PNAS

Supporting Information for CDCA7 facilitates MET1-mediated CG DNA methylation maintenance in centromeric heterochromatin via linker histone H1

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This PDF file includes:

Figures S1 to S4
Tables S1 to S2

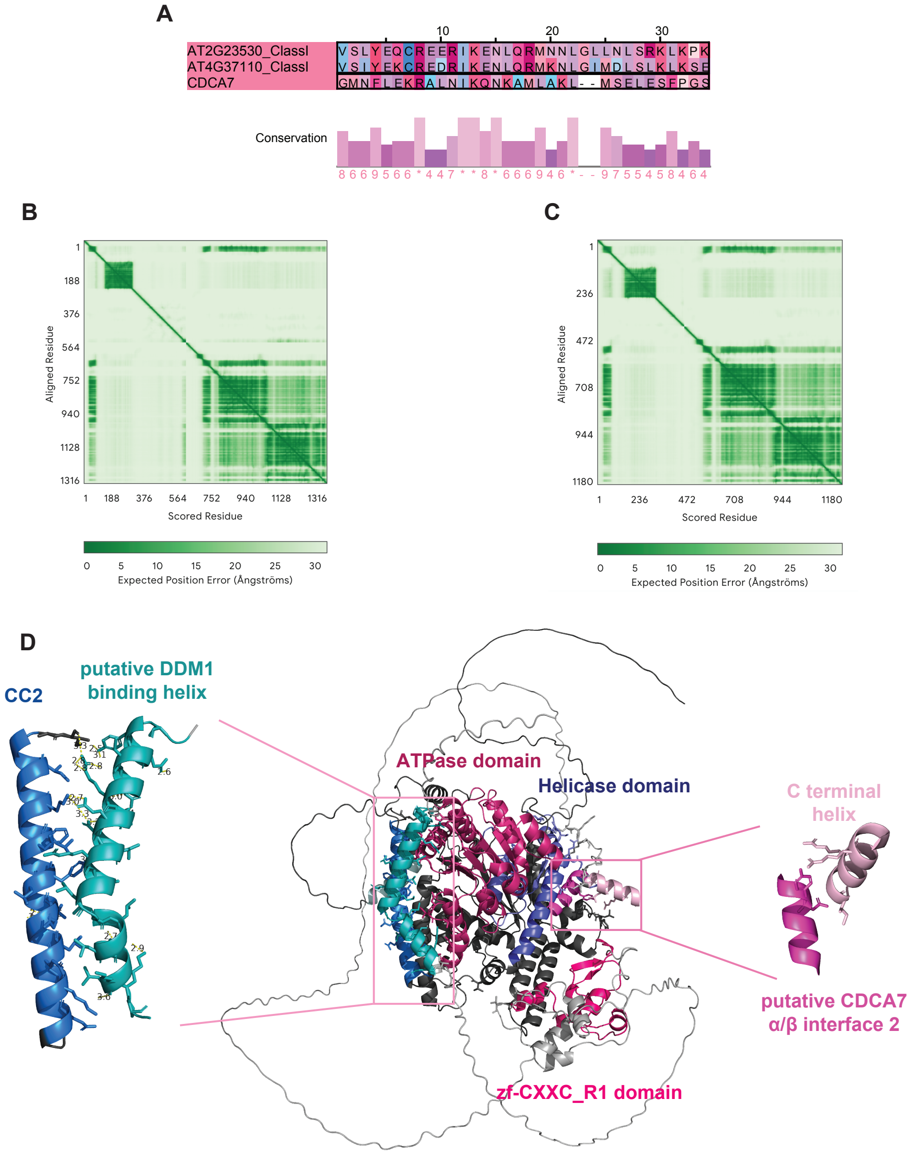
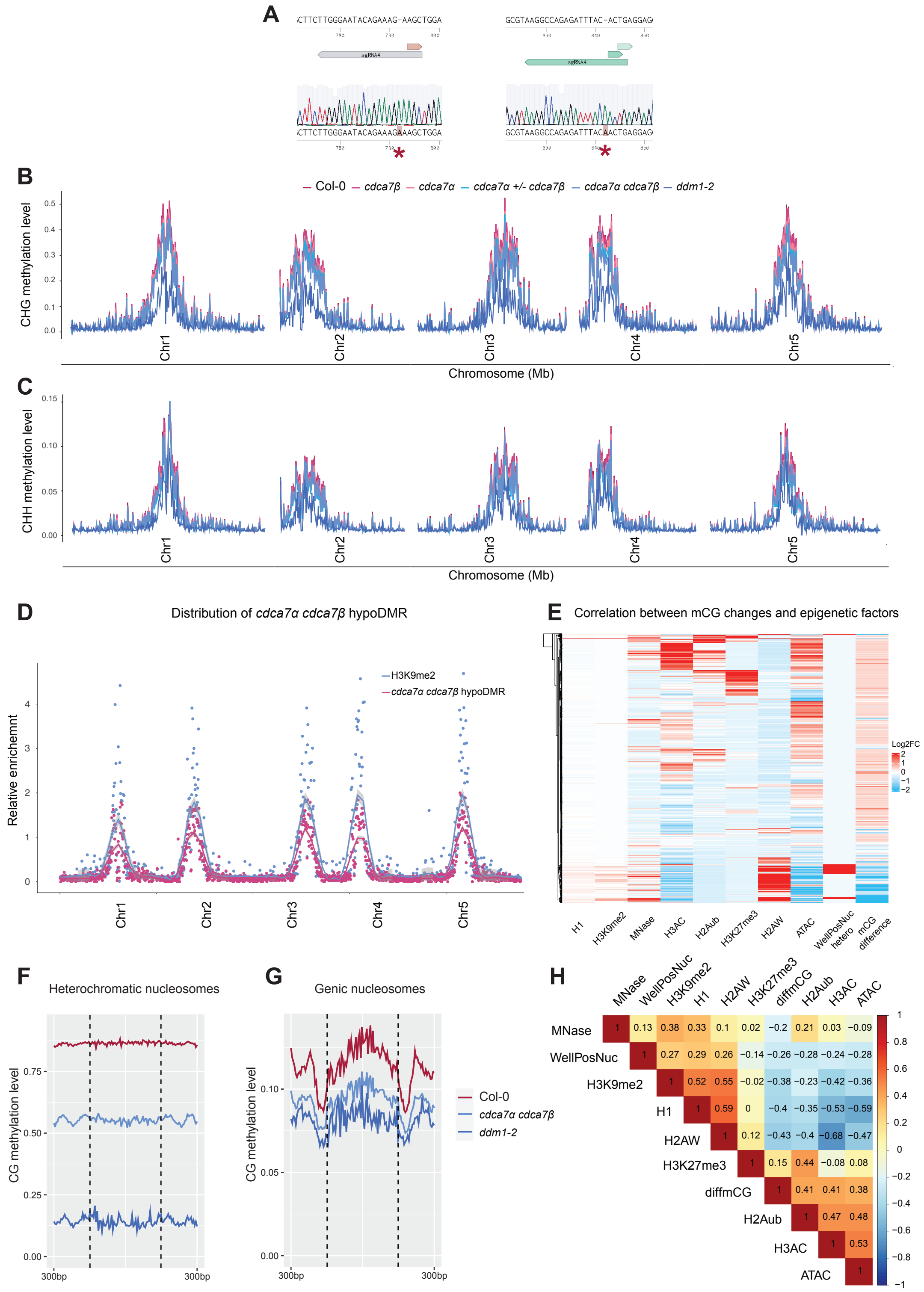


