	A	664	ASP
1	A	666	ARG
1	A	668	ILE
1	A	690	LEU
1	A	691	SER
1	A	693	ILE
1	A	694	ARG
1	A	721	ASP
1	A	725	THR
1	A	726	LEU
1	A	740	ARG
1	A	742	CYS
1	A	744	VAL
1	A	746	MET
1	A	747	ARG
1	A	763	ARG
1	A	766	LYS
1	A	769	SER
1	A	770	ASP
1	A	772	ILE
1	A	796	LEU
1	A	797	ARG
1	A	798	LYS
1	A	804	THR
1	A	806	LEU
1	A	810	LYS
1	A	816	ILE
1	A	851	LEU
1	A	854	ASP
1	A	859	LEU
1	A	870	LYS
1	A	1017	LEU
1	A	1020	GLU
1	A	1022	LEU
1	A	1024	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1025	SER
1	A	1039	SER
1	A	1040	LEU
1	A	1212	ILE
1	A	1214	LYS
1	A	1224	ARG
1	A	1225	PHE
1	A	1257	ASP
1	A	1261	GLN
1	A	1262	LYS
1	A	1263	TYR
1	A	1313	LEU
1	A	1314	CYS
1	A	1369	GLN
1	A	1373	CYS
1	A	1428	GLN
1	A	1495	ARG
1	A	1502	LEU
1	A	1504	ASP
1	A	1524	HIS
1	A	1657	LEU
1	A	1659	LYS
1	A	1742	CYS
1	A	1743	GLN
1	A	1745	GLN
1	A	1764	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	GLN
1	A	538	ASN
1	A	850	GLN
1	A	886	ASN
1	A	1103	ASN
1	A	1261	GLN
1	A	1272	GLN
1	A	1523	ASN
1	A	1633	ASN
1	A	1647	HIS
1	A	1669	GLN
1	A	1758	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1775	GLN
1	A	1789	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	79/89 (88%)	33 (41%)	2 (2%)

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	3	A
2	G	9	G
2	G	10	C
2	G	14	G
2	G	16	U
2	G	18	G
2	G	19	A
2	G	20	G
2	G	21	A
2	G	26	U
2	G	28	A
2	G	30	U
2	G	31	C
2	G	33	C
2	G	34	A
2	G	35	U
2	G	36	G
2	G	37	A
2	G	49	U
2	G	57	A
2	G	66	A
2	G	71	G
2	G	72	G
2	G	73	A
2	G	74	C
2	G	76	A
2	G	77	G
2	G	82	C
2	G	84	U
2	G	85	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	86	C
2	G	88	C
2	G	89	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	13	G
2	G	25	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.

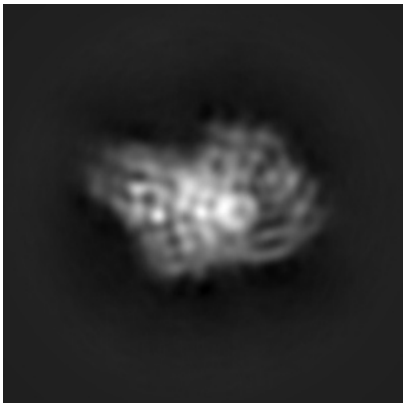
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31182. 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.

