

# Structure Factor Check

## 3VR8

Title: MITOCHONDRIAL RHODOQUINOL-FUMARATE REDUCTASE FROM THE PARASI  
NEMATODE ASCARIS SUUM  
Date: 07-APR-12  
PDB code: 3VR8

### Crystal

Cell parameters:

a: 123.71 A    b: 129.09 A    c: 221.17 A  
 $\alpha$ : 90.00     $\beta$ : 90.00     $\gamma$ : 90.00

Space group: P 21 21 21

### Structure Factors

#### Input

Nominal resolution range: 48.6 – 2.81 A  
 Reflections in file: 80036  
 Unique reflections above 0: 80036  
                                   above 1 $\sigma$ : 78869  
                                   above 3 $\sigma$ : 48126

#### SFCHECK

Nominal resolution range: 48.6 – 2.81 A  
\05max. from input data, min. from author\05  
 Used reflections: 80028  
 Reflections out of resolution: 8  
 Completeness: 92.2 %  
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$  : 0.082  
 Anisotropic distribution of Structure Factors  
     ratio of eigen values: 1.0000 0.9302 0.9688  
 $B_{\text{overall}}$  (by Patterson): 57. A<sup>2</sup>  
 Optical resolution: 2.21 A  
 Expected opt. resol. for complete data set: 2.21 A  
 Estimated minimal error: 0.074 A

### Model

18232 atoms  
 Number of chains: 24  
 Volume not occupied by model: 55.8 %  
 $\langle B \rangle$  (for atomic model): 92.2 A<sup>2</sup>  
 $\sigma(B)$ : 7.56 A<sup>2</sup>  
 Matthews coefficient: 3.46  
 Corresponding solvent % : 64.16

### Model vs. Structure Factors

R-factor for all reflections: 0.298  
 Correlation factor: 0.868  
 R-factor: 0.309  
     for  $F > 2.0\sigma$   
         nom. resolution range: 48.56 – 2.81A  
         reflections used: 78861  
 Rfree: 0.358  
 Nfree: 3965  
 R-factor without free-refl.: 0.306  
 Non free-reflections: 74896  
 $\langle u \rangle$  (error in coords by Luzzati plot): 0.546 A  
 Estimated maximal error: 0.223 A  
 DPI: 0.409 A

#### Scaling

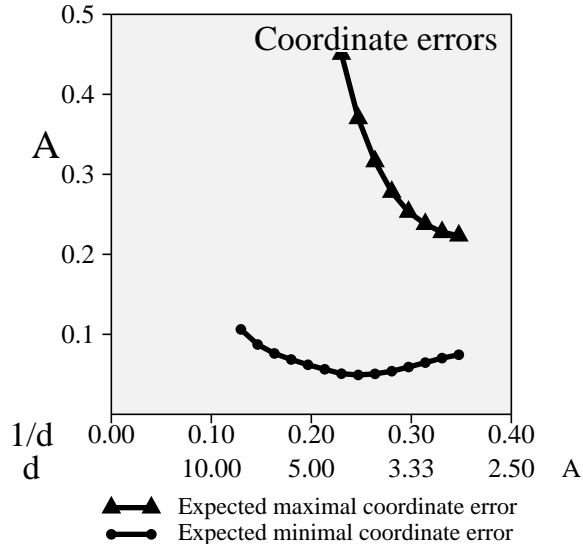
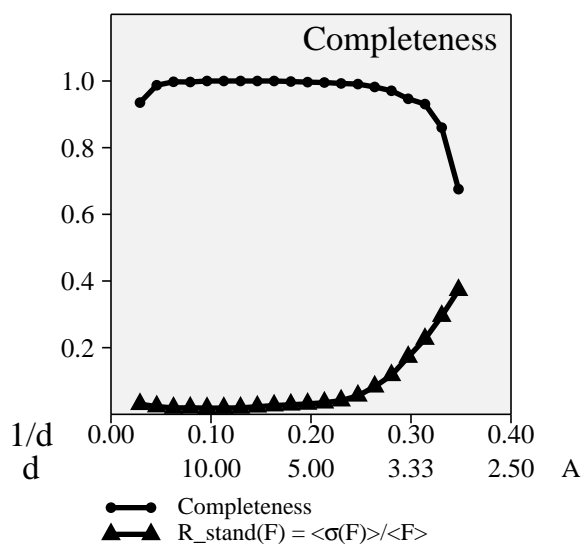
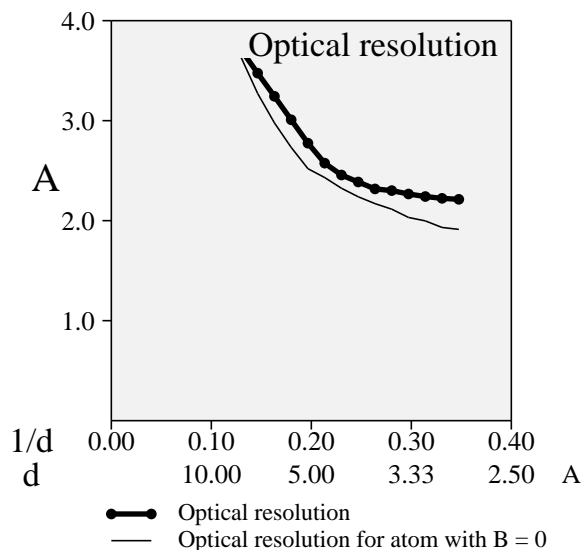
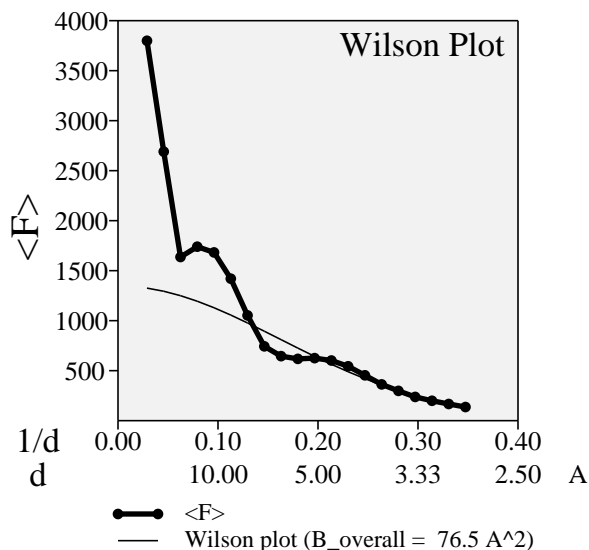
Scale: 0.797  
 Bdiff: -9.60  
 Anisothermal Scaling (Beta):  
     2.0022 1.0755 1.1452 0.0000 -0.0000 -0.0000  
 Solvent correction – Ks,Bs: 0.497 250.099

### Refinement

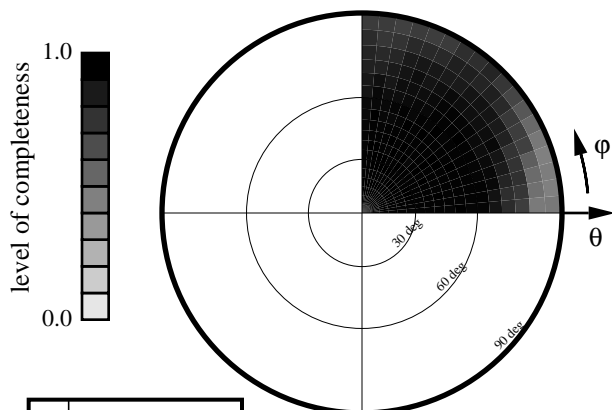
Program: REFMAC 5.5.0109  
 Nominal resolution range: 48.6 – 2.81 A  
 Reported R-factor: 0.231  
 Number of reflections used: 76011  
 Reported Rfree: 0.30  
 Sigma cut-off: N.A.

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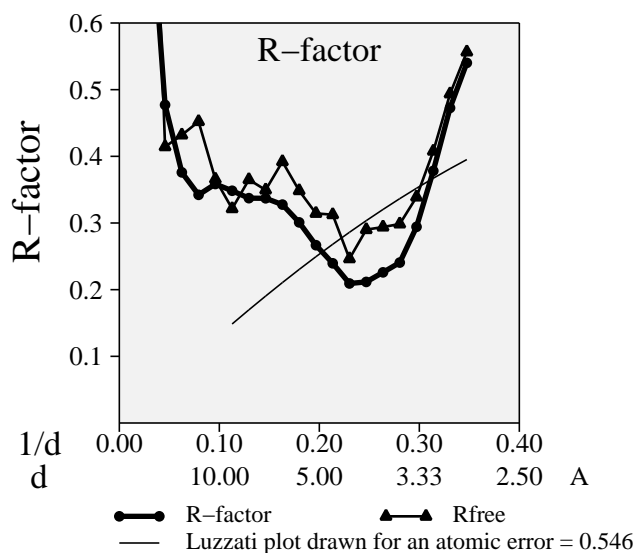


Stereographic projection of the averaged radial completeness



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

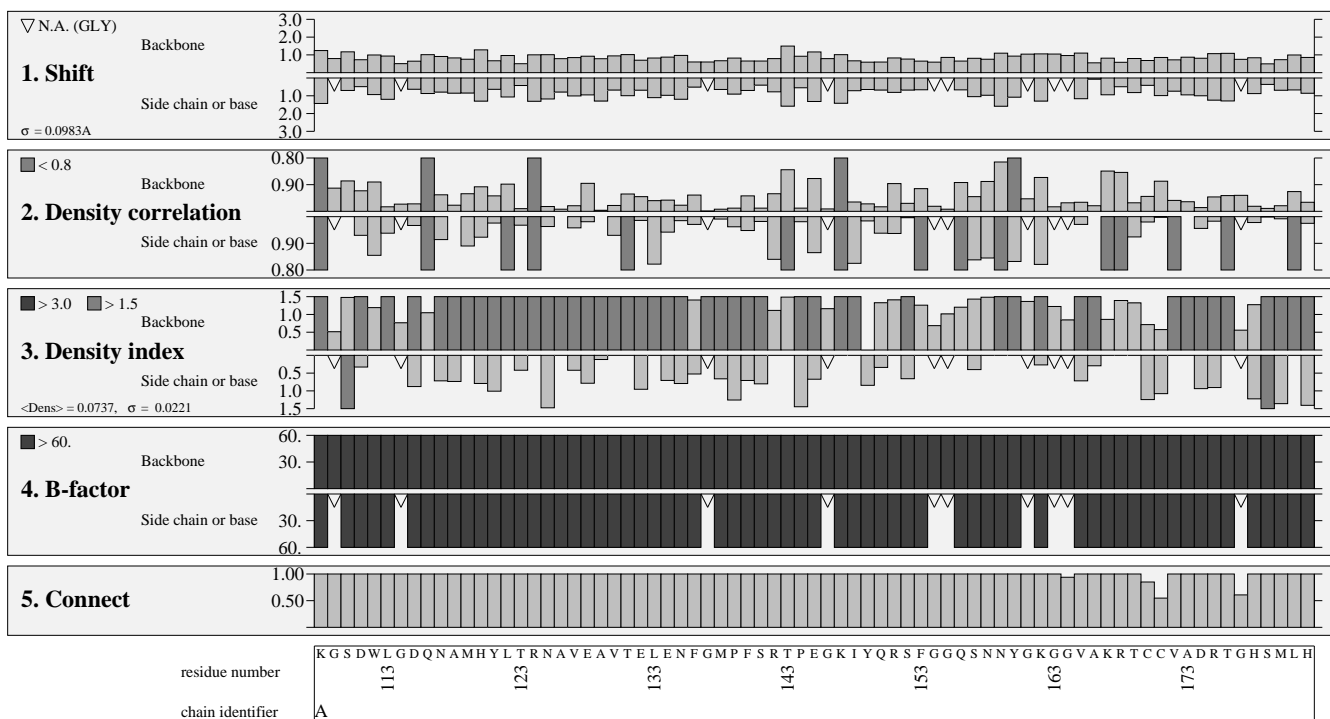
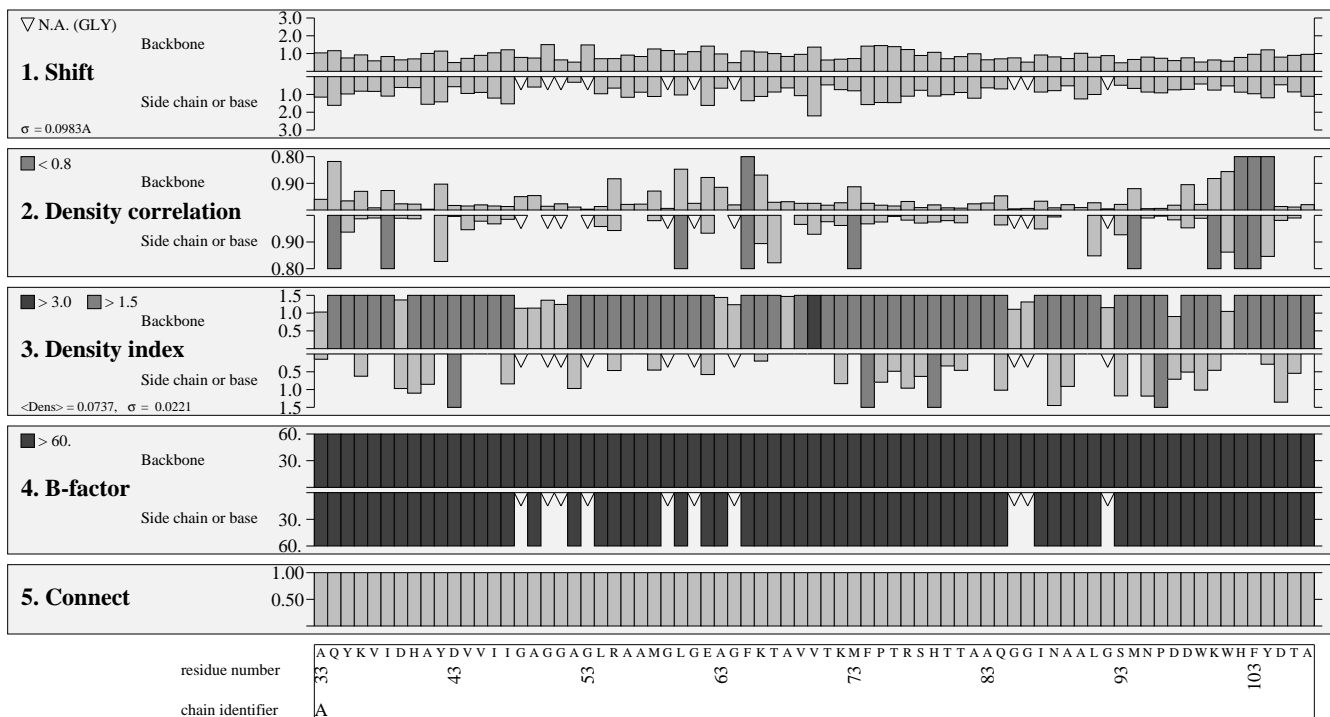
polar coordinates of the crystallographical axes



