



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:31 AM UTC

PDB ID : 6DNH / pdb_00006dnh
EMDB ID : EMD-7112
Title : Cryo-EM structure of human CPSF-160-WDR33-CPSF-30-PAS RNA complex
at 3.4 Å resolution
Authors : Sun, Y.; Zhang, Y.; Hamilton, K.; Walz, T.; Tong, L.
Deposited on : 2018-06-06
Resolution : 3.40 Å (reported)
Based on initial model : 2RHK

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

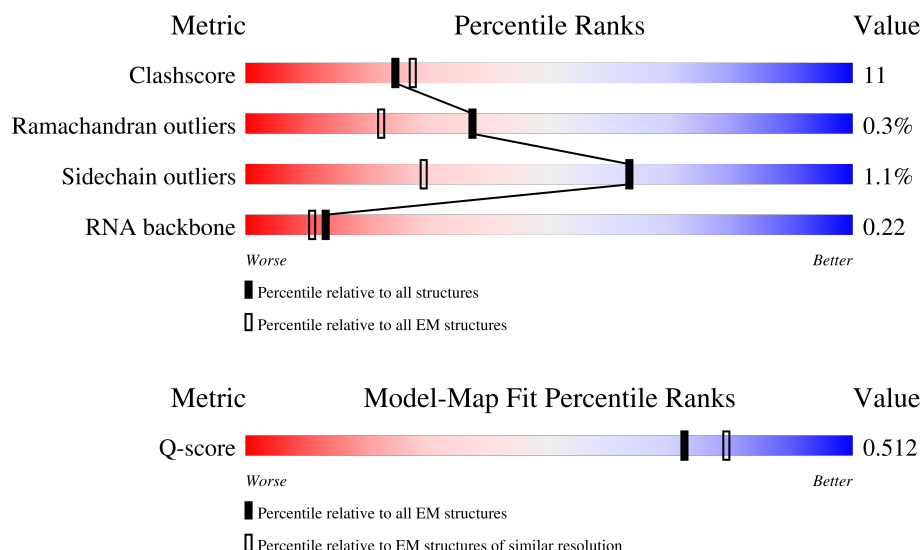
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	1443	
2	B	587	
3	C	245	

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Mol	Chain	Length	Quality of chain
4	E	17	6%24%18%59%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13442 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 Cleavage and polyadenylation specificity factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1177	Total	C	N	O	S	0	0
			9337	6003	1600	1679	55		

- Molecule 2 is a protein called pre-mRNA 3' end processing protein WDR33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	376	Total	C	N	O	S	0	0
			3035	1916	557	542	20		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	MET	-	expression tag	UNP Q9C0J8
B	-13	GLY	-	expression tag	UNP Q9C0J8
B	-12	SER	-	expression tag	UNP Q9C0J8
B	-11	SER	-	expression tag	UNP Q9C0J8
B	-10	HIS	-	expression tag	UNP Q9C0J8
B	-9	HIS	-	expression tag	UNP Q9C0J8
B	-8	HIS	-	expression tag	UNP Q9C0J8
B	-7	HIS	-	expression tag	UNP Q9C0J8
B	-6	HIS	-	expression tag	UNP Q9C0J8
B	-5	HIS	-	expression tag	UNP Q9C0J8
B	-4	SER	-	expression tag	UNP Q9C0J8
B	-3	SER	-	expression tag	UNP Q9C0J8
B	-2	GLY	-	expression tag	UNP Q9C0J8
B	-1	LEU	-	expression tag	UNP Q9C0J8
B	0	VAL	-	expression tag	UNP Q9C0J8

- Molecule 3 is a protein called Cleavage and polyadenylation specificity factor subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	117	Total	C	N	O	S	0	0
			917	587	151	165	14		

There is a discrepancy between the modelled and reference sequences:

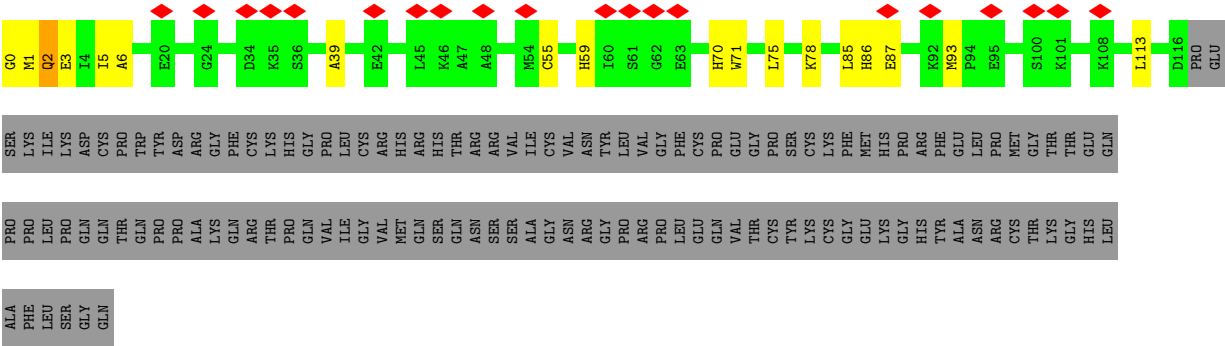
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP O95639

- Molecule 4 is a RNA chain called RNA (5'-R(P*AP*AP*UP*AP*AP*AP*C)-3').

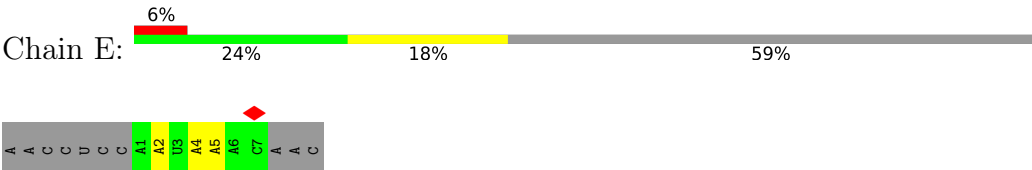
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	7	Total	C	N	O	P	0	0
			150	68	30	45	7		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	C	3	Total	Zn	0
			3	3	



● Molecule 4: RNA (5'-R(P*AP*AP*UP*AP*AP*AP*C)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	173632	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	46729	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.315	Depositor
Minimum map value	-0.177	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	205.44, 205.44, 205.44	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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

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	0.42	0/9553	0.64	10/12967 (0.1%)
2	B	0.44	1/3120 (0.0%)	0.66	2/4224 (0.0%)
3	C	0.32	0/941	0.69	0/1261
4	E	0.29	0/168	0.35	0/259
All	All	0.42	1/13782 (0.0%)	0.64	12/18711 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	57	ILE	C-N	5.14	1.40	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	CYS	N-CA-C	9.02	120.88	111.14
1	A	200	LEU	N-CA-C	8.23	119.88	111.07
2	B	266	SER	N-CA-C	6.26	118.10	111.28
1	A	1273	ASP	N-CA-C	5.96	118.67	109.07
1	A	331	SER	CB-CA-C	-5.87	109.83	116.63
1	A	518	SER	CA-C-N	-5.62	116.22	123.19
1	A	518	SER	C-N-CA	-5.62	116.22	123.19
1	A	631	GLY	N-CA-C	-5.52	103.22	110.29
1	A	377	MET	N-CA-C	-5.32	99.46	110.80
2	B	369	GLY	N-CA-C	5.18	118.67	111.10
1	A	1314	THR	CA-C-N	5.05	124.81	119.76
1	A	1314	THR	C-N-CA	5.05	124.81	119.76

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	9337	0	9390	191	0
2	B	3035	0	2949	82	0
3	C	917	0	889	18	0
4	E	150	0	77	2	0
5	C	3	0	0	0	0
All	All	13442	0	13305	284	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 11.