Fig. S1. *CDCA7α* and *CDCA7β* retain the HLBH domain for interacting with DDM1.

A. Sequence alignment calculated by Clustal Omega of the HLBH domains of *homo sapiens* CDCA7 and *Arabidopsis* Class I homologs. The red asterisk indicated the point mutations. Predicted Aligned Error (PAE) from AF3 structural modeling of **B.** *CDCA7β* or **C.** *CDCA7α* and DDM1 interactions. **D.** Close illustration of the AF3 predicted interface between *CDCA7α* and DDM1. Cyan represents the putative DDM1-binding helix of *CDCA7α*. Blue represents CC2 of DDM1. Light pink represents the C-terminal helix of *CDCA7α*. Pink represents putative CDCA7 interface 2 of DDM1. Dark pink represents the ATPase domain of DDM1. Purple indicates the Helicase C term domain of DDM1. Bright pink represents the zf-CXXC_R1 domain of *CDCA7α*.



	MNase	WellPosNuc	H3K9me2	H1	H2AW	H3K27me3	diffmCG	H2Aub	H3AC	ATAC
MNase	1	0.13	0.38	0.33	0.1	0.02	−0.2	0.21	0.03	−0.09
WellPosNuc		1	0.27	0.29	0.26	−0.14	−0.26	−0.28	−0.24	−0.28
H3K9me2			1	0.52	0.55	−0.02	−0.38	−0.23	−0.42	−0.36
H1				1	0.59	0	−0.4	−0.35	−0.53	−0.59
H2AW					1	0.12	−0.43	−0.4	−0.68	−0.47
H3K27me3						1	0.15	0.44	−0.08	0.08
diffmCG							1	0.41	0.41	0.38
H2Aub								1	0.47	0.48
H3AC									1	0.53
ATAC										1

Fig. S2. *CDCA7α* and *CDCA7β* promote DNA methylation at heterochromatic nucleosomes.

A. Sanger sequencing confirmation of CRISPR-Cas9 introduced A insertions at the *CDCA7β* and *CDCA7α* coding regions. **B.** Genome-wide CHG methylation landscape of Col-0, *cdca7α, cdca7β, cdca7α+/- cdca7β, cdca7α cdca7β*, and *ddm1-2*. **C.** Genome-wide CHH methylation landscape of Col-0, *cdca7α, cdca7β, cdca7α$^{+/-}$ cdca7β, cdca7α cdca7β*, and *ddm1-2*. **D.** Distribution of the *cdca7α cdca7β* hypoDMR. H3K9me2 enrichment marks the location of heterochromatin. **E.** Heatmaps showing the log2 fold change of epigenetic features and CG methylation at the *cdca7α cdca7β* DMR in the *cdca7α cdca7β* mutant compared to wild type. Metaplots showing CG methylation levels at **F.** heterochromatic well-positioned nucleosomes and **G.** genic well-positioned nucleosomes of Col-0, *cdca7α cdca7β*, and *ddm1-2*. **H.** Spearman correlation matrix among epigenetic features and changes in CG methylation level in the *cdca7α cdca7β* mutants.