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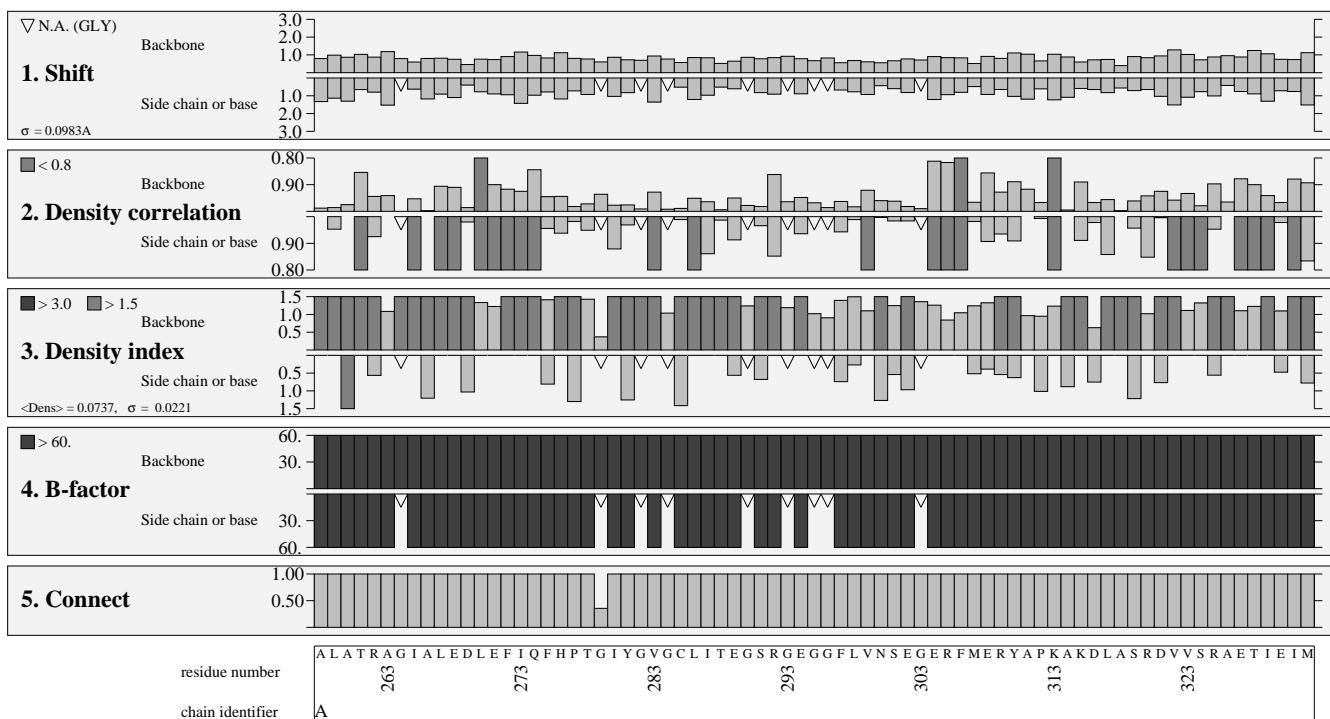
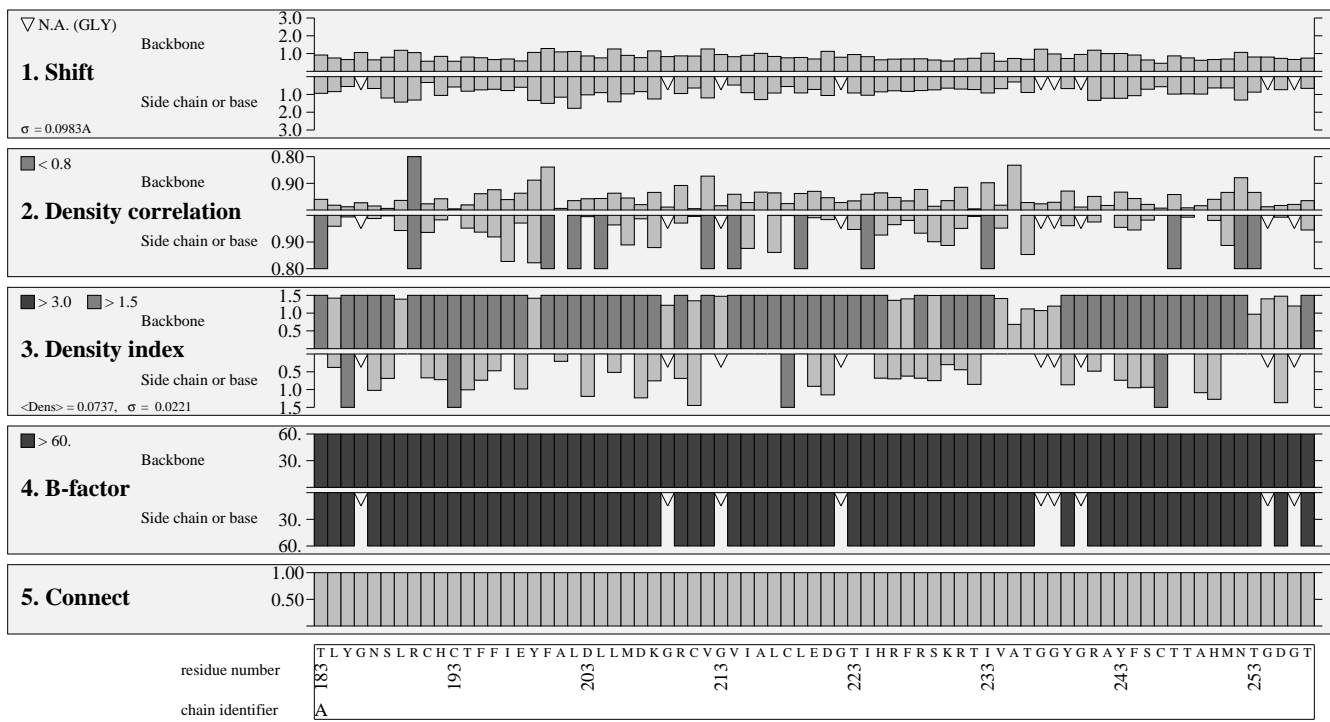
### Local estimation



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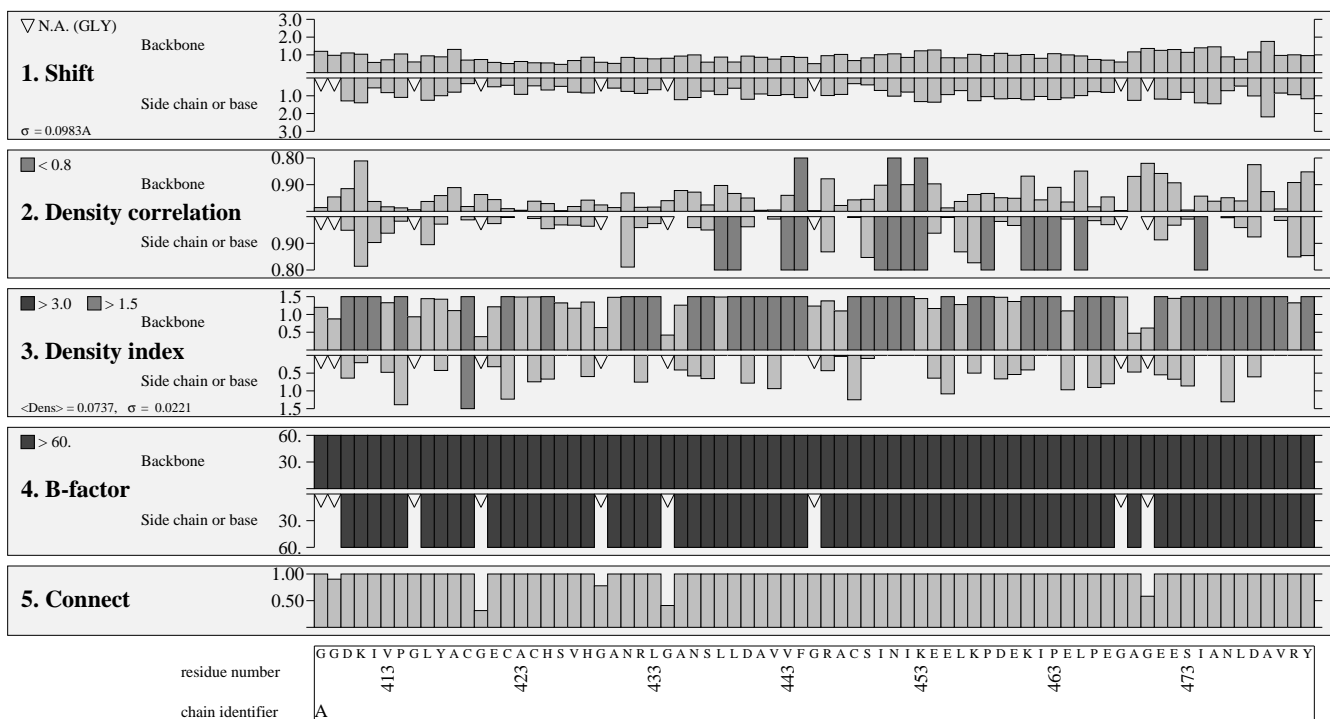
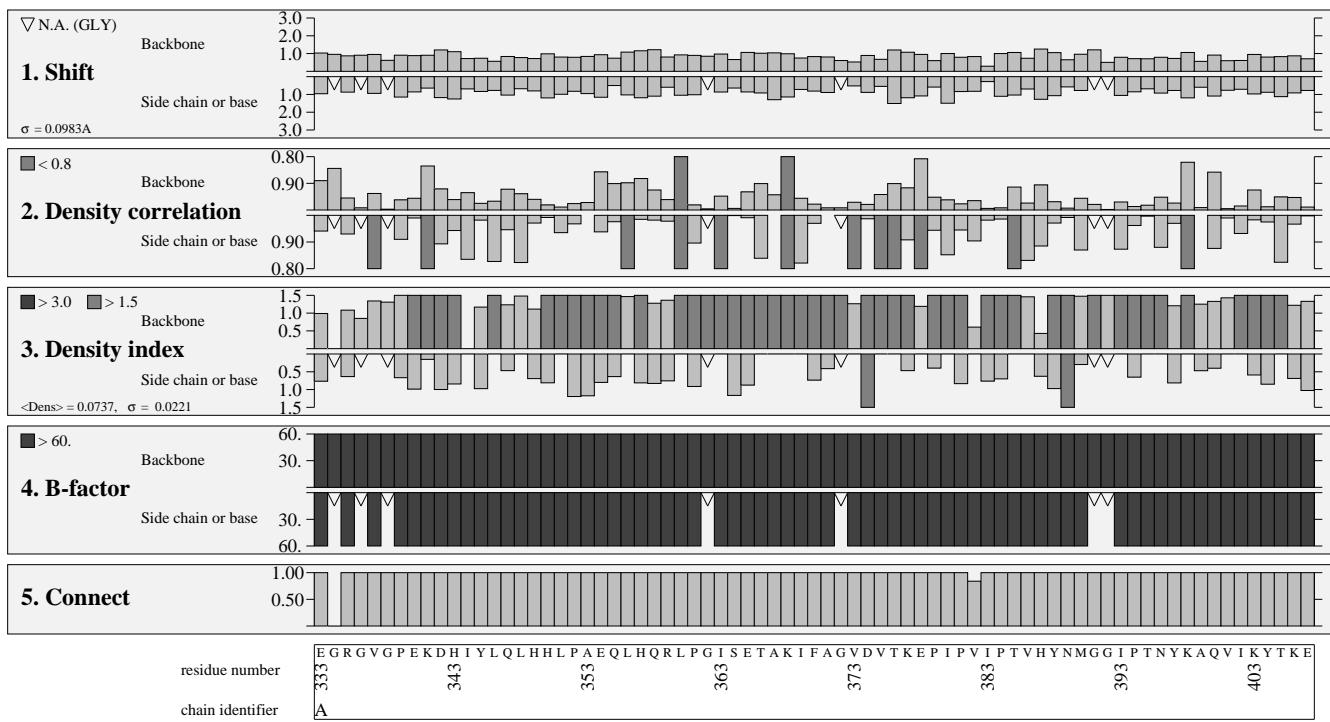
### Local estimation (2)



