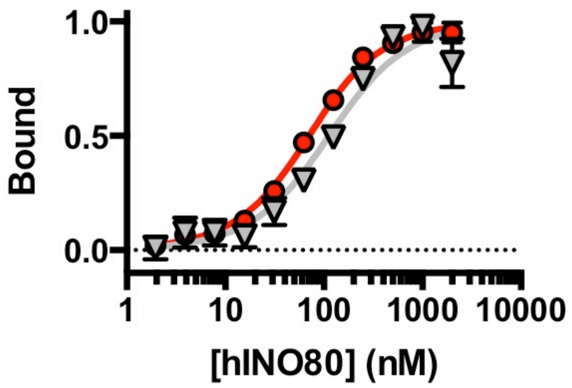
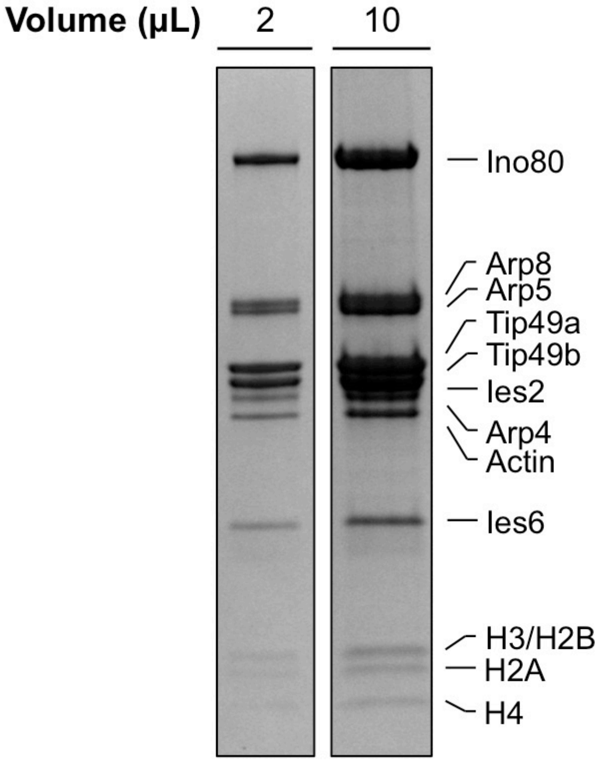
	INO80 nucleosome complex (EMDB-3954) (PDB 6ETX)
Data collection and processing	
Magnification	129,000
Voltage (kV)	300
Electron exposure (e–/Å^2)	80
Defocus range (µm)	-2.0 to -4.0
Pixel size (Å)	1.13
Symmetry imposed	C1
Initial particle images (no.)	775,804
Final particle images (no.)	26,416
Map resolution (Å)	4.8
FSC threshold	0.143
Map resolution range (Å)	4.0 to 8.0
Refinement	
Initial model used (PDB code)	2YQQ, 3LZ0, 5AV9, 5O9G, 50AF
Model resolution (Å)	4.8
Map sharpening *B* factor (Å^2)	-100
Refinement (Phenix)	
Map correlation coefficient (whole unit cell)	0.88
Map correlation coefficient (around atoms)	0.74
Model composition	
Non-hydrogen atoms	38,759
Protein residues	4,753
Nucleic acid residues	300
Ligands	7
R.m.s. deviations	
Bond lengths (Å)	0.002
Bond angles (°)	0.447
Validation	
MolProbity score	1.58 (93rd percentile*(0Å - 99Å))
Clashscore	8.4
Poor rotamers (%)	1.5
Ramachandran plot	
Favored (%)	98.2
Allowed (%)	1.75
Disallowed (%)	0.02

a



	Ligand	$k_{½}$ (nM)	h
▽	Apo	93.0 ± 11.0	1.6 ± 0.1
●	ADP.BeF$_3$	51.0 ± 2.9	1.6 ± 0.2