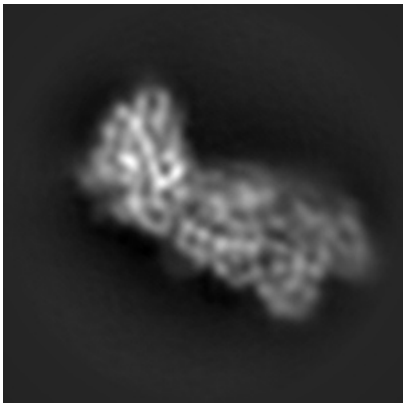
6.1 Orthogonal projections

6.1.1 Primary map



X

Y

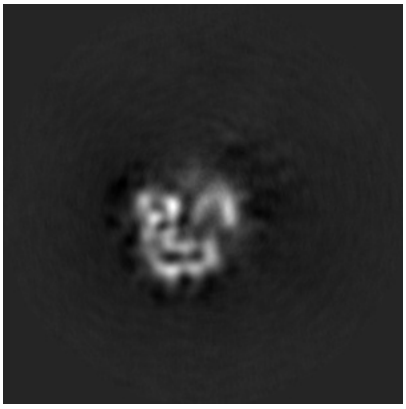


Z

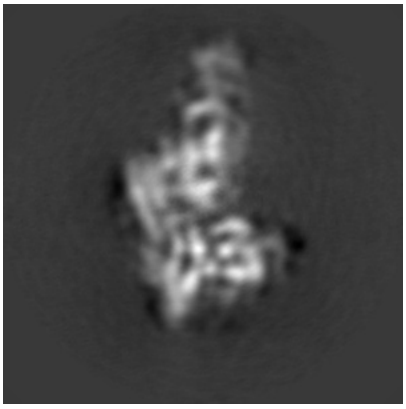
The images above show the map projected in three orthogonal directions.

6.2 Central slices

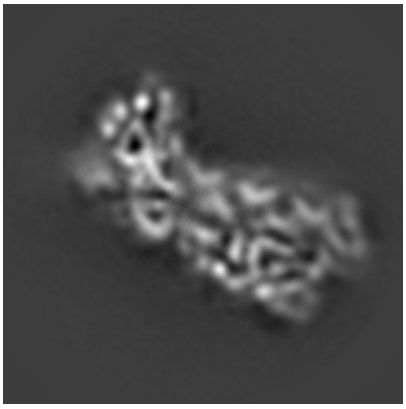
6.2.1 Primary map



X Index: 100



Y Index: 100

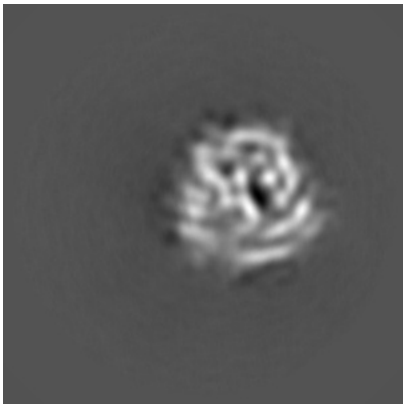


Z Index: 100

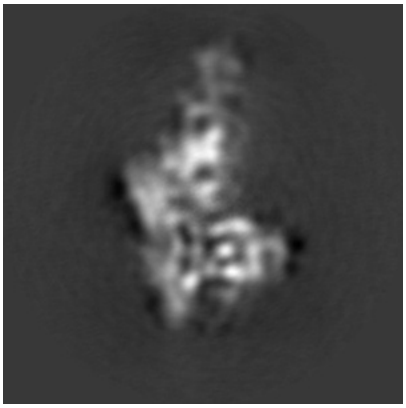
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

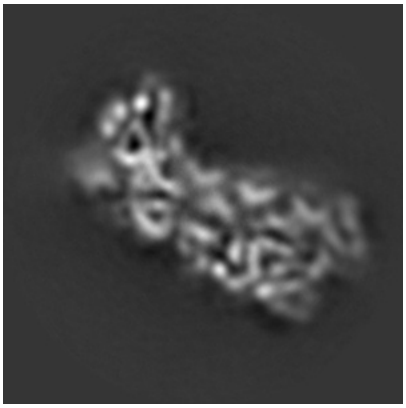
6.3.1 Primary map



X Index: 66



Y Index: 102

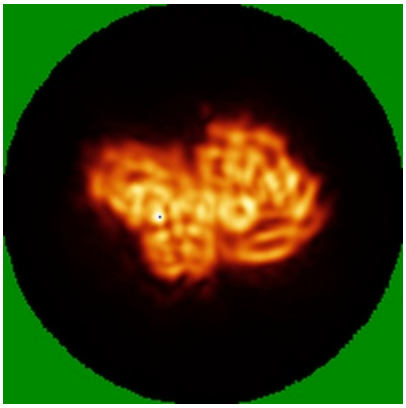


Z Index: 99

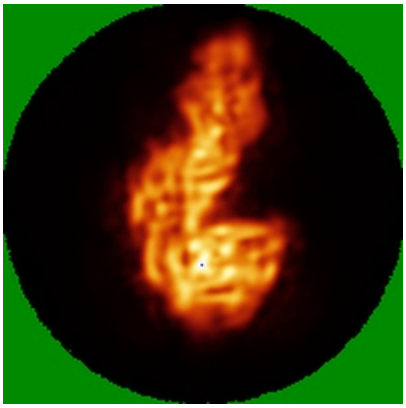
The images above show the largest variance slices of the map in three orthogonal directions.