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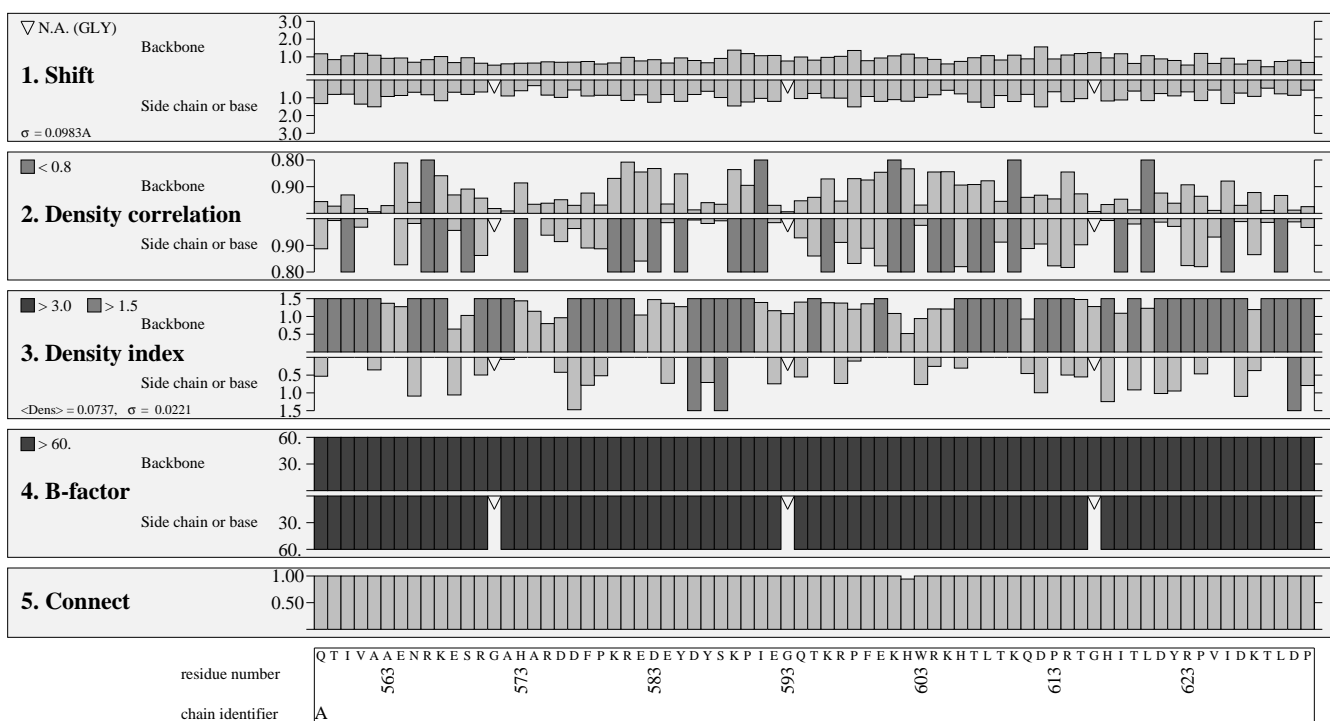
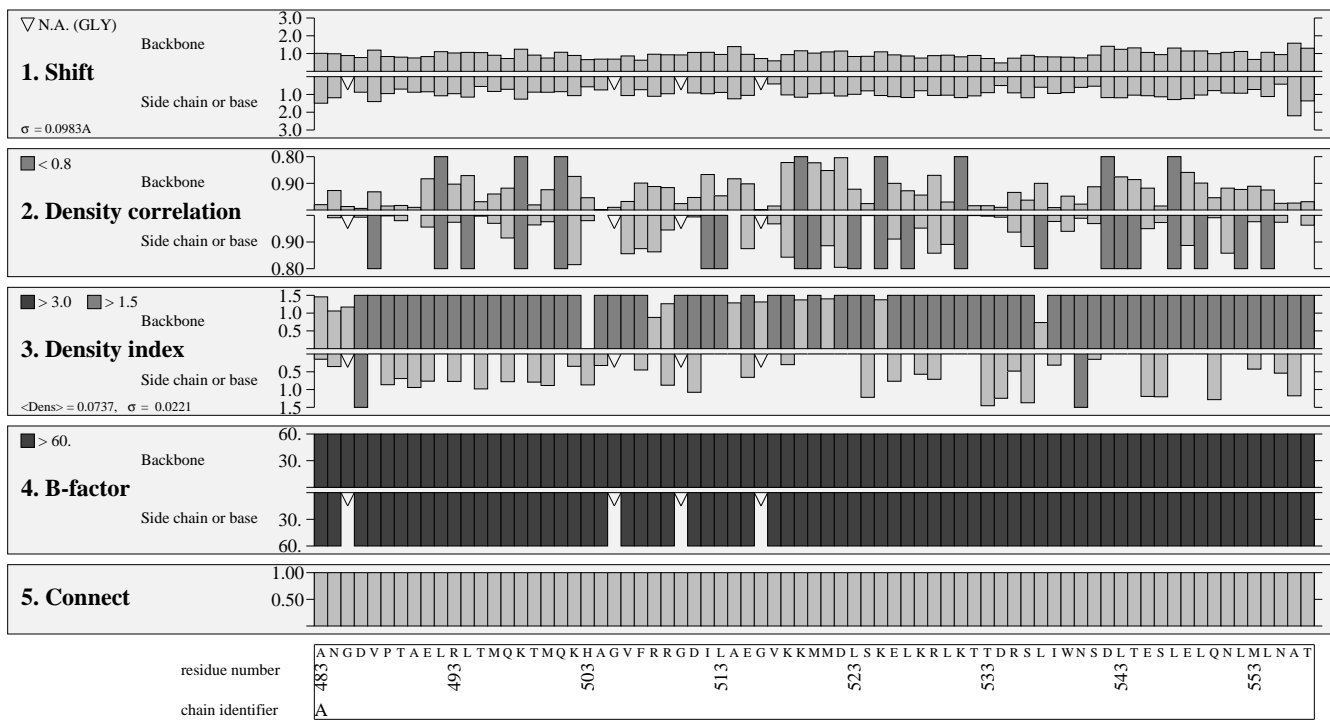
### Local estimation (3)



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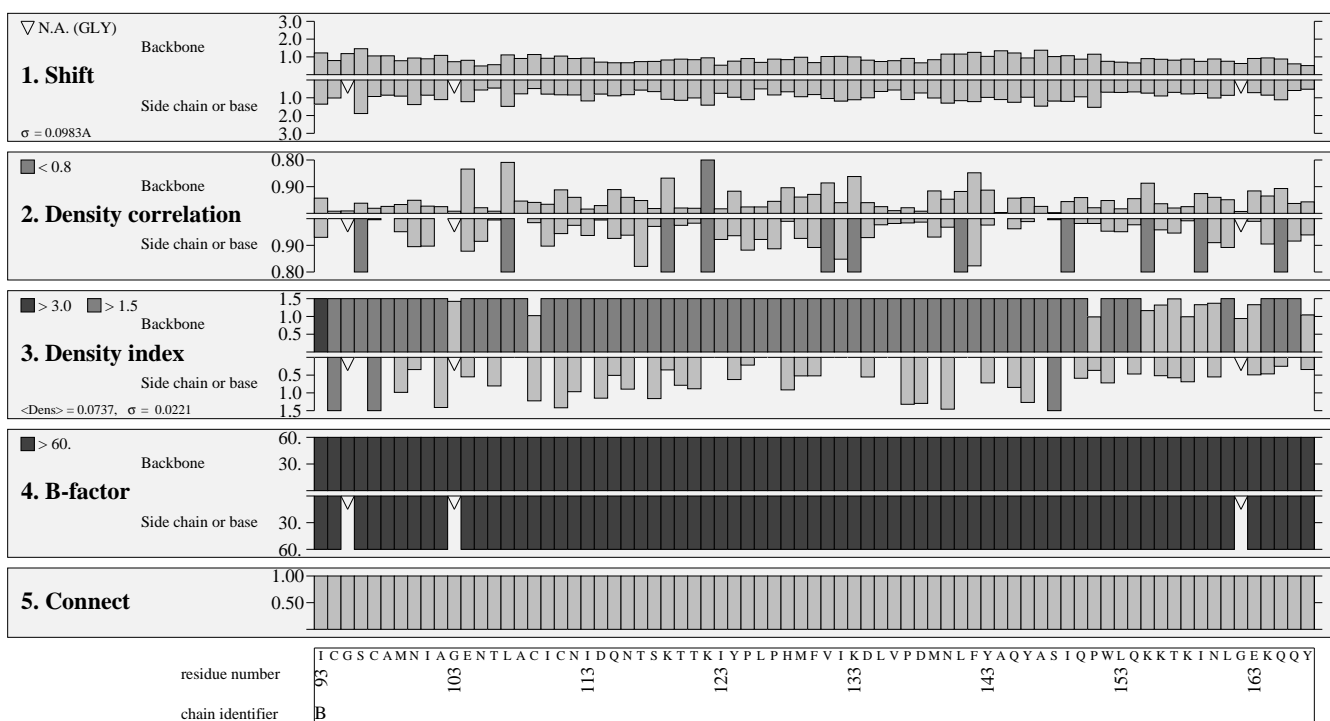
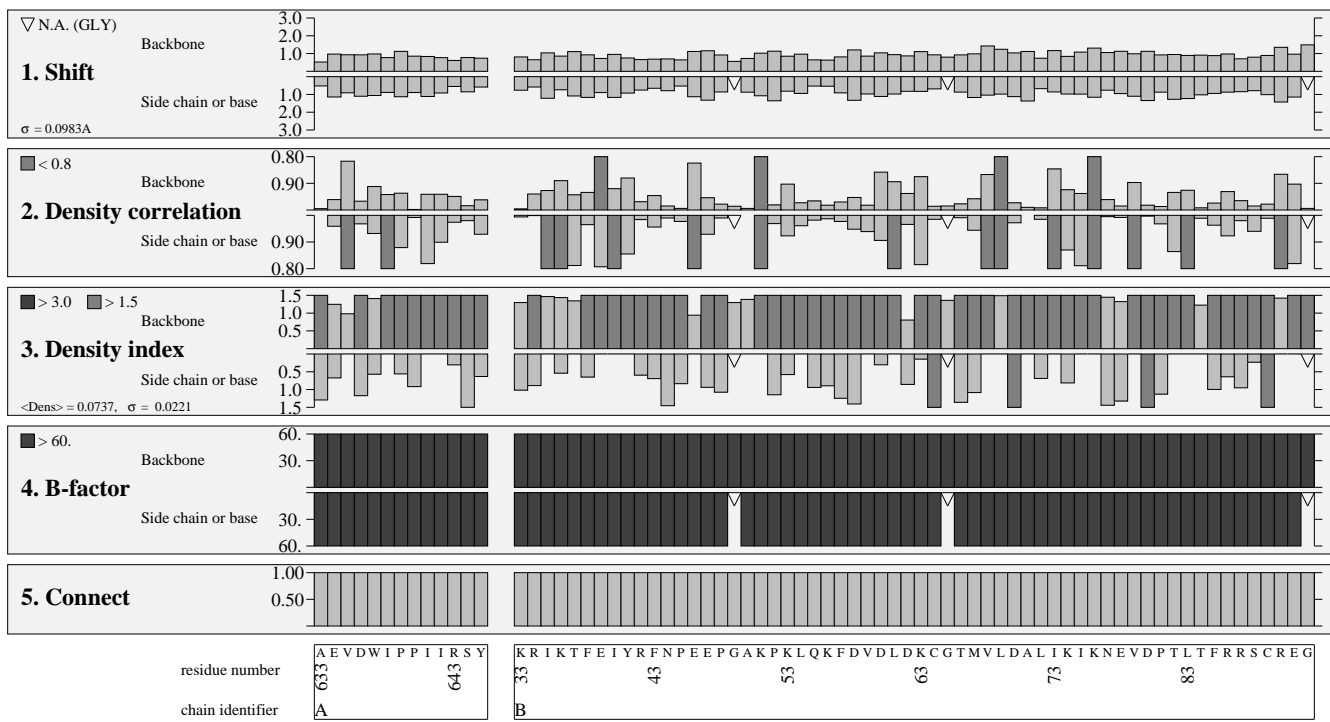
### Local estimation (4)



