

# Structure Factor Check

## 1BCC

Title: CYTOCHROME BC1 COMPLEX FROM CHICKEN  
 Date: 23-MAR-98  
 PDB code: 1BCC

### Crystal

Cell parameters:

a: 169.59 A    b: 182.52 A    c: 240.57 A  
 $\alpha$ : 90.00     $\beta$ : 90.00     $\gamma$ : 90.00

Space group: P 21 21 21

Number of NCS-operators: 2  
 NC-symmetry only for information

### Structure Factors

#### Input

Nominal resolution range: 27.9 – 3.16 A  
 Reflections in file: 123759  
 Unique reflections above 0: 115803  
                                   above 1 $\sigma$ : 108713  
                                   above 3 $\sigma$ : 93617  
 Reflections > 0: 7956

#### SFCHECK

Nominal resolution range: 27.9 – 3.16 A  
\05max. from input data, min. from author\05  
 Used reflections: 115803  
 Completeness: 90.7 %  
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$  : 0.061  
 Anisotropic distribution of Structure Factors  
     ratio of eigen values: 1.0000 0.4535 0.4561  
 B<sub>overall</sub> (by Patterson): 57. A<sup>2</sup>  
 Optical resolution: 2.33 A  
 Expected opt. resol. for complete data set: 2.33 A  
 Estimated minimal error: 0.149 A

### Model

15719 atoms  
 Number of chains: 18  
 Volume not occupied by model: 63.0 %  
 $\langle B \rangle$  (for atomic model): 80.2 A<sup>2</sup>  
 $\sigma(B)$ : 16.24 A<sup>2</sup>  
 Matthews coefficient: 8.46  
 Corresponding solvent % : 85.35

### Model vs. Structure Factors

R-factor for all reflections: 0.344  
 Correlation factor: 0.785  
 R-factor: 0.338  
     for  $F > 2.0\sigma$   
         nom. resolution range: 12.00 – 3.16A  
         reflections used: 107152  
 $\langle u \rangle$  (error in coords by Luzzati plot): 0.715 A  
 Estimated maximal error: 0.553 A  
 DPI: 0.373 A

### Refinement

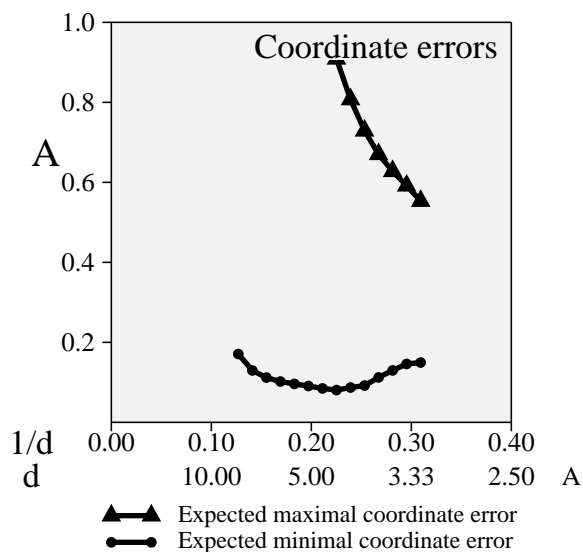
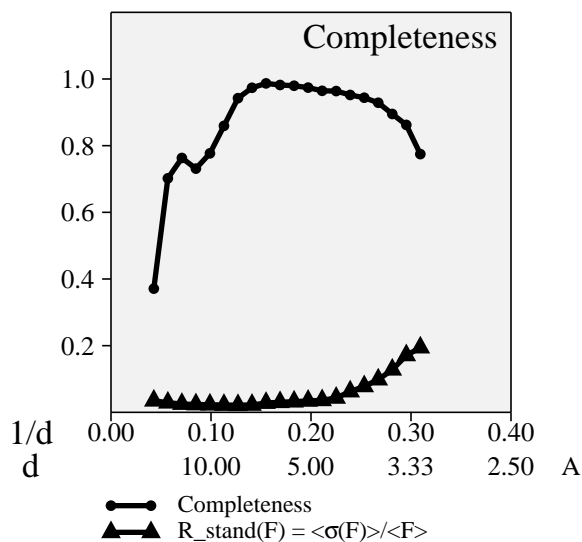
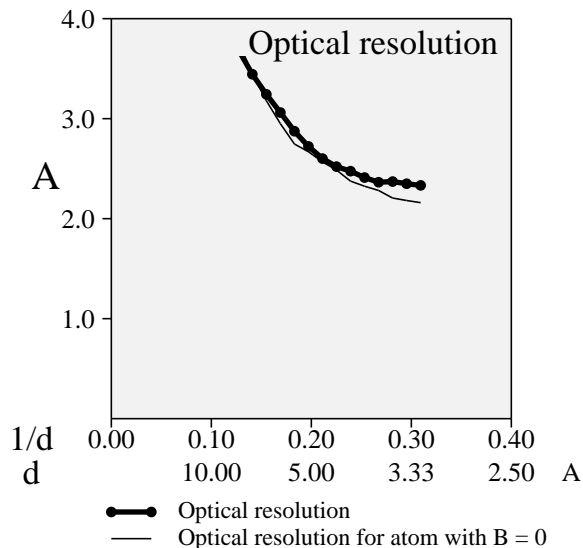
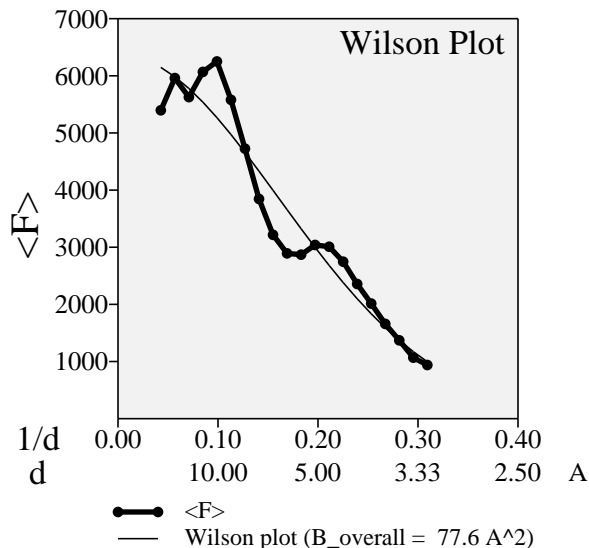
Program: CNS 0.1  
 Nominal resolution range: 12.0 – 3.16 A  
 Reported R-factor: 0.270  
 Number of reflections used: 107167  
 Reported Rfree: 0.31  
 Sigma cut-off (F): 2.00

#### Scaling

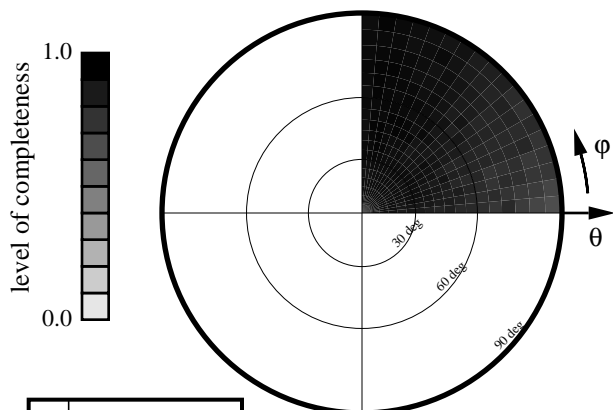
Scale: 1.554  
 Bdiff: -9.23  
 Anisothermal Scaling (Beta):  
 17.8401 -1.1807 -1.3339 0.0000 0.0000 0.0000  
 Solvent correction – Ks,Bs: 0.594 250.288

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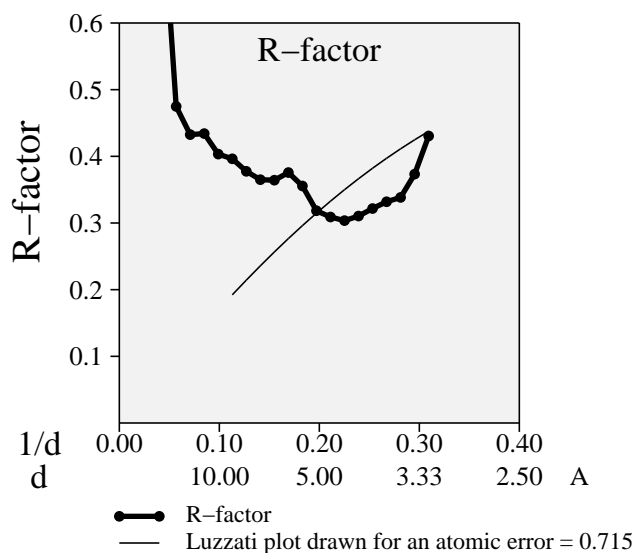


