

# Structure Factor Check

## 3L74

Title: CYTOCHROME BC1 COMPLEX FROM CHICKEN WITH FAMOXADONE BOUND  
 Date: 28-DEC-09  
 PDB code: 3L74

### Crystal

Cell parameters:

a: 171.89 A    b: 181.69 A    c: 240.75 A  
 $\alpha$ : 90.00     $\beta$ : 90.00     $\gamma$ : 90.00

Space group: P 21 21 21

### Structure Factors

#### Input

Nominal resolution range: 58.7 – 2.70 A  
 Reflections in file: 199233  
 Unique reflections above 0: 199233  
                                   above 1 $\sigma$ : 194835  
                                   above 3 $\sigma$ : 123637

#### SFCHECK

Nominal resolution range: 58.7 – 2.76 A  
\05max. from input data, min. from author\05  
 Used reflections: 189274  
 Reflections out of resolution: 9959  
 Completeness: 98.0 %  
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$  : 0.076  
 Anisotropic distribution of Structure Factors  
     ratio of eigen values: 1.0000 0.5632 0.7439  
 $B_{\text{overall}}$  (by Patterson): 45. A<sup>2</sup>  
 Optical resolution: 2.06 A  
 Expected opt. resol. for complete data set: 2.06 A  
 Estimated minimal error: 0.076 A

### Model

32703 atoms (28 water molecules)

Number of chains: 51  
 Volume not occupied by model: 62.5 %  
 $\langle B \rangle$  (for atomic model): 61.9 A<sup>2</sup>  
 $\sigma(B)$ : 21.35 A<sup>2</sup>  
 Matthews coefficient: 4.11  
 Corresponding solvent % : 69.81

### Model vs. Structure Factors

R-factor for all reflections: 0.296  
 Correlation factor: 0.857  
 R-factor: 0.299  
     for  $F > 2.0\sigma$   
         nom. resolution range: 58.66 – 2.76A  
         reflections used: 185359

Rfree: 0.319  
 Nfree: 3624  
 R-factor without free-refl.: 0.299  
 Non free-reflections: 181735  
 $\langle u \rangle$  (error in coords by Luzzati plot): 0.451 A  
 Estimated maximal error: 0.246 A  
 DPI: 0.315 A

#### Scaling

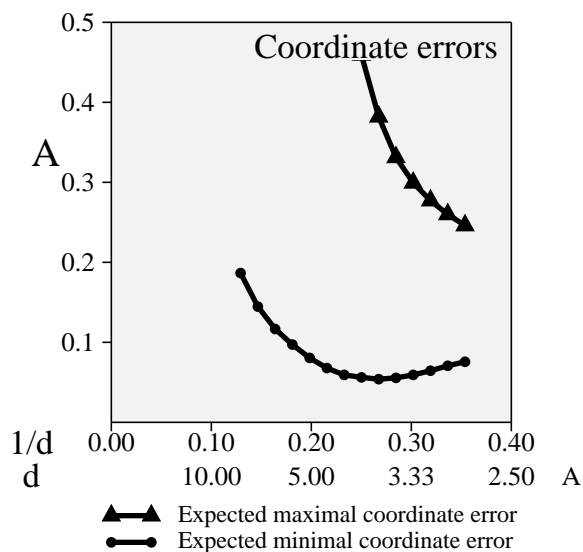
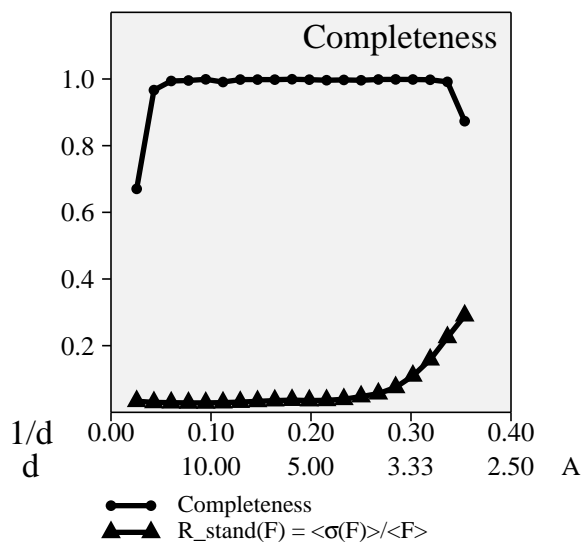
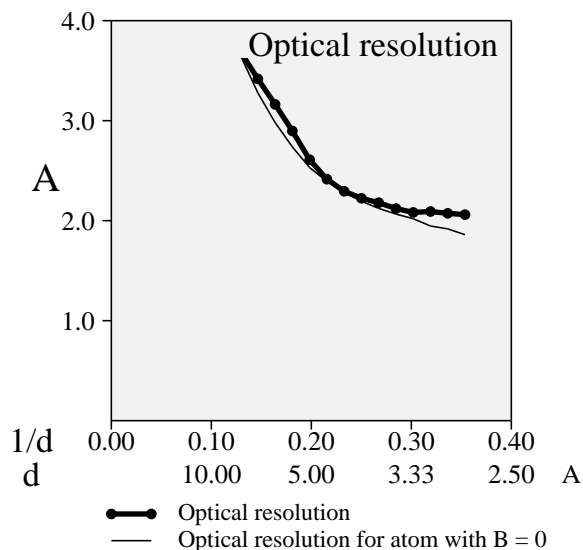
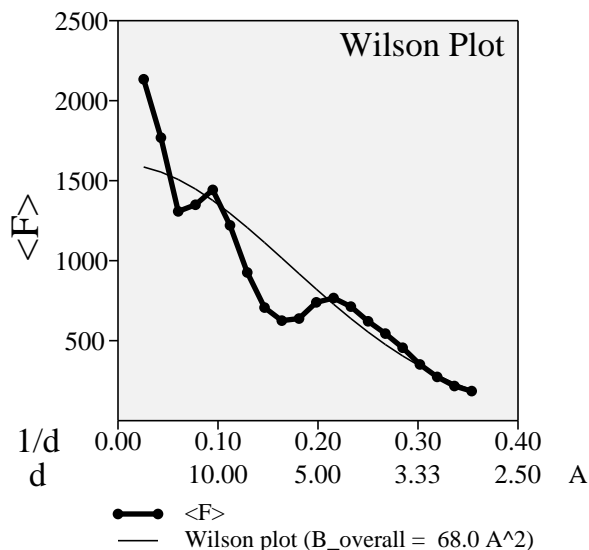
Scale: 0.528  
 Bdiff: -6.52  
 Anisothermal Scaling (Beta):  
     6.7160 -2.6140 1.8346 0.0000 0.0000 0.0000  
 Solvent correction – Ks,Bs: 0.710 250.093

### Refinement

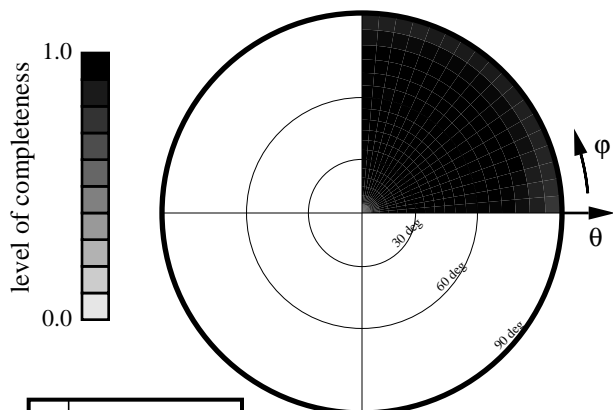
Program: CNS 1.1  
 Nominal resolution range: 58.7 – 2.76 A  
 Reported nominal resolution: 2.00 A  
 Reported R-factor: 0.259  
 Number of reflections used: 189275  
 Reported Rfree: 0.29  
 Sigma cut-off: N.A.

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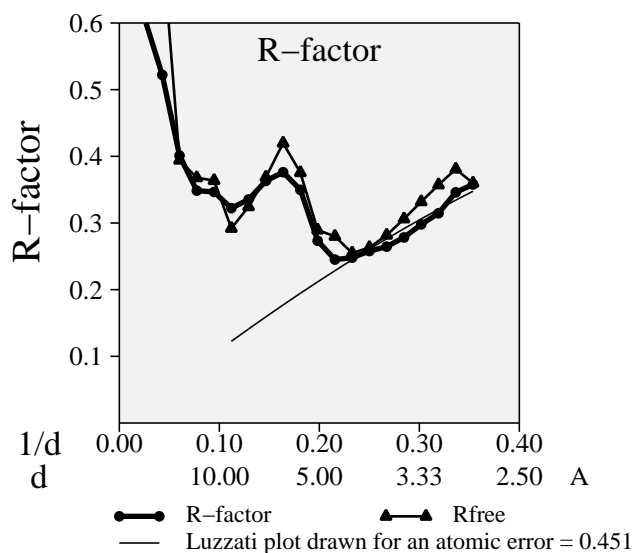


Stereographic projection of the averaged radial completeness



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

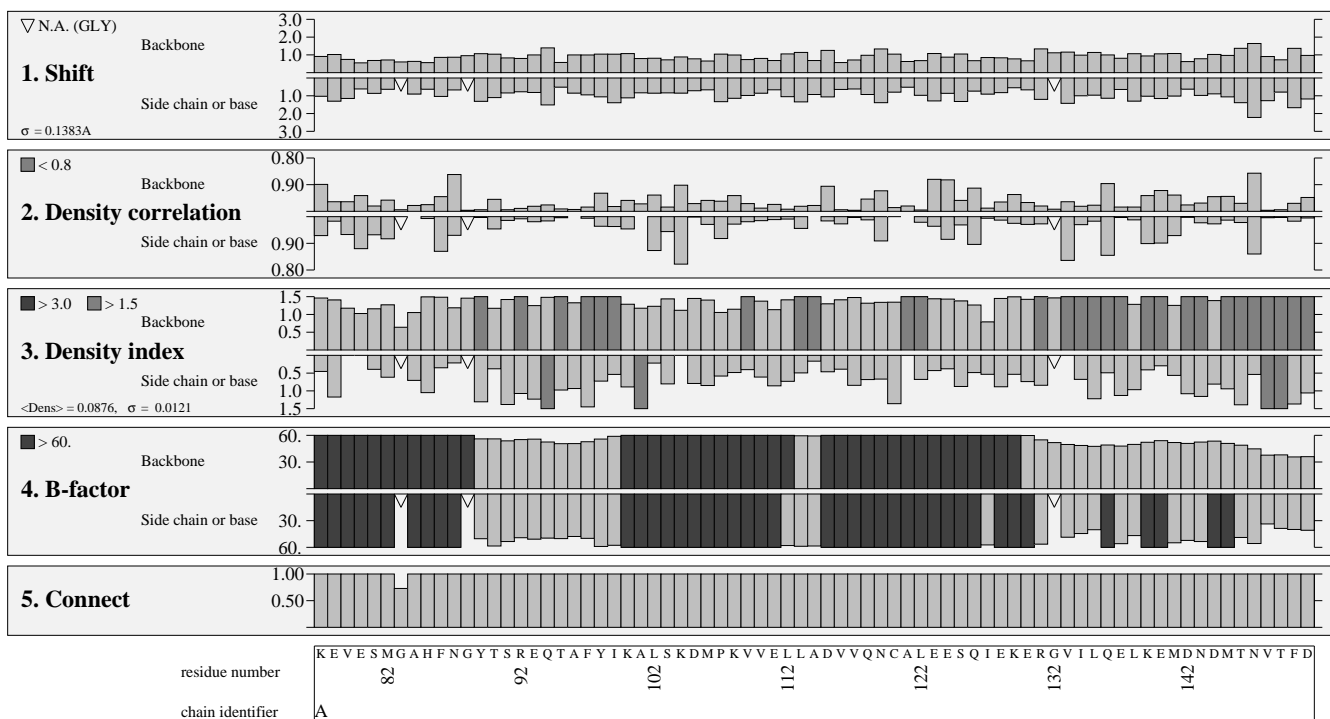
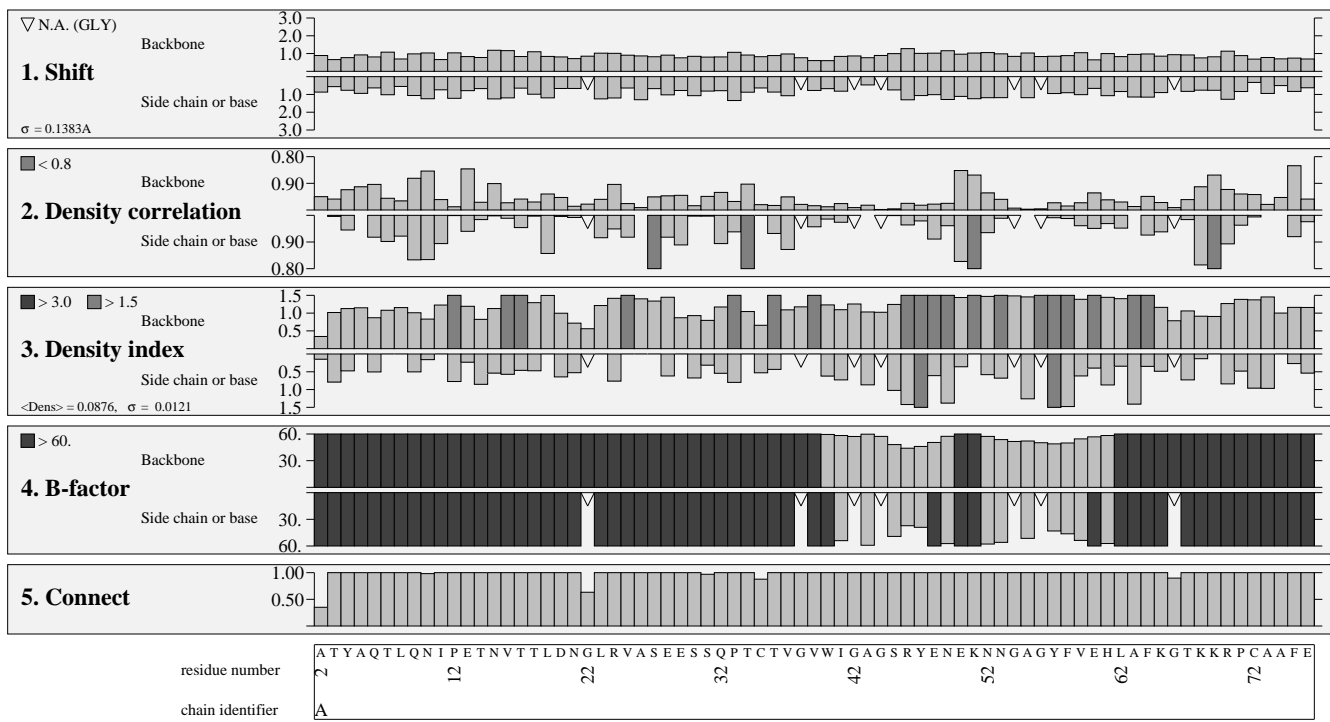
polar coordinates of the crystallographical axes



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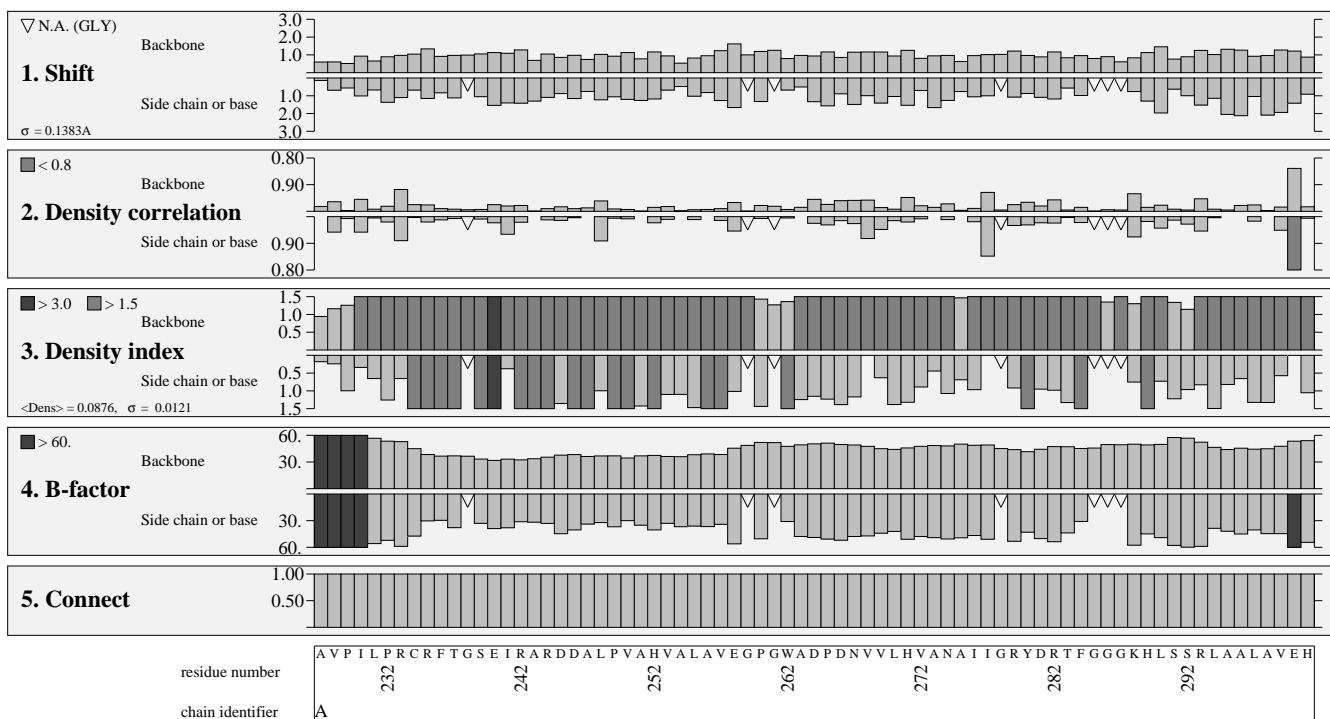
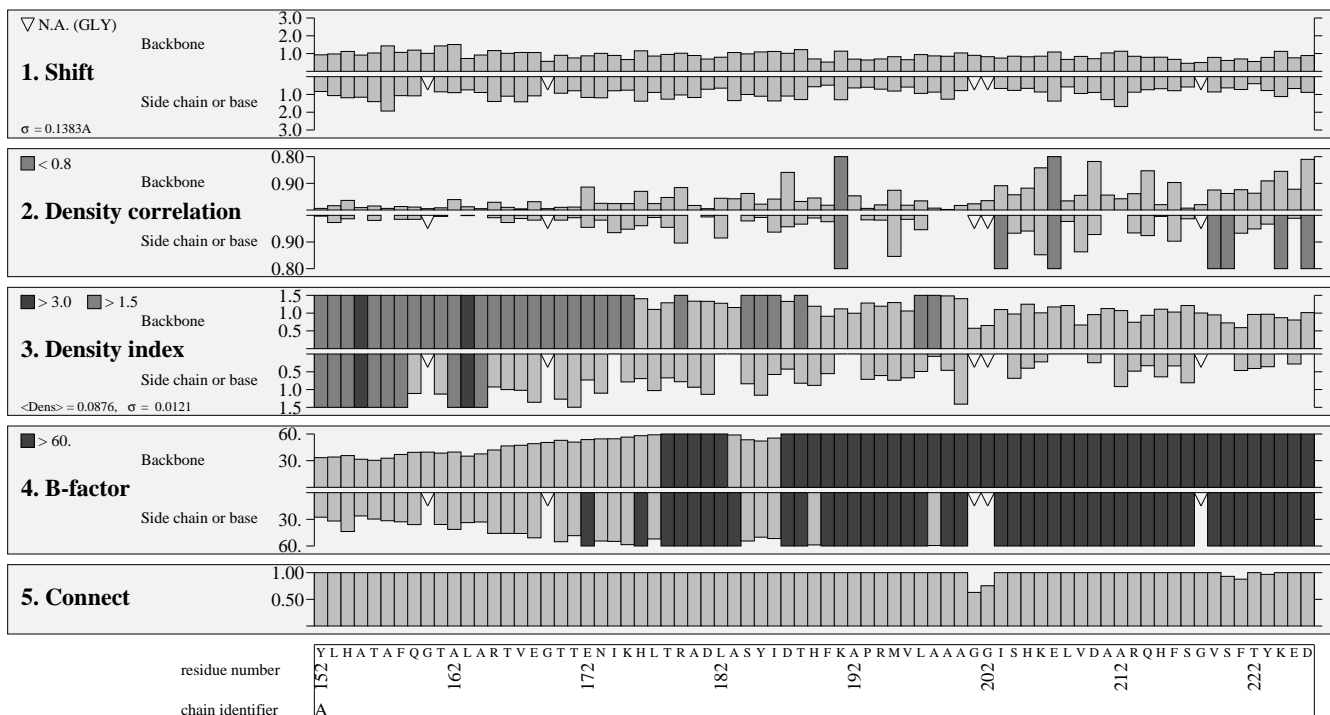
### Local estimation



