

# Structure Factor Check

## 3L72

Title: CHICKEN CYTOCHROME BC1 COMPLEX WITH KRESOXYM-I-DIMETHYL  
BOUND  
Date: 27-DEC-09  
PDB code: 3L72

### Crystal

Cell parameters:

a: 172.61 A    b: 181.55 A    c: 241.03 A  
 $\alpha$ : 90.00     $\beta$ : 90.00     $\gamma$ : 90.00

Space group: P 21 21 21

### Structure Factors

#### Input

Nominal resolution range: 49.9 – 3.00 A  
 Reflections in file: 141090  
 Unique reflections above 0: 141090  
                           above 1 $\sigma$ : 136498  
                           above 3 $\sigma$ : 67537

#### SFCHECK

Nominal resolution range: 49.9 – 3.06 A  
\05max. from input data, min. from author\05  
 Used reflections: 133914  
 Reflections out of resolution: 7176  
 Completeness: 93.7 %  
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$  : 0.110  
 Anisotropic distribution of Structure Factors  
     ratio of eigen values: 1.0000 0.4881 0.5169  
 $B_{\text{overall}}$  (by Patterson): 52. A<sup>2</sup>  
 Optical resolution: 2.24 A  
 Expected opt. resol. for complete data set: 2.24 A  
 Estimated minimal error: 0.148 A

### Model

32648 atoms (18 water molecules)

Number of chains: 51  
 Volume not occupied by model: 62.6 %  
 $\langle B \rangle$  (for atomic model): 75.1 A<sup>2</sup>  
 $\sigma(B)$ : 20.12 A<sup>2</sup>  
 Matthews coefficient: 4.13  
 Corresponding solvent % : 69.99

### Model vs. Structure Factors

R-factor for all reflections: 0.315  
 Correlation factor: 0.833  
 R-factor: 0.315  
     for  $F > 2.0\sigma$   
         nom. resolution range: 28.93 – 3.06A  
         reflections used: 130194

Rfree: 0.345  
 Nfree: 2577  
 R-factor without free-refl.: 0.315  
 Non free-reflections: 127617  
 $\langle u \rangle$  (error in coords by Luzzati plot): 0.635 A  
 Estimated maximal error: 0.355 A  
 DPI: 0.433 A

#### Scaling

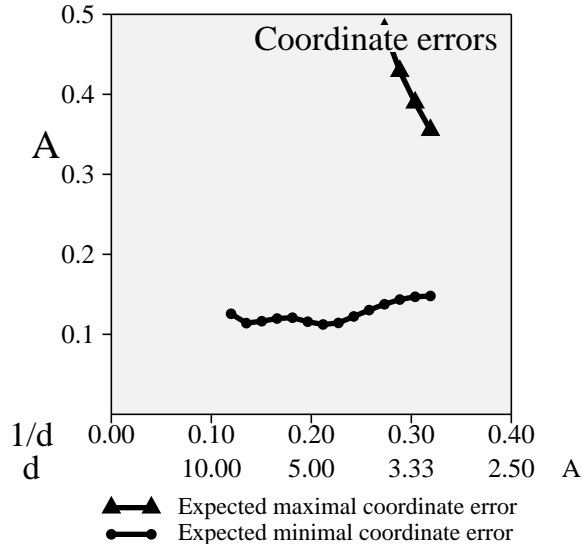
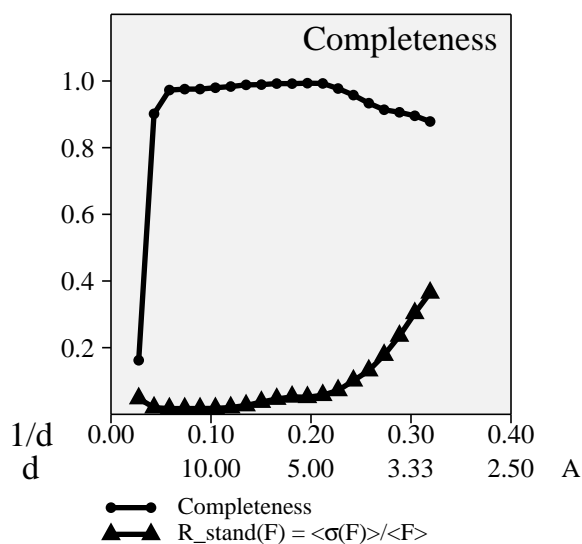
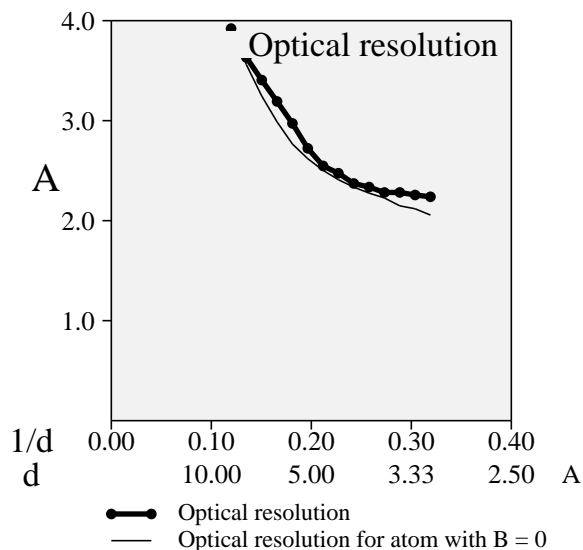
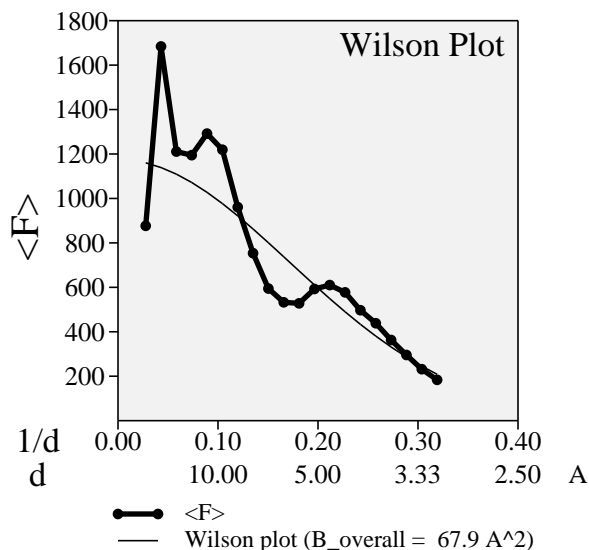
Scale: 0.477  
 Bdiff: -6.65  
 Anisothermal Scaling (Beta):  
     9.7787 -2.1367 -0.8959 0.0000 0.0000 0.0000  
 Solvent correction – Ks,Bs: 0.695 250.139

### Refinement

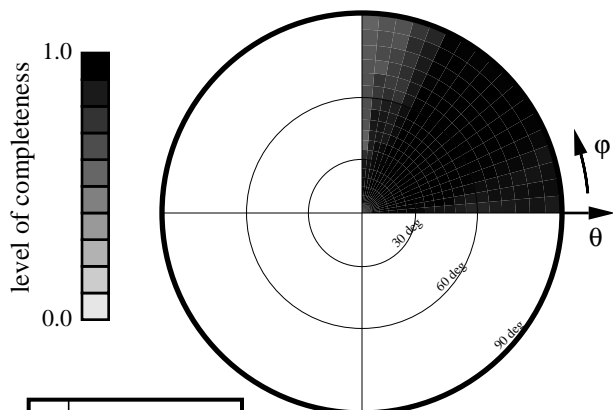
Program: CNS 1.1  
 Nominal resolution range: 28.9 – 3.06 A  
 Reported nominal resolution: 3.00 A  
 Reported R-factor: 0.264  
 Number of reflections used: 133892  
 Reported Rfree: 0.29  
 Sigma cut-off: N.A.

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## 3L72

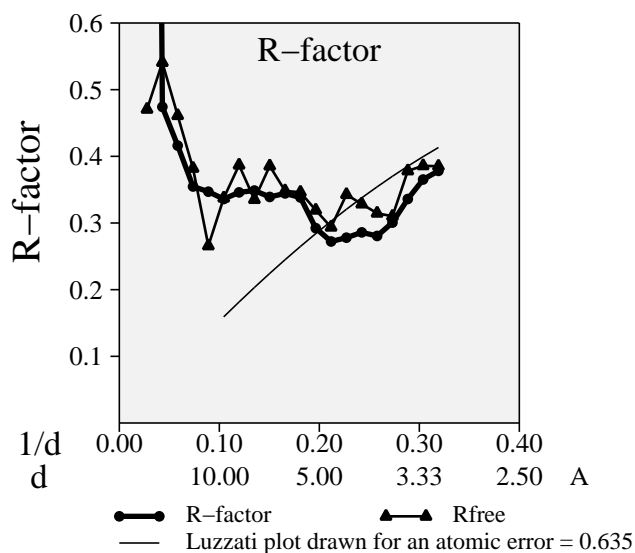


Stereographic projection of the averaged radial completeness



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

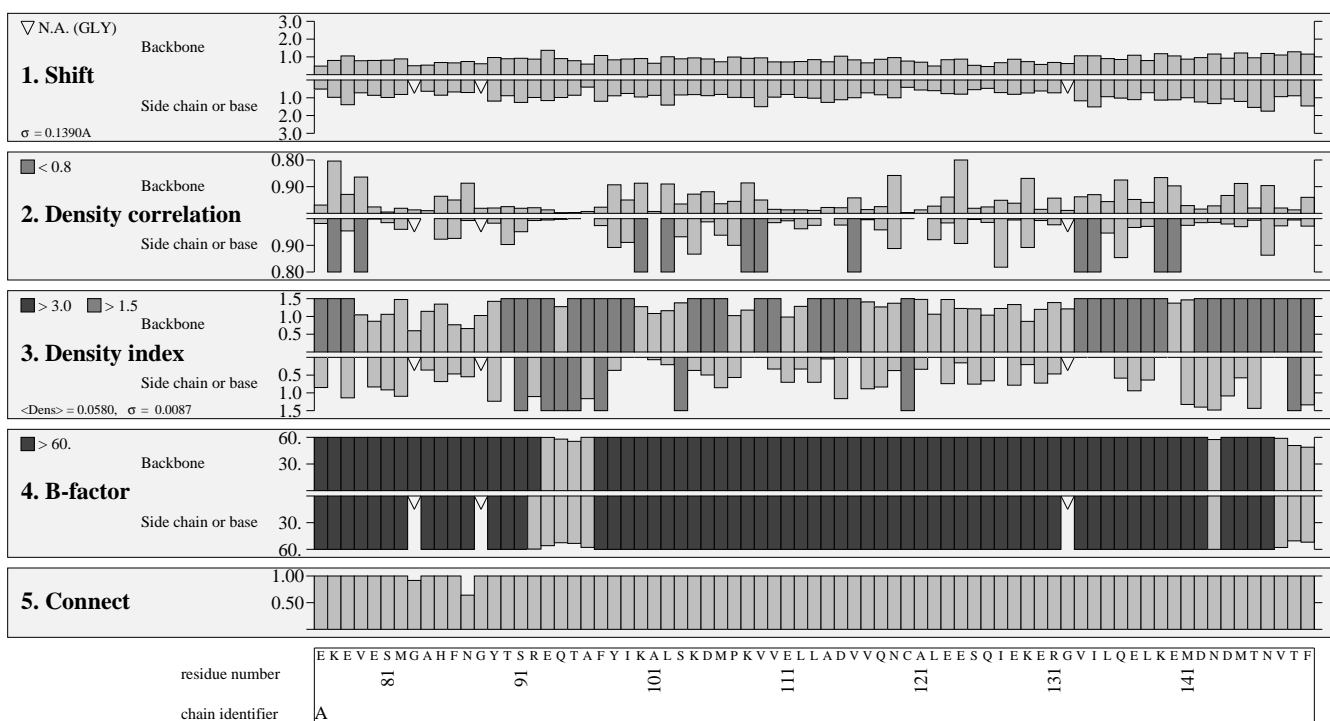
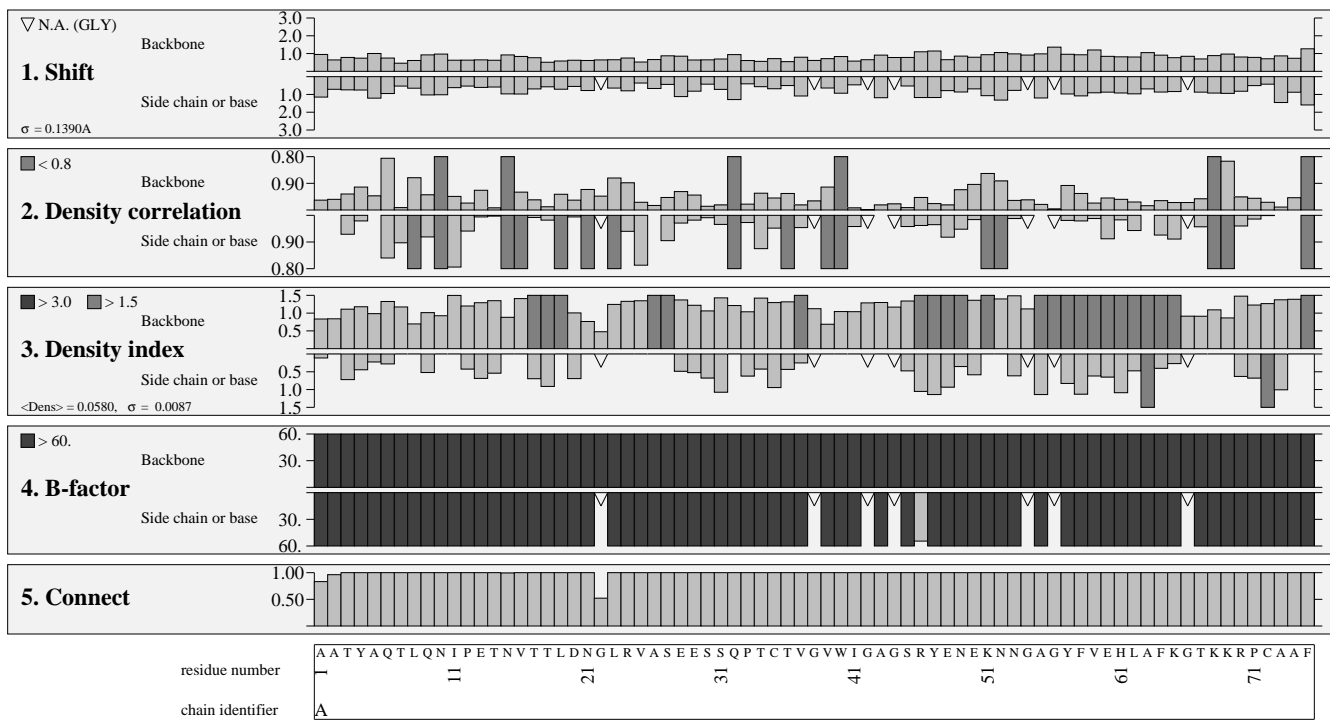
polar coordinates of the crystallographical axes



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## 3L72

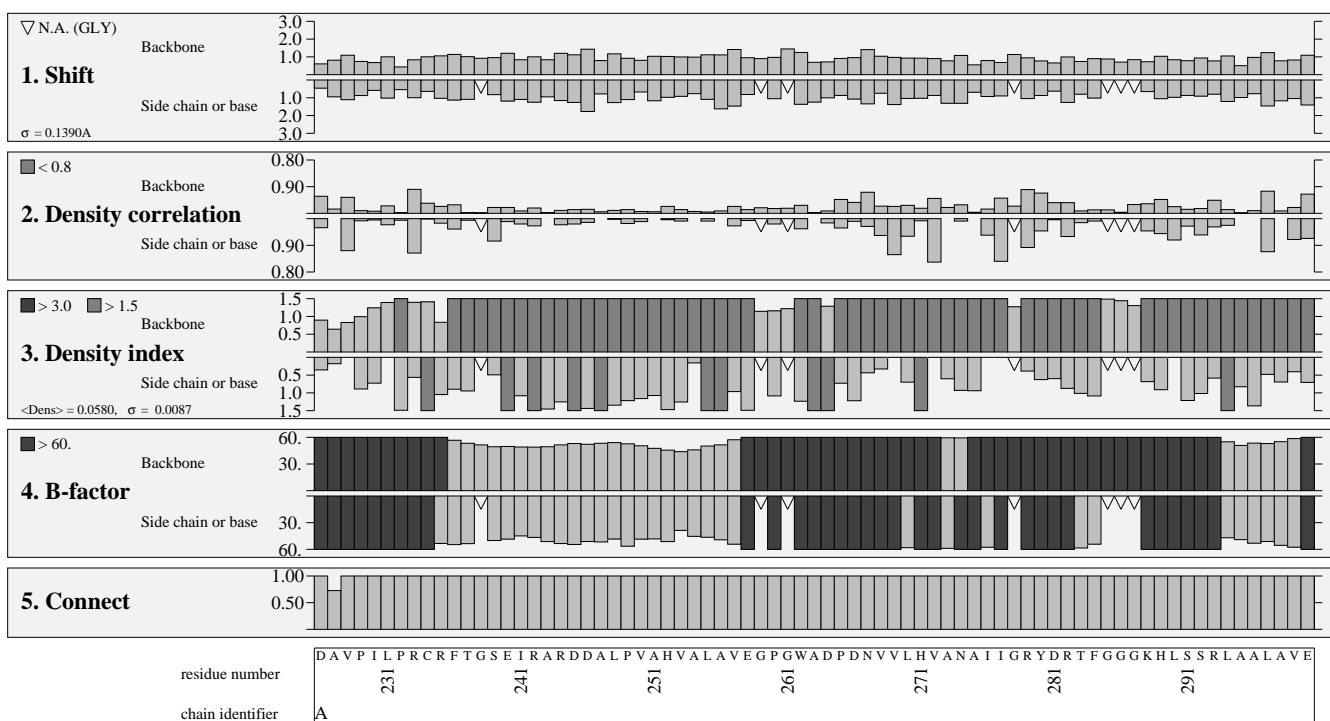
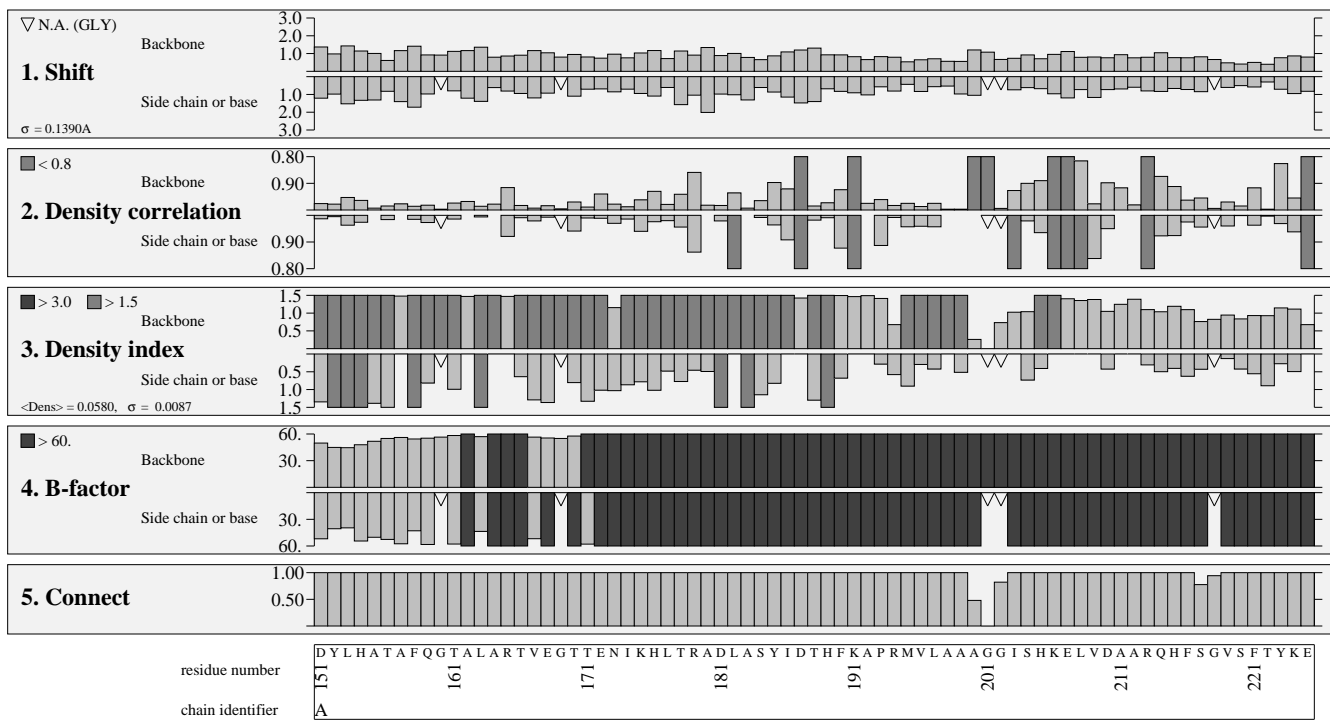
### Local estimation