All (284) 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)
2:B:245:ALA:HB2	2:B:265:ASP:HB2	1.27	1.16
1:A:653:ASP:HB3	1:A:654:PRO:CD	1.76	1.15
1:A:653:ASP:HB3	1:A:654:PRO:HD3	1.24	1.13
2:B:245:ALA:HB2	2:B:265:ASP:CB	1.84	1.07
1:A:653:ASP:CG	1:A:702:ARG:HD3	1.80	1.05
1:A:1273:ASP:O	1:A:1275:ASP:N	1.88	1.05
1:A:202:ASN:ND2	1:A:225:GLN:OE1	1.91	1.03
1:A:1273:ASP:C	1:A:1275:ASP:H	1.68	1.02
1:A:653:ASP:CB	1:A:654:PRO:CD	2.38	1.01
2:B:246:ASP:OD1	2:B:264:LYS:HB3	1.63	0.99
2:B:245:ALA:CB	2:B:265:ASP:CB	2.42	0.97
1:A:608:PHE:HZ	1:A:651:VAL:CG1	1.77	0.96
2:B:245:ALA:CB	2:B:265:ASP:HB3	1.97	0.94
1:A:14:LEU:HD13	1:A:32:VAL:HB	1.47	0.93
1:A:653:ASP:OD2	1:A:702:ARG:HD3	1.66	0.93
2:B:243:HIS:NE2	2:B:263:SER:HB2	1.83	0.93
1:A:330:ILE:HD12	1:A:336:VAL:HG23	1.50	0.91
1:A:608:PHE:HZ	1:A:651:VAL:HG11	1.34	0.91
2:B:54:ARG:NE	2:B:152:ASN:HD21	1.70	0.90
1:A:651:VAL:O	1:A:651:VAL:HG13	1.72	0.87
1:A:65:LYS:HG3	1:A:467:ASP:OD2	1.75	0.87
2:B:245:ALA:HB3	2:B:265:ASP:HB3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:ASP:OD1	1:A:702:ARG:NE	2.09	0.85
1:A:608:PHE:CZ	1:A:651:VAL:CG1	2.59	0.85
2:B:246:ASP:OD1	2:B:264:LYS:CB	2.25	0.85
1:A:653:ASP:OD1	1:A:702:ARG:HD3	1.78	0.84
1:A:1258:VAL:HG12	1:A:1271:VAL:HG22	1.58	0.84
2:B:245:ALA:CB	2:B:265:ASP:HB2	2.05	0.84
2:B:297:ASN:CB	2:B:299:ASN:OD1	2.26	0.84
2:B:54:ARG:HE	2:B:152:ASN:HD21	1.26	0.83
1:A:14:LEU:HD13	1:A:32:VAL:CB	2.10	0.82
1:A:330:ILE:CD1	1:A:336:VAL:HG23	2.08	0.82
1:A:653:ASP:OD1	1:A:702:ARG:CD	2.30	0.80
1:A:653:ASP:OD1	1:A:702:ARG:CZ	2.31	0.78
1:A:653:ASP:CB	1:A:654:PRO:HD2	2.12	0.77
2:B:357:LEU:HD23	2:B:369:GLY:HA3	1.64	0.77
2:B:54:ARG:HG2	2:B:152:ASN:OD1	1.84	0.76
3:C:78:LYS:HG2	4:E:2:A:N6	2.01	0.76
1:A:113:HIS:HB3	1:A:893:LYS:HD2	1.68	0.75
1:A:200:LEU:N	1:A:200:LEU:HD23	2.01	0.75
1:A:330:ILE:HD11	1:A:336:VAL:CG2	2.16	0.74
1:A:330:ILE:CD1	1:A:336:VAL:CG2	2.64	0.74
2:B:54:ARG:CZ	2:B:152:ASN:HD21	2.00	0.74
2:B:43:PHE:HE1	2:B:47:ARG:HH12	1.36	0.74
2:B:346:LEU:HD12	2:B:346:LEU:C	2.14	0.72
1:A:653:ASP:OD2	1:A:702:ARG:HB3	1.89	0.72
1:A:495:GLU:HB3	1:A:1317:ARG:HH21	1.52	0.72
1:A:495:GLU:HB3	1:A:1317:ARG:NH2	2.05	0.72
2:B:297:ASN:HB3	2:B:299:ASN:OD1	1.91	0.71
2:B:354:GLY:CA	2:B:376:GLY:O	2.38	0.71
2:B:54:ARG:NE	2:B:152:ASN:ND2	2.40	0.70
1:A:1273:ASP:C	1:A:1275:ASP:N	2.38	0.70
1:A:608:PHE:CZ	1:A:651:VAL:HG12	2.27	0.69
1:A:330:ILE:HD11	1:A:336:VAL:HG21	1.73	0.69
1:A:620:GLN:HE21	1:A:627:ARG:HD2	1.58	0.68
3:C:2:GLN:CD	3:C:2:GLN:H	2.01	0.68
1:A:653:ASP:HB2	1:A:654:PRO:HD2	1.76	0.68
3:C:1:MET:O	3:C:3:GLU:N	2.26	0.67
1:A:1274:ARG:O	1:A:1274:ARG:HG2	1.95	0.65
3:C:1:MET:O	3:C:1:MET:HG3	1.97	0.65
1:A:1237:GLN:HE22	3:C:39:ALA:HB1	1.61	0.65
2:B:243:HIS:NE2	2:B:262:GLY:O	2.30	0.65
2:B:374:HIS:NE2	2:B:394:SER:OG	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:MET:HB3	2:B:373:ALA:HB3	1.81	0.63
1:A:202:ASN:ND2	1:A:225:GLN:CD	2.57	0.63
2:B:54:ARG:NH2	2:B:152:ASN:HD21	1.96	0.63
1:A:14:LEU:HD13	1:A:32:VAL:CG2	2.29	0.63
1:A:473:GLY:H	1:A:504:SER:HB2	1.64	0.62
2:B:248:LYS:NZ	2:B:264:LYS:HB2	2.14	0.61
1:A:14:LEU:CD1	1:A:32:VAL:HG21	2.31	0.61
2:B:384:HIS:HB2	2:B:389:ILE:HG22	1.83	0.60
2:B:113:THR:HG22	2:B:400:LYS:HG2	1.82	0.60
2:B:297:ASN:HB2	2:B:299:ASN:OD1	2.01	0.60
2:B:54:ARG:HE	2:B:152:ASN:ND2	1.95	0.60
1:A:229:GLY:HA2	2:B:407:PRO:HA	1.84	0.59
1:A:577:LEU:HB2	1:A:584:MET:HB2	1.84	0.59
1:A:656:VAL:HB	1:A:668:PHE:HB2	1.84	0.59
1:A:692:GLN:OE1	1:A:789:ARG:NH1	2.35	0.59
1:A:1106:VAL:HG13	1:A:1177:HIS:HB3	1.84	0.59
1:A:202:ASN:HD22	1:A:225:GLN:HB2	1.68	0.59
1:A:298:VAL:HG12	1:A:313:ARG:HB2	1.85	0.59
1:A:651:VAL:CG1	1:A:651:VAL:O	2.44	0.59
1:A:378:GLU:OE1	1:A:378:GLU:HA	2.01	0.59
2:B:354:GLY:O	2:B:374:HIS:HB3	2.03	0.58
2:B:377:MET:O	2:B:395:ASN:N	2.35	0.58
1:A:378:GLU:OE1	1:A:379:PRO:CD	2.52	0.58
1:A:1044:CYS:HB3	1:A:1069:PRO:HG2	1.85	0.58
3:C:0:GLY:N	3:C:5:ILE:HD11	2.18	0.57
1:A:653:ASP:OD2	1:A:702:ARG:CD	2.46	0.57
2:B:75:ASP:HB2	2:B:77:ARG:HG2	1.87	0.57
1:A:640:VAL:HG21	1:A:646:ILE:HD11	1.86	0.57
2:B:344:GLU:O	2:B:344:GLU:HG3	2.05	0.57
3:C:55:CYS:HB3	3:C:59:HIS:HE1	1.69	0.57
1:A:378:GLU:OE1	1:A:379:PRO:HD2	2.05	0.57
1:A:652:ALA:HB2	1:A:700:LEU:HB2	1.86	0.56
1:A:1028:HIS:ND1	1:A:1030:GLU:O	2.35	0.56
1:A:1273:ASP:HB2	1:A:1277:ASN:HB2	1.88	0.56
1:A:1104:LYS:NZ	1:A:1215:MET:O	2.39	0.56
1:A:202:ASN:ND2	1:A:225:GLN:HB2	2.20	0.56
2:B:308:ARG:HE	2:B:333:GLU:HG2	1.70	0.56
1:A:387:ARG:O	1:A:471:ASN:ND2	2.37	0.55
1:A:811:PHE:HZ	1:A:865:VAL:HG11	1.71	0.55
2:B:325:GLN:HE22	2:B:362:GLY:H	1.53	0.55
3:C:78:LYS:CG	4:E:2:A:N6	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:MET:HB3	2:B:188:TRP:HB2	1.88	0.55
1:A:785:CYS:HB2	1:A:799:LEU:HD13	1.87	0.55
2:B:76:GLN:NE2	2:B:79:MET:SD	2.80	0.55
2:B:243:HIS:CE1	2:B:262:GLY:O	2.60	0.54
1:A:480:VAL:HG22	1:A:500:ILE:HG22	1.89	0.54
1:A:1231:ILE:HG21	1:A:1271:VAL:HG21	1.90	0.54
1:A:601:ALA:H	1:A:620:GLN:HE22	1.56	0.54
1:A:267:GLN:NE2	1:A:325:ALA:O	2.40	0.54
1:A:163:PRO:HB2	1:A:186:LEU:HB2	1.90	0.54
1:A:1408:LEU:HA	1:A:1415:ARG:HH12	1.73	0.54
1:A:621:VAL:HG22	1:A:626:ILE:HG23	1.88	0.54
1:A:1188:GLN:OE1	2:B:59:TYR:OH	2.26	0.54
1:A:98:PHE:HB2	1:A:102:LYS:HB2	1.90	0.53
1:A:330:ILE:C	1:A:331:SER:HG	2.13	0.53
1:A:14:LEU:HD11	1:A:32:VAL:HG21	1.89	0.53
2:B:57:ILE:HG22	2:B:57:ILE:O	2.08	0.53
2:B:133:ARG:HD3	2:B:145:LEU:HD23	1.90	0.53
2:B:54:ARG:NH2	2:B:152:ASN:ND2	2.57	0.53
1:A:808:VAL:HG21	1:A:818:LEU:HD13	1.91	0.52
2:B:352:SER:HA	2:B:377:MET:HG3	1.91	0.52
1:A:888:LEU:HB3	1:A:890:VAL:HG22	1.91	0.52
1:A:652:ALA:HB3	1:A:700:LEU:CD1	2.39	0.52
2:B:54:ARG:CZ	2:B:152:ASN:ND2	2.70	0.52
1:A:380:GLY:O	1:A:395:LYS:HA	2.09	0.52
1:A:962:ARG:NE	1:A:1008:ASP:O	2.38	0.52
2:B:162:SER:HB3	2:B:181:HIS:HB3	1.90	0.52
1:A:608:PHE:CZ	1:A:651:VAL:HG11	2.27	0.52
2:B:122:VAL:HA	2:B:138:ALA:HA	1.92	0.52
1:A:21:ASN:HB2	1:A:92:ASP:HB2	1.93	0.51
1:A:786:LEU:HD13	1:A:796:ILE:HG12	1.93	0.51
1:A:1313:ARG:HG2	1:A:1336:THR:HG22	1.92	0.51
1:A:1276:ARG:O	1:A:1304:VAL:O	2.29	0.51
1:A:318:VAL:HG21	1:A:362:PHE:HD2	1.76	0.51
2:B:354:GLY:HA2	2:B:376:GLY:O	2.11	0.51
1:A:687:PRO:HB3	1:A:802:TRP:CE2	2.46	0.51
1:A:652:ALA:HB3	1:A:700:LEU:HD13	1.93	0.50
2:B:335:THR:HG21	2:B:377:MET:HE3	1.92	0.50
1:A:1384:LEU:O	1:A:1385:HIS:ND1	2.44	0.50
1:A:575:LEU:HB3	1:A:586:LEU:HB2	1.94	0.50
3:C:71:TRP:CZ3	3:C:86:HIS:O	2.65	0.50
3:C:71:TRP:CH2	3:C:86:HIS:O	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:SER:HA	2:B:210:PHE:HZ	1.76	0.50
