method	b	b^{+2}	detected		detected	y	y^{+2}	method
	---	---		**A**		---	---	
HCD	159.0764	---	159.9769	**S**		3957.7121	1979.3597	
HCD	256.1292	---	256.1298	**P**	1290.9012(3+);968.4276(4+)	3870.6801	1935.8437	CID
HCD	384.1878	---	384.1890	**Q**		3773.6274	1887.3173	
	512.2463	---	512.2478	**Q**		3645.5688	1823.2880	
	583.2835	---	583.2851	**A**	1173.1779(3+)	3517.5102	1759.2587	CID
both	711.3784	356.1928	711.3808	**K**		3446.4731	1723.7402	
HCD	874.4417	437.7245	874.4445	**Y**		3318.3781	1659.6927	
	1034.4724	517.7398		$\mathbf{C^{AM}}$	1578.6184[1]	3155.3148	1578.1610	
both	1197.5357	599.2715	1197.5382	**Y**		2995.2841	1498.1457	
both	1326.5783	663.7928	1326.5819; 663.7944	**E**		2832.2208	1416.6140	
both	1454.6369	727.8221	1454.6404; 727.8242	**Q**	1352.0967; 901.7330(3+)	2703.1782	1352.0927	CID
both	1614.6675	807.8374	807.8394	$\mathbf{C^{AM}}$	1288.0667	2575.1196	1288.0635	both
CID	1728.7105	864.8589	864.8613	**N**		2415.0890	1208.0481	
both	1827.7789	914.3931	914.3953	**V**	1151.0287	2301.0461	1151.0267	CID
both	1941.8218	971.4145	971.4173	**N**	1101.4950	2201.9777	1101.4925	both
both	2069.9168	1035.4620	1035.4635	**K**	1044.4753	2087.9347	1044.4710	both
both	2168.9852	1084.9962	1984.9987	**V**		1959.8398	980.4235	
	2266.0379	1133.5226		**P**	1860.7755; 930.8919	1860.7714	930.8893	both
both	2413.1064	1207.0568	1207.0595	**F**		1763.7186	882.3629	
both	2528.1333	1264.5703	1264.5737	**D**	1616.6542; 808.8302	1616.6502	808.8287	CID
both	2656.1919	1328.5996	1328.6040	**Q**	751.3171	1501.6232	751.3153	both
both	2816.2225	1408.6149	1408.6191	$\mathbf{C^{AM}}$	1373.5683; 687.2877	1373.5647	687.2860	both
CID	2979.2859	1490.1466	1490.1507	**Y**	1213.5372; 607.2721	1213.5340	607.2706	half each
CID	3107.3444	1554.1759	1554.1780	**Q**	1050.4731; 525.7402	1050.4707	525.7390	both
CID	3238.3849	1619.6961	1080.1356(3+)	**M**	944.4146	922.4121	461.7097	both
CID	3341.3941	1671.2007	1114.4717(3+)	**C**	791.3736	791.3716	396.1894	both
CID	3428.4261	1714.7167	1714.7219	**S**	688.3641	688.3624	344.6849	both
CID	3525.4789	1763.2431	1175.8357(3+)	**P**	601.3318	601.3304	301.1688	both
CID	3638.5630	1819.7851	1213.5343(3+)	**L**	504.2792	504.2776	252.6425	both
CID	3767.6056	1884.3064	1256.5428(3+)	**E**	391.1947	391.1936	196.1004	both
CID	3923.7067	1962.3570	981.684(4+)	**R**	262.1518	262.1510	131.5791	HCD
	---	---		**S**		106.0499	---	

[1]Single isotope

Table S1, related to Figure 1 Summary of WaTx fragment ions detected in ion trap collision-induced dissociation (CID) or beam-type Higher-energy C-trap dissociation (HCD) spectra of partially cysteine carbamidomethylated (C^{AM}) m/z 1007.9457 (4^+) and assigned in the manual de novo sequencing process. We measured all masses in the Orbitrap.

Resonance assignments[1]	
[^{1}H,^{1}H] NOESY (10% D_2O)	
Backbone	29/30 (97%)
Side chain	134/138 (97%)
[^{1}H,^{1}H] NOESY (100% D_2O)	
Backbone	0/30 (0%)
Side chain	121/138 (88%)
[^{1}H, ^{13}C] HSQC (100% D_2O)	
Backbone	27/33 (82%)
Side chain	72/90 (80%)
Restraints[2]	
Total NOE constraints	538
Intraresidue (i=j)	275
Sequential (|i=j|=1)	125
Medium range (1<|i=j|<5)	91
Long range (1<|i=j|≥5)	47
Dihedral	58
Disulfide	2
Residual restraint violations[2] (Mean ± SD)	
*Avg. distance violation / structure (*Å)	0.10 ± 0.30
Avg. dihedral violation / structure (°)	0.53 ± 1.9
Model quality	
RMSD all atoms[1] (Å)	0.332
RMSD bond lengths[2] (Å)	0.005
RMSD bond angles[2] (°)	0.7
Number of close contacts[3]	0
Ramachandran statistics[2] (%)	
Most favored	84
Additionally allowed	12
Generously allowed	4
Disallowed	0
Model contents	
Total no. of residues	33
Total no. models calculated	200
Total no. models deposited	50
PDB/BMRB code	6OFA/30597

Table S2, related to Figure 2 NMR data collection and refinement statistics for WaTx.

[1]Determined with CCPN Analysis

[2]Calculated with PSVS; average distance violations were calculated using sum over r^2

[3]Defined as being within 1.6Å for Hydrogen atoms