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## 3L72

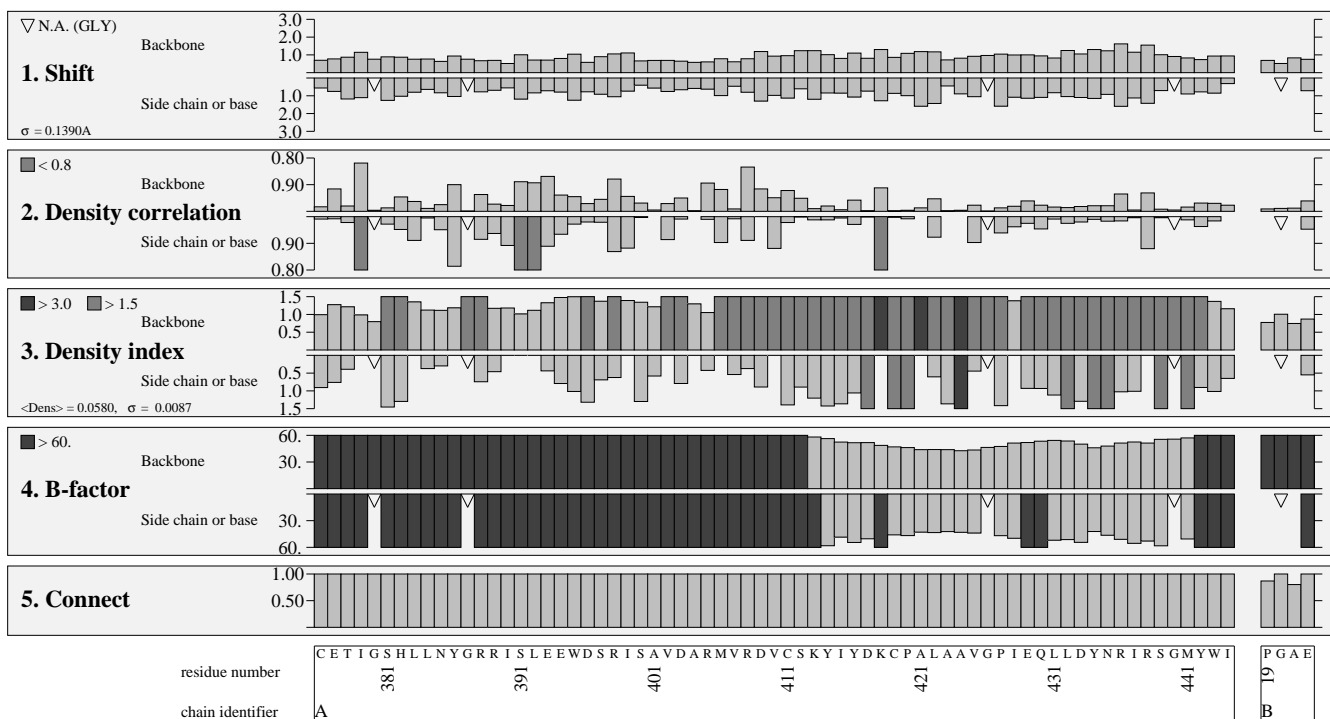
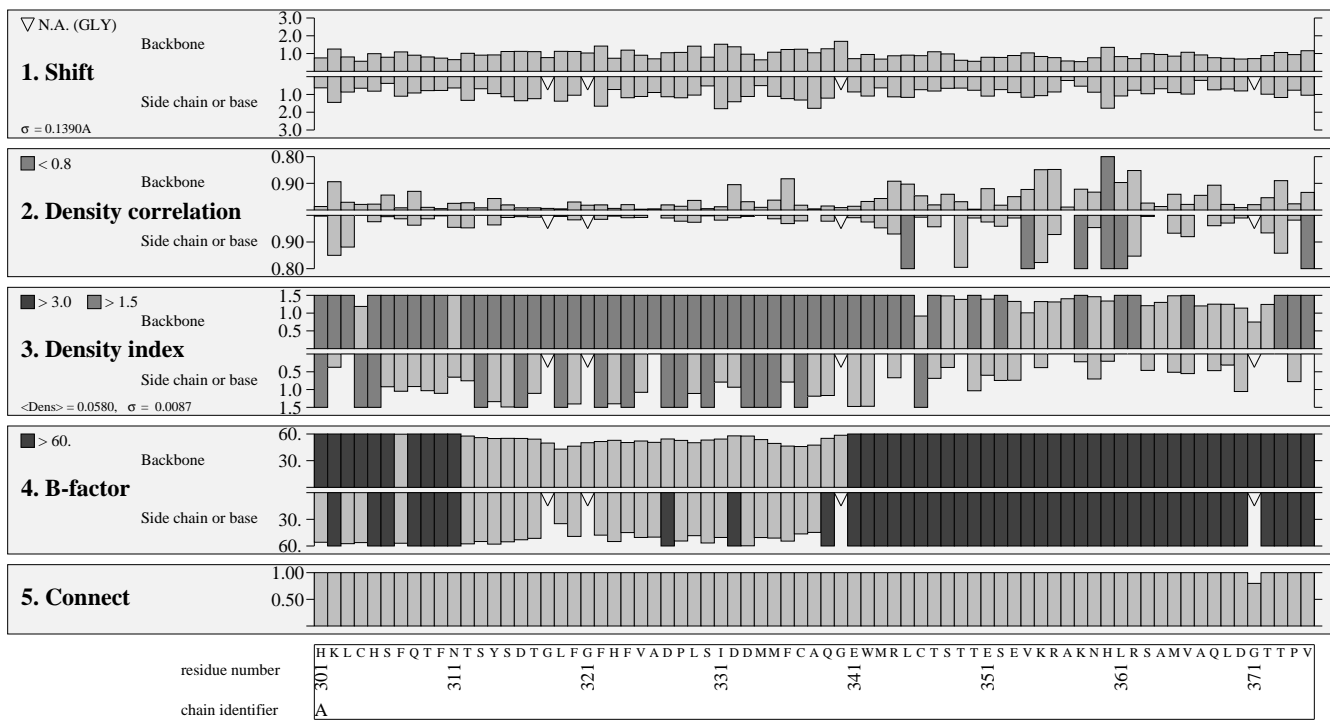
### Local estimation (2)



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## 3L72

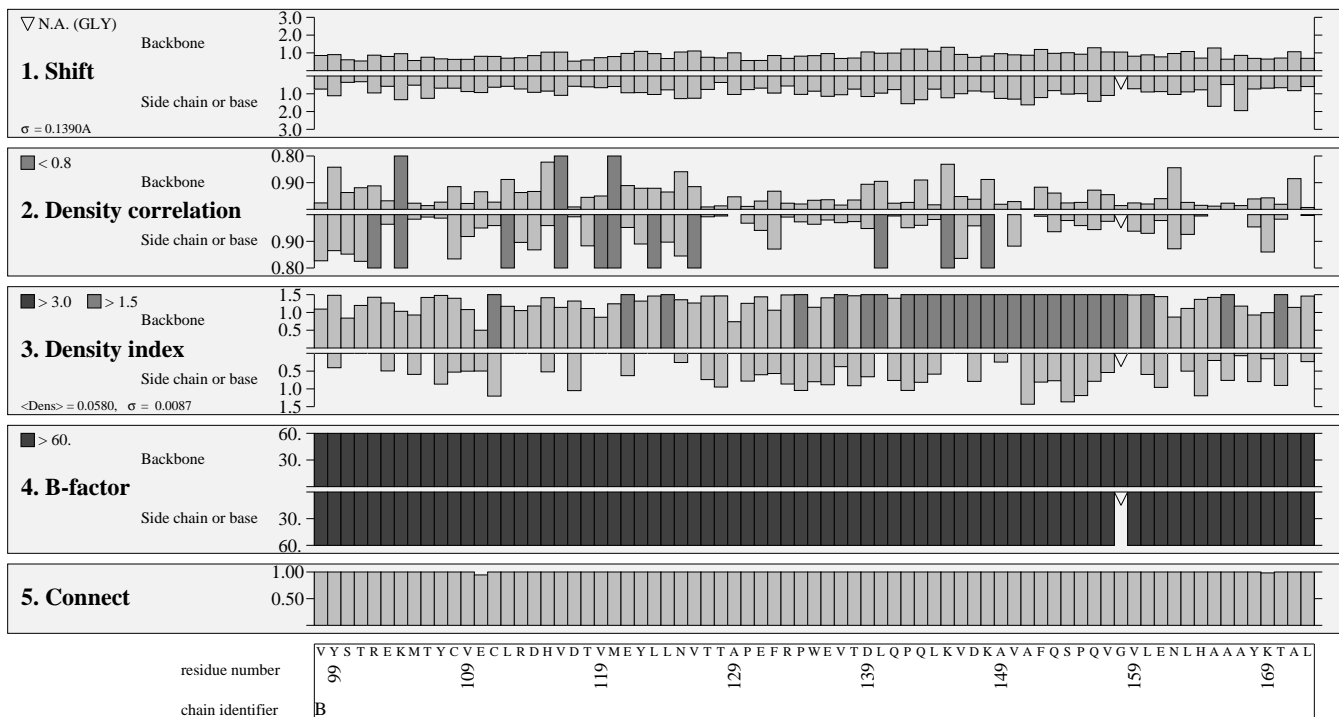
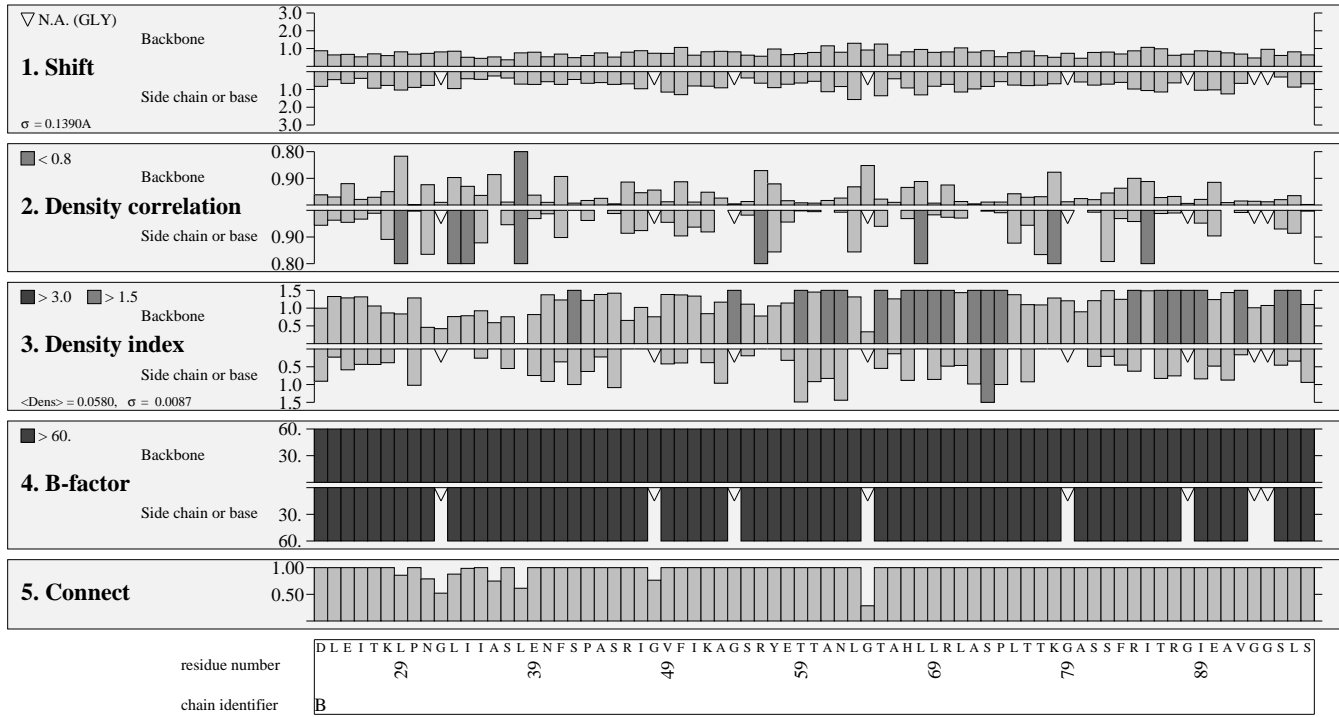
### Local estimation (3)



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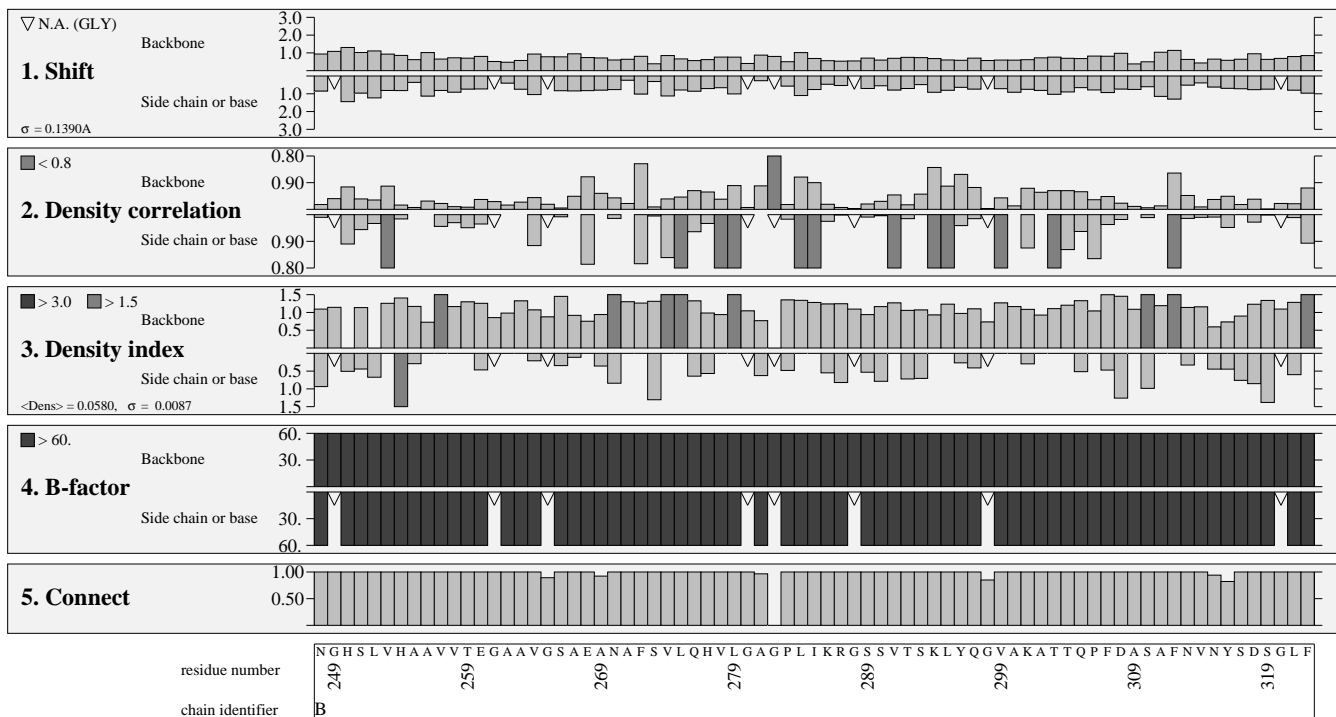
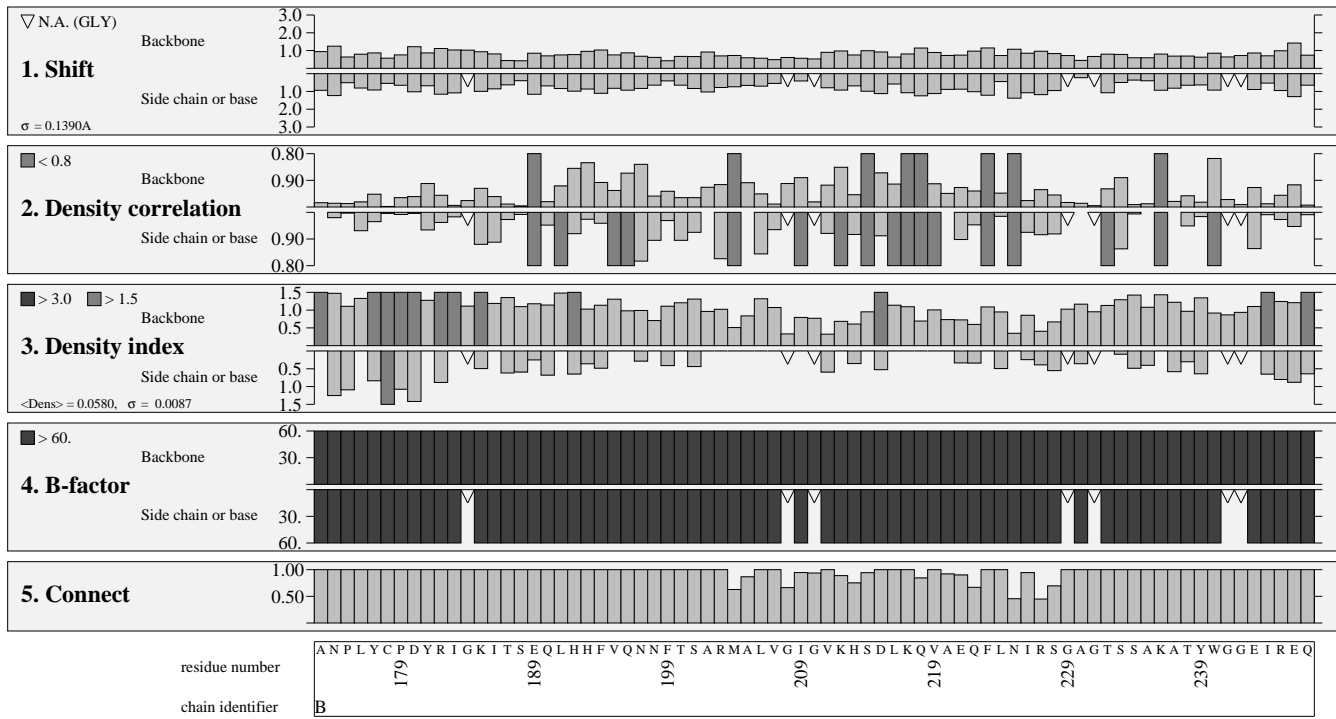
### Local estimation (4)



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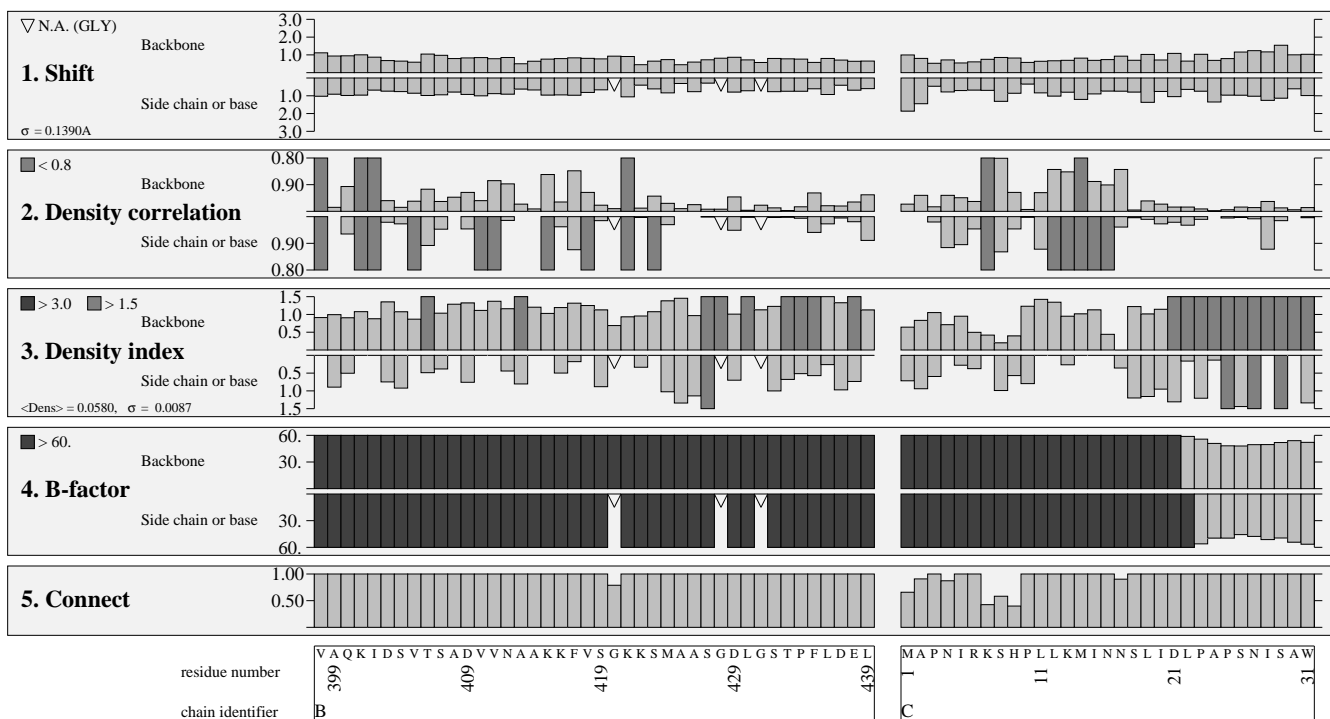
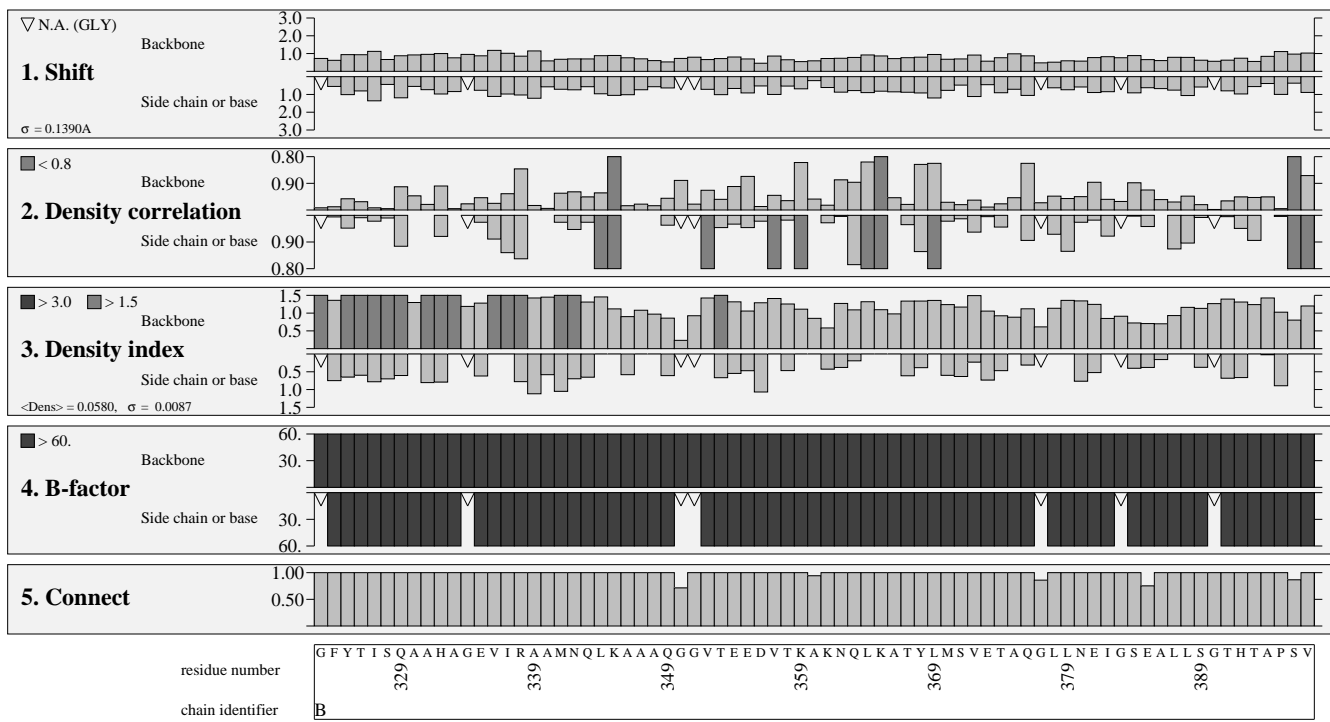
### Local estimation (5)



