Supplementary Tables for "Sub-ångstrom cryo-EM structure of a prion protofibril reveals a polar clasp"

Supplementary Table 1. Crystallographic structure determination of proto-PrP^{Sc}.

proto-PrP^{sc}	X-ray	MicroED (Phenix)	MicroED (Refmac)
Data collection			
Space group	P1	P1	
Cell dimensions			
a, *b*, *c* (Å)	4.87 10.11 30.42	4.94 10.34 31.15	
α, *β*, *γ* (°)	93.36 91.15 101.66	94.26 92.38 102.20	
Resolution (Å)	30.35 - 1.10 (1.14 - 1.10)	10.34-0.75 (0.78-0.75)[a]	
R_{merge}	0.099 (0.405)	0.232 (0.638)	
R_{meas}	0.142 (0.573)	0.250 (0.729)	
R_{pim}	0.098 (0.405)	0.090 (0.319)	
$I/\sigma(I)$	6.20 (1.92)	4.57 (1.77)	
$CC_{1/2}$	0.986 (0.546)	0.982 (0.209)	
Completeness (%)	80.75 (46.22)	96.95 (96.17)	
No. Reflections	3059 (127)	43252 (2359)	
Redundancy	1.6 (1.2)	5.8 (4.4)	
Refinement			
No. reflections	1866 (110)	7473 (720)	6800 (470)
R_{work}	0.139 (0.29)	0.242 (0.37)	0.233 (0.36)
R_{free}	0.162 (0.23)	0.246 (0.39)	0.254 (0.35)
No. atoms			
Total	85	152	152
Waters	4	2	2
Hydrogens Possible	70	69	69
Hydrogens Modeled[b]	0	51	61
B factors			
Protein	12.27	6.00	5.88
Water	23.09	11.59	11.56
R.m.s. deviations			
Bond lengths (Å)	0.007	0.014	0.034
Bond angles (°)	0.99	1.01	2.21

[a] Values in parentheses are for the highest-resolution shell.

[b] Hydrogens modelled include only those for which density is observed in 2Fo-Fc maps at 0.70σ or higher.

Supplementary Table 2. Hydrogen bonds in proto-PrP^{Sc}.

	Donor name[a]	Atom type	Acceptor name[a]	Atom type	DA dist.	DA pair[b]	Gap	CA-CA dist.	DHA angle	H-A dist.	H-A-AA angle	D-A-AA angle
1	A**0168-**GLN	NE2	B**0168-**GLN	OE1	3.02	SS	-	4.90	136.7	2.21	137.7	150.8
2	A**0170-**ASN	ND2	A**0168-**GLN	OE1	3.11	SS	2	6.48	176.4	2.11	108.9	109.4
3	A**0169-**TYR	N	B**0168-**GLN	O	3.00	MM	-	6.32	164.6	2.17	163.5	167.8
4	B**0170-**ASN	N	A**0169-**TYR	O	2.85	MM	-	6.00	163.4	2.01	166	170.9
5	B**0170-**ASN	ND2	A**0170-**ASN	OD1	2.90	SS	-	4.90	159.5	1.94	160.1	167.0
6	A0171-ASN	N	B**0170-**ASN	O	3.01	MM	-	6.24	144.0	2.27	151.4	161.1
7	B0172-GLN	N	A0171-ASN	O	3.19	MM	-	6.48	142.2	2.46	139.6	149.0
8	A0171-ASN	ND2	B0171-ASN	OD1	2.87	SS	-	4.90	151.1	1.95	153.7	163.4
9	A0173-ASN	ND2	A0171-ASN	OD1	3.09	SS	2	6.93	146.1	2.21	106.4	99.4
10	A0172-GLN	NE2	A0174-ASN	OD1	2.99	SS	2	7.07	173.3	2.00	108.7	110.9
11	A0172-GLN	NE2	B0172-GLN	OE1	2.92	SS	-	4.90	164.1	1.95	162.3	167.7
12	C0171-ASN	ND2	A0172-GLN	OE1	3.04	SS	-	8.49	131.4	2.28	113.5	102.0
13	B0174-ASN	N	A0173-ASN	O	3.06	MM	-	6.48	160.0	2.24	159.1	164.6
14	A0173-ASN	ND2	B0173-ASN	OD1	3.07	SS	-	4.90	156.0	2.13	154.3	161.9
15	A0174-ASN	ND2	D0173-ASN	OD1	3.13	SS	-	8.77	150.1	2.22	120.7	119.4
16	B0174-ASN	ND2	A0174-ASN	OD1	2.98	SS	-	4.90	161.9	2.01	162.2	168.1
17	A0175-PHE	N	B0174-ASN	O	2.93	MM	-	6.16	158.8	2.11	158.6	164.7
18	B0176-VAL	N	A0175-PHE	O	2.87	MM	-	6.08	170.4	2.02	174.9	177.7
19	C0169-TYR	O4	B0171-ASN	O	2.95	SM	-	9.90	142.5	2.23	119.8	128.8
20	A0171-ASN	N	A0171-ASN	O	2.80	MM	0	0	103.8	2.50	76.9	59.7
21	A0172-GLN	N	A0172-GLN	O	2.80	MM	0	0	107.2	2.42	77.2	60.6
22	A0173-ASN	N	A0173-ASN	O	2.81	MM	0	0	103.3	2.48	78.6	61.3

[a] Donor and acceptor names are abbreviated as the chain name followed by a four-digit residue number, a dash and the residue three letter code. A four-chain assembly (A-D) was used that encompass all unique hydrogen bonds in proto-PrPSc; two sheets, with two strands each. Chains A and B make up one sheet, C and D make up the mating sheet.