b



c

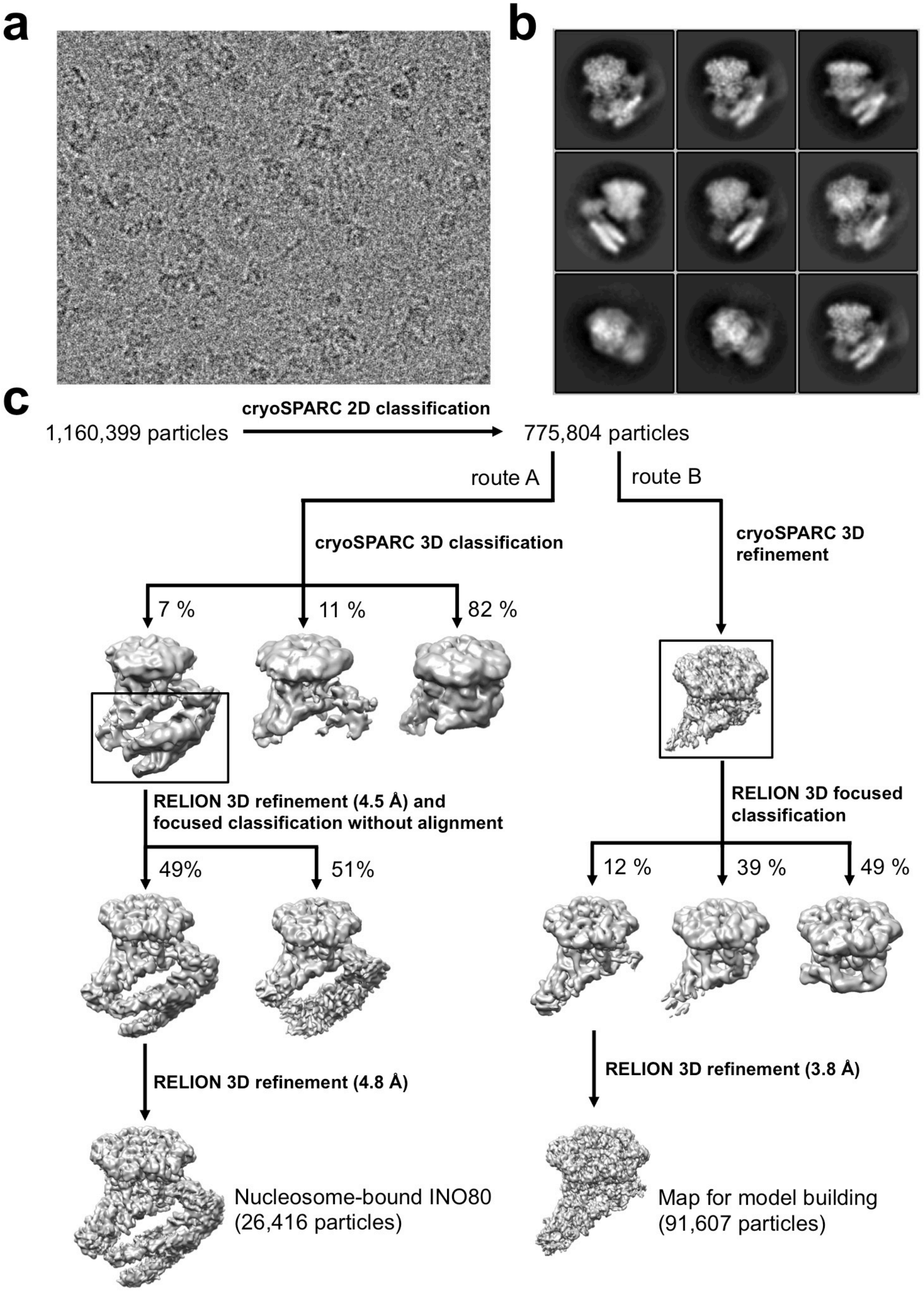
1 GTCTTGAGTCCAACCCGGTAAGACACGACTTATCGCCACCCCGAGTA 47

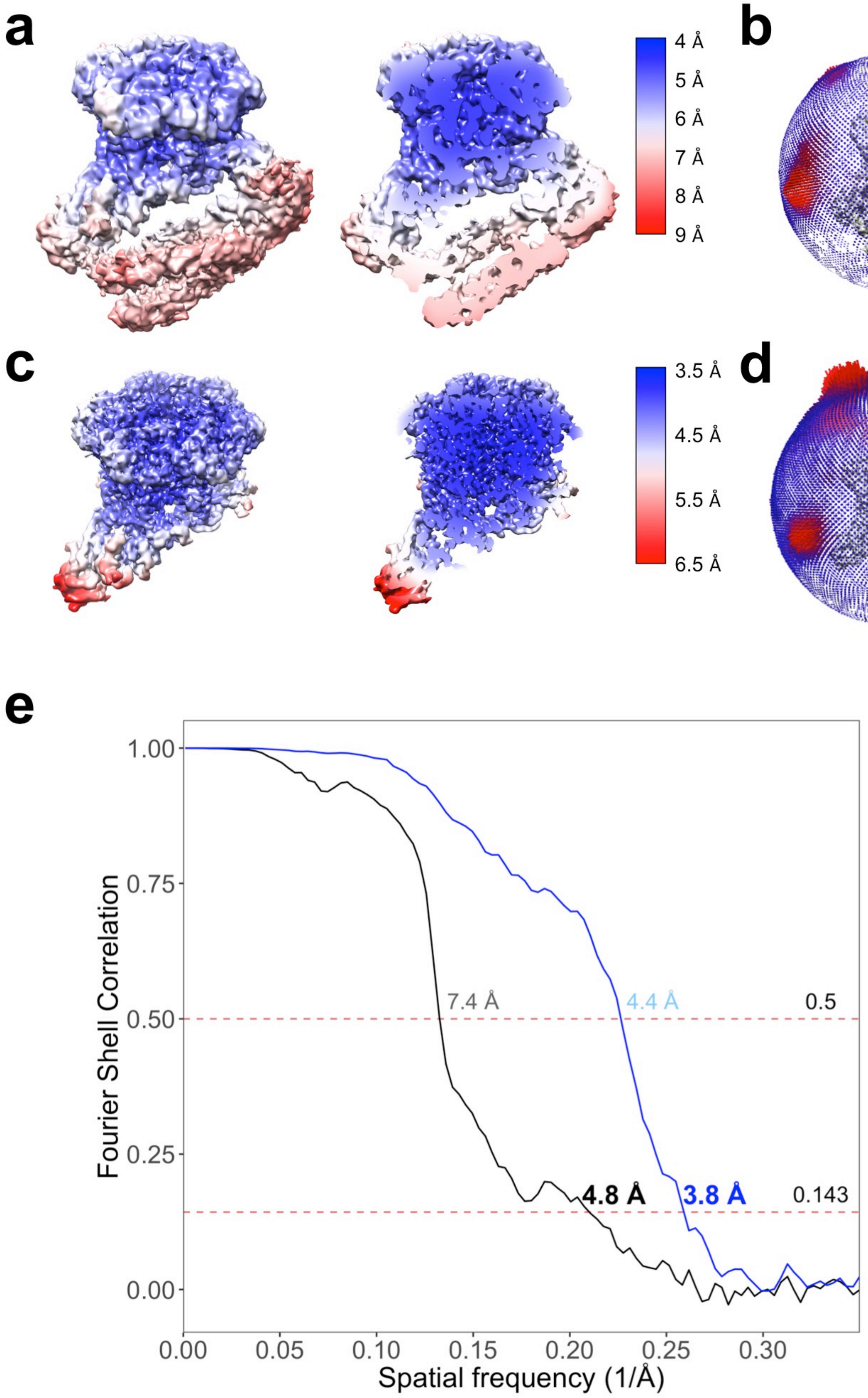
48 CATGCACAGGATGTATATATCTGACACGTGCCTGGAGACTAGGGAGT 94

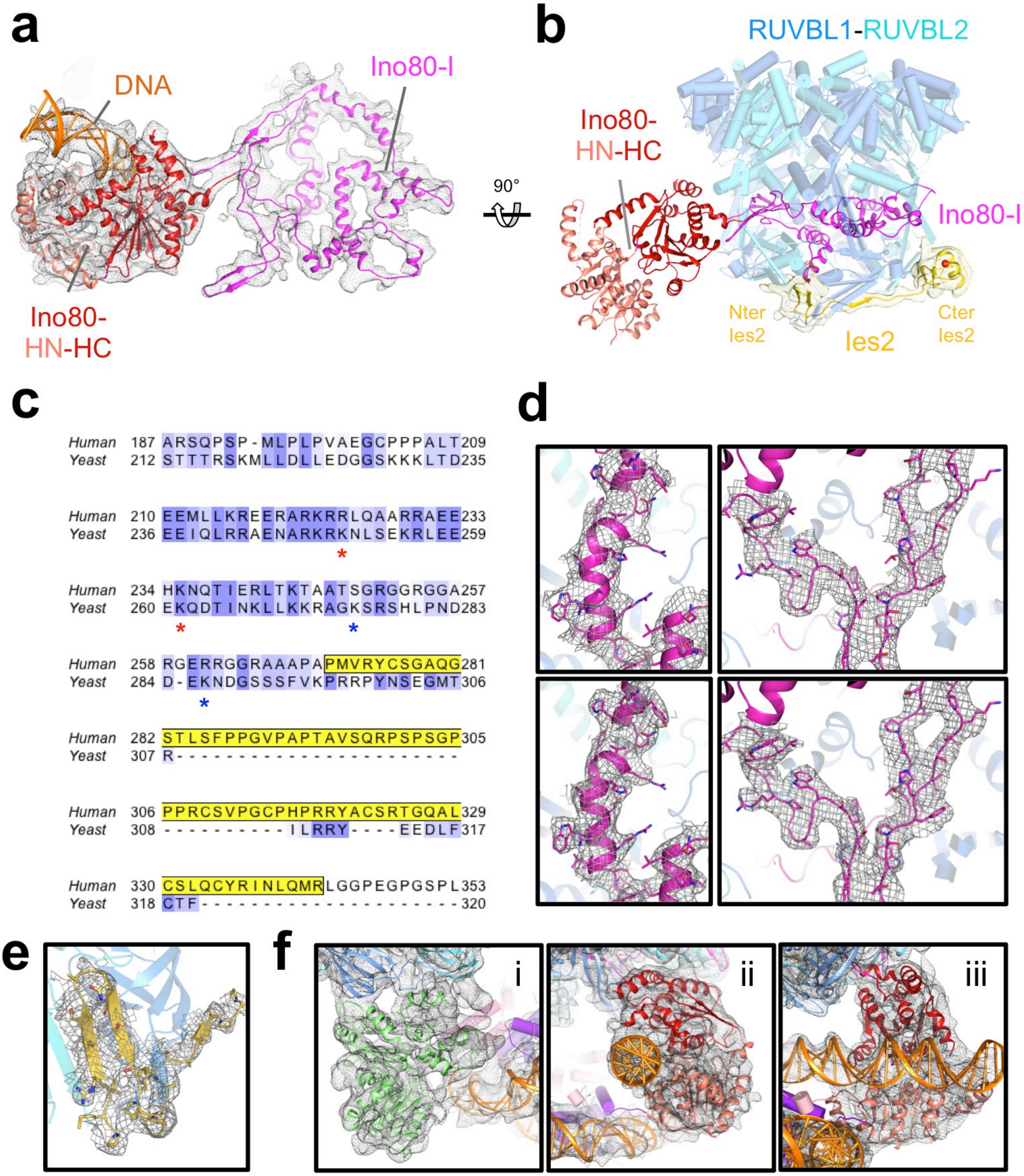
95 AATCCCCTTGGCGGTTAAAACGCGGGGGACAGCGCGTACGTGCGTTT 141

