Supplementary Information

Visualization of Results: In SSEhunter, the composite score is mapped to the B-factor column of the pseudoatom PDB file, allowing for software programs to represent the actual score using a variety of rendering options. In this work, we have chosen to represent α-helices using a red color while β-sheets are shown as blue. In Chimera, the lowest scoring pseudoatoms from SSEhunter were set to blue. Conversely the highest scoring pseudoatoms were set to red, while pseudoatoms near zero were colored grey. Thus, the intensity of color reflects the reliability of the prediction. Strong α-helices will appear bright red, while less reliable α-helices are pale red; similarly strong β-sheet regions are bright blue, while less reliable β-sheets are pale blue. This and other types of similar renderings can be used to quickly focus user attention and provide an intuitive visual interface for identifying secondary structure elements.

Beyond pseudoatoms, SSEhunter and SSEbuilder support a number of visualization and analysis formats. Rendering of β-sheets and α-helices are primarily done using VRML geometries. This type of rendering is rather simplistic, but is quite useful in displaying structural features. As α-helices are more regular, they can be rendered as prototypical PDB style α-helices; i.e. they contain atoms with coordinate. This representation is more common in molecular visualization software and thus more portable. In addition to the graphical displays, pseudoatoms containing the individual, annotated α-helices and β-sheets can be saved as coordinate data (PDB files). Furthermore, α-helices can be represented in the DejaVu format (Kleywegt and Jones, 1997), which can in turn be used for identifying similar secondary structure distributions in the PDB (Jiang et al., 2001).

Supplementary Table 1. Assessment of SSEhunter results on the representative structures from the top ten most commonly occurring folds.

Structure	**Helix ≤ 4aa**	**5-8aa helix**	**helix > 8aa**	**sheet ≤ 2 strands**	**sheet > 2 strands**
1AJW	0/0	1/1	0/0	0/0	2/2
1AJZ	0/1	3/3	7/7	0/1	1/1
1AL7	1/3	4/4	10/10	0/2	1/1
1CV1	1/1	0/2	8/8	0/0	1/1
1DAI	2/2	2/2	5/5	0/2	1/1
1ENY	0/0	1/1	9/9	0/0	1/1
1WAB	1/3	0/0	6/6	0/0	1/1
2AW0	0/0	0/0	2/2	0/0	1/1
2ITG	0/0	1/1	5/5	0/0	1/1
3LCK	1/4	0/2	6/6	1/1	1/1
Total	6/14	12/16	58/58	1/6	11/11

Supplementary Figure 1. Skeletonization. Shown in (A) is the complete skeleton generated by SSEhunter in a simulated 8 Å resolution density map (2BTV monomer). This skeleton is classified into two parts: surfaces (blue) that approximate β-sheets and lines (green) that correspond to loops and α-helices (B). Based on the skeleton and the density features of the skeleton, individual pseudoatoms can be assigned a score based on the pseudoatoms position on the skeleton (C). In this representation, β-sheet regions are colored blue and α-helical/loop regions are red.

Supplementary Figure 2. BTV VP7 Skeleton. The skeleton generated by SSEhunter for the 8Å resolution simulated BTV VP7 monomer (A, B). The density is shown in grey, while the skeleton is shown in red. In (B), a zoomed in view of the lower domain of VP7 is shown with the X-ray structure (light grey) superimposed on the density map and skeleton, illustrating the ability of the skeleton to approximate the polypeptide chain.

Supplementary Figure 3. Graphical interface. SSEhunter and SSEbuilder utilize the graphical interface in UCSF's Chimera. SSEhunter produces a set of pseudoatoms, scored based on the likely hood of being a α-helix or sheet, while SSEbuilder produces an annotated representation of the SSEhunter results as VRML or PDB-style α-helices.

