

# Structure Factor Check

## 3H1I

Title: STIGMATELLIN AND ANTIMYCIN BOUND CYTOCHROME BC1 COMPLEX  
FROM CHICKEN  
Date: 12-APR-09  
PDB code: 3H1I

### Crystal

Cell parameters:

a: 174.69 A b: 181.67 A c: 240.73 A  
 $\alpha$ : 90.00  $\beta$ : 90.00  $\gamma$ : 90.00

Space group: P 21 21 21

### Structure Factors

#### Input

Nominal resolution range: 49.5 – 3.53 A  
 Reflections in file: 85472  
 Unique reflections above 0: 85472  
 above 1 $\sigma$ : 82734  
 above 3 $\sigma$ : 38800

#### SFCHECK

Nominal resolution range: 49.5 – 3.53 A  
\05max. from input data, min. from author\05  
 Used reflections: 85472  
 Completeness: 90.5 %  
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$  : 0.149  
 Anisotropic distribution of Structure Factors  
 ratio of eigen values: 1.0000 0.5035 0.5470  
 $B_{\text{overall}}$  (by Patterson): 60. A<sup>2</sup>  
 Optical resolution: 2.50 A  
 Expected opt. resol. for complete data set: 2.50 A  
 Estimated minimal error: 0.224 A

### Model

32701 atoms  
 Number of chains: 51  
 Volume not occupied by model: 62.7 %  
 $\langle B \rangle$  (for atomic model): 78.7 A<sup>2</sup>  
 $\sigma(B)$ : 21.96 A<sup>2</sup>  
 Matthews coefficient: 4.17  
 Corresponding solvent % : 70.29

### Model vs. Structure Factors

R-factor for all reflections: 0.321  
 Correlation factor: 0.777  
 R-factor: 0.319  
 for  $F > 2.0\sigma$   
 nom. resolution range: 19.99 – 3.53A  
 reflections used: 82388

Rfree: 0.351  
 Nfree: 2477  
 R-factor without free-refl.: 0.318  
 Non free-reflections: 79911  
 $\langle u \rangle$  (error in coords by Luzzati plot): 0.715 A  
 Estimated maximal error: 0.470 A  
 DPI: 0.691 A

#### Scaling

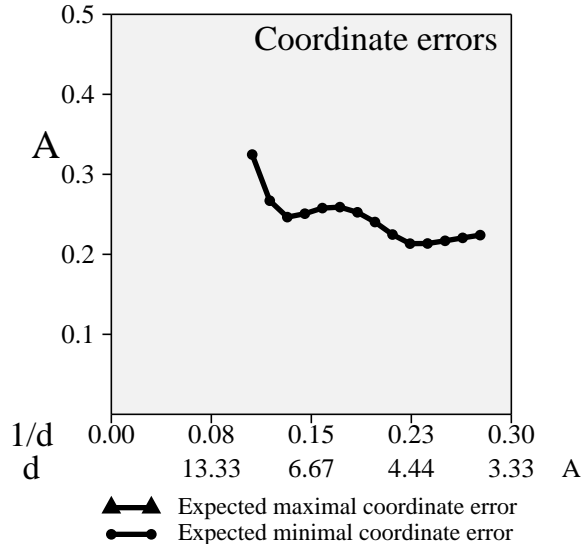
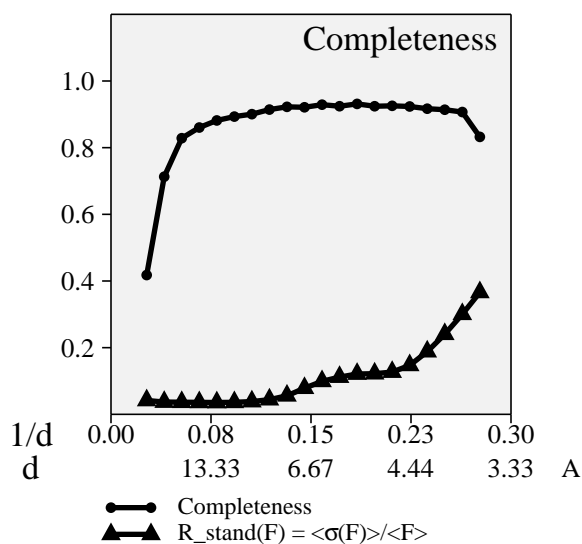
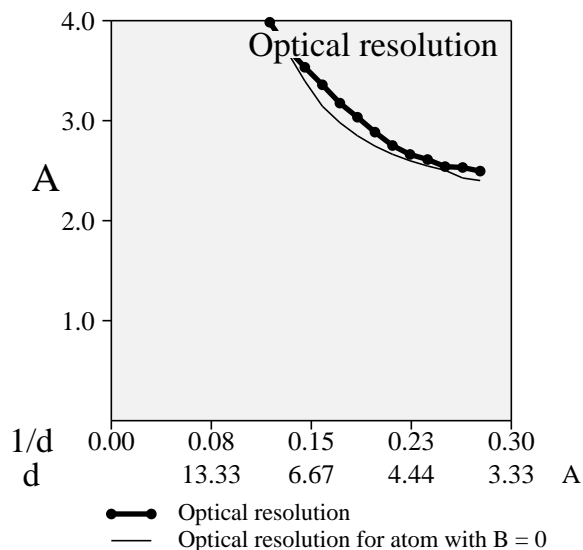
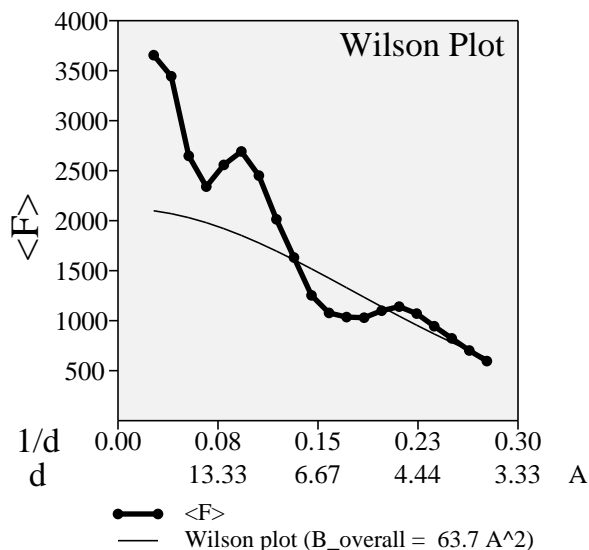
Scale: 0.883  
 Bdiff: -7.32  
 Anisothermal Scaling (Beta):  
 13.0667 0.6487 2.3764 0.0000 0.0000 0.0000  
 Solvent correction – Ks,Bs: 0.655 250.453

### Refinement

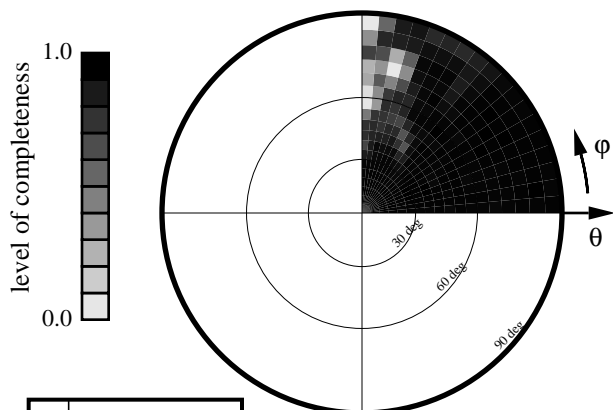
Program: CNS 1.1  
 Nominal resolution range: 20.0 – 3.53 A  
 Reported nominal resolution: 3.00 A  
 Reported R-factor: 0.263  
 Number of reflections used: 85111  
 Reported Rfree: 0.31  
 Sigma cut-off: N.A.

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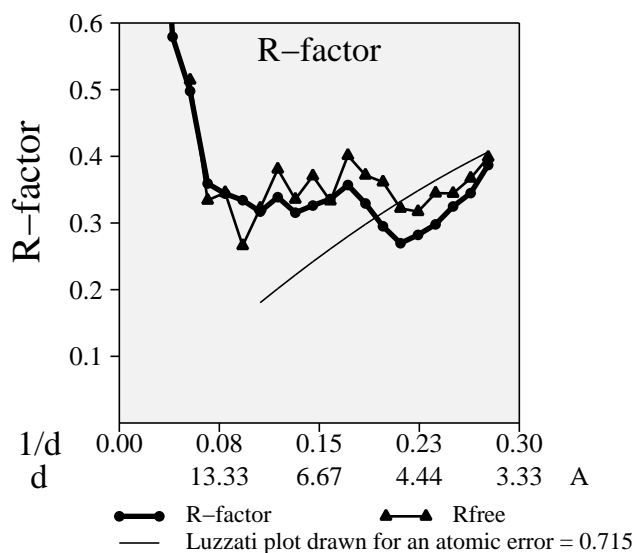


Stereographic projection of the averaged radial completeness



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

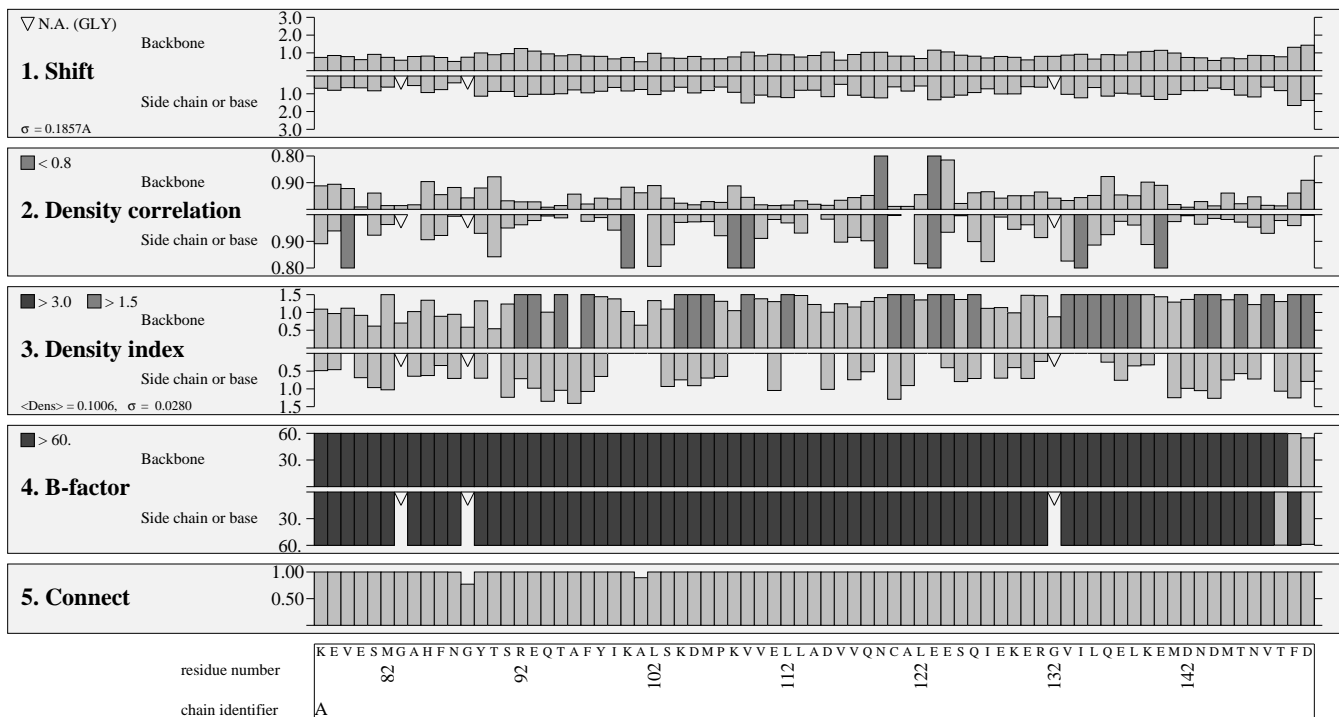
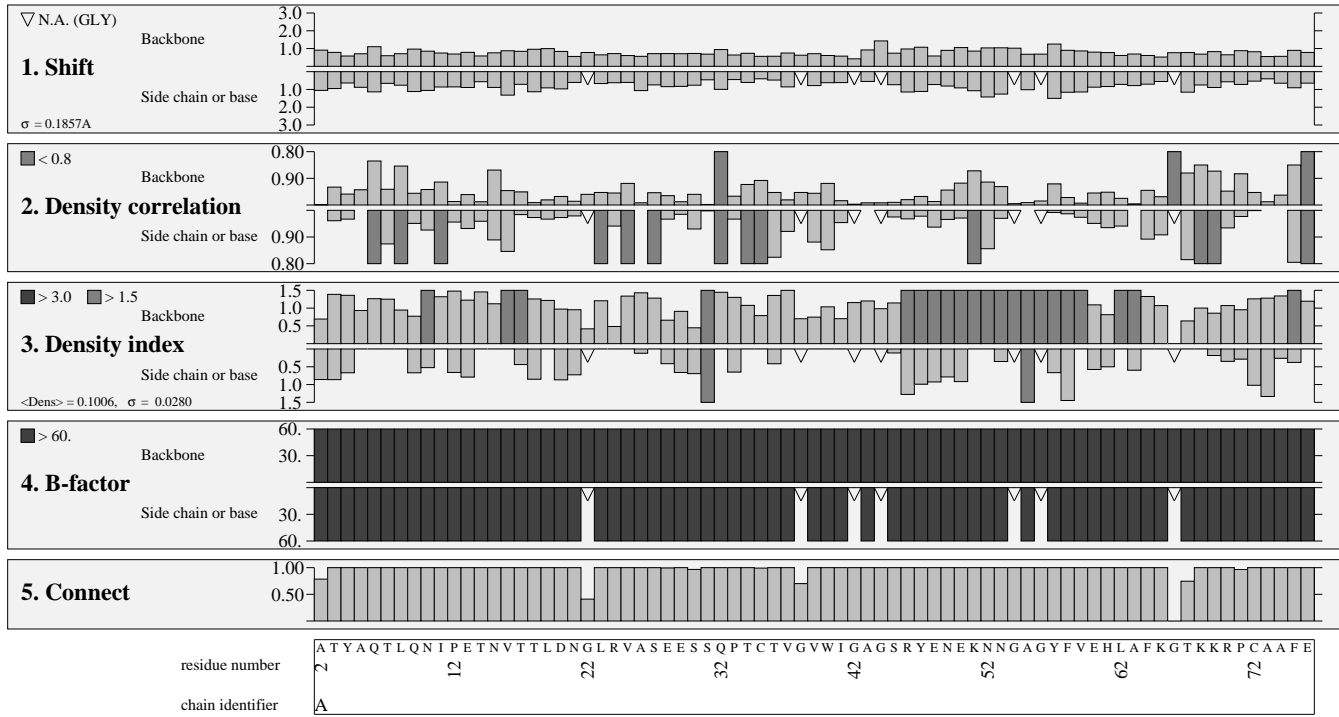
polar coordinates of the crystallographical axes



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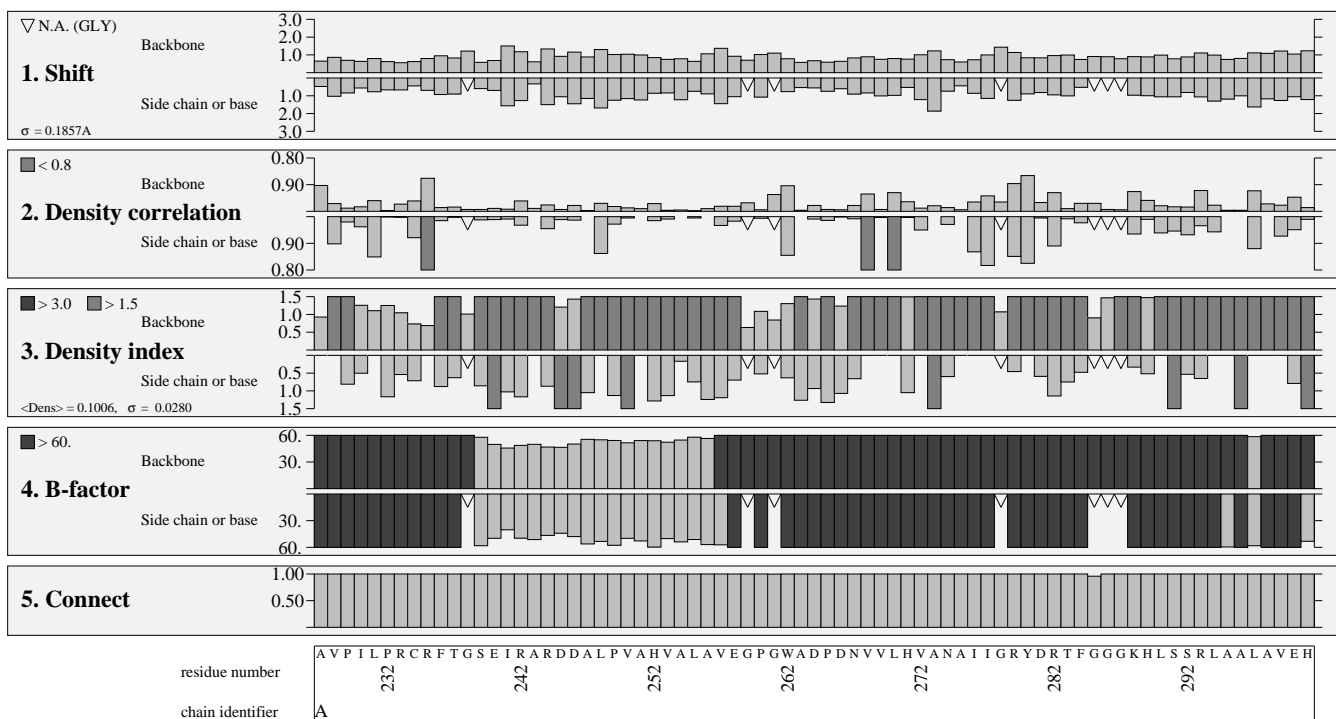
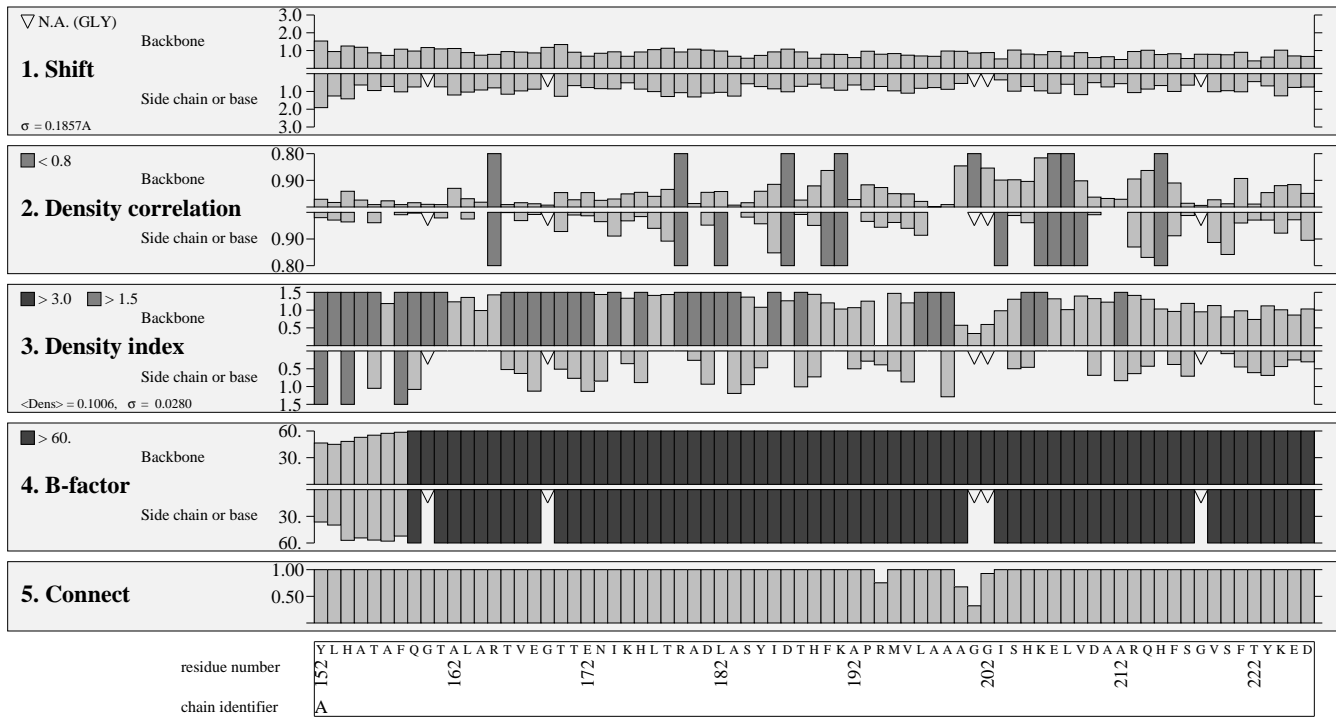
### Local estimation