Stereographic projection of the averaged radial completeness



	$\theta$	$\phi$
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

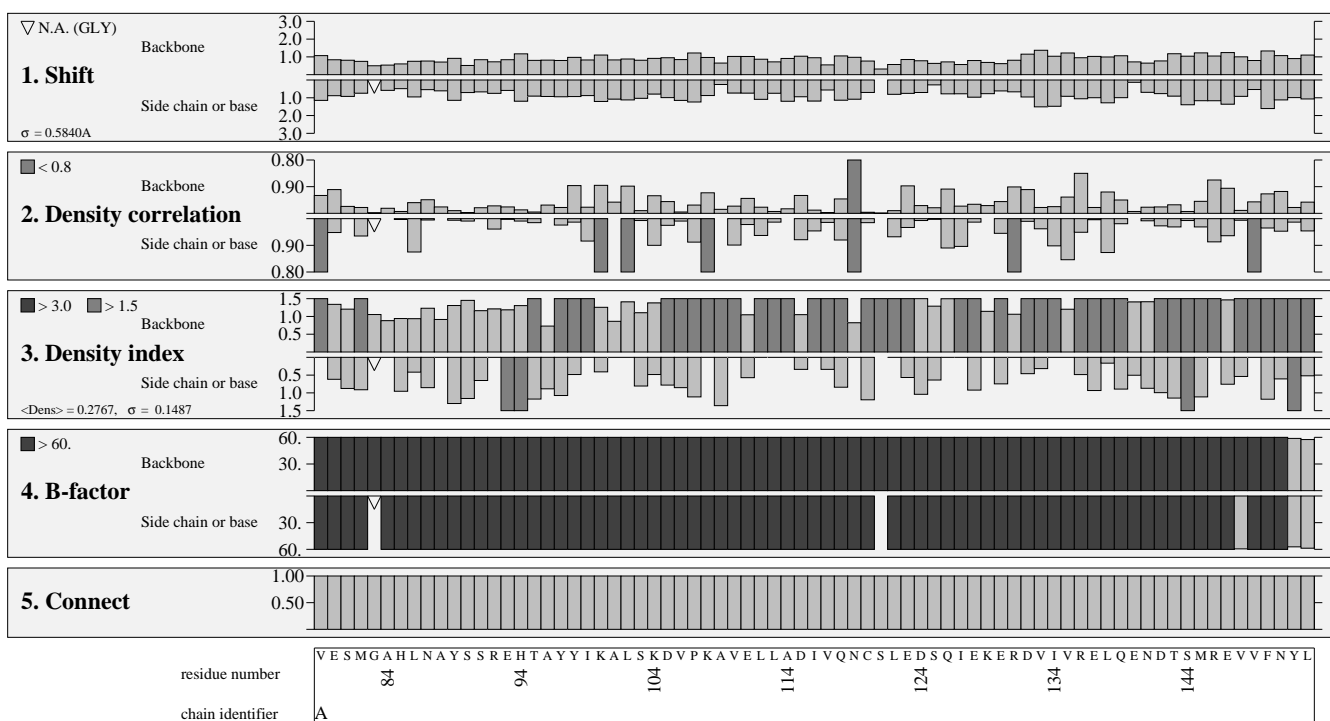
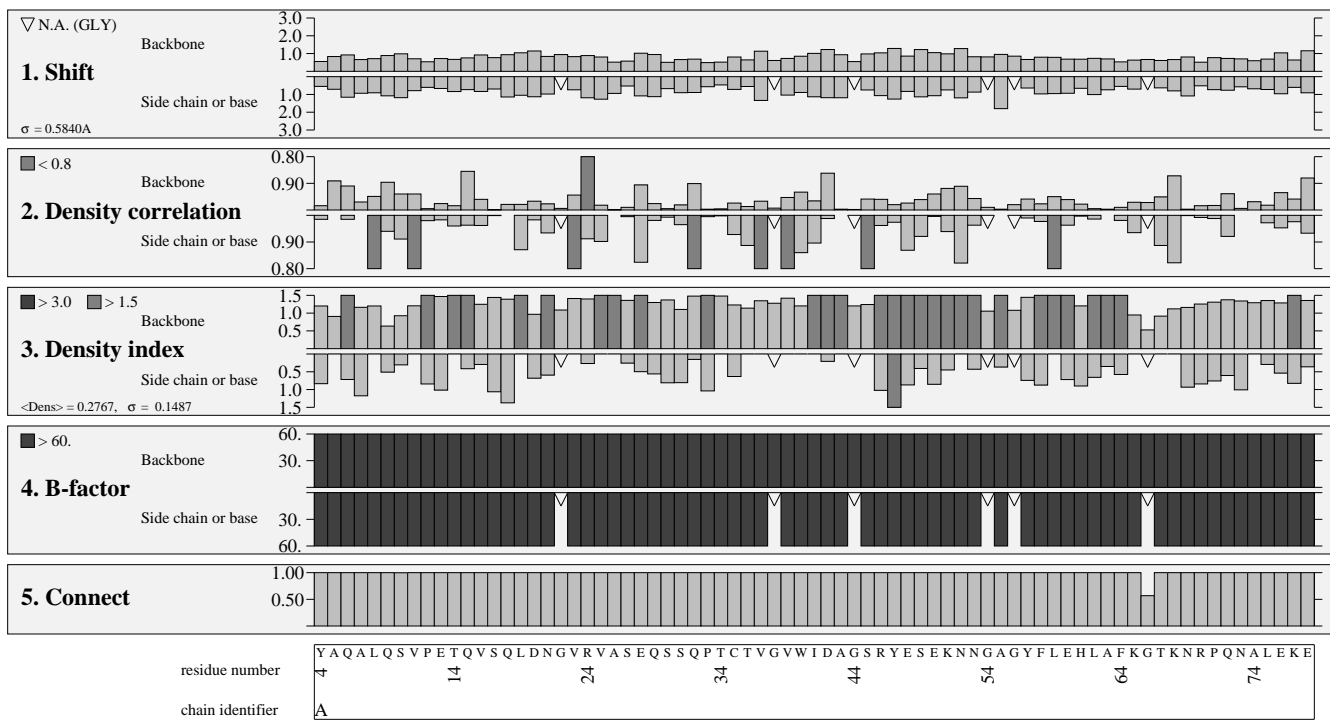
polar coordinates of the crystallographical axes



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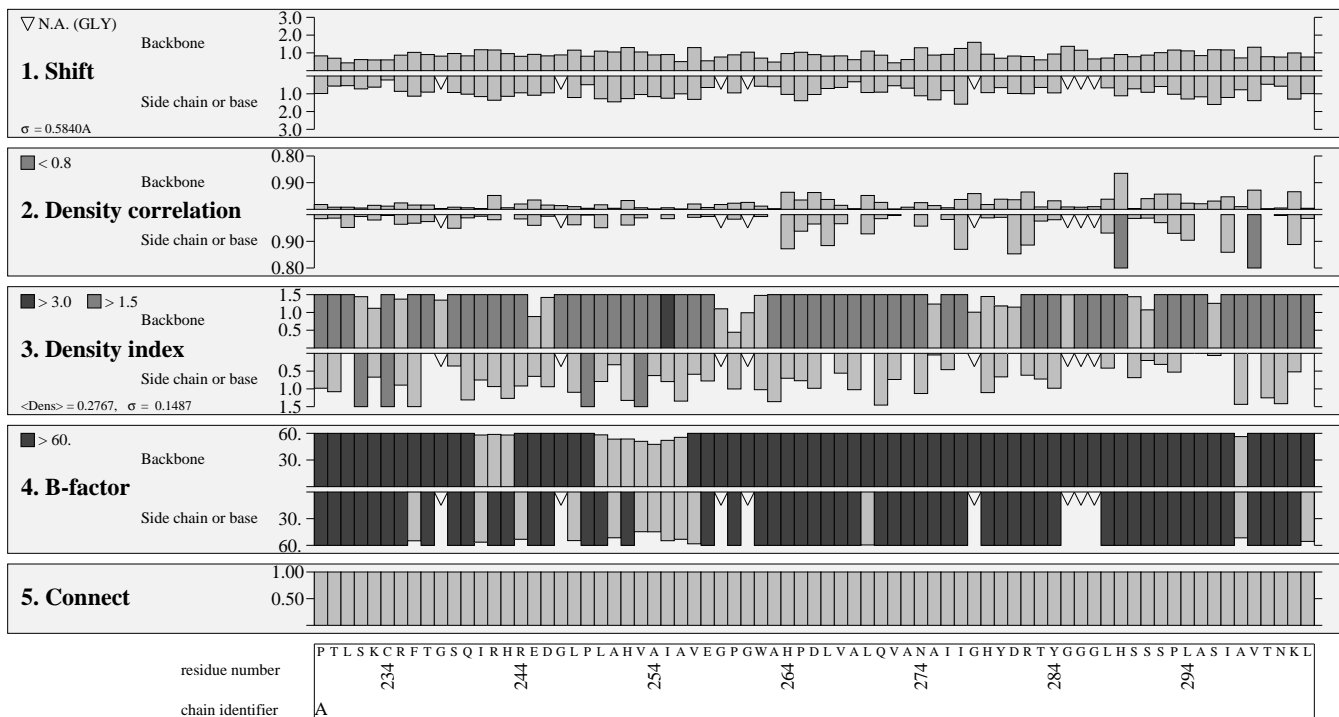
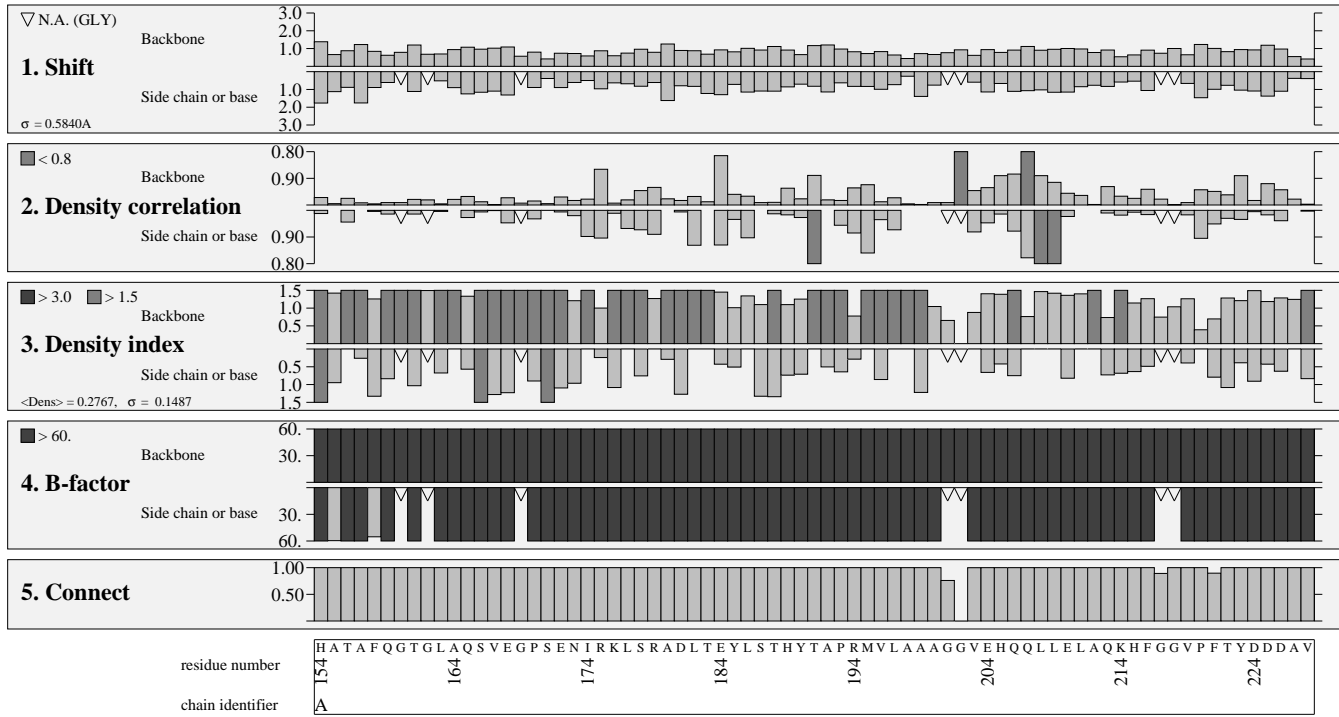
### Local estimation