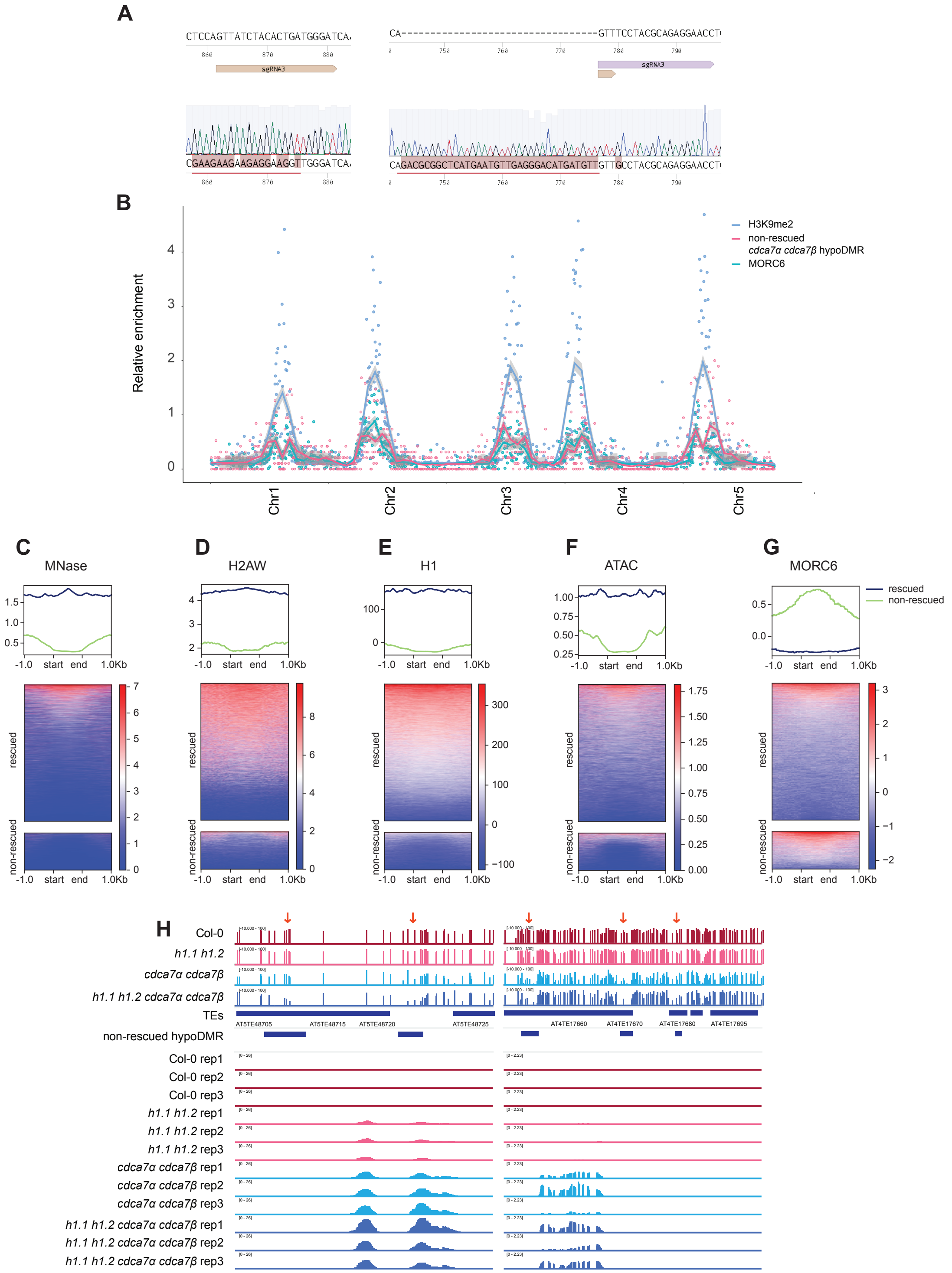


Fig. S3. *CDCA7α* and *CDCA7β* maintain CG methylation independently of H1.

A. Sanger sequencing confirmation of CRISPR-Cas9 introduced mutations at *CDCA7β* and *CDCA7α* coding regions. The red lines indicated the region where mutations were introduced. **B.** Distribution of the non-rescued *cdca7α cdca7β* hypoDMR (regions with CG methylation levels not recovered in *h1.1 h1.2 cdca7α cdca7β*). Relative enrichment of H3K9me2 indicates heterochromatin. Metaplots showing **C.** MNase-seq signal, **D.** H2A.W ChIP-seq signal, **E.** H1

ChIP-seq signal, **F.** ATAC-seq signal, and **G.** MORC6 ChIP-seq signal at non-rescued *cdca7α cdca7β* hypoDMR sites. **H.** Genome browser examples showing CG methylation and gene expression across Col-0, *h1.1 h1.2, cdca7α cdca7β,* and *h1.1 h1.2 cdca7α cdca7β* at non-rescued hypoDMRs in *h1.1 h1.2 cdca7α cdca7β* mutants. The red arrows indicate the locations of the hypoDMRs in the *h1.1 h1.2 cdca7α cdca7β* mutants.

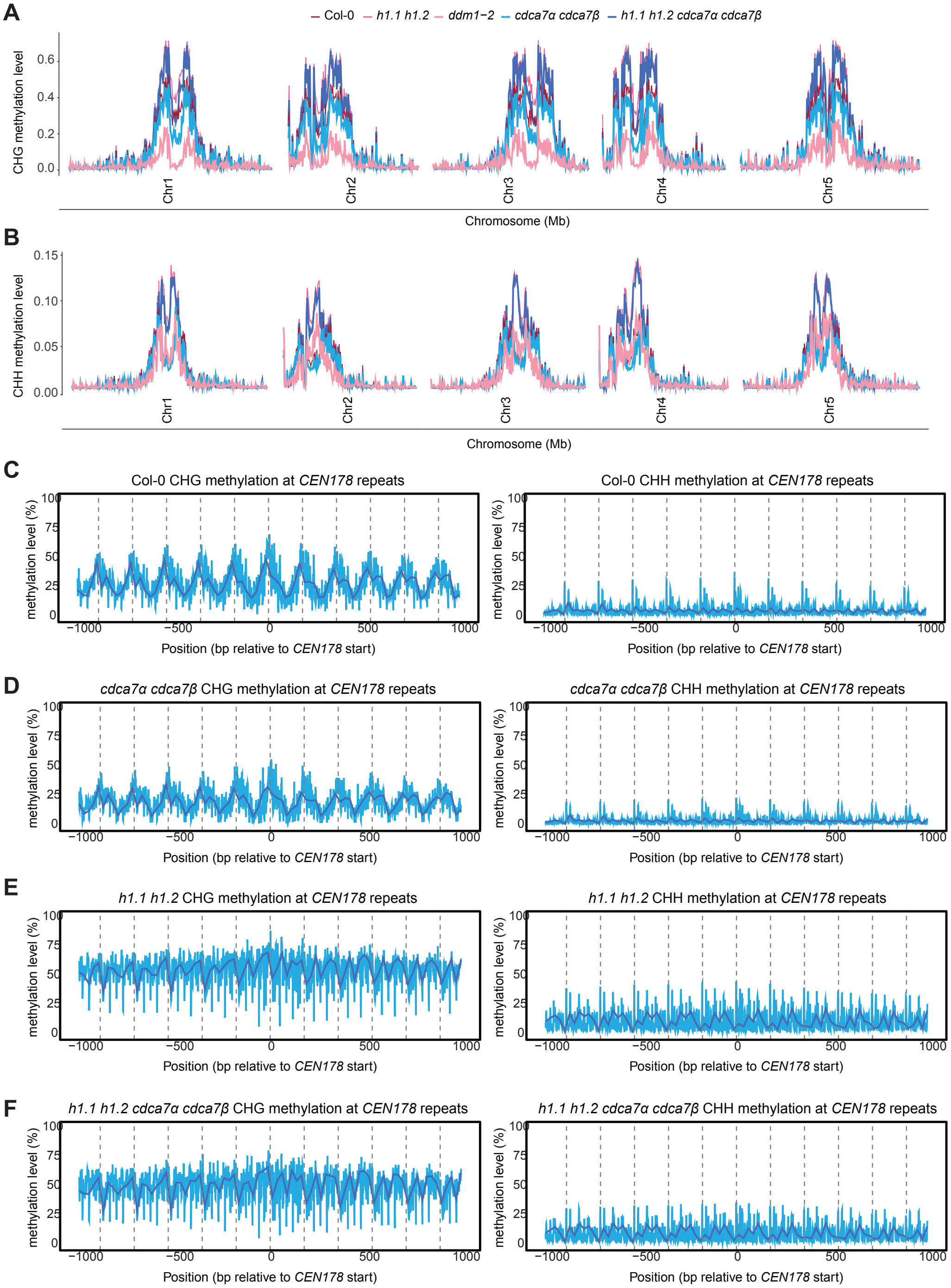
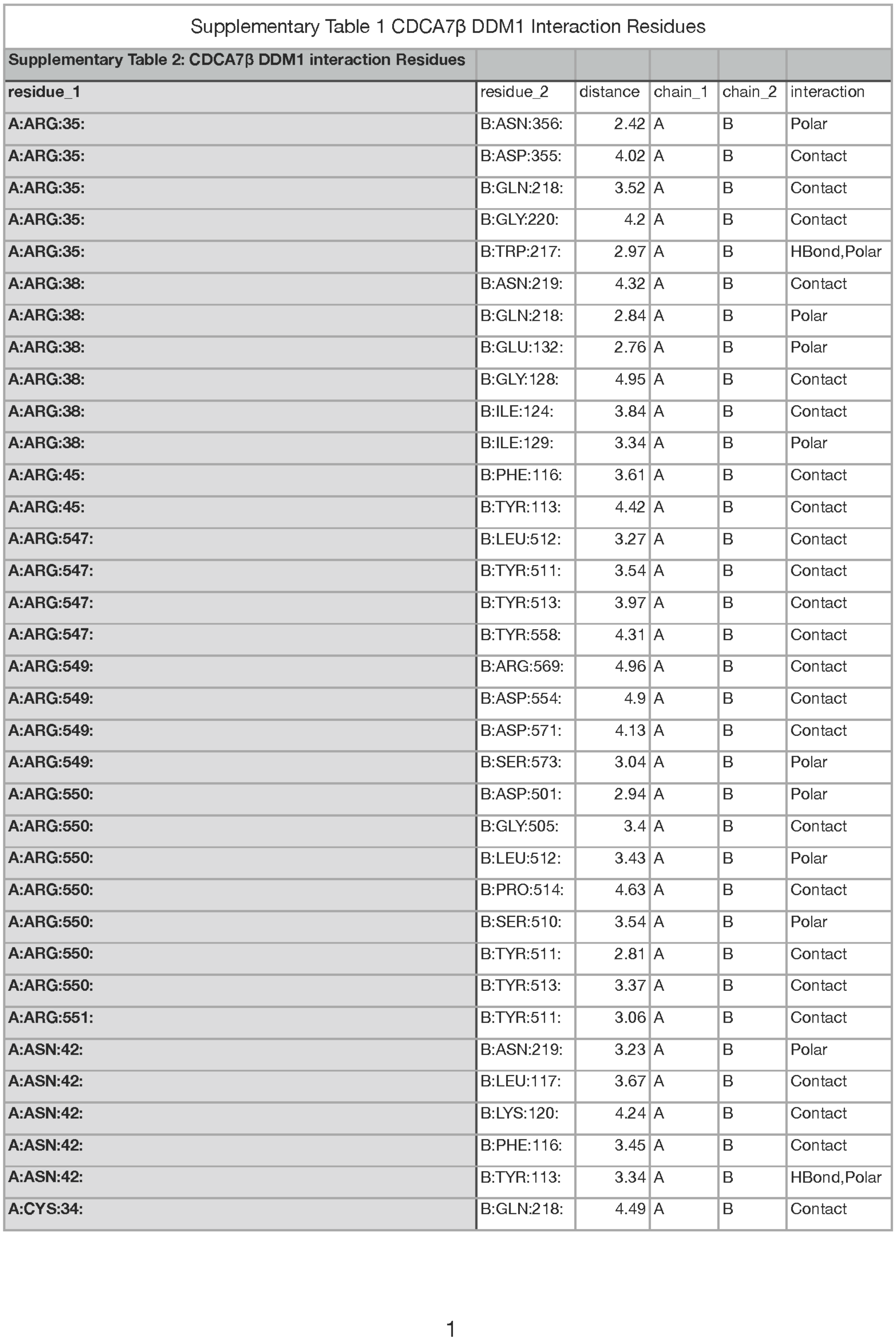