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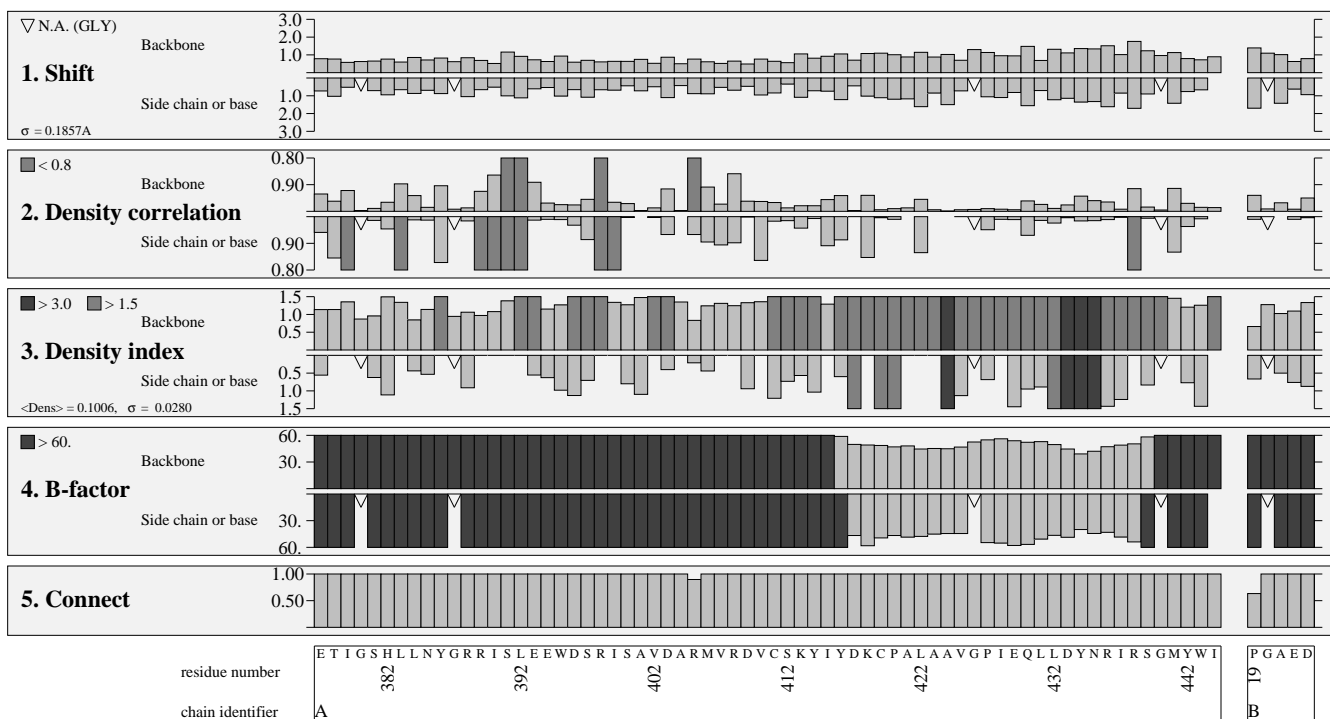
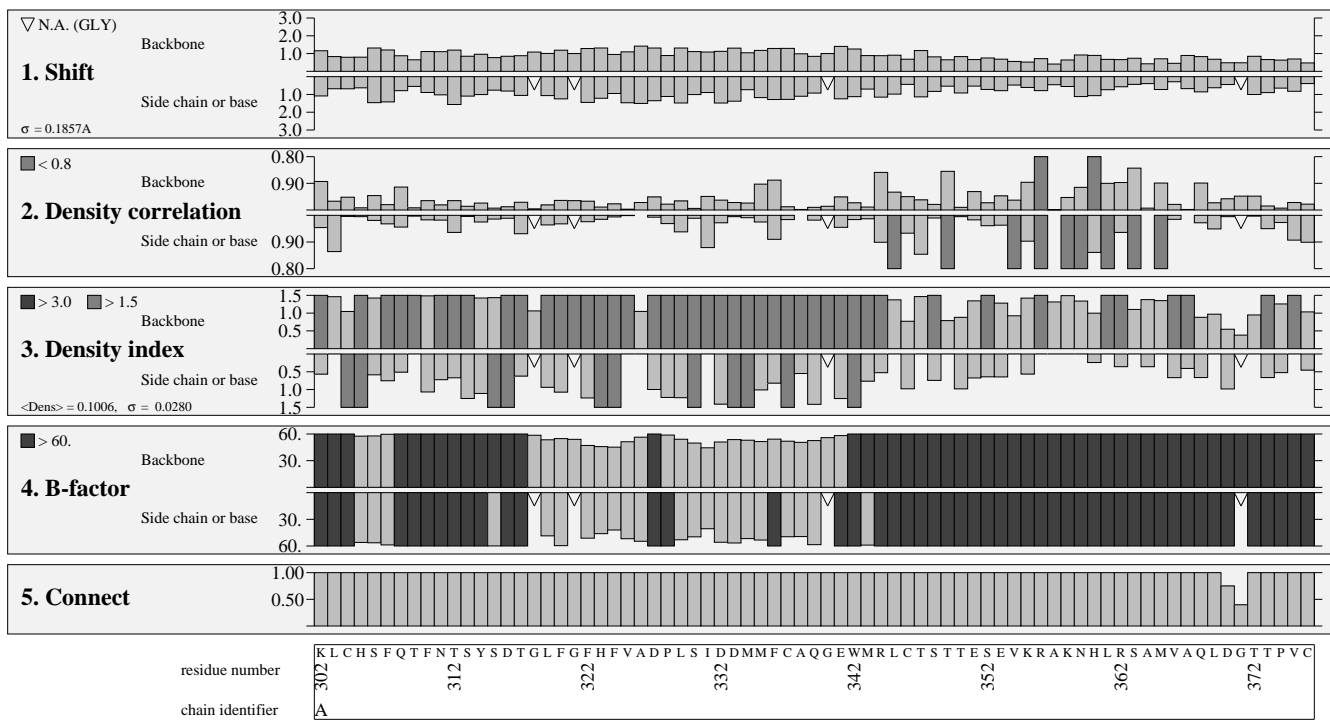
### Local estimation (2)



# Structure Factor Check

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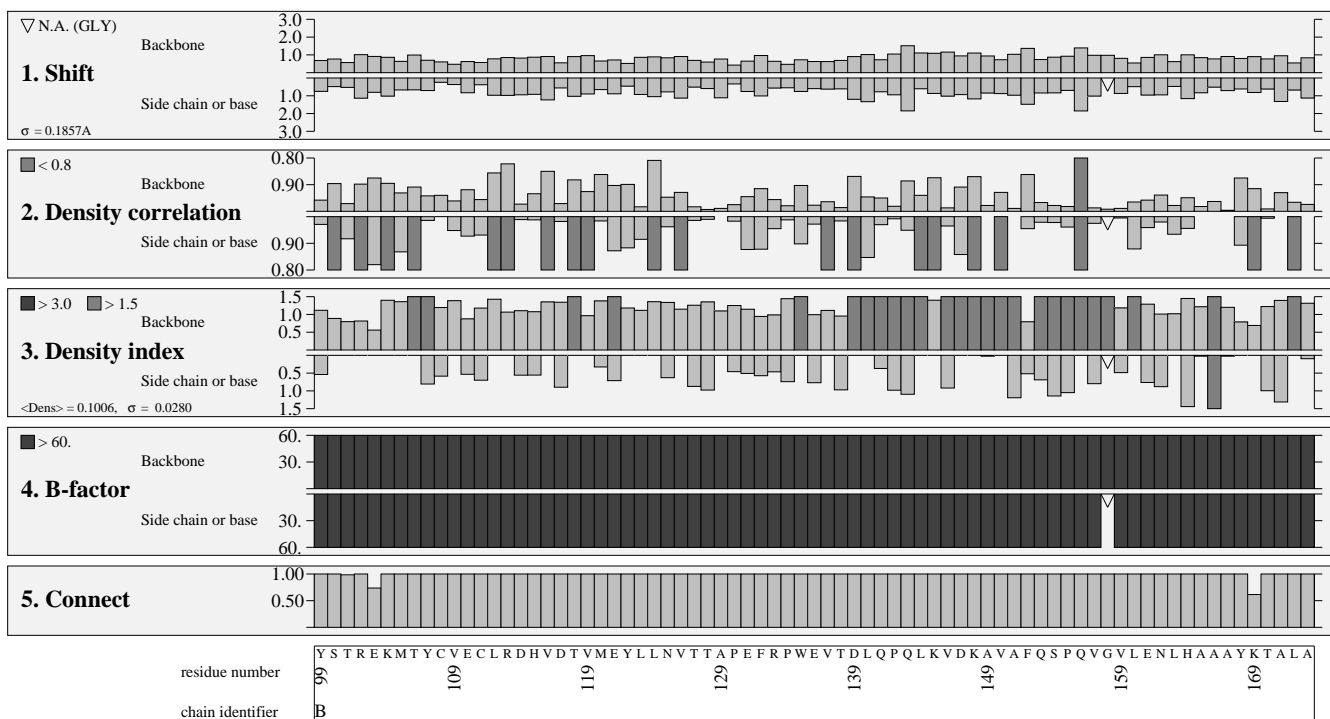
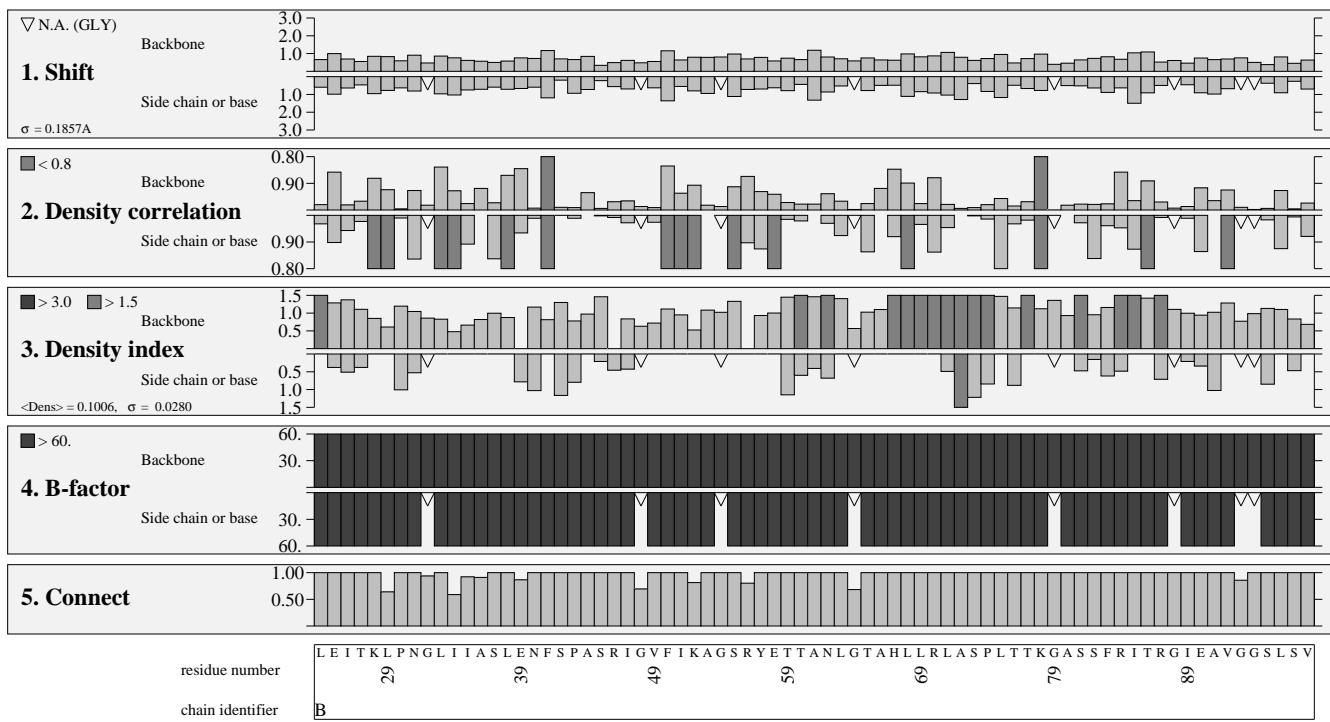
### Local estimation (3)



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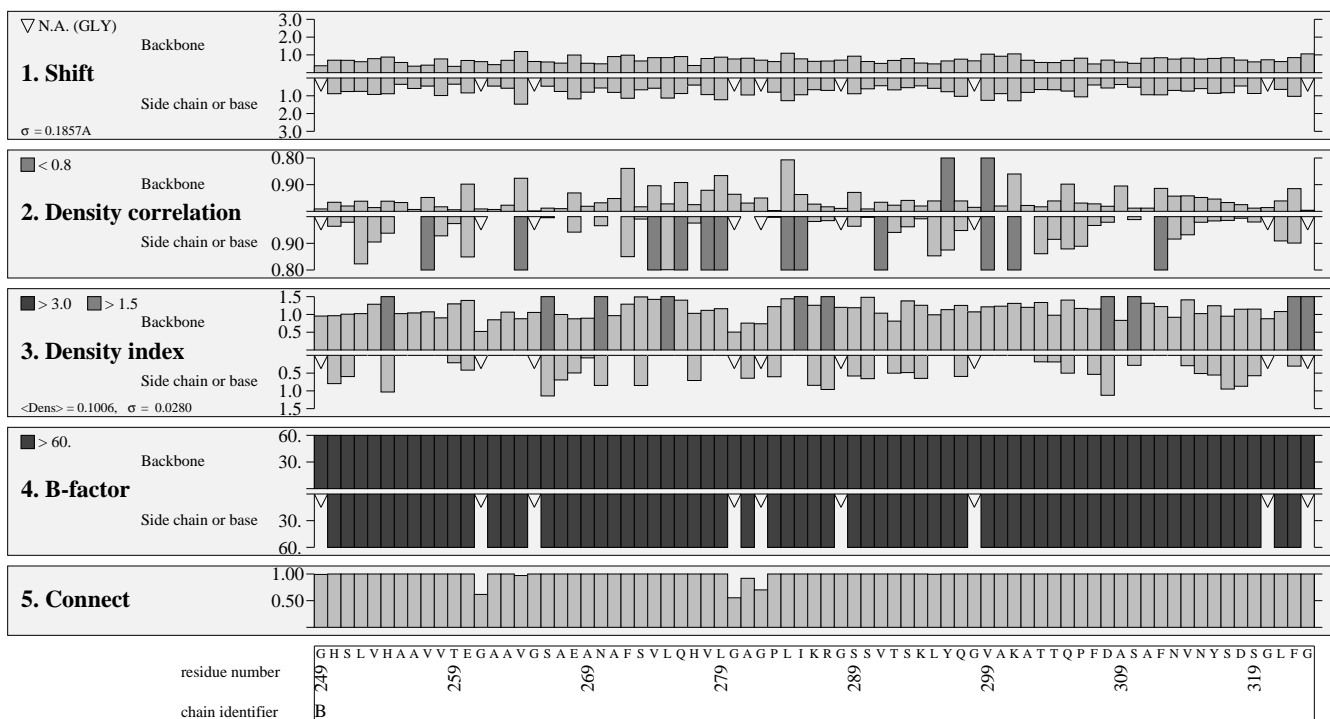
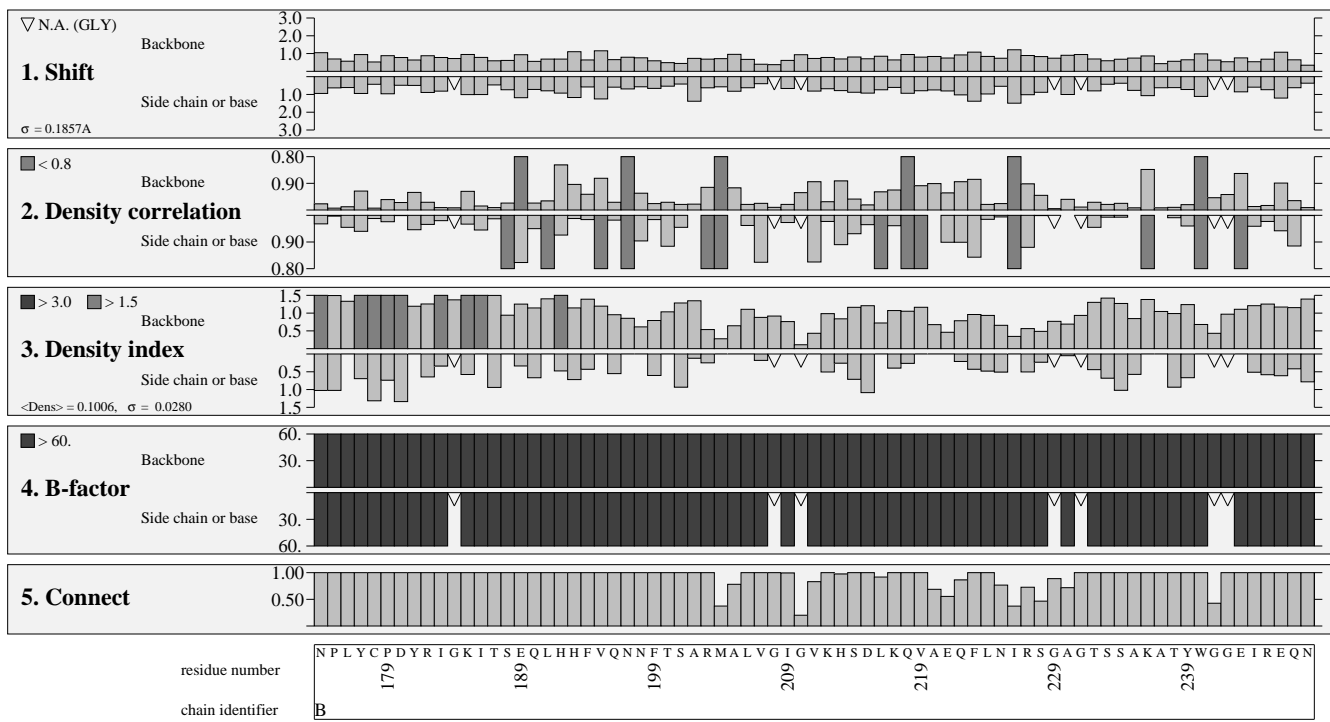
### Local estimation (4)