2:B:313:LYS:HG2	2:B:326:VAL:HG12	1.93	0.50
1:A:103:LEU:HD12	1:A:152:MET:HE3	1.94	0.49
1:A:381:TYR:HB3	1:A:393:LEU:HD11	1.94	0.49
2:B:346:LEU:C	2:B:346:LEU:CD1	2.85	0.49
1:A:1222:ILE:HB	1:A:1234:LEU:HB2	1.94	0.49
1:A:1275:ASP:HB3	1:A:1277:ASN:ND2	2.27	0.49
2:B:248:LYS:HZ3	2:B:264:LYS:HB2	1.76	0.49
1:A:608:PHE:CE2	1:A:651:VAL:HB	2.46	0.49
1:A:646:ILE:HA	1:A:660:SER:HA	1.94	0.49
1:A:854:LEU:HB3	1:A:955:VAL:HB	1.93	0.49
1:A:214:GLU:OE2	1:A:246:ASN:ND2	2.45	0.49
1:A:948:PRO:HA	1:A:971:PRO:HB3	1.94	0.49
1:A:607:VAL:HG22	1:A:621:VAL:O	2.13	0.49
1:A:269:LEU:HB2	1:A:279:VAL:HG23	1.93	0.49
1:A:1077:GLN:HE22	1:A:1091:ARG:HH21	1.61	0.49
1:A:140:ARG:NH1	1:A:204:ILE:O	2.44	0.48
1:A:477:ASN:HD22	1:A:1024:TYR:HD1	1.61	0.48
1:A:301:ASN:OD1	1:A:301:ASN:N	2.45	0.48
3:C:0:GLY:H1	3:C:5:ILE:HD11	1.77	0.48
2:B:54:ARG:CG	2:B:152:ASN:OD1	2.59	0.48
2:B:54:ARG:HH21	2:B:152:ASN:HD21	1.61	0.48
2:B:125:VAL:HG22	2:B:136:THR:HG23	1.94	0.48
1:A:703:ASP:HB3	1:A:706:GLY:HA3	1.94	0.48
2:B:221:SER:OG	2:B:223:ASP:OD1	2.28	0.48
1:A:241:VAL:HG13	1:A:254:VAL:HG13	1.96	0.48
2:B:259:VAL:HG23	2:B:275:PRO:HG3	1.96	0.48
1:A:271:VAL:HB	1:A:276:GLY:O	2.14	0.48
1:A:1411:SER:O	1:A:1415:ARG:N	2.46	0.48
2:B:162:SER:HB2	2:B:180:ASP:HB2	1.96	0.48
1:A:846:VAL:HG22	1:A:867:VAL:HG22	1.96	0.48
2:B:301:ASN:O	2:B:302:TRP:CD1	2.67	0.48
1:A:378:GLU:HB3	1:A:379:PRO:HD2	1.95	0.47
1:A:1183:VAL:HG11	1:A:1222:ILE:HD13	1.97	0.47
1:A:653:ASP:OD2	1:A:702:ARG:CB	2.60	0.47
1:A:813:VAL:HG12	1:A:1411:SER:HB2	1.97	0.47
1:A:470:LEU:HD23	1:A:1009:ALA:HB2	1.95	0.47
1:A:1184:SER:O	1:A:1191:PHE:N	2.47	0.47
1:A:335:MET:HE2	1:A:347:LEU:HD23	1.97	0.47
1:A:653:ASP:CG	1:A:702:ARG:CD	2.66	0.47
1:A:1254:GLU:OE1	1:A:1274:ARG:CD	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:CYS:HB2	2:B:327:PHE:HB2	1.97	0.46
1:A:200:LEU:N	1:A:200:LEU:CD2	2.73	0.46
2:B:43:PHE:HE1	2:B:47:ARG:NH1	2.07	0.46
1:A:230:ARG:NH1	2:B:108:THR:OG1	2.49	0.46
1:A:1263:ASP:HA	1:A:1333:LYS:HG2	1.98	0.46
2:B:170:SER:HA	2:B:210:PHE:CZ	2.50	0.46
1:A:158:ARG:NH1	1:A:192:ASP:OD1	2.49	0.46
3:C:2:GLN:OE1	3:C:2:GLN:N	2.43	0.46
1:A:330:ILE:CD1	1:A:336:VAL:HG21	2.40	0.46
1:A:1142:MET:HG2	1:A:1162:VAL:HG22	1.97	0.46
1:A:1433:LEU:O	1:A:1436:THR:OG1	2.33	0.46
1:A:1315:PRO:HD2	3:C:5:ILE:HG22	1.98	0.45
1:A:12:THR:O	1:A:1342:ASP:O	2.35	0.45
1:A:224:ASN:HB2	1:A:237:THR:HG21	1.98	0.45
1:A:536:TRP:CZ2	1:A:608:PHE:HA	2.51	0.45
1:A:656:VAL:O	1:A:668:PHE:N	2.39	0.45
1:A:18:MET:HE3	1:A:81:MET:HE3	1.97	0.45
2:B:106:VAL:HG21	2:B:367:VAL:HG11	1.99	0.45
2:B:210:PHE:HB3	2:B:217:PHE:HB3	1.99	0.45
1:A:937:ILE:HD13	1:A:987:PHE:HB3	1.99	0.45
1:A:1254:GLU:OE1	1:A:1274:ARG:HD2	2.16	0.45
1:A:193:VAL:HG13	1:A:200:LEU:HD12	1.98	0.45
1:A:502:VAL:HB	1:A:513:SER:HB2	1.99	0.45
1:A:626:ILE:HG21	1:A:668:PHE:HE2	1.82	0.45
1:A:160:VAL:HG22	1:A:190:ILE:HG12	1.99	0.44
1:A:385:GLY:HA2	1:A:391:SER:HB2	1.99	0.44
1:A:528:GLU:HG3	1:A:995:GLU:HG2	1.99	0.44
3:C:2:GLN:O	3:C:6:ALA:N	2.50	0.44
1:A:652:ALA:CB	1:A:700:LEU:HB2	2.47	0.44
1:A:1259:ASP:HB3	1:A:1270:LEU:HB3	1.98	0.44
1:A:1071:GLN:NE2	1:A:1096:GLU:O	2.50	0.44
1:A:1223:LEU:HD11	1:A:1231:ILE:HD12	1.99	0.44
1:A:1253:LEU:HD11	1:A:1273:ASP:CG	2.43	0.44
1:A:45:ARG:HA	1:A:64:GLU:HG3	2.00	0.44
2:B:253:HIS:HB2	2:B:258:LEU:HB2	2.00	0.44
1:A:870:GLU:OE2	1:A:1415:ARG:NH2	2.51	0.43
1:A:512:LEU:HD11	1:A:1036:VAL:HG21	1.99	0.43
1:A:874:TYR:HB3	1:A:892:PHE:HB3	1.99	0.43
1:A:940:TYR:HB3	1:A:954:LEU:HD22	2.00	0.43
1:A:654:PRO:HG2	1:A:655:TYR:CD2	2.54	0.43
1:A:995:GLU:OE1	1:A:997:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:MET:HB3	2:B:395:ASN:HB2	2.00	0.43
2:B:43:PHE:CE2	2:B:117:LYS:HG3	2.53	0.43
3:C:93:MET:HB2	3:C:113:LEU:HG	1.99	0.43
2:B:195:VAL:HG12	2:B:196:LYS:H	1.84	0.43
2:B:243:HIS:NE2	2:B:263:SER:CB	2.70	0.43
1:A:516:GLN:O	1:A:1011:TRP:HB3	2.18	0.43
1:A:44:ASN:ND2	1:A:67:GLU:OE1	2.51	0.43
1:A:900:ASN:HD22	1:A:1434:LEU:HD13	1.83	0.43
2:B:211:SER:OG	2:B:213:THR:O	2.36	0.43
1:A:652:ALA:CB	1:A:700:LEU:CB	2.97	0.43
1:A:1302:PHE:CZ	1:A:1382:ARG:HD2	2.54	0.43
2:B:340:HIS:CE1	2:B:387:GLY:HA3	2.54	0.42
1:A:863:LEU:HB3	1:A:874:TYR:HB2	2.01	0.42
1:A:1273:ASP:O	1:A:1276:ARG:N	2.52	0.42
1:A:630:GLU:CD	1:A:635:LEU:HD13	2.43	0.42
2:B:157:LEU:HD11	2:B:192:MET:HB3	2.01	0.42
2:B:246:ASP:OD1	2:B:264:LYS:HB2	2.17	0.42
3:C:71:TRP:HB2	3:C:86:HIS:CD2	2.54	0.42
1:A:1110:SER:N	1:A:1116:GLY:O	2.52	0.42
1:A:1300:ALA:HB1	1:A:1398:VAL:HG23	2.01	0.42
2:B:354:GLY:N	2:B:376:GLY:O	2.52	0.42
1:A:1108:LEU:HD21	1:A:1182:LEU:HB2	2.01	0.42
1:A:1118:LYS:HE3	1:A:1118:LYS:HB3	1.87	0.42
1:A:1233:LEU:HD23	1:A:1296:LEU:HD11	2.01	0.42
2:B:353:ASP:OD1	2:B:353:ASP:N	2.46	0.42
1:A:319:ARG:NH2	1:A:1066:TYR:O	2.53	0.41
1:A:1222:ILE:O	1:A:1234:LEU:N	2.42	0.41
1:A:1273:ASP:OD2	1:A:1279:MET:HE3	2.20	0.41
1:A:1214:GLN:HB2	1:A:1225:ALA:HB3	2.02	0.41
1:A:1290:SER:HB3	1:A:1297:LEU:HD11	2.02	0.41
1:A:1341:LEU:HD11	2:B:71:ILE:HG23	2.03	0.41
1:A:1074:PHE:HB2	1:A:1094:LEU:HD12	2.01	0.41
1:A:1118:LYS:HE3	1:A:1120:TYR:CZ	2.55	0.41
1:A:495:GLU:CB	1:A:1317:ARG:NH2	2.78	0.41
1:A:1052:GLY:HA2	2:B:53:ASN:HB2	2.03	0.41
1:A:1279:MET:HB3	1:A:1279:MET:HE2	1.81	0.41
2:B:358:PHE:HD2	2:B:368:GLY:O	2.04	0.41
1:A:873:ILE:HG12	1:A:897:HIS:NE2	2.36	0.41
1:A:1281:TYR:OH	1:A:1298:ARG:NH2	2.54	0.41
1:A:614:ASP:OD1	1:A:614:ASP:N	2.54	0.41
1:A:688:PRO:HD2	1:A:802:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:LEU:HD12	1:A:858:GLN:HG3	2.02	0.41
1:A:1175:LEU:HD23	1:A:1184:SER:HA	2.02	0.41
1:A:1364:ASN:OD1	1:A:1379:ARG:NH2	2.54	0.41
3:C:85:LEU:HG	3:C:87:GLU:H	1.86	0.41
1:A:308:THR:HG22	1:A:310:PHE:H	1.86	0.41
1:A:332:TYR:CD2	1:A:333:ASP:HB3	2.56	0.40
2:B:373:ALA:HB1	2:B:415:TYR:HD1	1.85	0.40
1:A:80:SER:HB3	1:A:97:SER:HB3	2.03	0.40
1:A:200:LEU:HD23	1:A:200:LEU:H	1.84	0.40
1:A:378:GLU:OE1	1:A:379:PRO:HD3	2.21	0.40
1:A:399:LYS:HD2	1:A:462:SER:HB3	2.03	0.40
2:B:226:VAL:HB	2:B:240:LEU:HB2	2.03	0.40
1:A:612:ILE:HG23	1:A:670:LEU:HD11	2.04	0.40
1:A:1261:MET:HA	1:A:1336:THR:HG21	2.03	0.40
1:A:1348:LEU:HD23	1:A:1348:LEU:HA	1.92	0.40
3:C:70:HIS:HB3	3:C:75:LEU:O	2.22	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	1151/1443 (80%)	1056 (92%)	92 (8%)	3 (0%)	36	65
2	B	374/587 (64%)	342 (91%)	31 (8%)	1 (0%)	36	65
3	C	115/245 (47%)	98 (85%)	16 (14%)	1 (1%)	14	42
All	All	1640/2275 (72%)	1496 (91%)	139 (8%)	5 (0%)	37	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	653	ASP