142 AAGCGGTGCTAGAGCTGTCTACGACCAATTGAGCGGCCTCGGCACCG 188

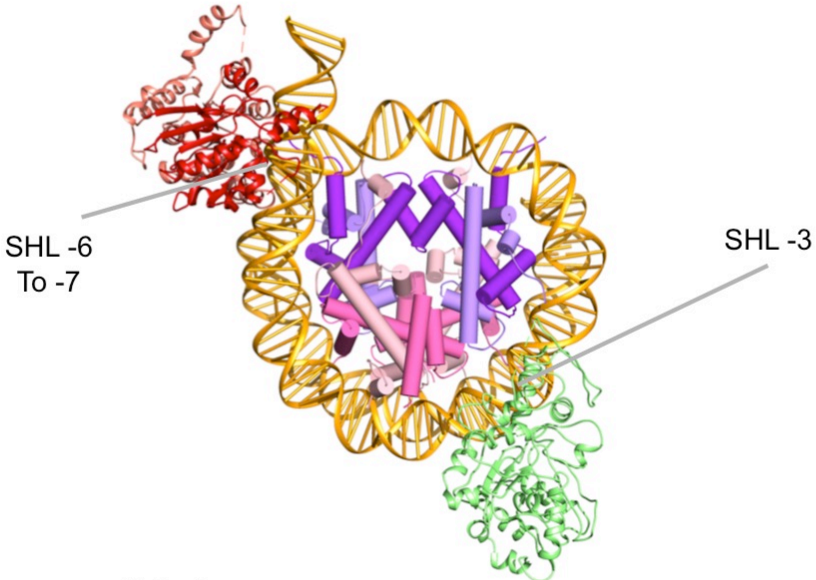
189 GGATTGTCCAGGGCGGCCGCGGATGCATTAATGCAGatt 227


a
b
c
1,160,399 particles
cryoSPARC 2D classification
775,804 particles
route A
route B
cryoSPARC 3D classification
cryoSPARC 3D refinement
7 %
11 %
82 %
RELION 3D refinement (4.5 Å) and focused classification without alignment
49%
51%
RELION 3D focused classification
12 %
39 %
49 %
RELION 3D refinement (4.8 Å)
RELION 3D refinement (3.8 Å)
Nucleosome-bound INO80 (26,416 particles)
Map for model building (91,607 particles)