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## 3L72

### Local estimation (6)

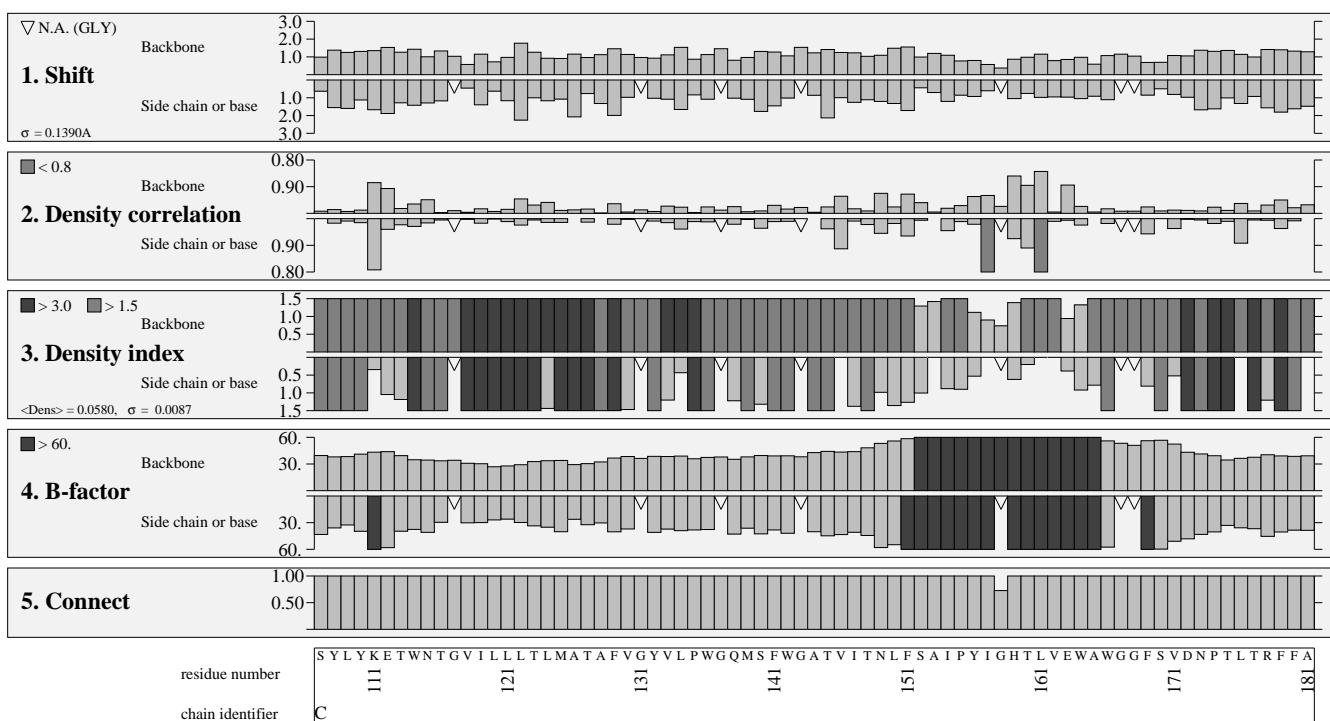
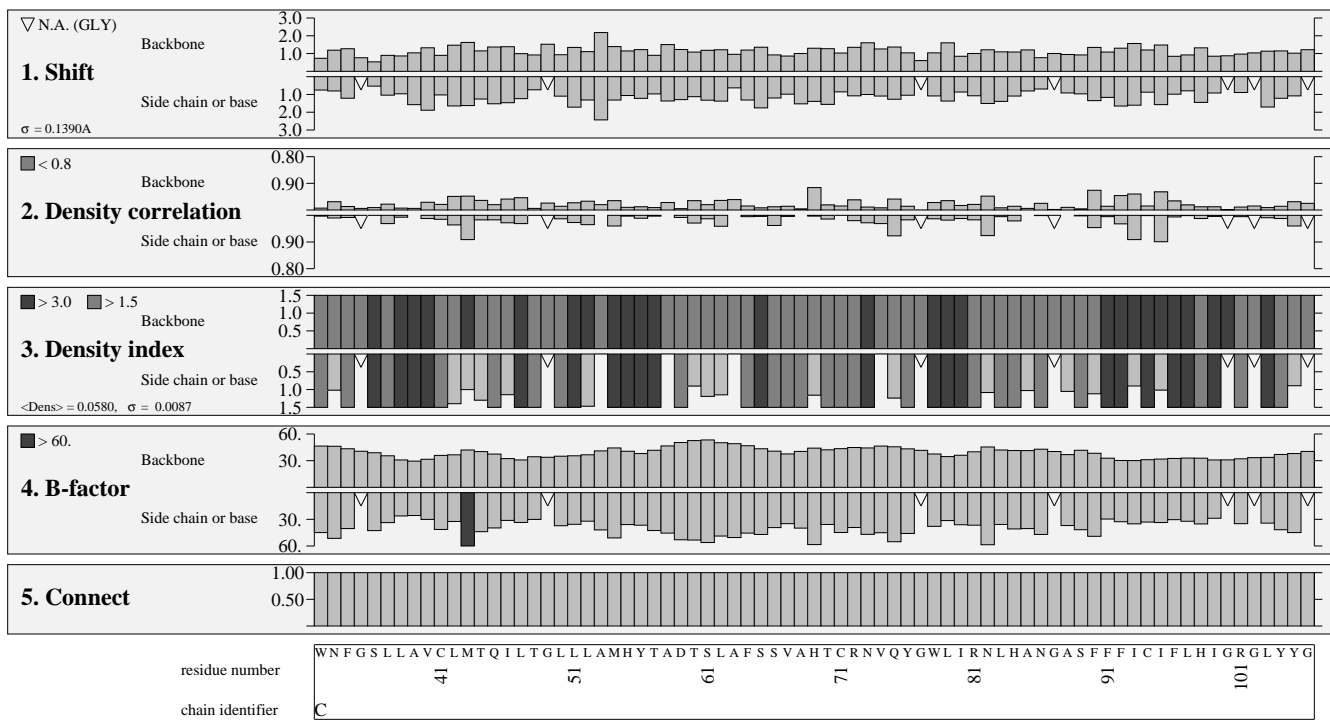




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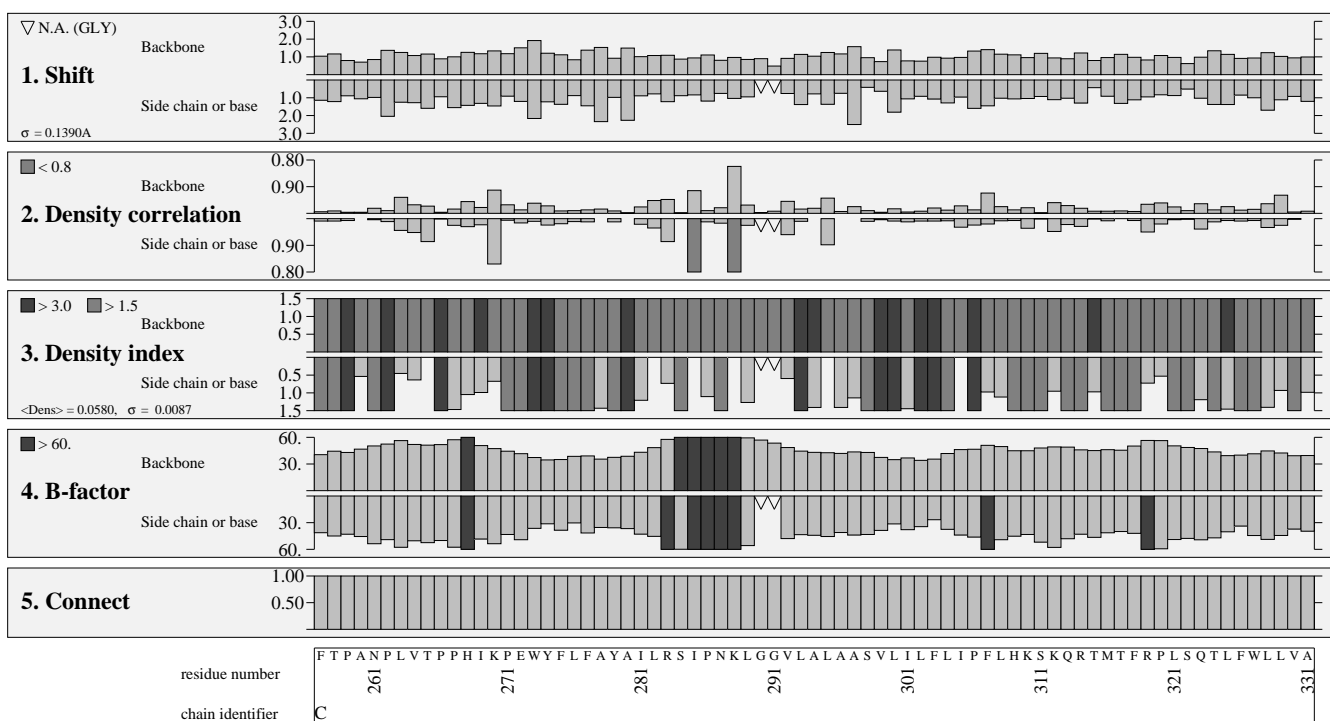
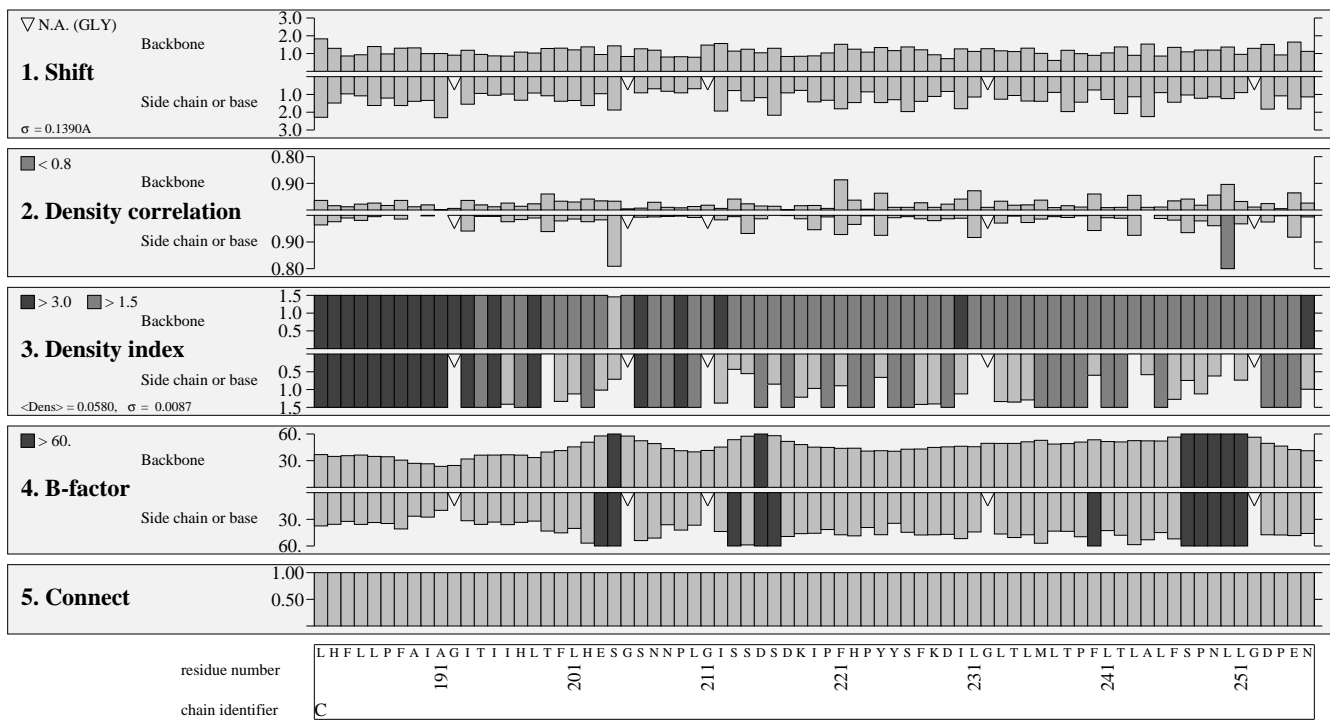
### Local estimation (7)



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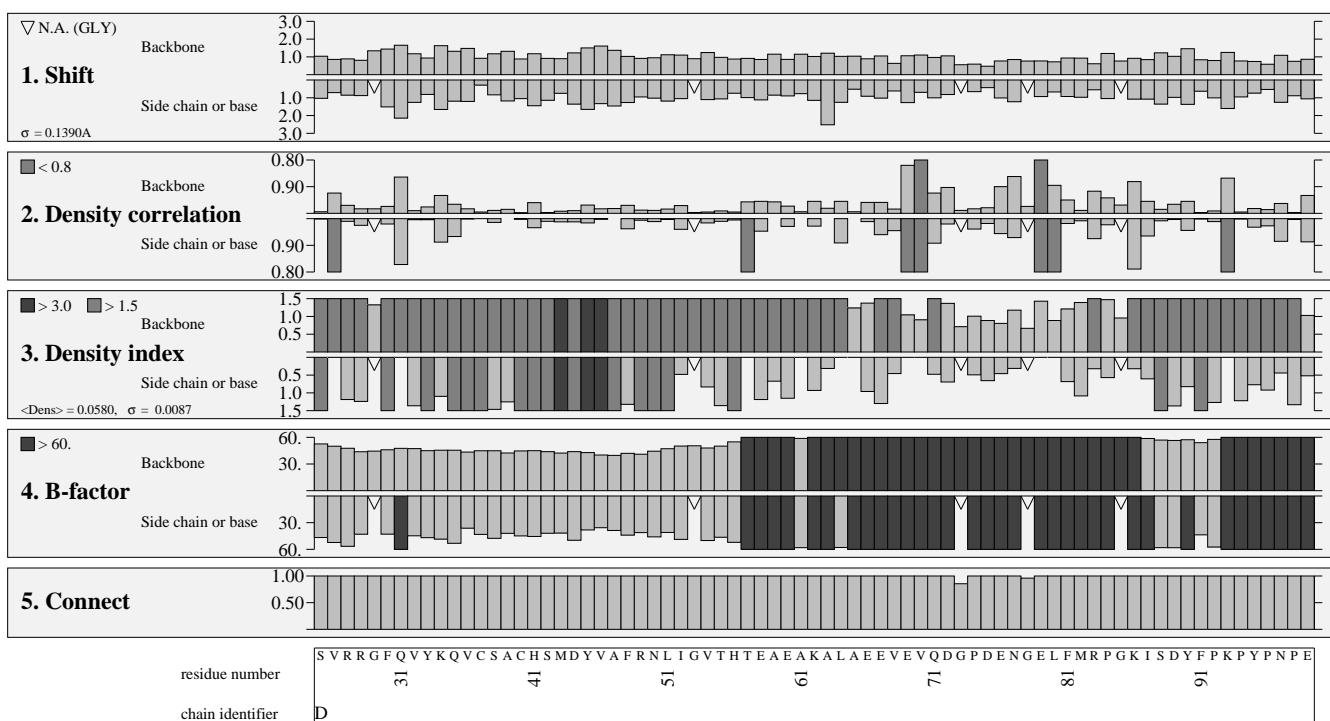
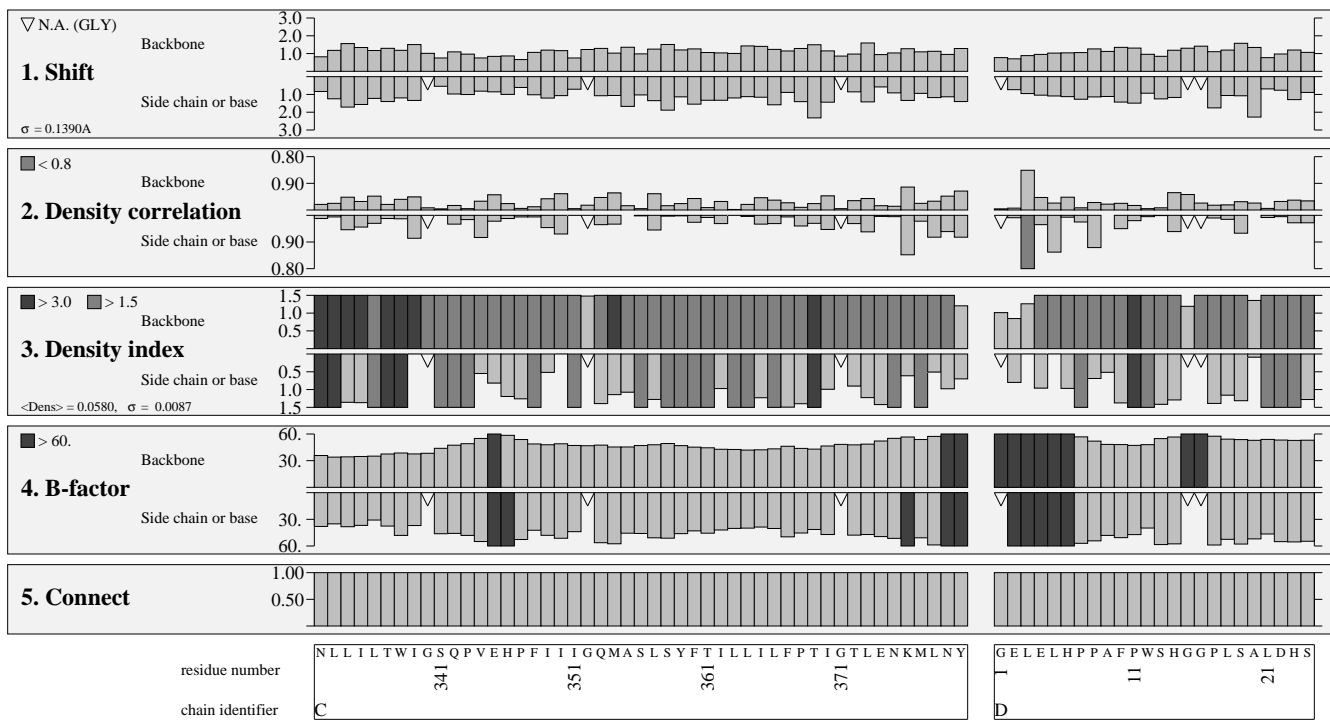
### Local estimation (8)



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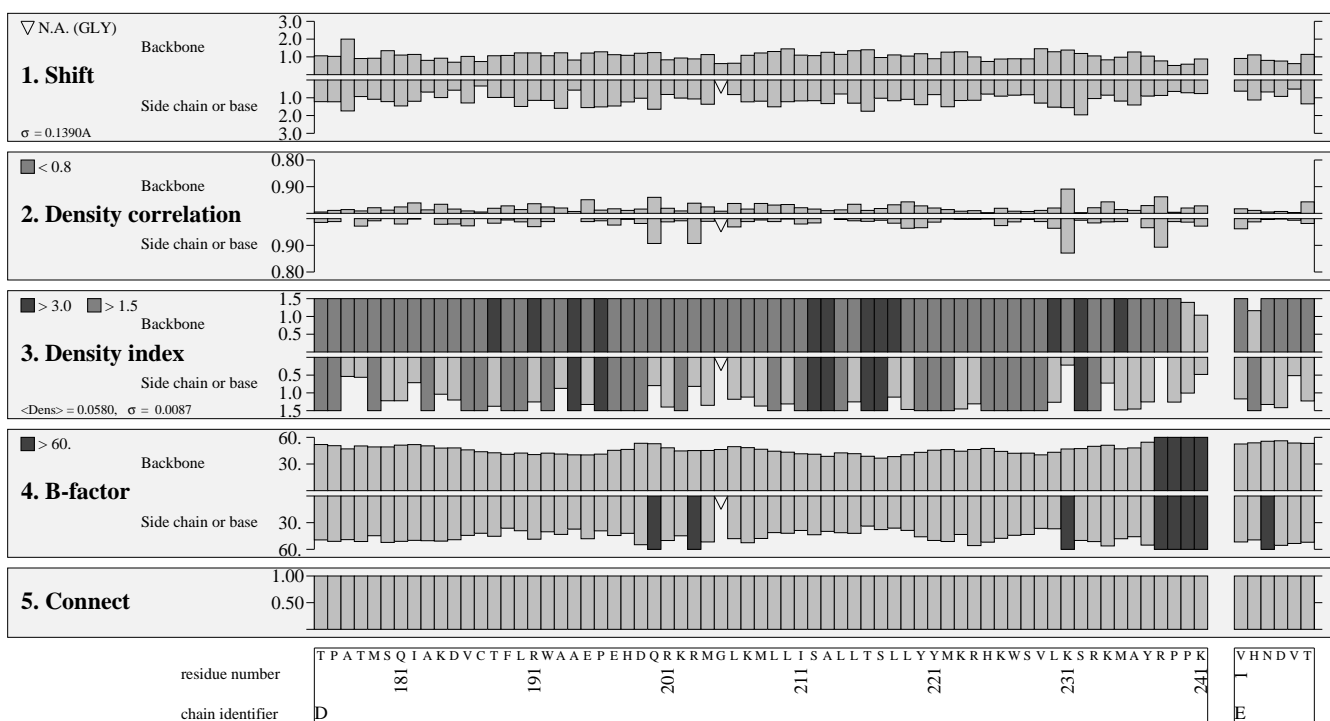
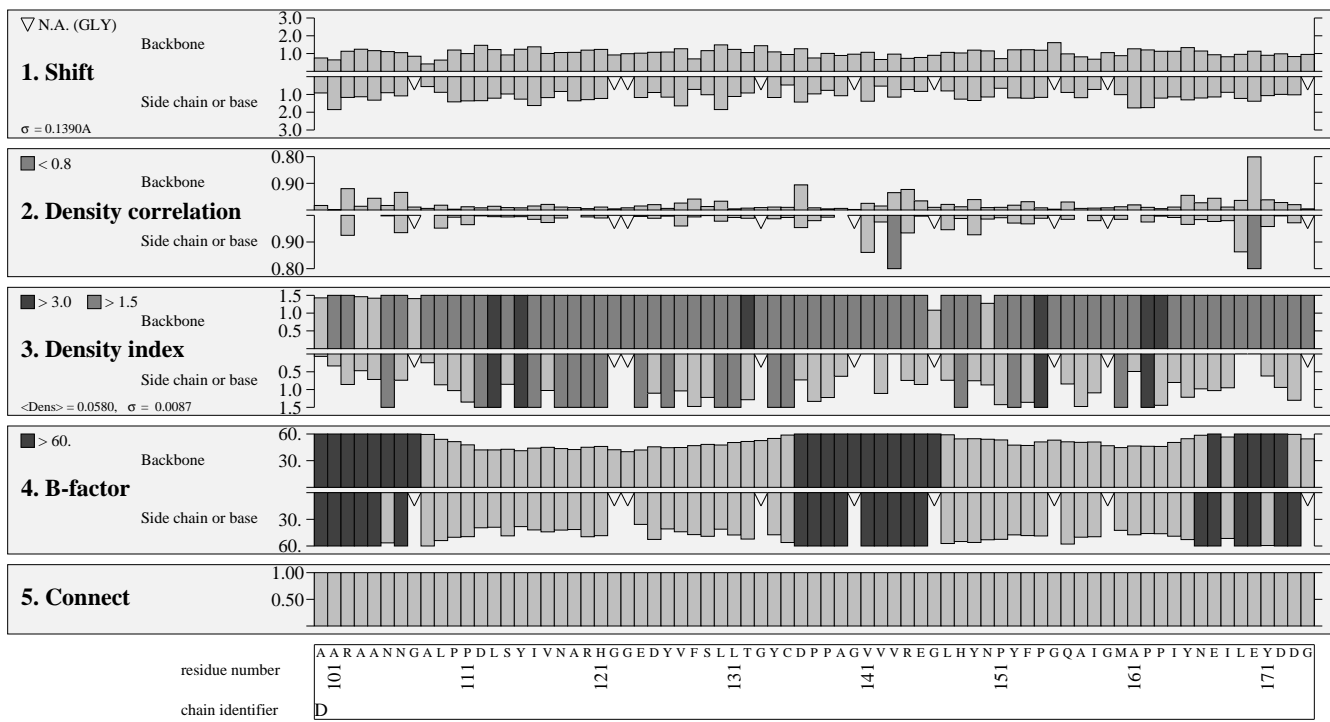
### Local estimation (9)