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Mol	Chain	Res	Type
1	A	1274	ARG
3	C	2	GLN
1	A	201	LEU
2	B	152	ASN

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	1030/1235 (83%)	1016 (99%)	14 (1%)	59	70
2	B	326/514 (63%)	324 (99%)	2 (1%)	78	80
3	C	99/211 (47%)	99 (100%)	0	100	100
All	All	1455/1960 (74%)	1439 (99%)	16 (1%)	63	74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	LEU
1	A	333	ASP
1	A	388	LEU
1	A	498	LEU
1	A	629	LEU
1	A	632	VAL
1	A	1118	LYS
1	A	1176	CYS
1	A	1206	ILE
1	A	1233	LEU
1	A	1275	ASP
1	A	1276	ARG
1	A	1316	CYS
1	A	1317	ARG
2	B	265	ASP
2	B	346	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	506	HIS
1	A	509	ASN
1	A	620	GLN
1	A	664	HIS
1	A	680	HIS
1	A	783	HIS
1	A	1023	HIS
1	A	1099	HIS
1	A	1168	GLN
1	A	1177	HIS
1	A	1309	ASN
1	A	1334	HIS
1	A	1363	GLN
2	B	60	ASN
2	B	152	ASN
2	B	181	HIS
2	B	325	GLN
2	B	343	HIS
2	B	416	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	E	6/17 (35%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	E	4	A
4	E	5	A