Fig. S4. *CDCA7α* and *CDCA7β* play a minor role in regulating non-CG methylation at centromeric regions.

Genome-wide **A.** CHG methylation, and **B.** CHH methylation landscapes of Col-0, *h1.1 h1.2, cdca7α cdca7β, h1.1 h1.2 cdca7α cdca7β,* and *ddm1-2.* Metaplots showing the non-CG methylation levels at *CEN178* satellite repeats of **C.** Col-0, **D.** *cdca7α cdca7β*, **E.** *h1.1 h1.2,* and **F.** *h1.1 h1.2 cdca7α cdca7β*.

Table S1. Details of the predicted interaction interfaces between *CDCA7β* and DDM1 from AF3.



Supplementary Table 1 CDCA7β DDM1 Interaction Residues

Supplementary Table 2: CDCA7β DDM1 interaction Residues					
residue_1	residue_2	distance	chain_1	chain_2	interaction
A:ARG:35:	B:ASN:356:	2.42	A	B	Polar
A:ARG:35:	B:ASP:355:	4.02	A	B	Contact
A:ARG:35:	B:GLN:218:	3.52	A	B	Contact
A:ARG:35:	B:GLY:220:	4.2	A	B	Contact
A:ARG:35:	B:TRP:217:	2.97	A	B	HBond,Polar
A:ARG:38:	B:ASN:219:	4.32	A	B	Contact
A:ARG:38:	B:GLN:218:	2.84	A	B	Polar
A:ARG:38:	B:GLU:132:	2.76	A	B	Polar
A:ARG:38:	B:GLY:128:	4.95	A	B	Contact
A:ARG:38:	B:ILE:124:	3.84	A	B	Contact
A:ARG:38:	B:ILE:129:	3.34	A	B	Polar
A:ARG:45:	B:PHE:116:	3.61	A	B	Contact
A:ARG:45:	B:TYR:113:	4.42	A	B	Contact
A:ARG:547:	B:LEU:512:	3.27	A	B	Contact
A:ARG:547:	B:TYR:511:	3.54	A	B	Contact
A:ARG:547:	B:TYR:513:	3.97	A	B	Contact
A:ARG:547:	B:TYR:558:	4.31	A	B	Contact
A:ARG:549:	B:ARG:569:	4.96	A	B	Contact
A:ARG:549:	B:ASP:554:	4.9	A	B	Contact
A:ARG:549:	B:ASP:571:	4.13	A	B	Contact
A:ARG:549:	B:SER:573:	3.04	A	B	Polar
A:ARG:550:	B:ASP:501:	2.94	A	B	Polar
A:ARG:550:	B:GLY:505:	3.4	A	B	Contact
A:ARG:550:	B:LEU:512:	3.43	A	B	Polar
A:ARG:550:	B:PRO:514:	4.63	A	B	Contact
A:ARG:550:	B:SER:510:	3.54	A	B	Polar
A:ARG:550:	B:TYR:511:	2.81	A	B	Contact
A:ARG:550:	B:TYR:513:	3.37	A	B	Contact
A:ARG:551:	B:TYR:511:	3.06	A	B	Contact
A:ASN:42:	B:ASN:219:	3.23	A	B	Polar
A:ASN:42:	B:LEU:117:	3.67	A	B	Contact
A:ASN:42:	B:LYS:120:	4.24	A	B	Contact
A:ASN:42:	B:PHE:116:	3.45	A	B	Contact
A:ASN:42:	B:TYR:113:	3.34	A	B	HBond,Polar
A:CYS:34:	B:GLN:218:	4.49	A	B	Contact