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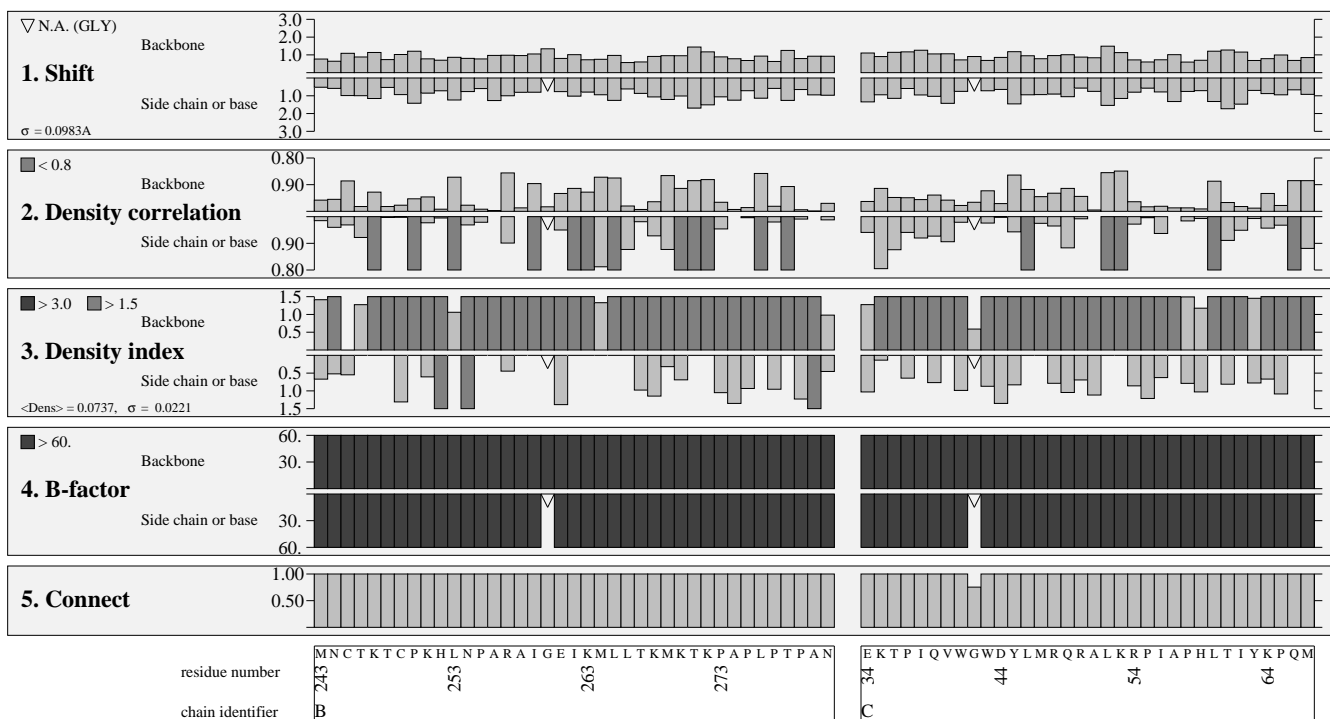
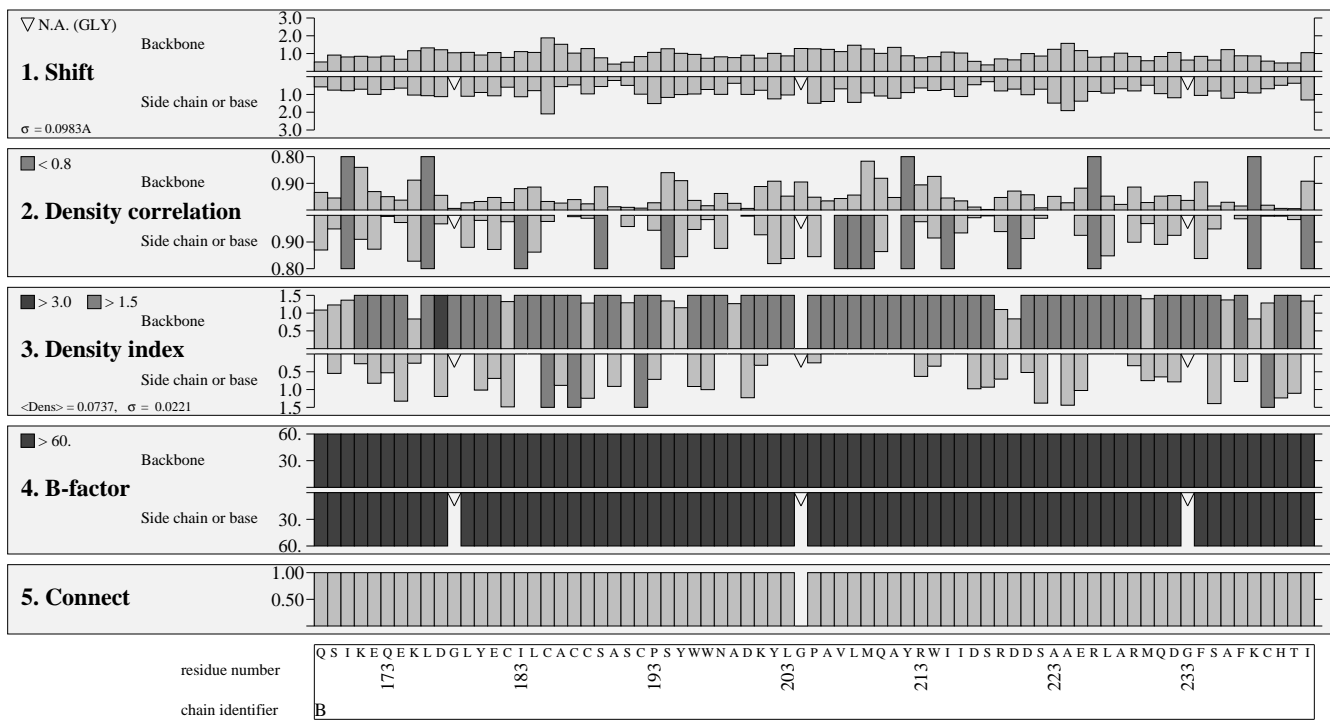
### Local estimation (5)



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### Local estimation (6)

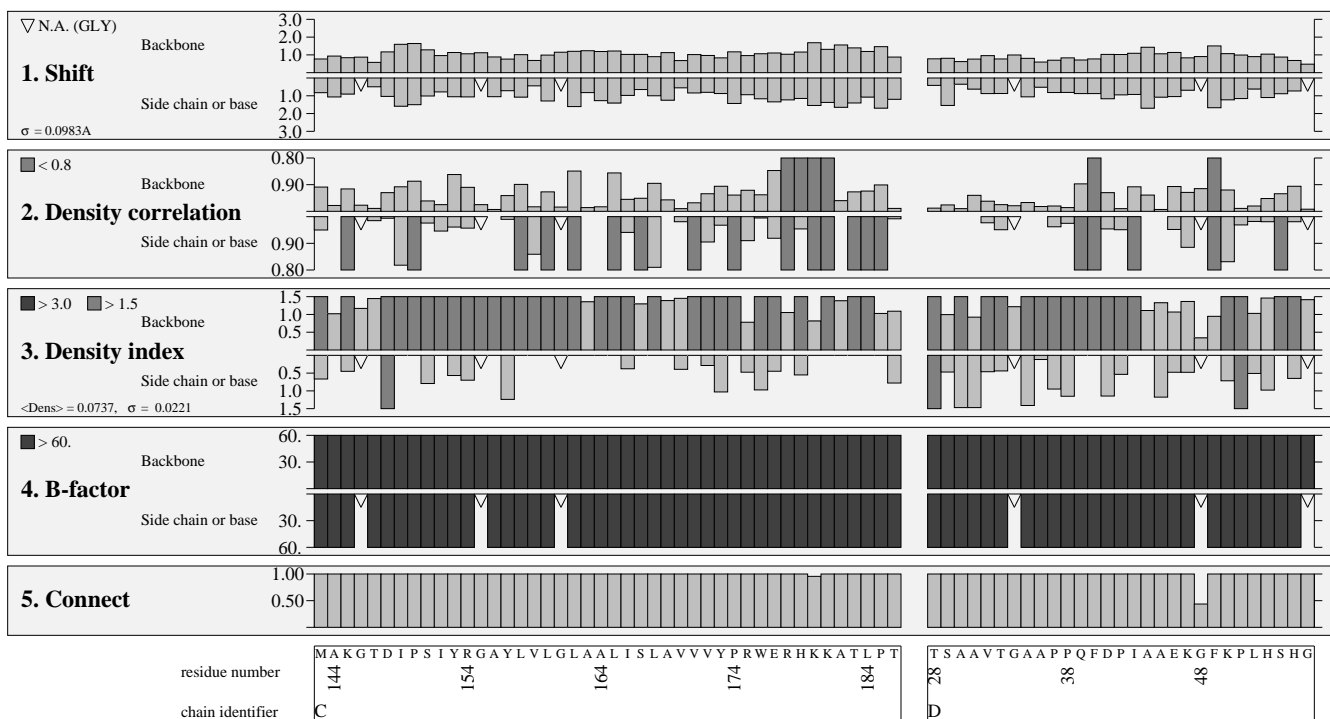
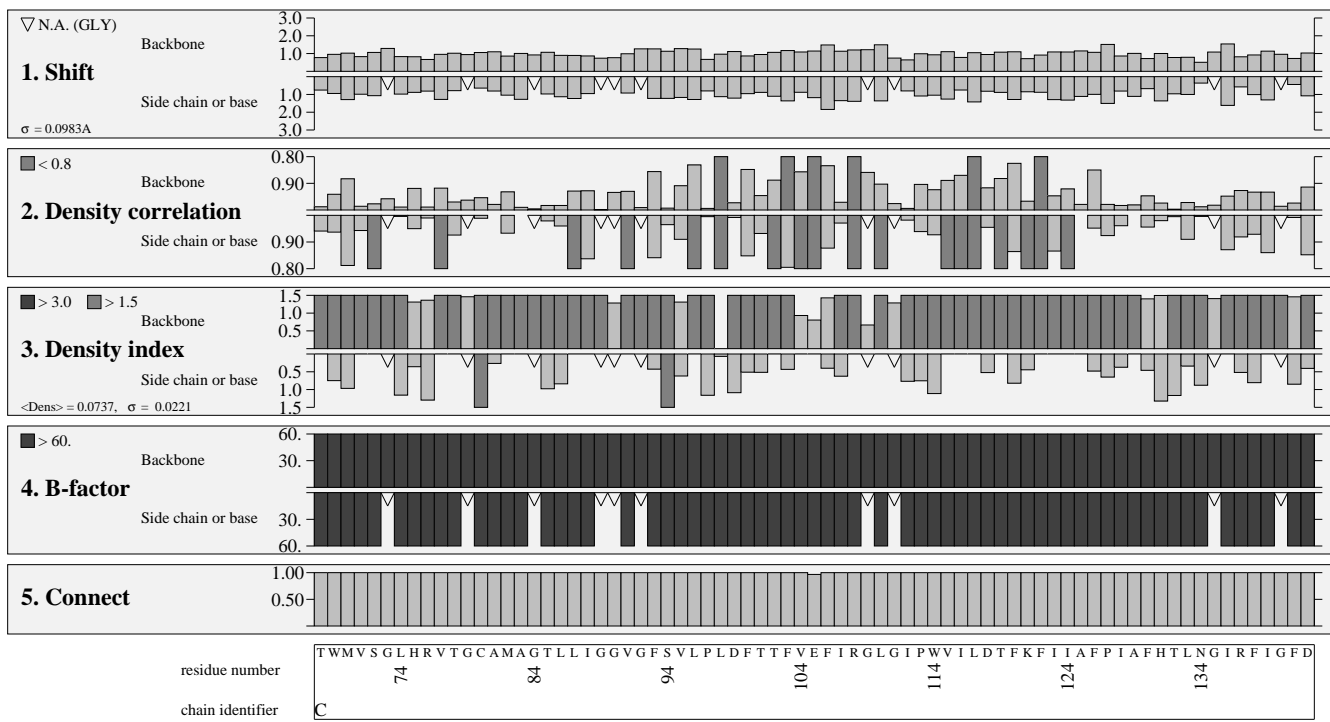