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

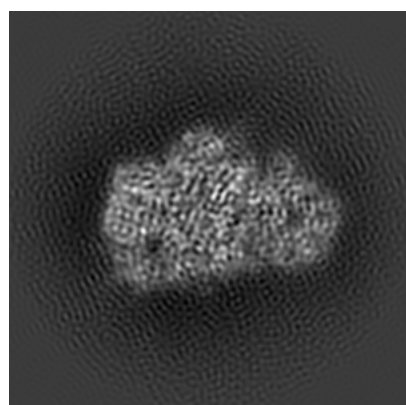
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7112. These allow visual inspection of the internal detail of the map and identification of artifacts.

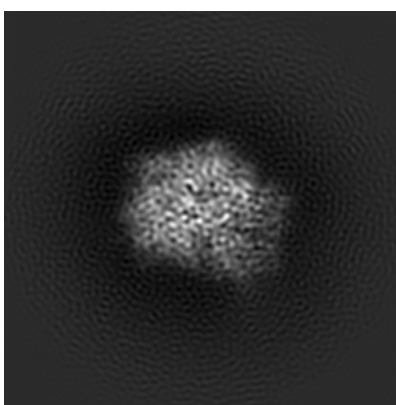
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

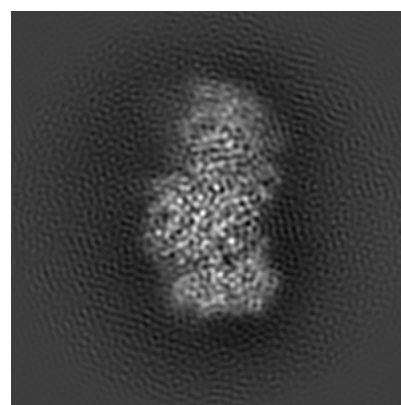
6.1.1 Primary map



X



Y

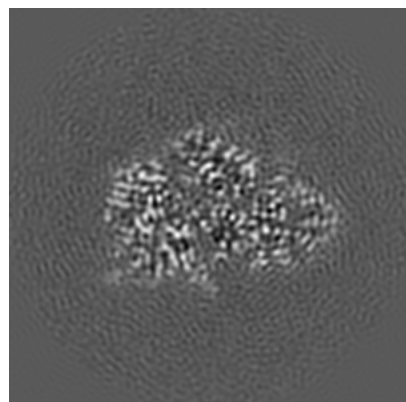


Z

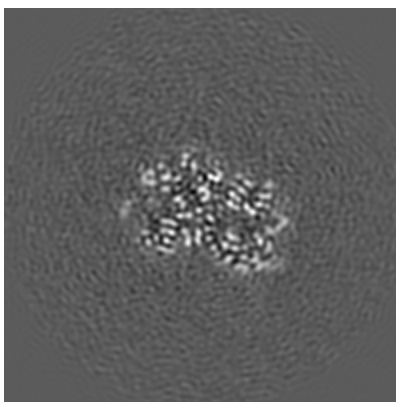
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