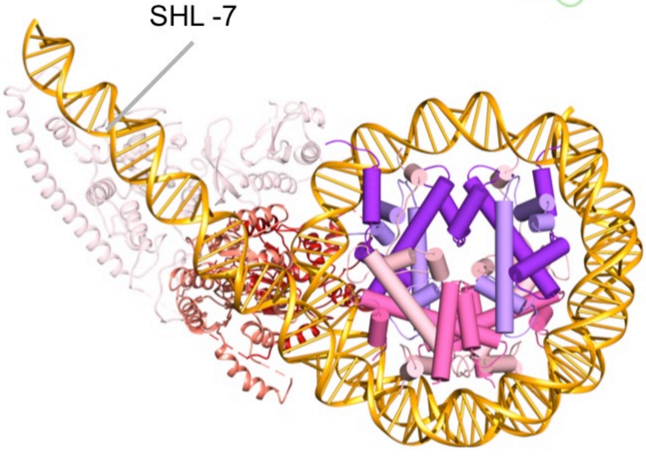

a
4 Å
5 Å
6 Å
7 Å
8 Å
9 Å
b
c
3.5 Å
4.5 Å
5.5 Å
6.5 Å
d
e
Fourier Shell Correlation
1.00
0.75
0.50
0.25
0.00
7.4 Å
4.4 Å
0.5
4.8 Å
3.8 Å
0.143
0.00
0.05
0.10
0.15
0.20
0.25
0.30
Spatial frequency (1/Å)


a
DNA
Ino80-I
Ino80-HN-HC
90°
b
RUVBL1-RUVBL2
Ino80-HN-HC
Ino80-I
Nter Ies2
Ies2
Cter Ies2
c
Human 187 ARSQPSP-MLPLPVAEGCPPPALT 209
Yeast 212 STTTRSKMLLDLLEDGGSKKKLTD 235
Human 210 EEMLLKREERARKRRLQAARRAEE 233
Yeast 236 EEIQLRRAENARKRKNLSEKRLEE 259
*
Human 234 HKNQTIERLTKTAATSGRGGRGGA 257
Yeast 260 EKQDTINKLLKKRAGKSRSHLPND 283
*
*
Human 258 RGERRGGRAAAPAPMVRYCSGAQG 281
Yeast 284 D-EKNDGSSSFVKPRRPYNSEGMT 306
*
Human 282 STLSFPPGVPAPTAVSQRPSPSGP 305
Yeast 307 R-----------------------
Human 306 PPRCSVPGCPHPRRYACSRTGQAL 329
Yeast 308 -----------ILRRY---EEDLF 317
Human 330 CSLQCYRINLQMRLGGPEGPGSPL 353
Yeast 318 CTF--------------------- 320
d
e
f
i
ii
iii