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

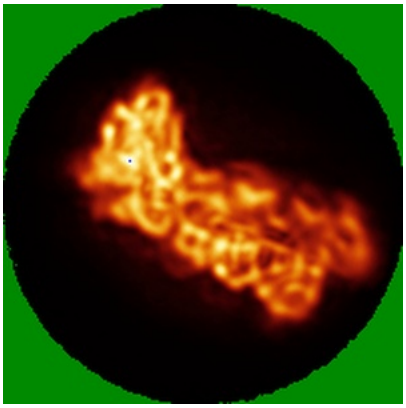
6.4.1 Primary map



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 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

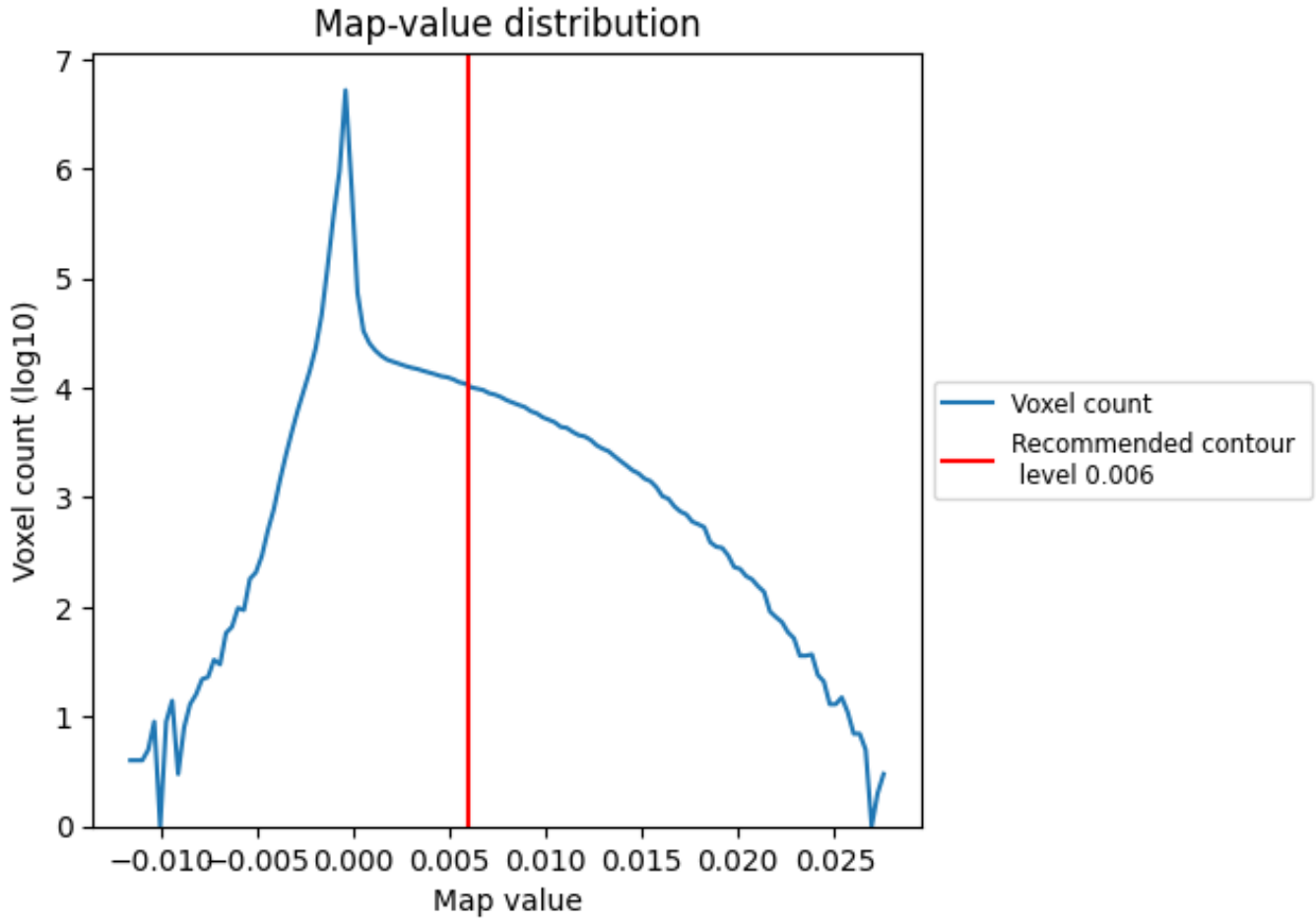
6.6 Mask visualisation (i)