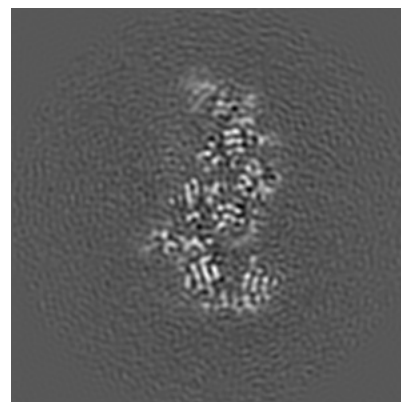
6.2.1 Primary map



X Index: 96



Y Index: 96

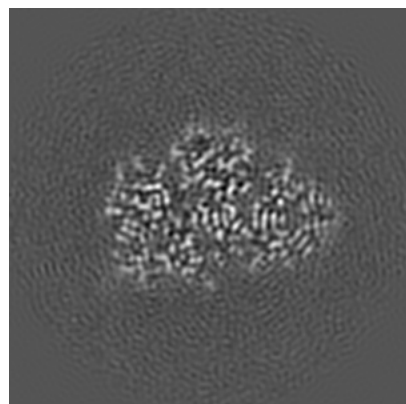


Z Index: 96

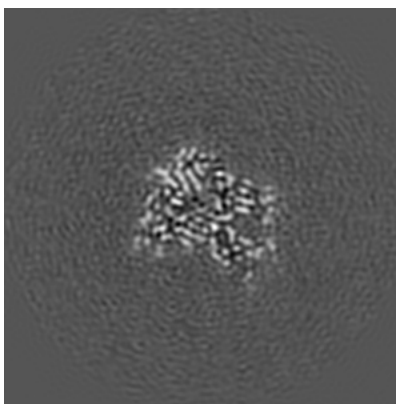
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

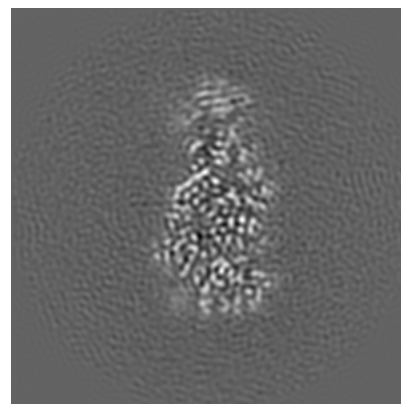
6.3.1 Primary map



X Index: 98



Y Index: 101

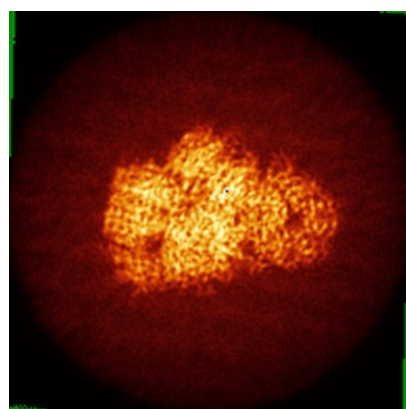


Z Index: 87

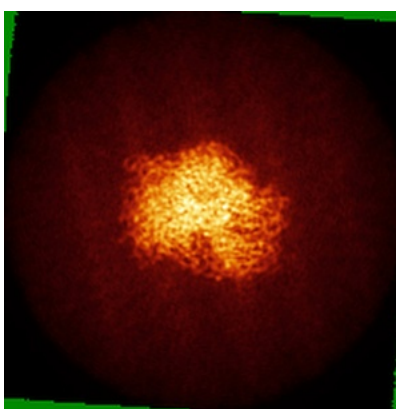
The images above show the largest variance slices of the map in three orthogonal directions.

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

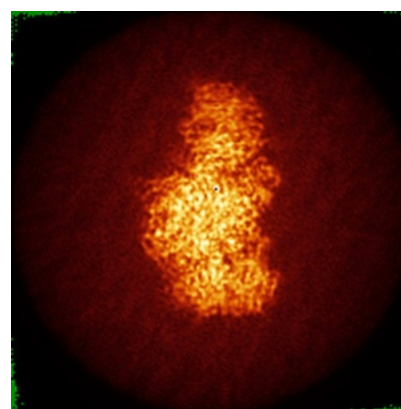
6.4.1 Primary map



X



Y

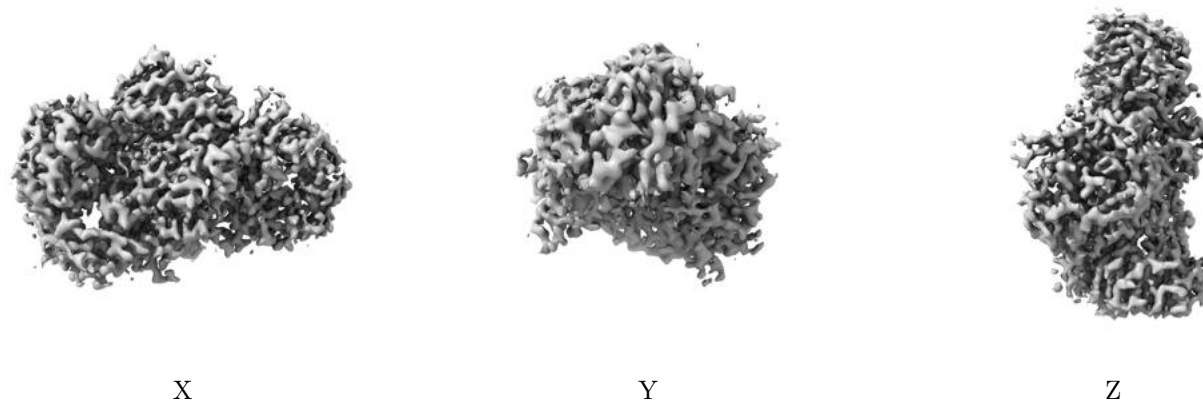


Z

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

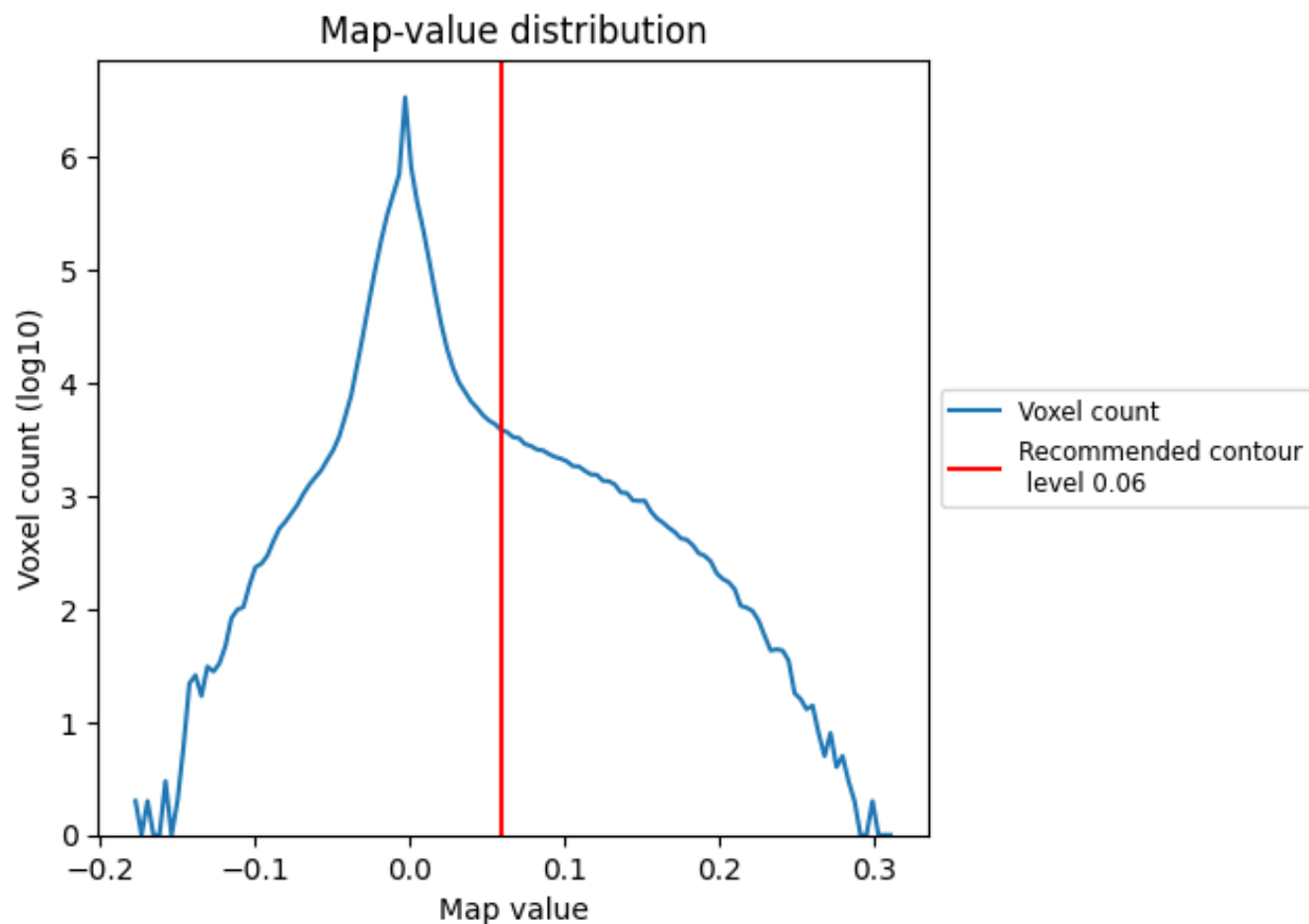
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