1

A:GLU:32:	B:LEU:249:	3.17	A	B	Contact
A:GLU:32:	B:LYS:328:	2.62	A	B	Polar
A:GLU:41:	B:LYS:120:	2.72	A	B	Polar
A:GLU:41:	B:PHE:116:	4.3	A	B	Contact
A:GLU:536:	B:LEU:512:	3.83	A	B	Contact
A:GLY:543:	B:SER:561:	3.72	A	B	Contact
A:GLY:543:	B:TYR:513:	4.92	A	B	Contact
A:GLY:543:	B:TYR:558:	3.99	A	B	Contact
A:ILE:39:	B:ASN:219:	3.8	A	B	Contact
A:ILE:39:	B:GLN:218:	4.53	A	B	Contact
A:ILE:39:	B:GLY:220:	3.61	A	B	Contact
A:ILE:542:	B:ASP:557:	3.03	A	B	Contact
A:ILE:542:	B:SER:561:	4.35	A	B	Contact
A:ILE:542:	B:VAL:567:	4.43	A	B	Contact
A:LEU:43:	B:ASP:382:	4.79	A	B	Contact
A:LEU:43:	B:TYR:113:	4.46	A	B	Contact
A:LEU:49:	B:GLN:109:	3.52	A	B	Contact
A:LEU:49:	B:LEU:112:	4.55	A	B	Contact
A:LEU:49:	B:TYR:113:	3.62	A	B	Contact
A:LEU:51:	B:GLN:109:	3.44	A	B	Contact
A:LEU:51:	B:ILE:383:	3.68	A	B	Contact
A:LEU:51:	B:LEU:106:	3.83	A	B	Contact
A:LEU:51:	B:THR:110:	3.42	A	B	Contact
A:LEU:51:	B:TYR:113:	3.6	A	B	Contact
A:LEU:52:	B:ASP:382:	3.44	A	B	Contact
A:LEU:52:	B:ILE:383:	4.79	A	B	Contact
A:LEU:546:	B:ARG:569:	3.45	A	B	Contact
A:LEU:546:	B:ASP:554:	3.4	A	B	Contact
A:LEU:546:	B:ASP:557:	3.48	A	B	Contact
A:LEU:546:	B:TYR:513:	4.07	A	B	Contact
A:LEU:546:	B:TYR:558:	3.6	A	B	Contact
A:LEU:54:	B:GLN:109:	3.68	A	B	Contact
A:LEU:54:	B:GLU:105:	3.54	A	B	Contact
A:LEU:54:	B:LEU:106:	3.7	A	B	Contact
A:LEU:58:	B:GLN:99:	3.89	A	B	Contact
A:LEU:58:	B:LEU:103:	3.67	A	B	Contact
A:LEU:58:	B:LEU:106:	3.18	A	B	Contact
A:LEU:58:	B:LYS:102:	3.74	A	B	Contact

A:LEU:58:	B:TRP:393:	3.23	A	B	Polar
A:LYS:57:	B:LYS:102:	4.04	A	B	Contact
A:LYS:59:	B:GLU:389:	3.34	A	B	Contact
A:LYS:59:	B:THR:385:	2.92	A	B	Polar
A:LYS:59:	B:TRP:393:	4.23	A	B	Contact
A:MET:46:	B:ASP:382:	4.54	A	B	Contact
A:MET:46:	B:ILE:383:	3.85	A	B	Contact
A:MET:46:	B:TYR:113:	3.74	A	B	Contact
A:PRO:537:	B:GLU:562:	3.58	A	B	Contact
A:PRO:537:	B:TYR:558:	4.1	A	B	Contact
A:PRO:60:	B:GLU:389:	4.35	A	B	Contact
A:PRO:60:	B:TRP:393:	4.7	A	B	Contact
A:SER:29:	B:ASN:247:	4.11	A	B	Contact
A:SER:541:	B:SER:561:	4.52	A	B	Contact
A:SER:55:	B:ASP:382:	4.52	A	B	Contact
A:SER:55:	B:ILE:383:	2.67	A	B	HBond,Polar
A:SER:55:	B:LEU:106:	3.87	A	B	Contact
A:SER:55:	B:PHE:384:	4.88	A	B	Contact
A:SER:55:	B:THR:385:	4.47	A	B	Contact
A:TYR:31:	B:ASN:247:	3.97	A	B	Contact
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A:TYR:31:	B:HIS:243:	2.52	A	B	Polar
A:TYR:31:	B:ILE:129:	3.51	A	B	Contact
A:TYR:31:	B:ILE:214:	3.78	A	B	Contact
A:TYR:31:	B:LEU:244:	4.74	A	B	Contact
A:TYR:31:	B:LEU:249:	4.2	A	B	Contact
A:TYR:31:	B:TRP:217:	3.16	A	B	Contact
B:ARG:569:	A:ARG:549:	4.96	B	A	Contact
B:ARG:569:	A:LEU:546:	3.45	B	A	Contact
B:ASN:219:	A:ARG:38:	4.32	B	A	Contact
B:ASN:219:	A:ASN:42:	3.23	B	A	Polar
B:ASN:219:	A:ILE:39:	3.8	B	A	Contact
B:ASN:247:	A:SER:29:	4.11	B	A	Contact
B:ASN:247:	A:TYR:31:	3.97	B	A	Contact
B:ASN:356:	A:ARG:35:	2.42	B	A	Polar
B:ASP:355:	A:ARG:35:	4.02	B	A	Contact
B:ASP:382:	A:LEU:43:	4.79	B	A	Contact
B:ASP:382:	A:LEU:52:	3.44	B	A	Contact