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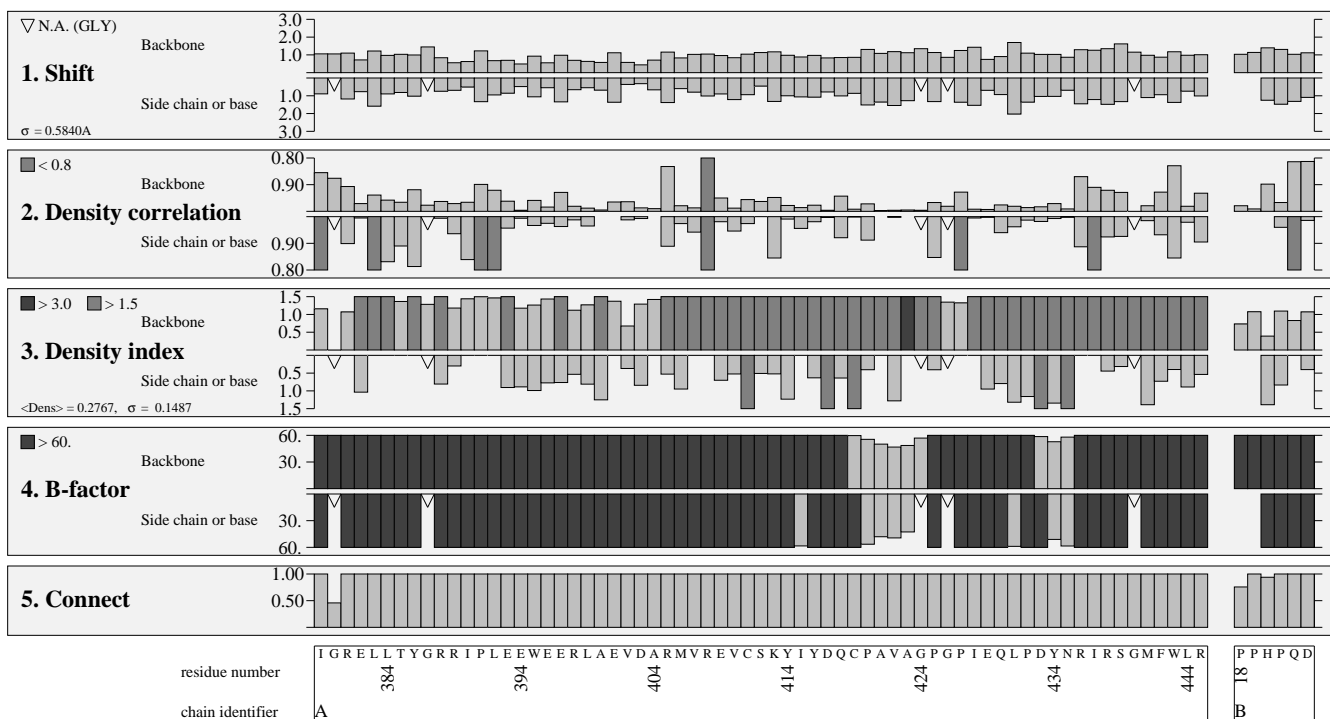
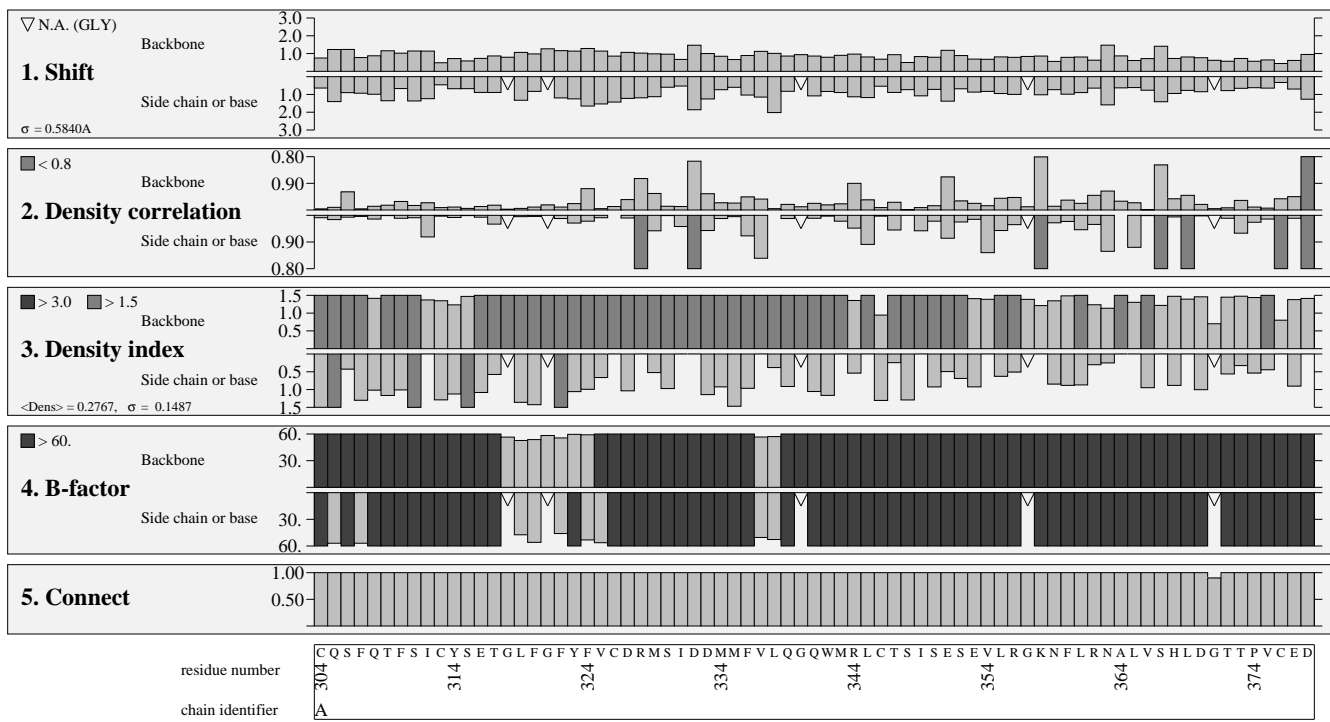
### Local estimation (2)



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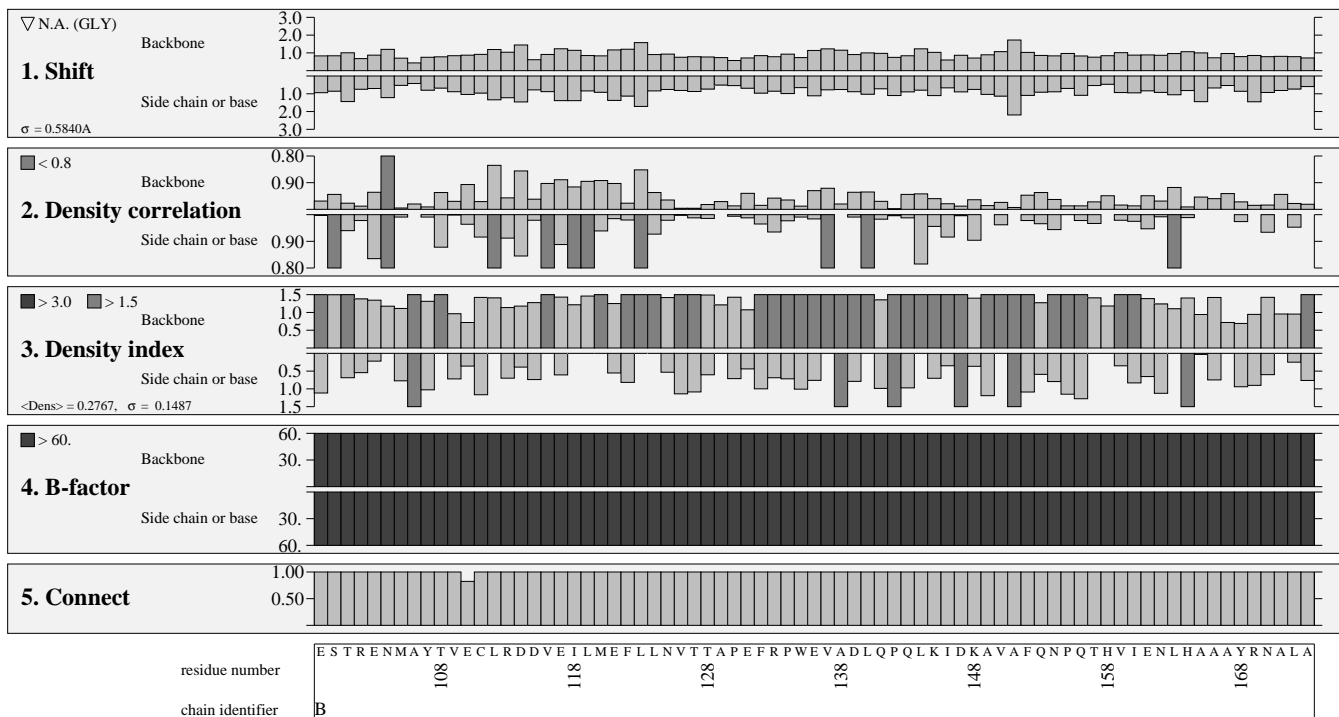
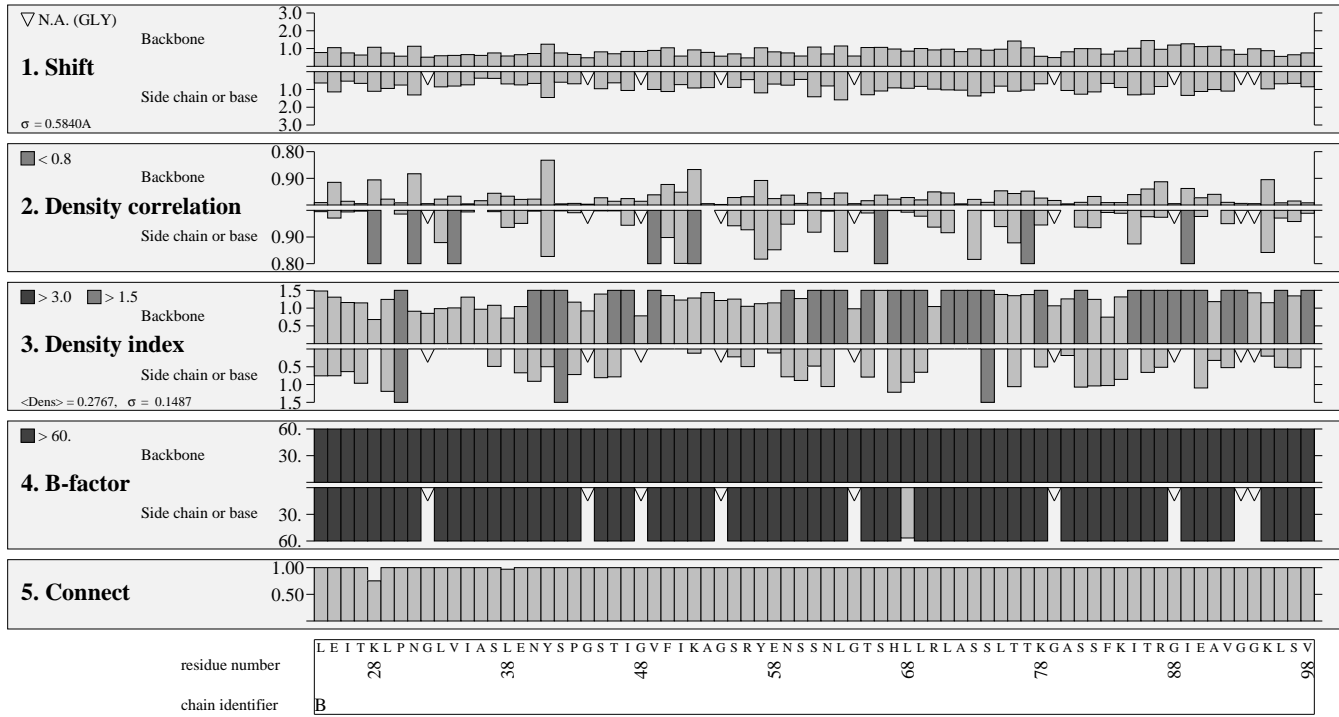
### Local estimation (3)