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## 3L72

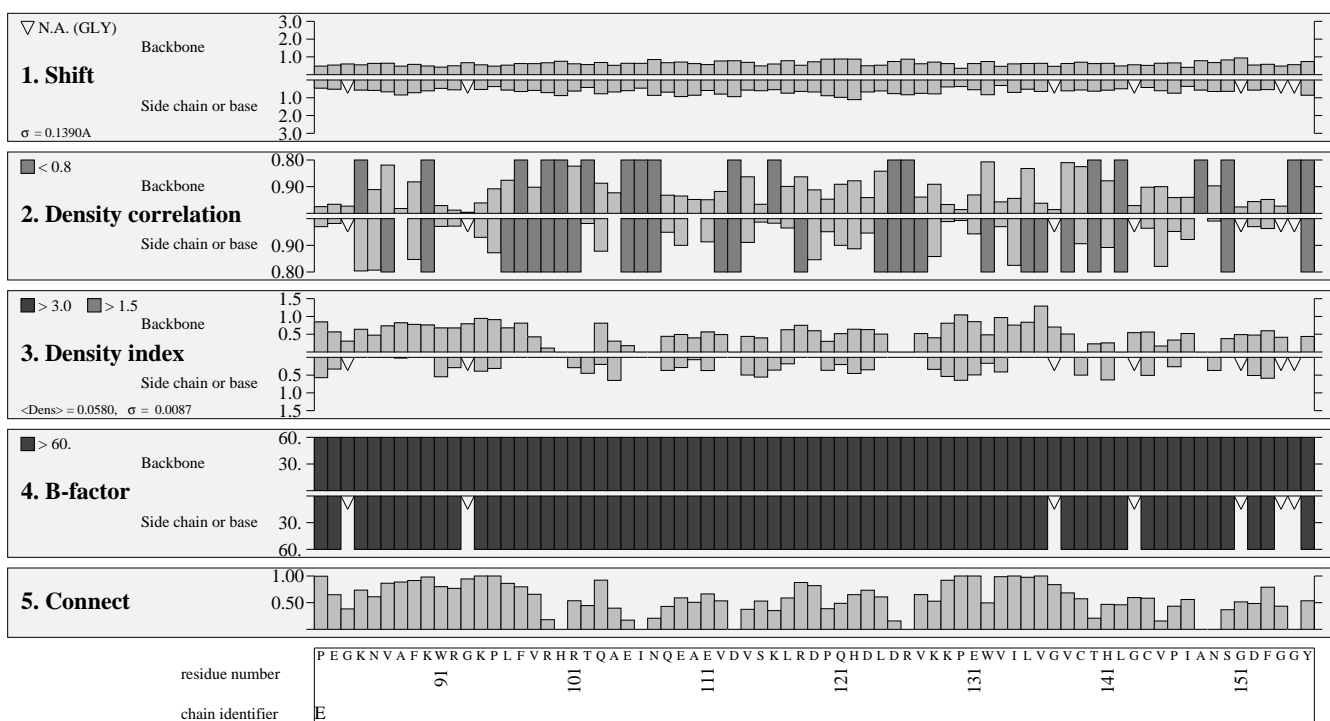
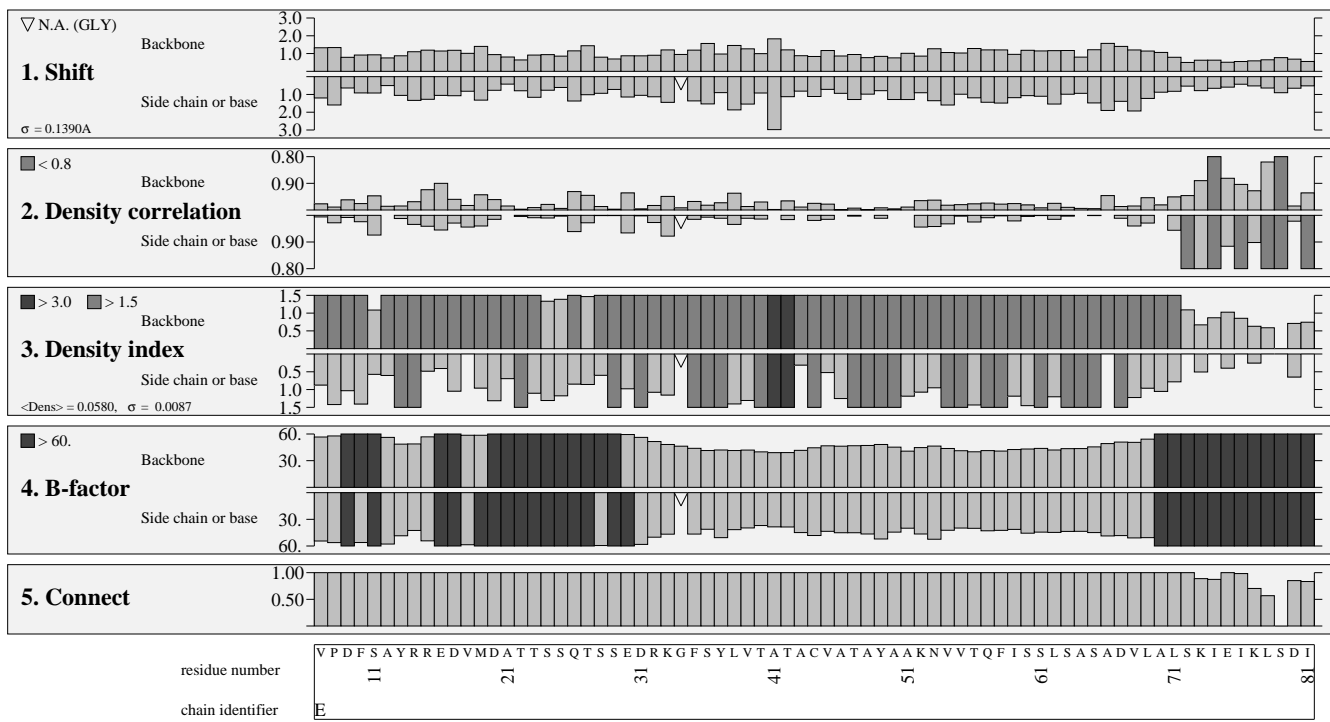
### Local estimation (10)



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## 3L72

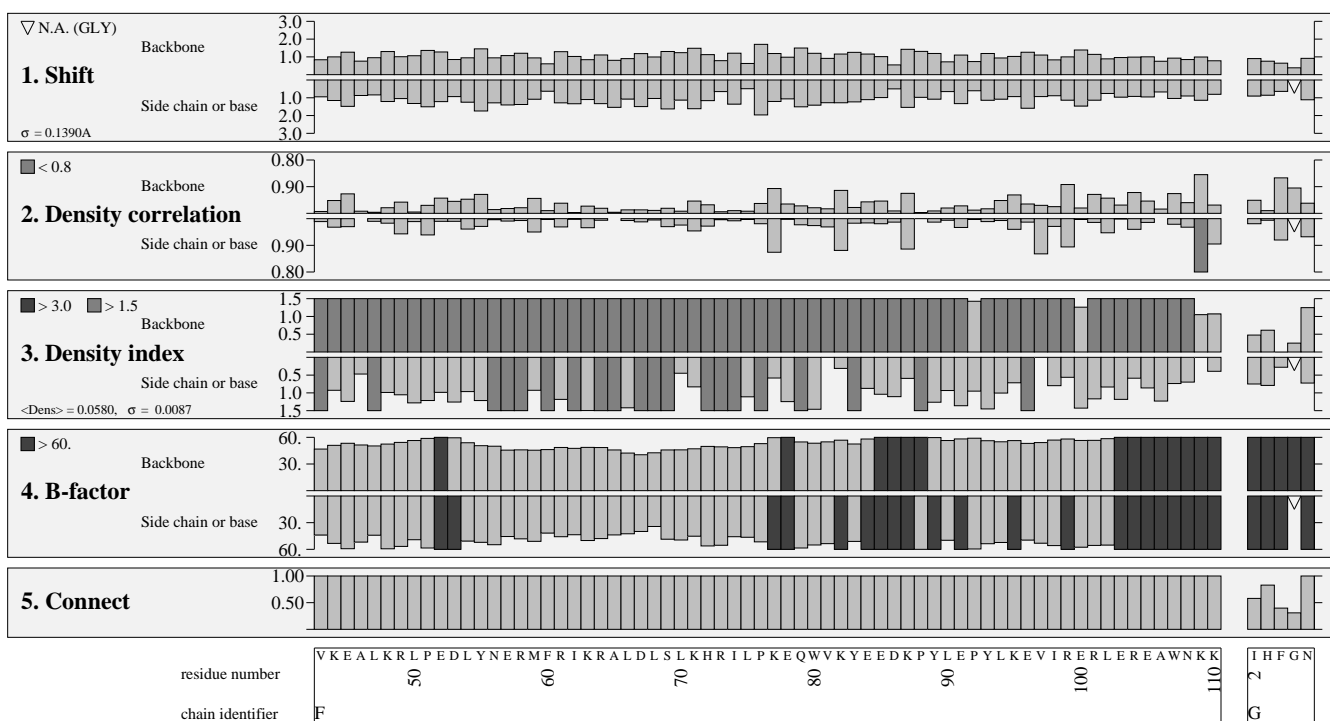
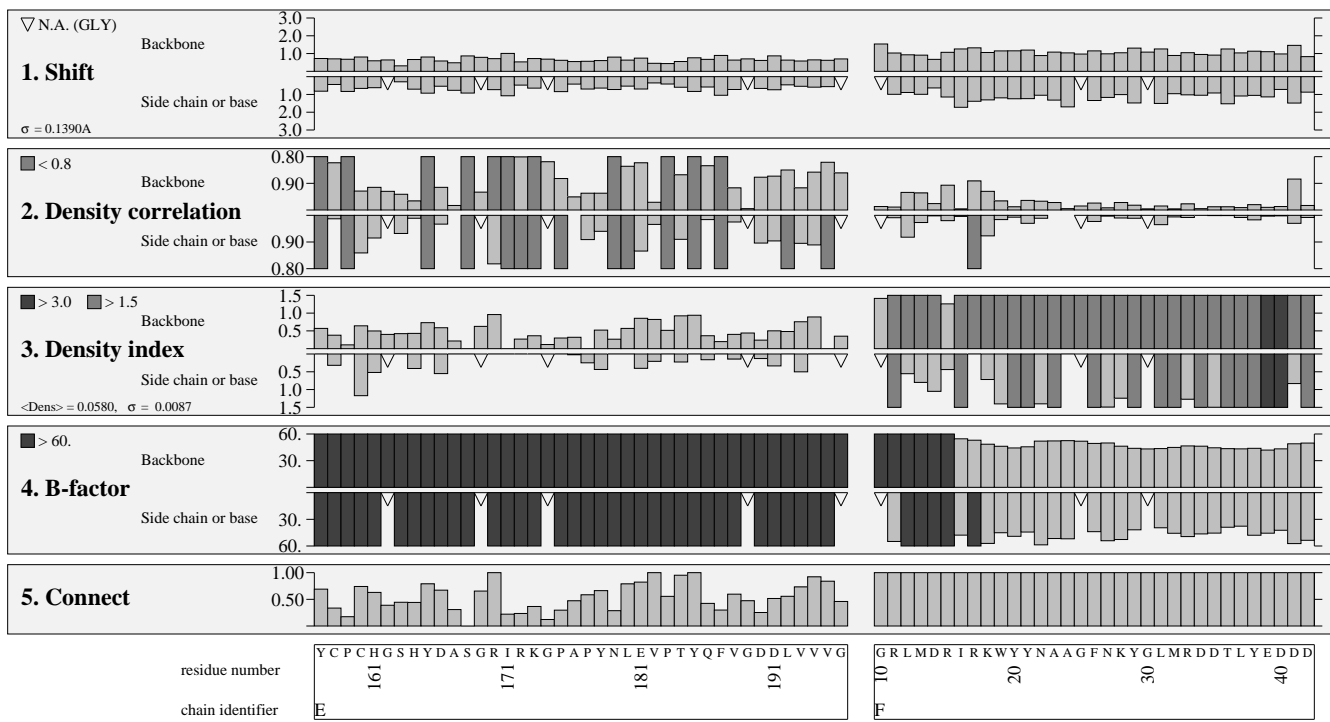
### Local estimation (11)



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## 3L72

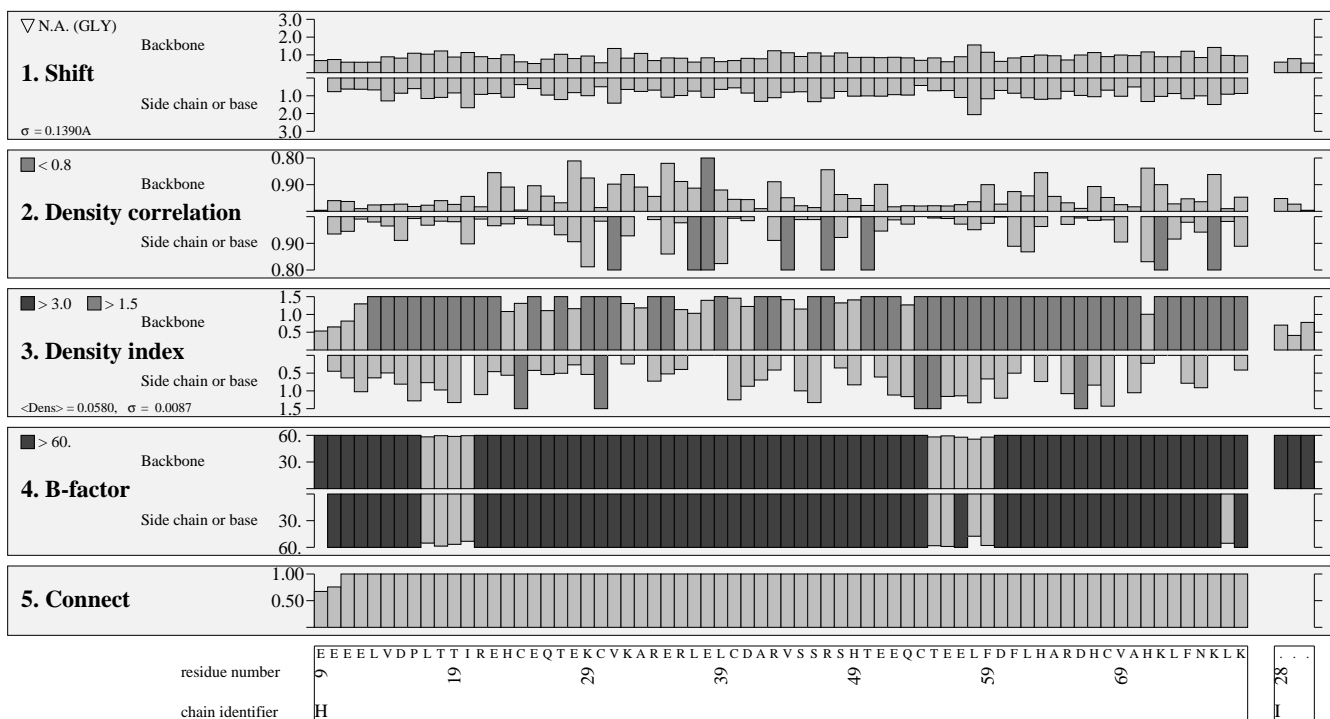
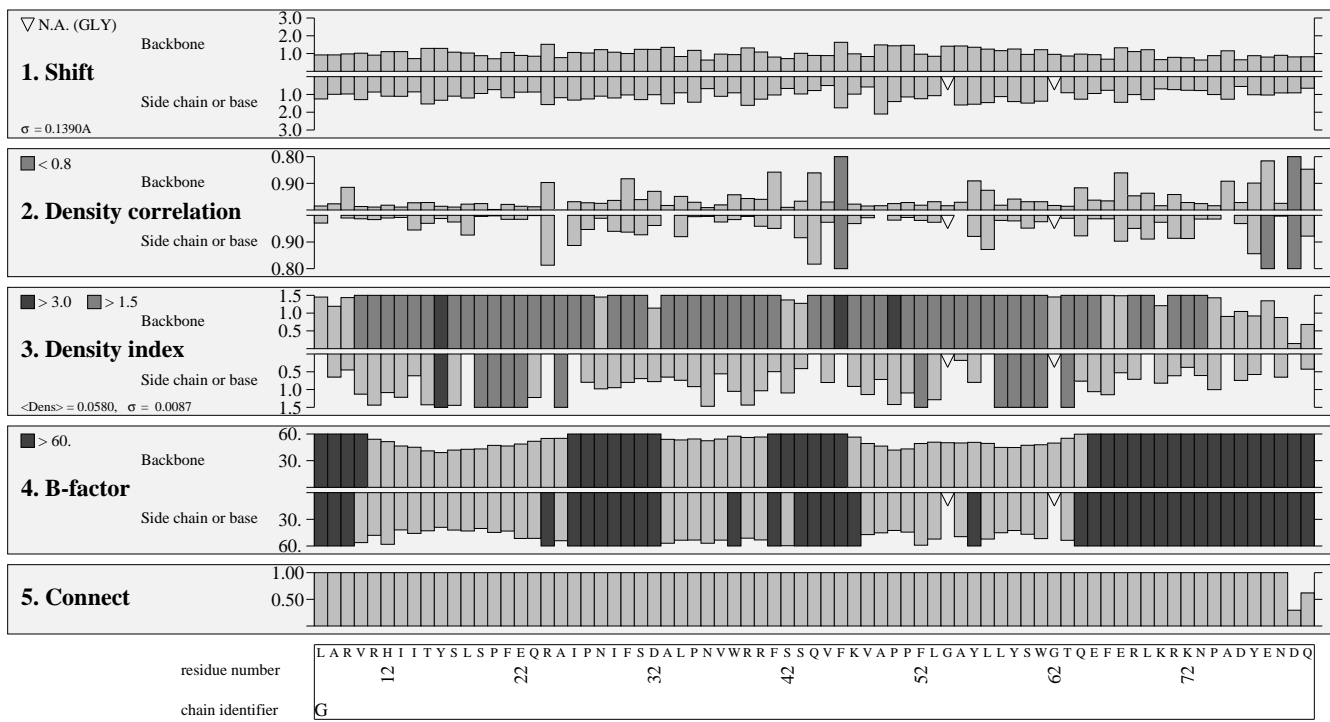
### Local estimation (12)