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B:ASP:382:	A:SER:55:	4.52	B	A	Contact
B:ASP:501:	A:ARG:550:	2.94	B	A	Polar
B:ASP:554:	A:ARG:549:	4.9	B	A	Contact
B:ASP:554:	A:LEU:546:	3.4	B	A	Contact
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B:GLY:220:	A:ILE:39:	3.61	B	A	Contact
B:GLY:505:	A:ARG:550:	3.4	B	A	Contact
B:HIS:243:	A:TYR:31:	2.52	B	A	Polar
B:ILE:124:	A:ARG:38:	3.84	B	A	Contact
B:ILE:129:	A:ARG:38:	3.34	B	A	Polar
B:ILE:129:	A:TYR:31:	3.51	B	A	Contact
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B:ILE:383:	A:LEU:52:	4.79	B	A	Contact
B:ILE:383:	A:MET:46:	3.85	B	A	Contact
B:ILE:383:	A:SER:55:	2.67	B	A	HBond,Polar
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B:LEU:106:	A:LEU:54:	3.7	B	A	Contact

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B:LEU:112:	A:LEU:49:	4.55	B	A	Contact
B:LEU:117:	A:ASN:42:	3.67	B	A	Contact
B:LEU:244:	A:TYR:31:	4.74	B	A	Contact
B:LEU:249:	A:GLU:32:	3.17	B	A	Contact
B:LEU:249:	A:TYR:31:	4.2	B	A	Contact
B:LEU:512:	A:ARG:547:	3.27	B	A	Contact
B:LEU:512:	A:ARG:550:	3.43	B	A	Polar
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B:LYS:102:	A:LEU:58:	3.74	B	A	Contact
B:LYS:102:	A:LYS:57:	4.04	B	A	Contact
B:LYS:120:	A:ASN:42:	4.24	B	A	Contact
B:LYS:120:	A:GLU:41:	2.72	B	A	Polar
B:LYS:328:	A:GLU:32:	2.62	B	A	Polar
B:PHE:116:	A:ARG:45:	3.61	B	A	Contact
B:PHE:116:	A:ASN:42:	3.45	B	A	Contact
B:PHE:116:	A:GLU:41:	4.3	B	A	Contact
B:PHE:384:	A:SER:55:	4.88	B	A	Contact
B:PRO:514:	A:ARG:550:	4.63	B	A	Contact
B:SER:510:	A:ARG:550:	3.54	B	A	Polar
B:SER:561:	A:GLY:543:	3.72	B	A	Contact
B:SER:561:	A:ILE:542:	4.35	B	A	Contact
B:SER:561:	A:SER:541:	4.52	B	A	Contact
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B:THR:110:	A:LEU:51:	3.42	B	A	Contact
B:THR:385:	A:LYS:59:	2.92	B	A	Polar
B:THR:385:	A:SER:55:	4.47	B	A	Contact
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B:TRP:217:	A:TYR:31:	3.16	B	A	Contact
B:TRP:393:	A:LEU:58:	3.23	B	A	Polar
B:TRP:393:	A:LYS:59:	4.23	B	A	Contact
B:TRP:393:	A:PRO:60:	4.7	B	A	Contact
B:TYR:113:	A:ARG:45:	4.42	B	A	Contact
B:TYR:113:	A:ASN:42:	3.34	B	A	HBond,Polar
B:TYR:113:	A:LEU:43:	4.46	B	A	Contact
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B:TYR:511:	A:ARG:550:	2.81	B	A	Contact
B:TYR:511:	A:ARG:551:	3.06	B	A	Contact
B:TYR:513:	A:ARG:547:	3.97	B	A	Contact
B:TYR:513:	A:ARG:550:	3.37	B	A	Contact
B:TYR:513:	A:GLY:543:	4.92	B	A	Contact
B:TYR:513:	A:LEU:546:	4.07	B	A	Contact
B:TYR:558:	A:ARG:547:	4.31	B	A	Contact
B:TYR:558:	A:GLY:543:	3.99	B	A	Contact
B:TYR:558:	A:LEU:546:	3.6	B	A	Contact
B:TYR:558:	A:PRO:537:	4.1	B	A	Contact
B:VAL:567:	A:ILE:542:	4.43	B	A	Contact

Table S2. Details of the predicted interaction interfaces between *CDCA7α* and DDM1 from AF3.

Supplementary Table 2 CDCA7α DDM1 Interaction Residues

Supplementary Table 2: CDCA7α DDM1 interaction Residues					
residue_1	residue_2	distance	chain_1	chain_2	interaction
A:ARG:35:	B:ASN:356:	2.8	A	B	Polar
A:ARG:35:	B:ASP:355:	3.94	A	B	Contact
A:ARG:35:	B:GLN:218:	3.53	A	B	Contact
A:ARG:35:	B:GLY:220:	4.24	A	B	Contact
A:ARG:35:	B:TRP:217:	3.03	A	B	HBond,Polar
A:ARG:38:	B:ASN:219:	4.19	A	B	Contact
A:ARG:38:	B:GLN:218:	3.56	A	B	Polar
A:ARG:38:	B:ILE:124:	3.76	A	B	Contact
A:ARG:38:	B:ILE:129:	4.47	A	B	Contact
A:ARG:394:	B:ASN:540:	4.43	A	B	Contact
A:ARG:394:	B:GLU:589:	4.01	A	B	Contact
A:ARG:394:	B:LYS:542:	4.51	A	B	Contact
A:ARG:394:	B:SER:591:	4.13	A	B	Contact
A:ARG:394:	B:SER:592:	4.89	A	B	Contact
A:ARG:394:	B:SER:594:	4.29	A	B	Contact
A:ARG:410:	B:GLU:562:	2.6	A	B	Polar
A:ARG:410:	B:LYS:563:	4.84	A	B	Contact
A:ARG:410:	B:SER:561:	3.02	A	B	Polar
A:ARG:412:	B:TYR:511:	4.52	A	B	Contact
A:ARG:413:	B:LEU:512:	3.06	A	B	Contact
A:ARG:413:	B:PRO:514:	4.94	A	B	Contact
A:ARG:413:	B:TYR:513:	3.06	A	B	Polar
A:ARG:413:	B:TYR:558:	2.92	A	B	Polar
A:ARG:45:	B:PHE:116:	3.58	A	B	Contact
A:ARG:45:	B:TYR:113:	4.34	A	B	Contact
A:ASN:42:	B:ASN:219:	3.21	A	B	Polar
A:ASN:42:	B:LEU:117:	3.57	A	B	Contact
A:ASN:42:	B:LYS:120:	4.24	A	B	Contact
A:ASN:42:	B:PHE:116:	3.42	A	B	Contact
A:ASN:42:	B:TYR:113:	3.35	A	B	HBond,Polar
A:CYS:34:	B:GLN:218:	4.9	A	B	Contact
A:GLN:416:	B:LEU:512:	4.63	A	B	Contact
A:GLU:32:	B:LEU:249:	2.51	A	B	Contact
A:GLU:32:	B:LYS:328:	2.64	A	B	Polar
A:GLU:32:	B:TRP:217:	4.84	A	B	Contact