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

7 Map analysis

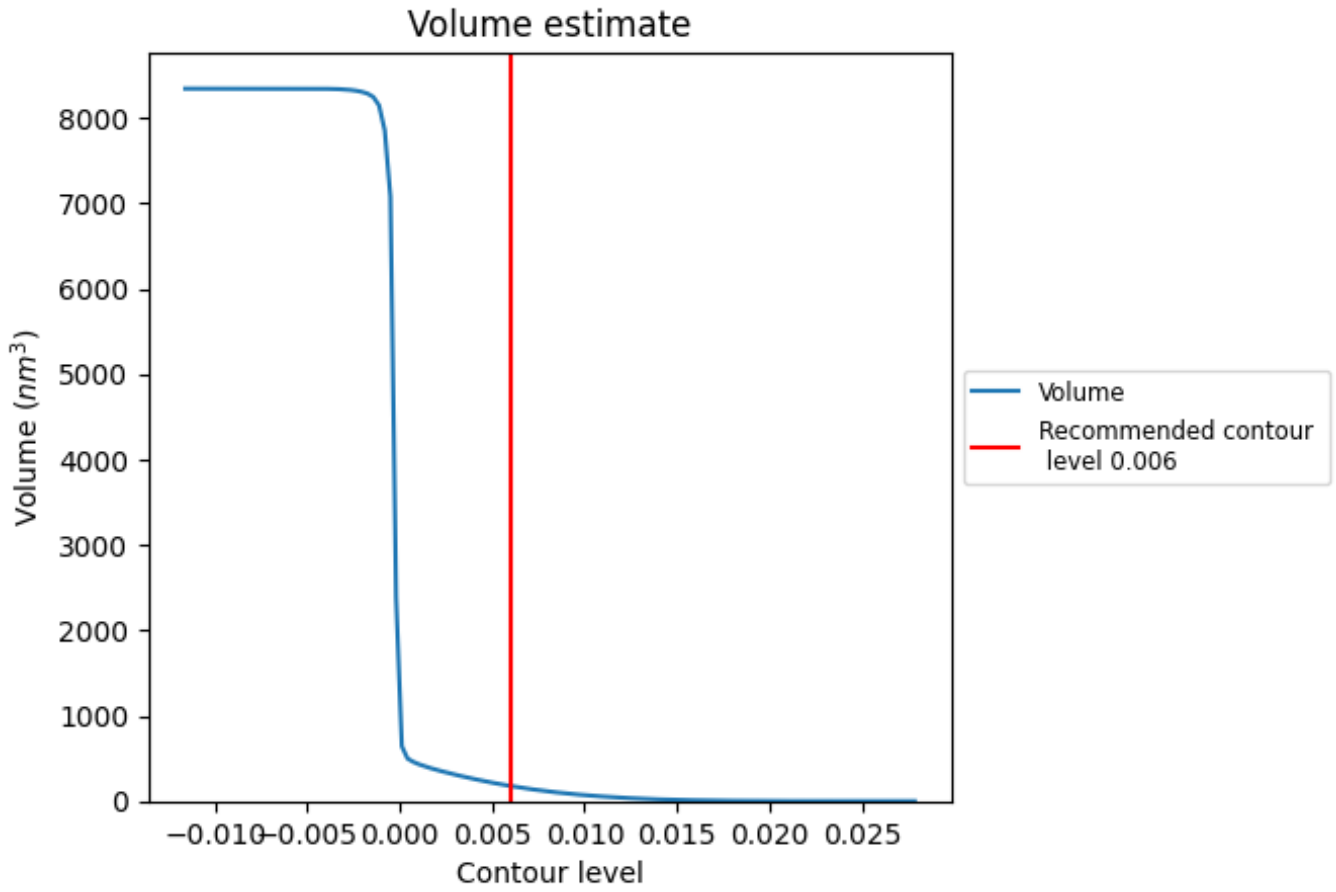
This section contains the results of statistical analysis of the map.