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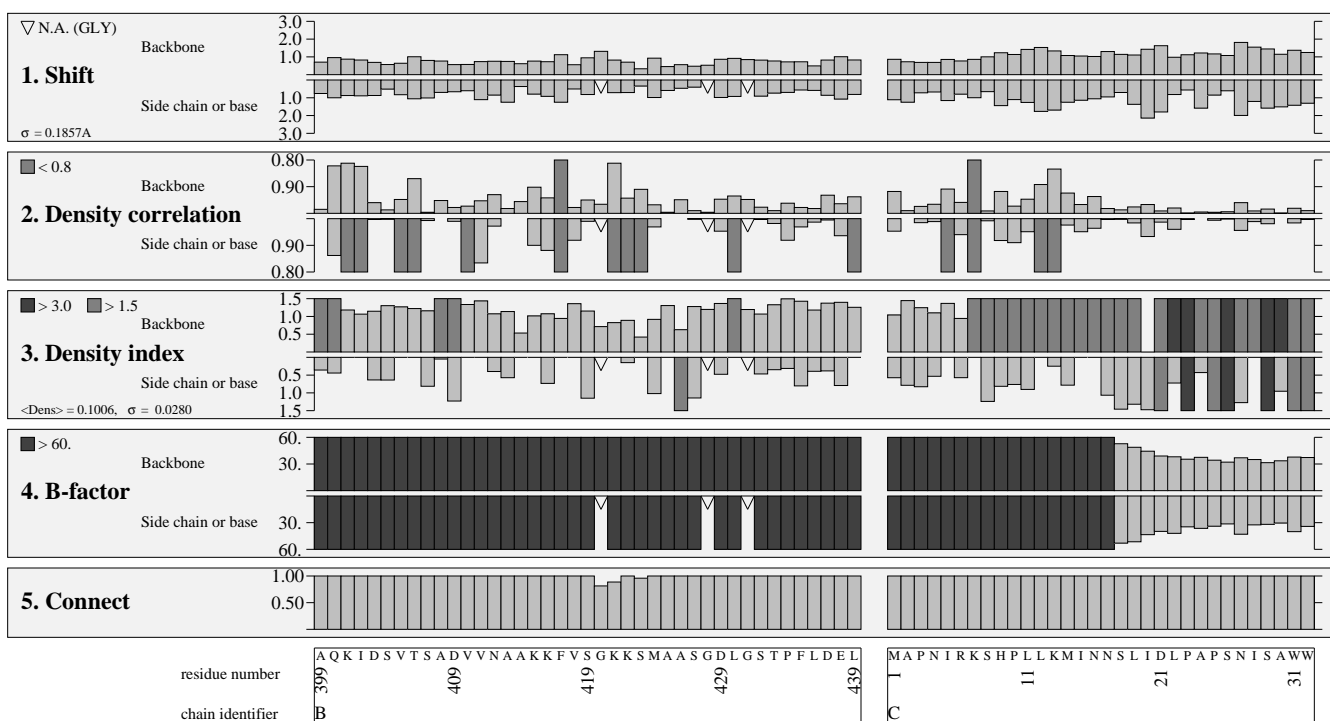
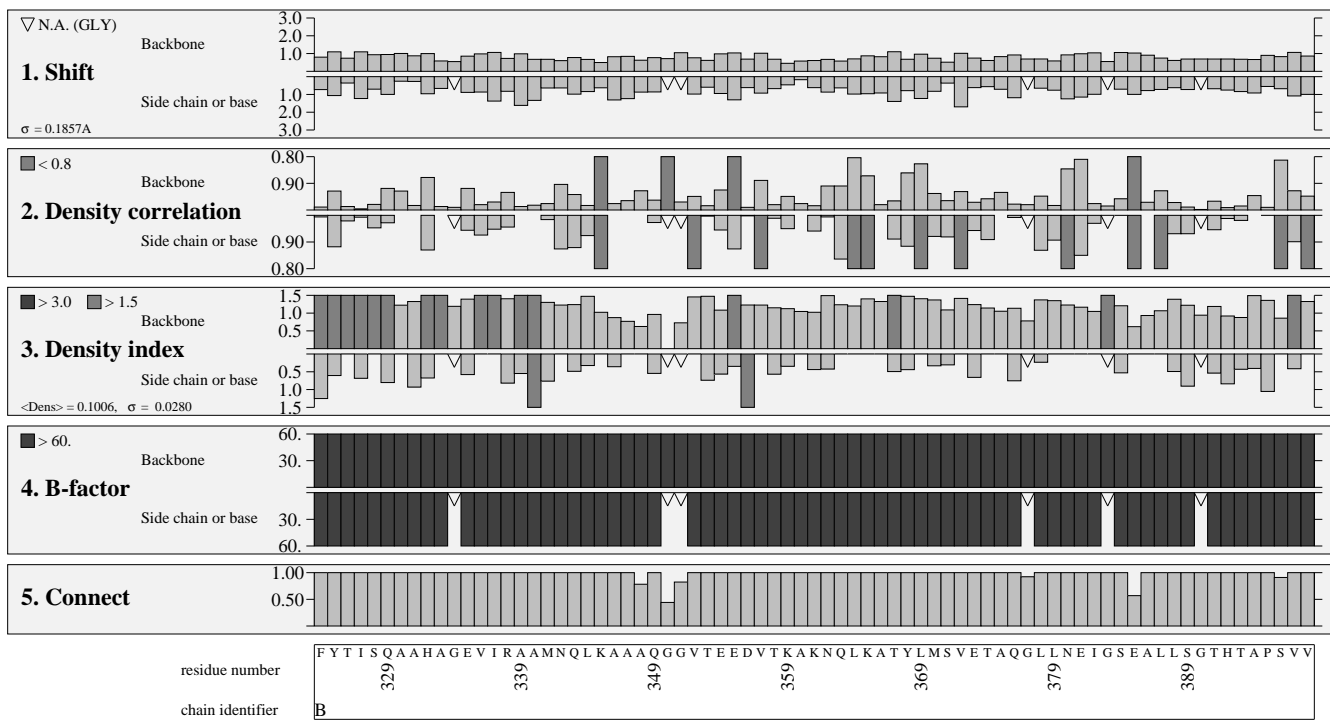
### Local estimation (5)



# Structure Factor Check

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### Local estimation (6)

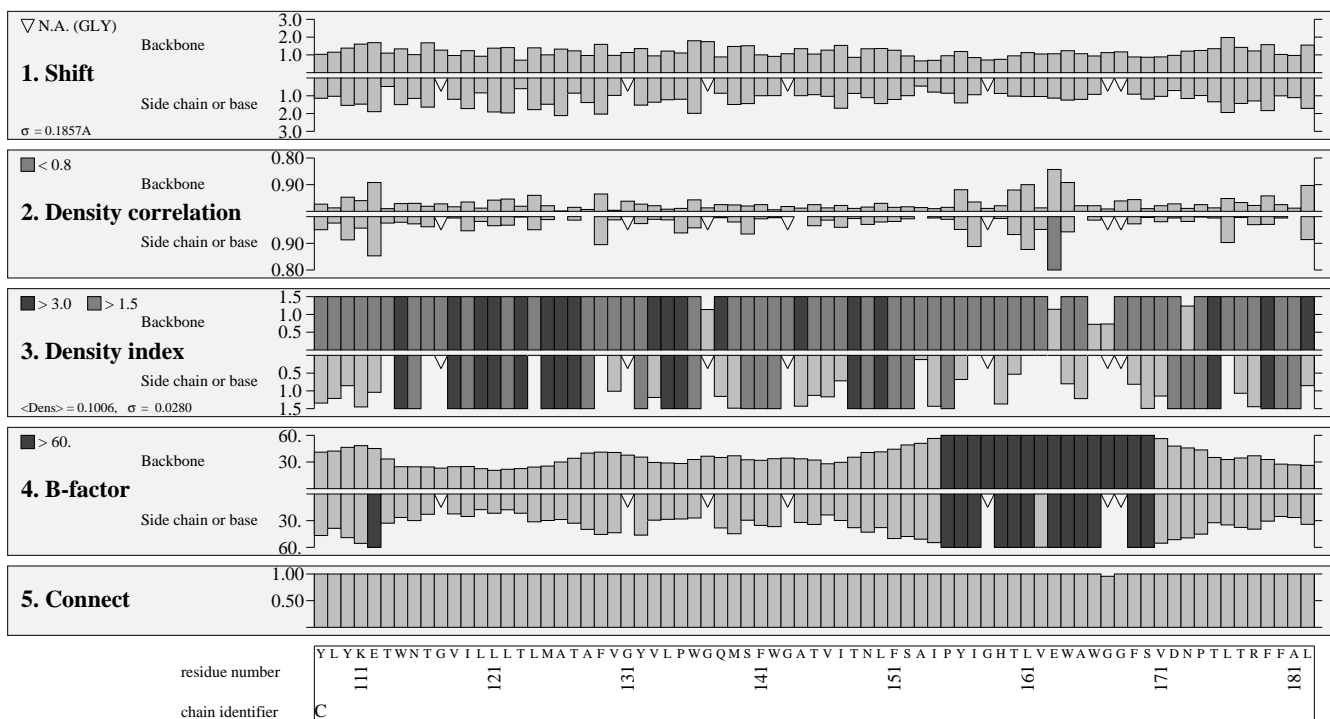
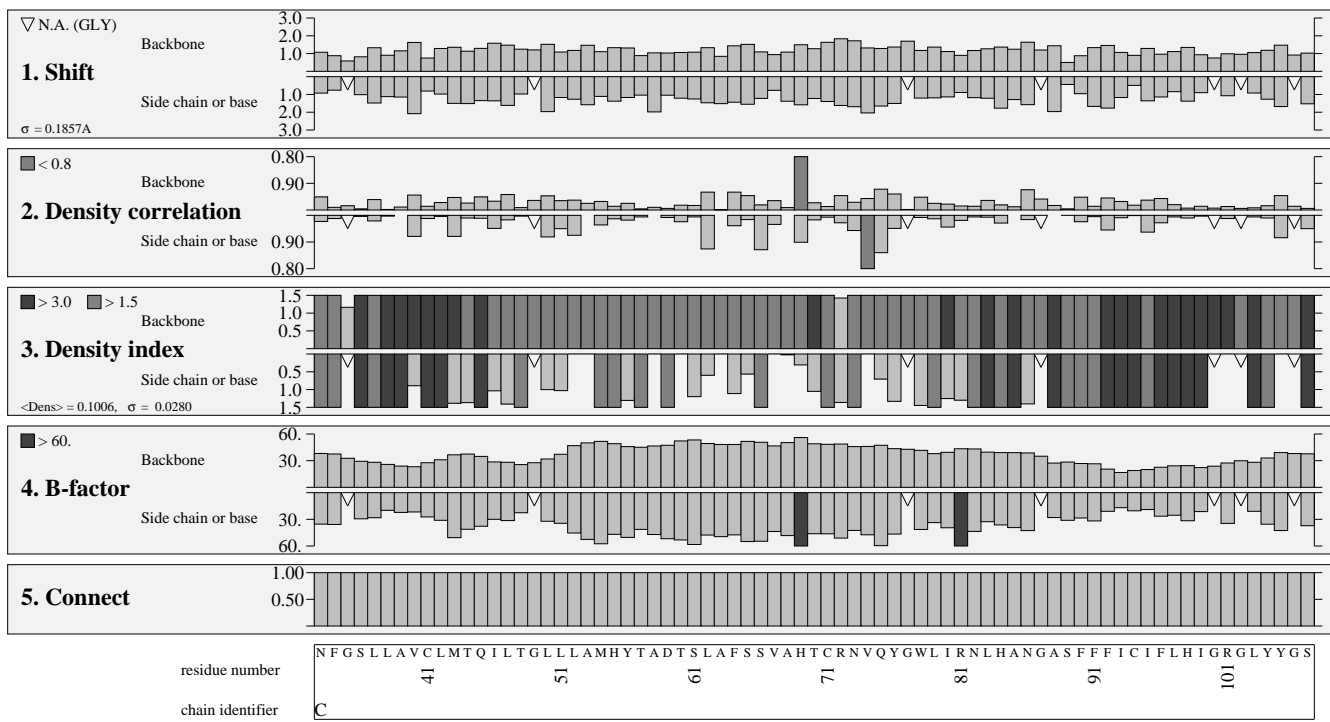




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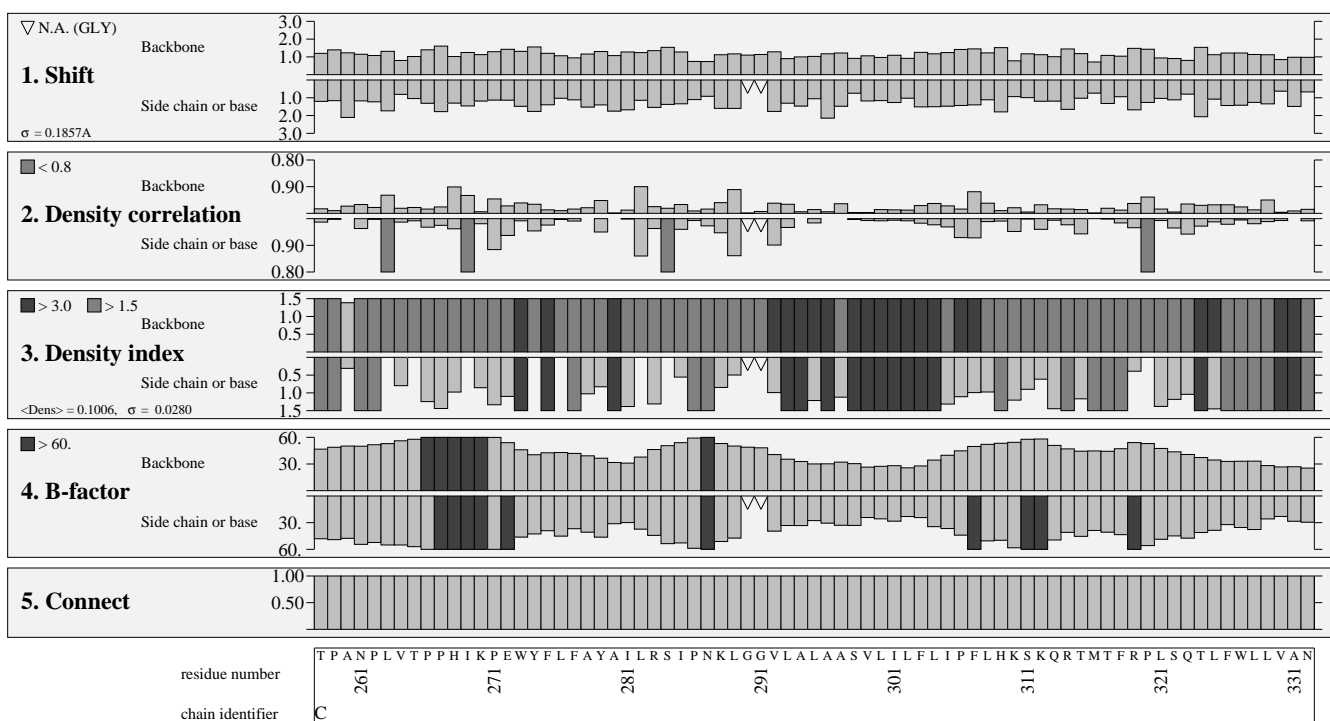
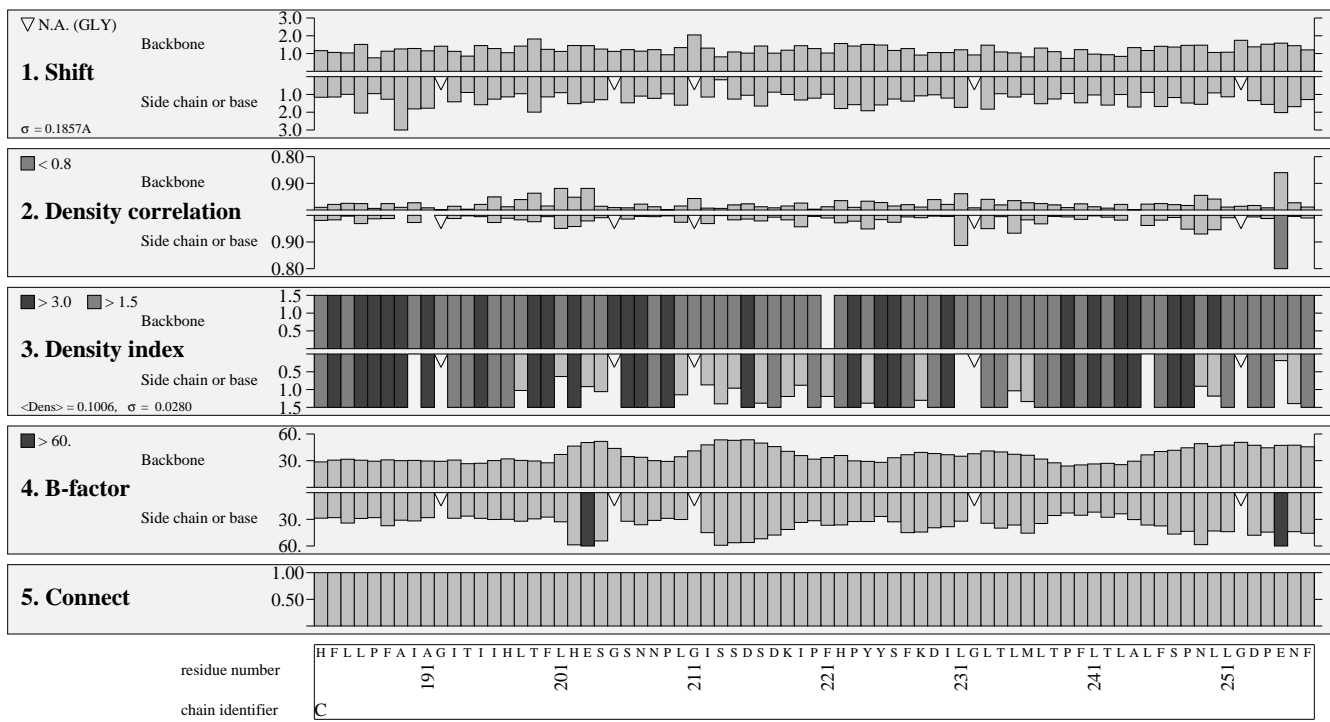
### Local estimation (7)