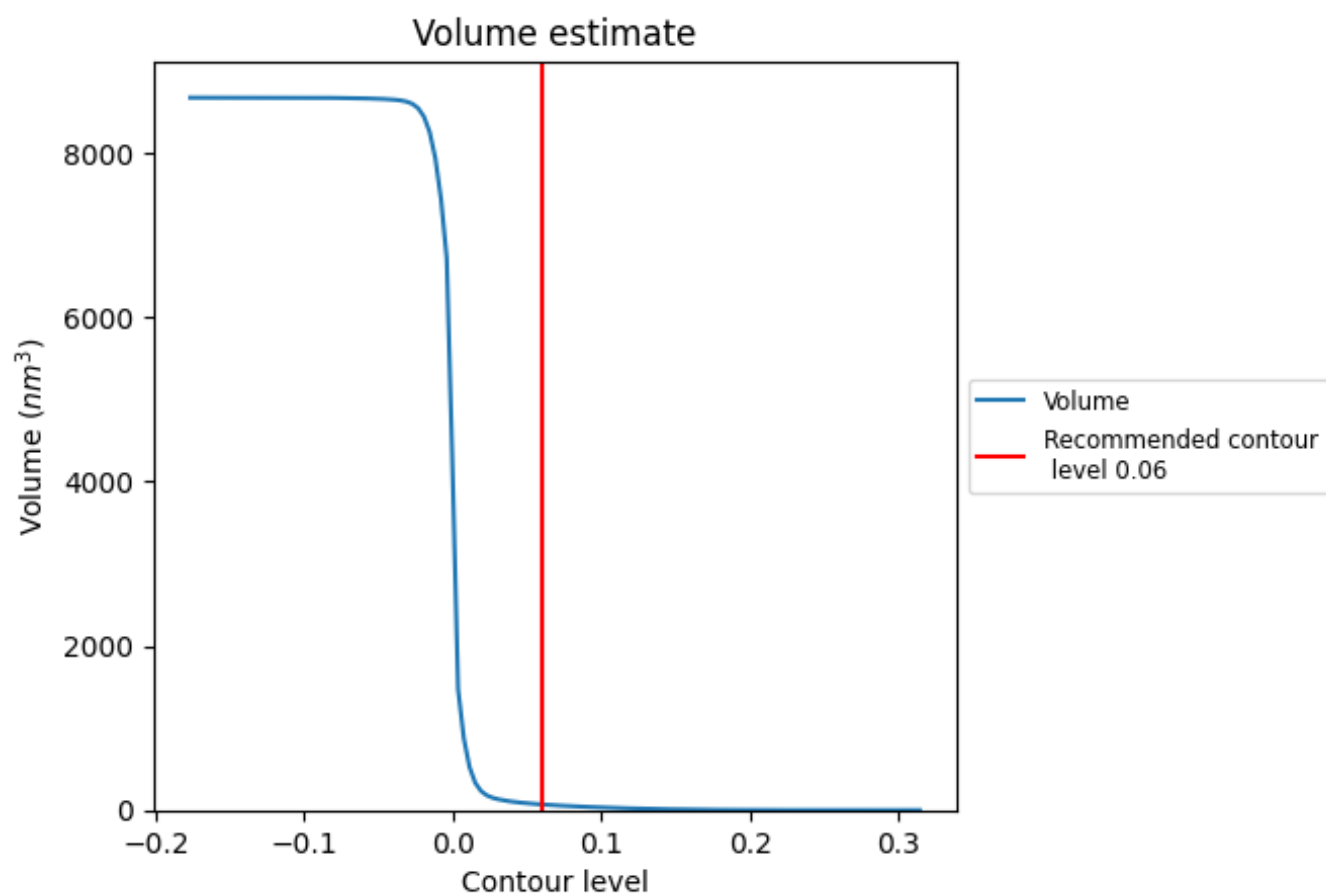
This section contains the results of statistical analysis of the map.

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.

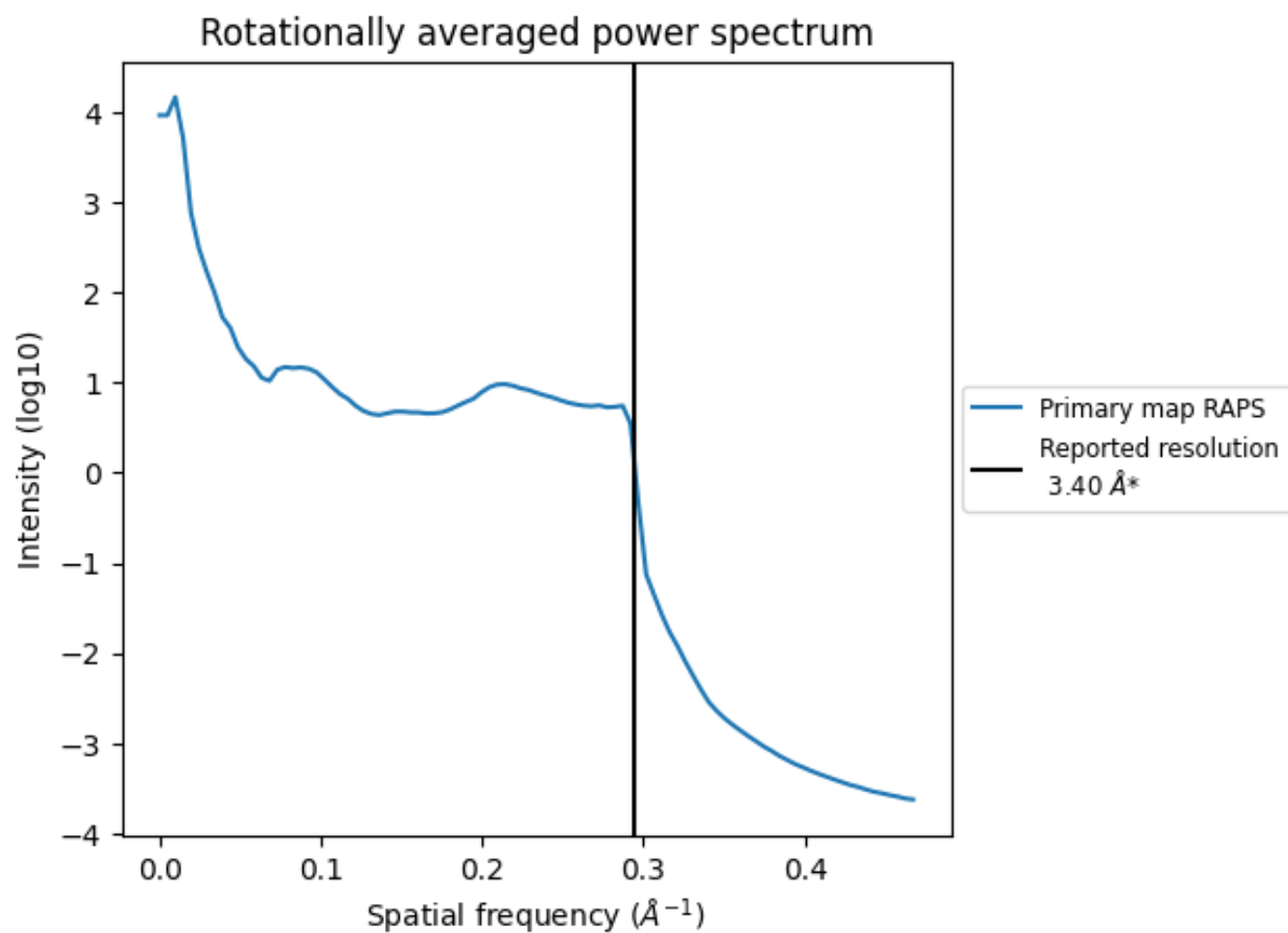
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm³; this corresponds to an approximate mass of 63 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 0.294 Å⁻¹