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.

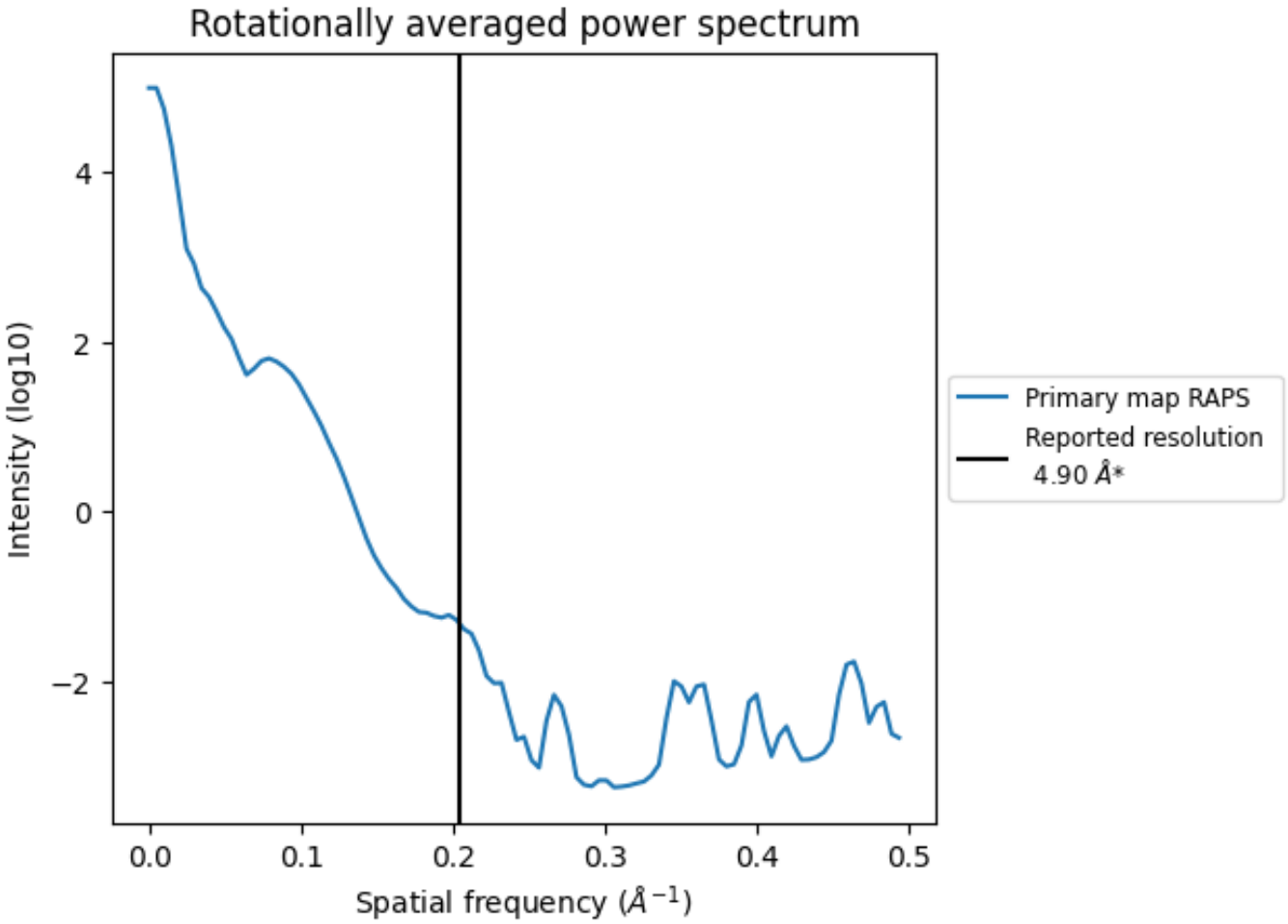
7.2 Volume estimate



The volume at the recommended contour level is 177 nm^3; this corresponds to an approximate mass of 160 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 0.204 $Å^{-1}$

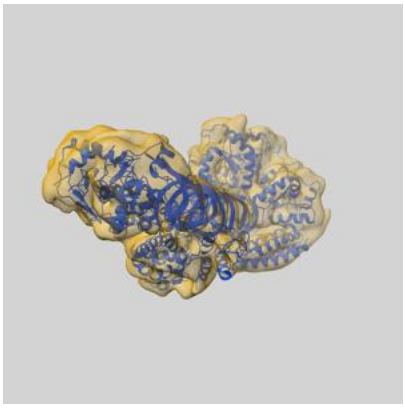
8 Fourier-Shell correlation

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

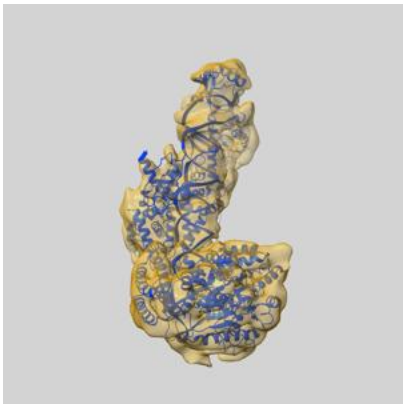
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31182 and PDB model 7ELE. Per-residue inclusion information can be found in section 3 on page 4.