# Structure Factor Check

## 3H1I

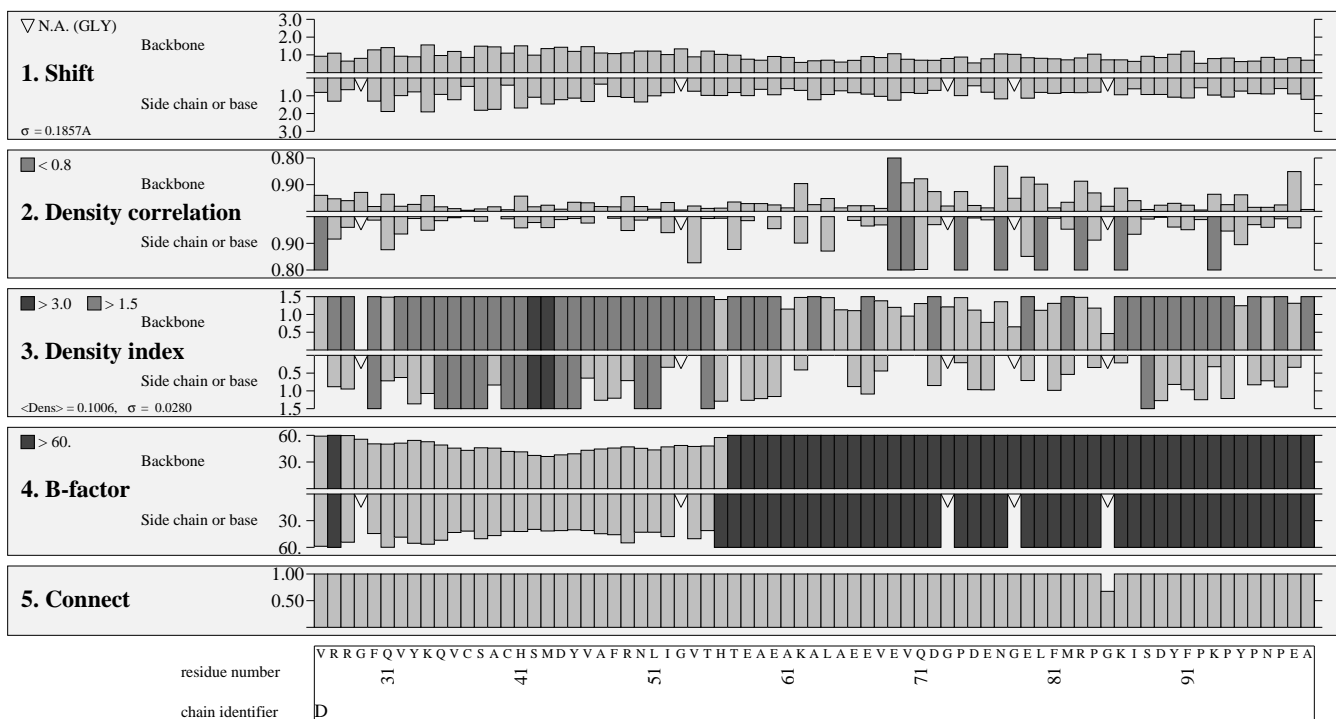
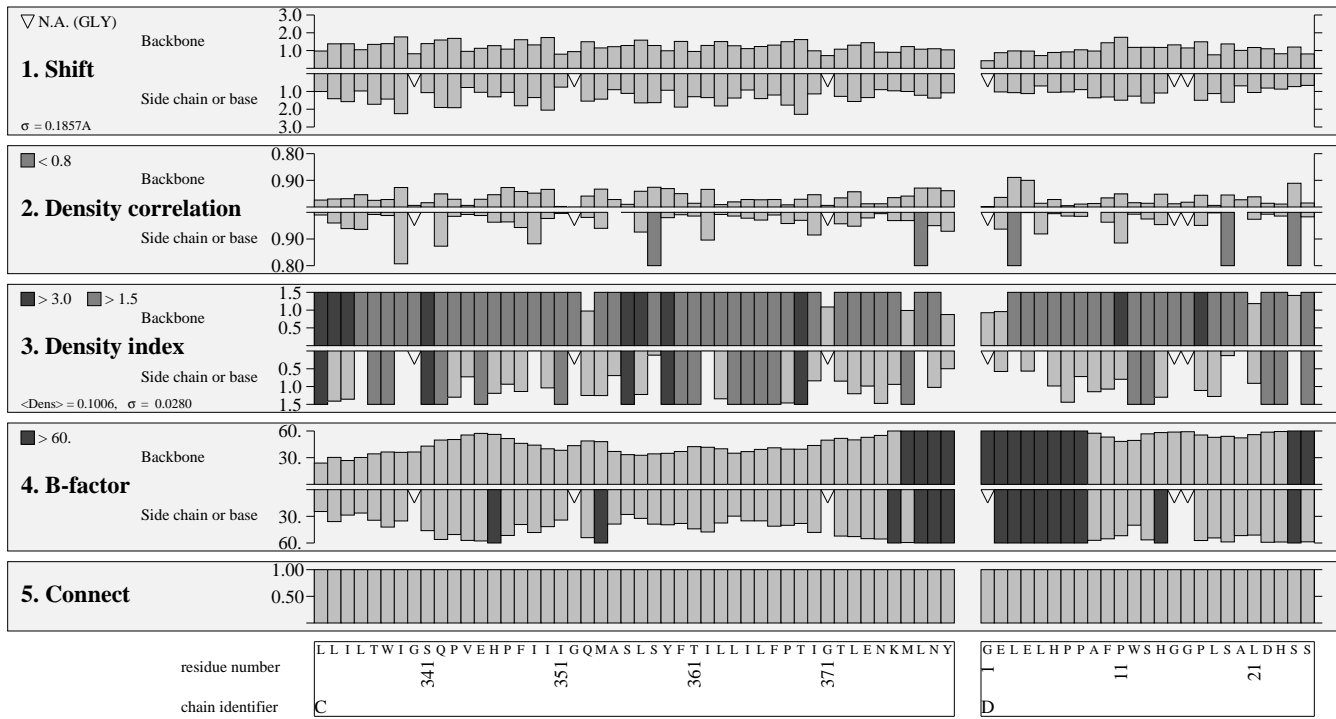
### Local estimation (8)



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## 3H1I

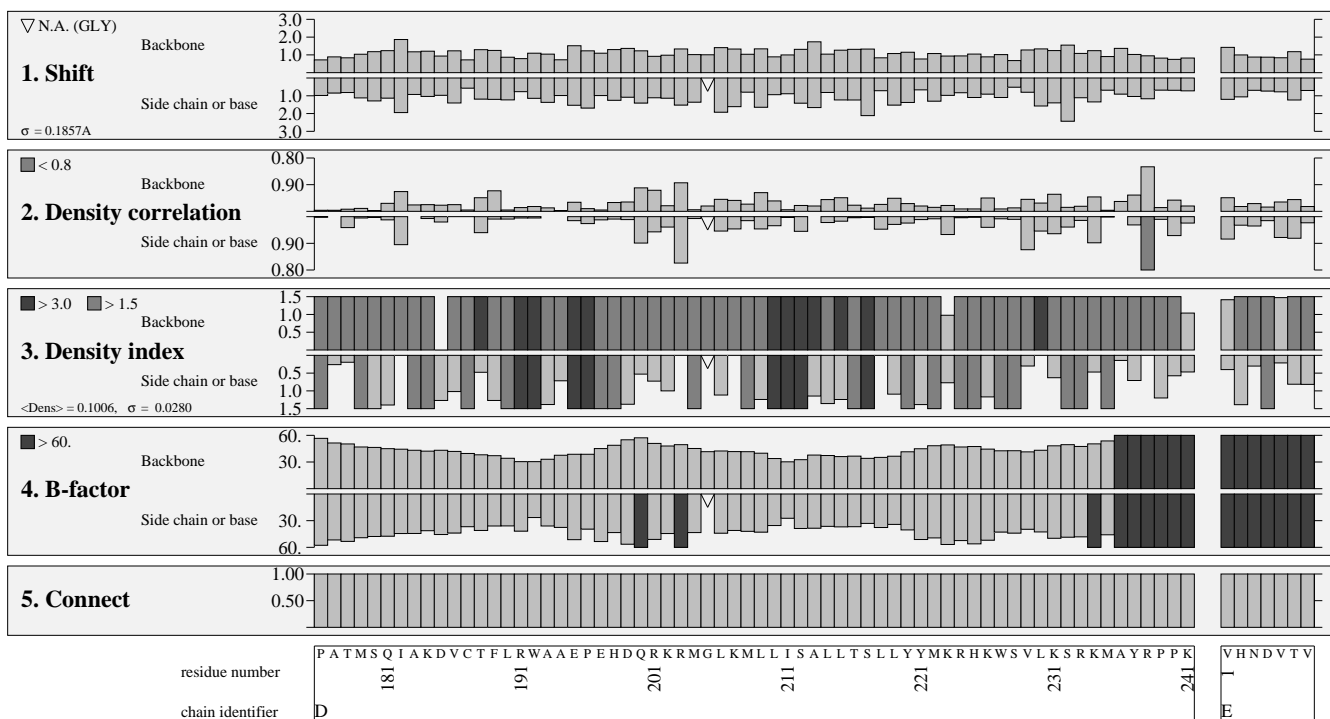
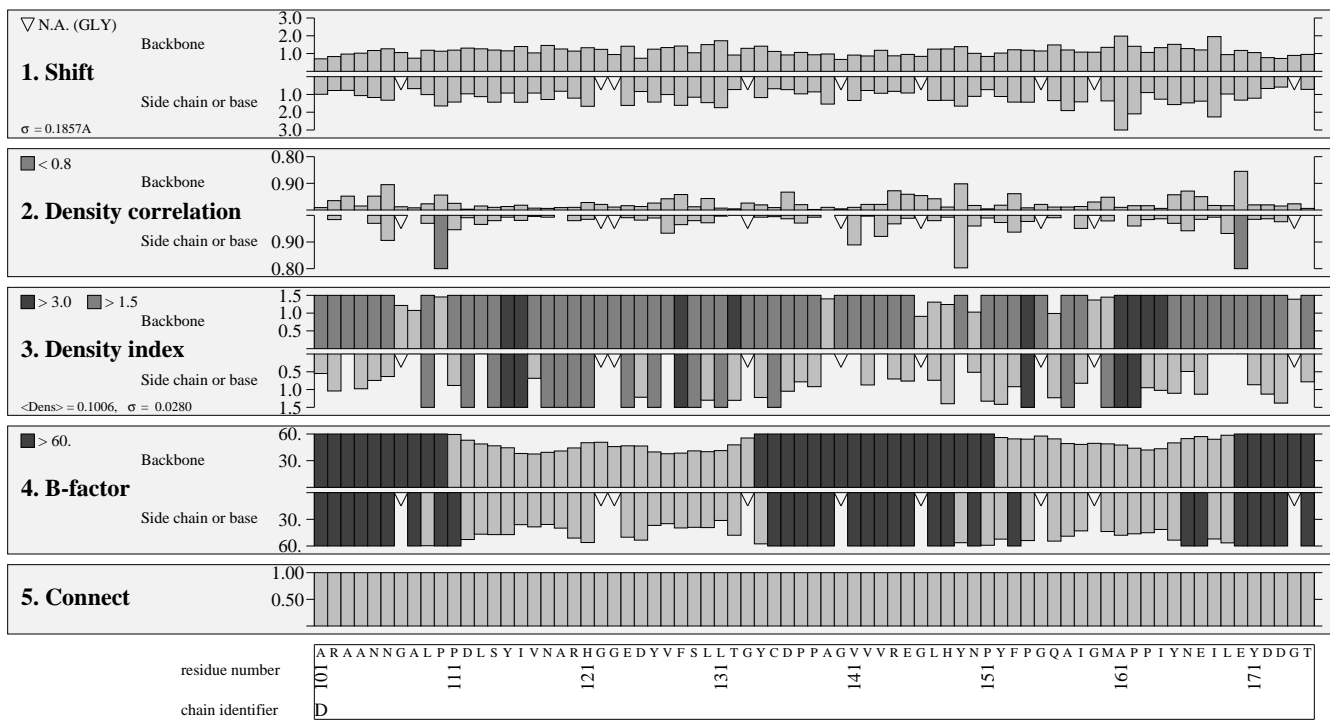
### Local estimation (9)



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## 3H1I

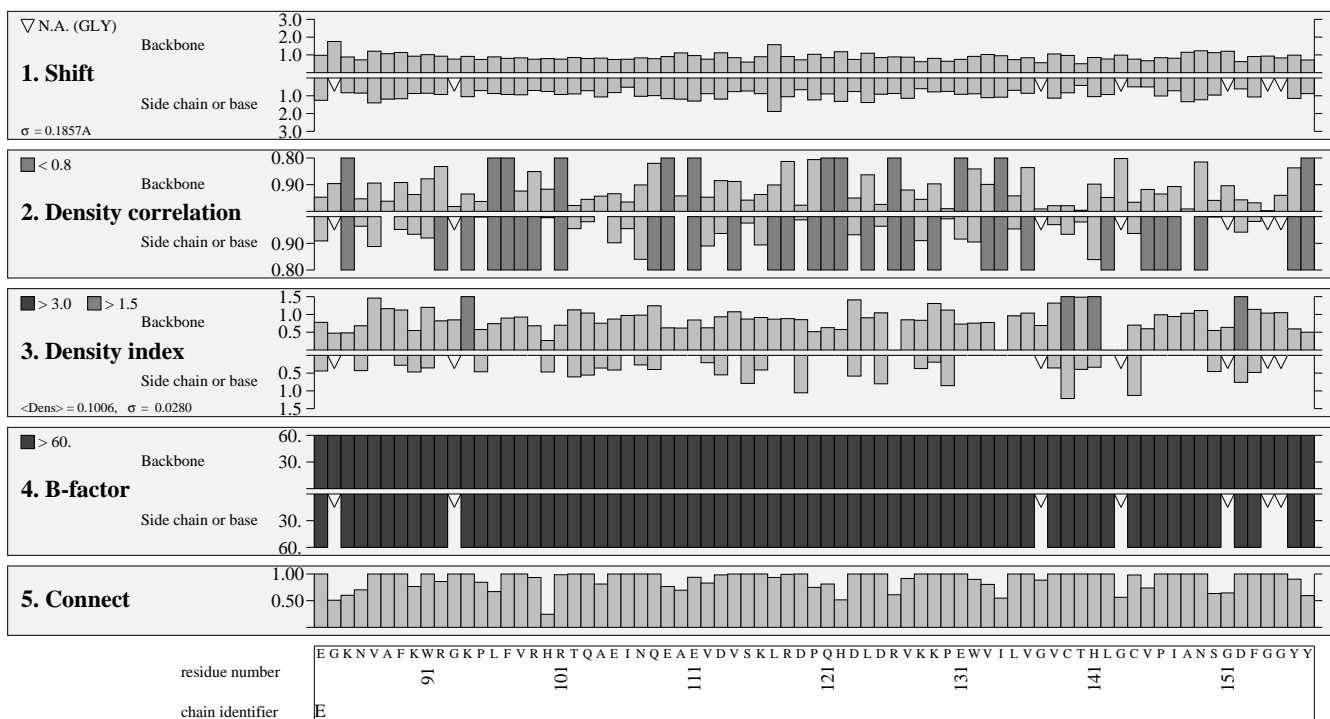
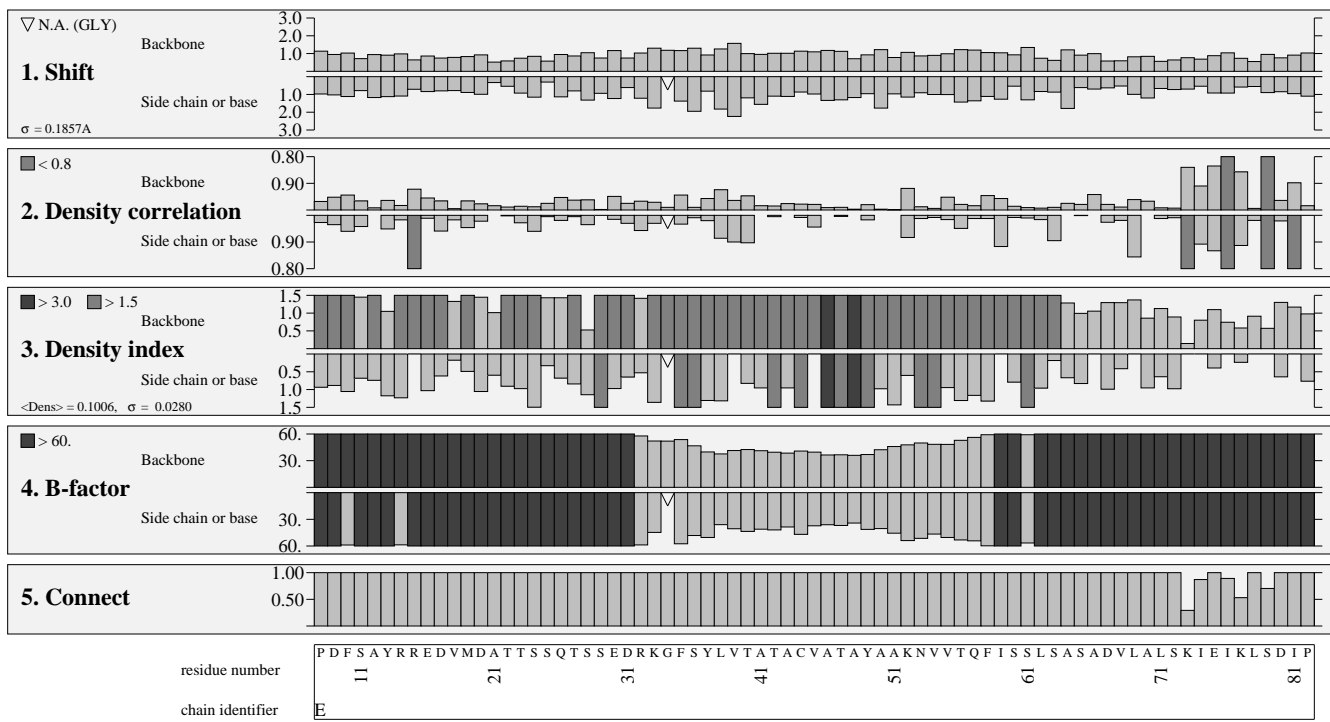
### Local estimation (10)