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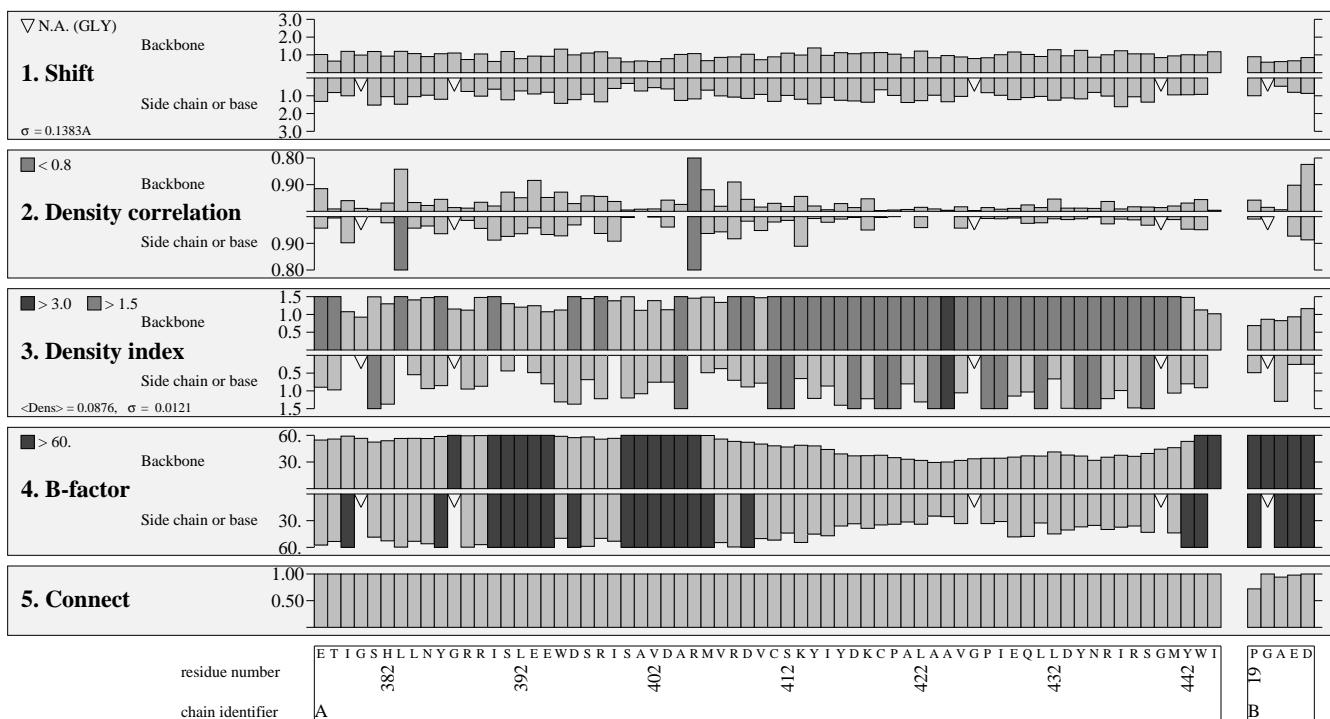
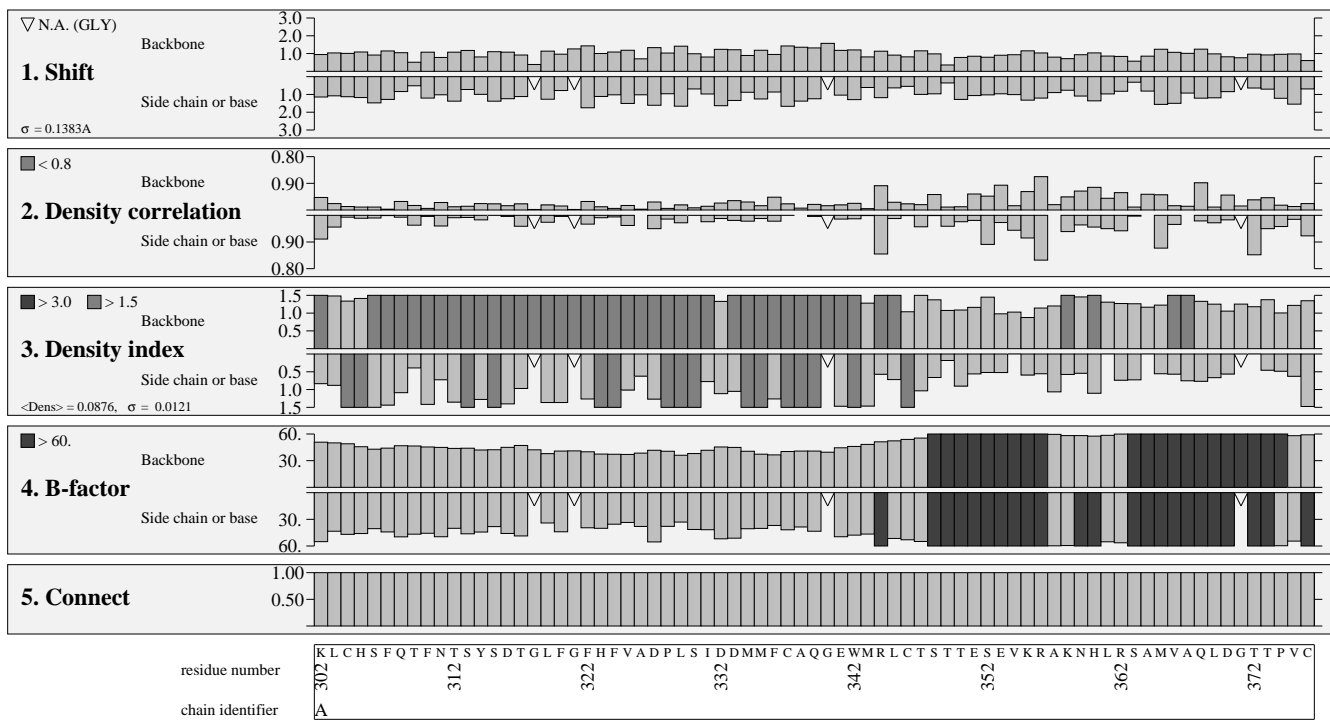
### Local estimation (2)



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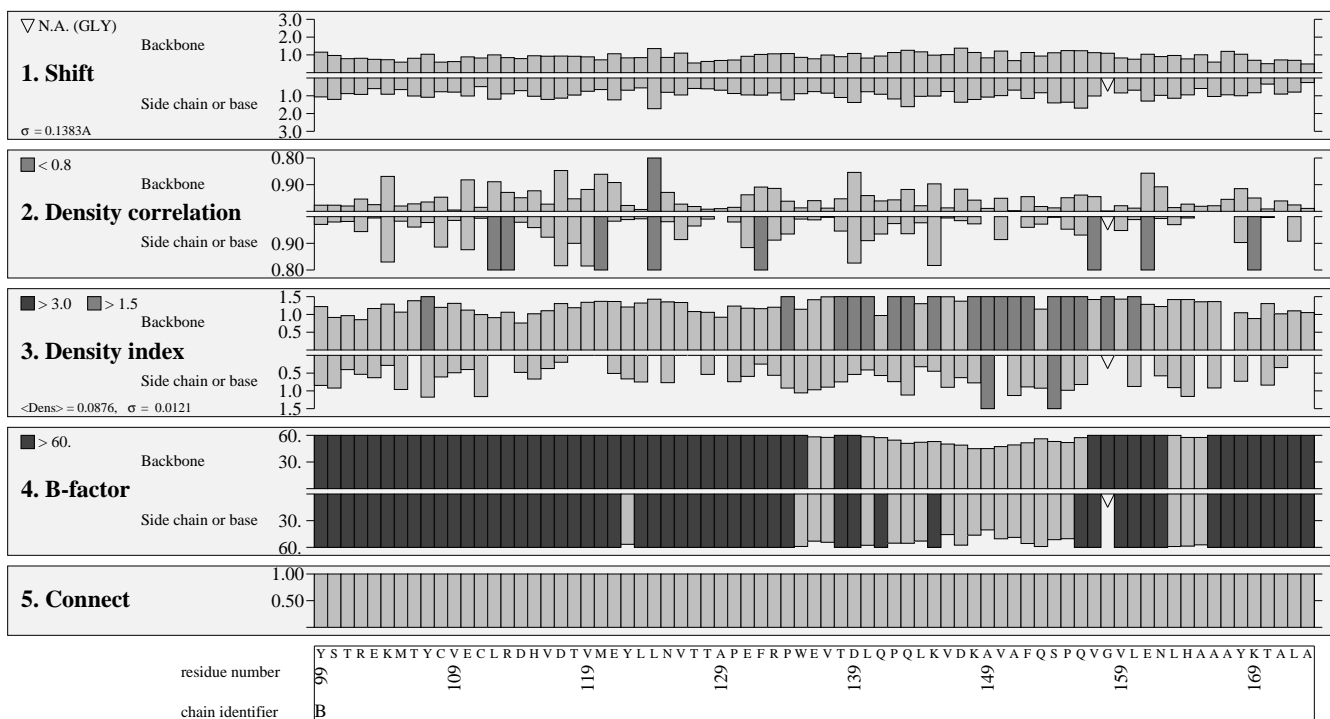
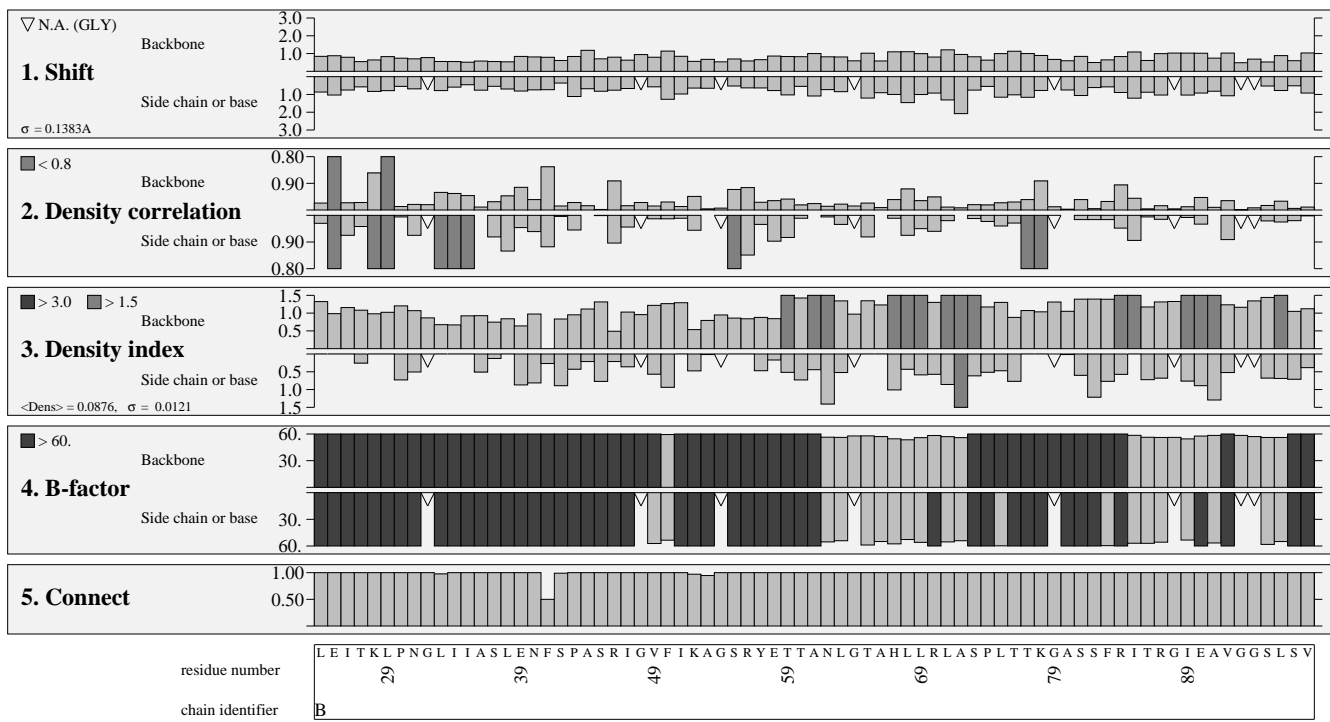
### Local estimation (3)



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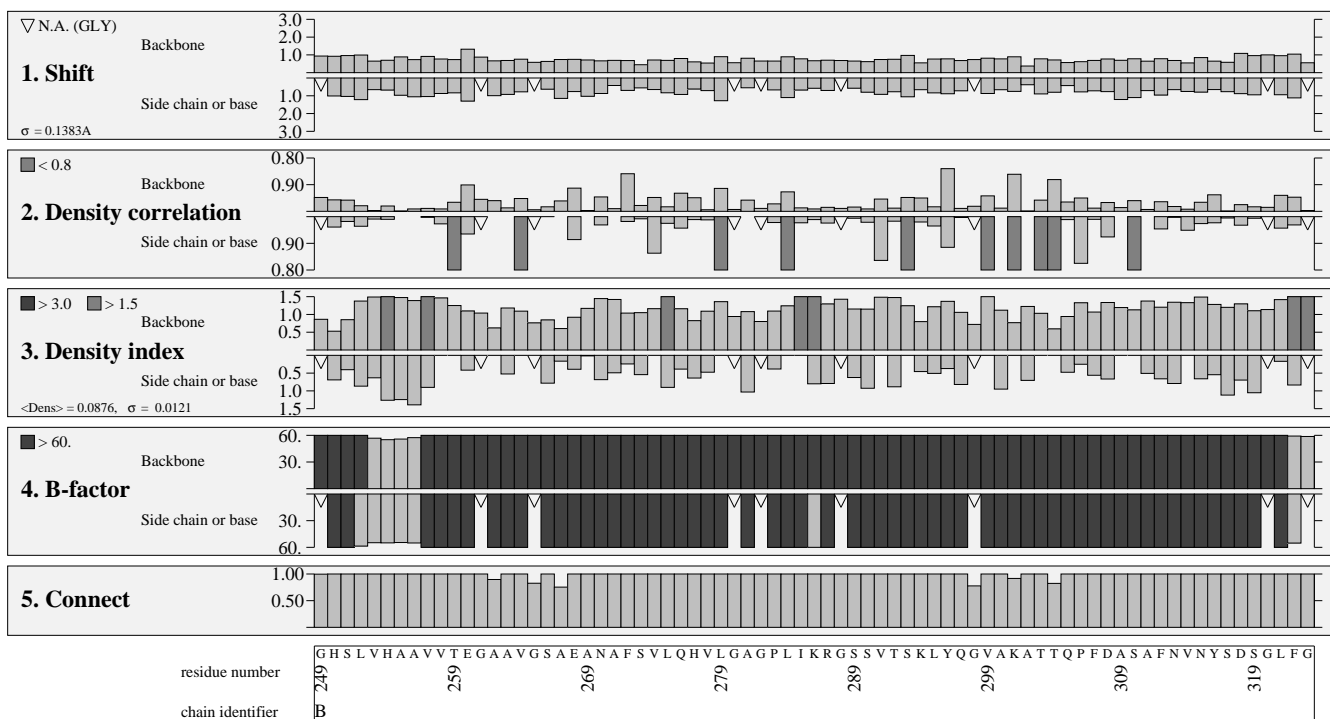
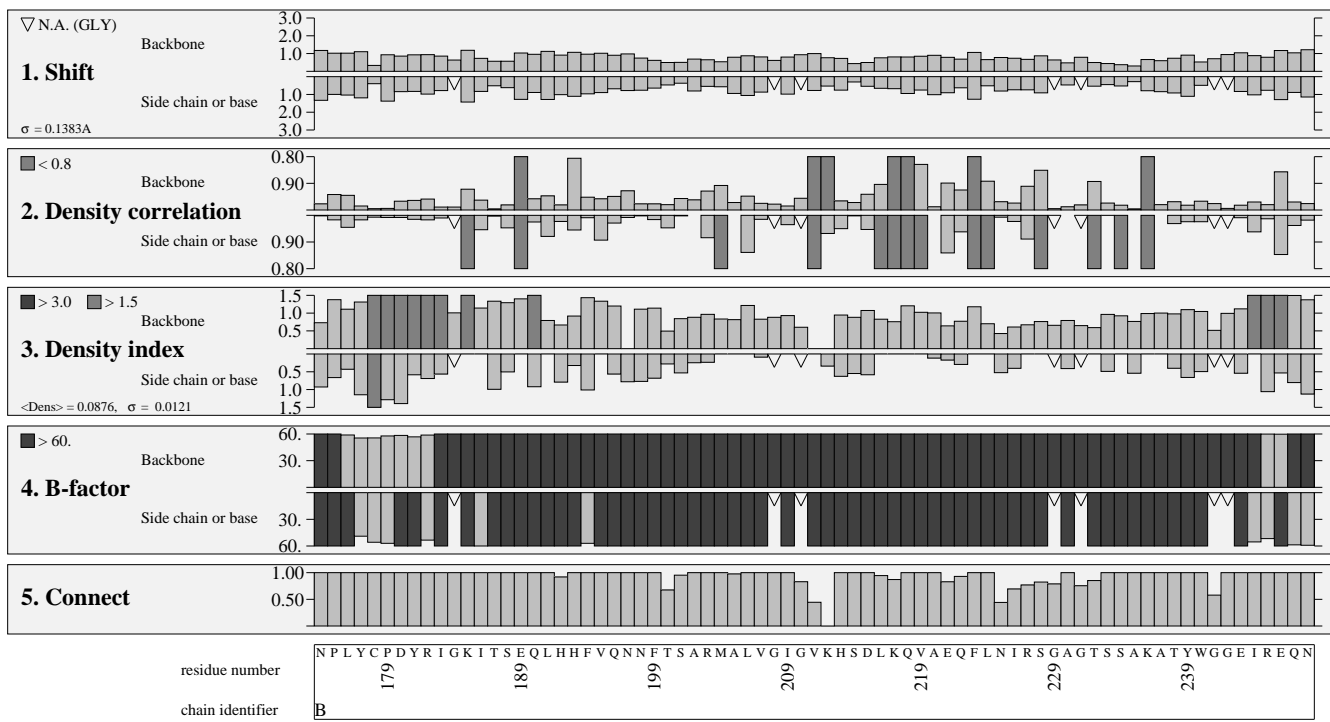
### Local estimation (4)



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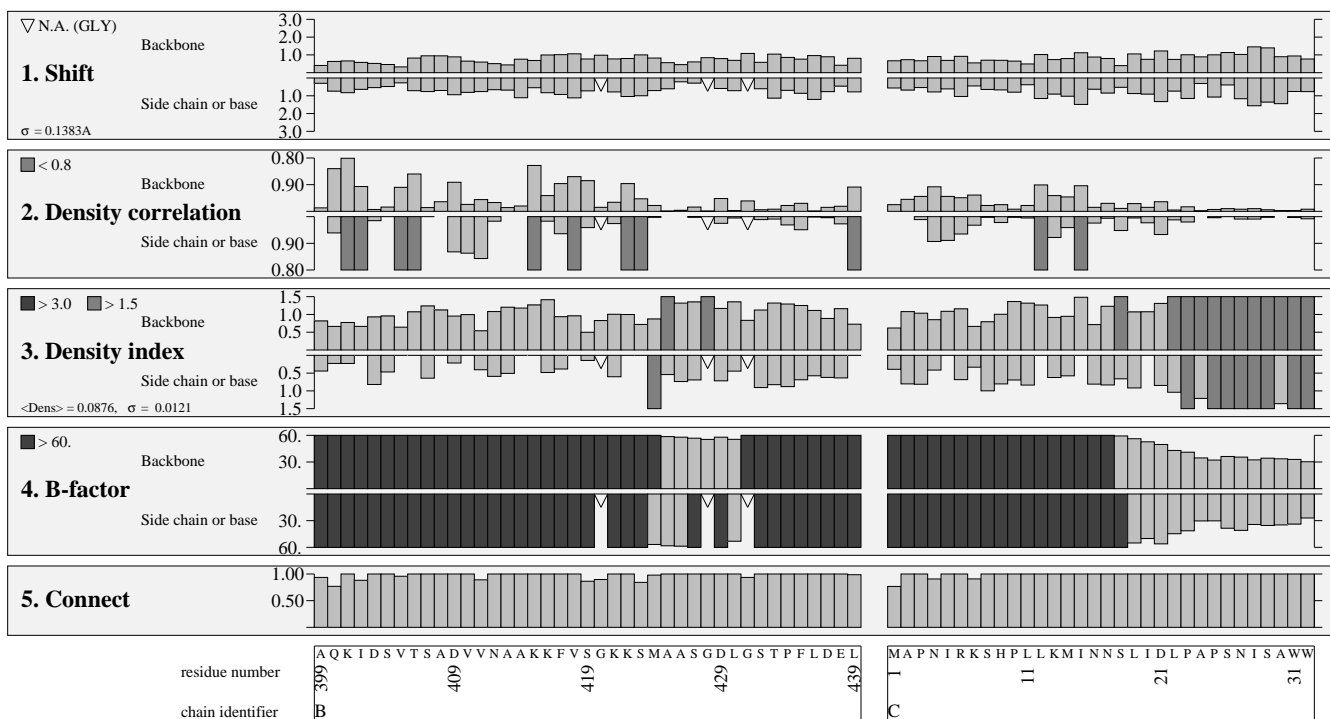
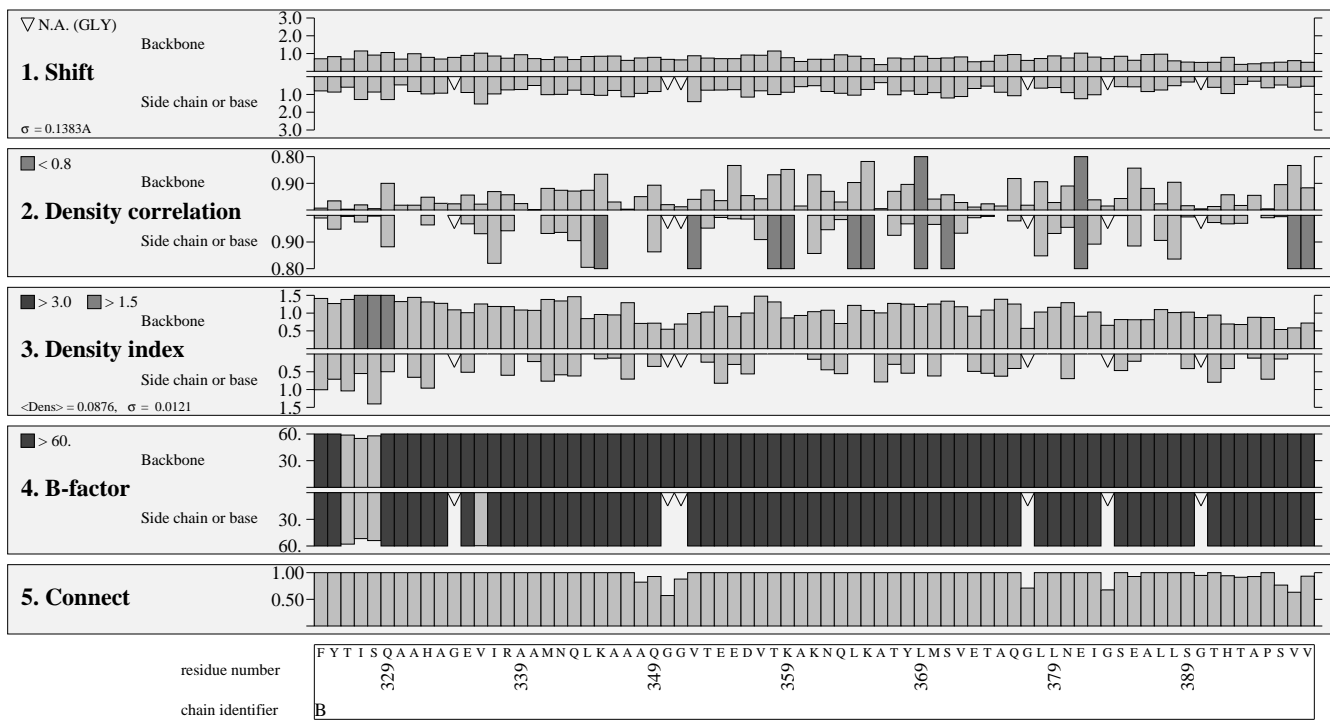
### Local estimation (5)