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## 3L72

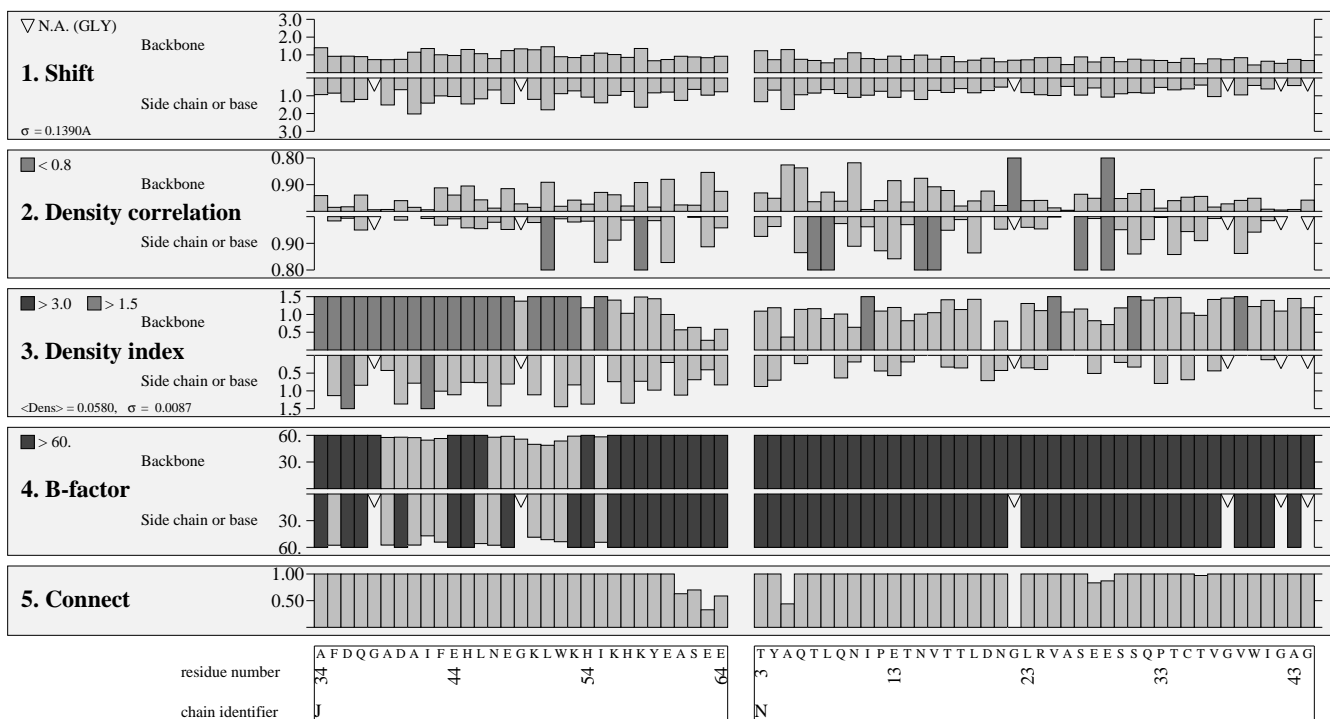
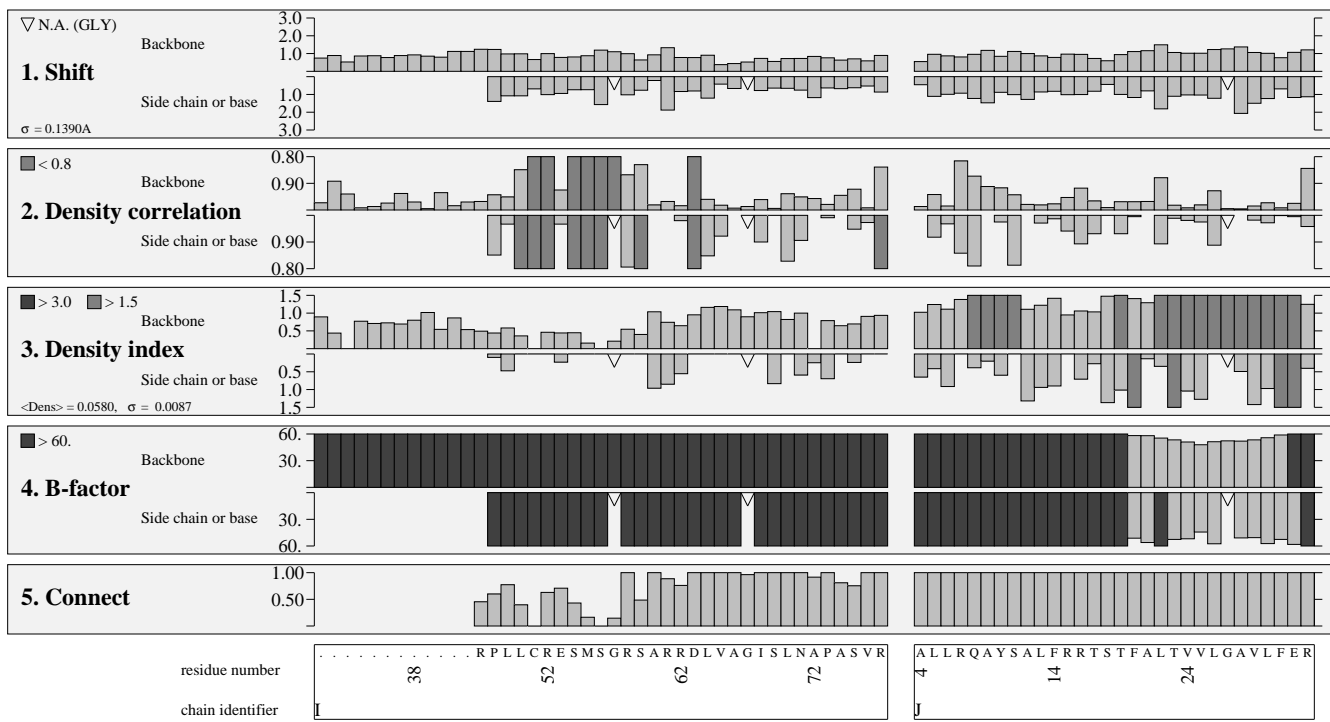
### Local estimation (13)



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## 3L72

### Local estimation (14)

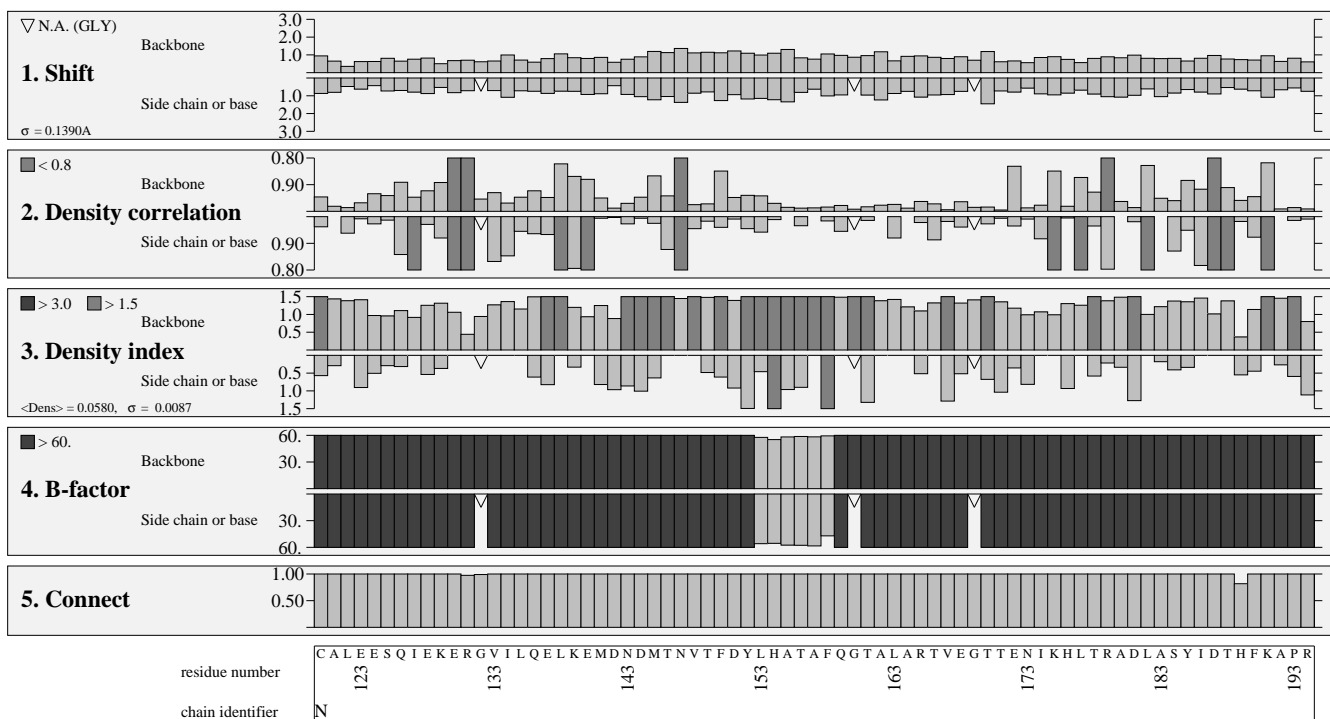
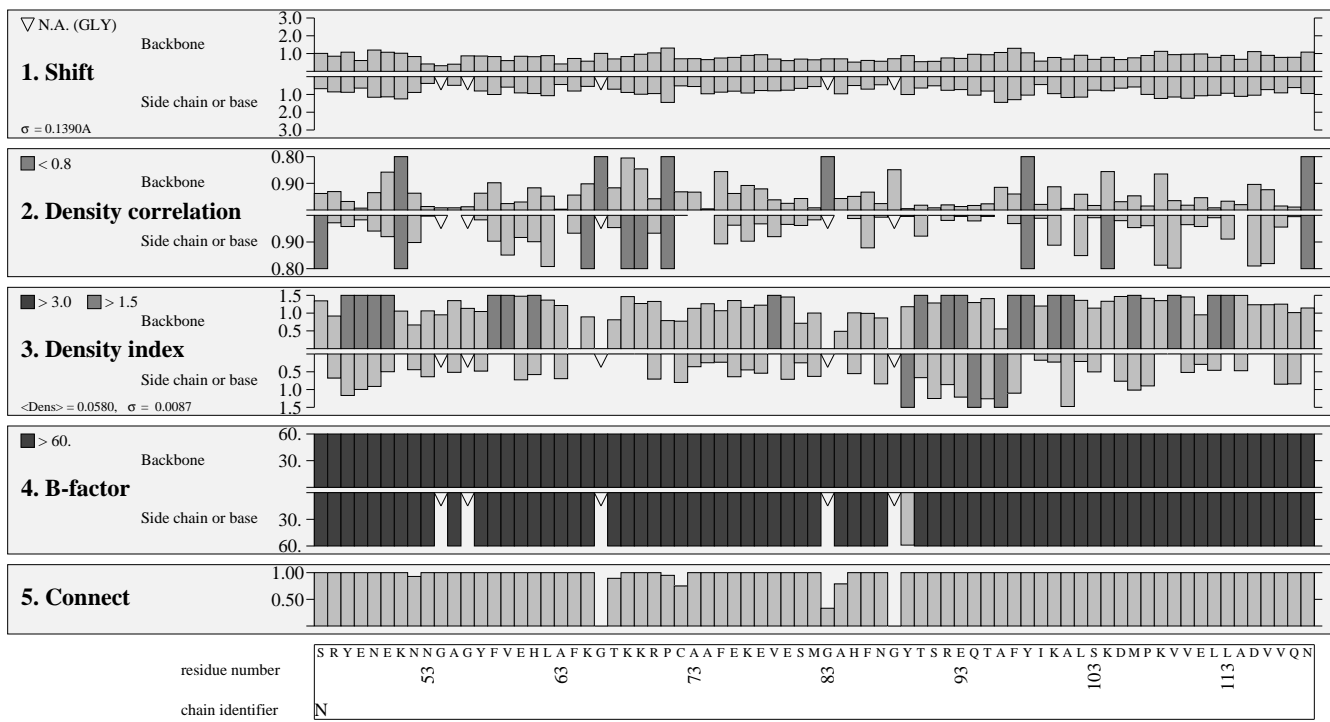




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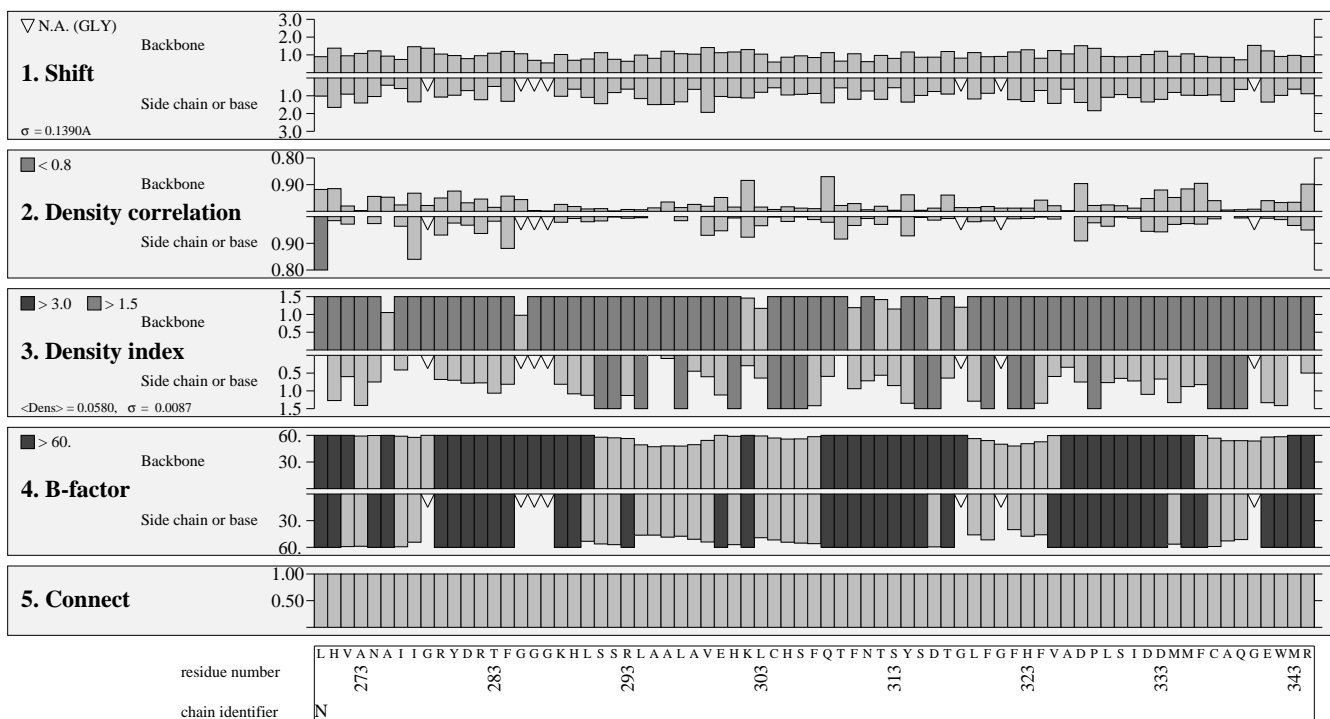
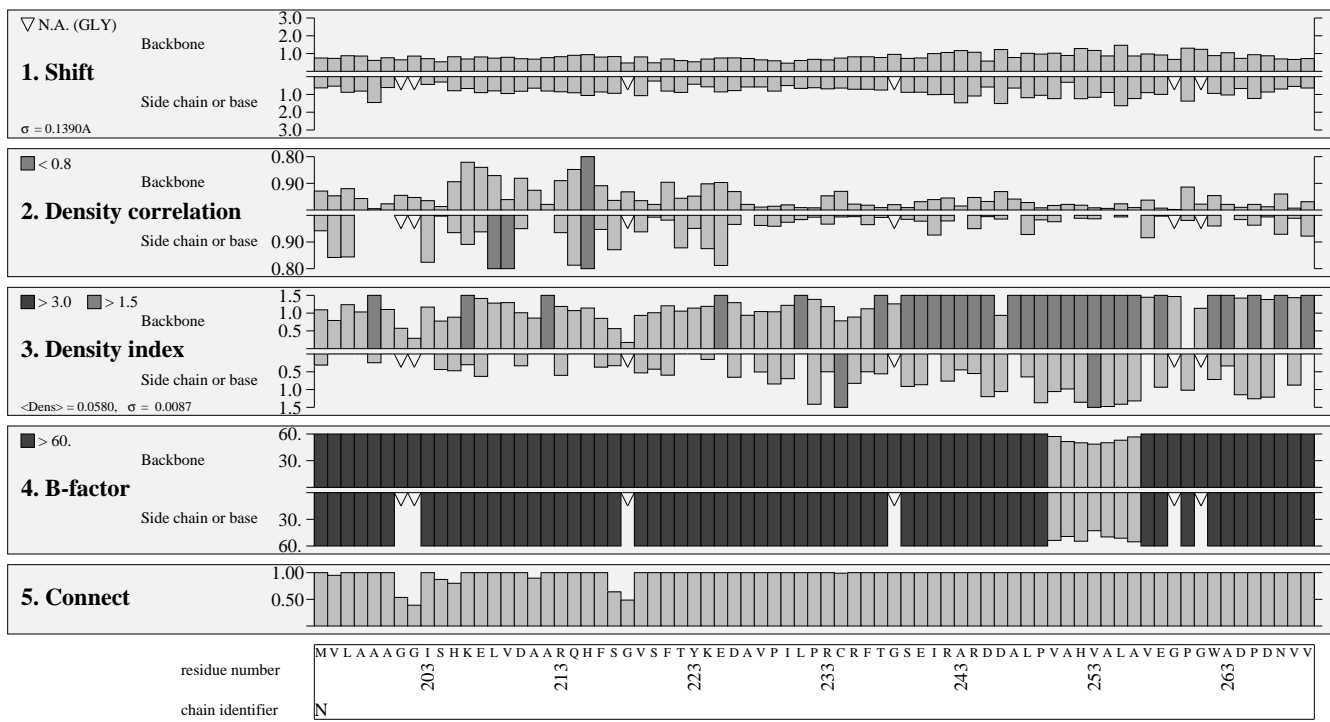
### Local estimation (15)



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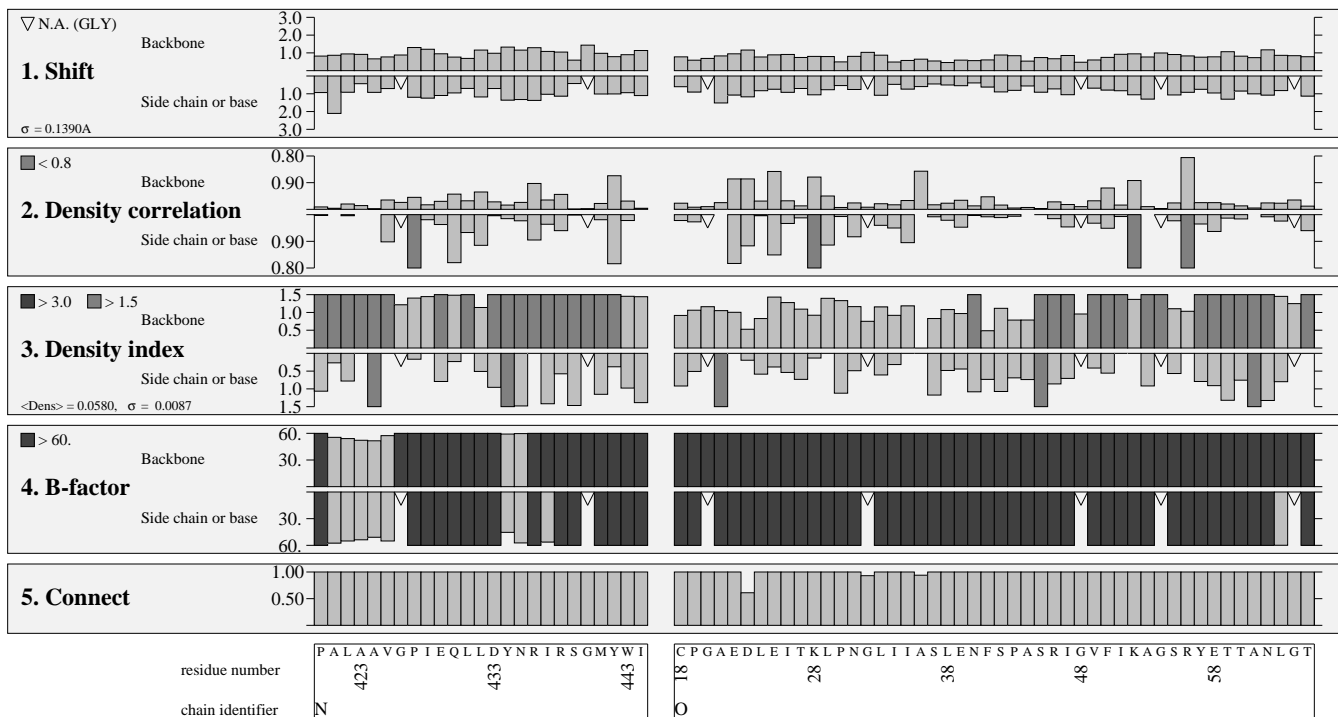
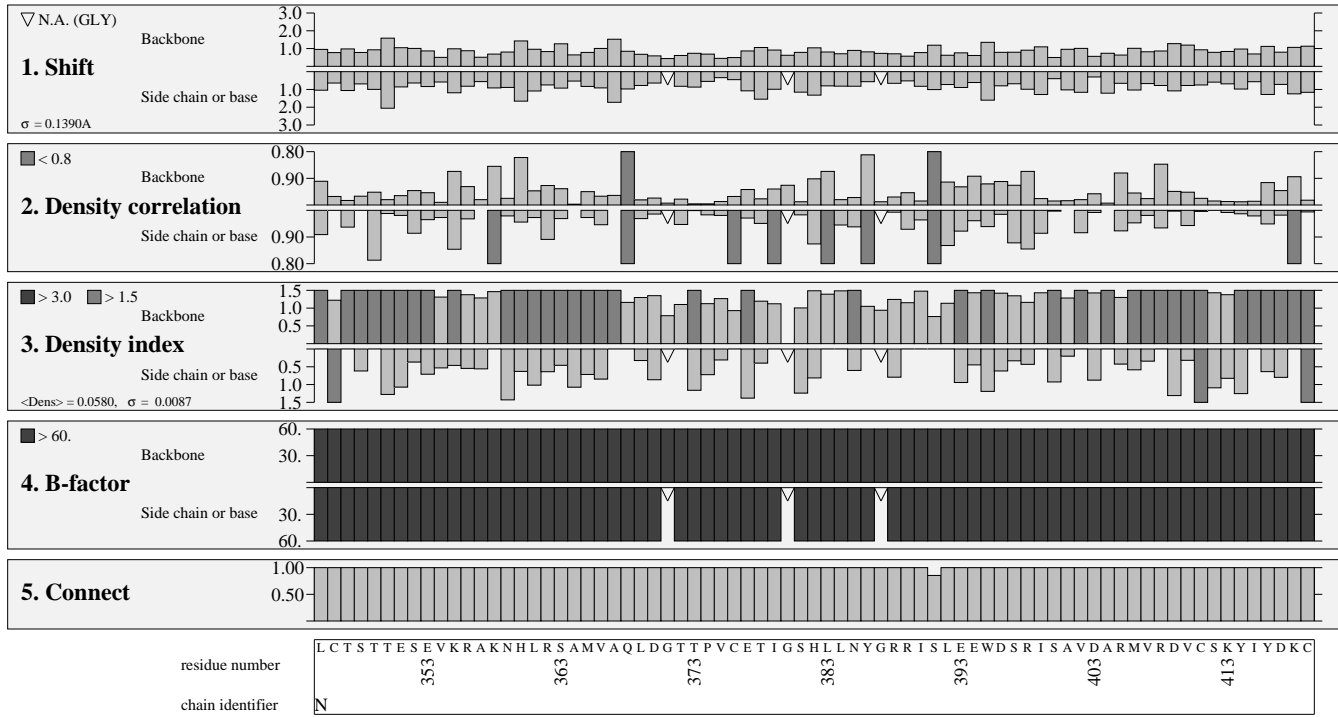
### Local estimation (16)