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## 3H1I

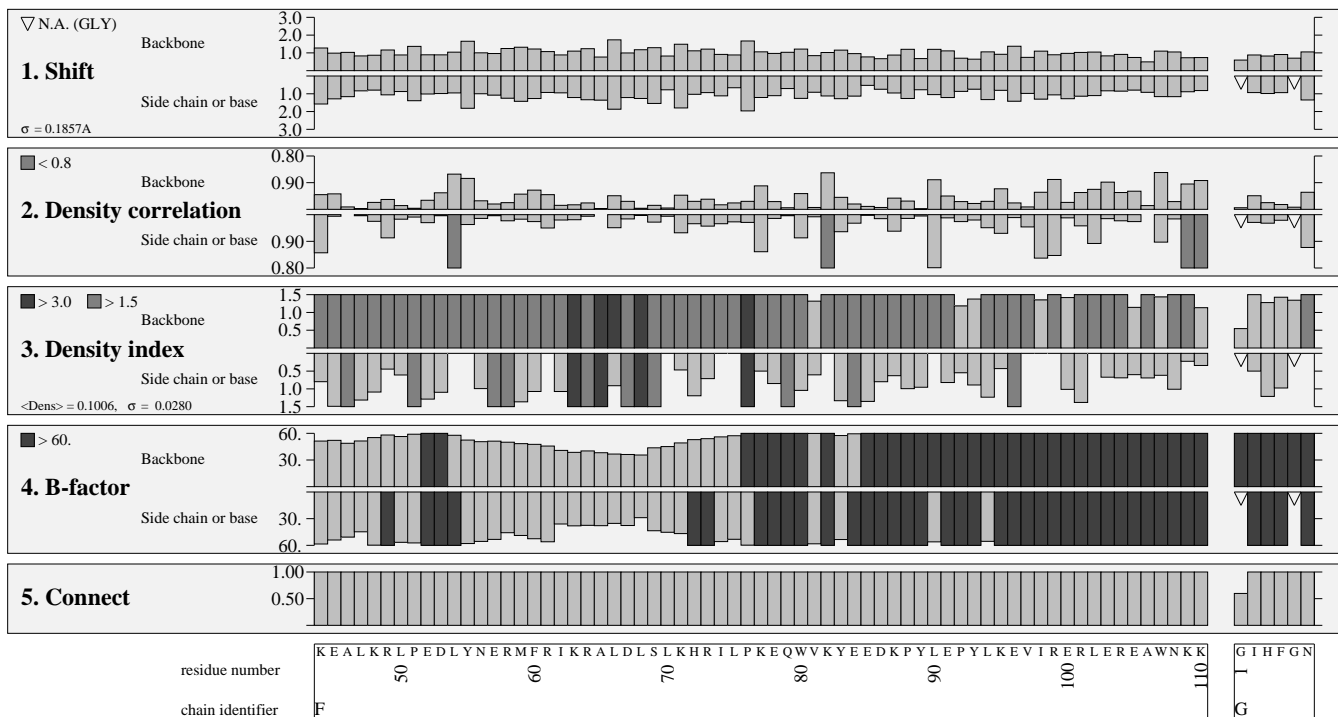
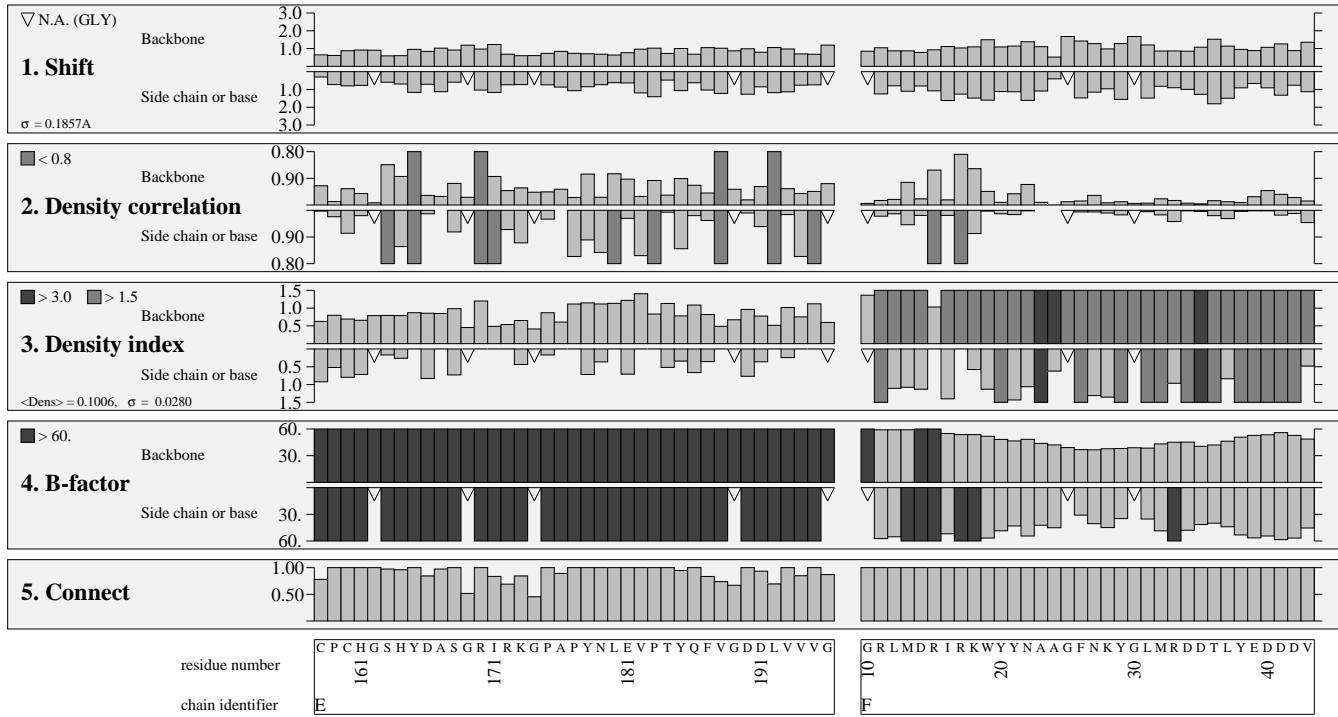
### Local estimation (11)



# Structure Factor Check

## 3H1I

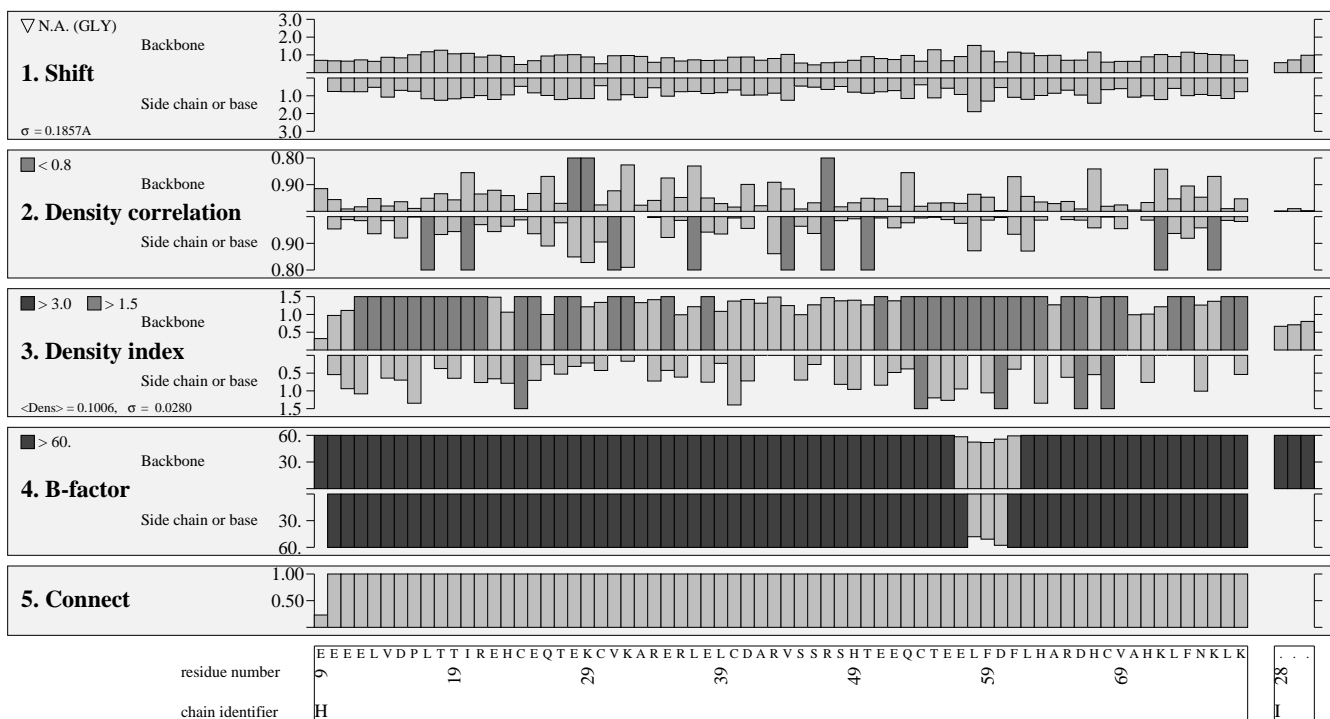
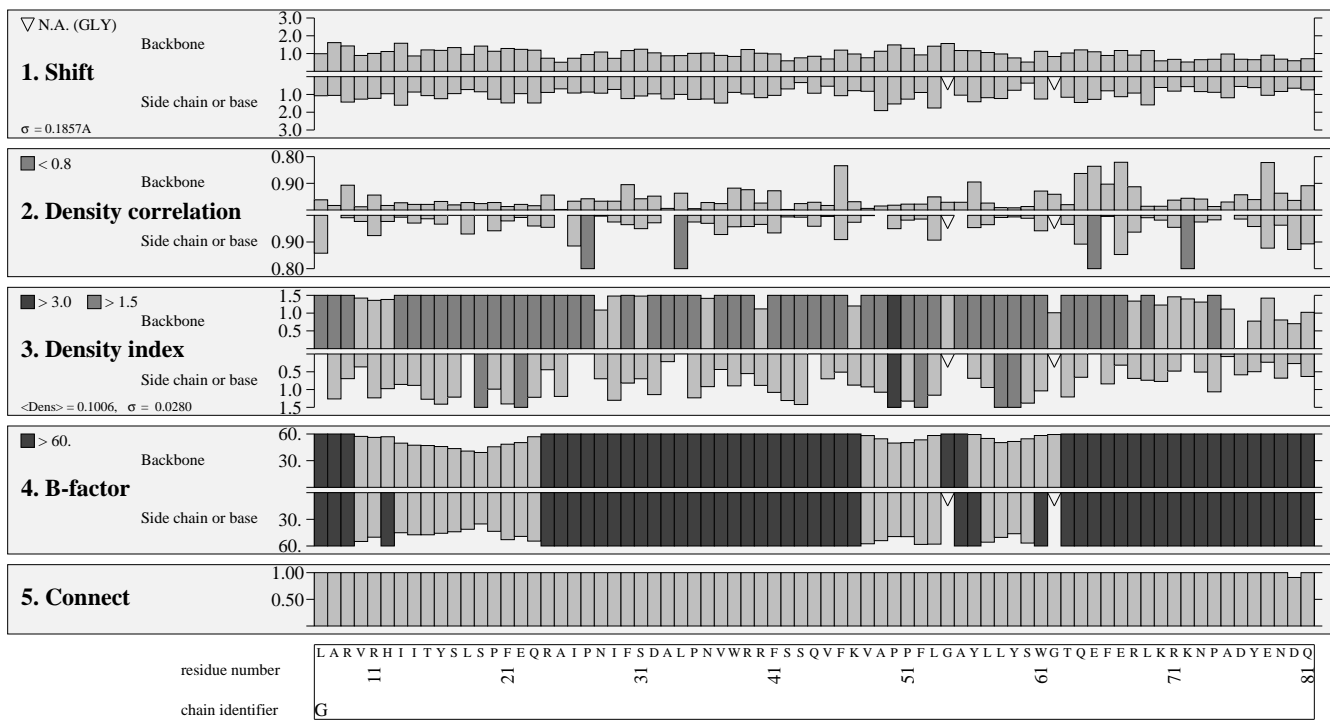
### Local estimation (12)



# Structure Factor Check

## 3H1I

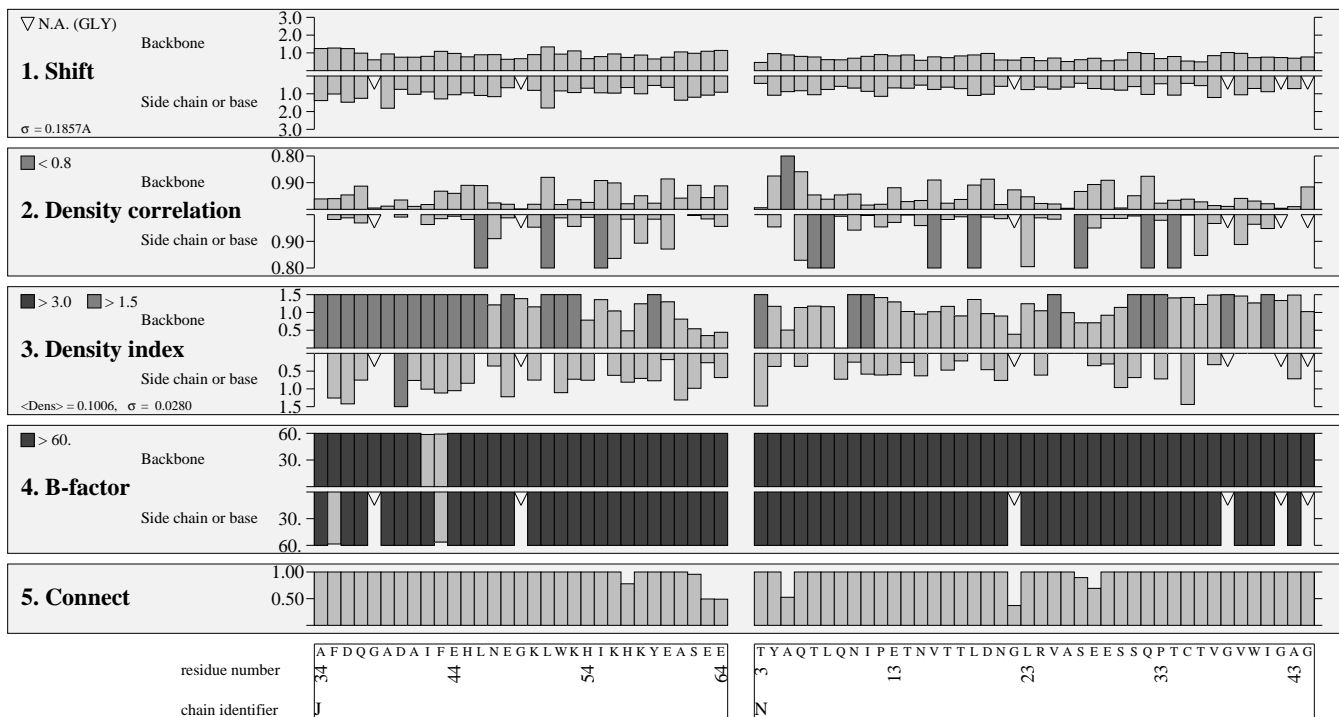
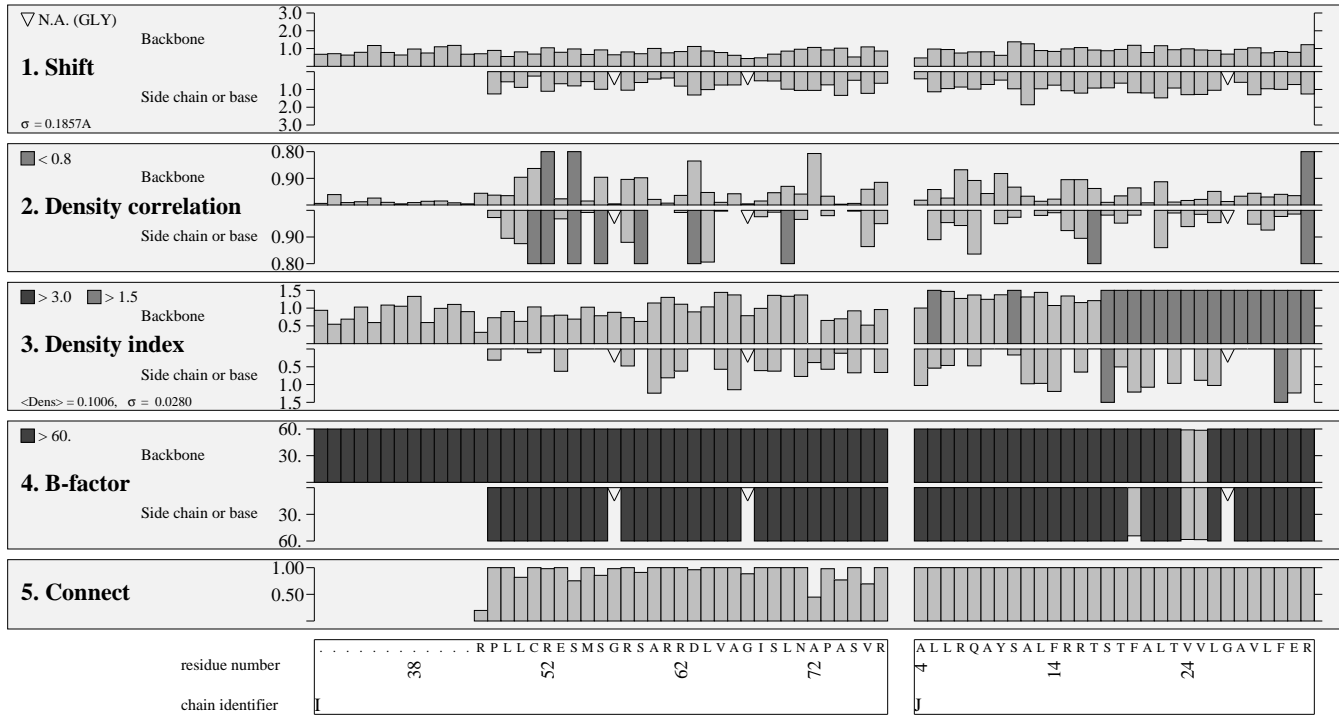
### Local estimation (13)