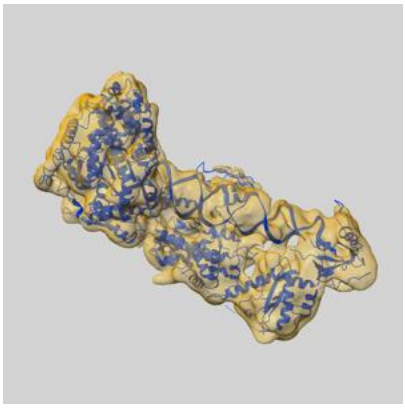
9.1 Map-model overlay



X



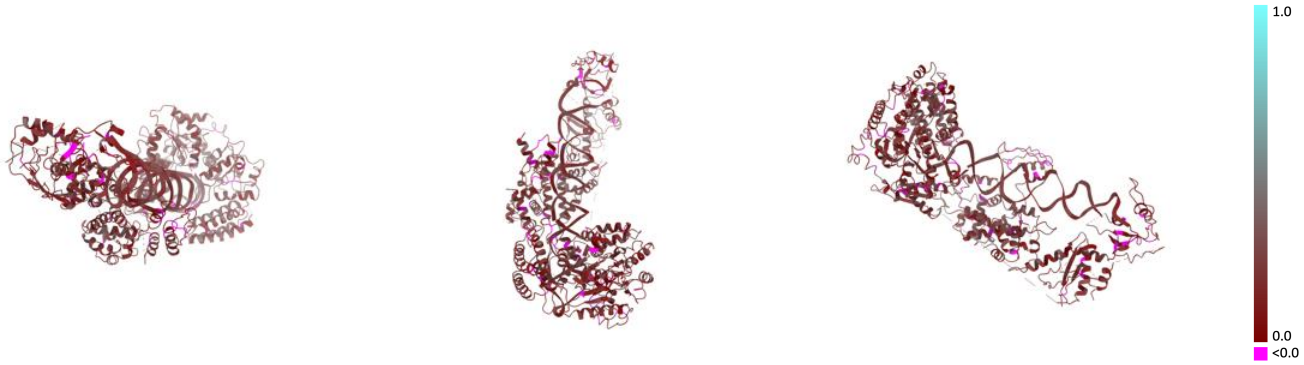
Y



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