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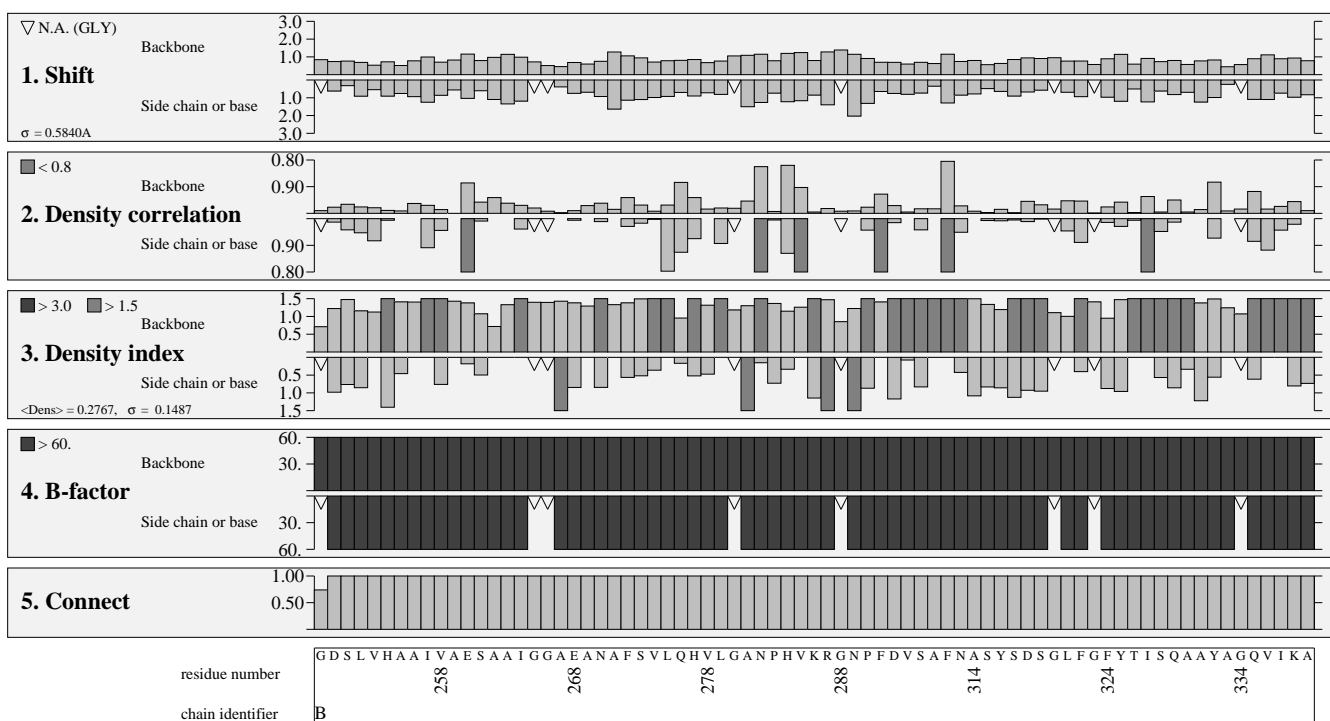
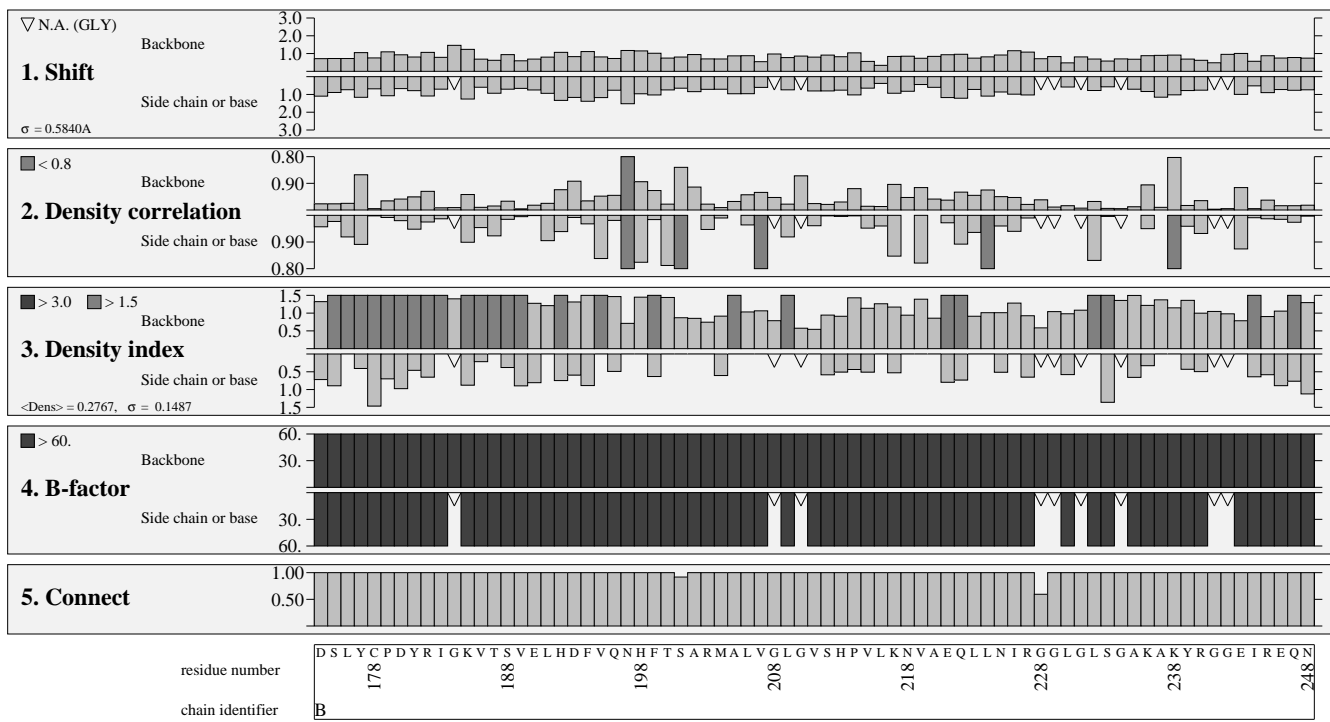
### Local estimation (4)