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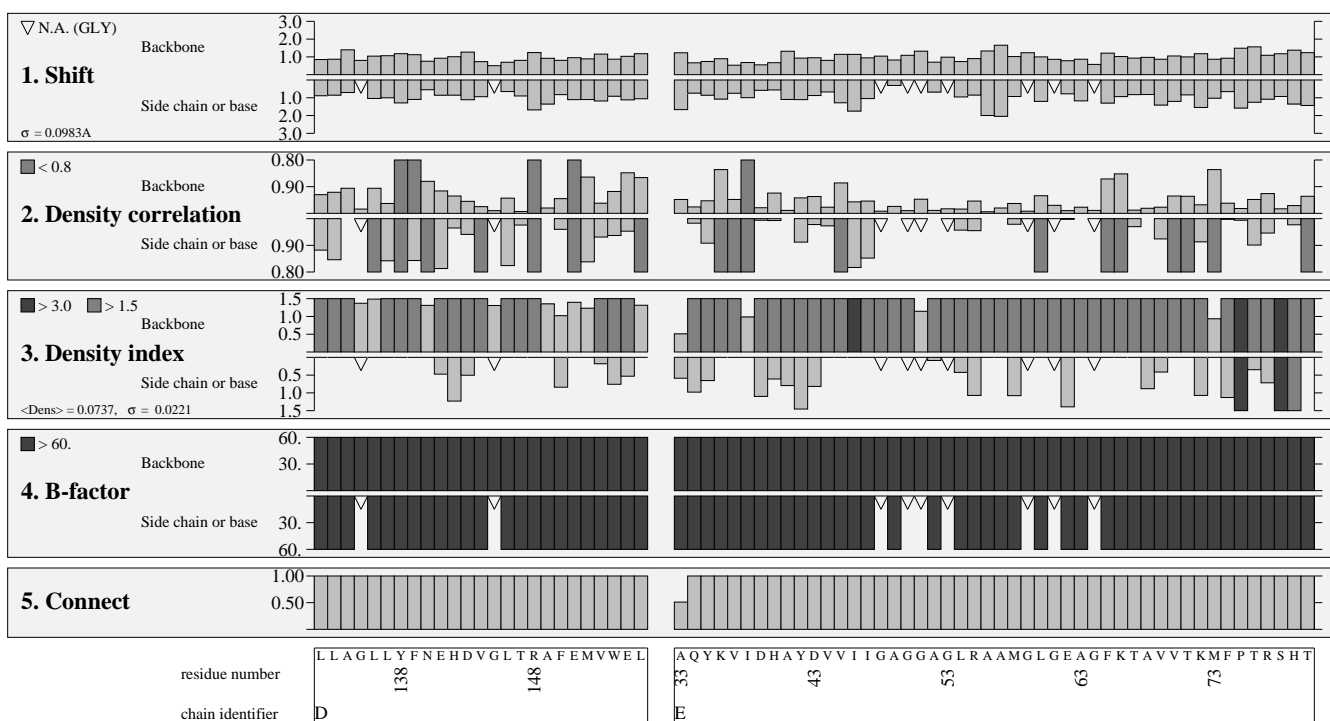
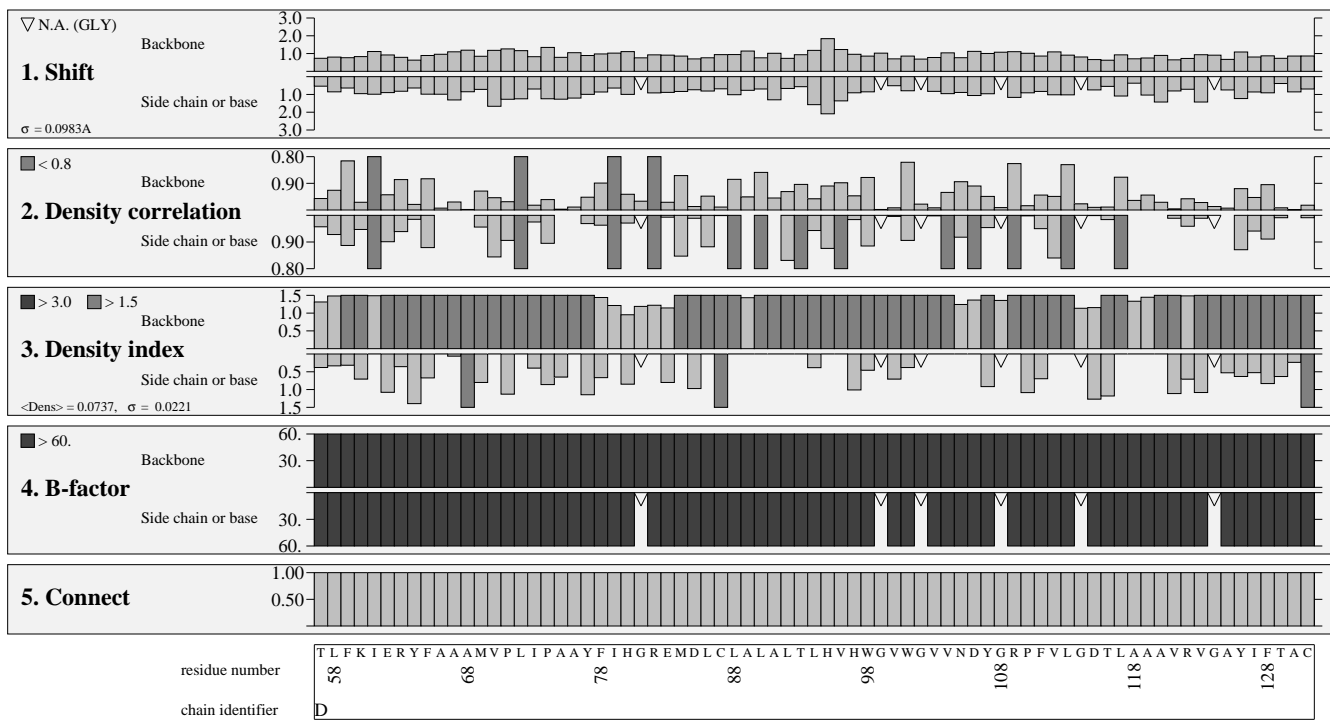
### Local estimation (7)



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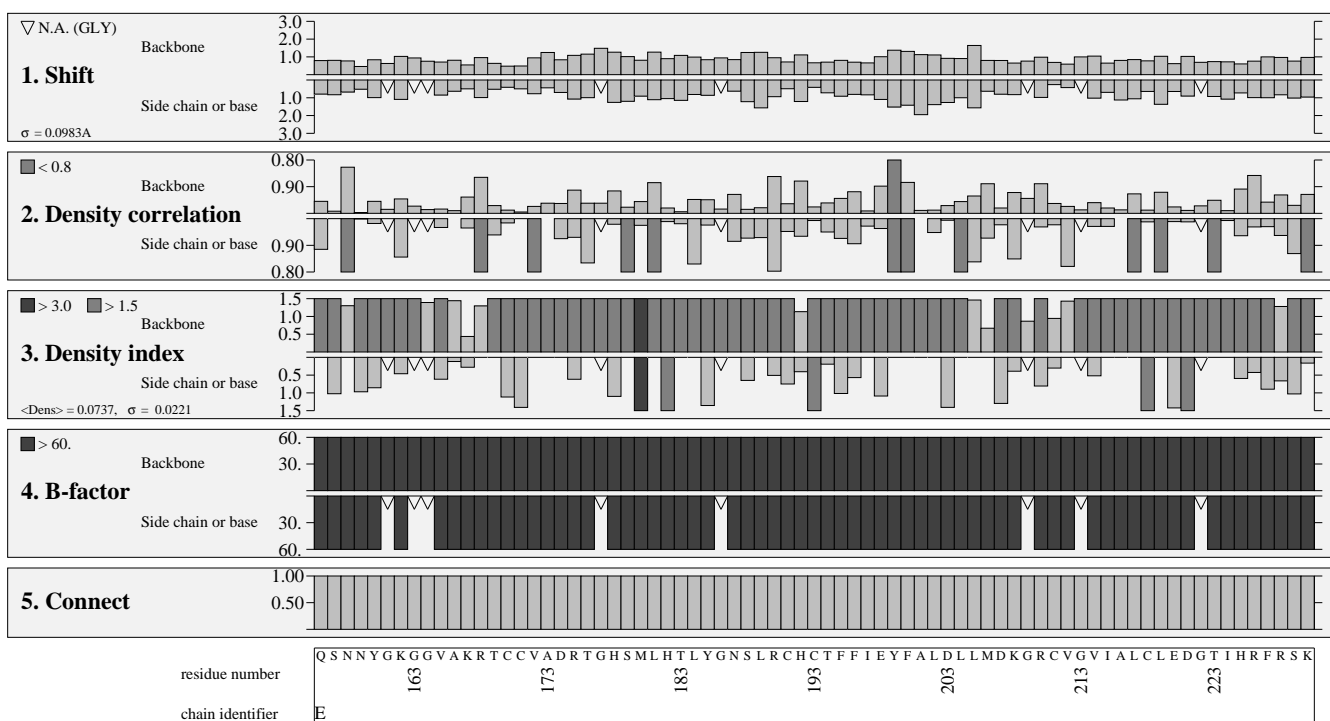
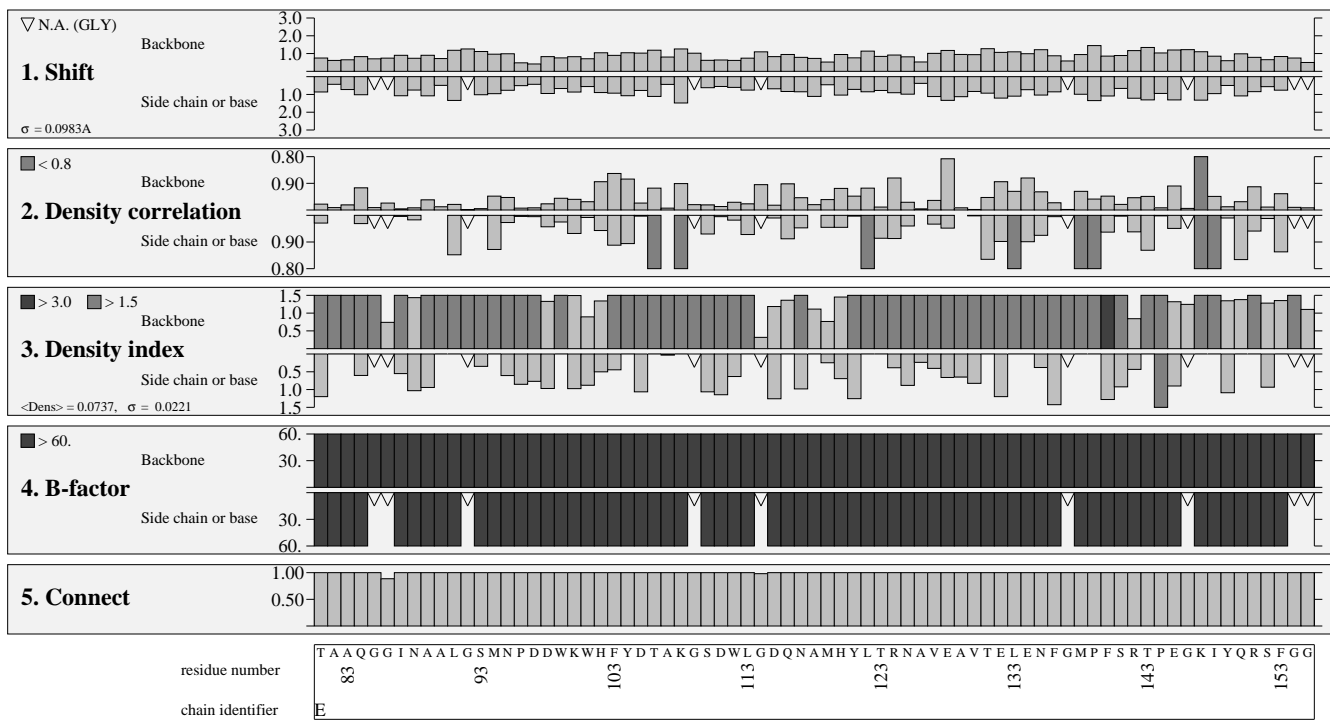
### Local estimation (8)



