The EPSR files for JCP “Is Water One Liquid or Two?” are contained in three zip files, namely AmorIce.zip, watercold2016.zip, and waterNIMRODxray2016.zip. When unpacked, these files should produce three folders with the same names. The AmorIce folder will itself be split into three subfolders, HDA80Kneutron, LDA80Kneutron, and VHDA80Kneutron. The other two files are self contained and should produce no subfolders.

The list of datasets used in this paper is shown in Table III of the main paper. It is reproduced below for information:-

TABLE III. Simulation box sizes, number of molecules and atomic number densities used in the EPSR simulation of liquid water and amorphous ices from 80K to 365K. The diffraction data for the states marked LDL and HDL were not measured but obtained by linear extrapolation to lower and higher density of the data at the three states LA, LB and LC, as described in[36]. A ‘*’ in the pressure column for LDL and HDL means undefined pressure, since these were extrapolated states.

State	T [K]	P [MPa]	Box size [nm]	N [molecules]	No. density [mols/nm^3]
LDA	80	0.1	4.57967	3000	31.23
HDA	80	0.1	4.25290	3000	39.00
VHDA	80	0.1	4.16017	3000	41.67
LD	258	410	3.74559	2000	38.06
LDL	268	*	4.07758	2000	29.50
LA	268	26	3.89408	2000	33.87
LB	268	209	3.80727	2000	36.24
LC	268	410	3.74559	2000	38.06
HDL	268	*	3.67791	2000	40.20
A1	280	0.1	3.10413	1000	33.43
A2	288	0.1	3.10413	1000	33.43
A3	295	0.1	3.10723	1000	33.33
A4	313	0.1	3.11139	1000	33.20
A5	343	0.1	3.12717	1000	32.70
A6	365	0.1	3.14110	1000	32.27

The first three cases are contained in the “AmorIce” folder, cases LD to HDL are contained in the folder watercold2016, and the cases A1 to A6 are contained in the folder “waterNIMRODxray2016”. For “watercold2016”, the relevant filenames are watera, waterb,…, waterh, and waterl. For waterNIMRODxray2016 case A1 is called h2o7c, case A2 is called h2o15c, and so on.

The filenames follow the standard filename convention for EPSR – see the EPSR documentation for list of these. Note that in the current version of EPSR, EPSR25, the mapgrentropy program may not be the latest, so that the mapgrentropy input files in the above folders will not run correctly. If this presents a problem, do please contact the author for the correct version. Currently running the EPSR program is the only reliable way of accessing these data files. However the software, both executables and source code, is freely available at the website listed in the supplementary information.

The files presented should be sufficient to run the EPSR simulations described in the paper, and perform some of the additional calculations, such as fluctuations and triangles distributions.