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## 3L72

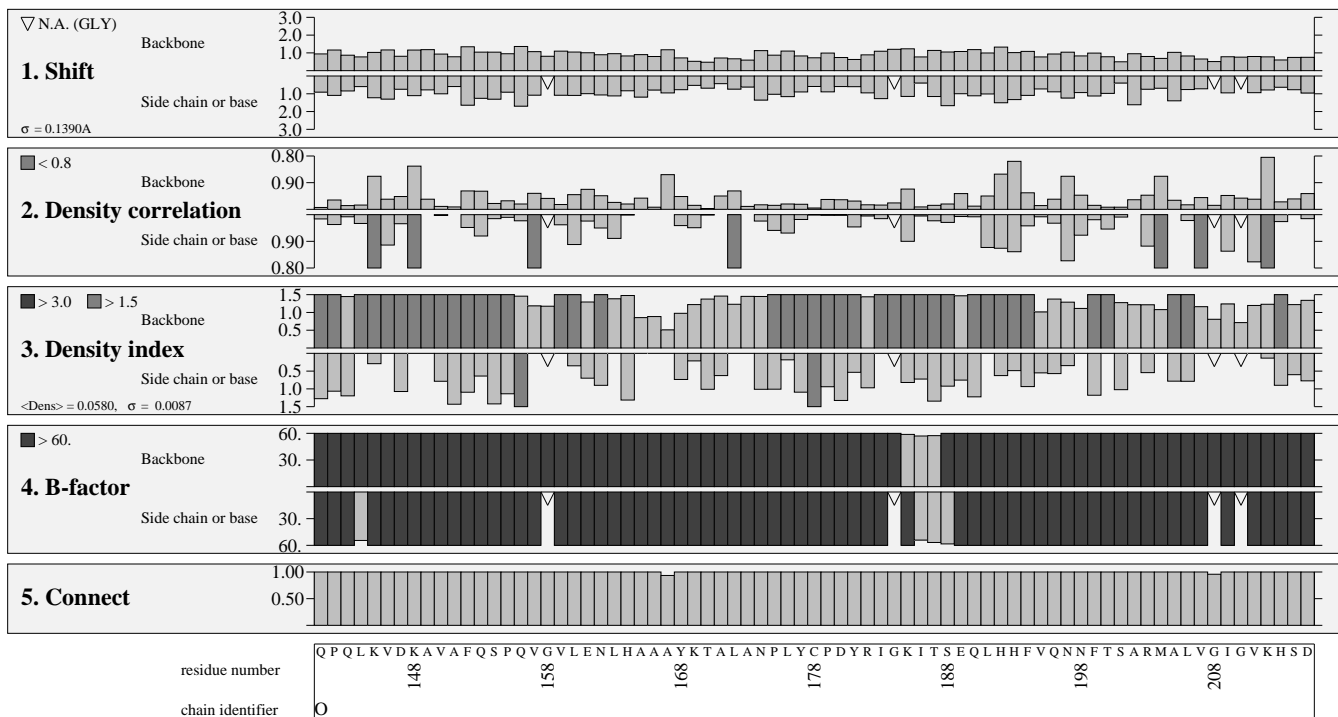
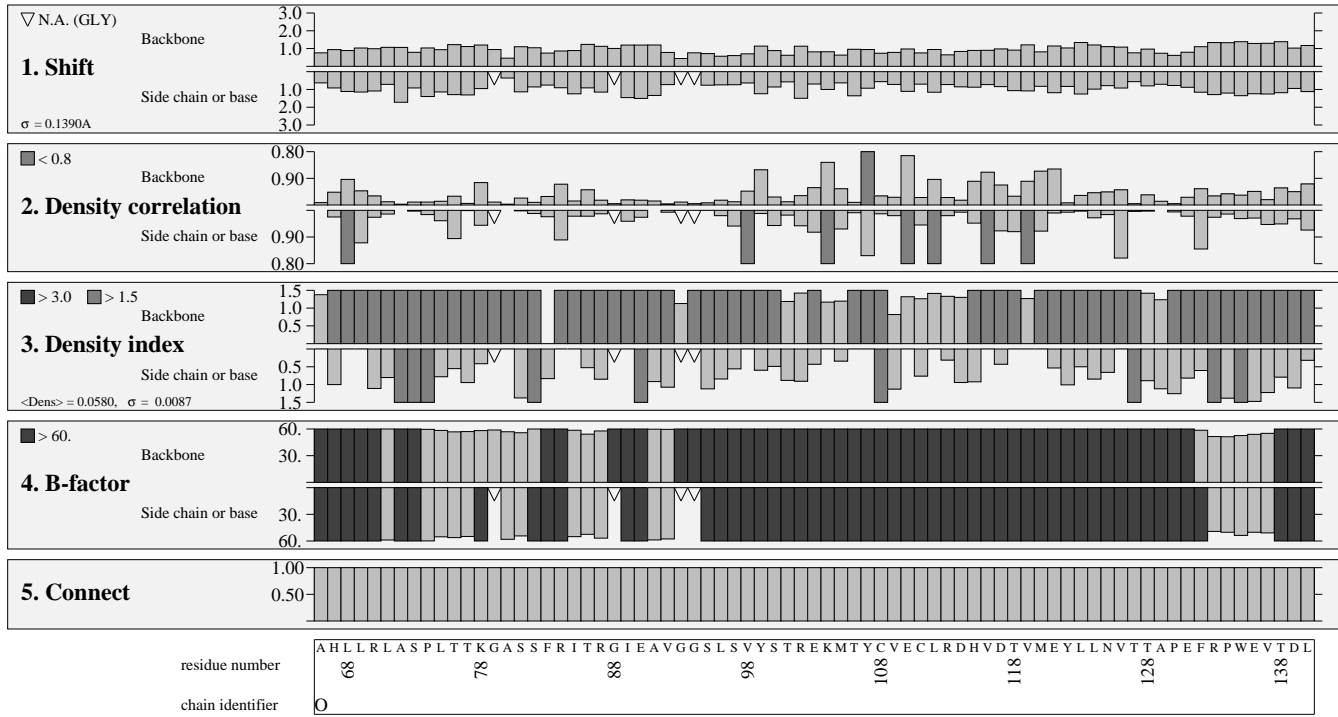
### Local estimation (17)



# Structure Factor Check

## 3L72

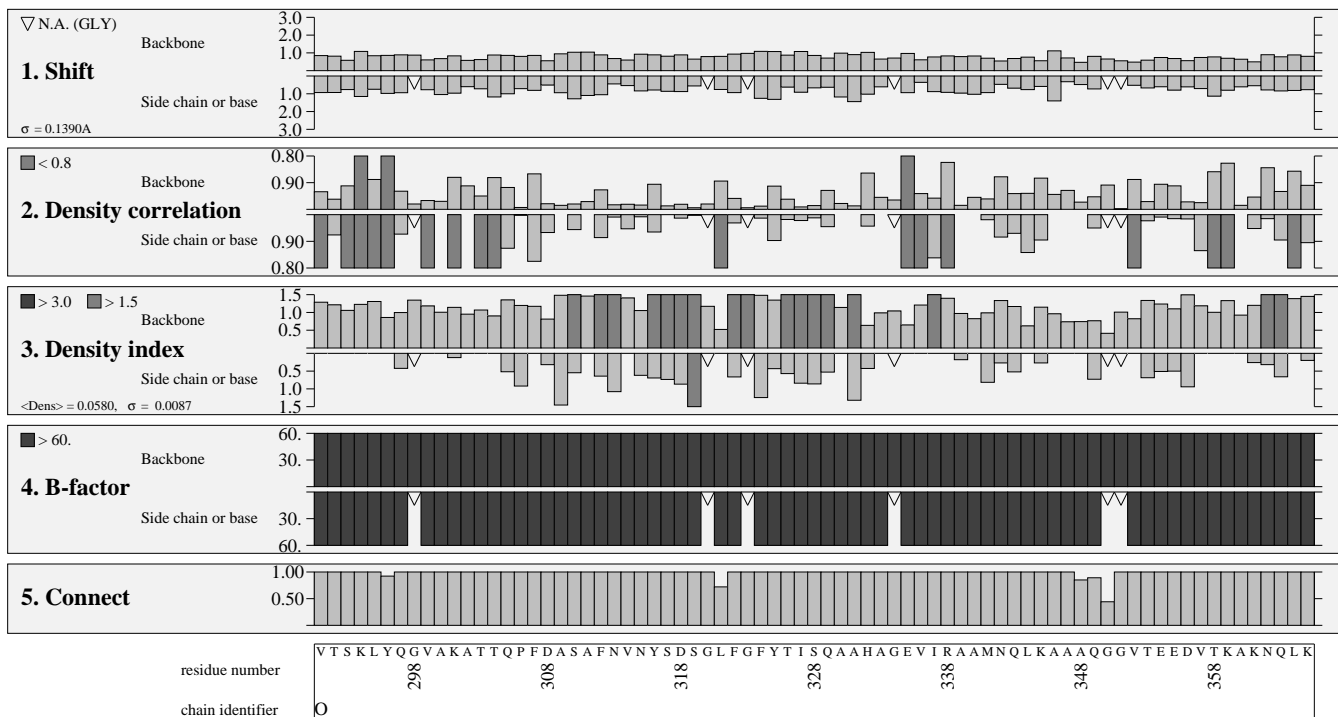
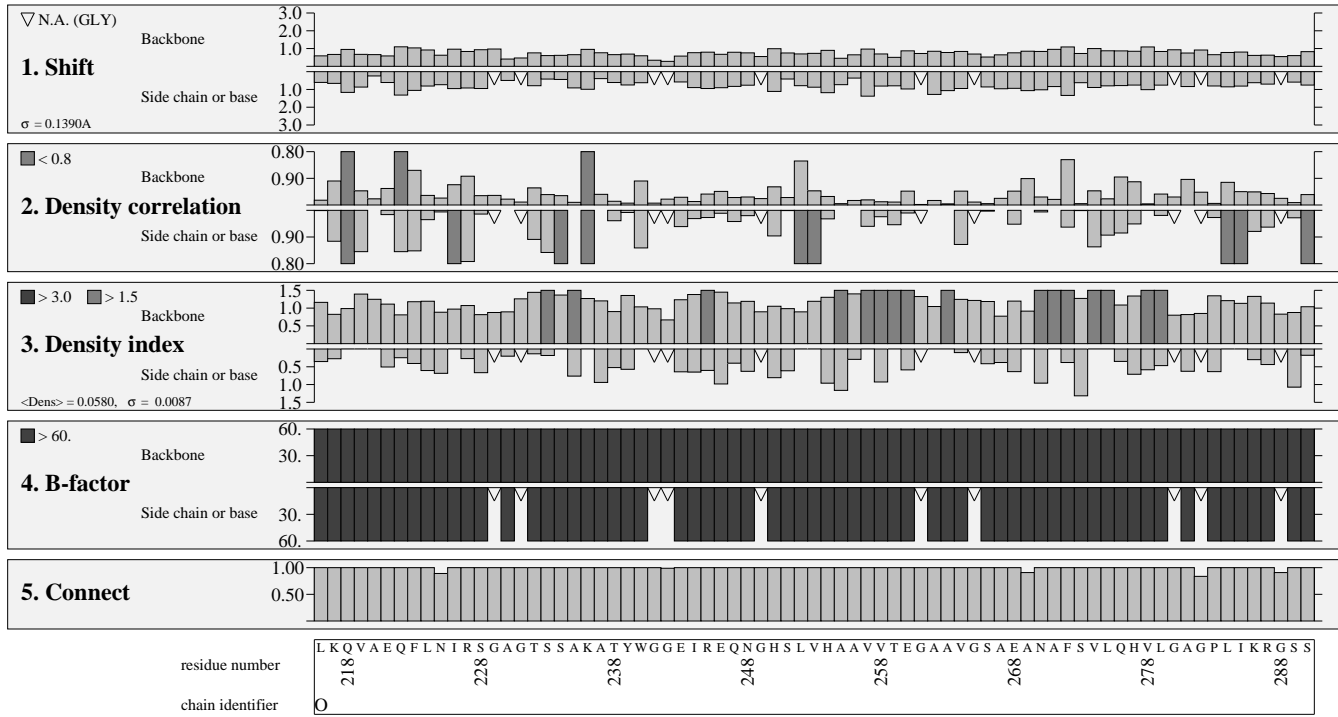
### Local estimation (18)



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## 3L72

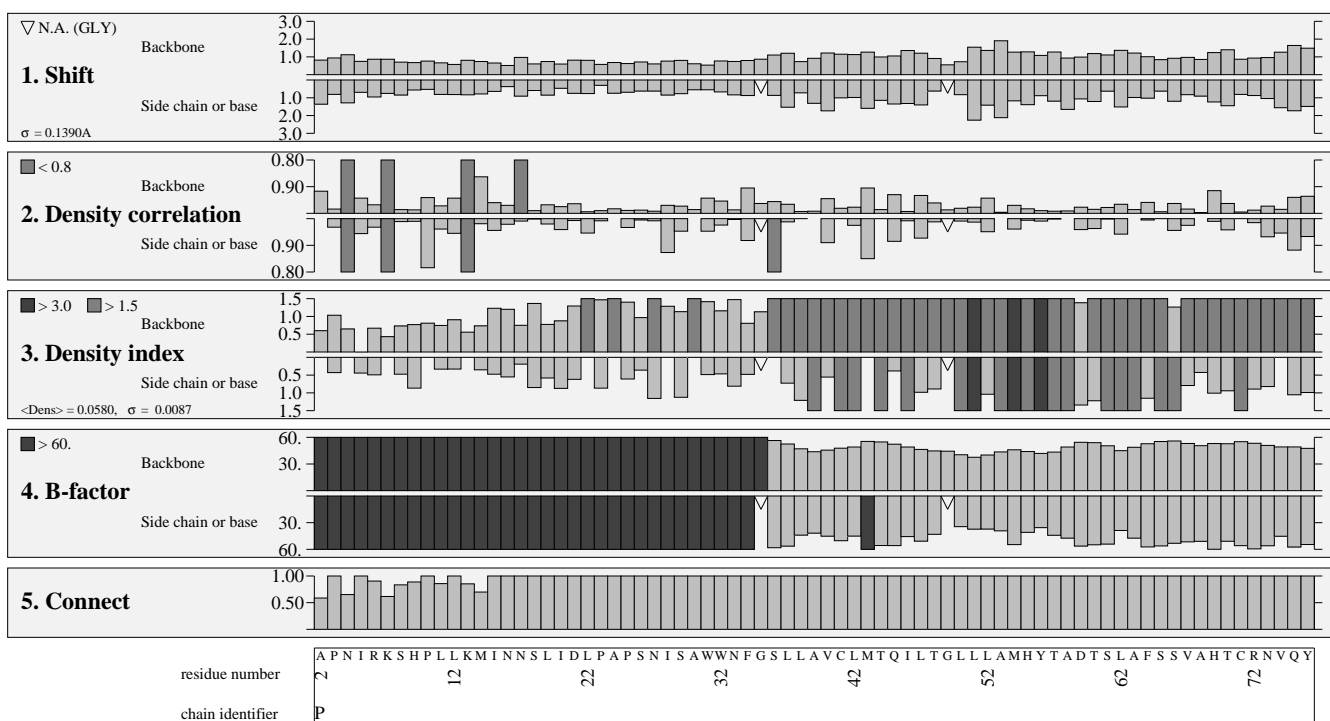
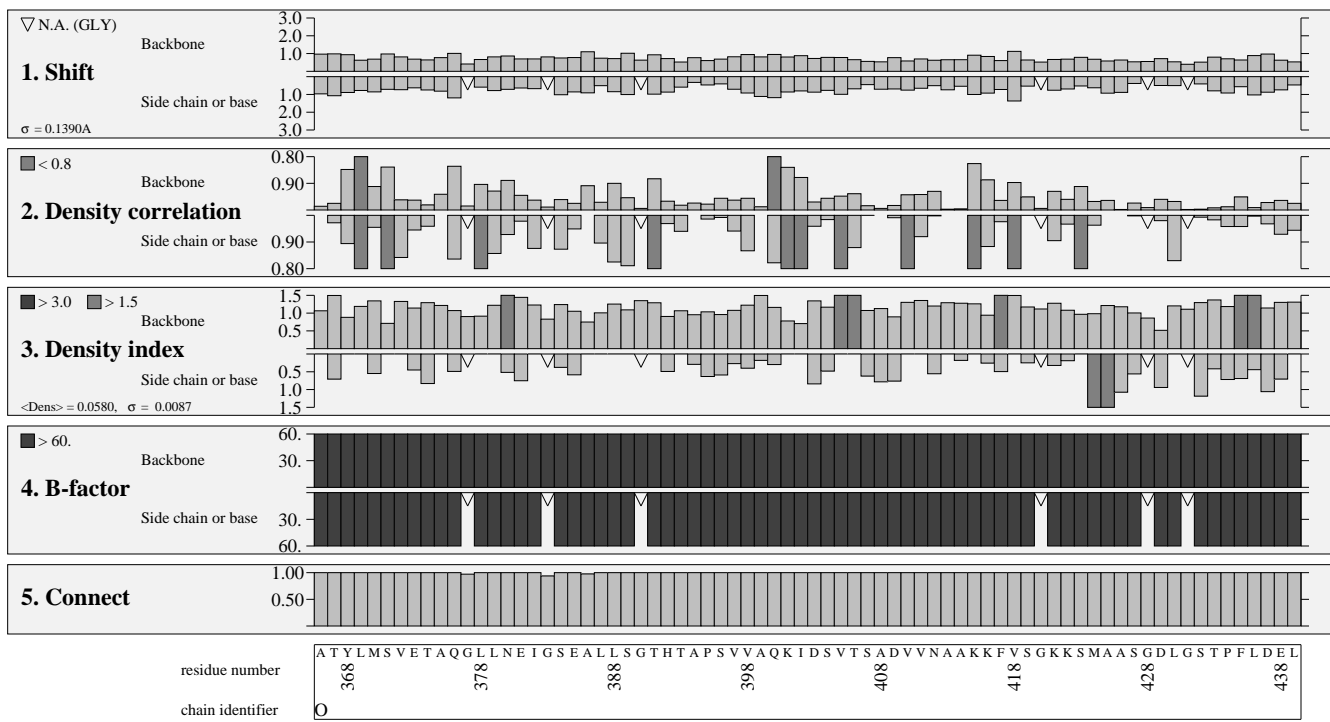
### Local estimation (19)



# Structure Factor Check

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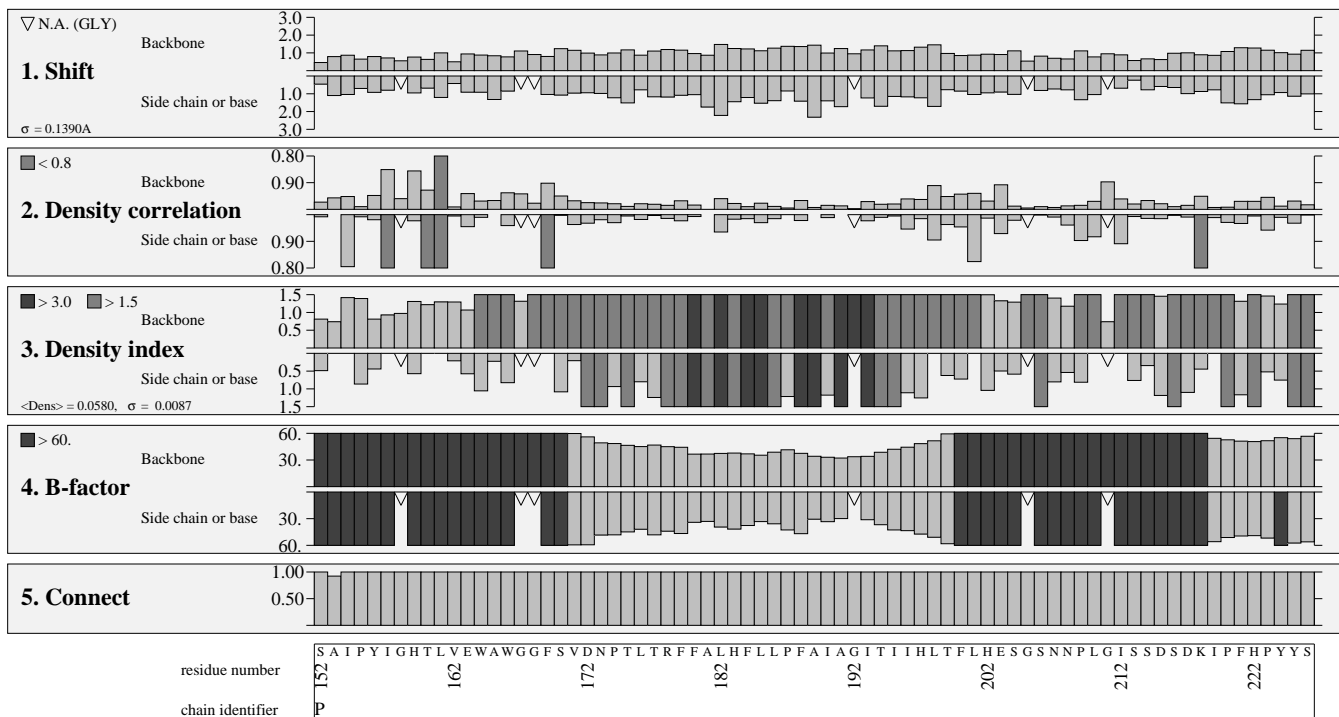
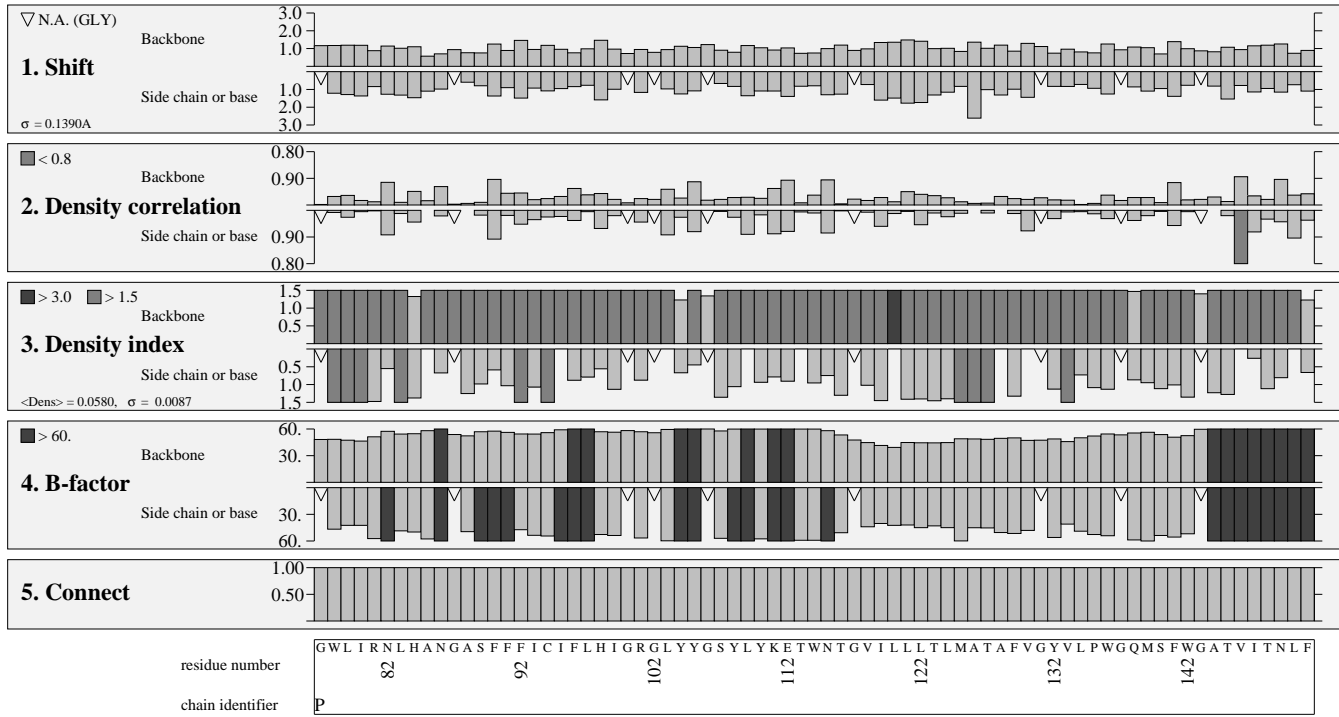
### Local estimation (20)