# Structure Factor Check

## 3H1I

### Local estimation (14)

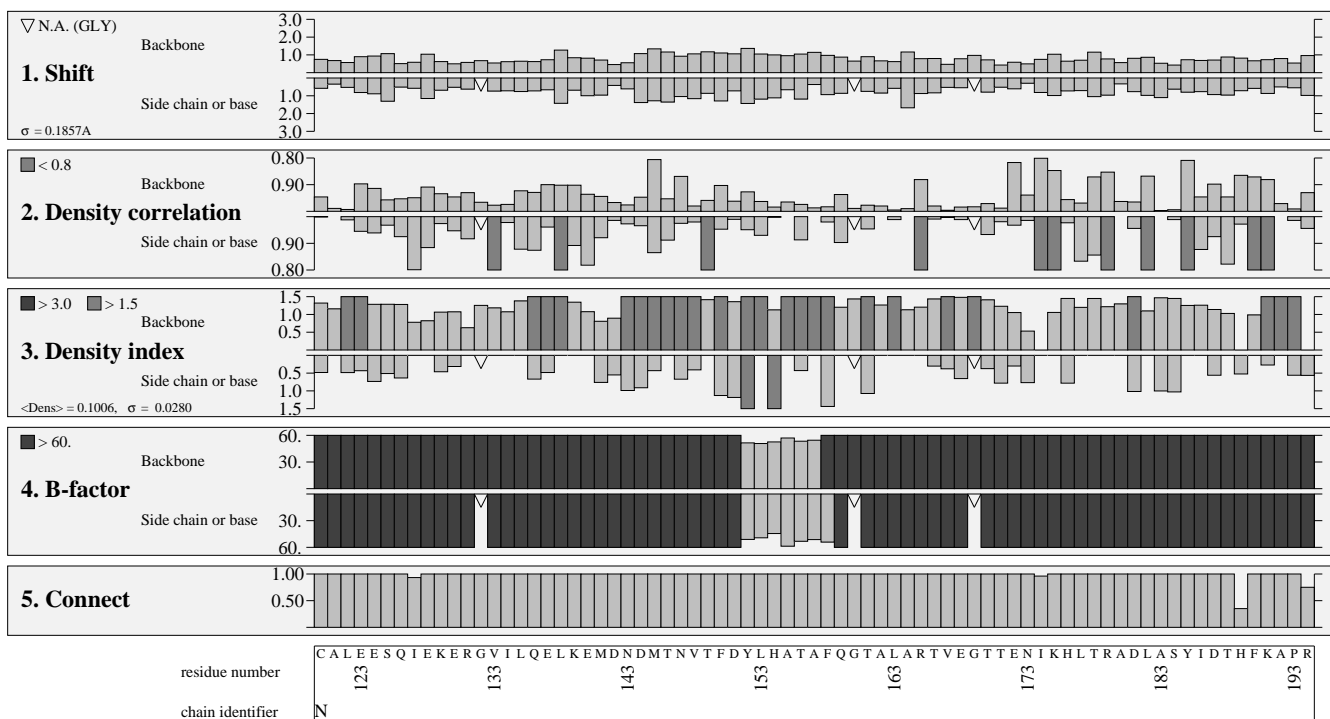
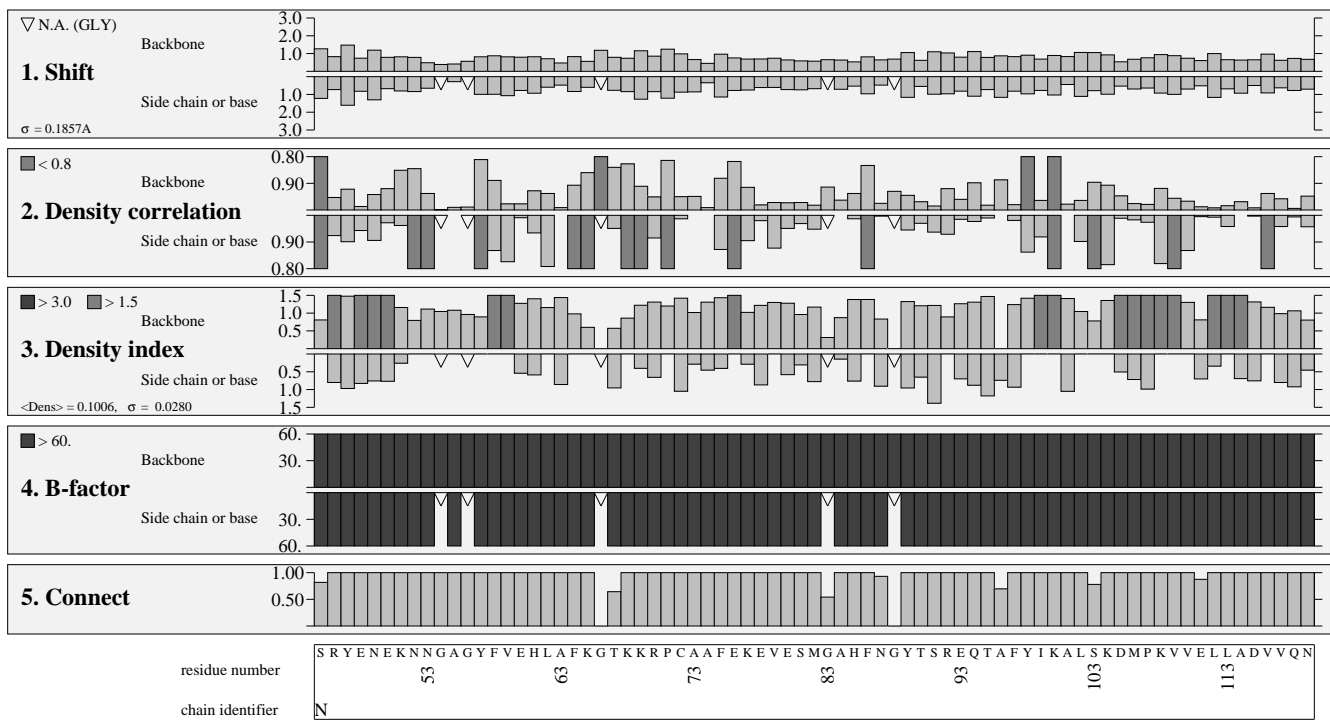




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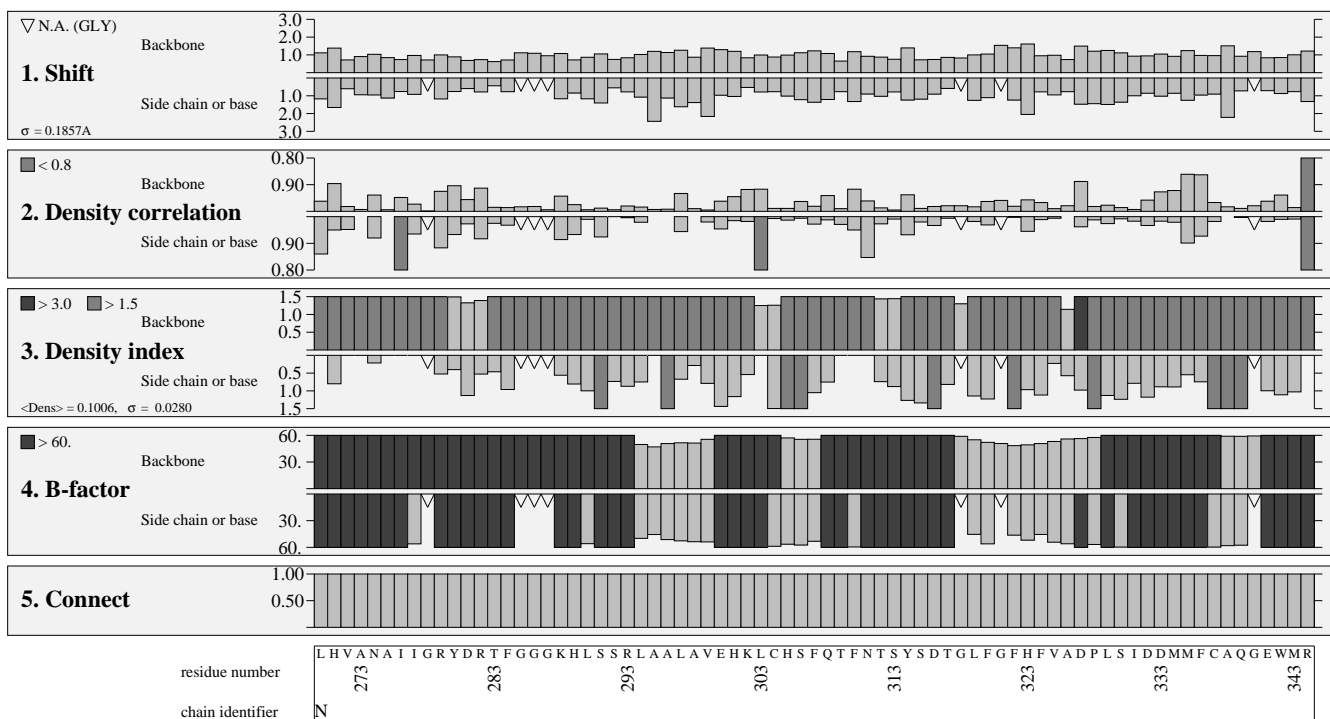
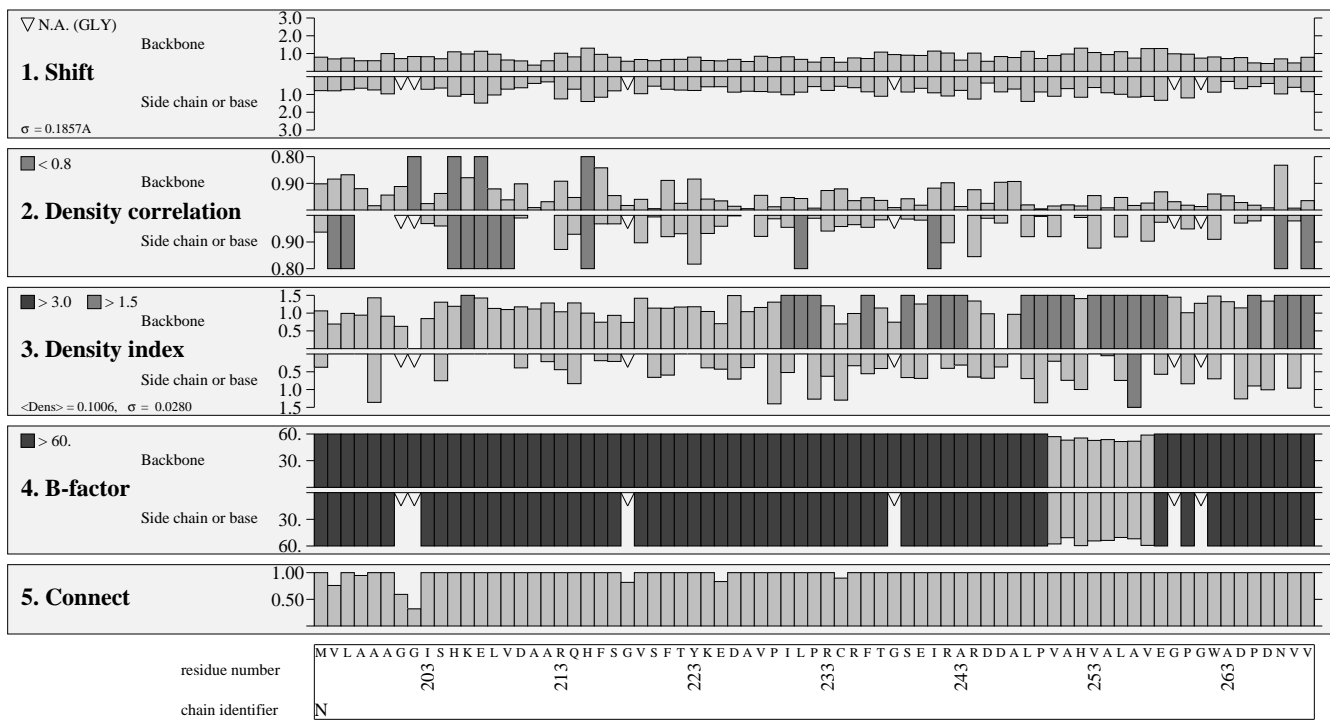
### Local estimation (15)



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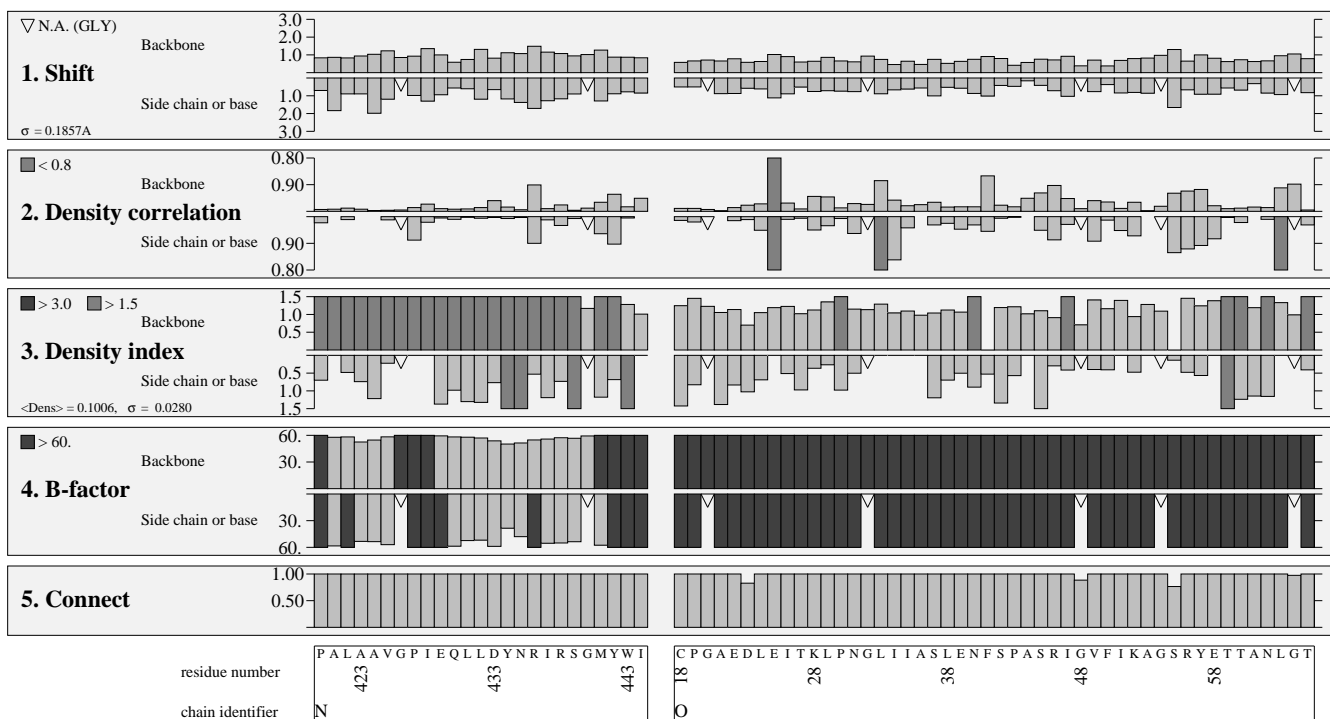
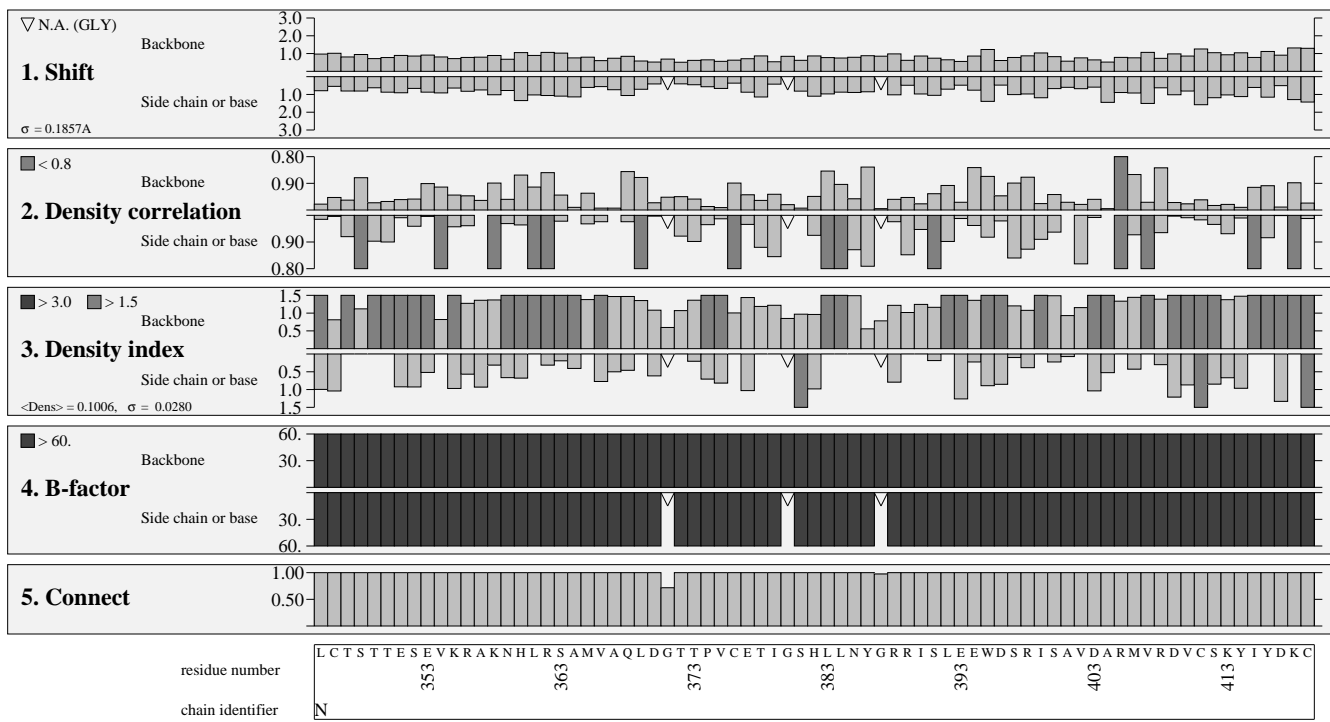
### Local estimation (16)