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### Local estimation (6)

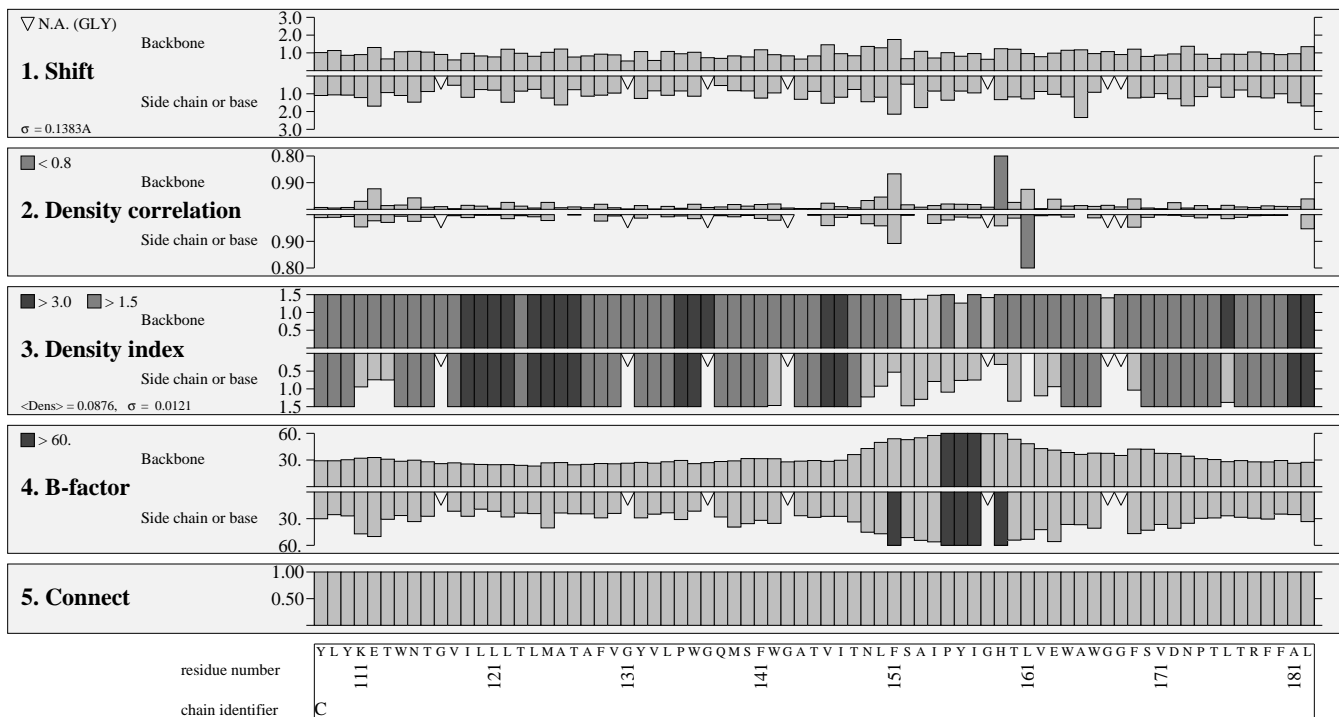
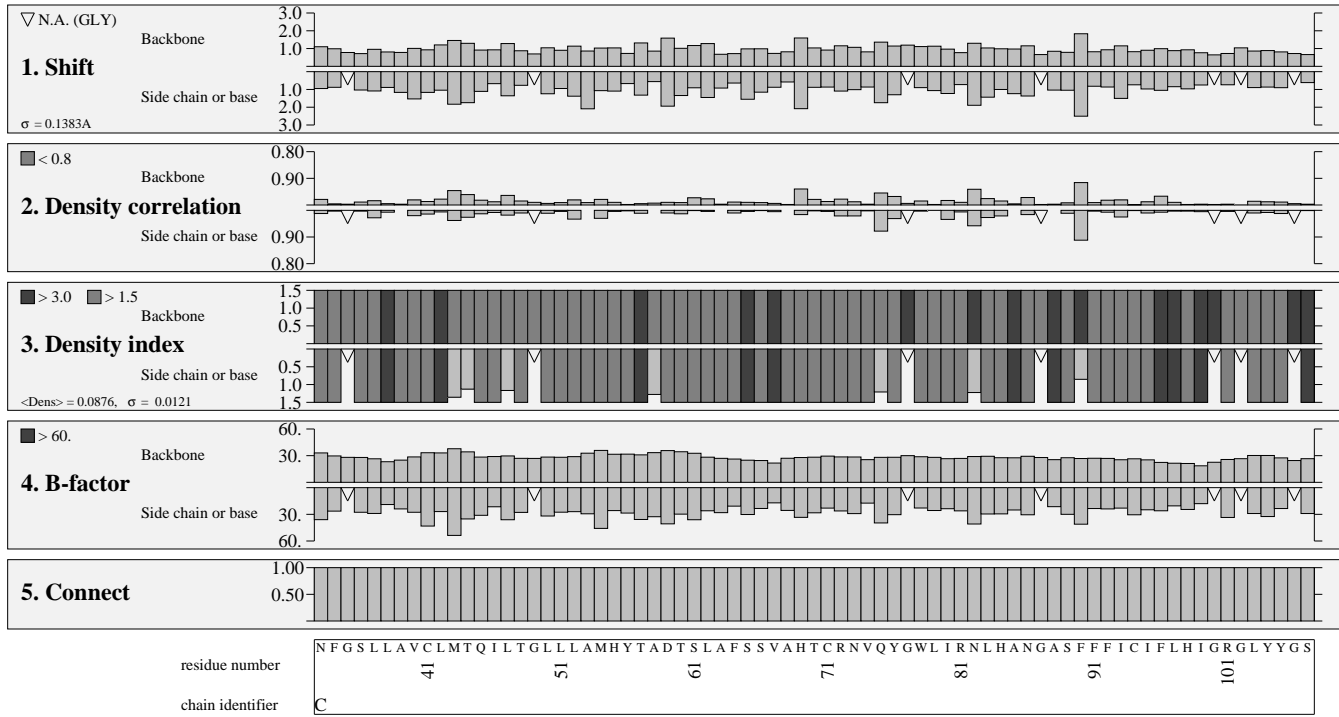




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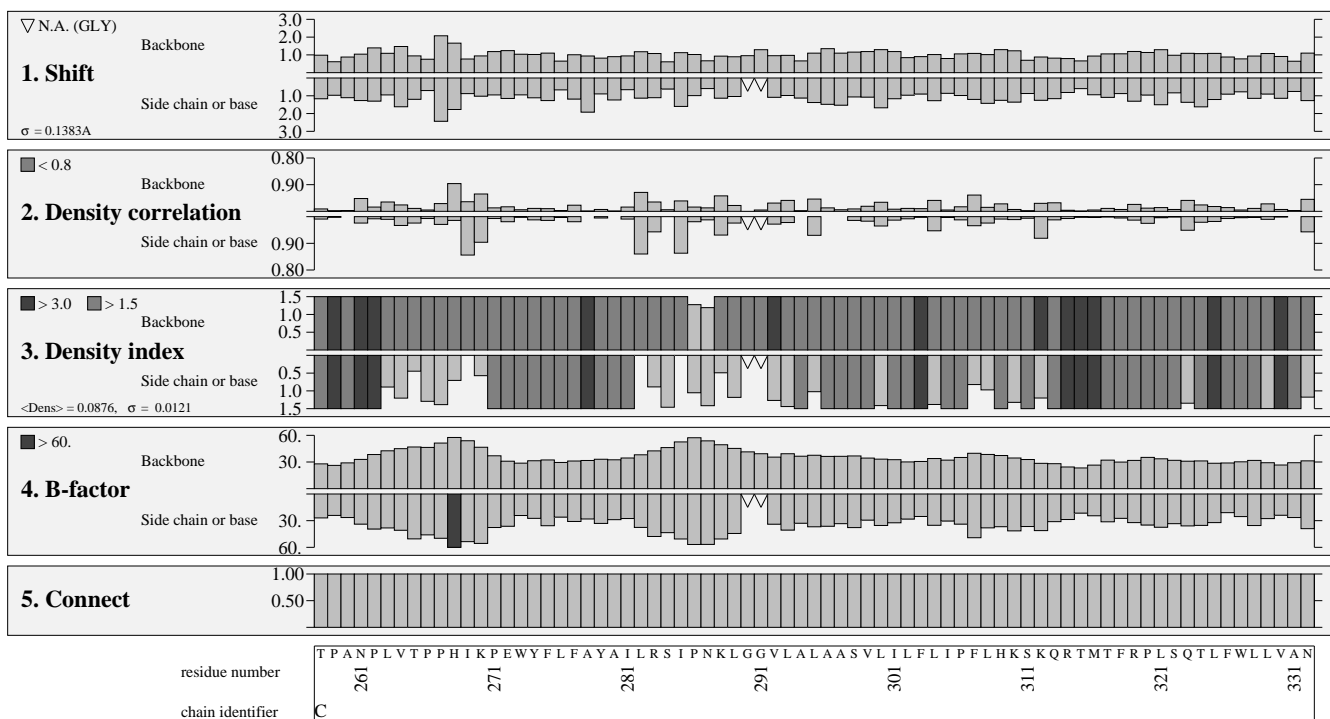
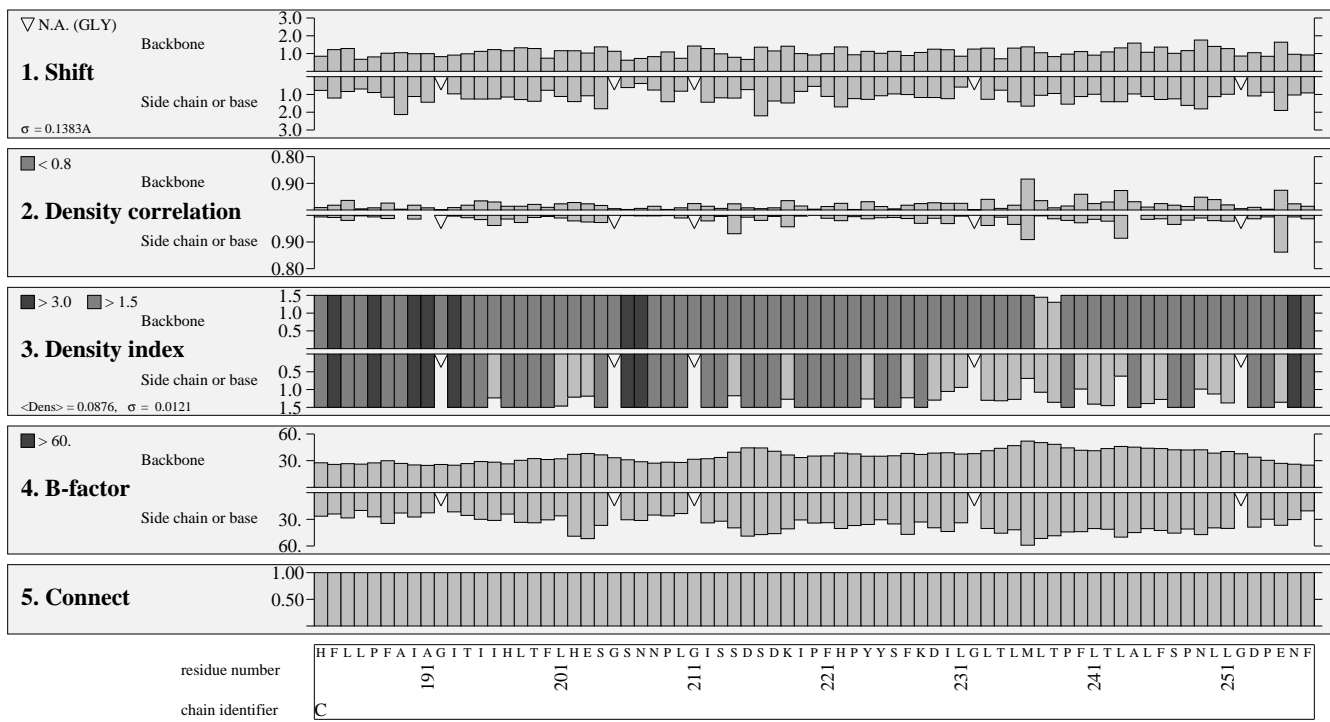
### Local estimation (7)



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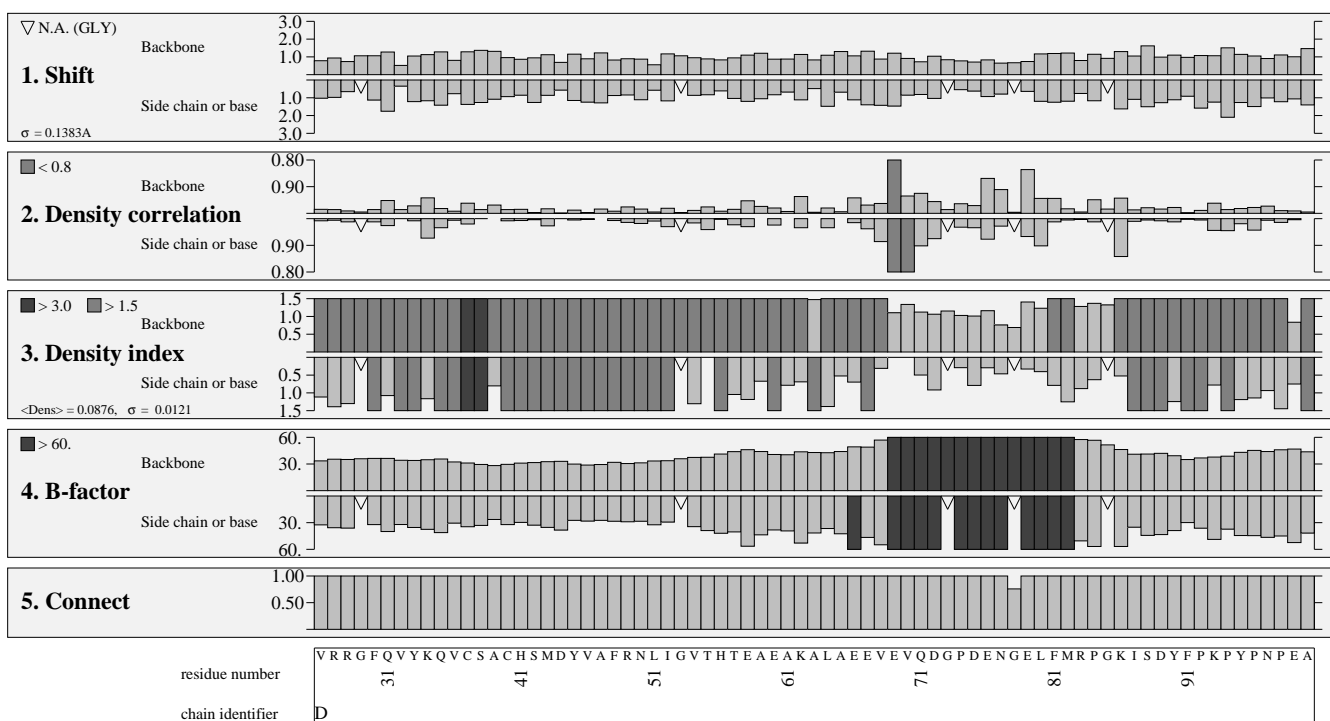
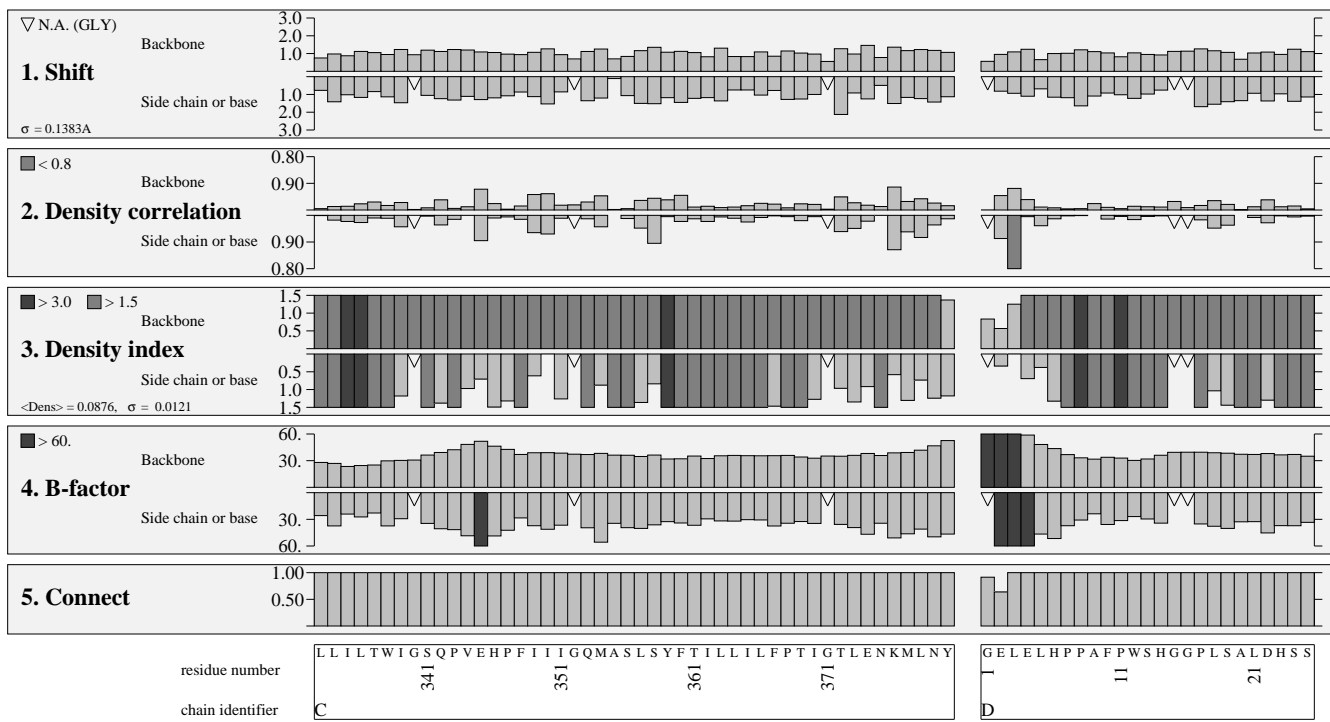
### Local estimation (8)