# Structure Factor Check

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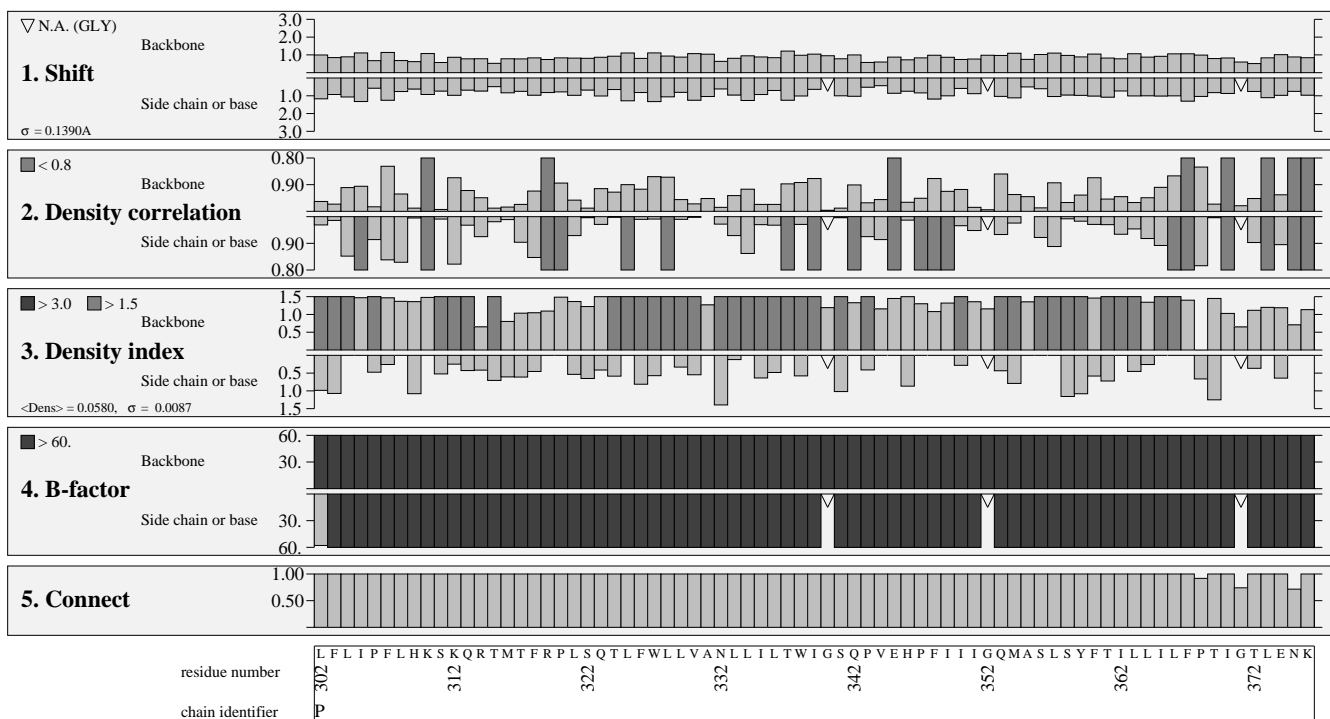
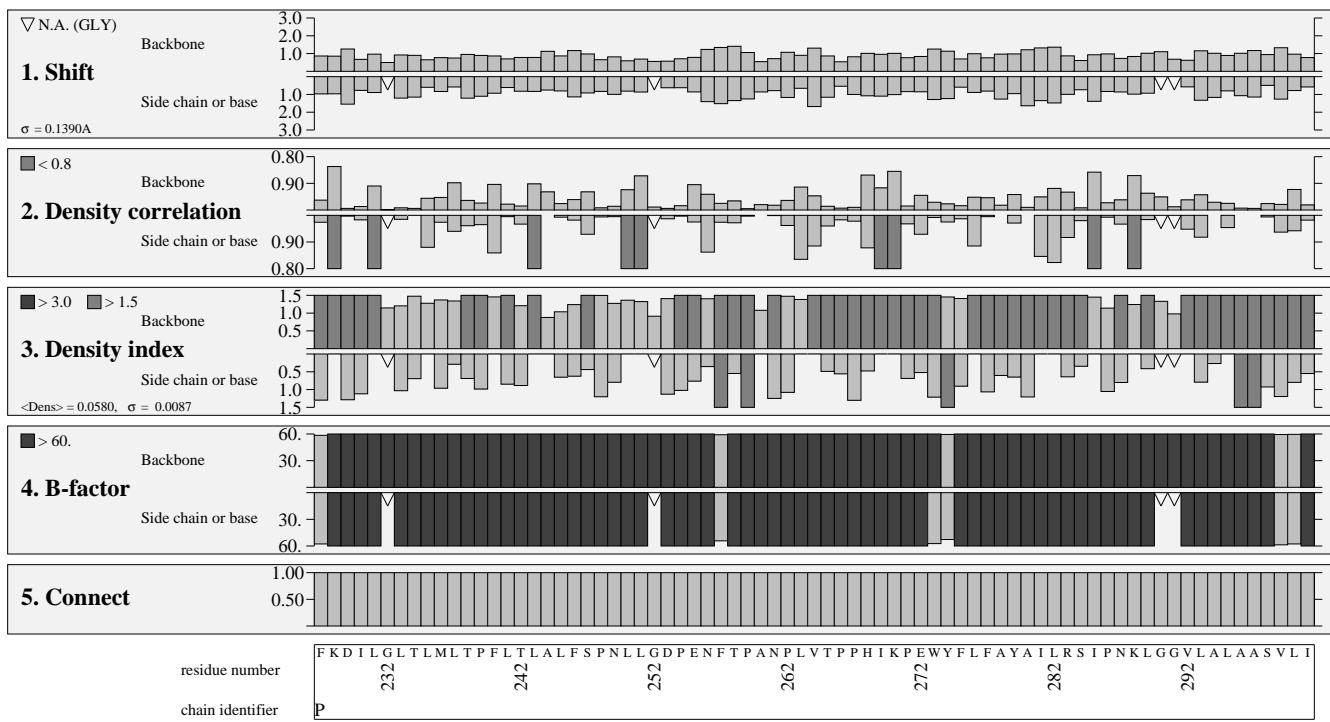
### Local estimation (21)



# Structure Factor Check

## 3L72

### Local estimation (22)

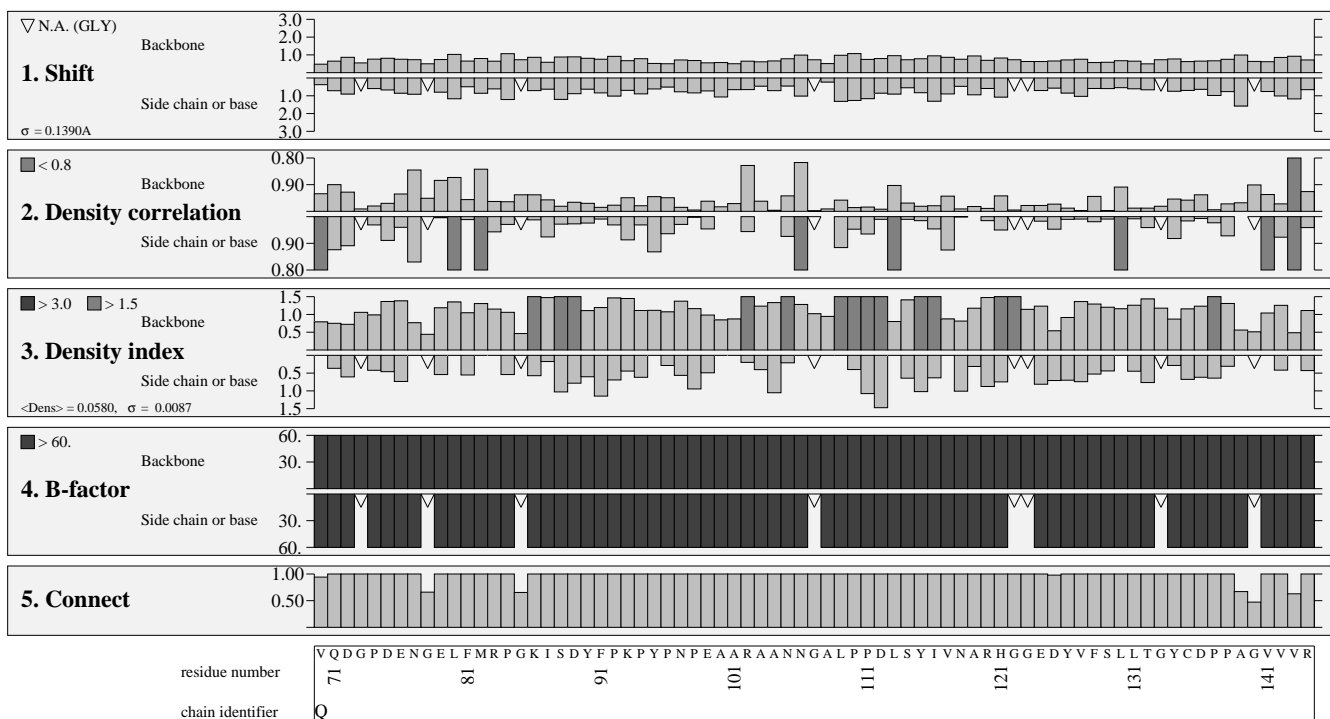
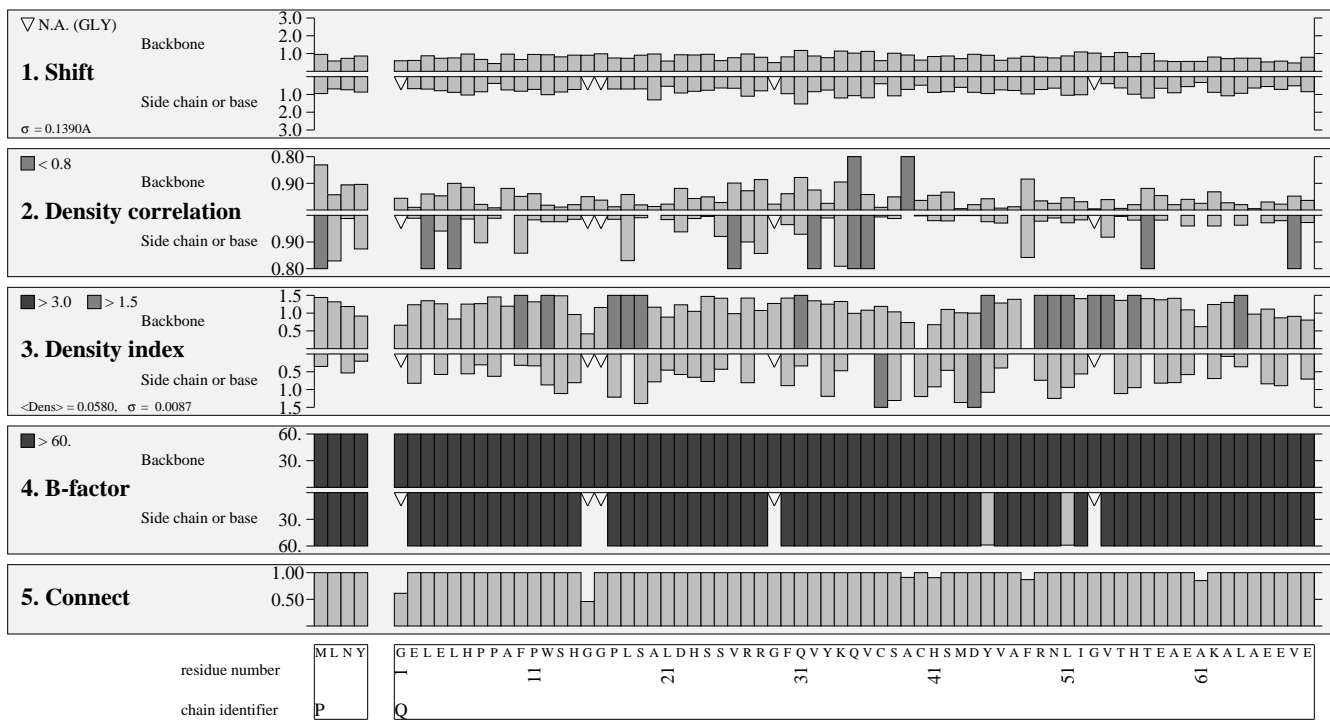




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## 3L72

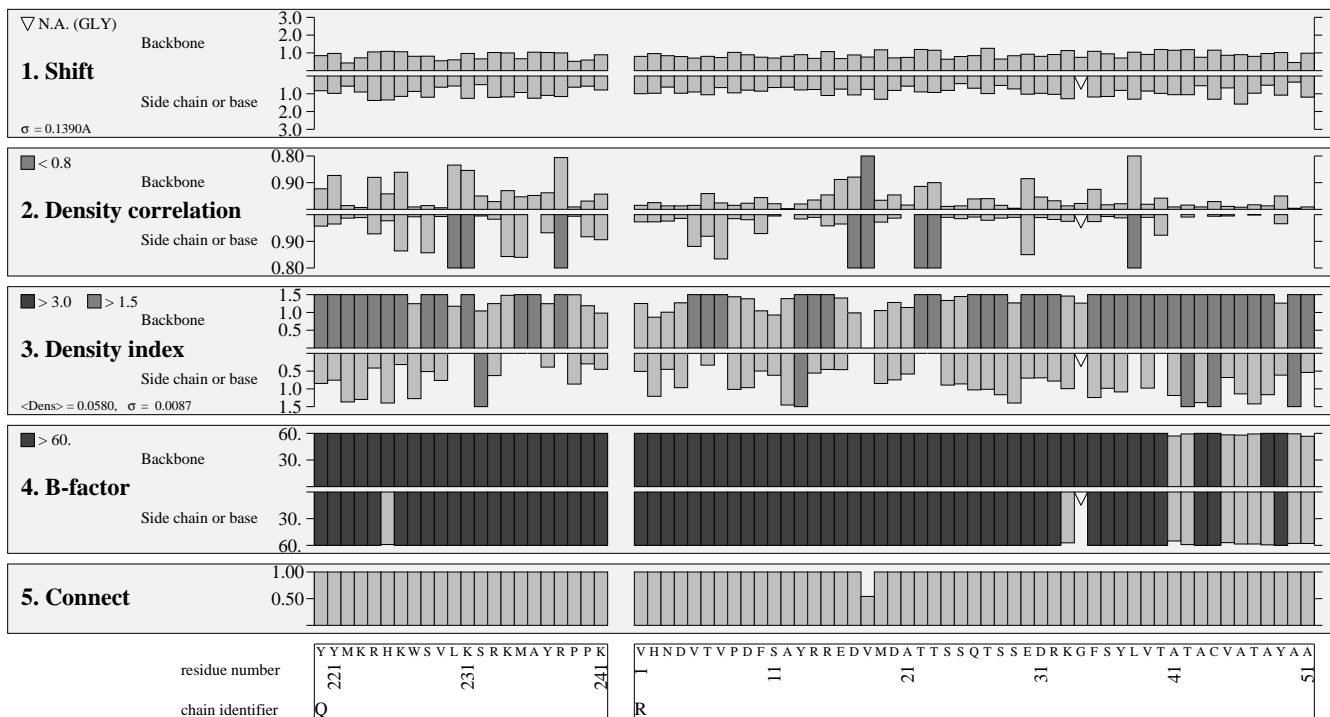
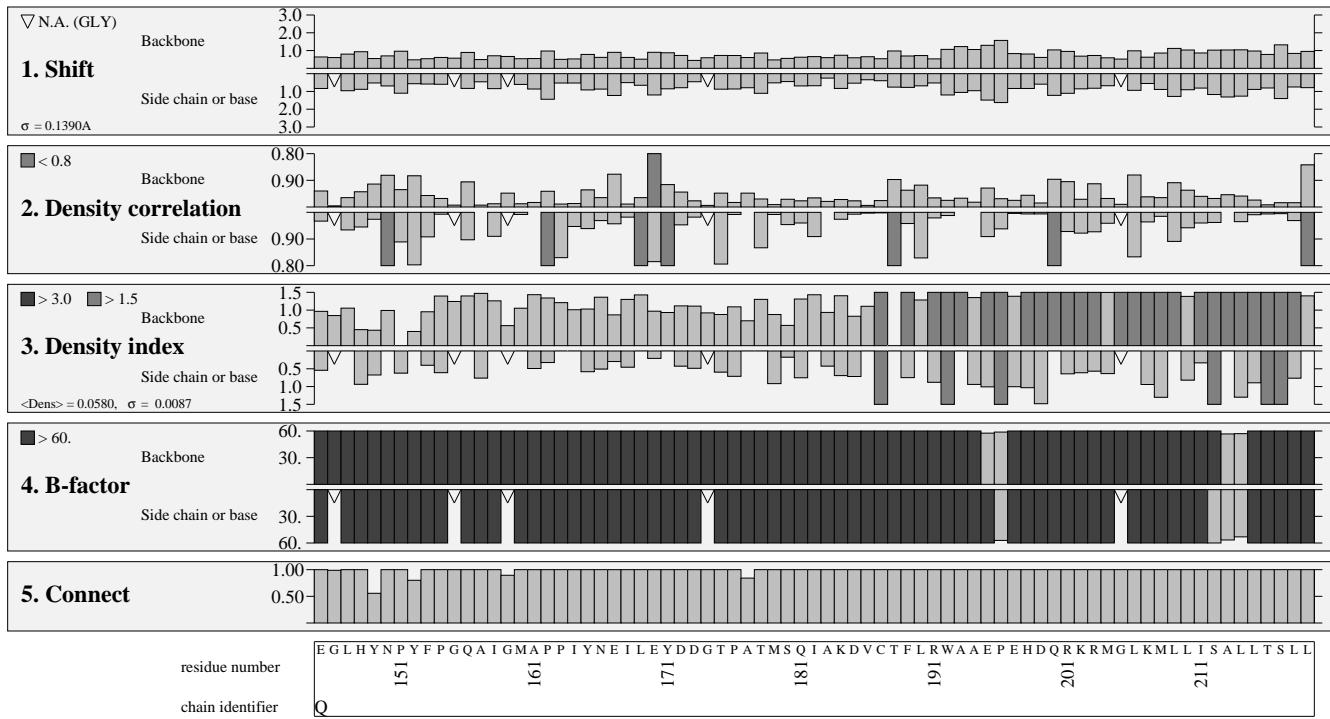
### Local estimation (23)