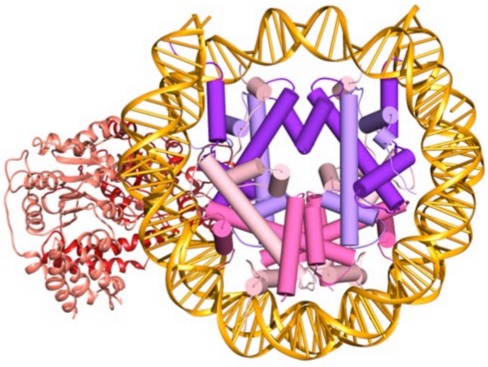
INO80



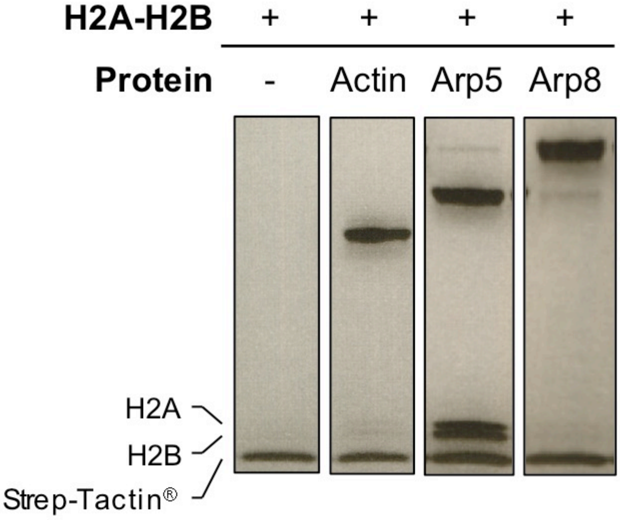
CHD1



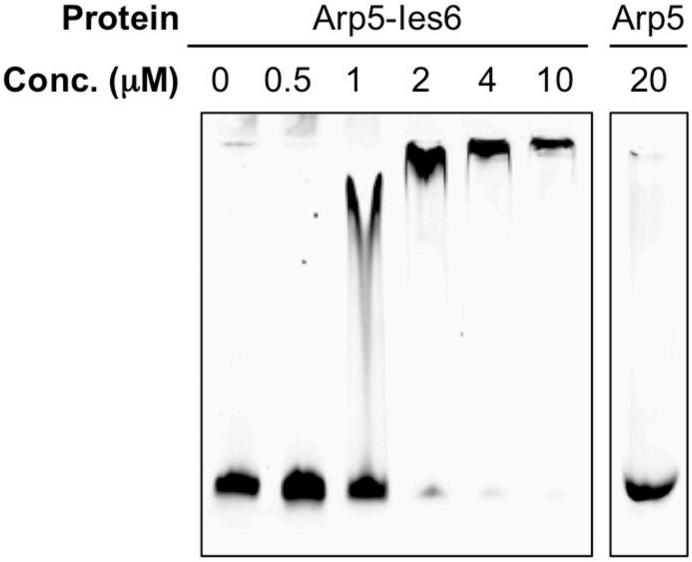
SNF2 (SHL2)



