Supporting information

S1. *DASH* running using Wine

Two locally operated computers with identical hardware running Windows 7 and Ubuntu 14.04 LTS were used to compare the performance of *DASH* running under Windows and Linux (using Wine) environments respectively. Identical *DASH* executables and *DASH* files were used in each case. 50 runs of 2×10^7 SA moves for VHCl were used as a test set. Results are summarised in Table S1. From these results, two important points are clear: (a) the use of Wine has a negligible impact on the performance of *DASH*, with only a few seconds difference between the runs in the different environments and (b) the results obtained in each case were identical and therefore the use of Wine does not affect the accuracy of results obtained by *DASH* when identical *DASH* files are used.

Table S1   Comparison of *DASH* performance when run on Windows and Linux (using Wine) operating systems. Identical *DASH* executables were used, and identical *DASH* run files consisting of 50 SA runs of 2×10^7 SA moves per run on the crystal structure VHCl were processed in each environment.

Parameter	Windows	Linux + Wine
Minimum run time / minutes	15.3	15.4
Maximum run time / minutes	16.6	16.9
Average run time / minutes	16.4	16.6
Minimum profile χ^2	12.28	12.28
Maximum profile χ^2	163.78	163.78
Number of solutions obtained	2	2

S2. *7zip* compression vs *zip* compression for *DASH* result files

The result files of 108 DASH SA runs for VHCl and 2160 DASH SA runs for ORN were compressed using the *7zip* and *zip* file compression packages. The resultant archive file sizes are listed in Table S2. For this particular file type, it is clear that the *7zip* algorithm offers a vastly superior compression ratio and hence its use is strongly recommended.

Table S2   Compression of results from 108 SA runs of VHCl and 2160 SA runs of ORN. The total file sizes are given for the uncompressed data and the resultant *7zip* and *zip* archives.

Results	Uncompressed / MB	*7zip* compression / MB	*zip* compression / MB
VHCl	10.9	0.064	5.44
ORN	245	0.792	123