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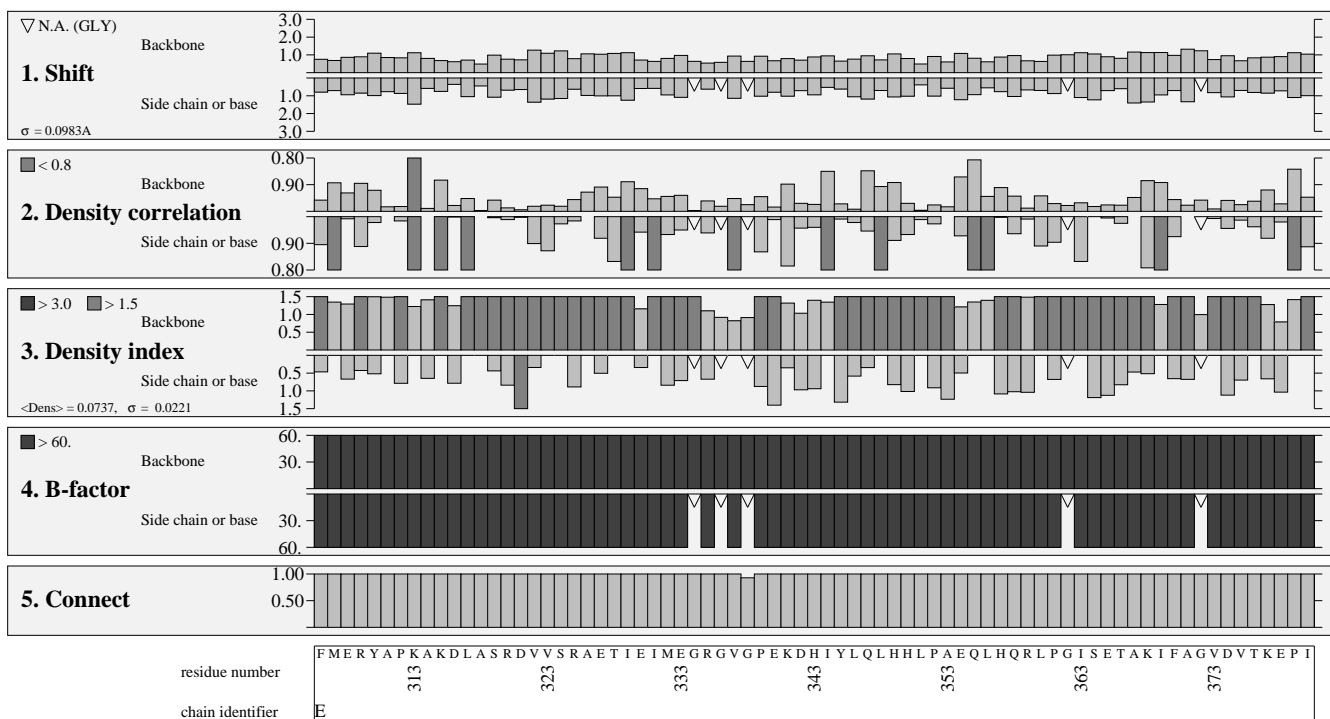
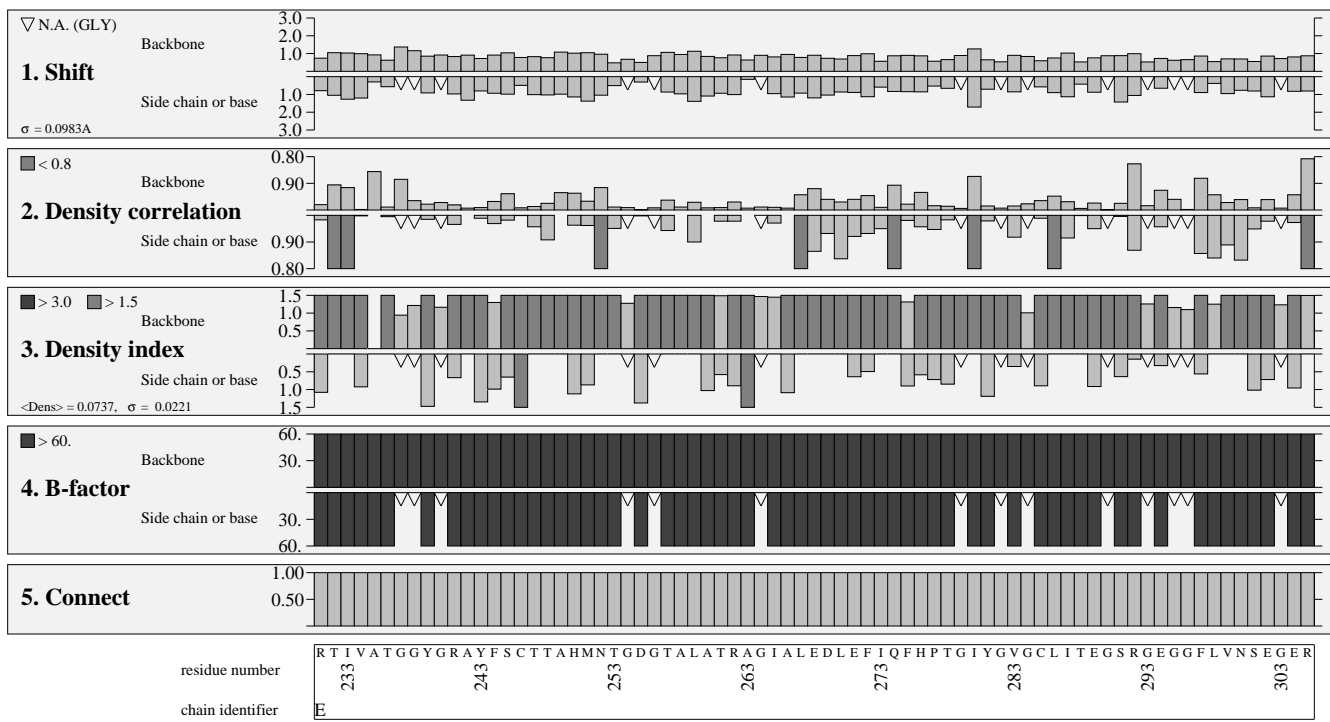
### Local estimation (9)



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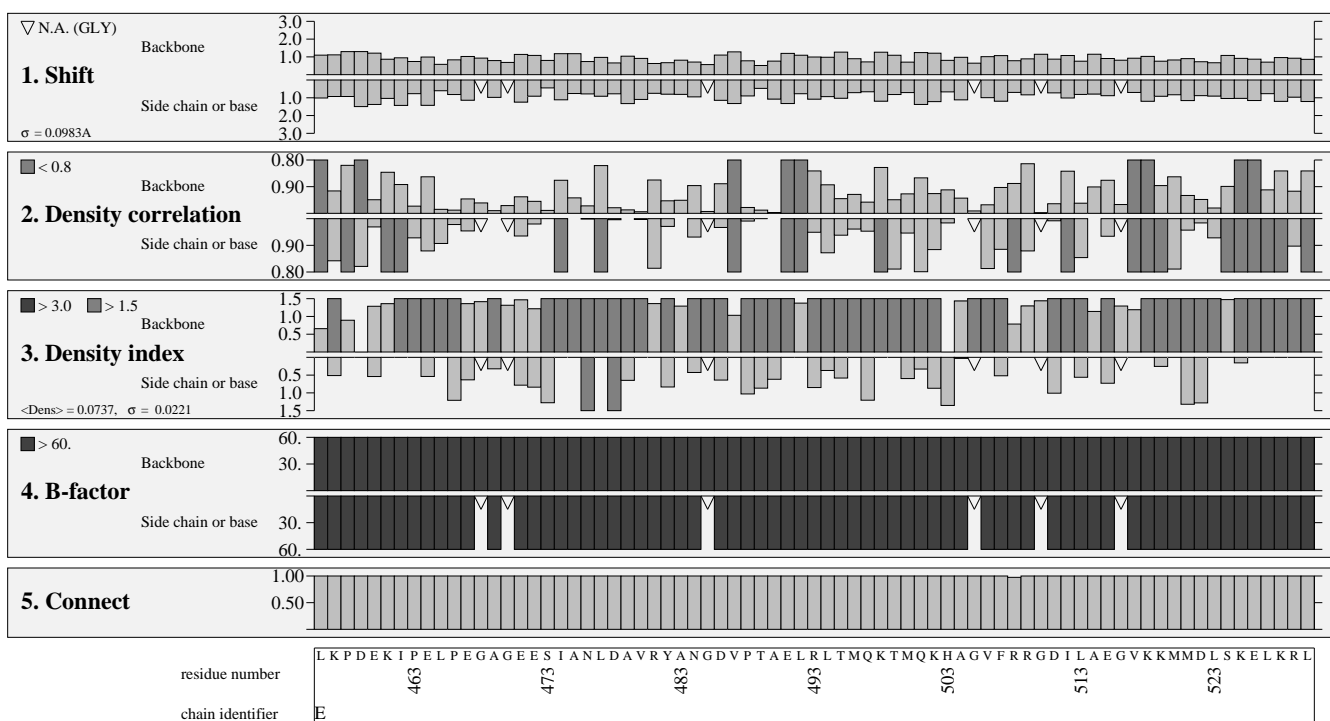
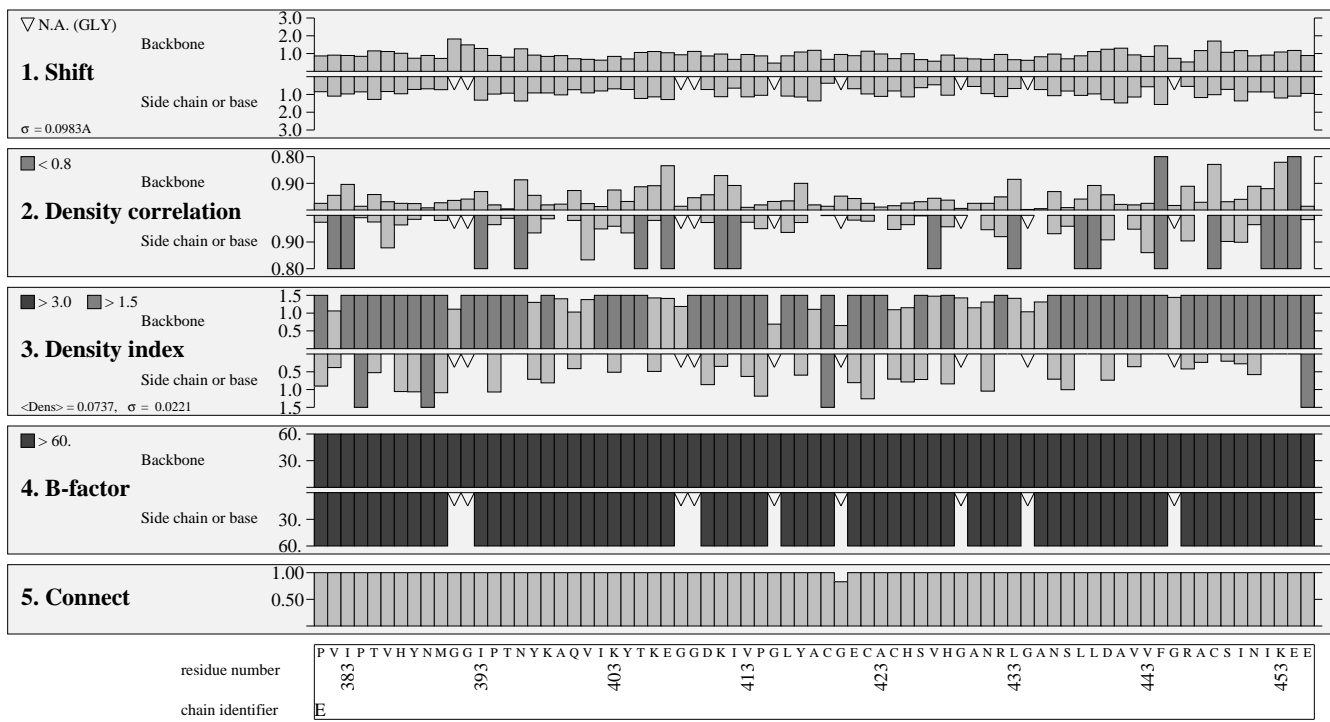
### Local estimation (10)