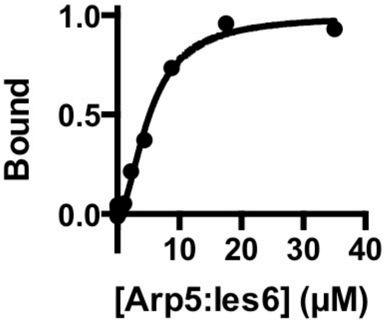
a



b

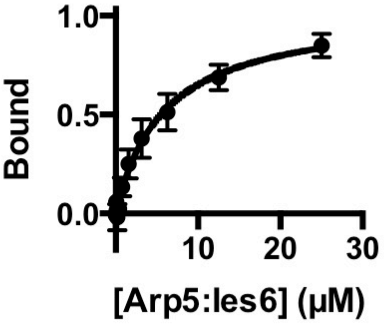


c

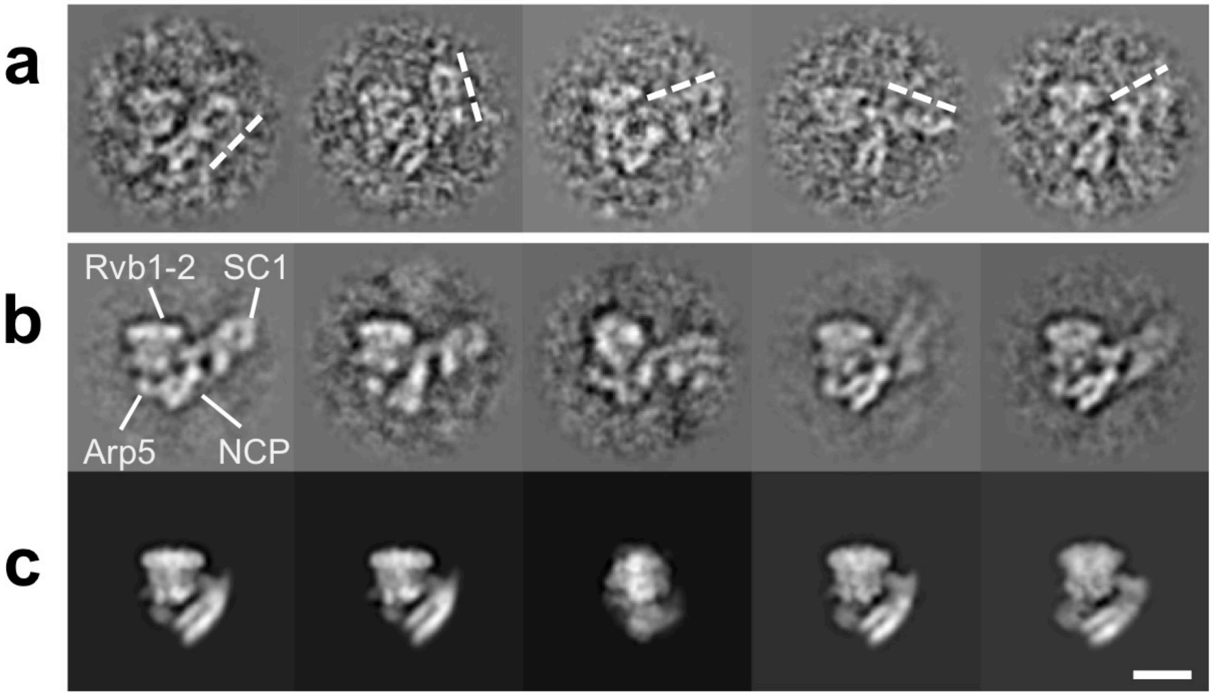


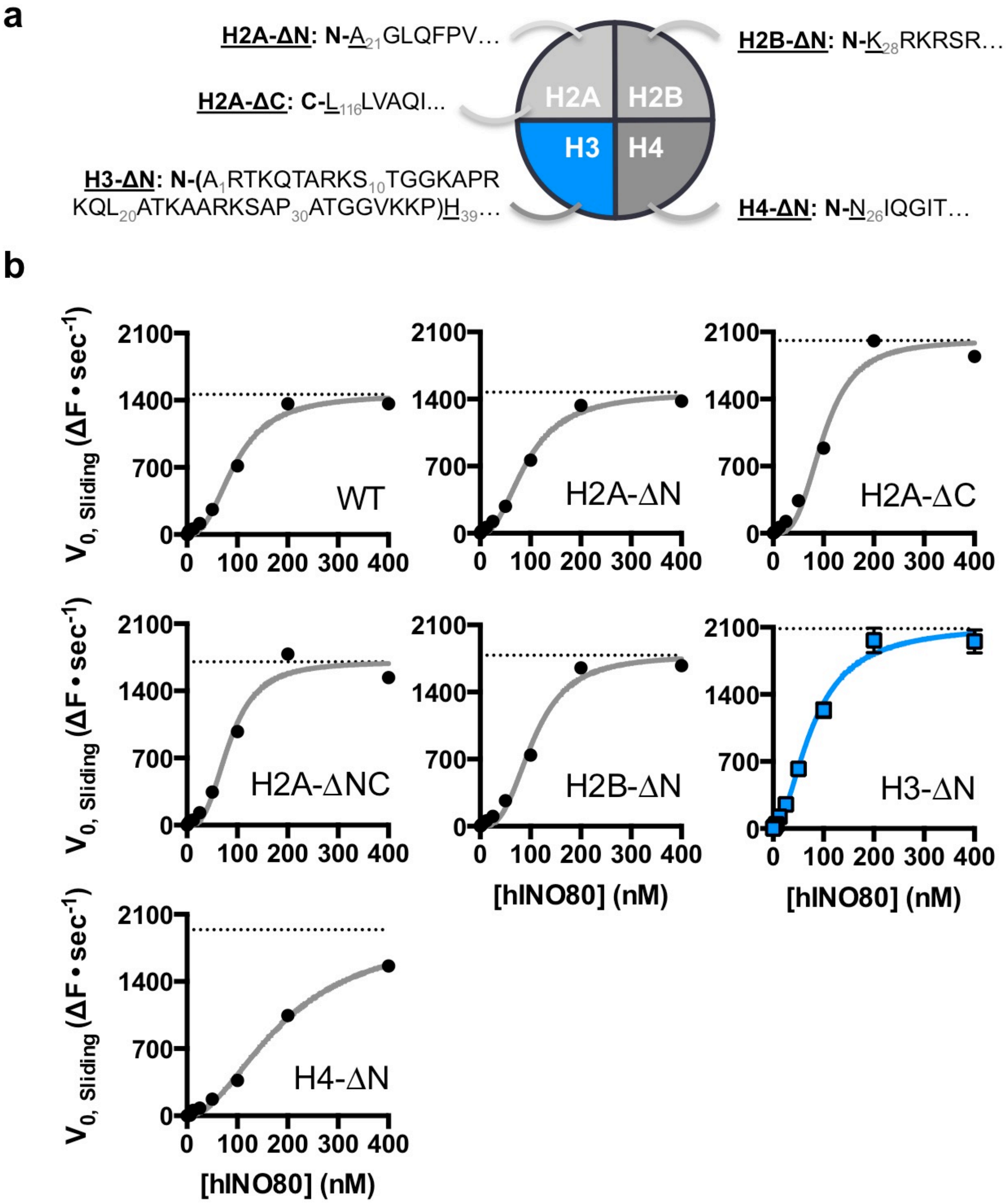
Substrate = 0N100
$k_{1/2}$ = 5.2 ±0.3 μM
r^2 = 0.99