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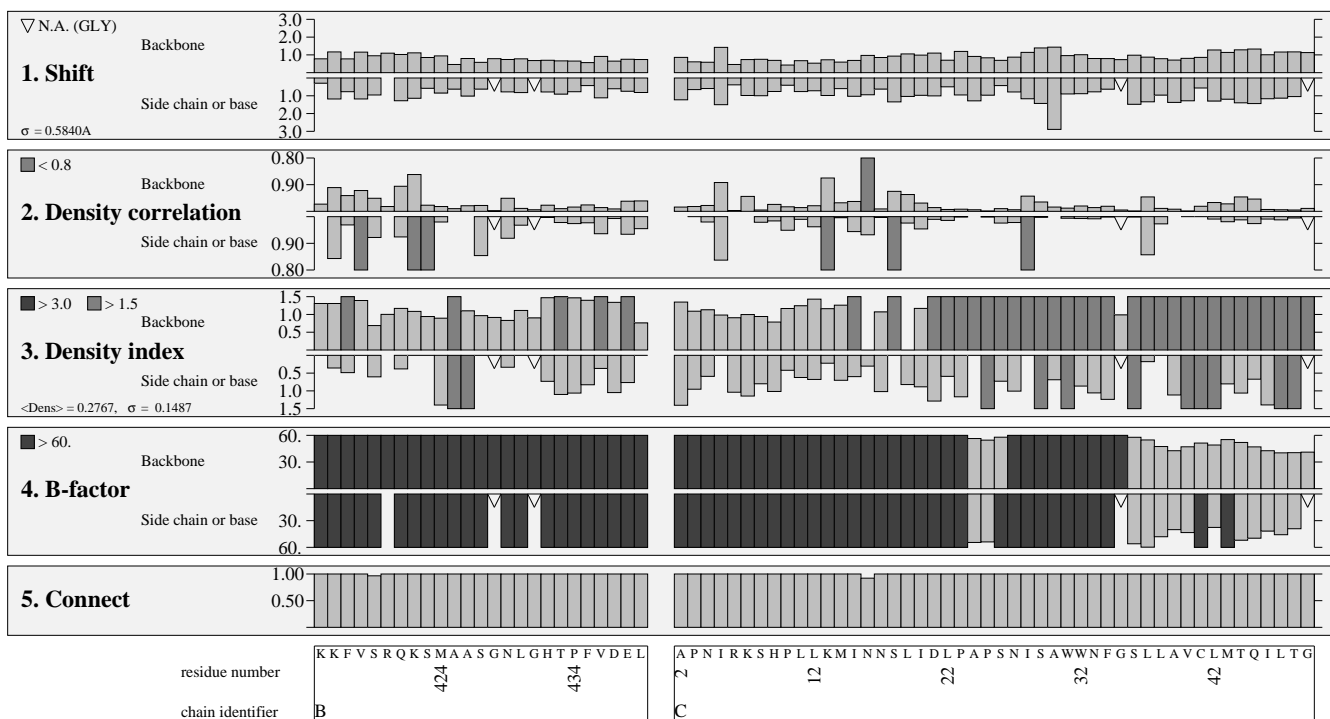
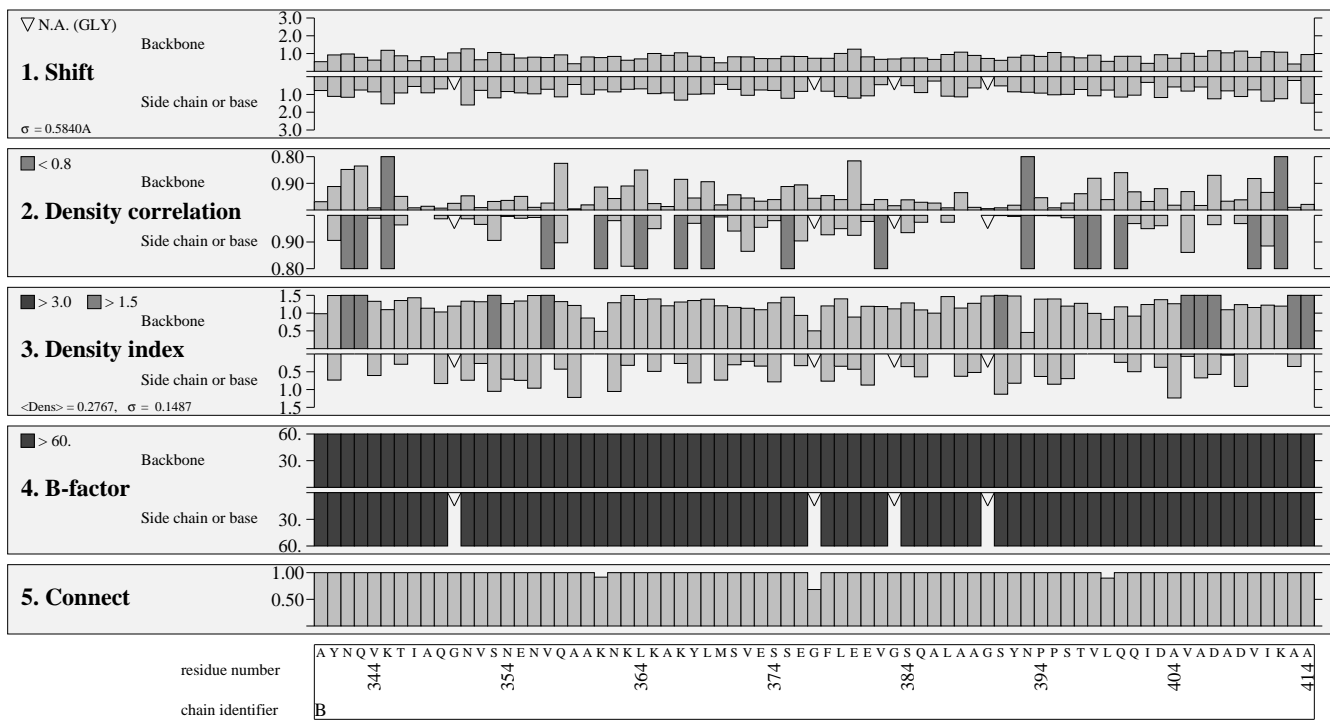
### Local estimation (5)



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### Local estimation (6)

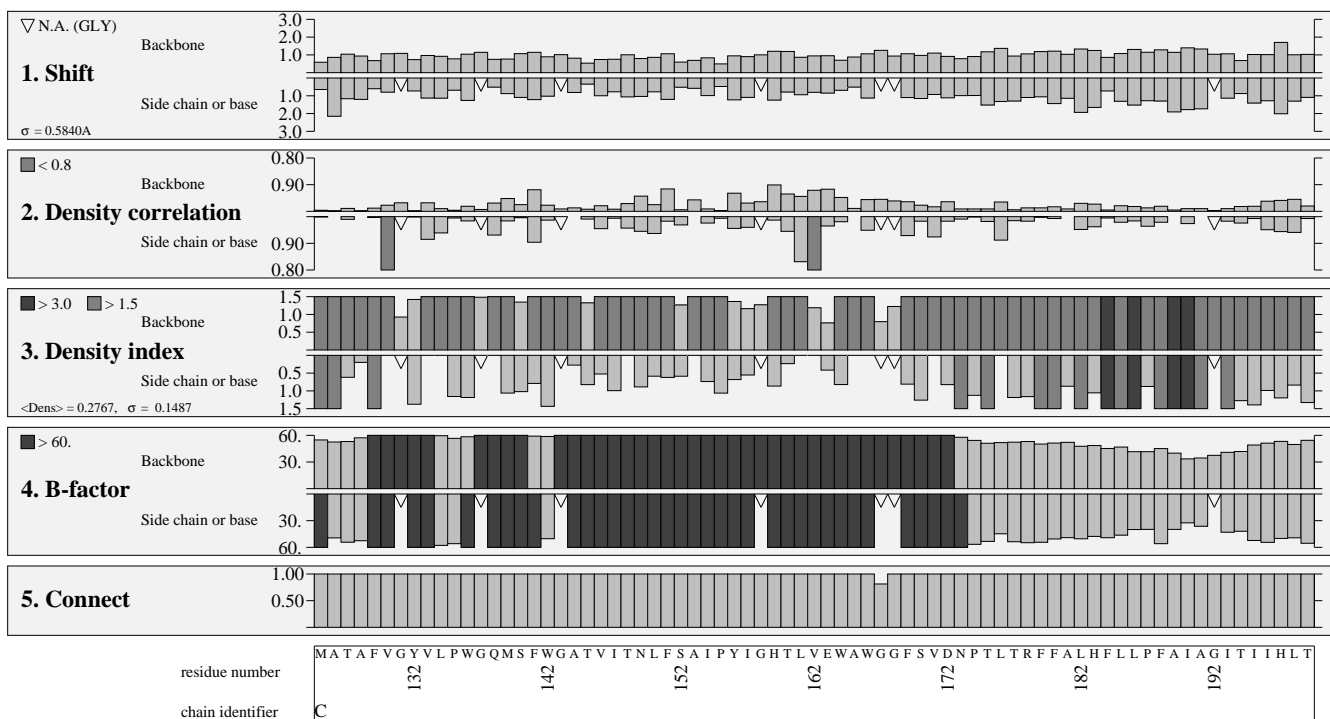
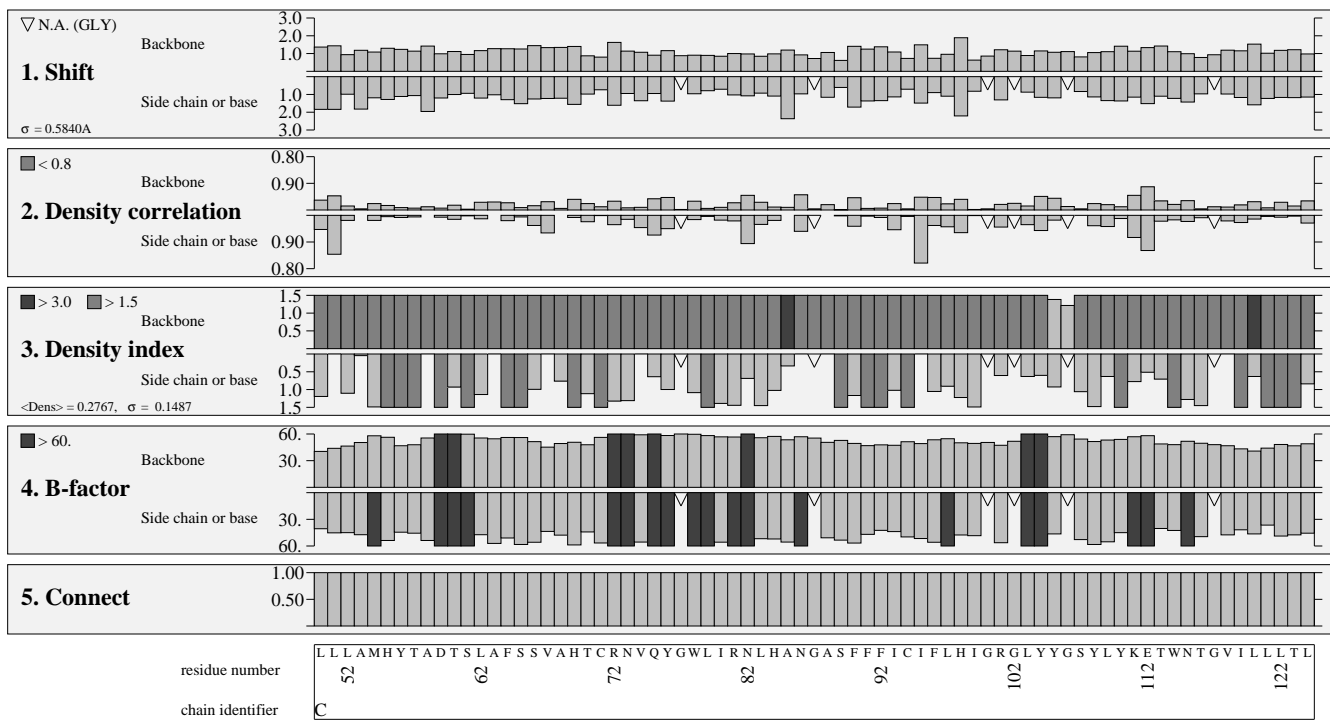