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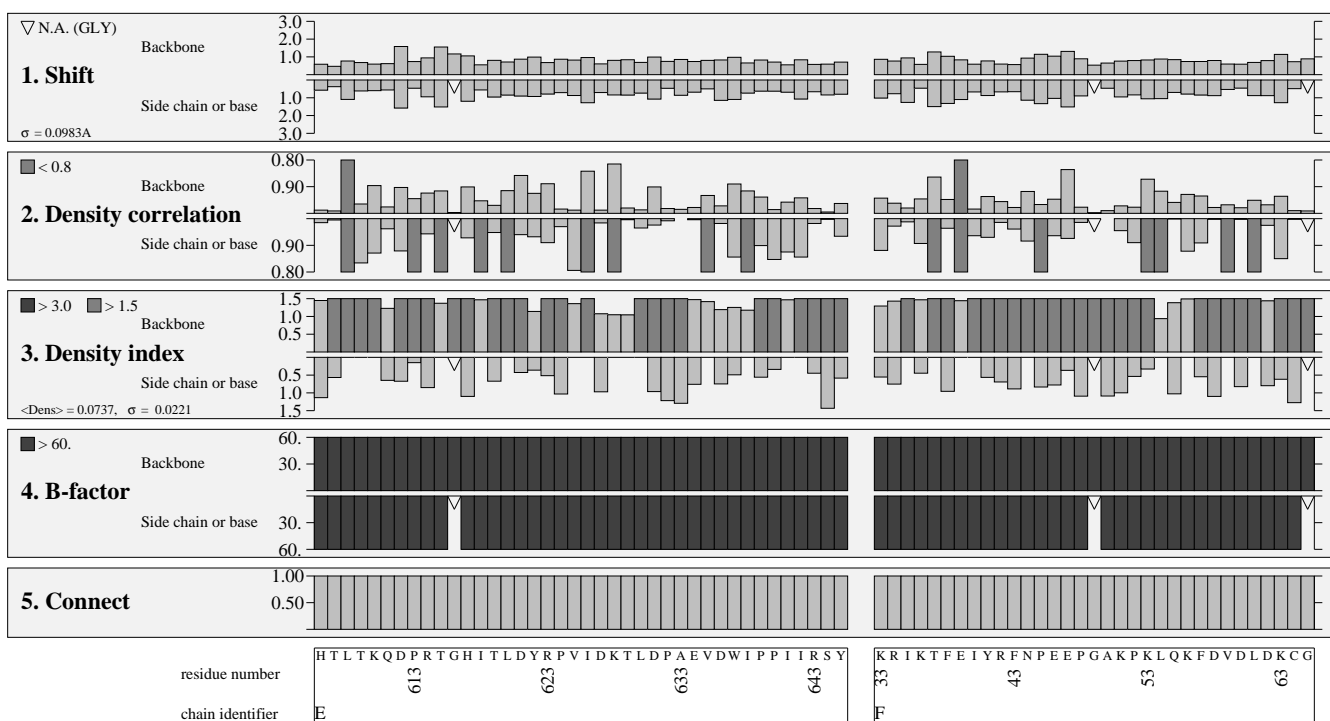
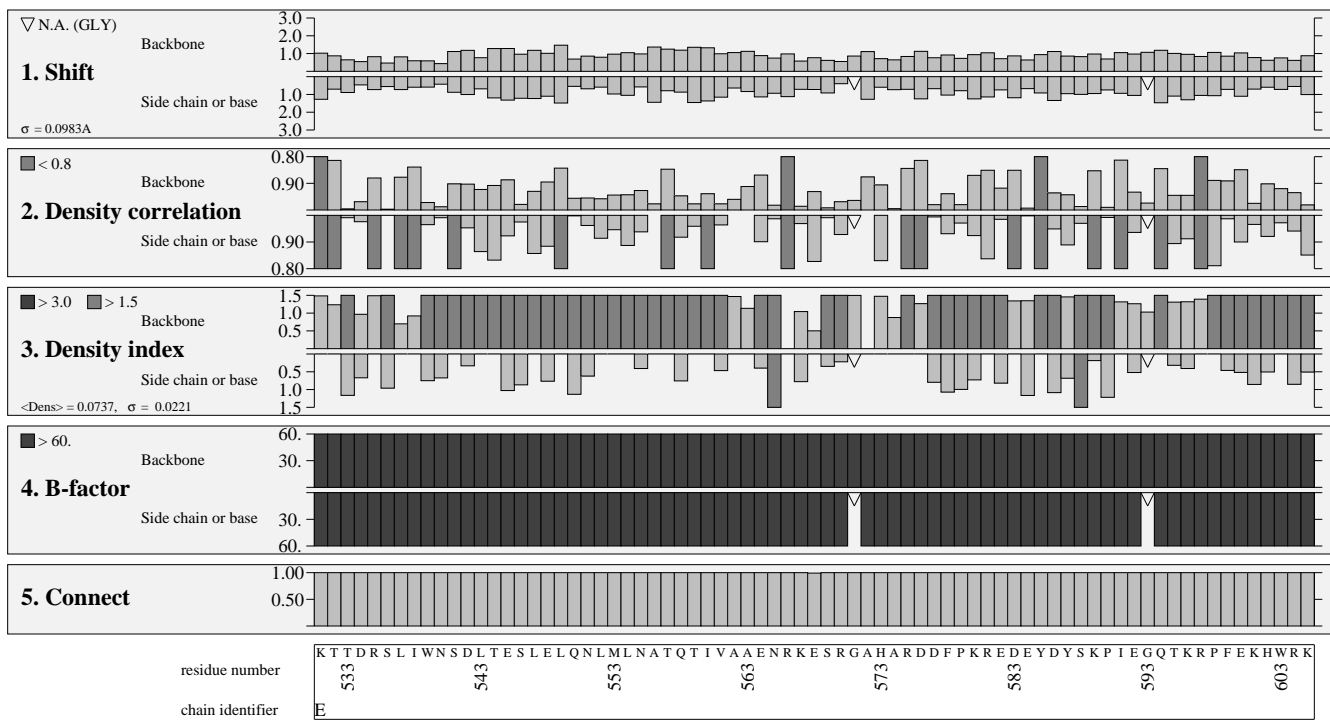
### Local estimation (11)



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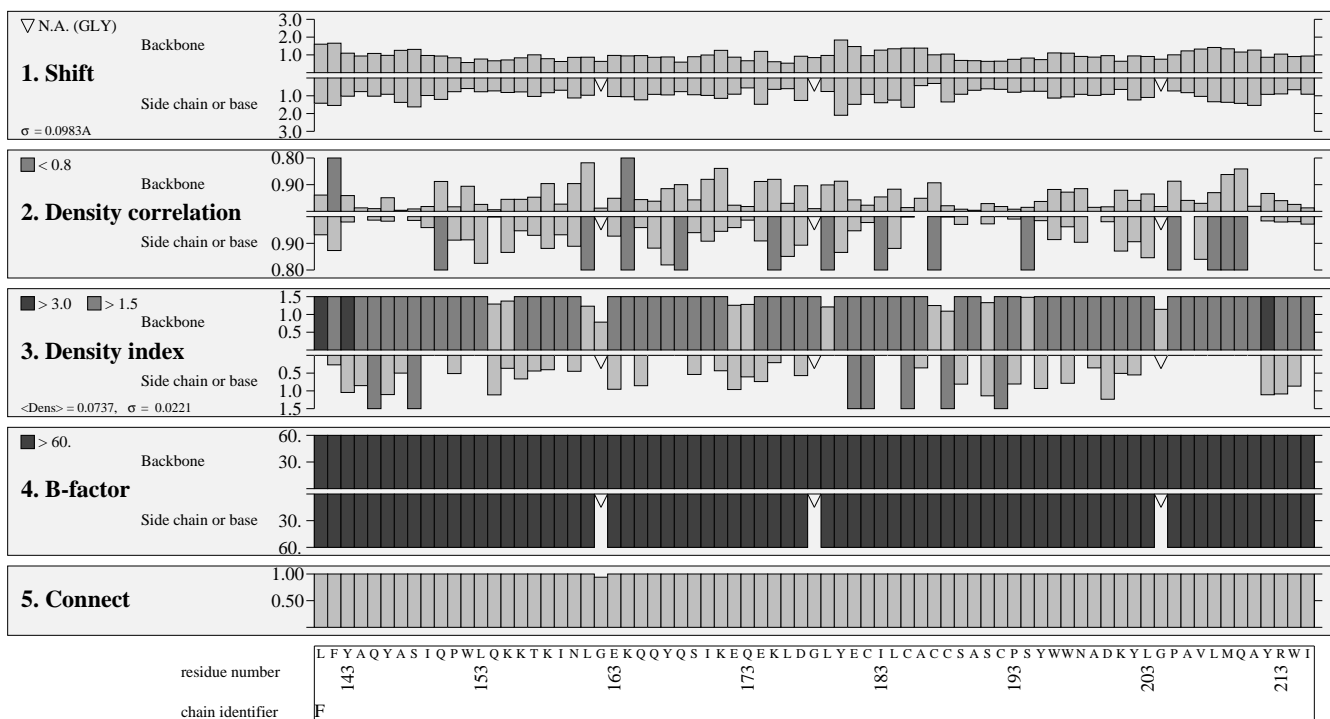
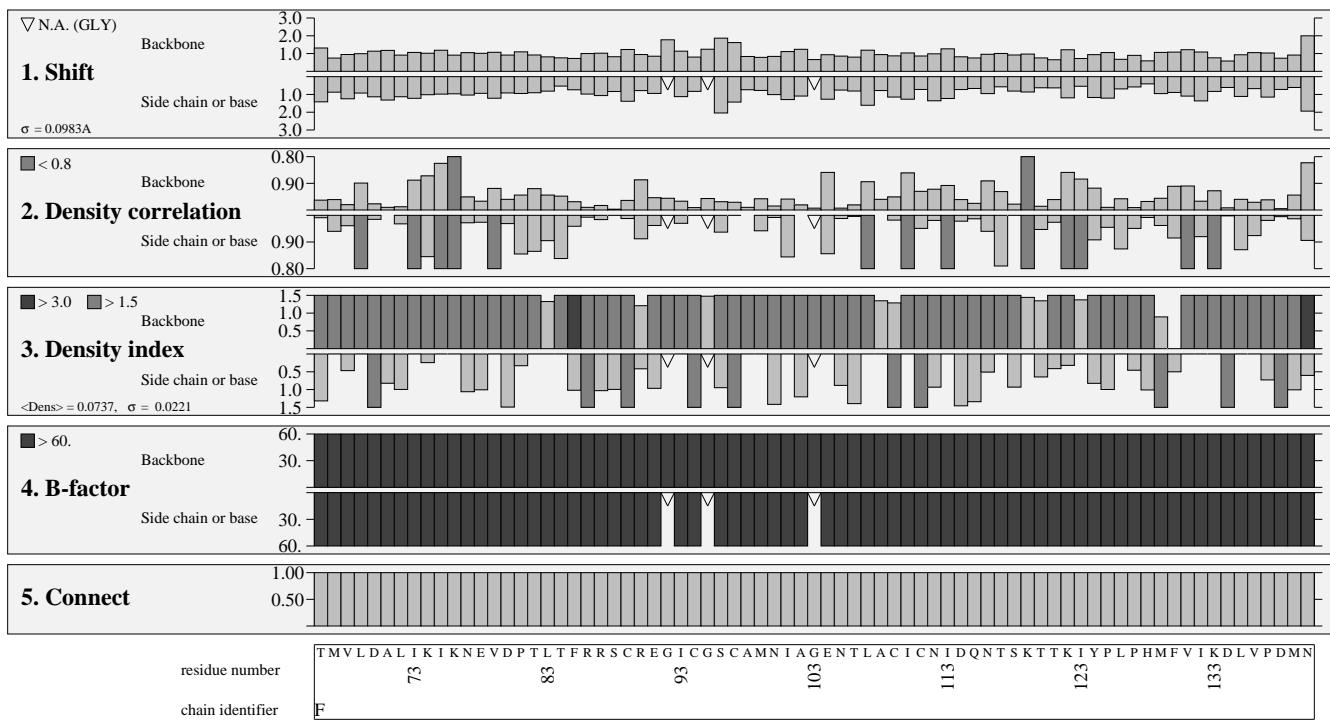
### Local estimation (12)