d



Substrate = H2A:H2B
$k_{1/2}$ = 5.9 ±2.0 μM
r^2 = 0.97


a
b
Rvb1-2
SC1
Arp5
NCP
c

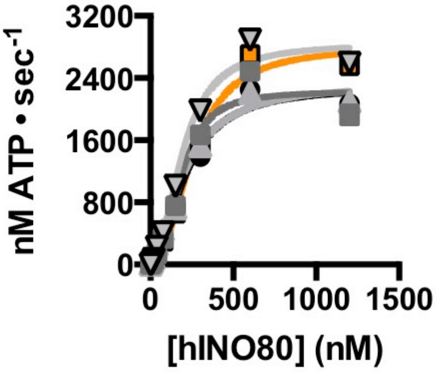

a
H2A-ΔN: N-A21GLQFPV…
H2B-ΔN: N-K28RKRSR…
H2A-ΔC: C-L116LVAQI...
H2A
H2B
H3
H4
H3-ΔN: N-(A1RTKQTARKS10TGGKAPR KQL20ATKAARKSAP30ATGGVKKP)H39…
H4-ΔN: N-N26IQGIT…
b
V0, Sliding (ΔF • sec-1)
2100
1400
700
0
0 100 200 300 400
WT
H2A-ΔN
H2A-ΔC
H2A-ΔNC
H2B-ΔN
H3-ΔN
H4-ΔN
[hINO80] (nM)

a

Nucleosome	V_{max} (nM ATP • sec^{-1})	h_{ATPase}
0N100 ($H3^{FL}$)	2430.0 ± 69.0	*1.4 ± 0.1*
0N100 ($H3^{L20}$)	2050.0 ± 82.0	*1.3 ± 0.1*
0N100 ($H3^{P30}$)	2660.0 ± 92.0	*1.4 ± 0.1*
0N100 ($H3^{H39}$)	3150.0 ± 160.0	*1.3 ± 0.1*

*__Bold__ = h > 1.5, _Italics_ = h < 1.5

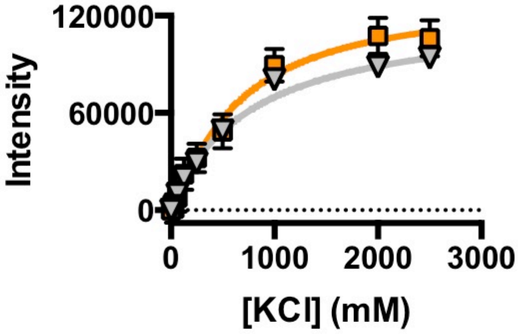
b



Nucleosome	$V_{max, ATPase}$ (ΔF • sec^{-1})	h_{ATPase}
▽ $H3^{WT}$	2850.0 ± 25.0	*1.3 ± 0.1*
■ $H3^{K27Q}$	2231.0 ± 174.0	*1.3 ± 0.1*
▲ $H3^{K36Q}$	2348.0 ± 177.0	*1.2 ± 0.1*
● $H3^{K37Q}$	2289.0 ± 151.0	*1.4 ± 0.1*
□ $H3^{K36Q, K37Q}$	2800.0 ± 174.0	*1.3 ± 0.1*

*__Bold__ = h > 1.5, _Italics_ = h < 1.5

c



Nucleosome	50% Unwrapped (mM)
▽ $H3^{WT}$	753 ± 100
□ $H3^{K36Q, K37Q}$	634 ± 199