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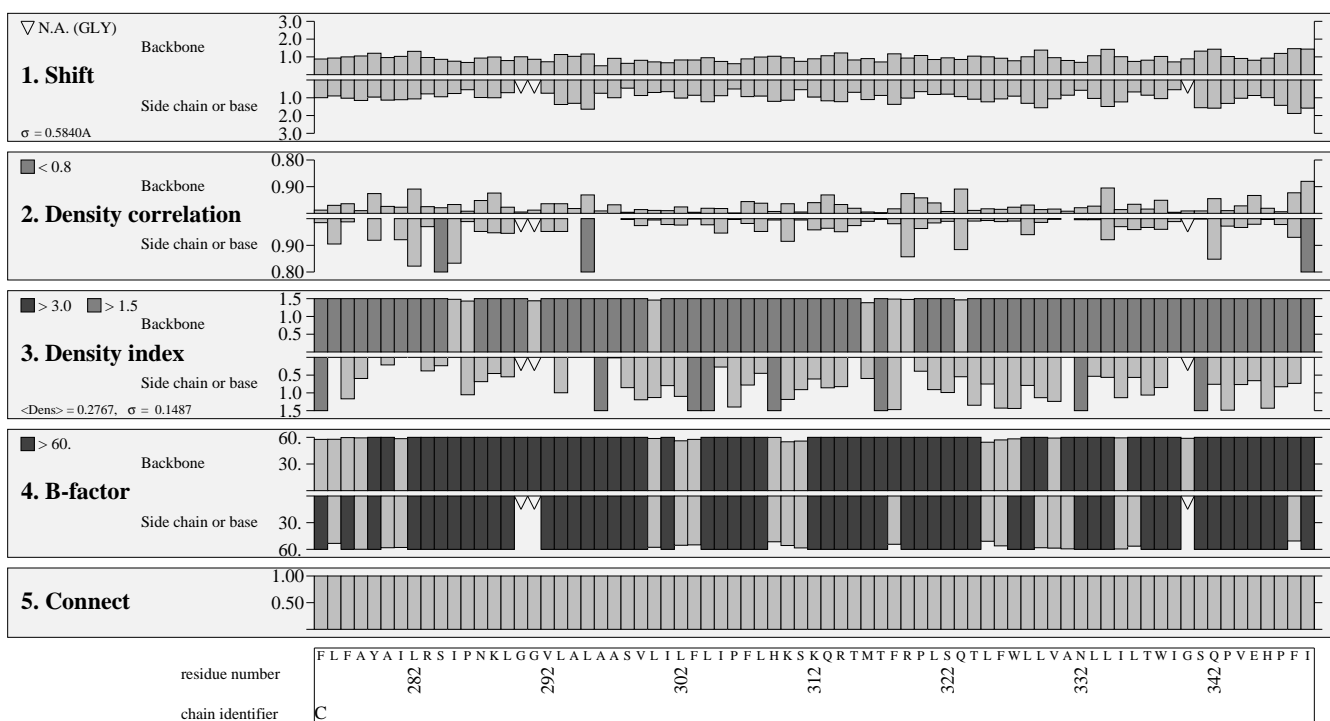
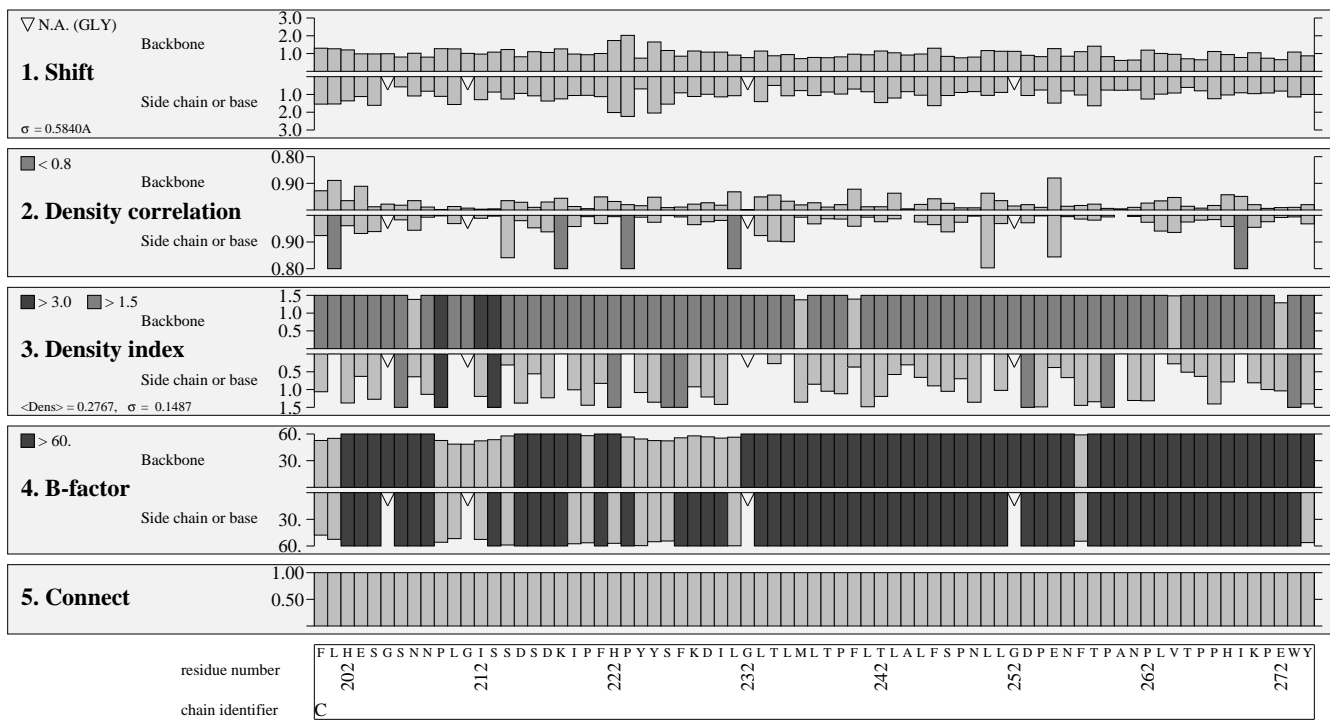
### Local estimation (7)



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### Local estimation (8)

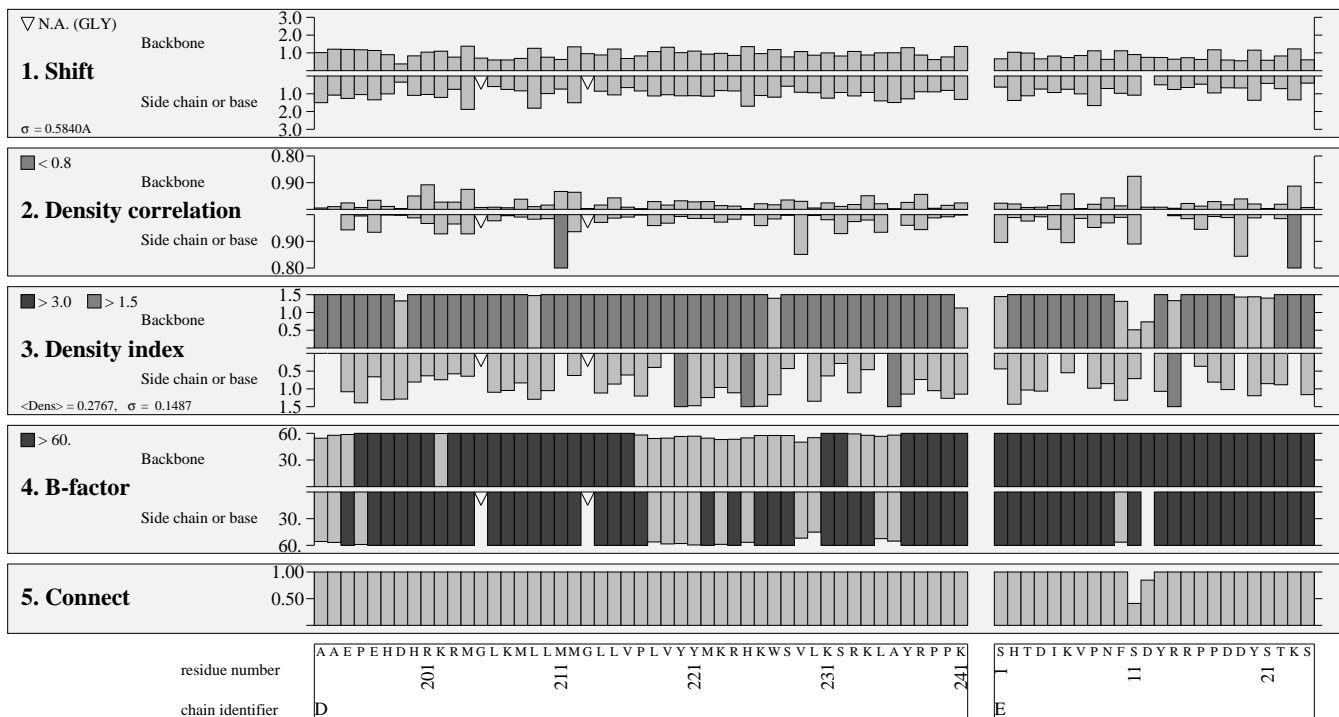
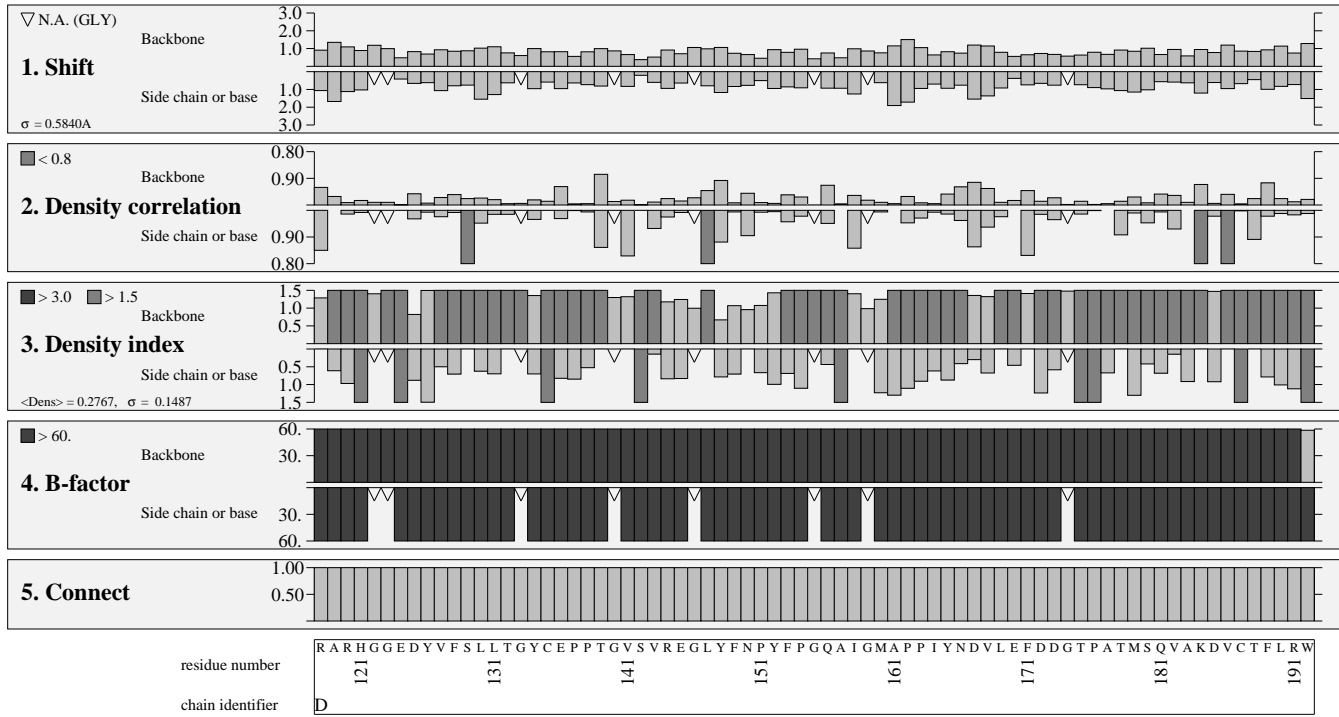