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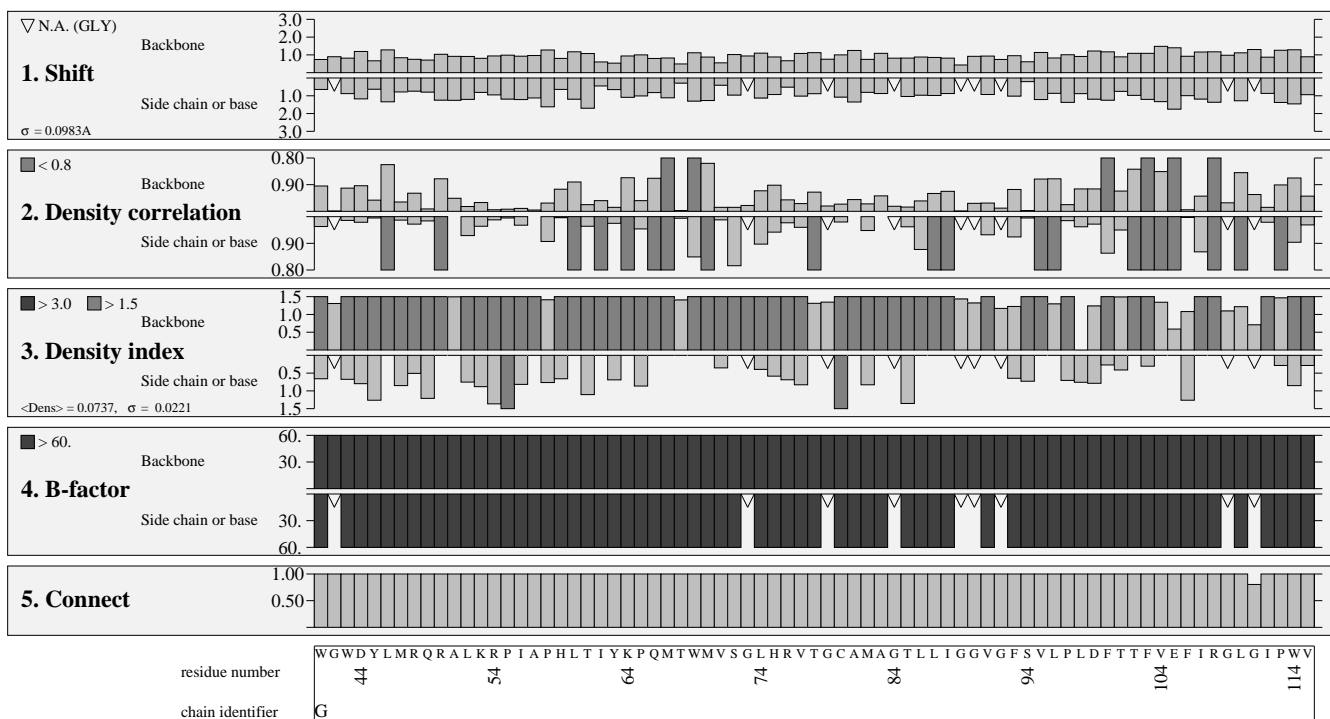
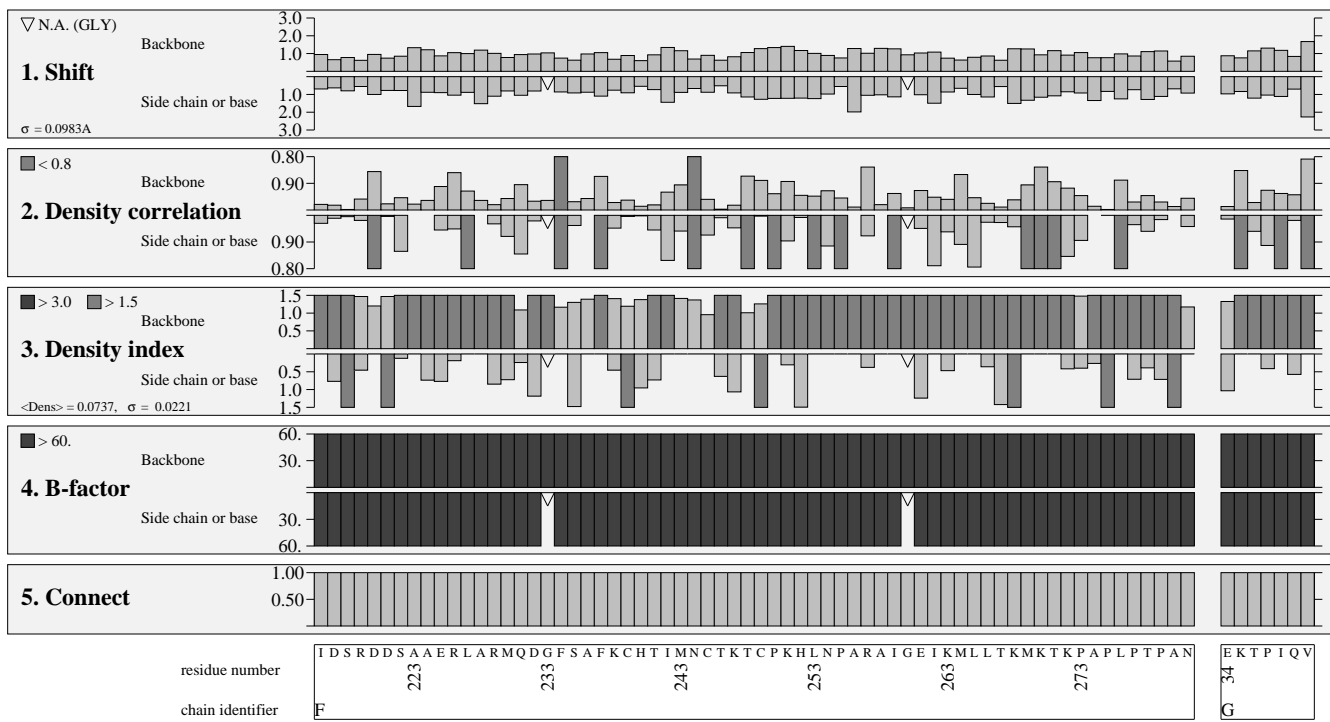
### Local estimation (13)



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### Local estimation (14)

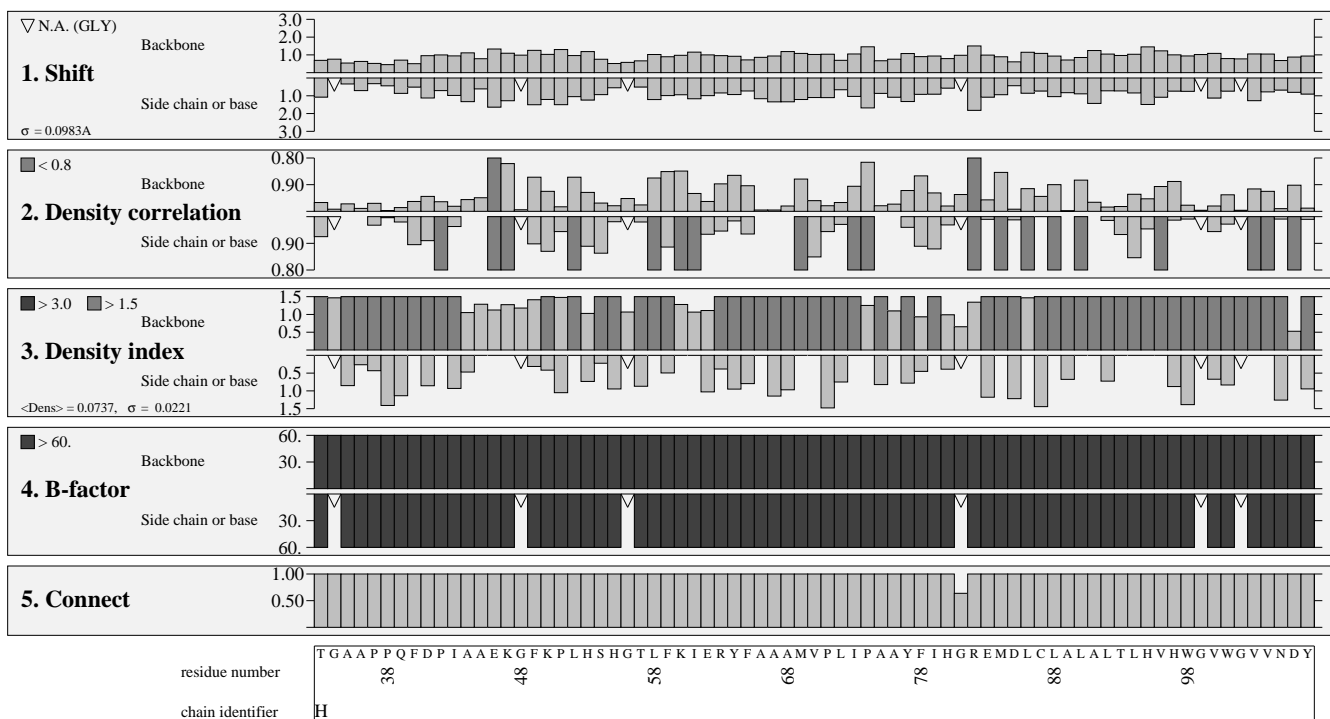
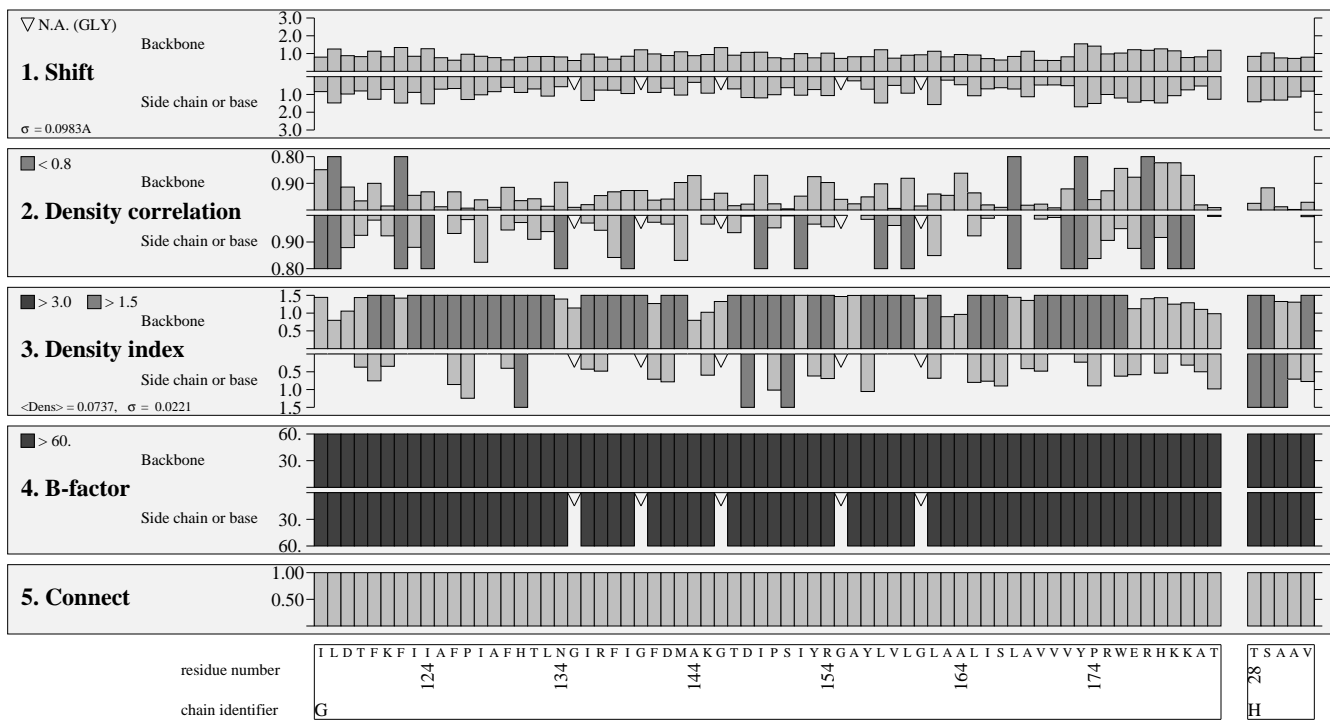




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### Local estimation (15)



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### Local estimation (16)