[b] M represents main chain, S represents side chain.

All distances are measured in ångstroms; angles in degrees.

Supplementary Table 3. Crystallographic structure determination of carbamazepine.

Carbamazepine	MicroED
Data collection	
Space group	P 1 21/m 1
Cell dimensions	
a, *b*, *c* (Å)	7.50, 11.00, 13.70
α, β, γ (°)	90.0, 93.2, 90.0
Resolution (Å)	7.49-0.849 (0.95-0.849)
R_{merge}	0.084 (0.149)
R_{meas}	0.104 (0.182)
R_{pim}	0.059 (0.103)
$I/\sigma(I)$	8.19 (4.55)
$CC_{1/2}$	0.992 (0.961)
Completeness (%)	49.8 (23.3)
No. Reflections	2739 (371)
Redundancy	2.71 (2.01)
Refinement	
No. reflections	2739 (371)
R_{work}	0.20
R_{free}	0.46
No. atoms	
Total	30
Waters	0
Hydrogens Possible	12
Hydrogens Modeled	12

[a] Values in parentheses are for the highest-resolution shell.

Supplementary Table 4. Refinement of proto-PrP^{Sc} as a function of resolution.

proto-PrP^{sc}	MicroED 0.75Å	MicroED 0.80Å	MicroED 0.90Å	MicroED 1.00Å	MicroED 1.10Å
Data collection					
Space group	P1	P1	P1	P1	P1
Cell dimensions					
a, *b*, *c* (Å)	4.94 10.34 31.15	4.94 10.34 31.15	4.94 10.34 31.15	4.94 10.34 31.15	4.94 10.34 31.15
α, *β*, *γ* (°)	94.21 92.38 102.20	94.26 92.38 102.20	94.26 92.38 102.20	94.26 92.38 102.20	94.26 92.38 102.20
Resolution (Å)[a]	10.34-0.75 (0.78-0.75)	10.34-0.80 (0.83-0.80)	10.34-0.90 (0.93-0.90)	10.34-1.0 (1.04-1.0)	10.34-1.10 (1.14-1.10)
R_{merge}	0.232 (0.638)	0.227 (0.524)	0.221 (0.373)	0.217 (0.335)	0.214 (0.265)
R_{meas}	0.250 (0.729)	0.245 (0.585)	0.238 (0.409)	0.233 (0.364)	0.229 (0.285)
R_{pim}	0.090 (0.319)	0.0872 (0.247)	0.0839 (0.159)	0.0823 (0.139)	0.0801 (0.0992)
$I/\sigma(I)$	4.57 (1.77)	5.05 (2.52)	5.82 (3.64)	6.30 (4.24)	6.71 (5.65)
$CC_{1/2}$	0.982 (0.209)	0.981 (0.549)	0.981 (0.847)	0.98 (0.92)	0.979 (0.938)
Completeness (%)	96.95 (96.17)	97.36 (95.54)	97.74 (95.48)	98.08 (97.40)	97.84 (99.24)
No. Reflections	43252 (2359)	36981 (3191)	27687 (2542)	20376 (1848)	15910 (1780)
Redundancy	5.8 (4.4)	6.0 (5.1)	6.3 (5.8)	6.4 (5.9)	6.6 (6.8)
***Ab initio* phasing**					
Atoms Placed[b]	62.4 ± 0.70	67.9 ± 1.37	66.5 ± 0.97	66.8 ± 0.42	66.9 ± 1.52
CFOM	97.0 ± 0.41	98.9 ± 0.41	102.0 ± 0.36	106.1 ± 0.56	99.0 ± 0.89
Refinement					
No. reflections	7473 (720)	6160 (623)	4377 (443)	3166 (314)	2408 (258)
R_{work}	0.243 (0.36)	0.233 (0.35)	0.218 (0.29)	0.205 (0.24)	0.197 (0.23)
R_{free}	0.252 (0.39)	0.247 (0.38)	0.222 (0.31)	0.217 (0.26)	0.215 (0.26)
No. atoms					
Total	152	152	152	152	152
Hydrogens Possible	69	69	69	69	69
Hydrogens Modelec	51	40	40	38	33
B factors					
Protein	6.00	6.51	6.01	5.79	5.45
Water	11.59	16.24	15.12	13.30	13.25
R.m.s. deviations					
Bond lengths (Å)	0.014	0.013	0.013	0.012	0.012
Bond angles (°)	1.01	1.00	1.06	1.06	1.08

[a] Values in parentheses are for the highest resolution shell

[b] Average number of atoms placed by ten independent runs of 10,000 placement tries in SHELX.

[c] Hydrogens modeled include only those for which density is observed in 2Fo-Fc maps at 0.70σ or higher.