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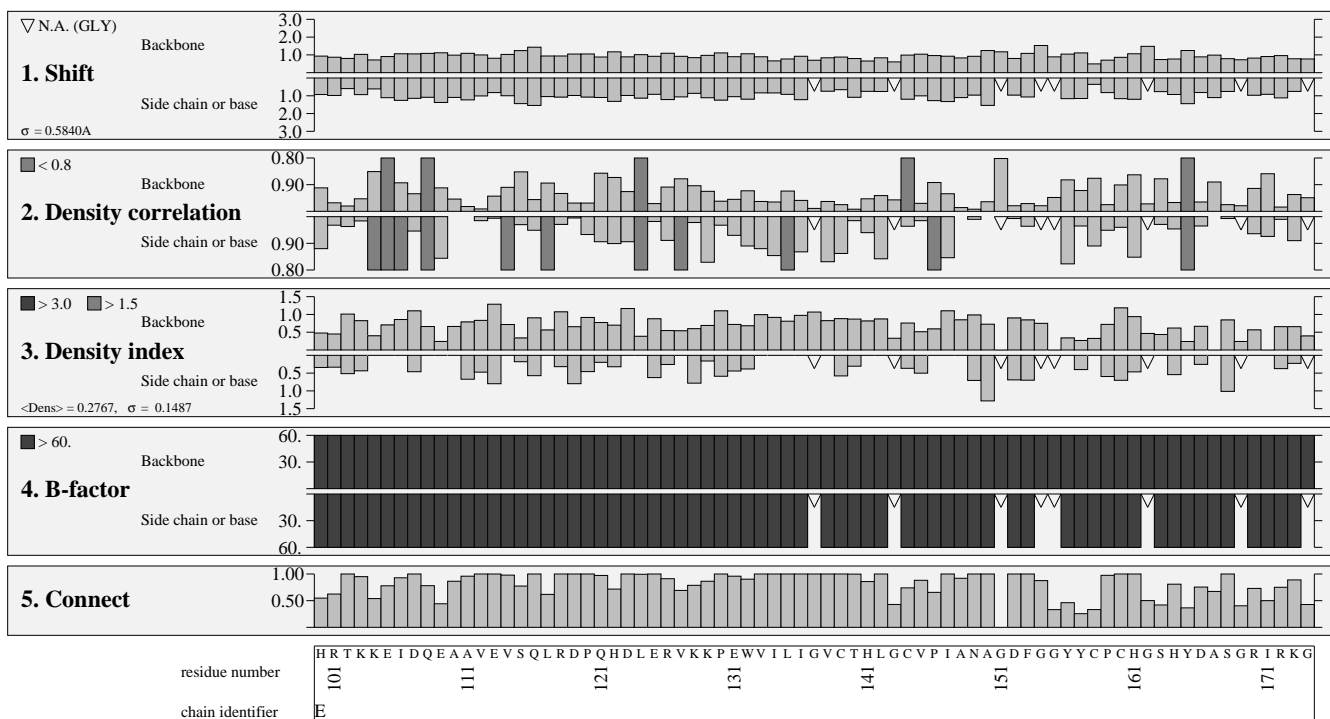
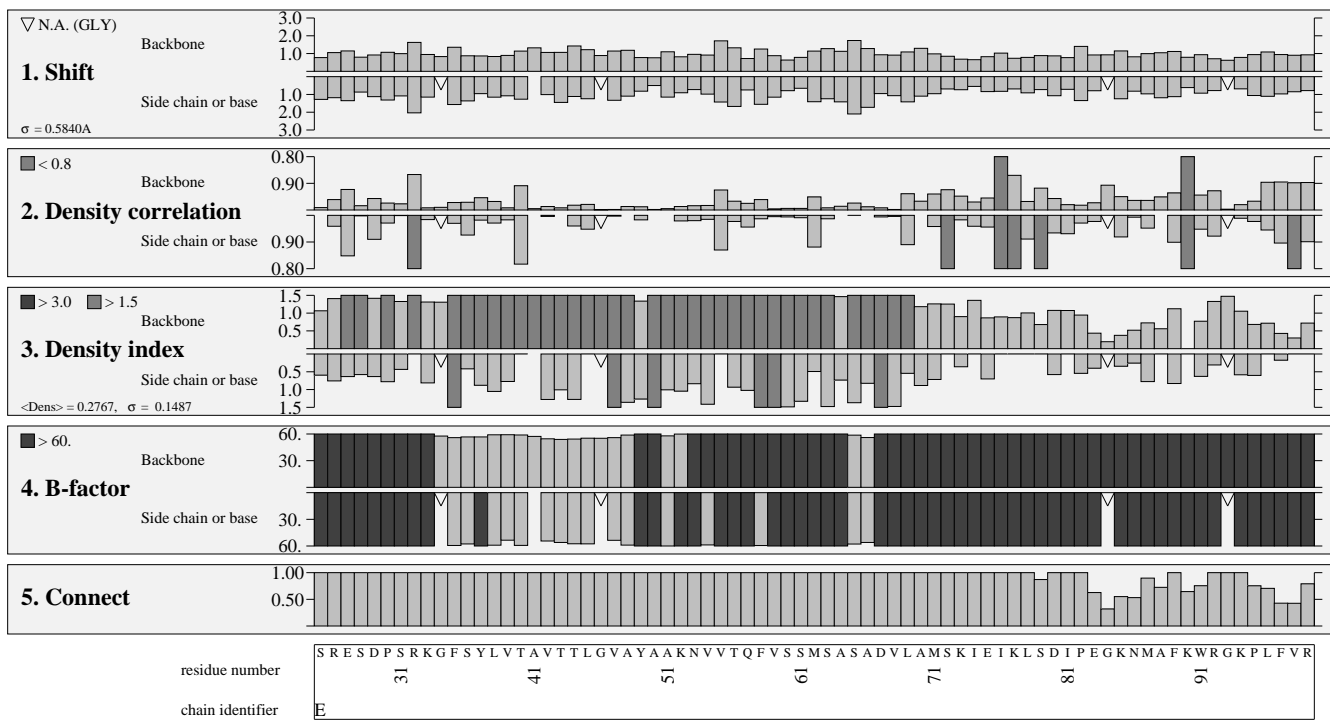
### Local estimation (10)