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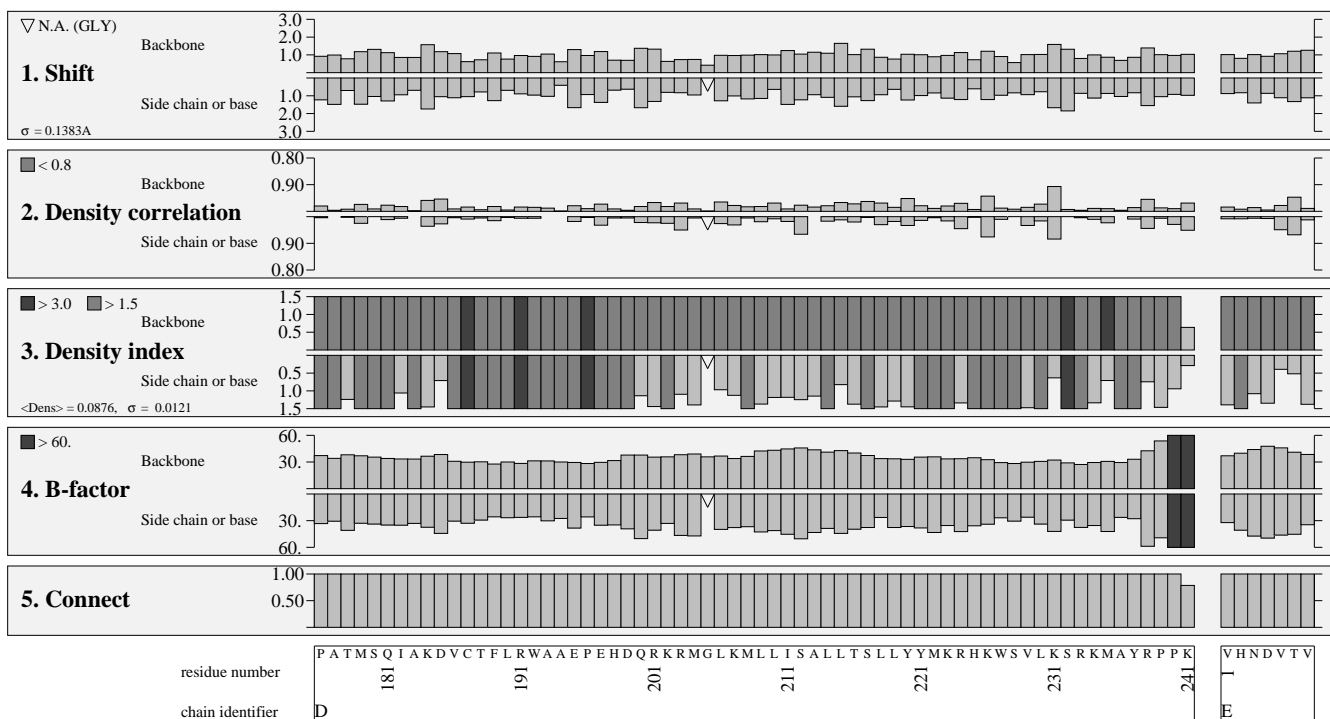
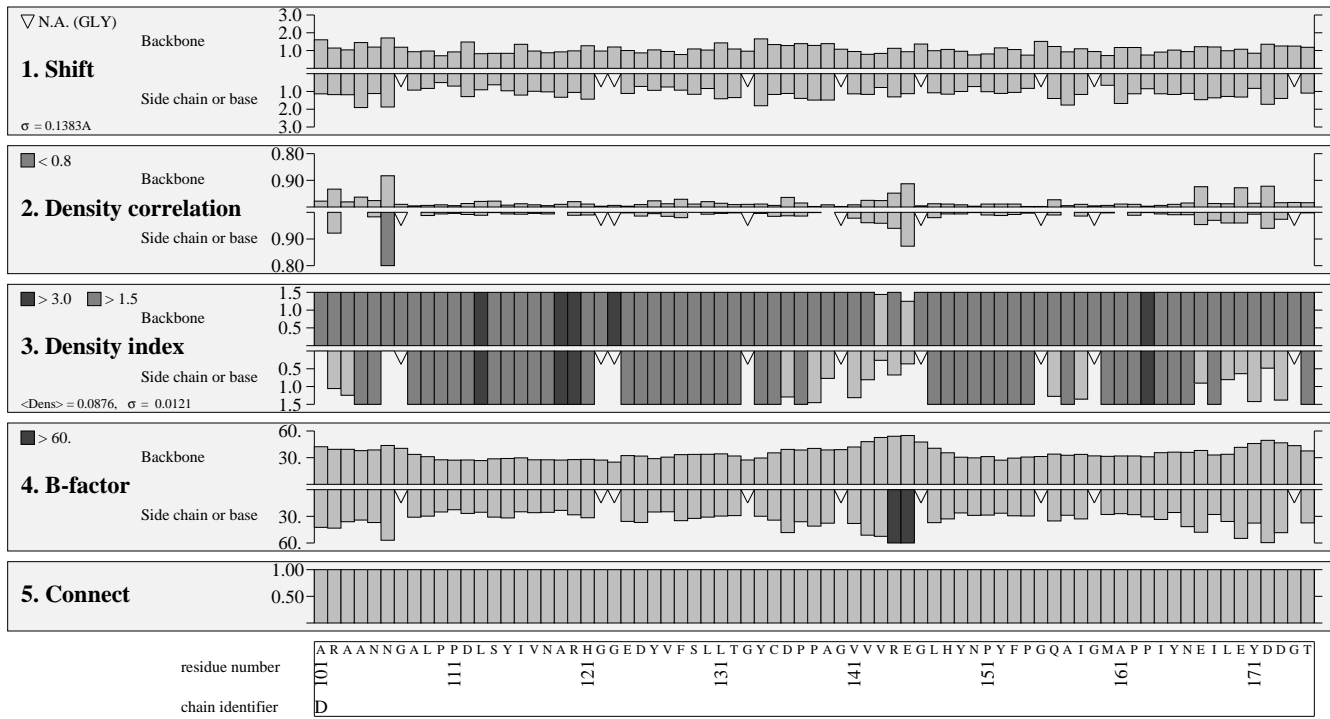
### Local estimation (9)



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### Local estimation (10)

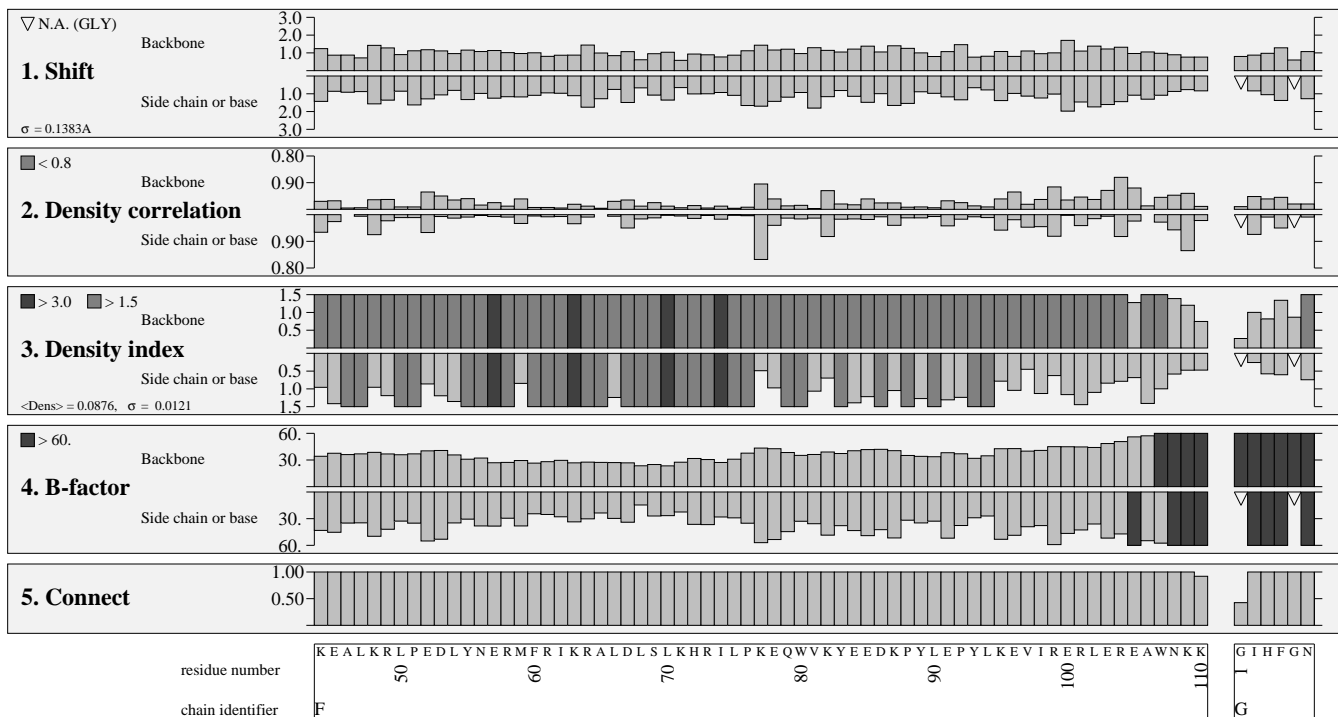
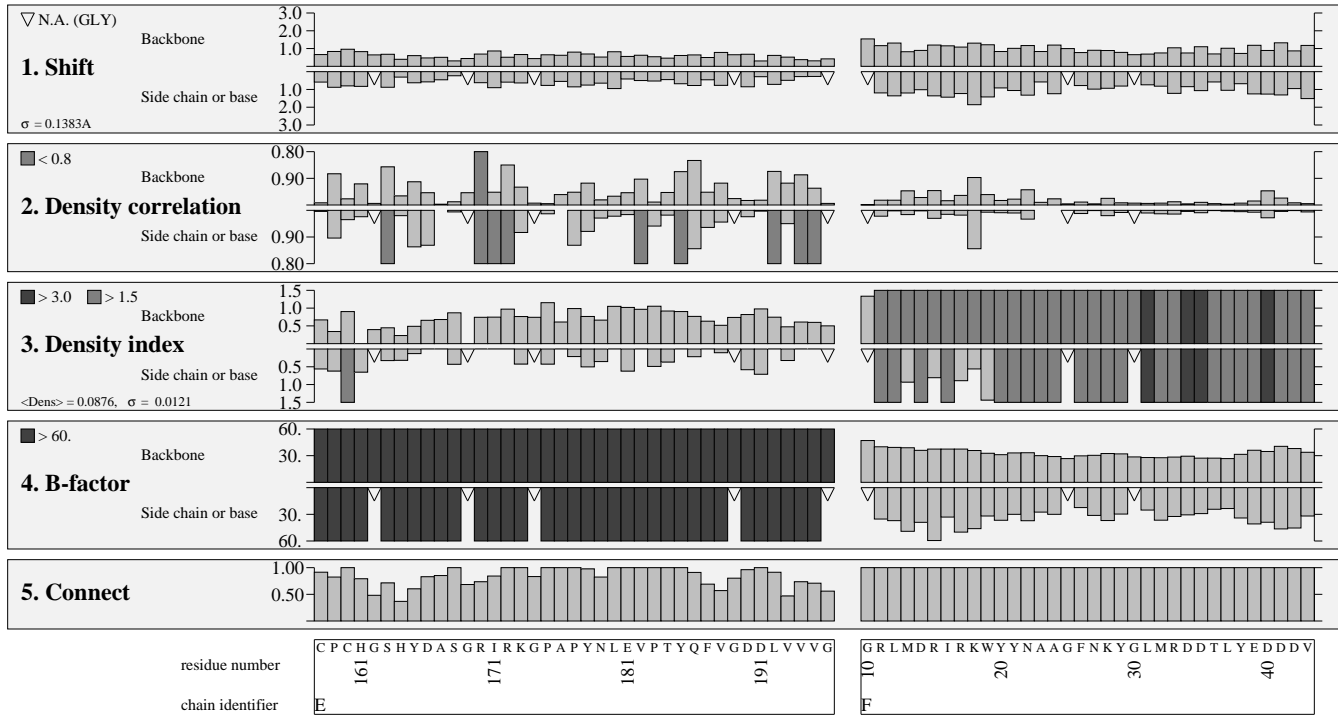




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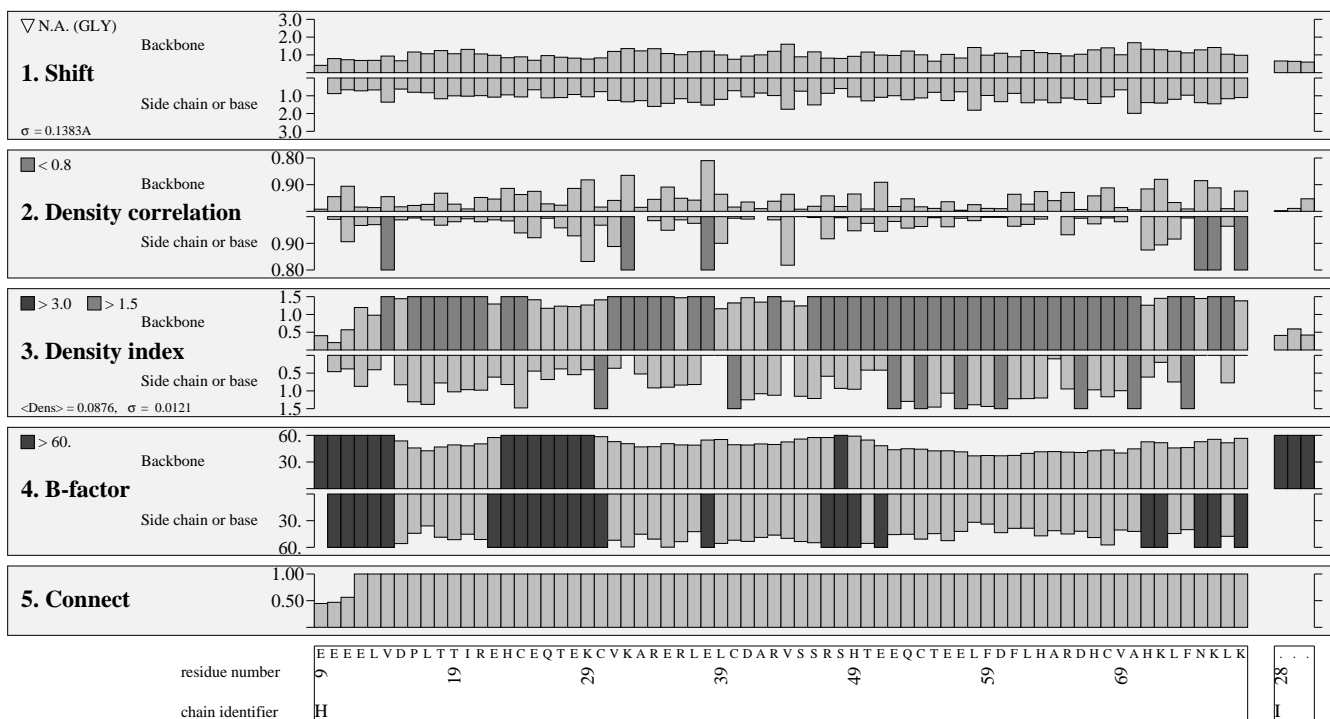
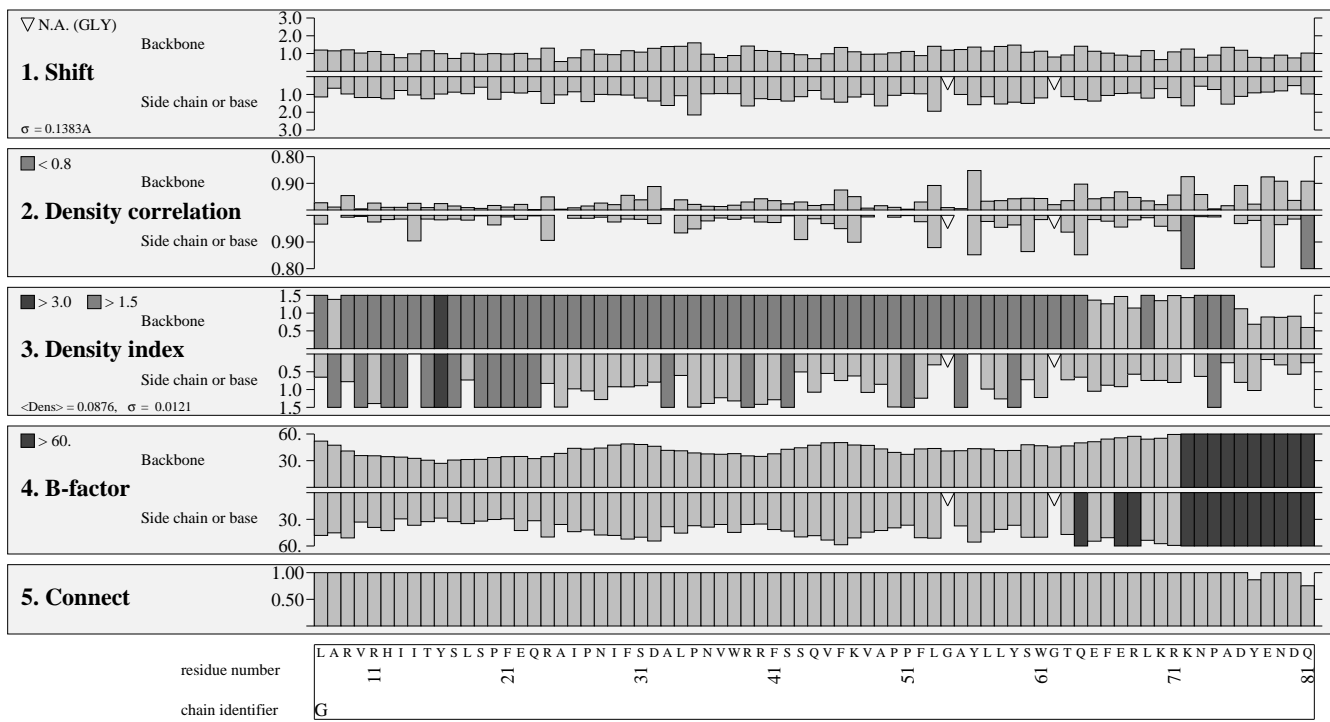
### Local estimation (12)



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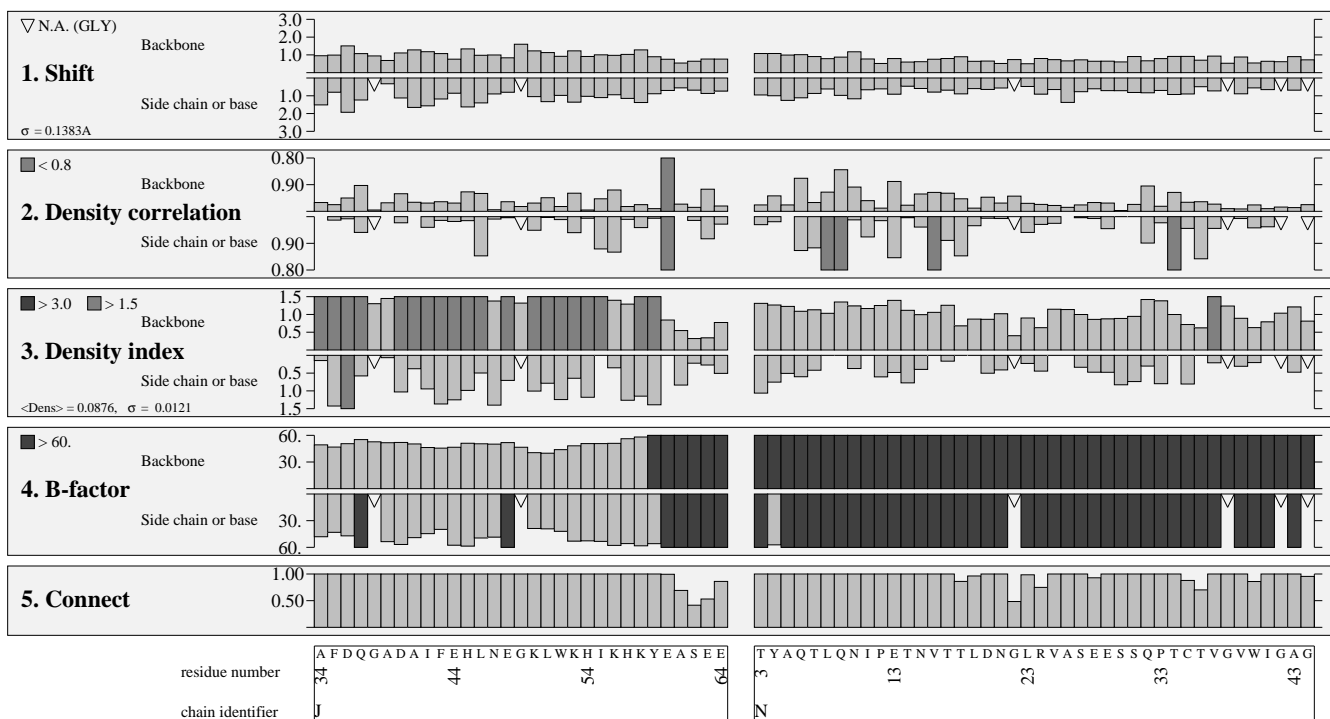
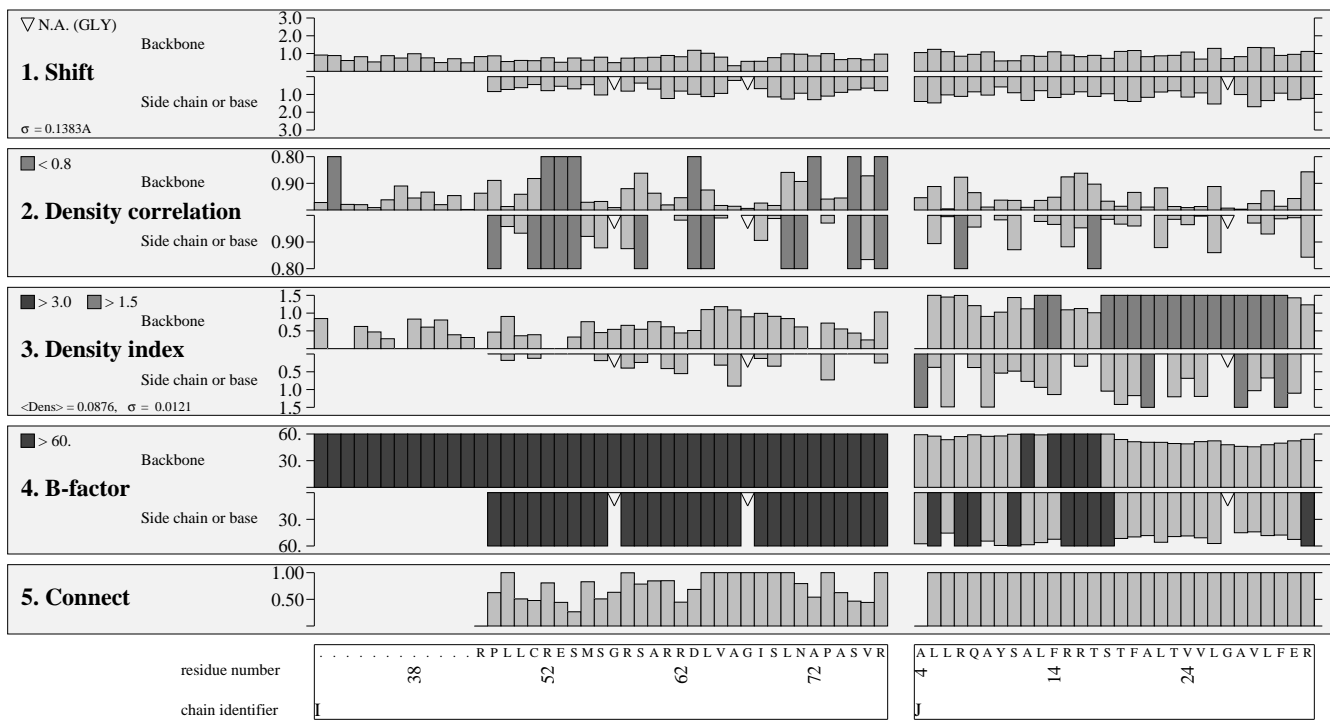
### Local estimation (13)