Supplemental Figure 1

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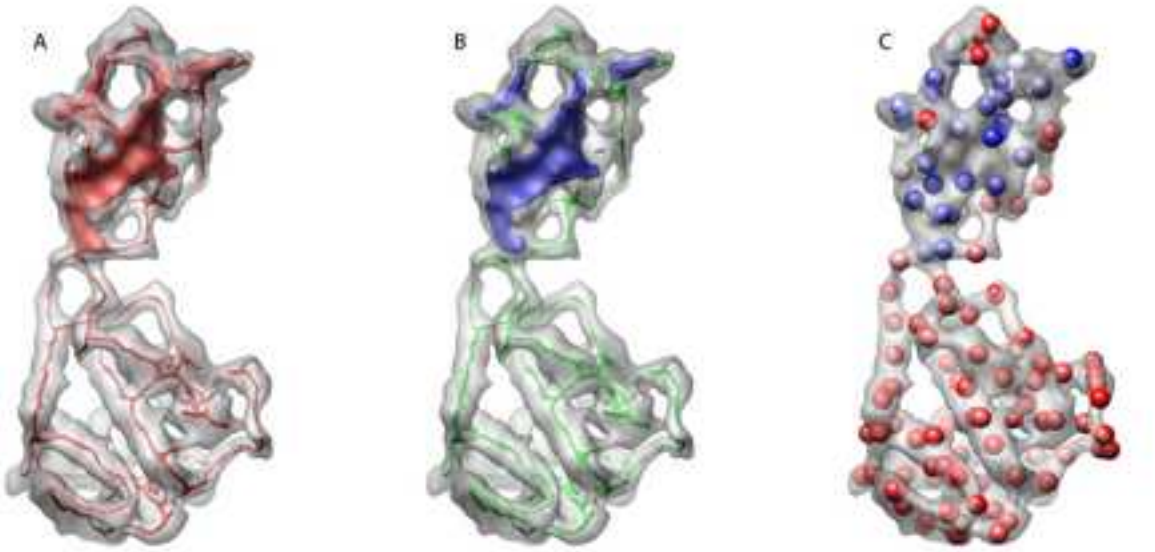

Supplemental Figure 2

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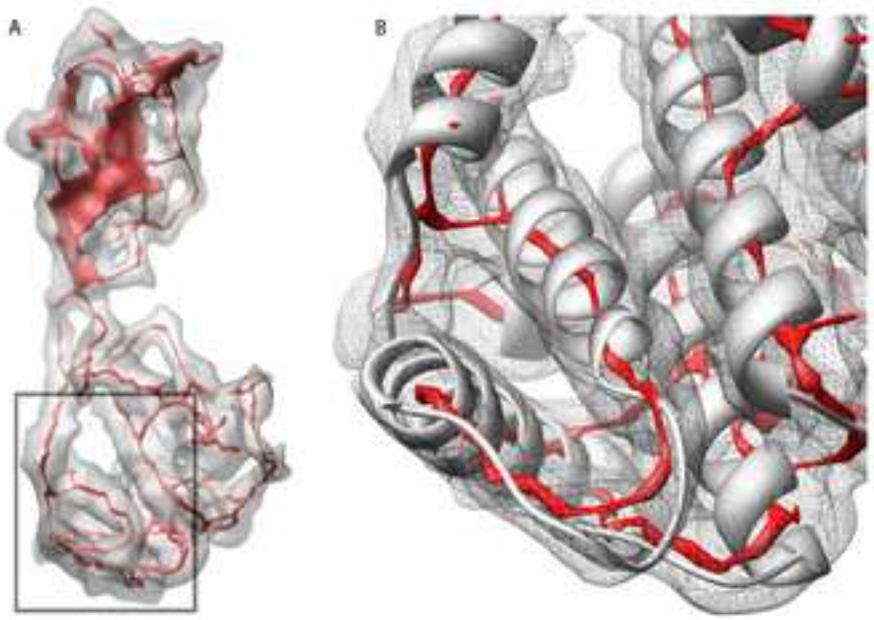

Supplemental Figure 3

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