# Structure Factor Check

## 3H1I

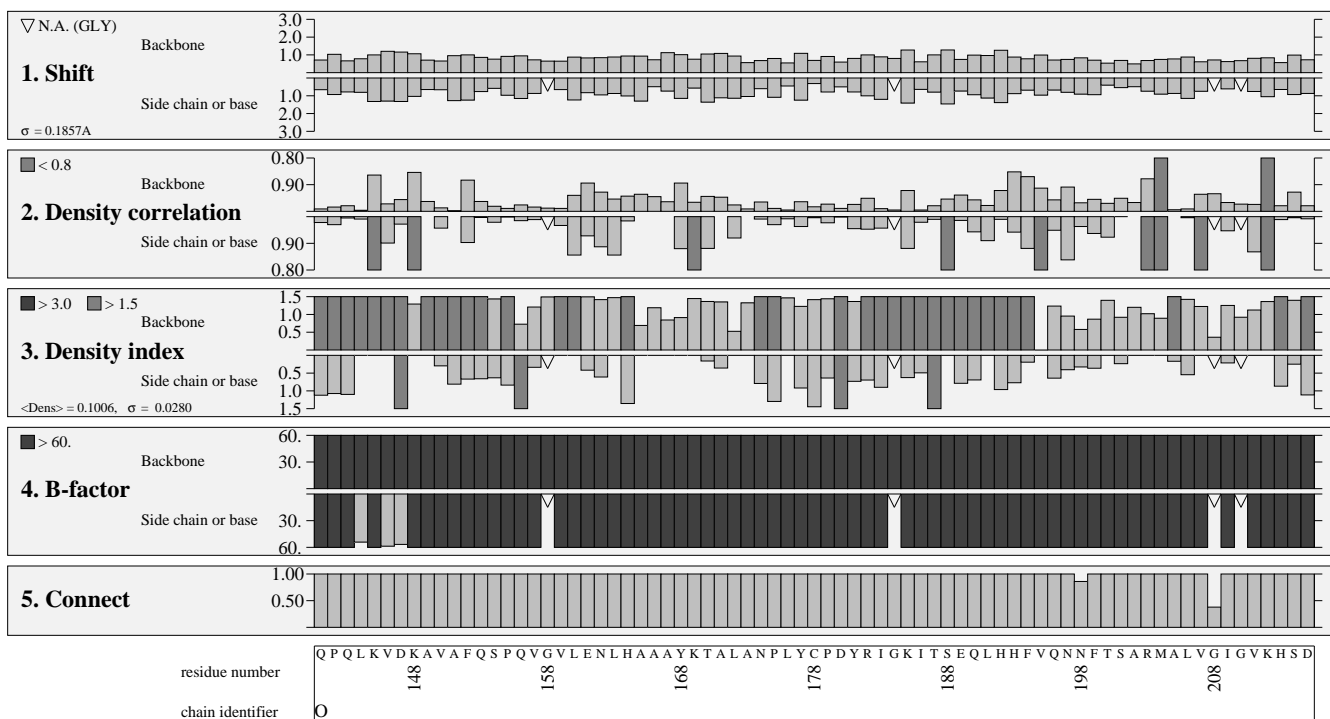
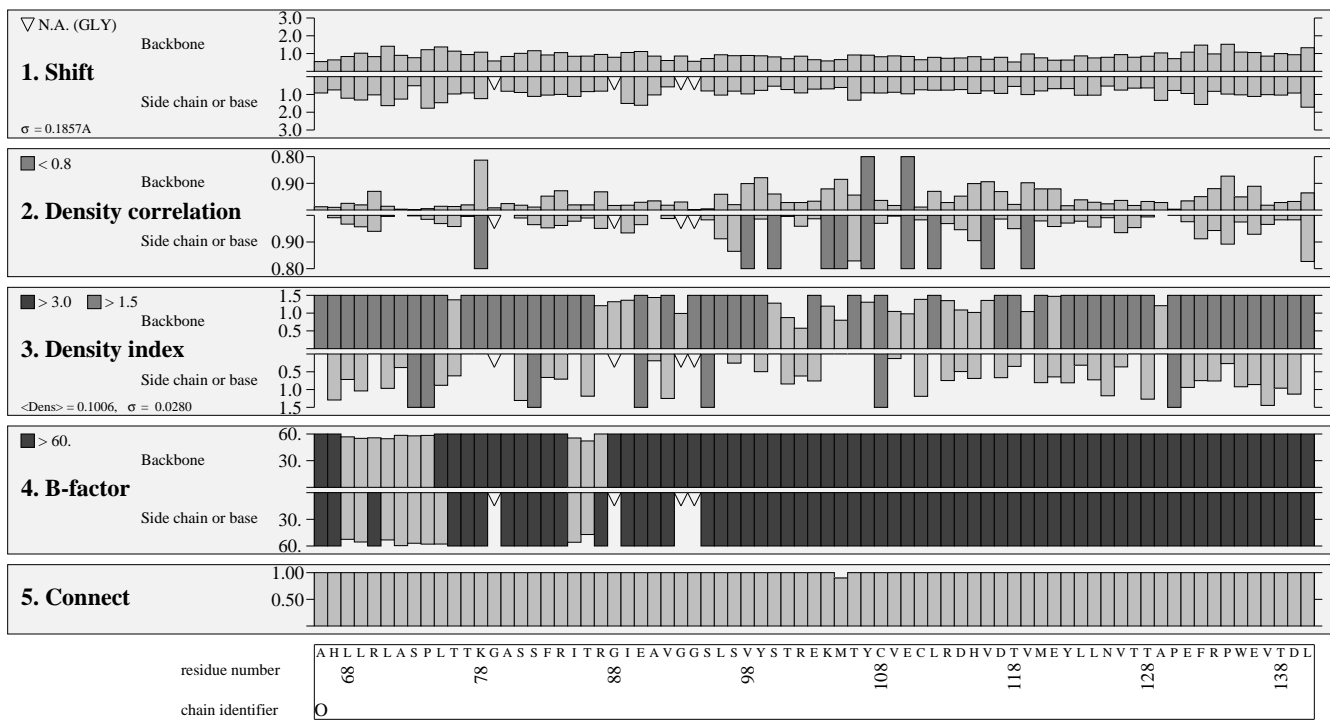
### Local estimation (17)



# Structure Factor Check

## 3H1I

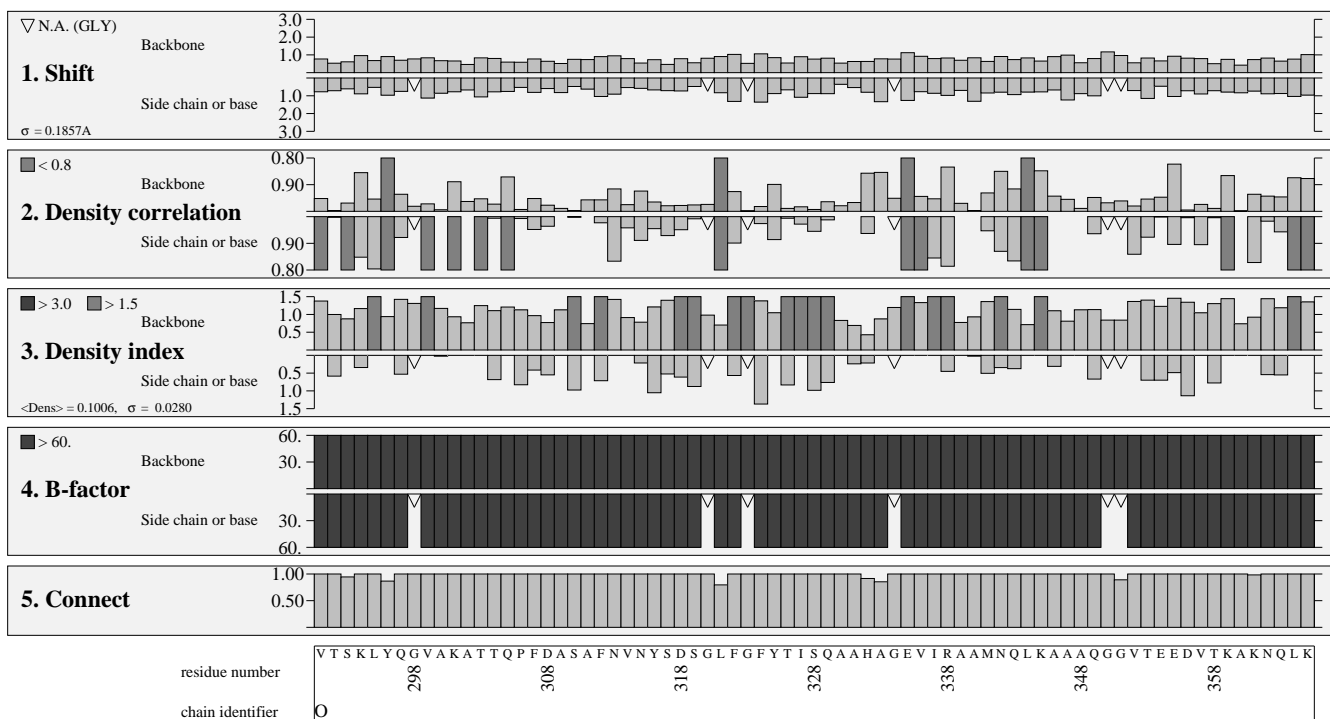
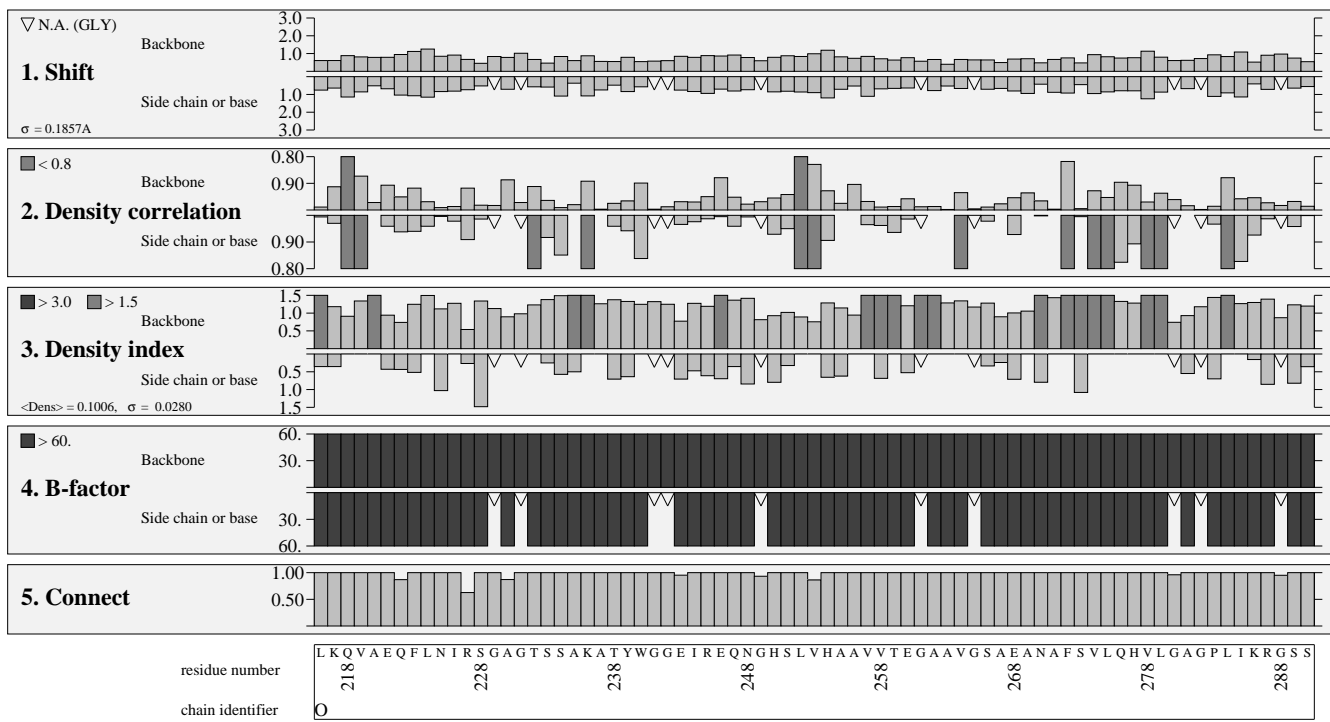
### Local estimation (18)



# Structure Factor Check

## 3H1I

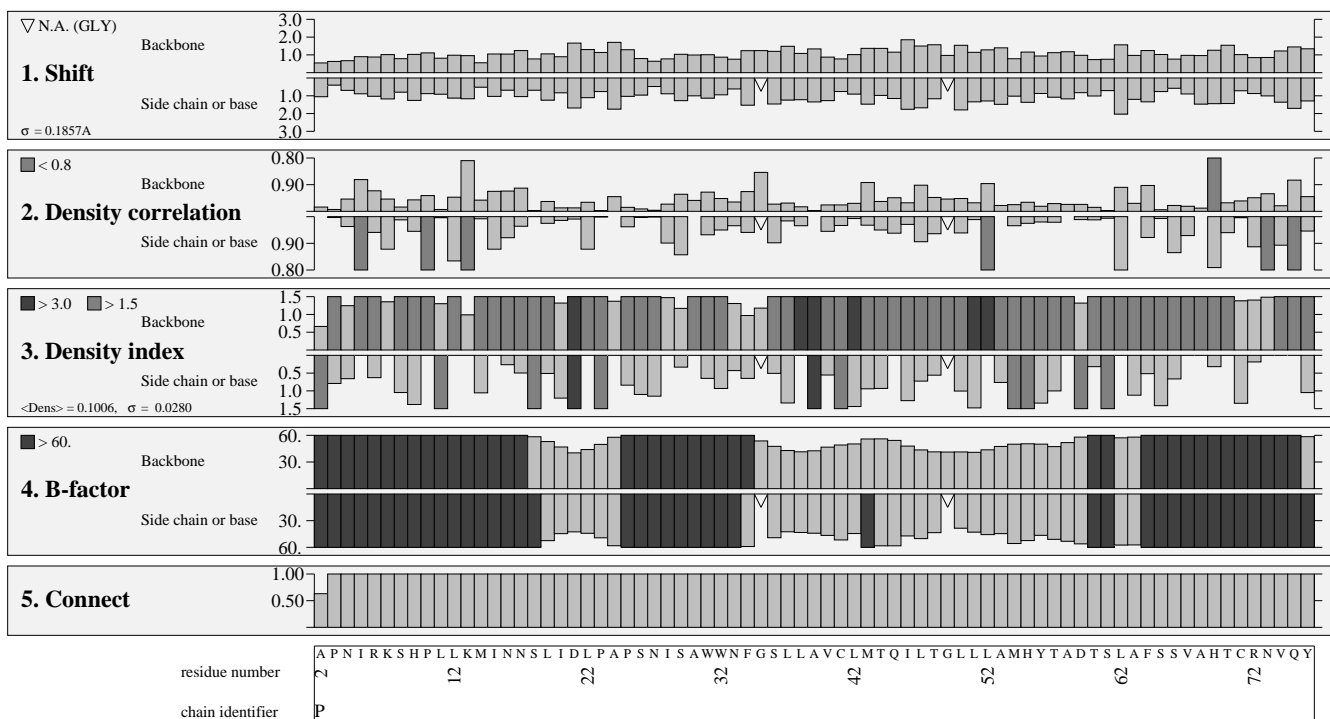
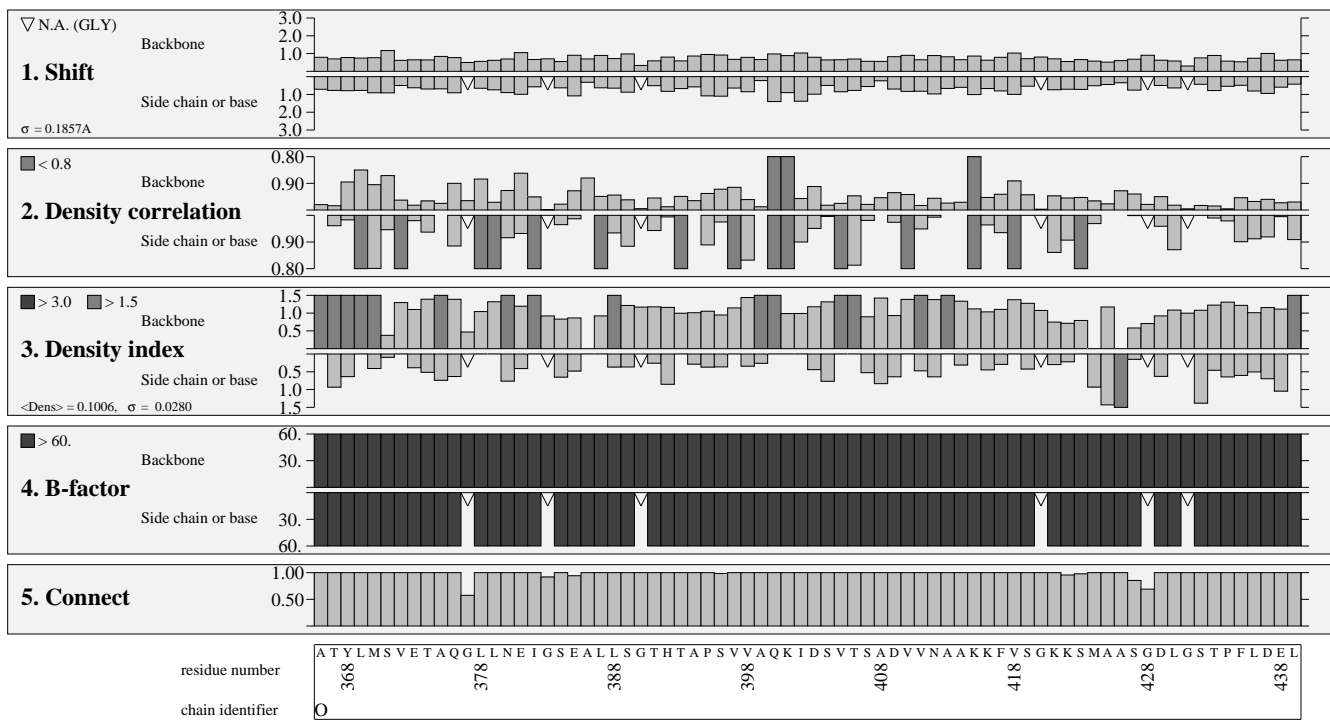
### Local estimation (19)