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### Local estimation (14)

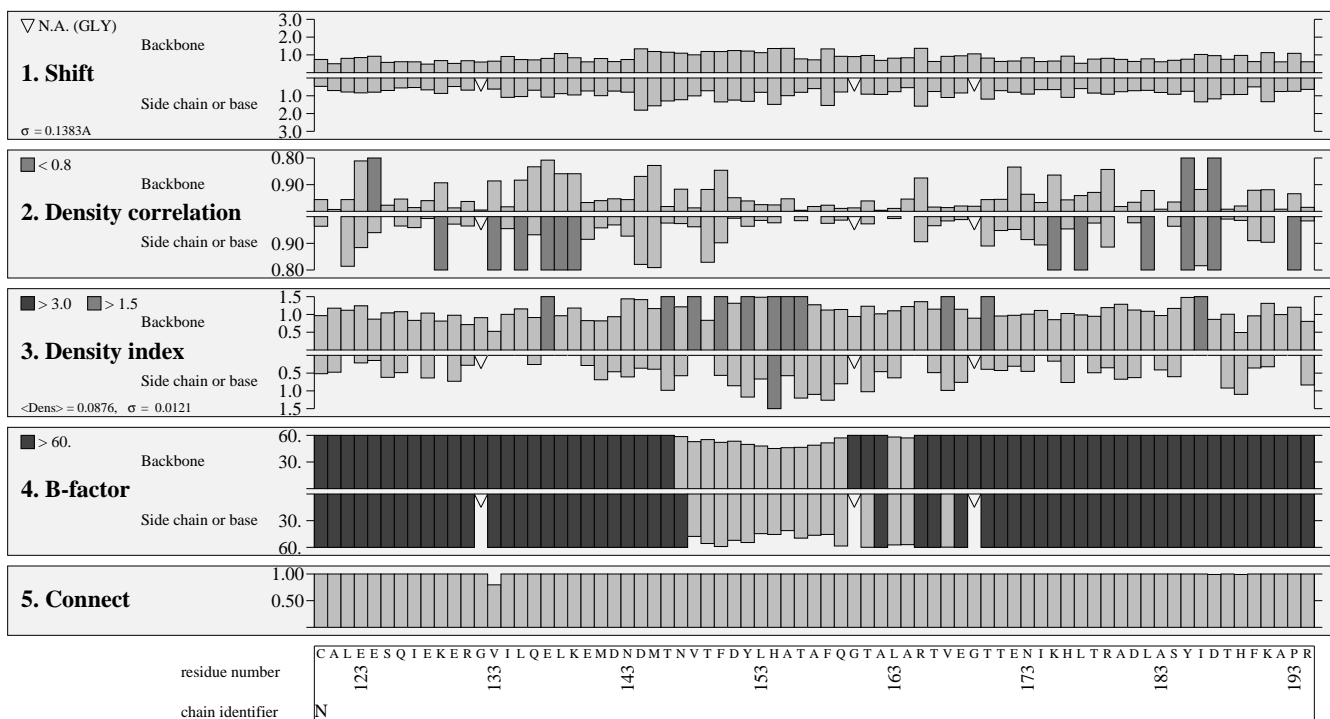
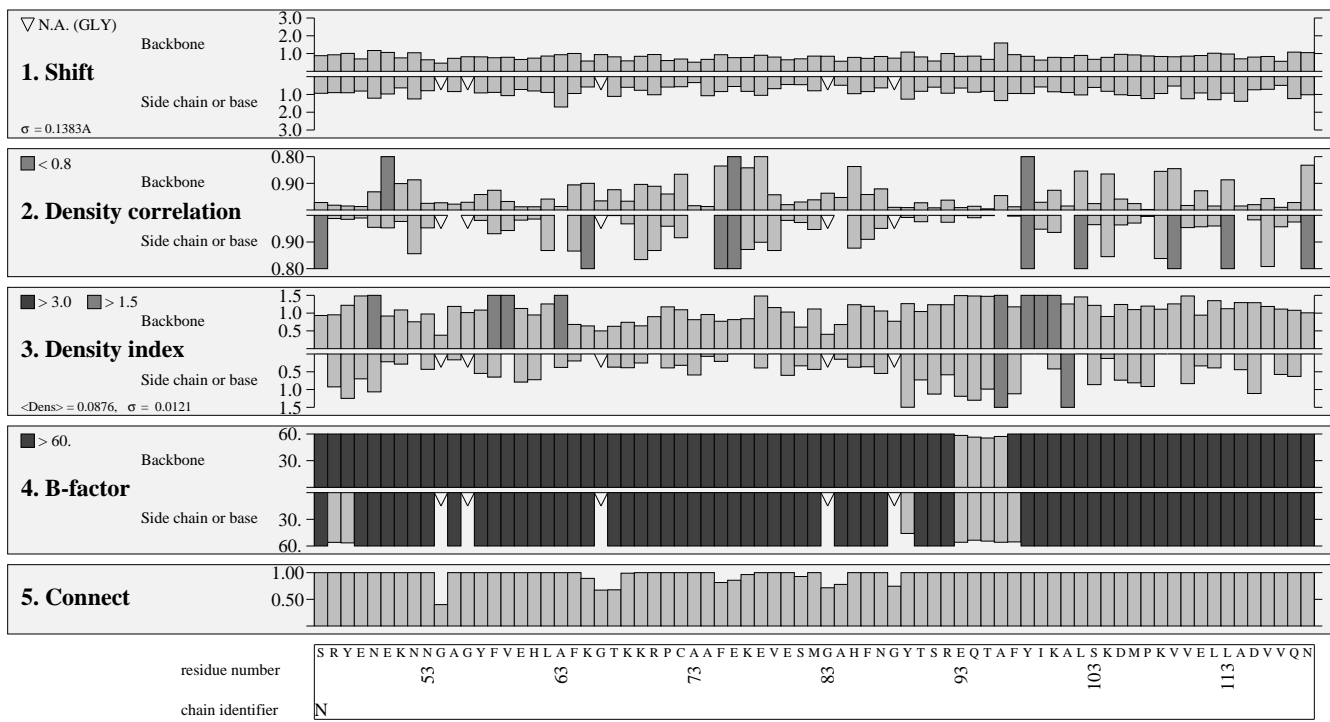




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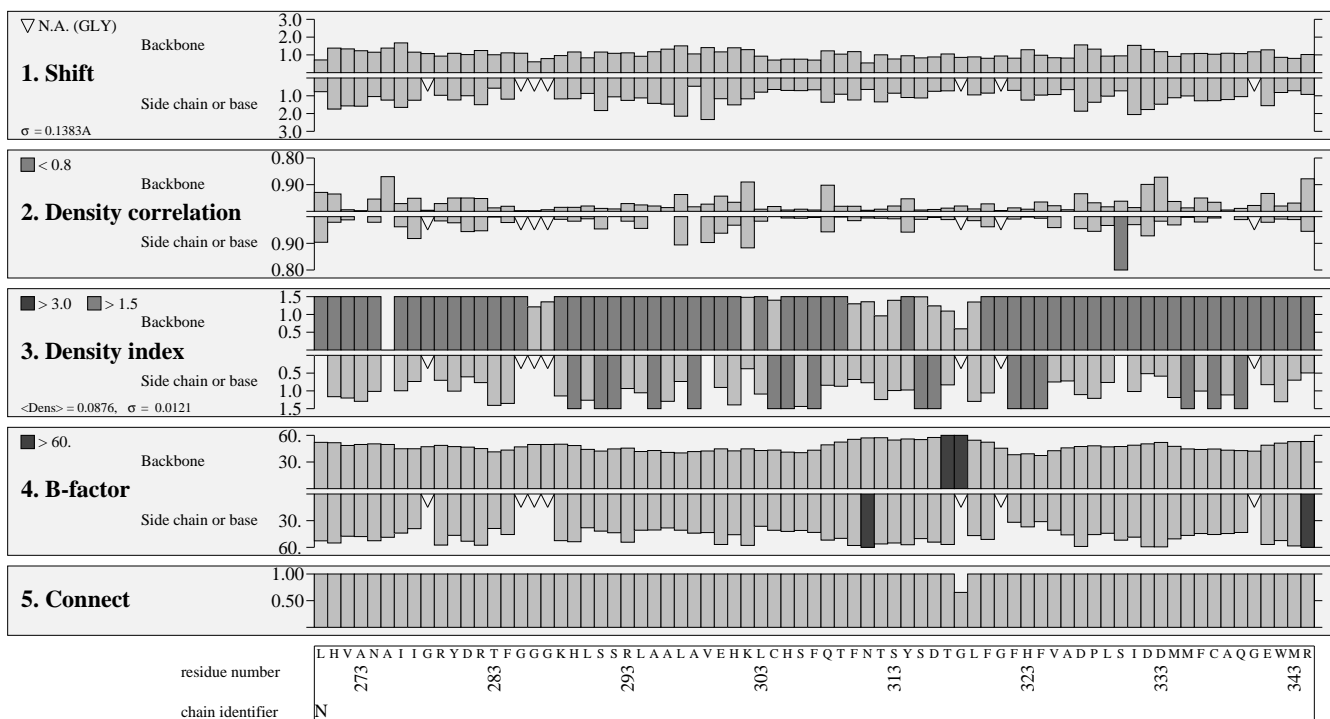
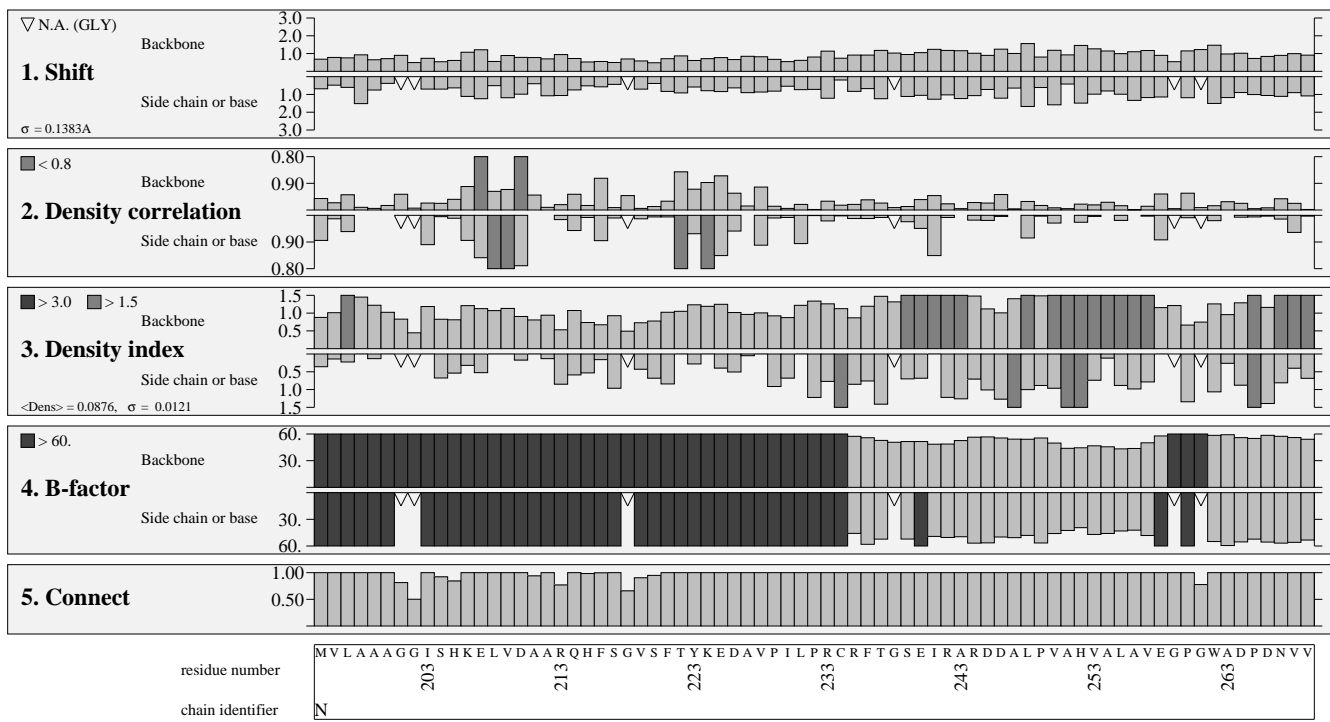
### Local estimation (15)



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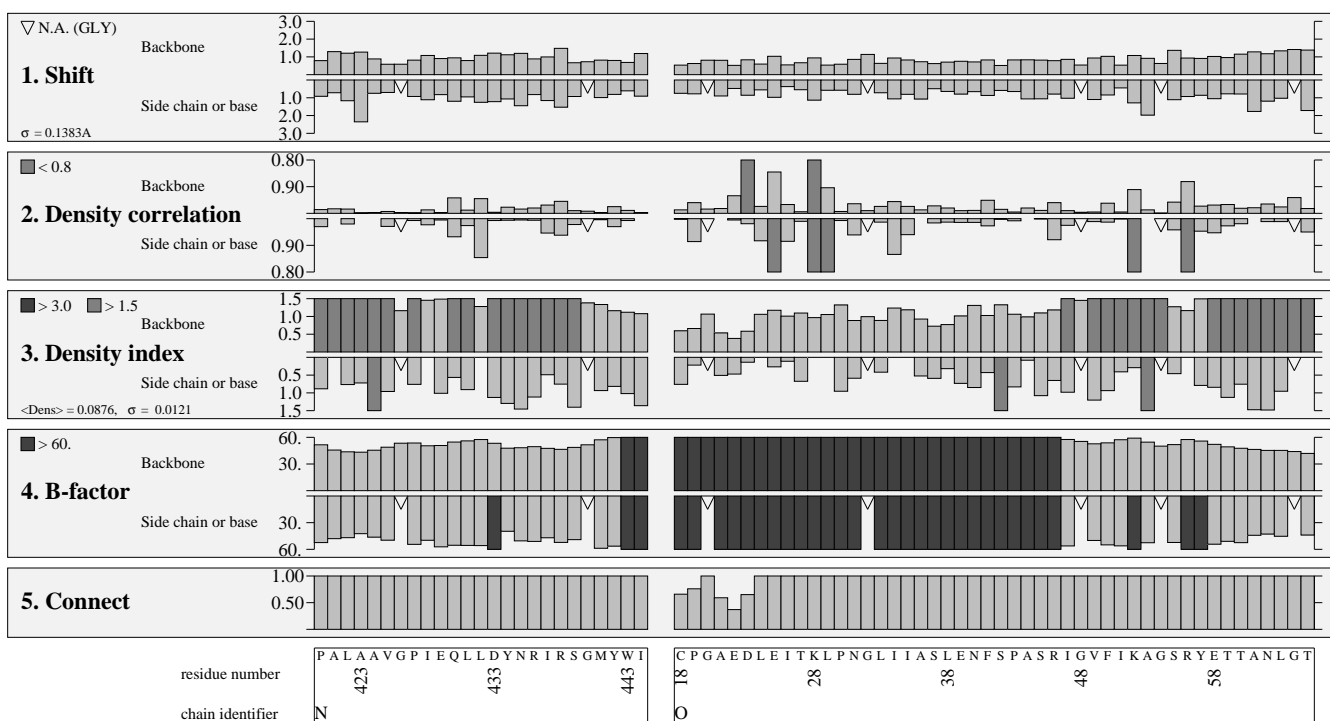
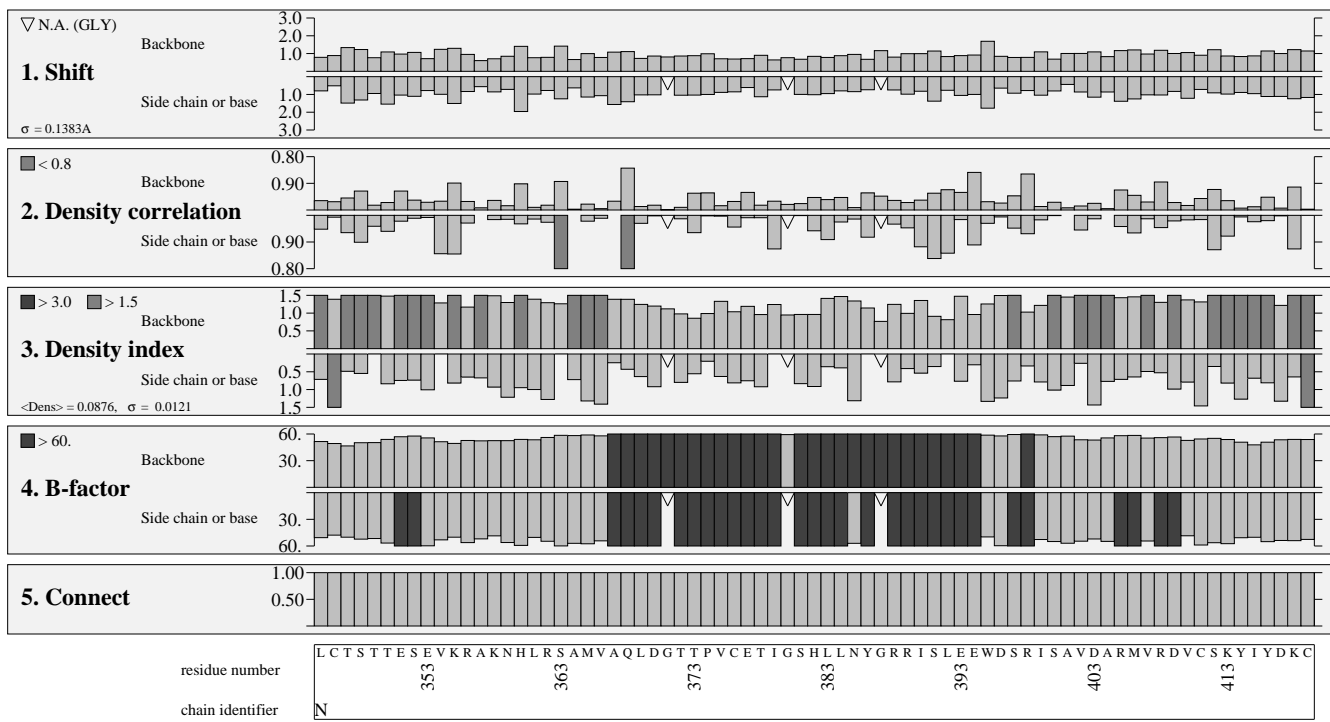
### Local estimation (16)



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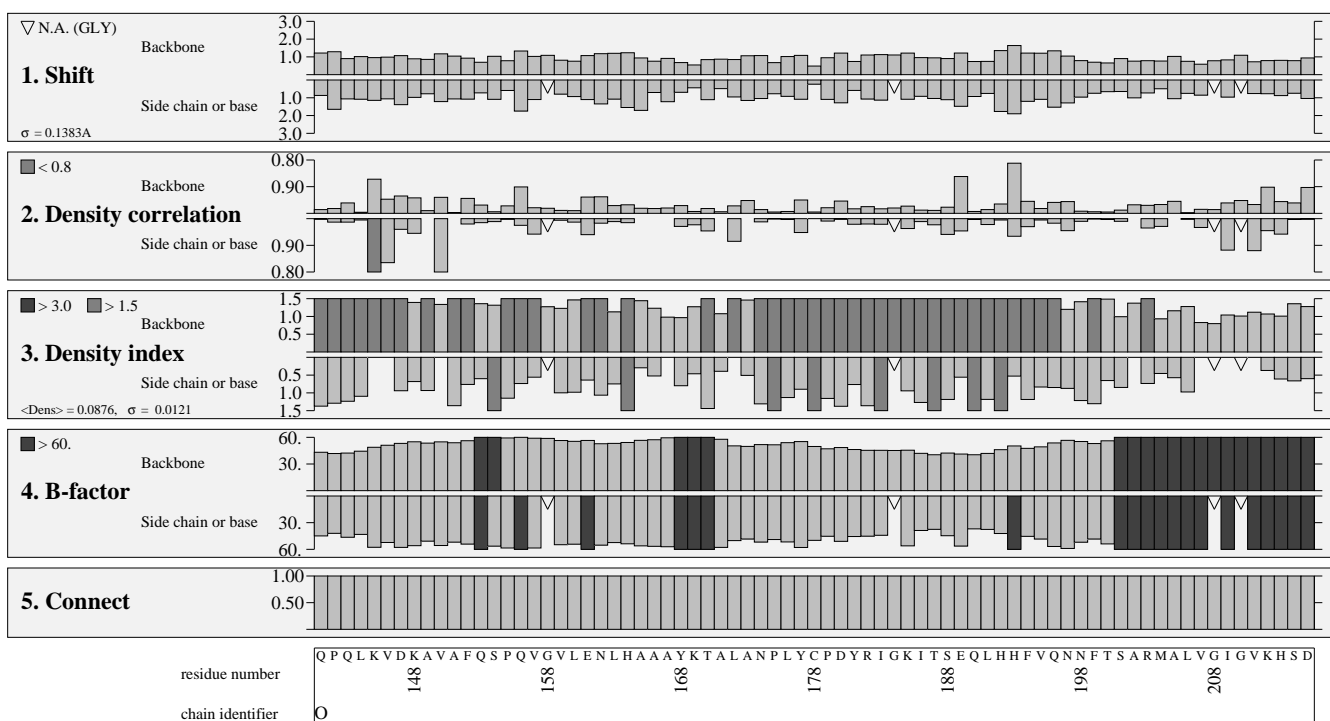
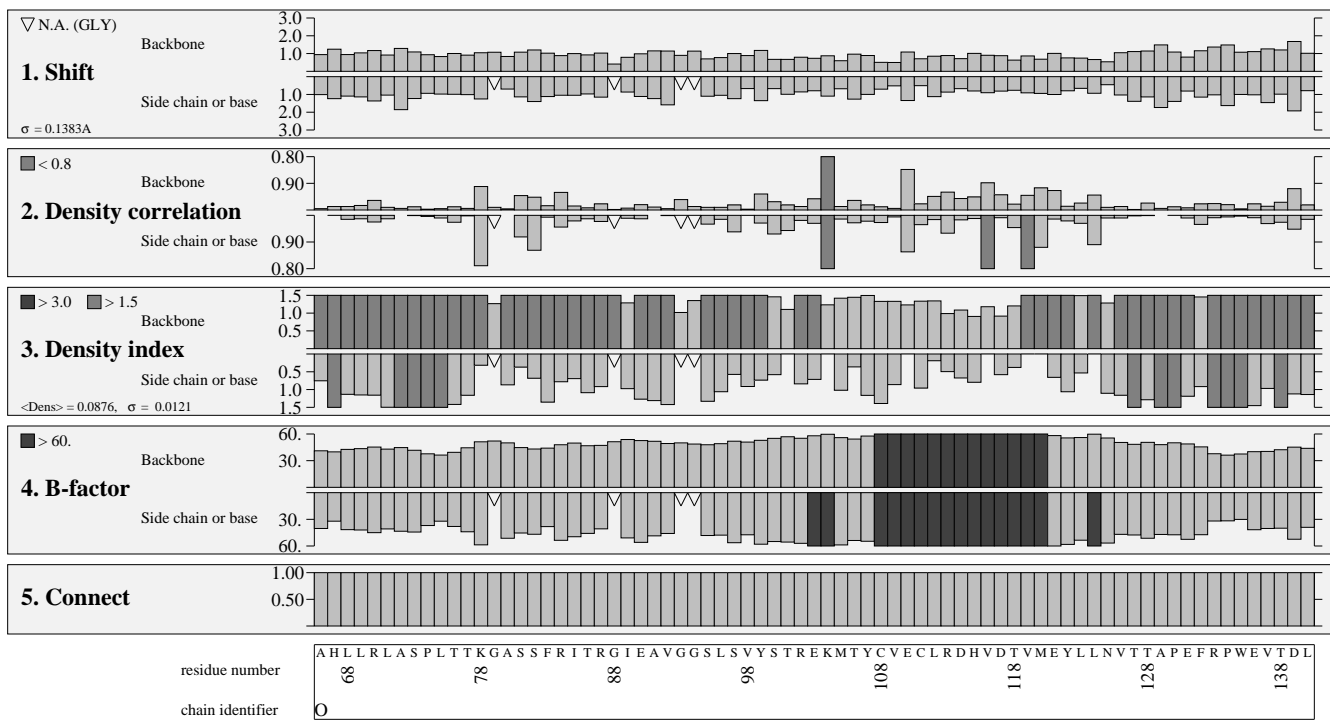
### Local estimation (17)