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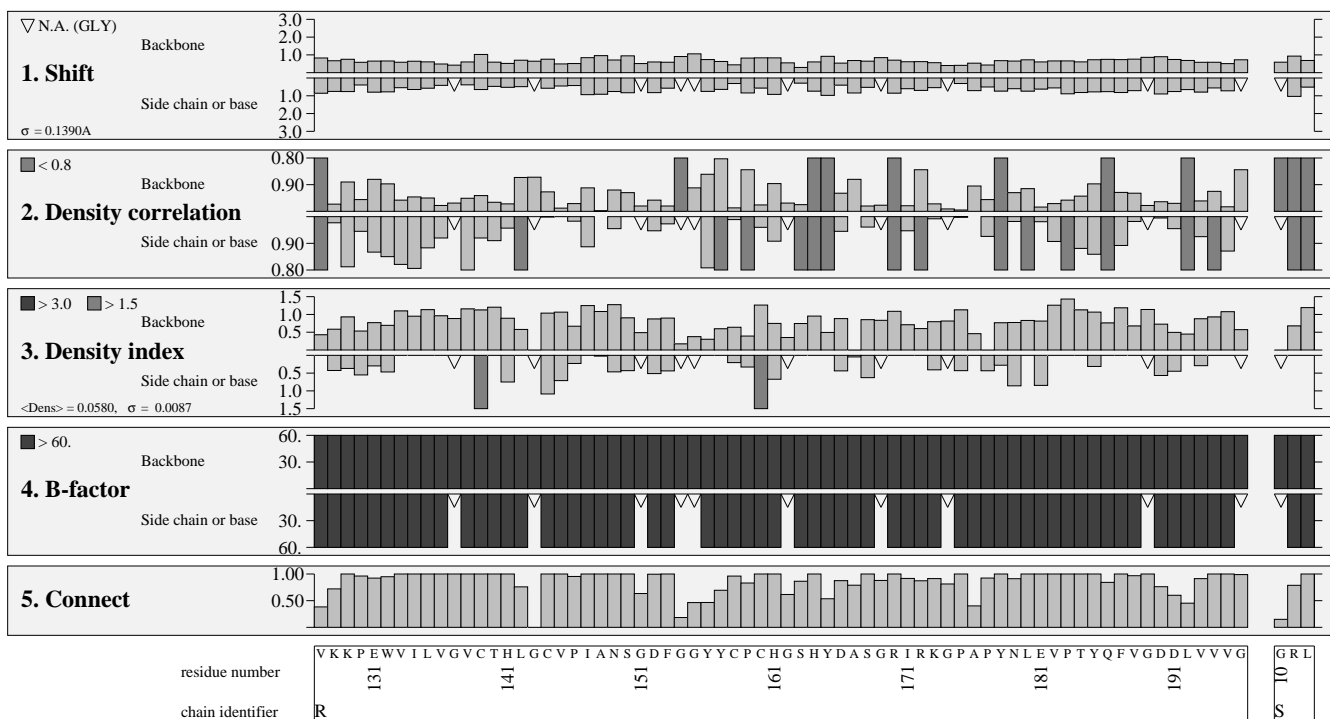
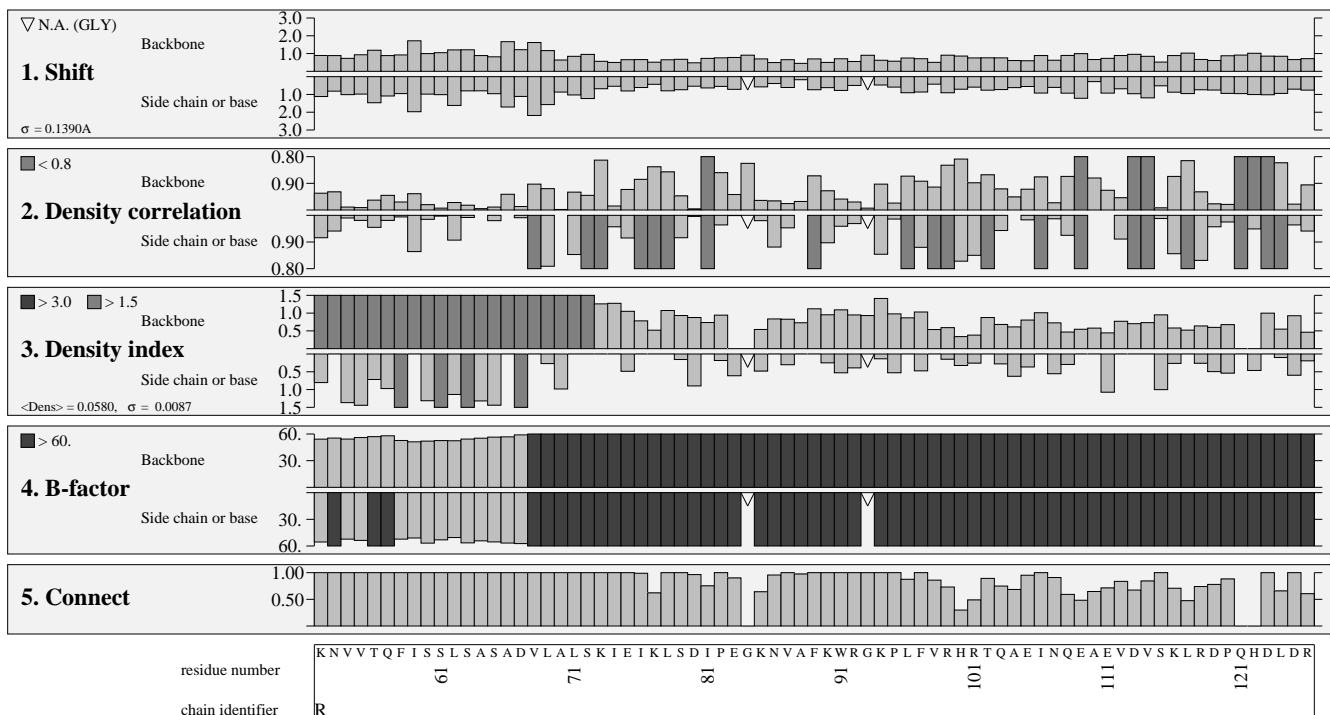
### Local estimation (24)



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## 3L72

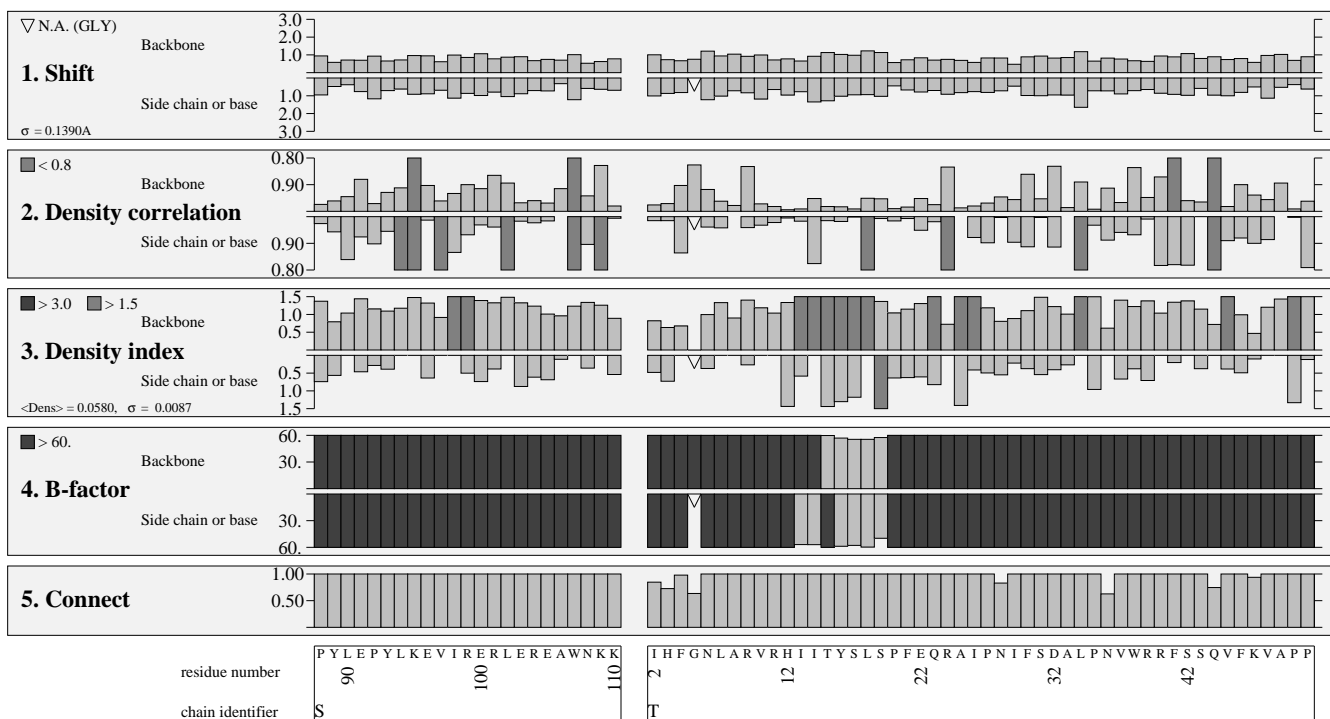
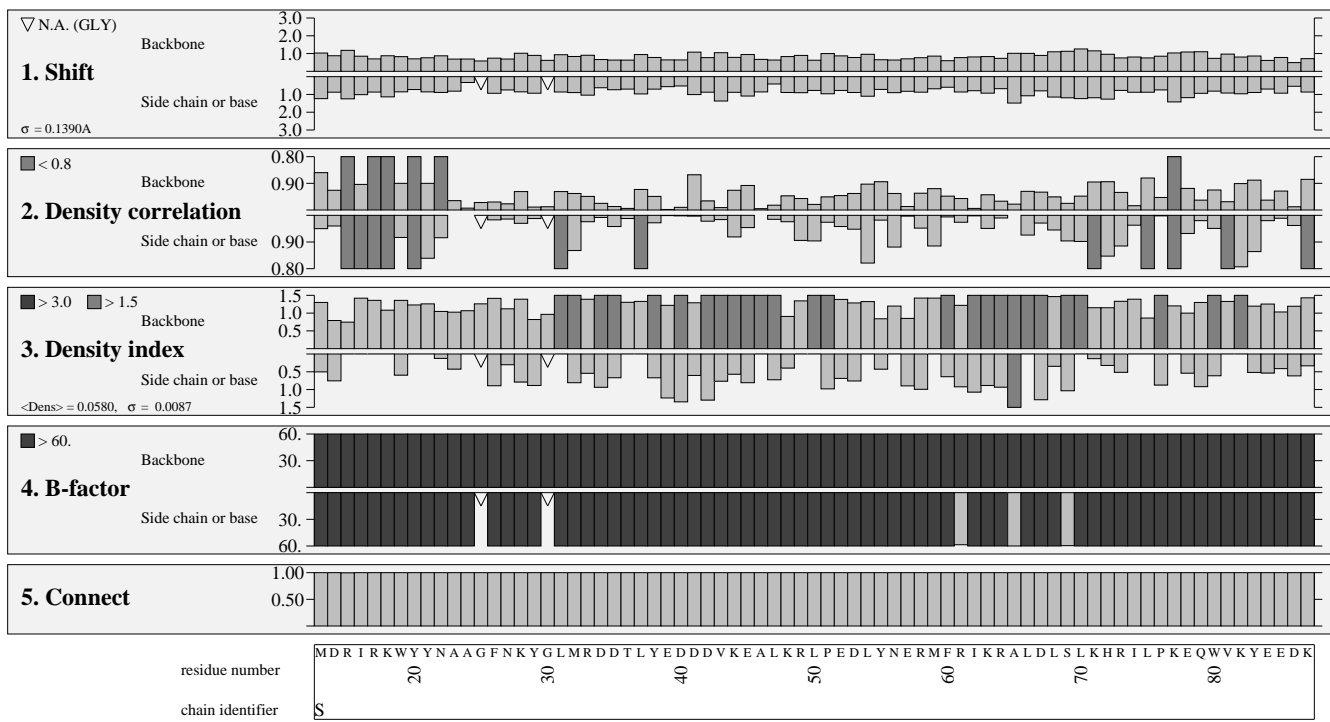
### Local estimation (25)



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## 3L72

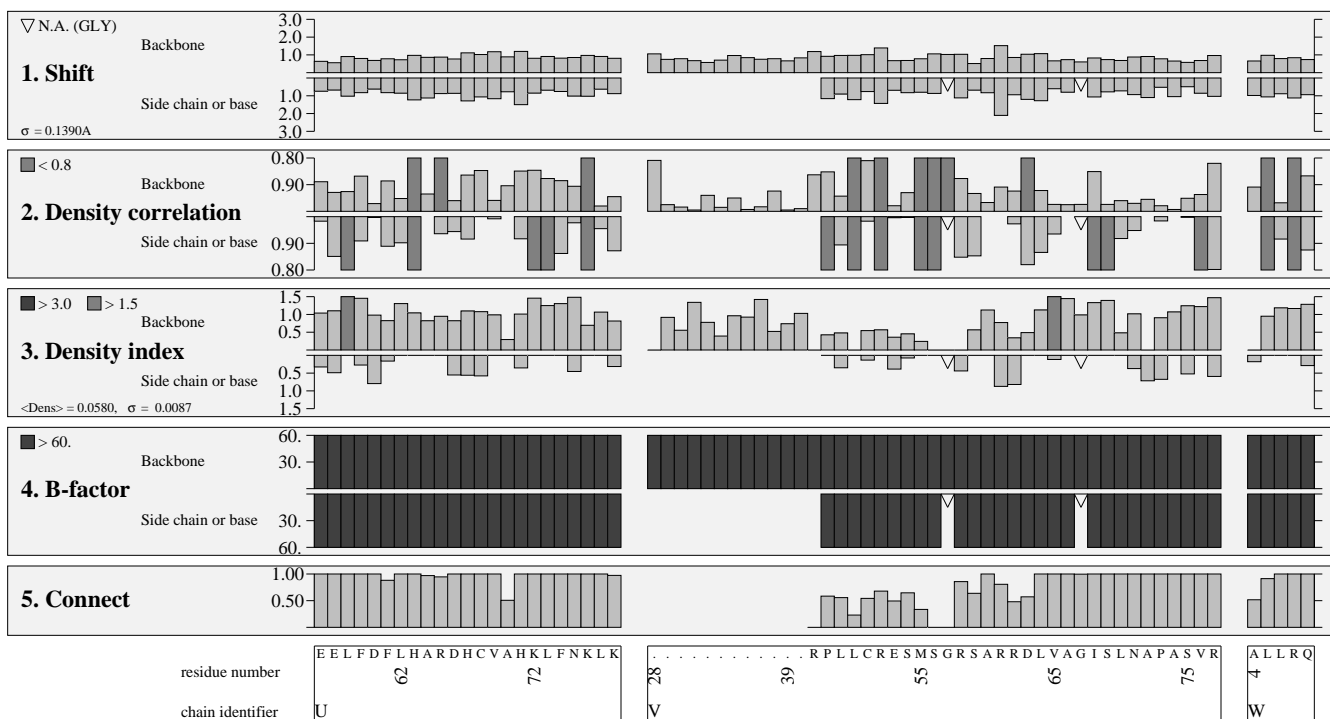
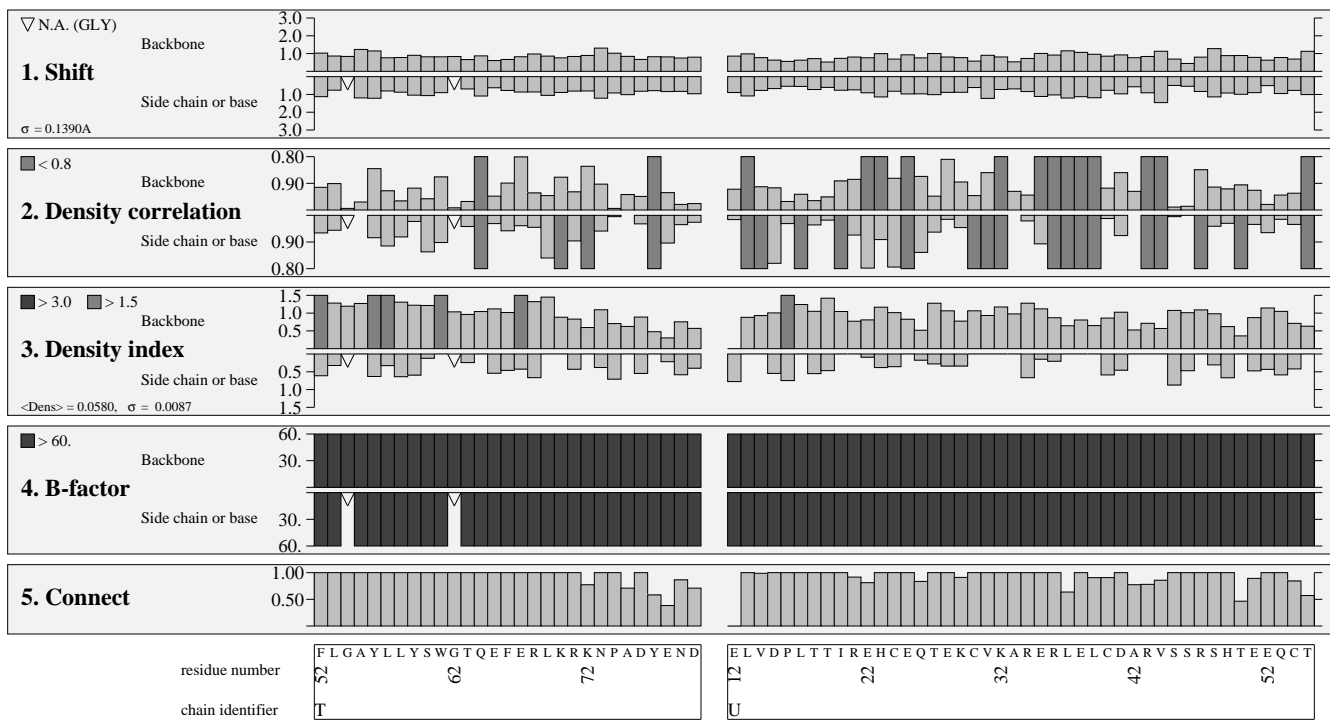
### Local estimation (26)



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## 3L72

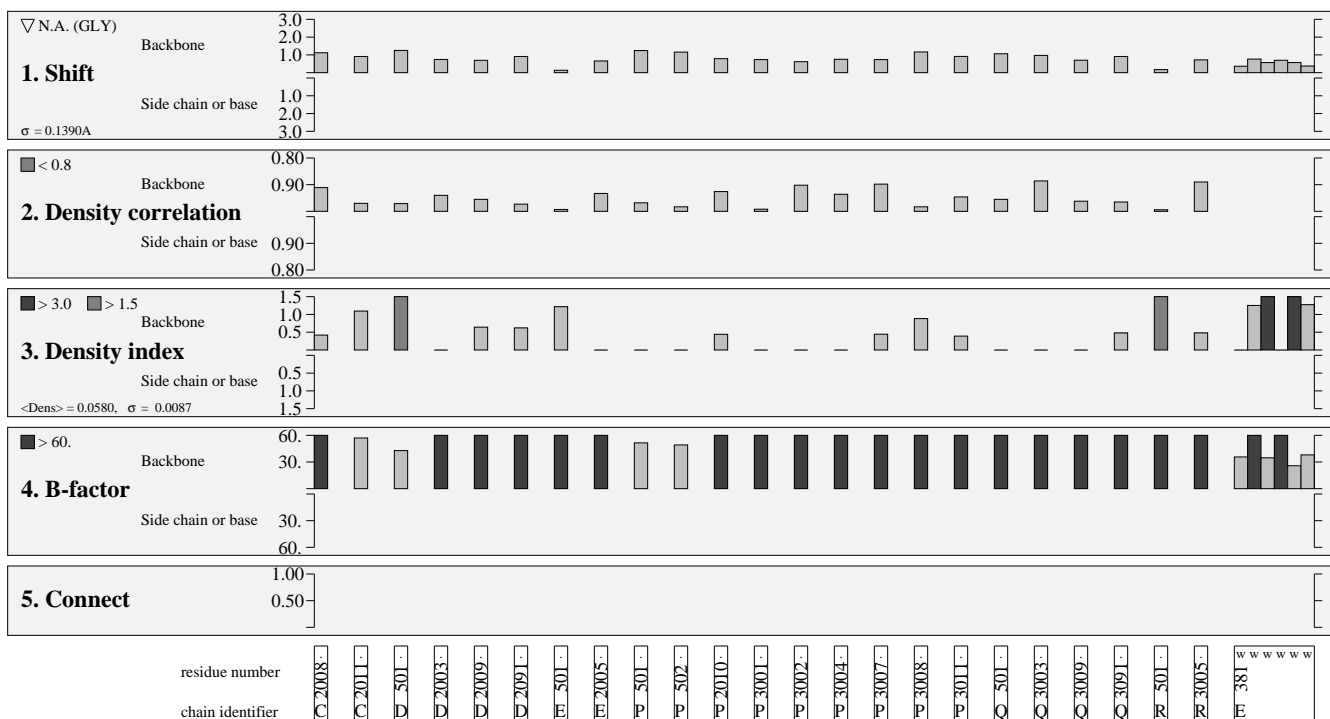
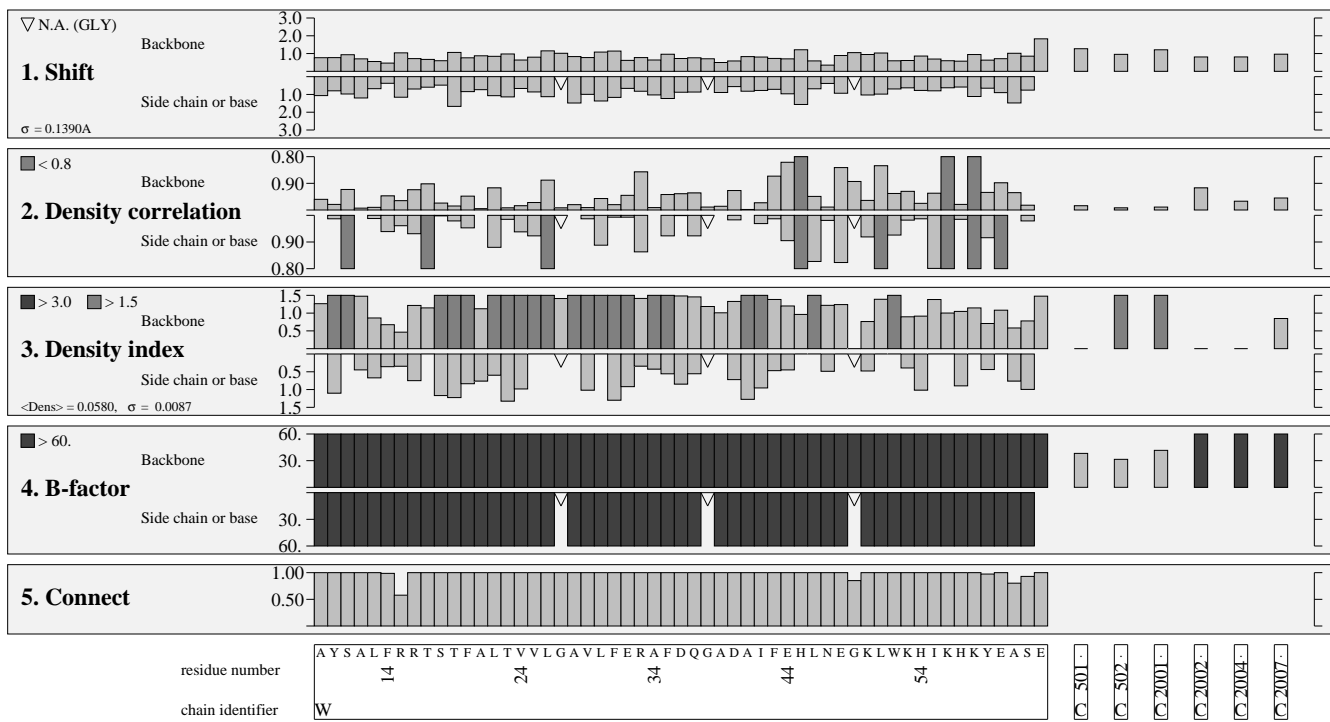
### Local estimation (27)



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## 3L72

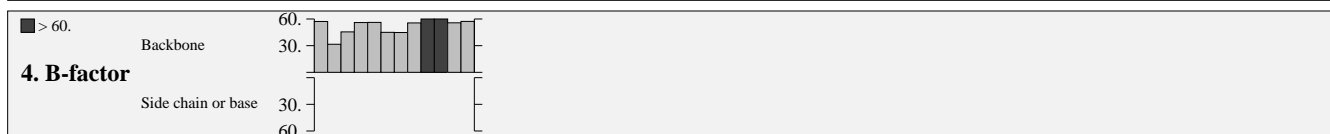
### Local estimation (28)



# Structure Factor Check

3L72

Local estimation (29)



residue number	www www www www www
chain identifier	E