A:GLU:41:	B:LYS:120:	2.62	A	B	Polar
A:GLU:41:	B:PHE:116:	4.21	A	B	Contact
A:GLU:61:	B:GLN:99:	4.28	A	B	Contact
A:GLU:61:	B:LYS:102:	2.38	A	B	Polar
A:GLY:406:	B:ASP:557:	3.75	A	B	Contact
A:GLY:406:	B:SER:561:	3.9	A	B	Contact
A:GLY:406:	B:TYR:558:	4.26	A	B	Contact
A:GLY:407:	B:SER:561:	3.99	A	B	Contact
A:ILE:39:	B:ASN:219:	3.82	A	B	Contact
A:ILE:39:	B:GLN:218:	4.7	A	B	Contact
A:ILE:39:	B:GLY:220:	3.69	A	B	Contact
A:ILE:405:	B:ARG:569:	2.76	A	B	Contact
A:ILE:405:	B:ASP:554:	3.42	A	B	Contact
A:ILE:405:	B:ASP:557:	3.13	A	B	HBond,Polar
A:ILE:51:	B:GLN:109:	3.52	A	B	Contact
A:ILE:51:	B:ILE:383:	3.5	A	B	Contact
A:ILE:51:	B:LEU:106:	3.69	A	B	Contact
A:ILE:51:	B:THR:110:	3.89	A	B	Contact
A:ILE:51:	B:TYR:113:	3.49	A	B	Contact
A:ILE:62:	B:GLN:99:	4.75	A	B	Contact
A:ILE:62:	B:GLU:389:	4.42	A	B	Contact
A:ILE:62:	B:SER:392:	3.29	A	B	Contact
A:ILE:62:	B:TRP:393:	2.25	A	B	Contact
A:LEU:251:	B:ALA:87:	4.04	A	B	Contact
A:LEU:409:	B:TYR:511:	3.73	A	B	Contact
A:LEU:409:	B:TYR:513:	3.1	A	B	Contact
A:LEU:409:	B:TYR:558:	4.42	A	B	Contact
A:LEU:43:	B:TYR:113:	4.43	A	B	Contact
A:LEU:49:	B:GLN:109:	3.58	A	B	Contact
A:LEU:49:	B:LEU:112:	4.41	A	B	Contact
A:LEU:49:	B:TYR:113:	3.66	A	B	Contact
A:LEU:54:	B:GLN:109:	3.83	A	B	Contact
A:LEU:54:	B:GLU:105:	3.72	A	B	Contact
A:LEU:54:	B:LEU:106:	3.88	A	B	Contact
A:LEU:58:	B:LEU:103:	3.93	A	B	Contact
A:LEU:58:	B:LEU:106:	3.84	A	B	Contact
A:LEU:58:	B:LYS:102:	3.82	A	B	Contact
A:LEU:58:	B:TRP:393:	2.97	A	B	Contact

A:LYS:247:	B:GLN:480:	3.61	A	B	Contact
A:LYS:395:	B:SER:592:	4.26	A	B	Contact
A:LYS:59:	B:ASP:382:	4.21	A	B	Contact
A:LYS:59:	B:GLU:389:	3.21	A	B	Contact
A:LYS:59:	B:ILE:383:	4.11	A	B	Contact
A:LYS:59:	B:THR:385:	2.8	A	B	Polar
A:MET:396:	B:GLY:564:	3.71	A	B	Contact
A:MET:396:	B:LYS:563:	4.52	A	B	Contact
A:MET:396:	B:PHE:565:	3.51	A	B	Contact
A:MET:46:	B:ASP:382:	4.98	A	B	Contact
A:MET:46:	B:ILE:383:	3.84	A	B	Contact
A:MET:46:	B:TYR:113:	3.79	A	B	Contact
A:MET:52:	B:ASP:382:	4.13	A	B	Contact
A:PRO:252:	B:ALA:87:	4.84	A	B	Contact
A:PRO:400:	B:SER:561:	3.87	A	B	Contact
A:SER:29:	B:ASN:247:	4.24	A	B	Contact
A:SER:397:	B:GLU:566:	2.16	A	B	Polar
A:SER:397:	B:GLY:564:	4.33	A	B	Contact
A:SER:404:	B:ASP:557:	4.28	A	B	Contact
A:SER:404:	B:SER:561:	4.19	A	B	Contact
A:SER:55:	B:ASP:382:	4.37	A	B	Contact
A:SER:55:	B:ILE:383:	2.85	A	B	HBond,Polar
A:SER:55:	B:LEU:106:	4.01	A	B	Contact
A:TYR:31:	B:ASN:247:	3.98	A	B	Contact
A:TYR:31:	B:GLN:218:	3.11	A	B	Polar
A:TYR:31:	B:HIS:243:	2.69	A	B	Polar
A:TYR:31:	B:ILE:129:	3.32	A	B	Contact
A:TYR:31:	B:ILE:214:	3.67	A	B	Contact
A:TYR:31:	B:LEU:244:	4.83	A	B	Contact
A:TYR:31:	B:LEU:249:	4.25	A	B	Contact
A:TYR:31:	B:TRP:217:	3	A	B	Contact
A:VAL:140:	B:VAL:91:	4.04	A	B	Contact
B:ALA:87:	A:LEU:251:	4.04	B	A	Contact
B:ALA:87:	A:PRO:252:	4.84	B	A	Contact
B:ARG:569:	A:ILE:405:	2.76	B	A	Contact
B:ASN:219:	A:ARG:38:	4.19	B	A	Contact
B:ASN:219:	A:ASN:42:	3.21	B	A	Polar
B:ASN:219:	A:ILE:39:	3.82	B	A	Contact