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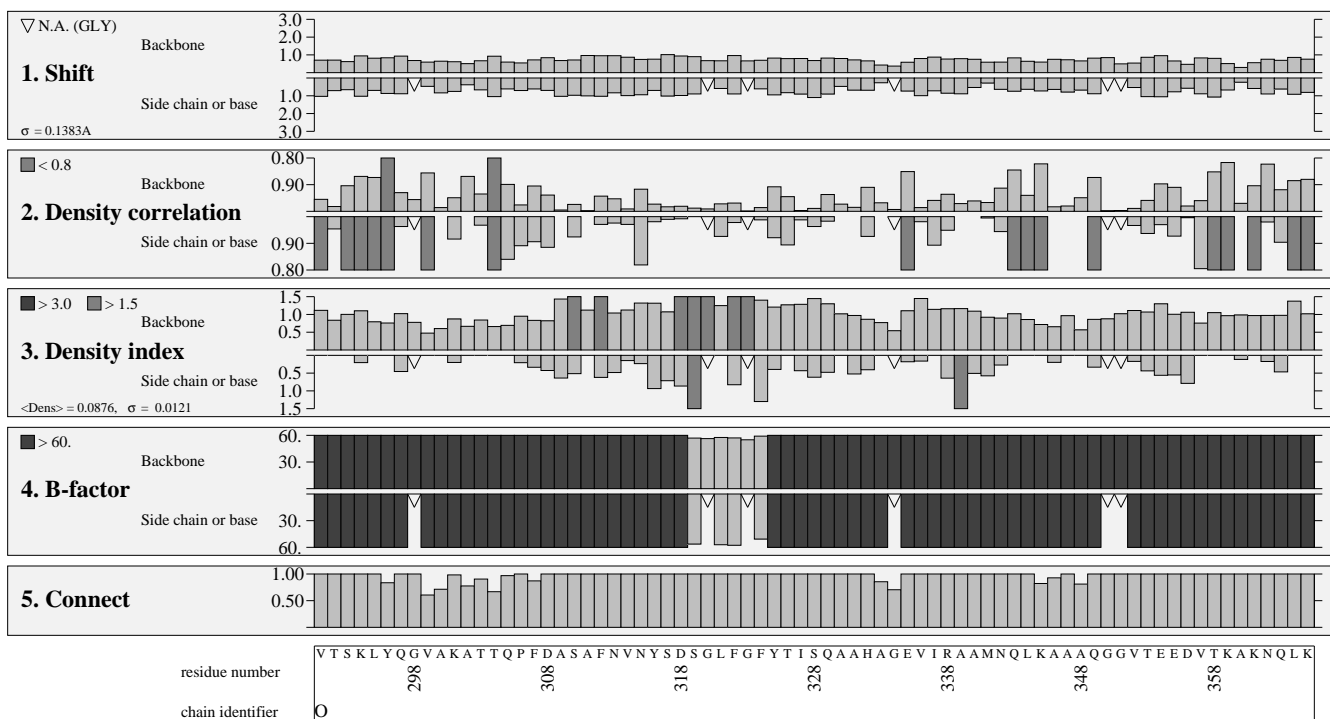
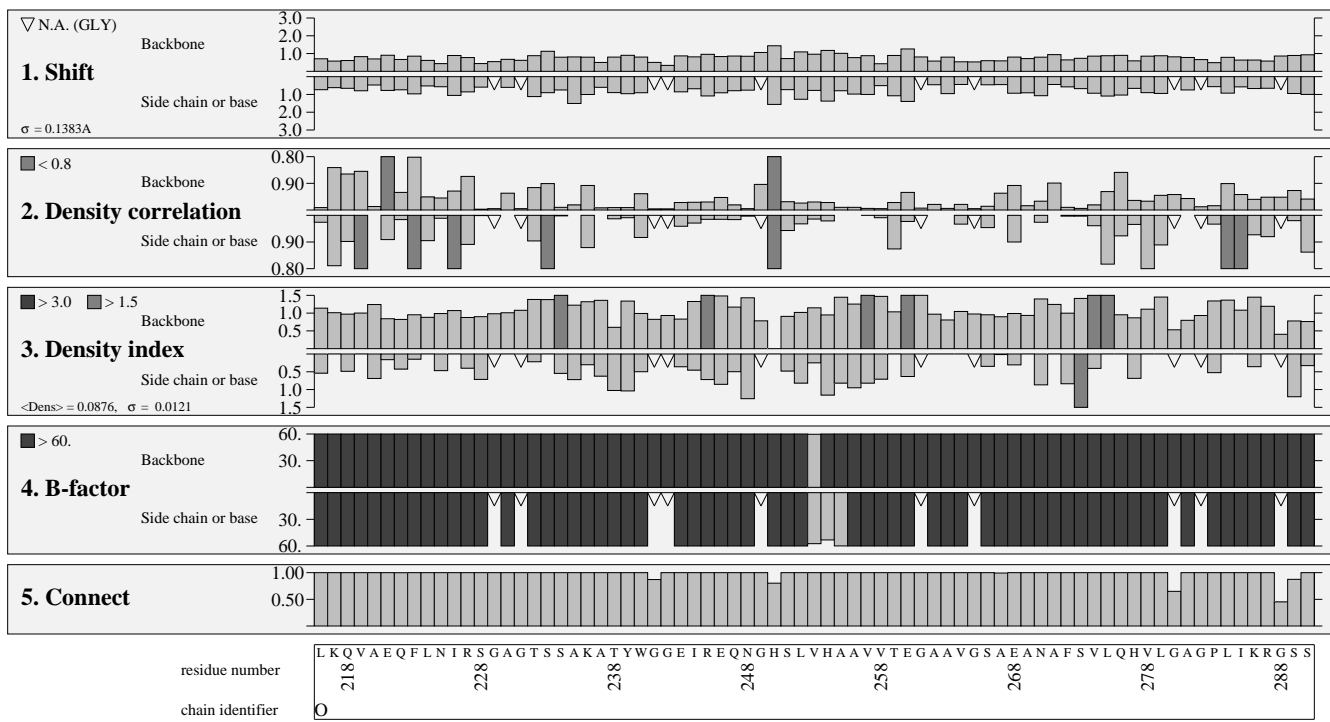
### Local estimation (18)



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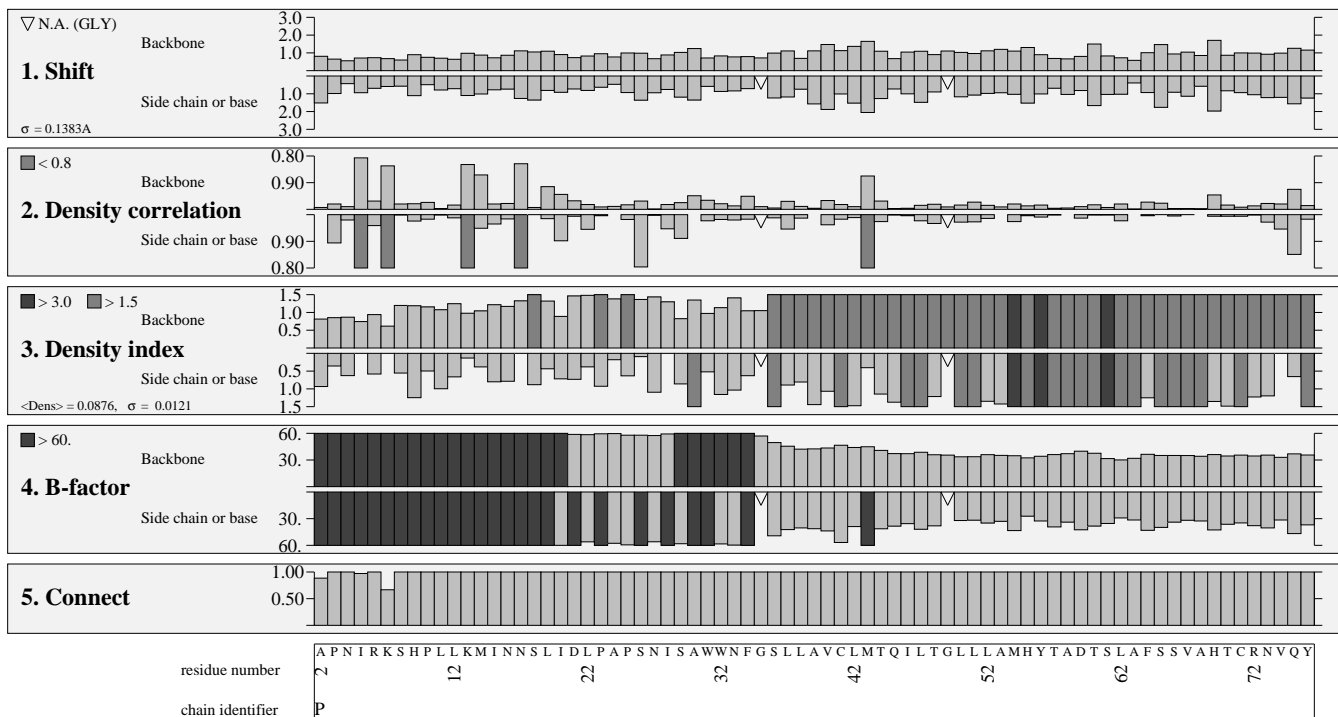
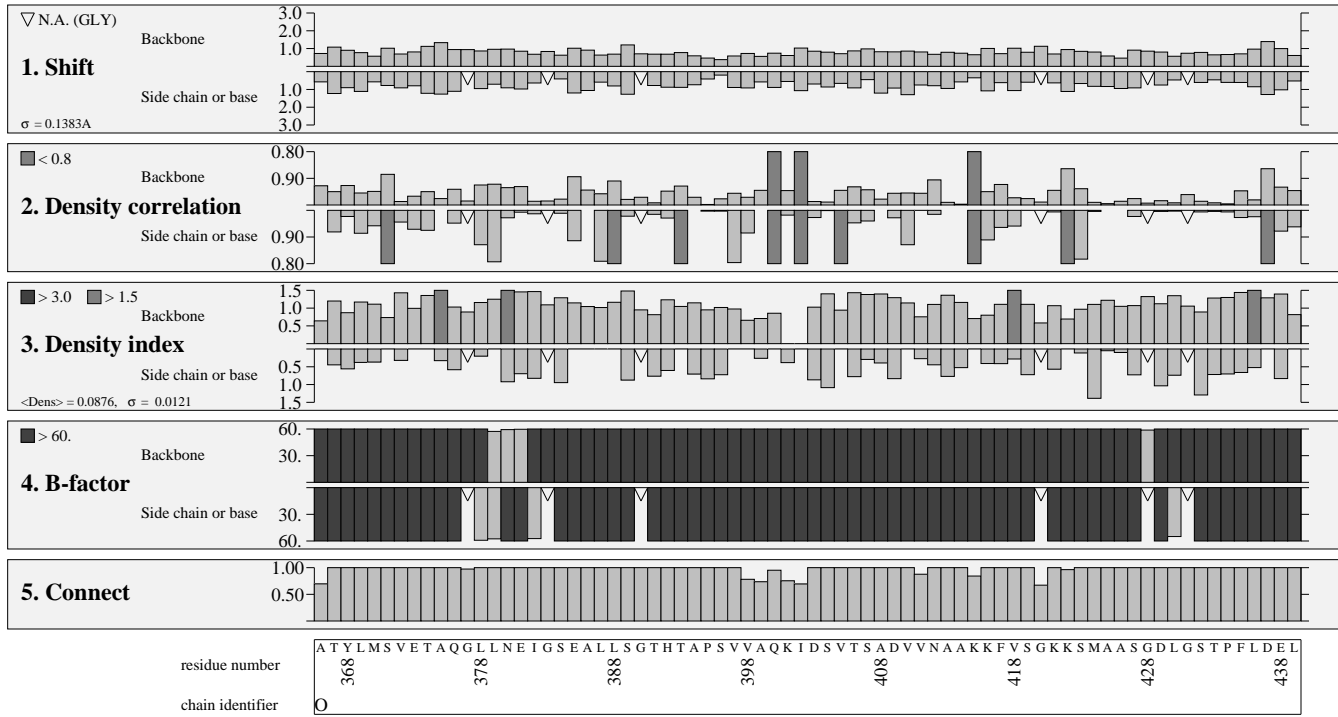
### Local estimation (19)



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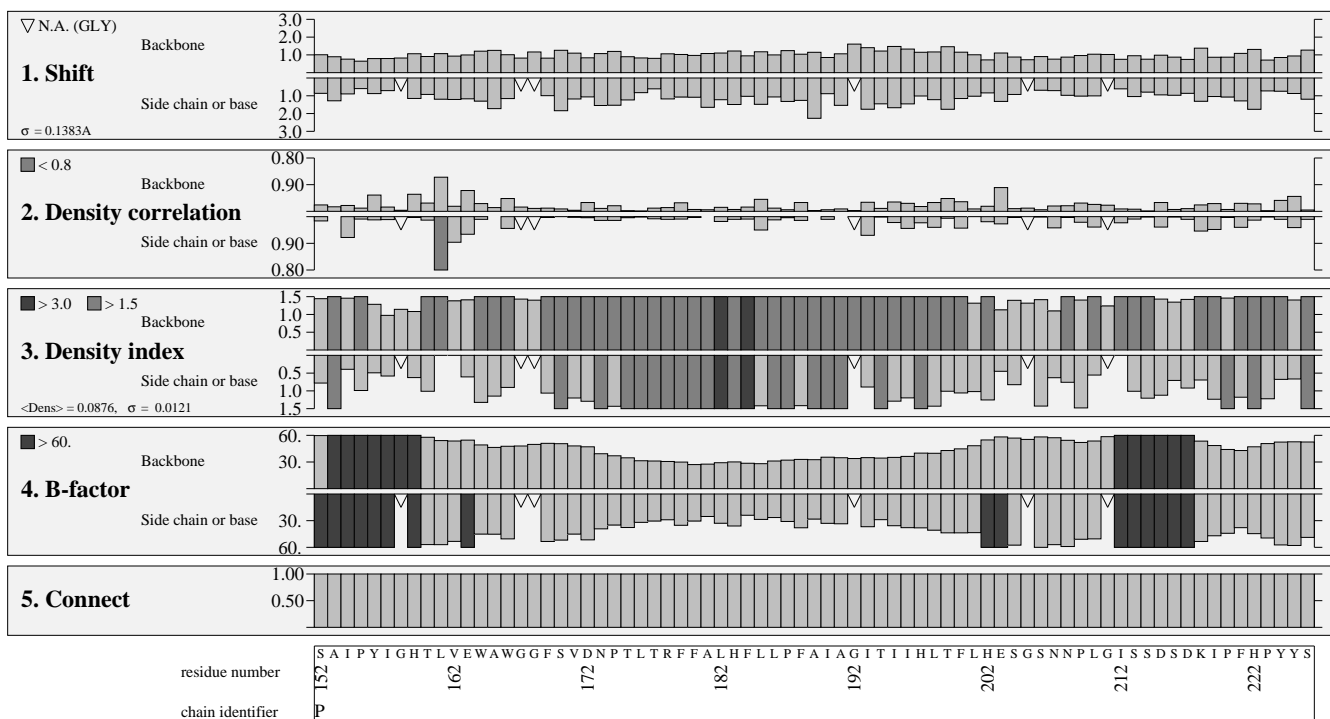
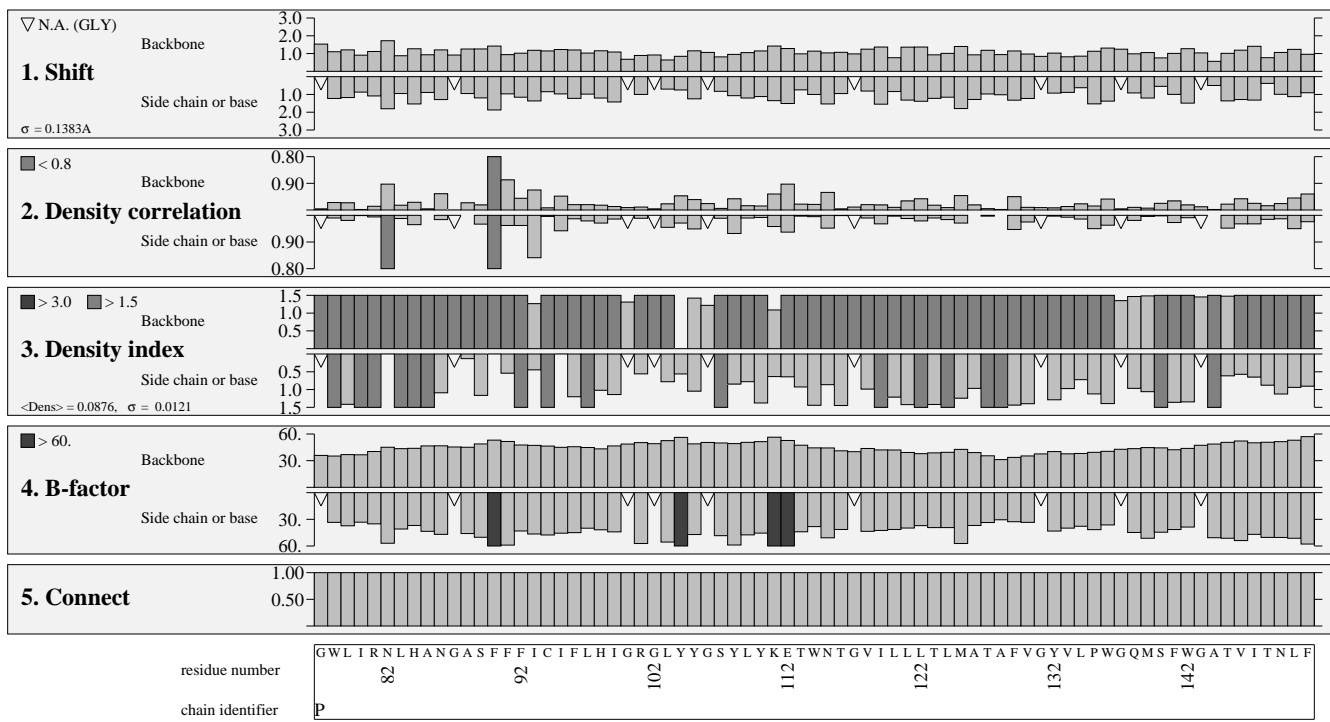
### Local estimation (20)