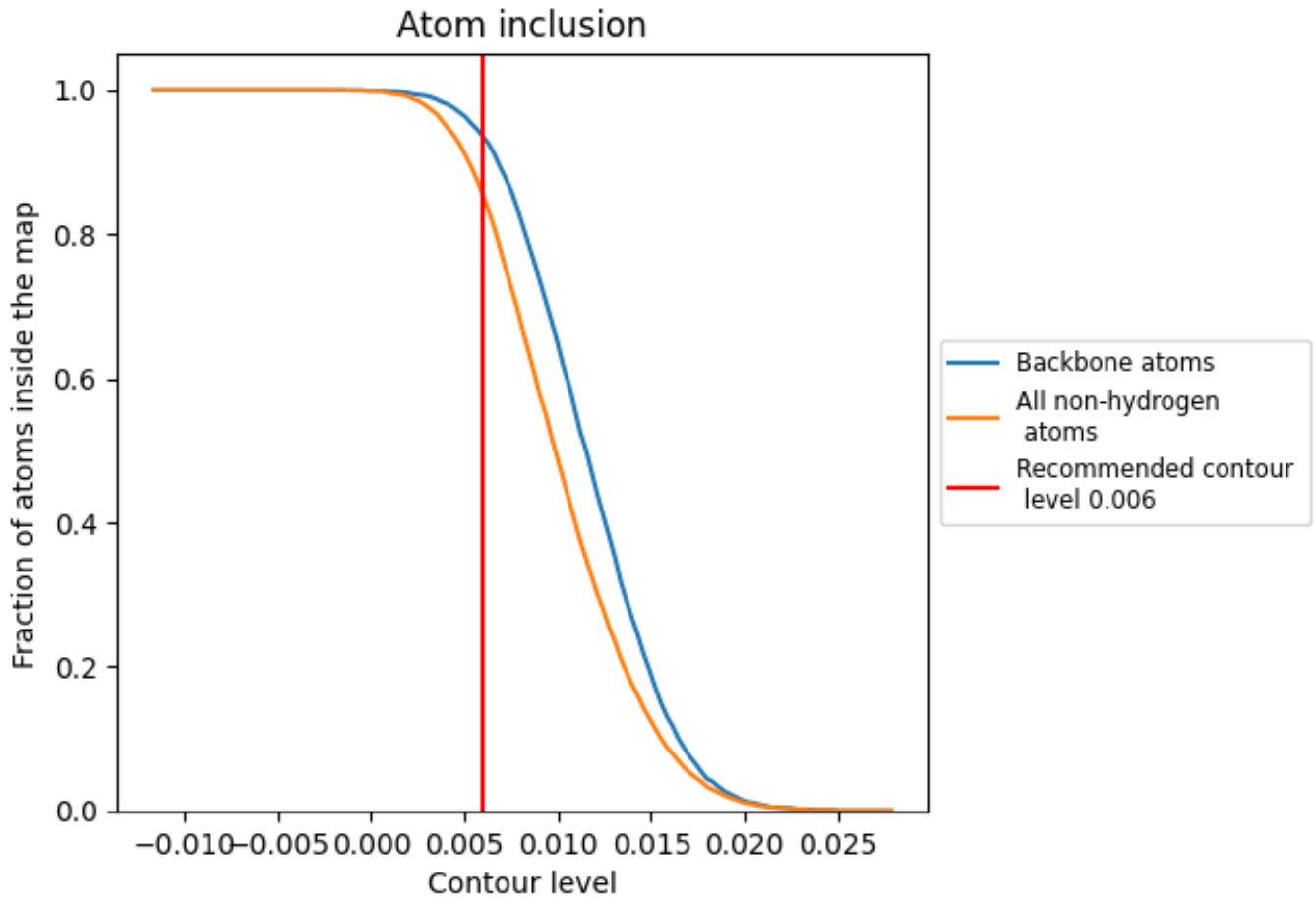
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	0.8540	0.1860
A	0.8360	0.1790
G	0.9440	0.2200