8 Fourier-Shell correlation

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

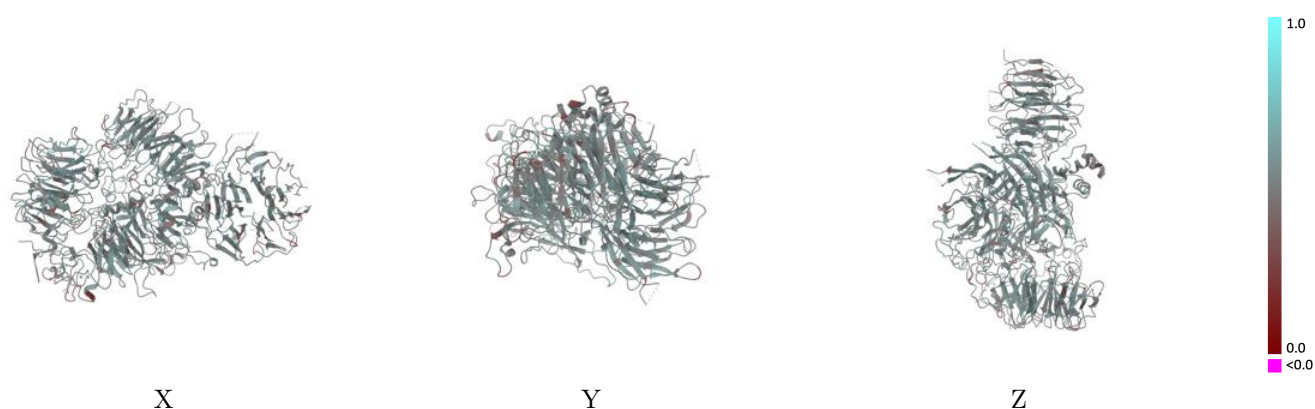
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7112 and PDB model 6DNH. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)

This section was not generated.

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

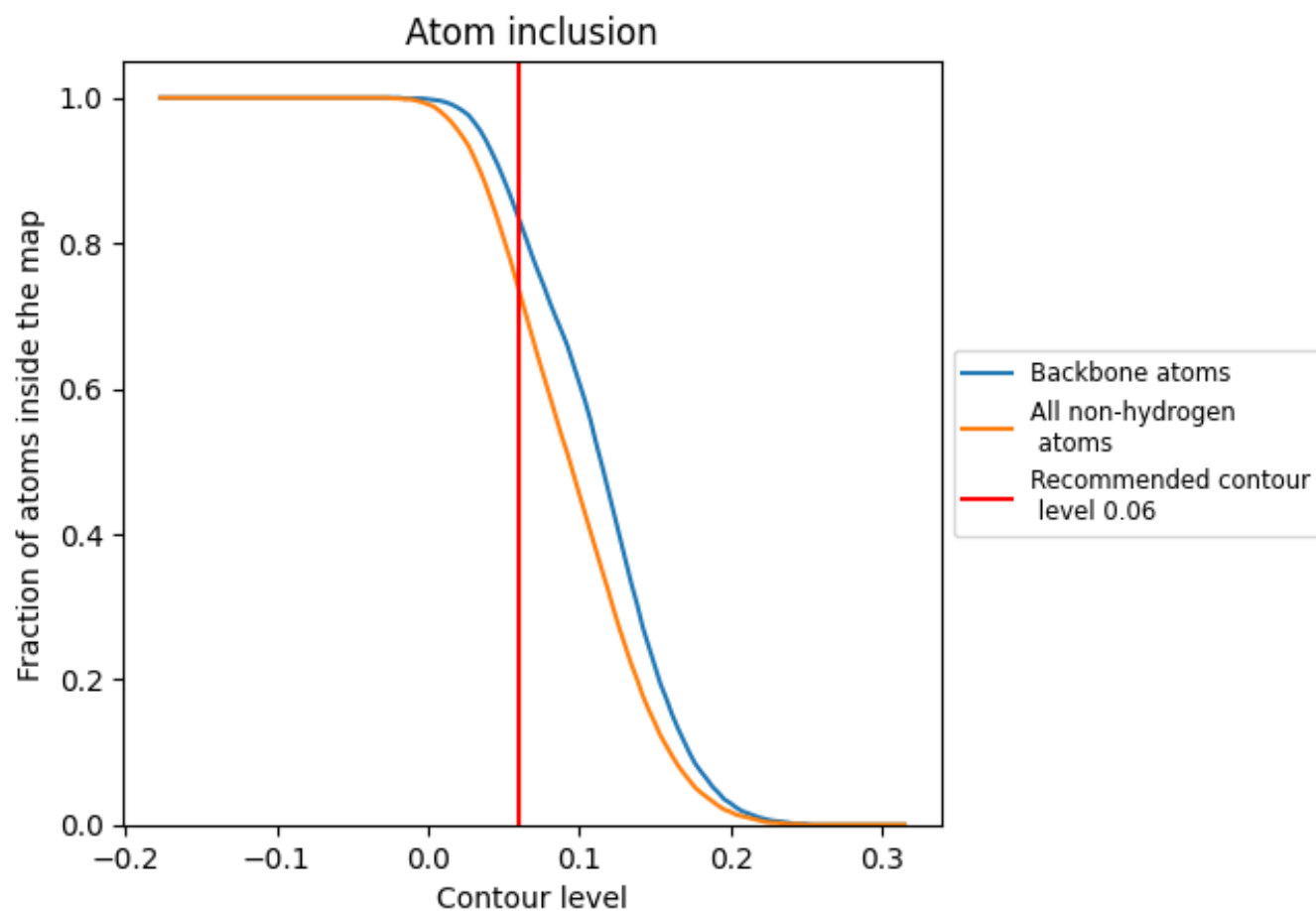


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 74% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.5120
A	0.7450	0.5140
B	0.7450	0.5160
C	0.6230	0.4760
E	0.7470	0.5020