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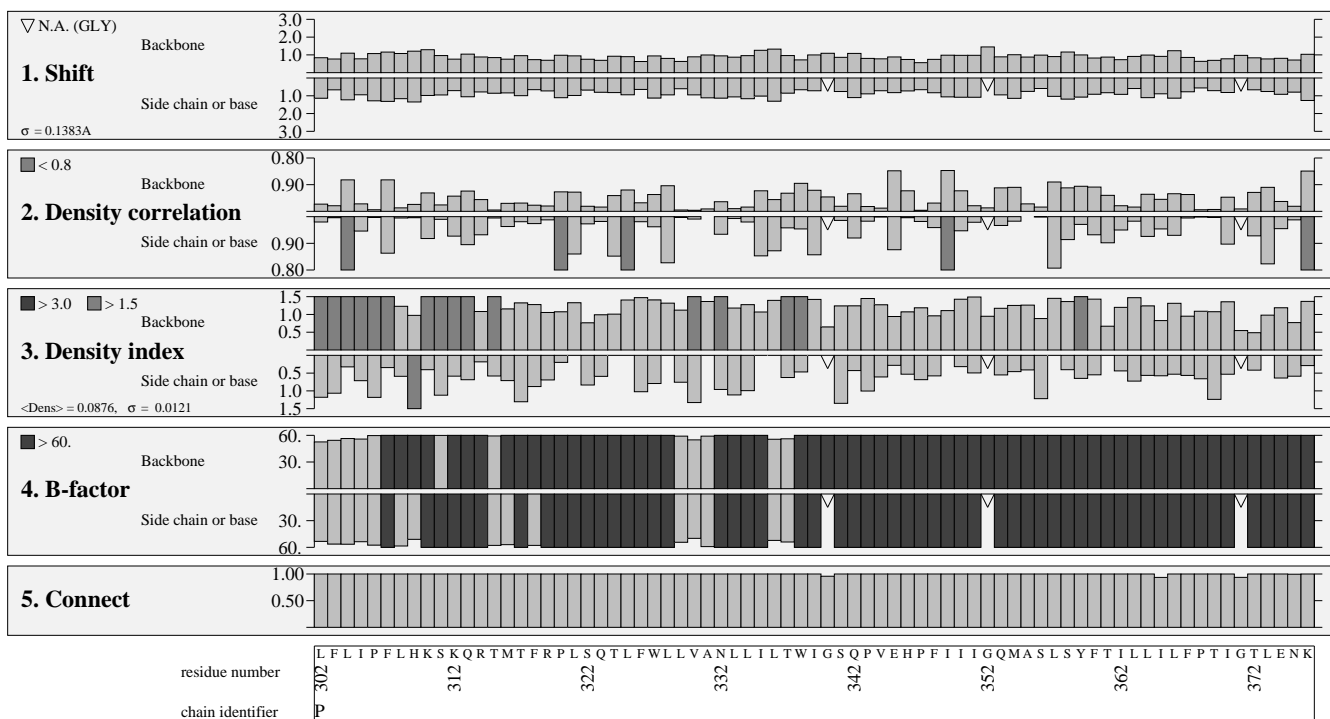
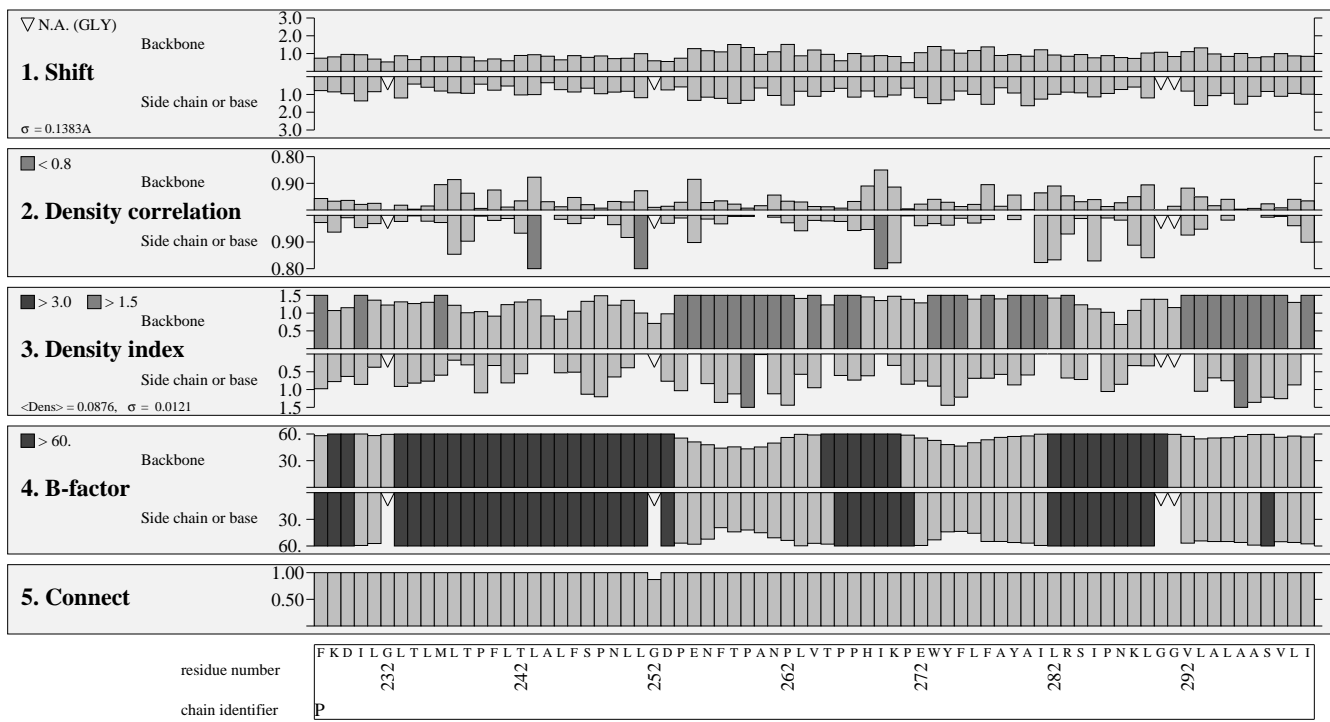
### Local estimation (21)



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### Local estimation (22)

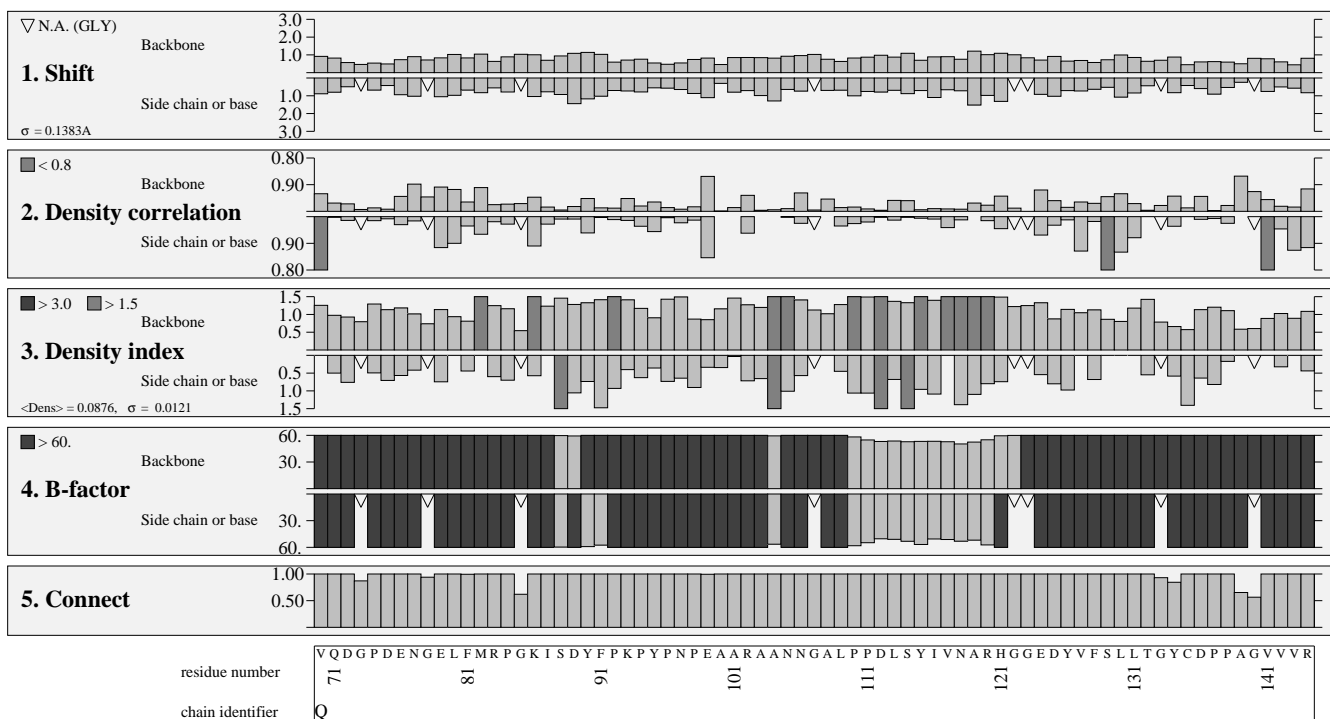
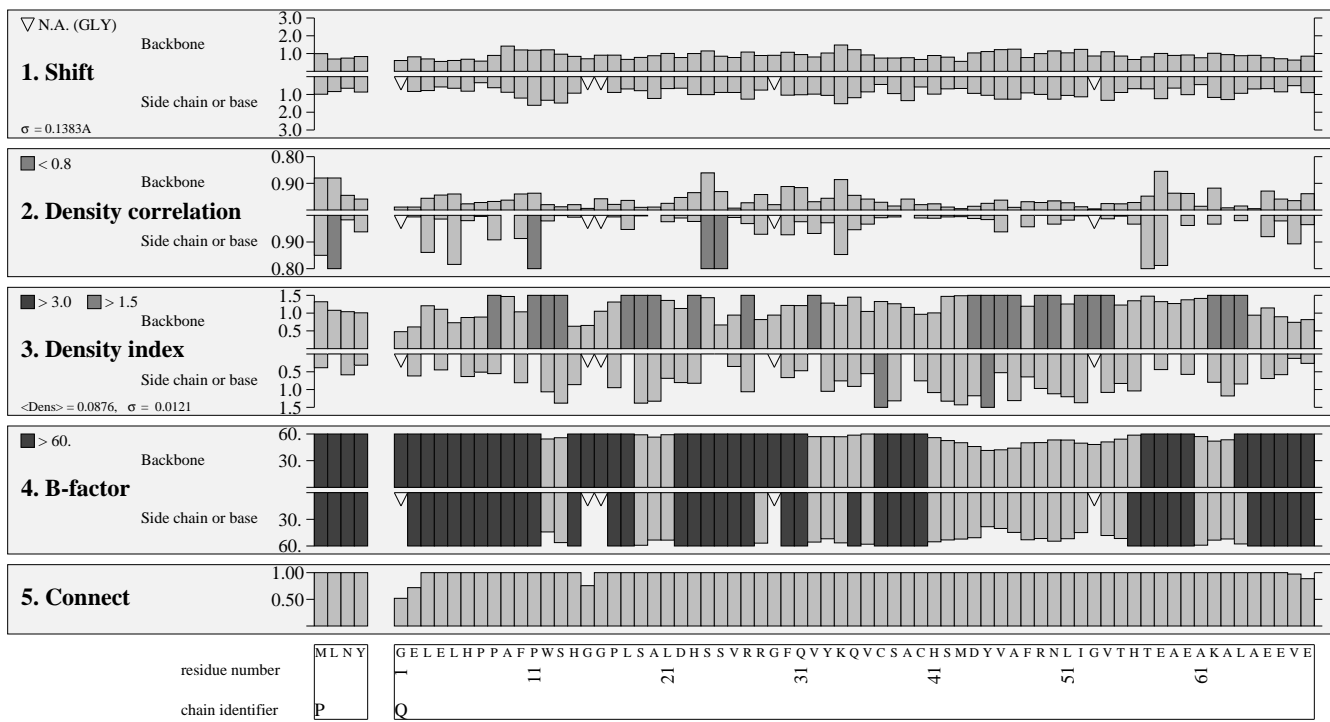




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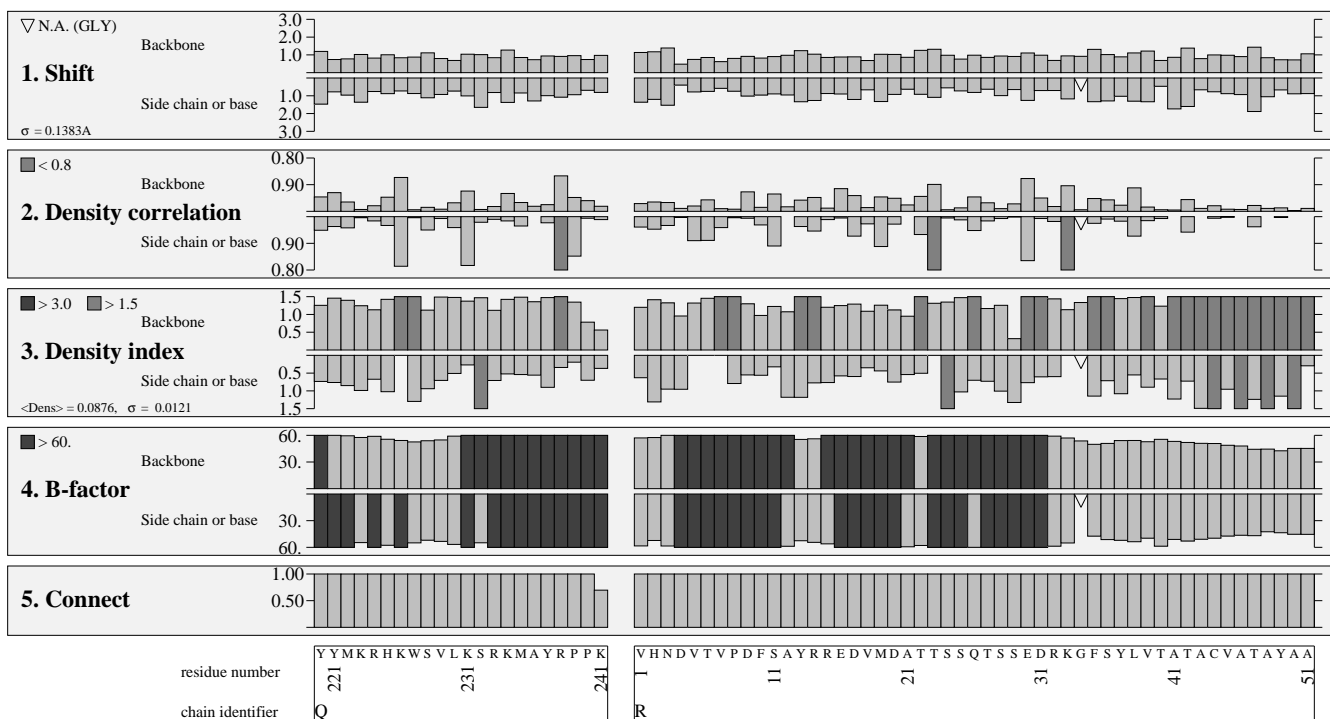
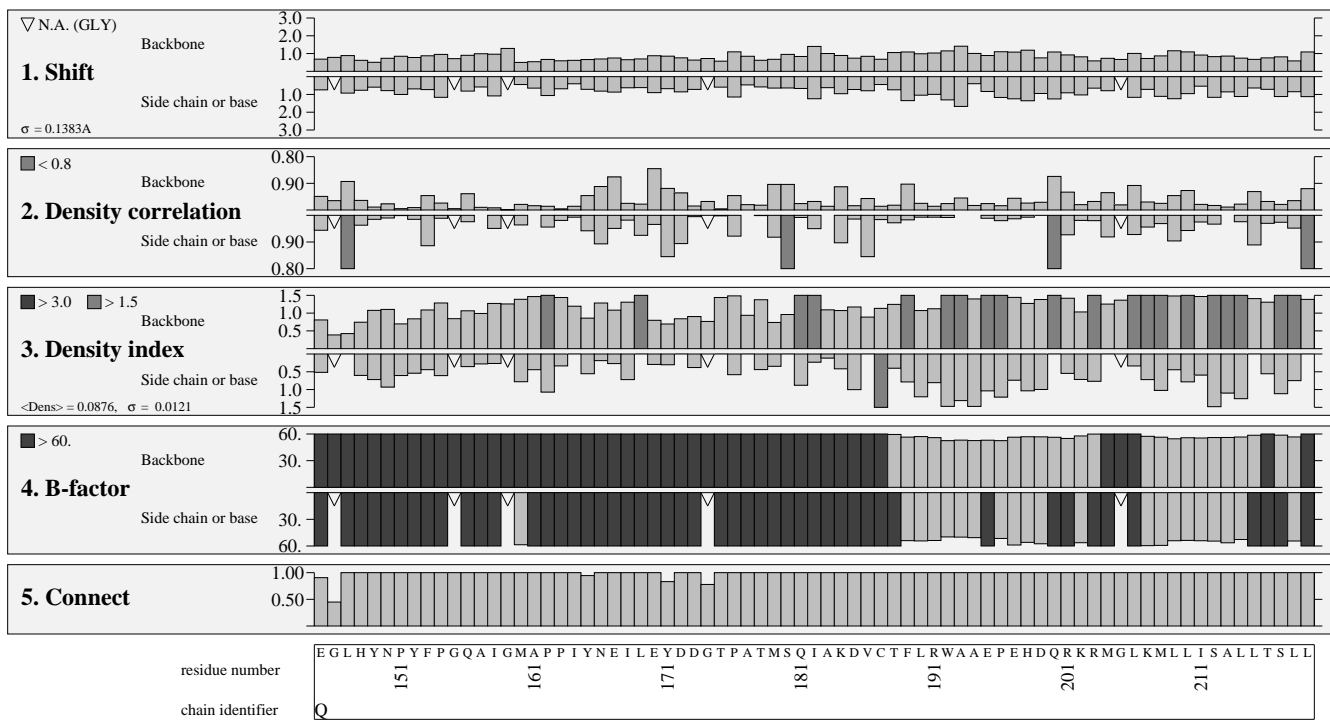
### Local estimation (23)



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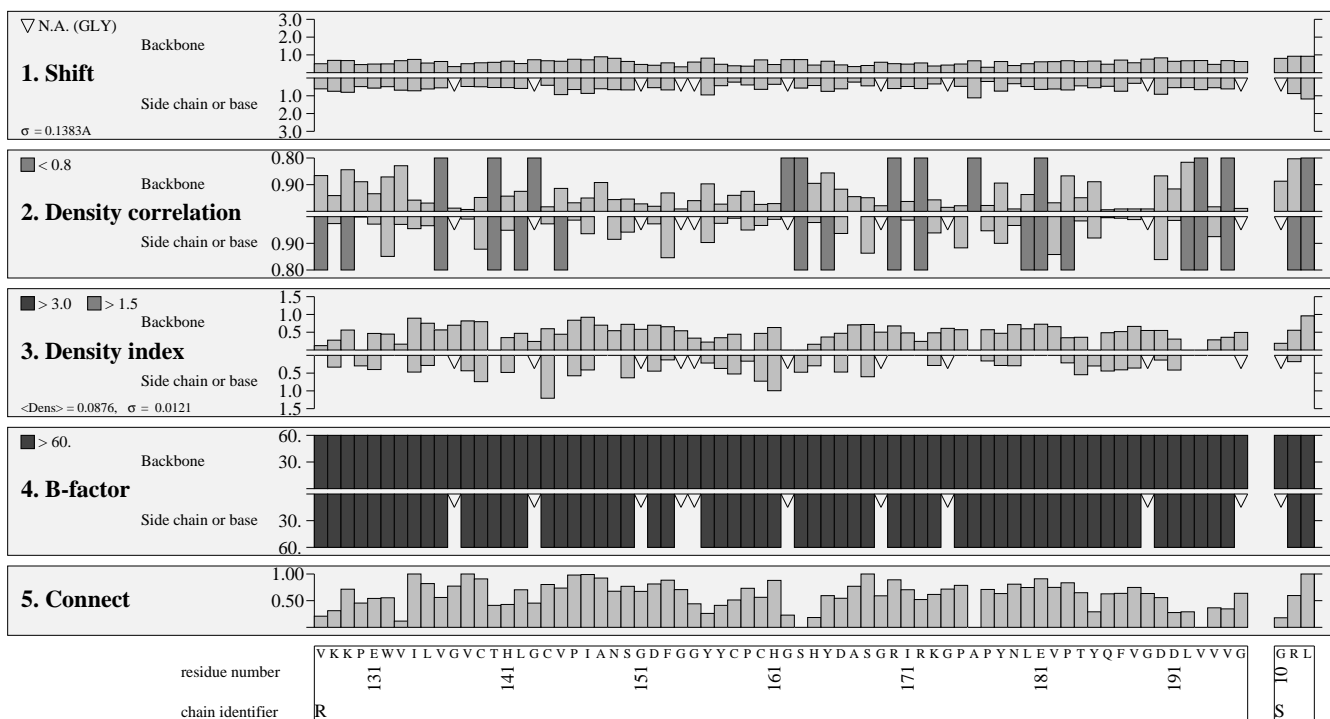
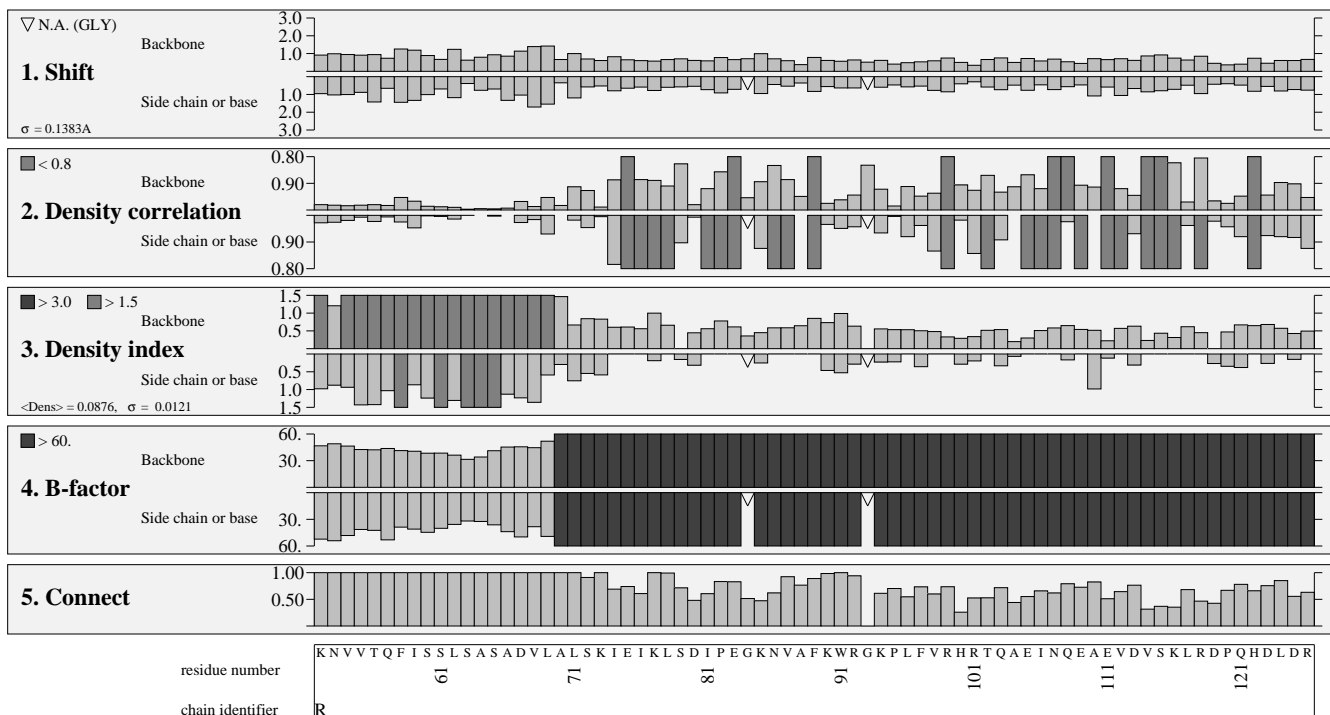
### Local estimation (24)



