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Supplemental Material to:

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Beta conformation of polyglutamine track revealed by a crystal structure of Huntingtin amino-terminal region with insertion of three histidine residues

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Supplementary Table 1. Results of MBP-HttPolyQ-EX1 crystallization trials.

Htt containing polyQ tracks of various length (17Q, 23Q, 36Q and 45Q) synthesized by GenScript, expressed and purified for crystallization. The crystallization of MBP-HttPolyQ-EX1 with XQXQX interrupters (X = G, A, H) introduced after 7th, 9th, 10th, 12th, and 15th glutamine residue within a polyQ region are summarized in the additional file1-Table 1.

XQXQX	First X at	17Q	23Q	36Q	45Q
AQAQA	7	▲ ■	▲	X	X
	10	X	X	X	X
GQGQG	7	X	X	X	X
HQHQH	7	▲	▲	▲ ■	X
	9	X	X	X	X
	12	NT	NT	X	X
	15	NT	NT	X	X

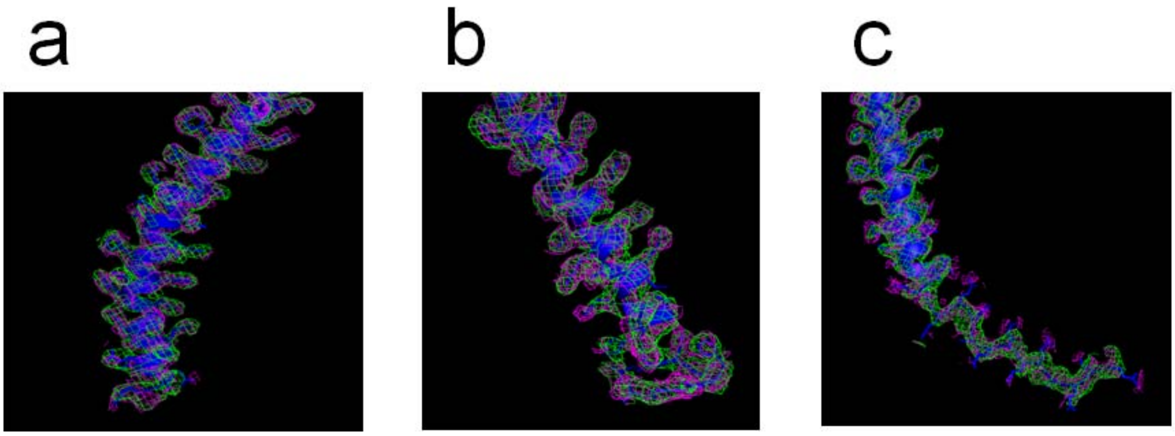
X = No crystal, ▲ =crystal, ■ =diffraction > 3A, NT = Not tested,

Supplementary Table 2 CC correlation coefficients : Electron density Map (2Fo-Fc) to Htt36Q3H Model fit

RESIDUE	X1				X2			
	A	B	C1	C2	A	B	C1	C2
MET 371	0.94	0.94	0.93	0.92	0.93	0.94	0.95	0.93
ALA 372	0.95	0.95	0.95	0.97	0.95	0.96	0.96	0.96
THR 373	0.95	0.92	0.93	0.94	0.93	0.92	0.96	0.96
LEU 374	0.97	0.96	0.97	0.97	0.95	0.98	0.96	0.97
GLU 375	0.97	0.97	0.98	0.98	0.96	0.98	0.97	0.98
LYS 376	0.92	0.98	0.96	0.97	0.96	0.98	0.96	0.99
LEU 377	0.97	0.98	0.98	0.98	0.95	0.98	0.97	0.98
MET 378	0.96	0.96	0.98	0.98	0.97	0.98	0.97	0.98
LYS 379	0.98	0.95	0.99	0.98	0.98	0.98	0.98	0.98
ALA 380	0.97	0.96	0.97	0.98	0.97	0.97	0.93	0.97
PHE 381	0.97	0.98	0.98	0.98	0.97	0.96	0.96	0.97
GLU 382	0.96	0.97	0.98	0.98	0.97	0.94	0.99	0.97
SER 383	0.94	0.93	0.93	0.97	0.90	0.95	0.93	0.95
LEU 384	0.98	0.98	0.98	0.99	0.97	0.98	0.97	0.97
LYS 385	0.97	0.97	0.98	0.99	0.95	0.96	0.98	0.98
SER 386	0.98	0.97	0.99	0.99	0.98	0.98	0.97	0.98
PHE 387	0.98	0.97	0.97	0.98	0.97	0.96	0.95	0.97
GLN 388	0.96	0.96	0.98	0.99	0.97	0.95	0.97	0.95
GLN 389	0.99	0.96	0.99	0.98	0.98	0.98	0.98	0.90
GLN 390	0.93	0.96	0.96	0.96	0.97	0.97	0.93	0.89
GLN 391	0.97	0.96	0.98	0.97	0.99	0.97	0.97	0.96
GLN 392	0.95	0.94	0.99	0.93	0.94	0.99	0.99	0.93
GLN 393	0.89	0.90	0.96	0.71	0.97	0.99	0.96	0.89
GLN 394	0.95	0.86	0.98	0.77	0.95	0.98	0.95	0.77
HIS 395	0.84	0.91	0.89	0.80	0.67	0.88	0.90	0.74
GLN 396	0.94	0.87	0.99	0.60	0.97	0.71	0.97	0.73
HIS 397	0.91	0.86	0.83	0.86	0.99	0.76	0.80	0.48
GLN 398	0.86	0.63	0.97	0.28	0.73	0.92	0.56	0.61
HIS 399	0.88	0.66	0.98	0.92	0.83	0.86	0.50	0.80
GLN 400	0.92	0.96	0.96	0.96	0.94	0.79	0.62	0.72
GLN 401	0.90	0.95	0.95	0.81	0.59	0.87	0.71	0.63
GLN 402	0.94	0.78	0.97	0.87	0.47	0.41	0.88	0.45
GLN 403			0.98				0.82	
GLN 404			0.98				0.83	
GLN 405			0.97				0.83	
GLN 406			0.97				0.67	
GLN 407			0.98				0.64	
GLN 408			0.98					
GLN 409			0.93					
GLN 410			0.89					

CC was calculated by Map to Model fit program in Phenix

Supplementary Figures



Supplementary Fig 1. Comparison of Omit and 2Fo-Fc maps for α-helical, beta and loop conformations of Htt-36Q3H.

a, Omit map (pink mesh) and 2Fo-Fc map (green mesh) are overlaid with the α-helical structure of Htt-polyQ (Q388-Q410) shown in blue (C1 molecule from crystal X1).

b, Omit map (pink mesh) and 2Fo-Fc map (green mesh) are overlaid with the α-helical structure of Htt-polyQ (Q388-Q394) followed by a β-hairpin (Q396-Q401) shown in blue (C2 molecule from crystal X1).

c, Omit map (pink mesh) and 2Fo-Fc map (green mesh) are overlaid with the α-helical structure of Htt-polyQ (Q388-Q394) followed by a loop (Q396-Q407) shown in blue (C1 molecule from crystal X2).