Supporting information for article:

Rigid-body motion is the main source of diffuse scattering in protein crystallography

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### Table S1. Statistics for lysozyme and CypA data.

|                         | Lysozyme-RT-ID30A-3 | CypA-RT-APS (PDB: 5f66) |
|-------------------------|---------------------|--------------------------|
| **Cell Dimensions:**    |                     |                          |
| a, b, c (Å)             | 78.83, 78.83, 38.23 | 42.91, 52.44, 89.12      |
| α, β, γ (°)             | 90.0, 90.0, 90.0    | 90.0, 90.0, 90.0         |
| **Data processing**     |                     |                          |
| Low resolution limit (Å)| 27.87               | 44.56                    |
| High resolution limit (Å)| 1.35 (1.3)          | 1.15 (1.18)              |
| Rmerge                  | 0.126 (3.813)       | 0.12 (0.58)              |
| Total number of observations | 319933 (11324)           | 68210                     |
| Total number unique     | 27088 (4928)        | 94.8 (86.0)              |
| Mean((I)/sd(I))         | 7.94 (0.98)         | 9.9 (2.1)                |
| CC(1/2)                 | 0.998 (0.101)       |                          |
| Completeness            | 100.0 (100.0)       | 94.8 (86.0)              |
| Multiplicity            | 11.8 (6.6)          | 5.8 (5.0)                |
| **Refinement**          |                     |                          |
| Resolution (Å)          | 1.4 - 27.87         | 1.15 - 44.56             |
| Reflections used in refinement | 24292 (2373)           | 68155 (6195)             |
| R-free reflections      | 1219 (110)          | 3464 (313)               |
| R-work                  | 0.158 (0.290)       | 0.140 (0.358)            |
| Rfree                   | 0.165 (0.314)       | 0.183 (0.376)            |
| Number of non-hydrogen atoms | 1185               | 1446                     |
| Macromolecules          | 1115                | 1272                     |
| Ligand                  | 2                   |                          |
| Solvent                 | 68                  | 174                      |
| Protein Residues        | 129                 | 164                      |
| RMS(bonds)              | 0.003               | 0.007                    |
| RMS(angles)             | 0.56                | 1.157                    |
| Ramachandran favored (%)| 98.43               | 96.91                    |
| Ramachandran allowed (%)| 1.57                | 3.09                     |
| Ramachandran outliers (%)| 0.00               | 0.00                     |
| Rotamer outliers (%)    | 1.68                | 1.49                     |
| Clashscore              | 4.97                | 0.79                     |
| Average B-factor (Å²)   | 26.05               | 21.42                    |
| Macromolecules          | 25.46               | 19.58                    |
| Ligands                 | 47.74               |                          |
| Solvent                 | 35.13               | 34.92                    |
| **Ensemble Refinement** |                     |                          |
| τₓ (ps)                 | 1.0                 | 1.5                      |
| pTLS                    | 0.2                 | 0.2                      |
| dTMP                    | 1.0                 | 2.5                      |
| R-work                  | 0.146               | 0.147                    |
| R-free                  | 0.166               | 0.166                    |
| Number of models        | 250                 | 250                      |

¹ Data from (Van Benschoten et al., 2016)
Fig. S1. Projections of 3D diffuse maps of CypA along $a^*$,$b^*$ and $c^*$ (A-C) and lysozyme (D-F).
Fig. S2. http://www.crystal.chem.uu.nl/diffusemaps. Sequential slices through maps along the l axis of data and the mixed models for both the CypA and the lysozyme data sets.
CypA:

\[
T = \begin{bmatrix}
0.1189 & -0.0069 & -0.0054 \\
0.1220 & -0.0083 & -0.0054 \\
0.1240 & & \\
\end{bmatrix}
\]

\[
L = \begin{bmatrix}
0.0148 & 0.0062 & -0.0119 \\
0.0288 & -0.0083 & -0.0112 \\
0.0288 & & \\
\end{bmatrix}
\]

Lysosome:

\[
T = \begin{bmatrix}
0.1135 & -0.1202 & -0.0093 \\
0.1007 & 0.0006 & -0.0093 \\
0.0668 & & \\
\end{bmatrix}
\]

\[
L = \begin{bmatrix}
0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 \\
0.0000 & & \\
\end{bmatrix}
\]

Fig. S3. T and L matrices fitted to the refined B-factors of the CypA and lysozyme structures

**References**

Van Benschoten, A. H., Liu, L., Gonzalez, A., Brewster, A. S., Sauter, N. K., Fraser, J. S. & Wall, M. E. (2016). Proc. Natl. Acad. Sci. 113(15), 201524048.