# Structure Factor Check

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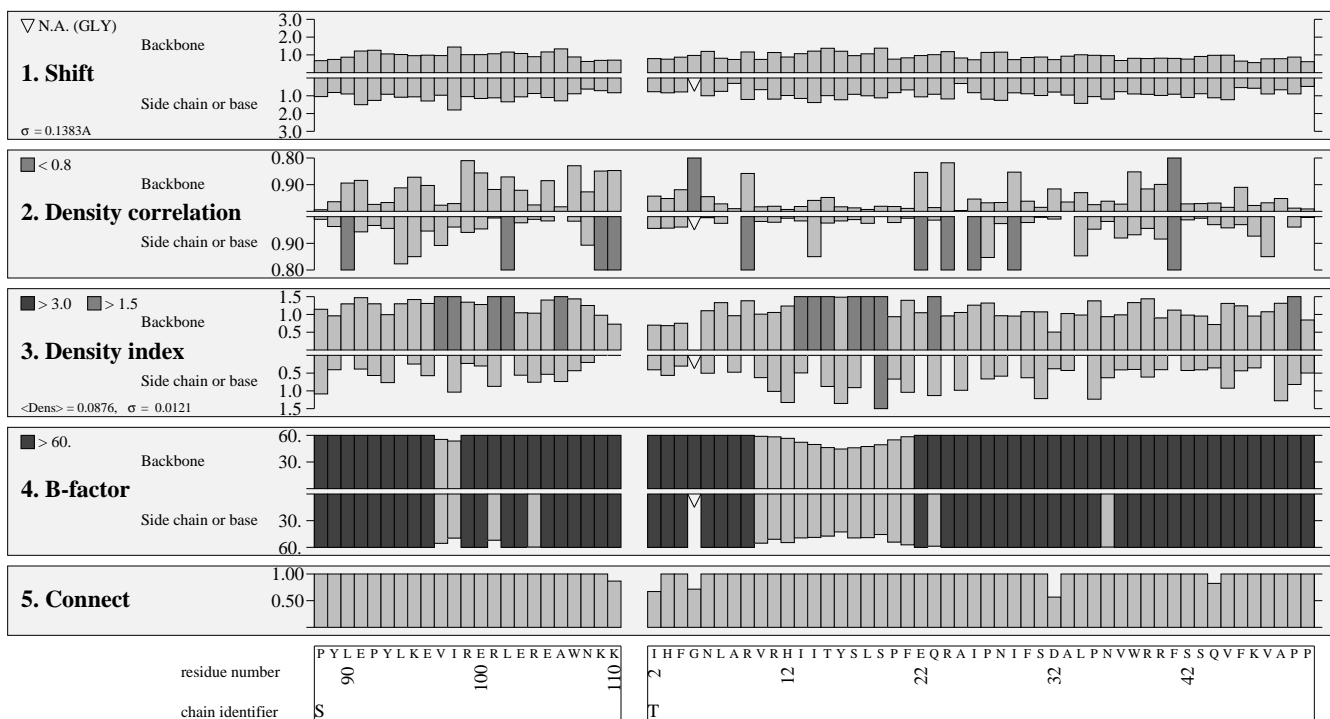
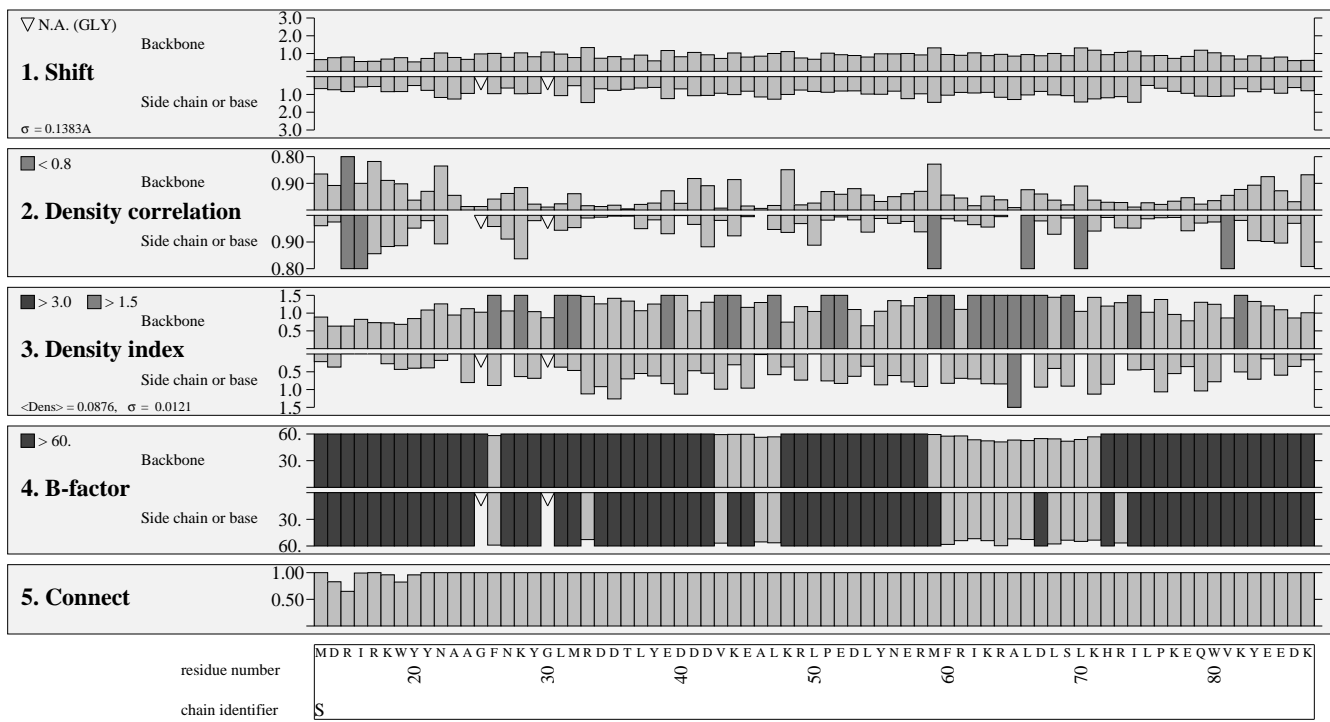
### Local estimation (25)



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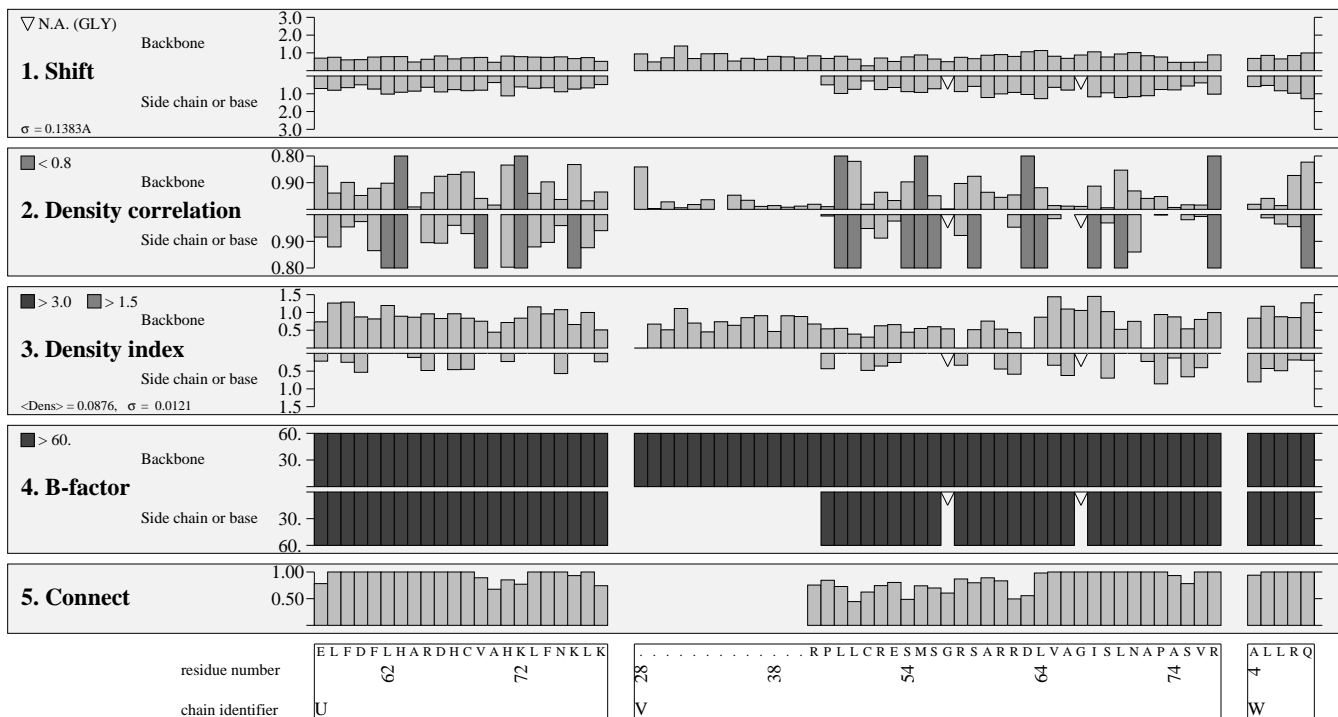
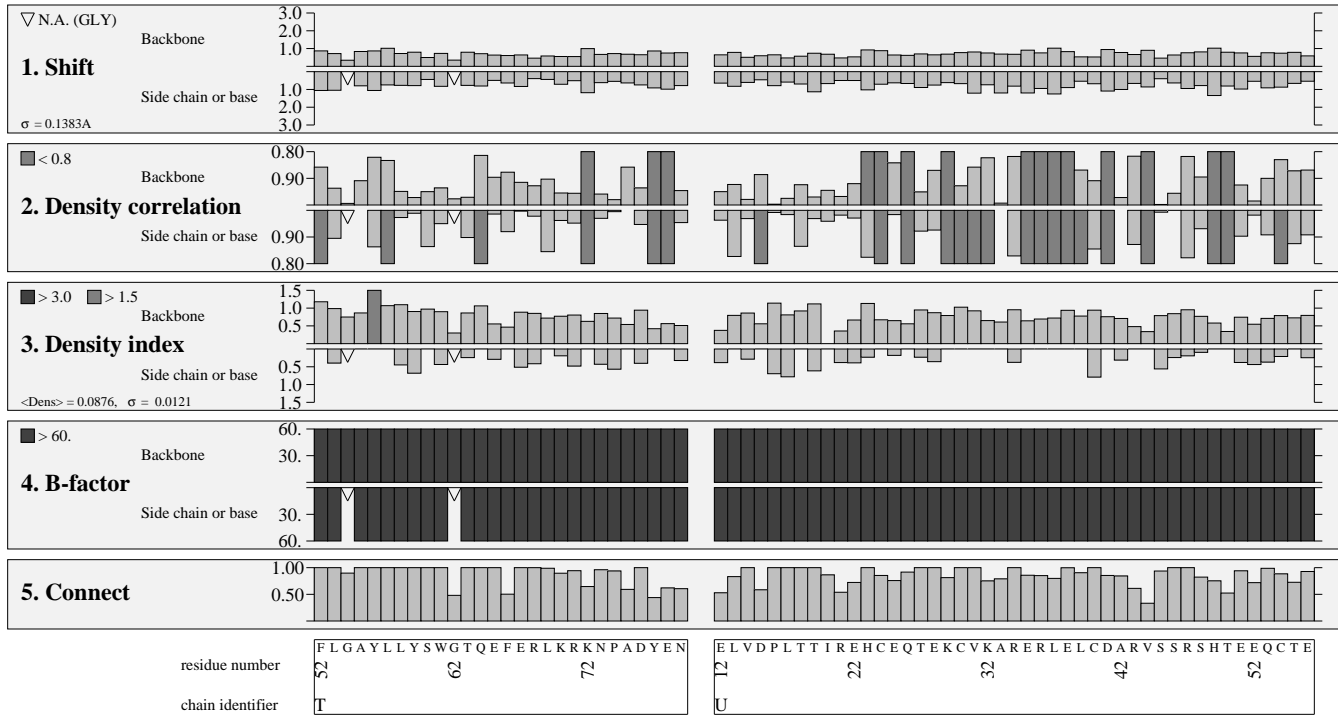
### Local estimation (26)



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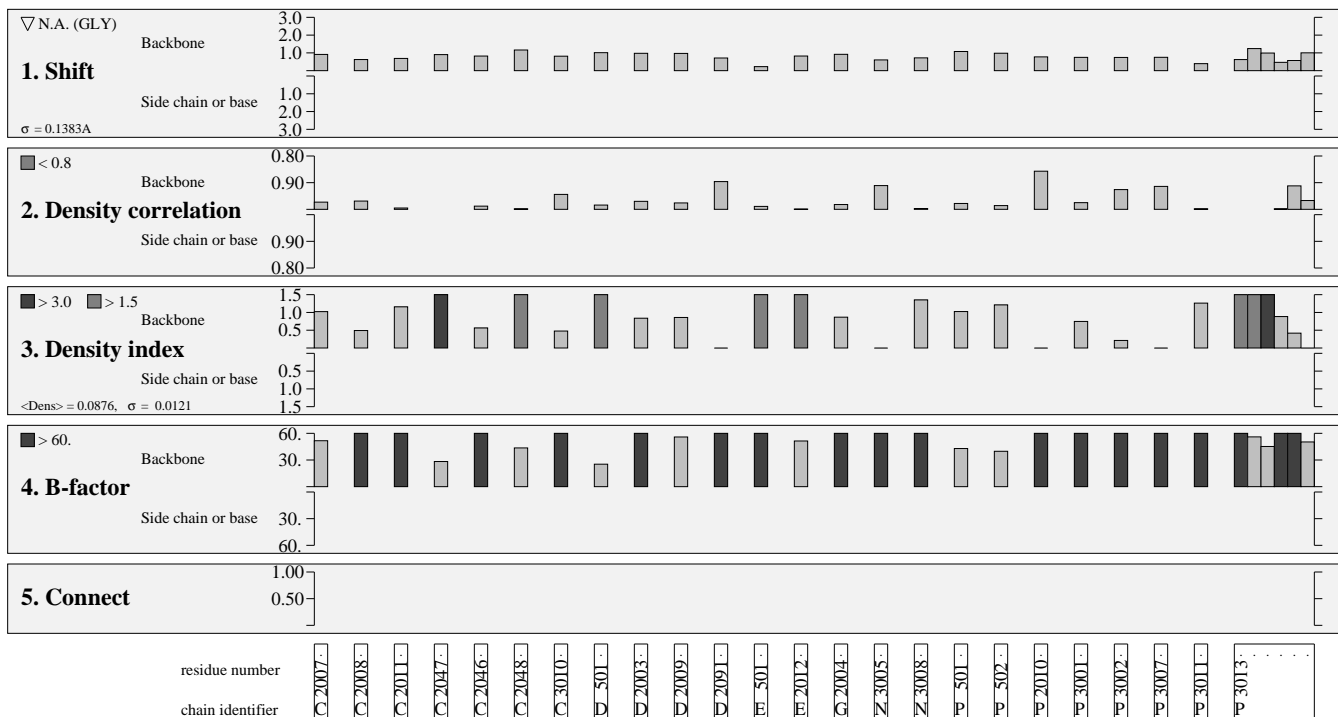
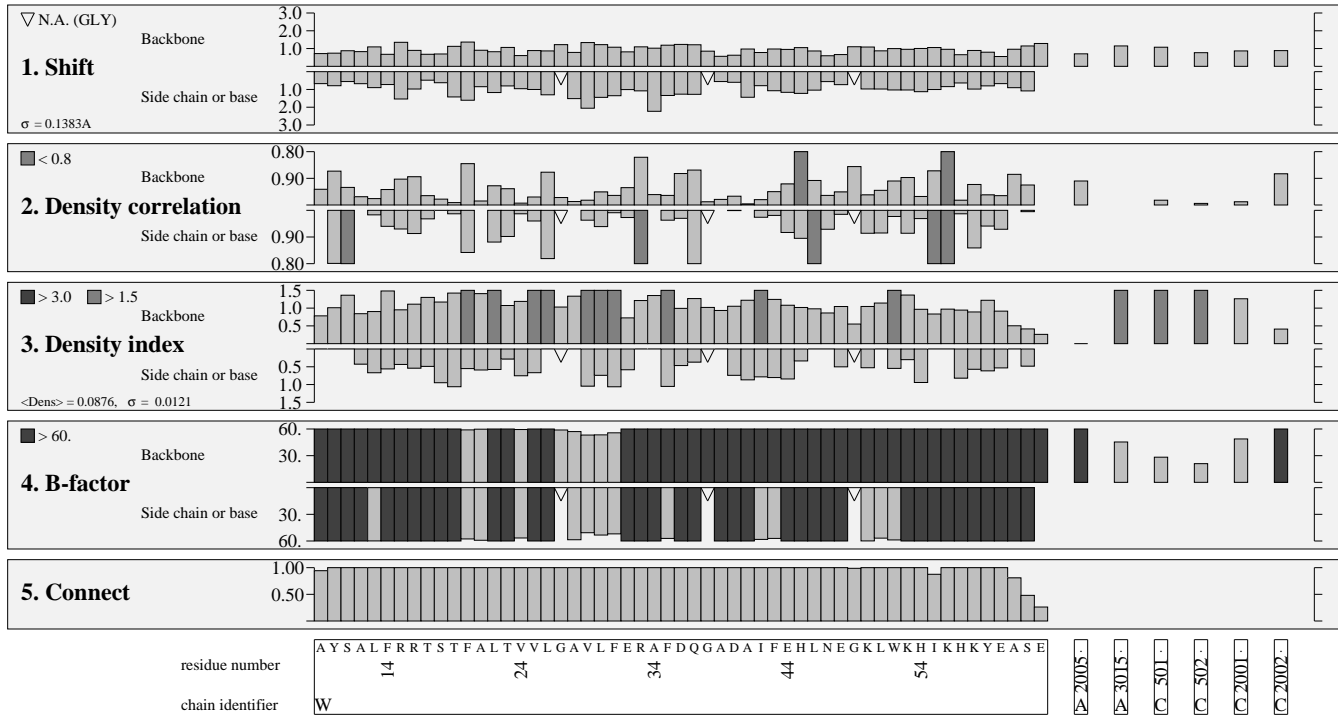
### Local estimation (27)



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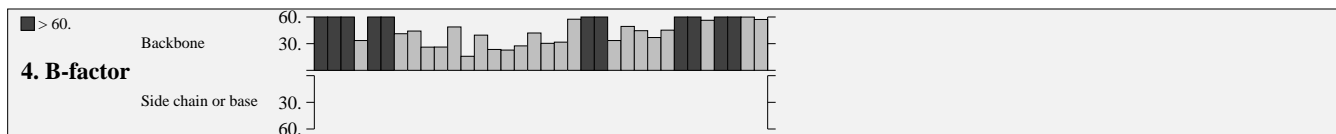
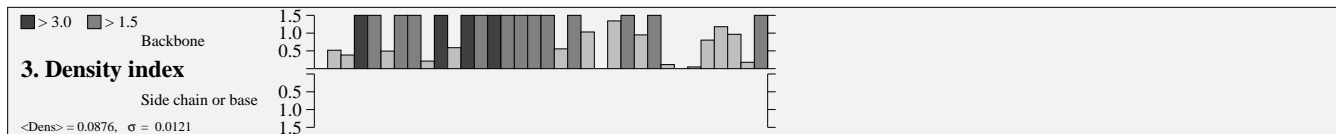
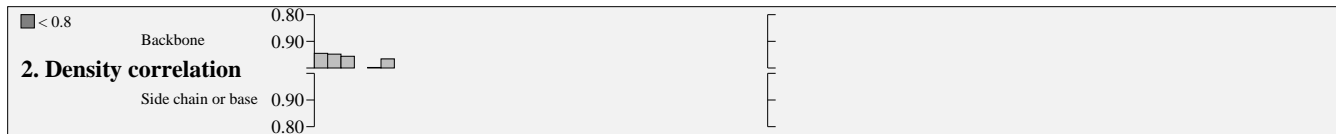
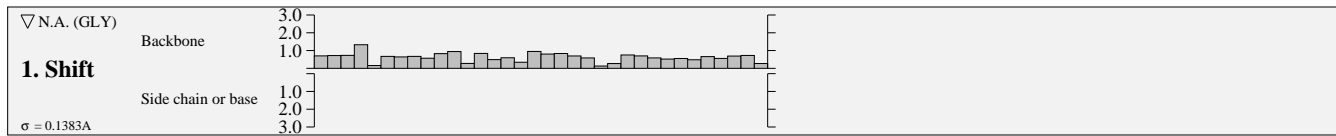
### Local estimation (28)



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### Local estimation (29)



residue number	chain identifier
501	P
387	P
387	P