B:ASN:247:	A:SER:29:	4.24	B	A	Contact
B:ASN:247:	A:TYR:31:	3.98	B	A	Contact
B:ASN:356:	A:ARG:35:	2.8	B	A	Polar
B:ASN:540:	A:ARG:394:	4.43	B	A	Contact
B:ASP:355:	A:ARG:35:	3.94	B	A	Contact
B:ASP:382:	A:LYS:59:	4.21	B	A	Contact
B:ASP:382:	A:MET:46:	4.98	B	A	Contact
B:ASP:382:	A:MET:52:	4.13	B	A	Contact
B:ASP:382:	A:SER:55:	4.37	B	A	Contact
B:ASP:554:	A:ILE:405:	3.42	B	A	Contact
B:ASP:557:	A:GLY:406:	3.75	B	A	Contact
B:ASP:557:	A:ILE:405:	3.13	B	A	HBond,Polar
B:ASP:557:	A:SER:404:	4.28	B	A	Contact
B:GLN:109:	A:ILE:51:	3.52	B	A	Contact
B:GLN:109:	A:LEU:49:	3.58	B	A	Contact
B:GLN:109:	A:LEU:54:	3.83	B	A	Contact
B:GLN:218:	A:ARG:35:	3.53	B	A	Contact
B:GLN:218:	A:ARG:38:	3.56	B	A	Polar
B:GLN:218:	A:CYS:34:	4.9	B	A	Contact
B:GLN:218:	A:ILE:39:	4.7	B	A	Contact
B:GLN:218:	A:TYR:31:	3.11	B	A	Polar
B:GLN:480:	A:LYS:247:	3.61	B	A	Contact
B:GLN:99:	A:GLU:61:	4.28	B	A	Contact
B:GLN:99:	A:ILE:62:	4.75	B	A	Contact
B:GLU:105:	A:LEU:54:	3.72	B	A	Contact
B:GLU:389:	A:ILE:62:	4.42	B	A	Contact
B:GLU:389:	A:LYS:59:	3.21	B	A	Contact
B:GLU:562:	A:ARG:410:	2.6	B	A	Polar
B:GLU:566:	A:SER:397:	2.16	B	A	Polar
B:GLU:589:	A:ARG:394:	4.01	B	A	Contact
B:GLY:220:	A:ARG:35:	4.24	B	A	Contact
B:GLY:220:	A:ILE:39:	3.69	B	A	Contact
B:GLY:564:	A:MET:396:	3.71	B	A	Contact
B:GLY:564:	A:SER:397:	4.33	B	A	Contact
B:HIS:243:	A:TYR:31:	2.69	B	A	Polar
B:ILE:124:	A:ARG:38:	3.76	B	A	Contact
B:ILE:129:	A:ARG:38:	4.47	B	A	Contact
B:ILE:129:	A:TYR:31:	3.32	B	A	Contact

B:ILE:214:	A:TYR:31:	3.67	B	A	Contact
B:ILE:383:	A:ILE:51:	3.5	B	A	Contact
B:ILE:383:	A:LYS:59:	4.11	B	A	Contact
B:ILE:383:	A:MET:46:	3.84	B	A	Contact
B:ILE:383:	A:SER:55:	2.85	B	A	HBond,Polar
B:LEU:103:	A:LEU:58:	3.93	B	A	Contact
B:LEU:106:	A:ILE:51:	3.69	B	A	Contact
B:LEU:106:	A:LEU:54:	3.88	B	A	Contact
B:LEU:106:	A:LEU:58:	3.84	B	A	Contact
B:LEU:106:	A:SER:55:	4.01	B	A	Contact
B:LEU:112:	A:LEU:49:	4.41	B	A	Contact
B:LEU:117:	A:ASN:42:	3.57	B	A	Contact
B:LEU:244:	A:TYR:31:	4.83	B	A	Contact
B:LEU:249:	A:GLU:32:	2.51	B	A	Contact
B:LEU:249:	A:TYR:31:	4.25	B	A	Contact
B:LEU:512:	A:ARG:413:	3.06	B	A	Contact
B:LEU:512:	A:GLN:416:	4.63	B	A	Contact
B:LYS:102:	A:GLU:61:	2.38	B	A	Polar
B:LYS:102:	A:LEU:58:	3.82	B	A	Contact
B:LYS:120:	A:ASN:42:	4.24	B	A	Contact
B:LYS:120:	A:GLU:41:	2.62	B	A	Polar
B:LYS:328:	A:GLU:32:	2.64	B	A	Polar
B:LYS:542:	A:ARG:394:	4.51	B	A	Contact
B:LYS:563:	A:ARG:410:	4.84	B	A	Contact
B:LYS:563:	A:MET:396:	4.52	B	A	Contact
B:PHE:116:	A:ARG:45:	3.58	B	A	Contact
B:PHE:116:	A:ASN:42:	3.42	B	A	Contact
B:PHE:116:	A:GLU:41:	4.21	B	A	Contact
B:PHE:565:	A:MET:396:	3.51	B	A	Contact
B:PRO:514:	A:ARG:413:	4.94	B	A	Contact
B:SER:392:	A:ILE:62:	3.29	B	A	Contact
B:SER:561:	A:ARG:410:	3.02	B	A	Polar
B:SER:561:	A:GLY:406:	3.9	B	A	Contact
B:SER:561:	A:GLY:407:	3.99	B	A	Contact
B:SER:561:	A:PRO:400:	3.87	B	A	Contact
B:SER:561:	A:SER:404:	4.19	B	A	Contact
B:SER:591:	A:ARG:394:	4.13	B	A	Contact
B:SER:592:	A:ARG:394:	4.89	B	A	Contact

B:SER:592:	A:LYS:395:	4.26	B	A	Contact
B:SER:594:	A:ARG:394:	4.29	B	A	Contact
B:THR:110:	A:ILE:51:	3.89	B	A	Contact
B:THR:385:	A:LYS:59:	2.8	B	A	Polar
B:TRP:217:	A:ARG:35:	3.03	B	A	HBond,Polar
B:TRP:217:	A:GLU:32:	4.84	B	A	Contact
B:TRP:217:	A:TYR:31:	3	B	A	Contact
B:TRP:393:	A:ILE:62:	2.25	B	A	Contact
B:TRP:393:	A:LEU:58:	2.97	B	A	Contact
B:TYR:113:	A:ARG:45:	4.34	B	A	Contact
B:TYR:113:	A:ASN:42:	3.35	B	A	HBond,Polar
B:TYR:113:	A:ILE:51:	3.49	B	A	Contact
B:TYR:113:	A:LEU:43:	4.43	B	A	Contact
B:TYR:113:	A:LEU:49:	3.66	B	A	Contact
B:TYR:113:	A:MET:46:	3.79	B	A	Contact
B:TYR:511:	A:ARG:412:	4.52	B	A	Contact
B:TYR:511:	A:LEU:409:	3.73	B	A	Contact
B:TYR:513:	A:ARG:413:	3.06	B	A	Polar
B:TYR:513:	A:LEU:409:	3.1	B	A	Contact
B:TYR:558:	A:ARG:413:	2.92	B	A	Polar
B:TYR:558:	A:GLY:406:	4.26	B	A	Contact
B:TYR:558:	A:LEU:409:	4.42	B	A	Contact
B:VAL:91:	A:VAL:140:	4.04	B	A	Contact