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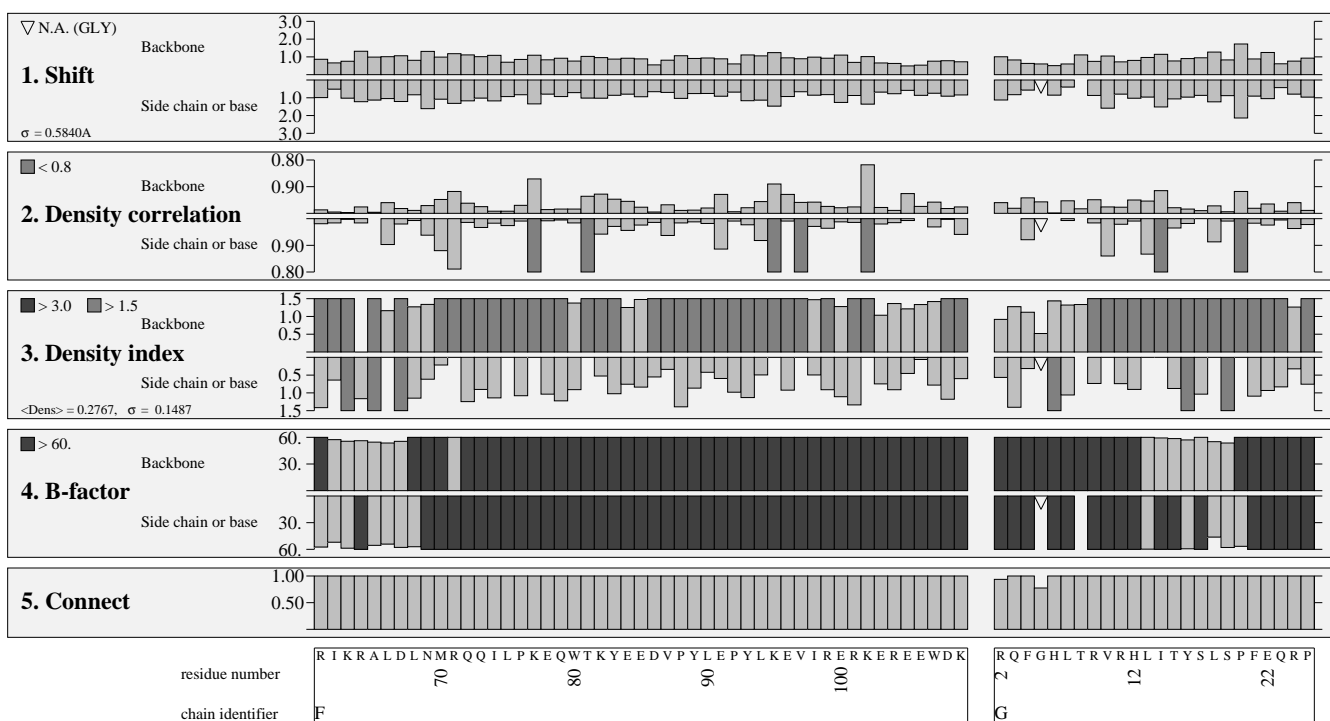
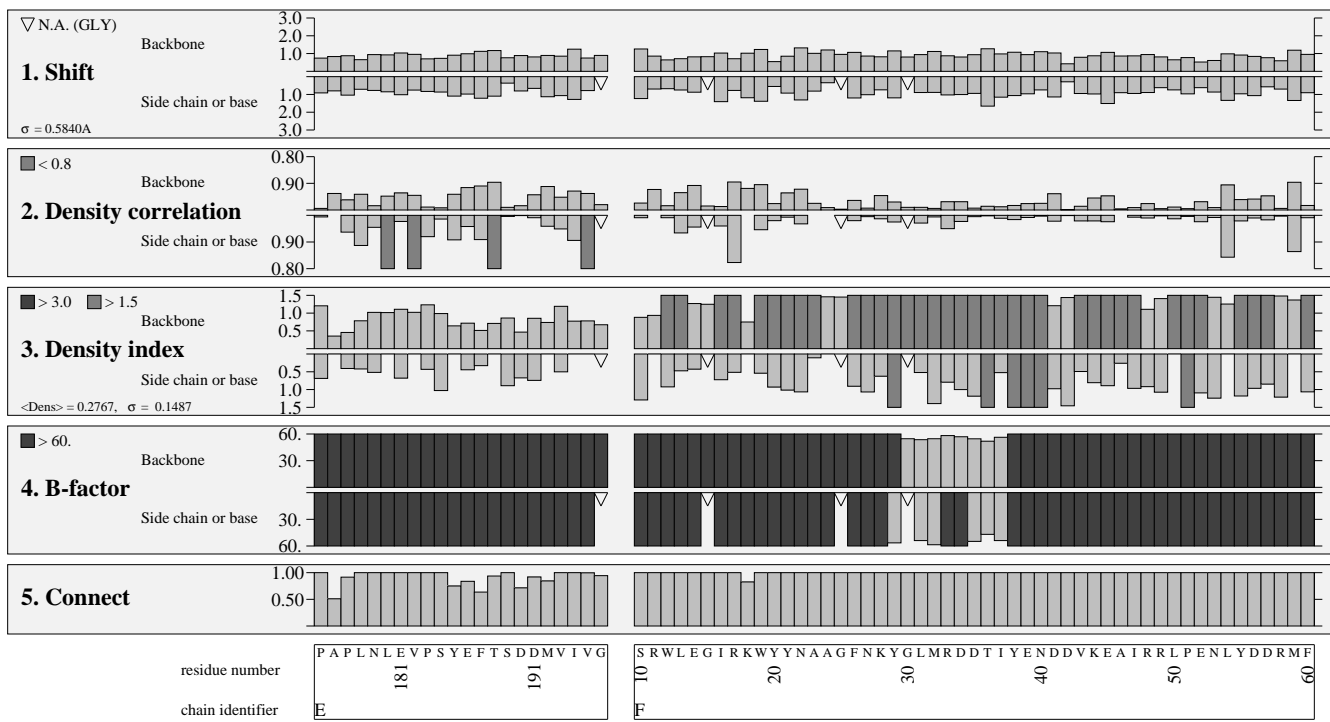
### Local estimation (11)



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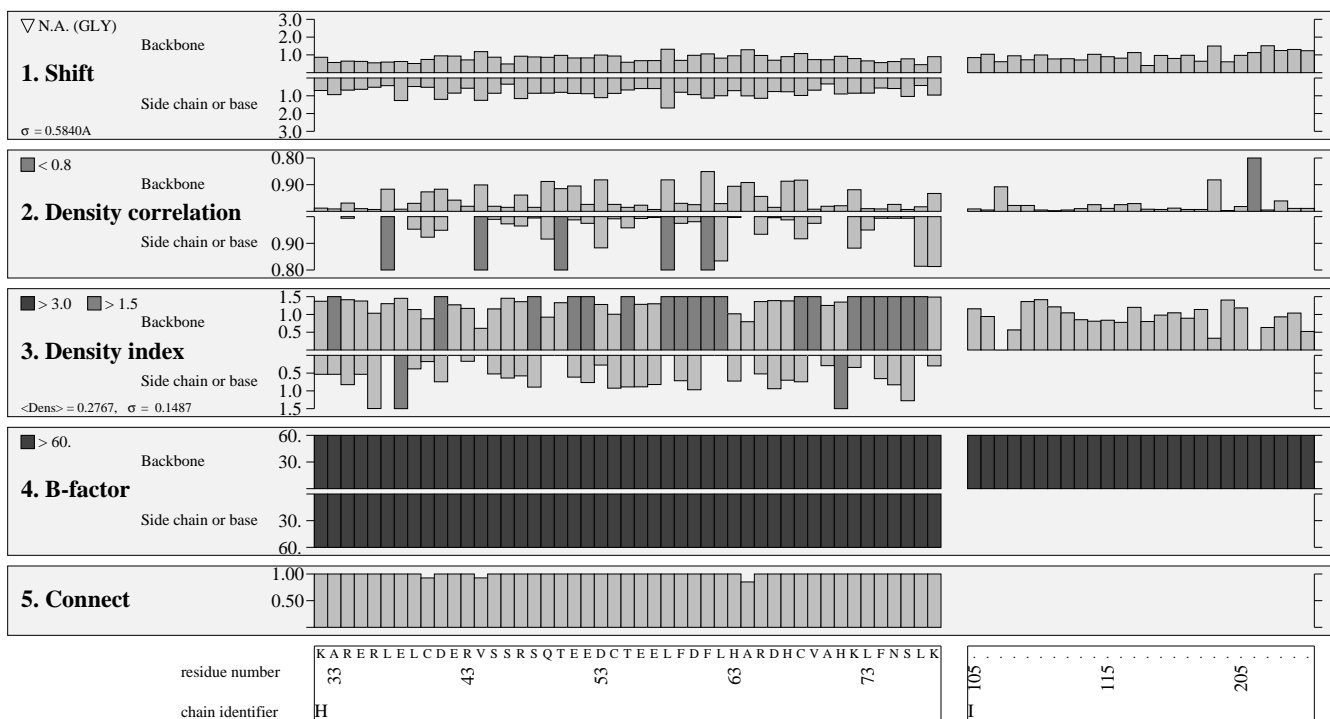
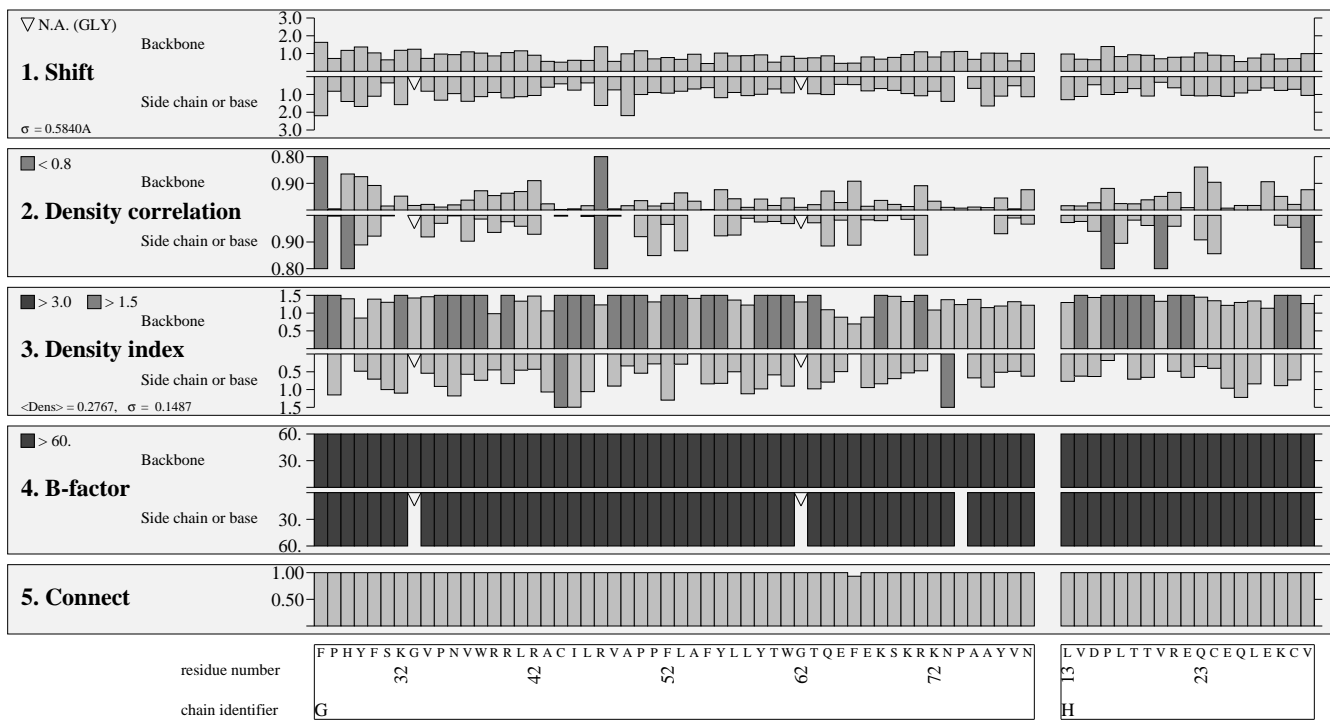
### Local estimation (12)



# Structure Factor Check

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### Local estimation (13)



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### Local estimation (14)