# Structure Factor Check

## 3H1I

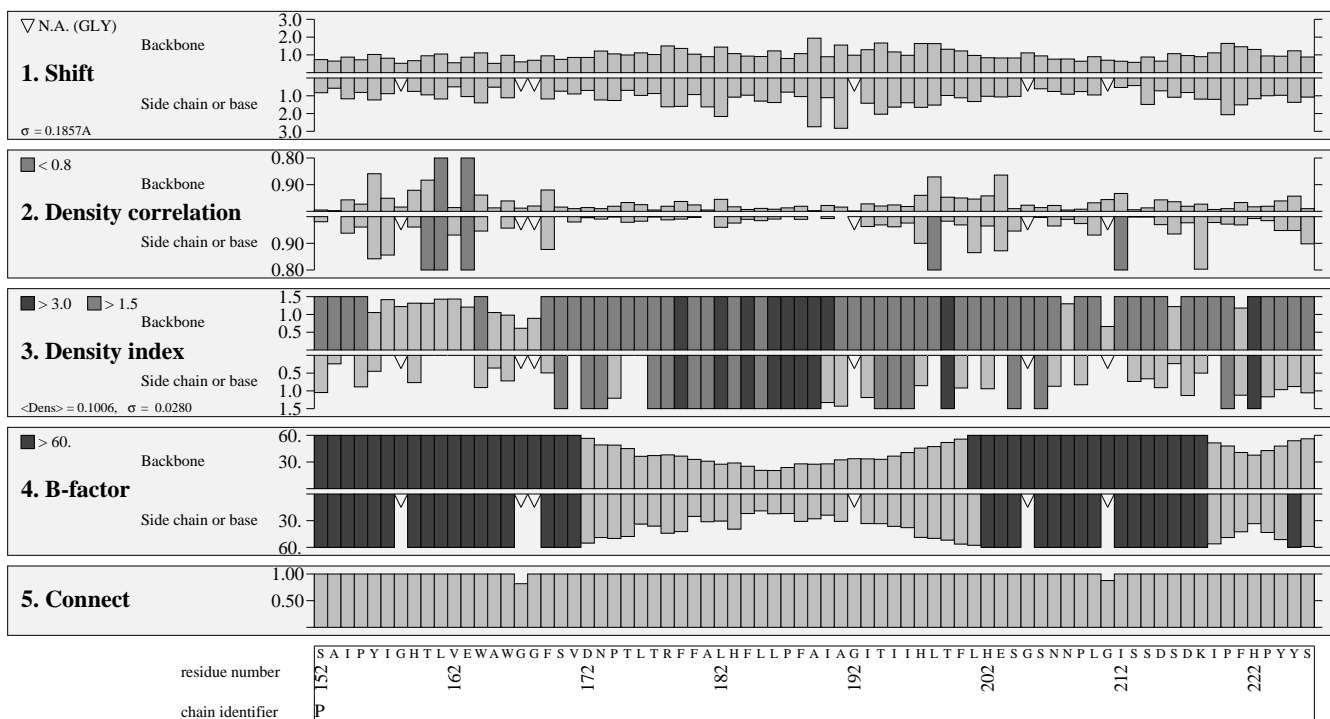
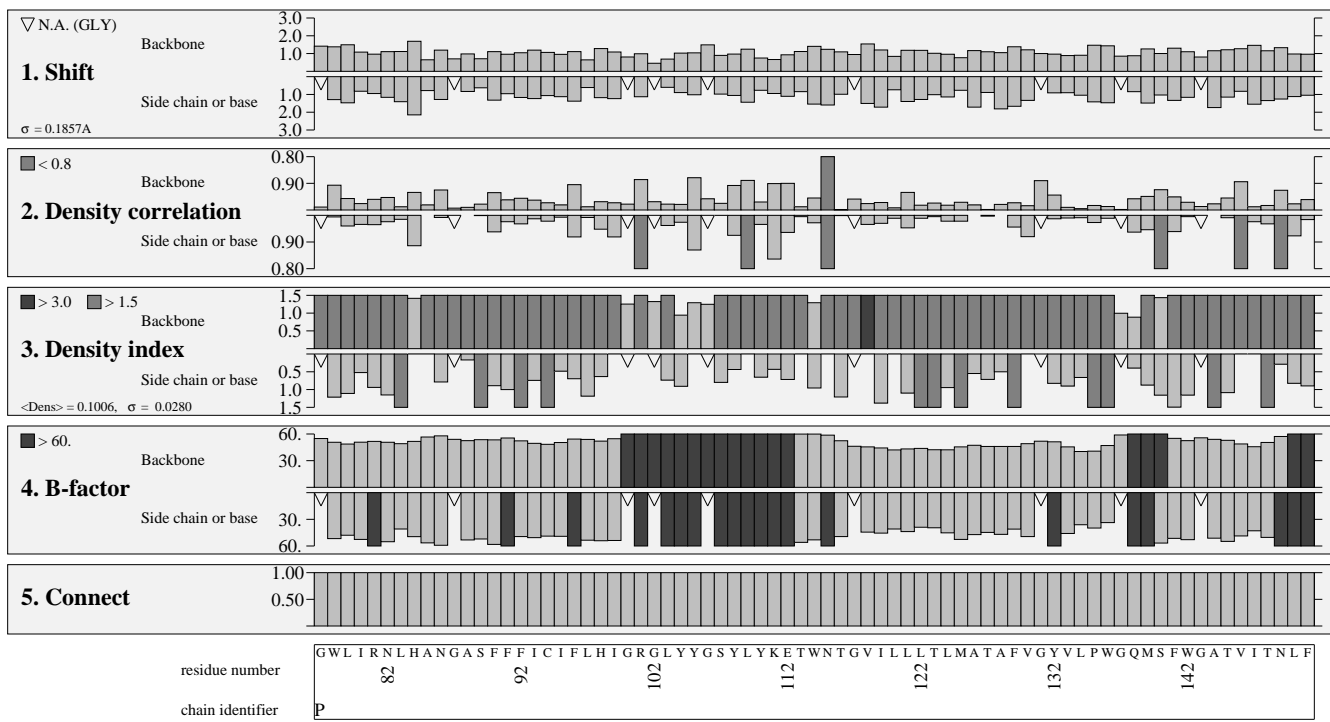
### Local estimation (20)



# Structure Factor Check

## 3H1I

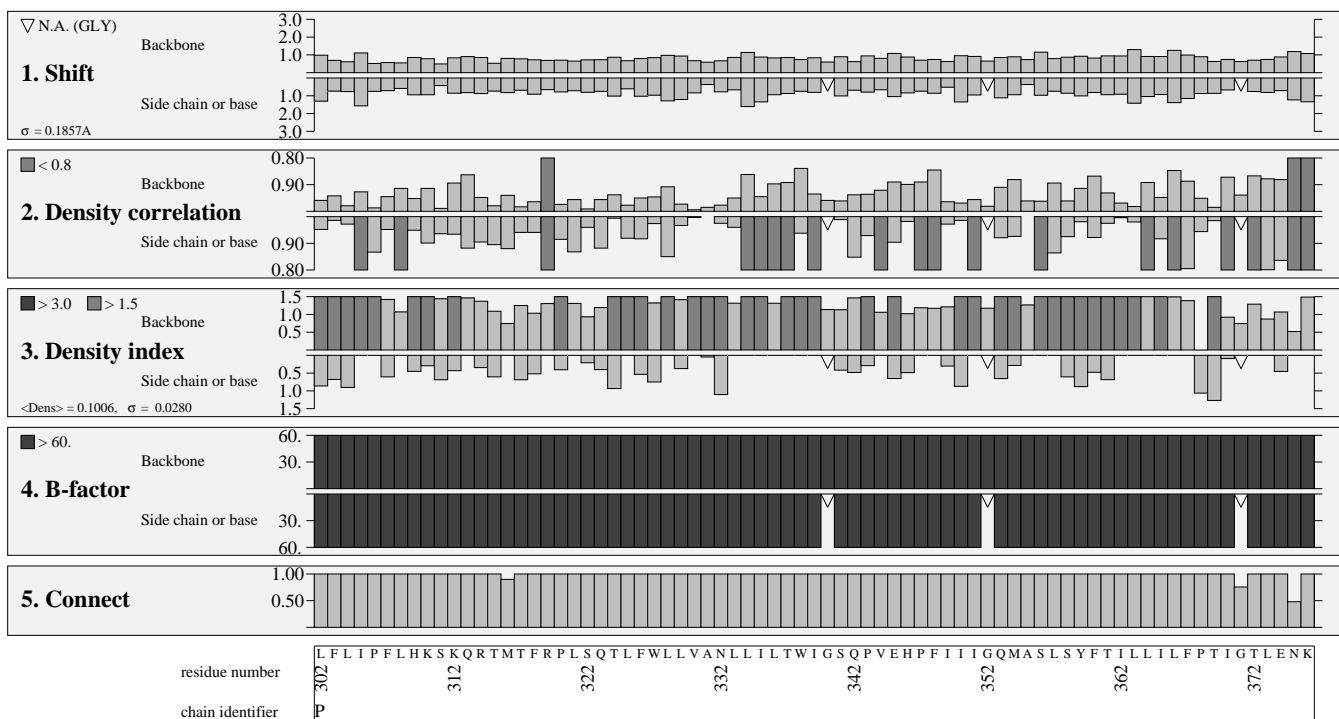
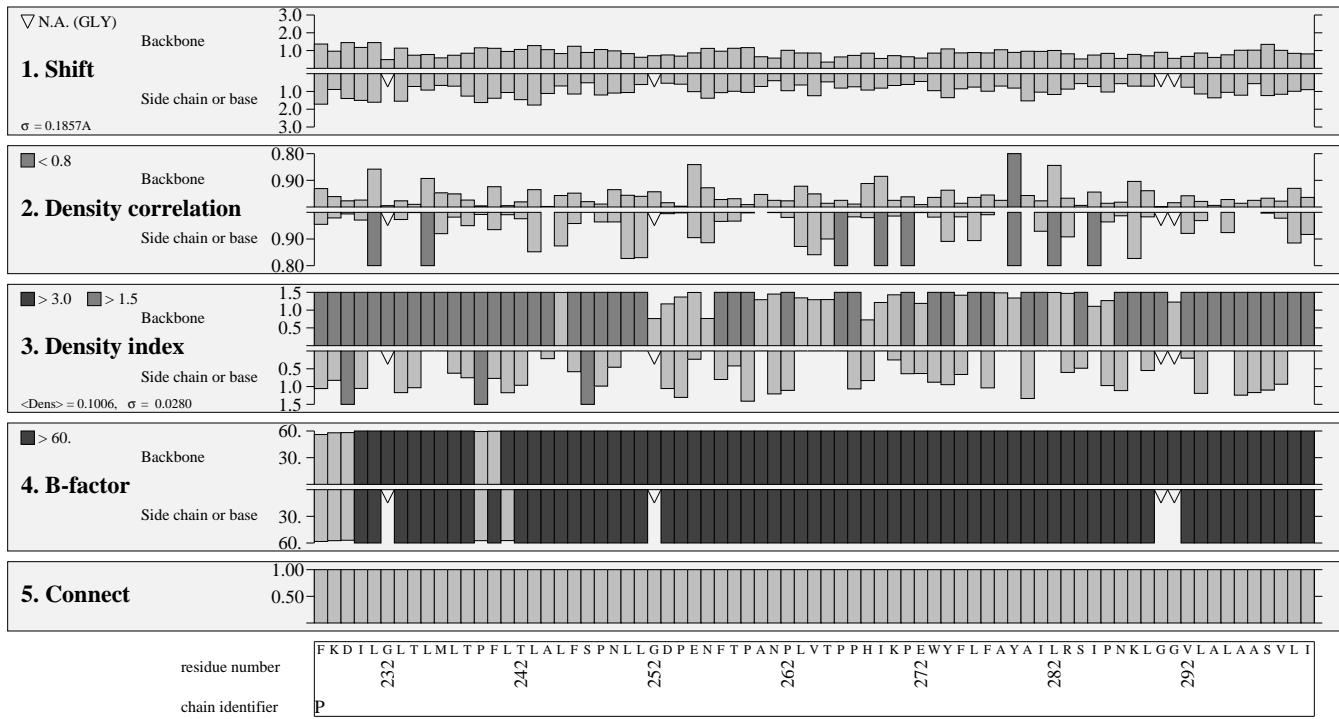
### Local estimation (21)



# Structure Factor Check

## 3H1I

### Local estimation (22)

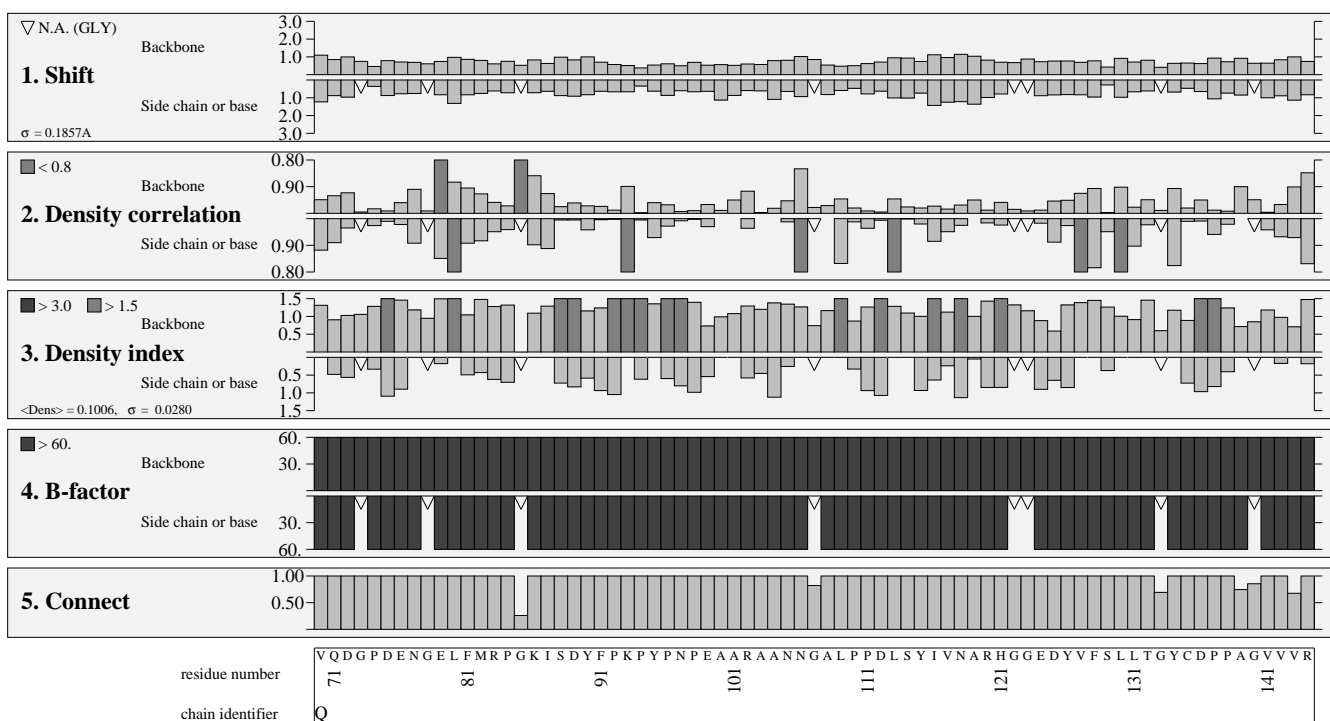
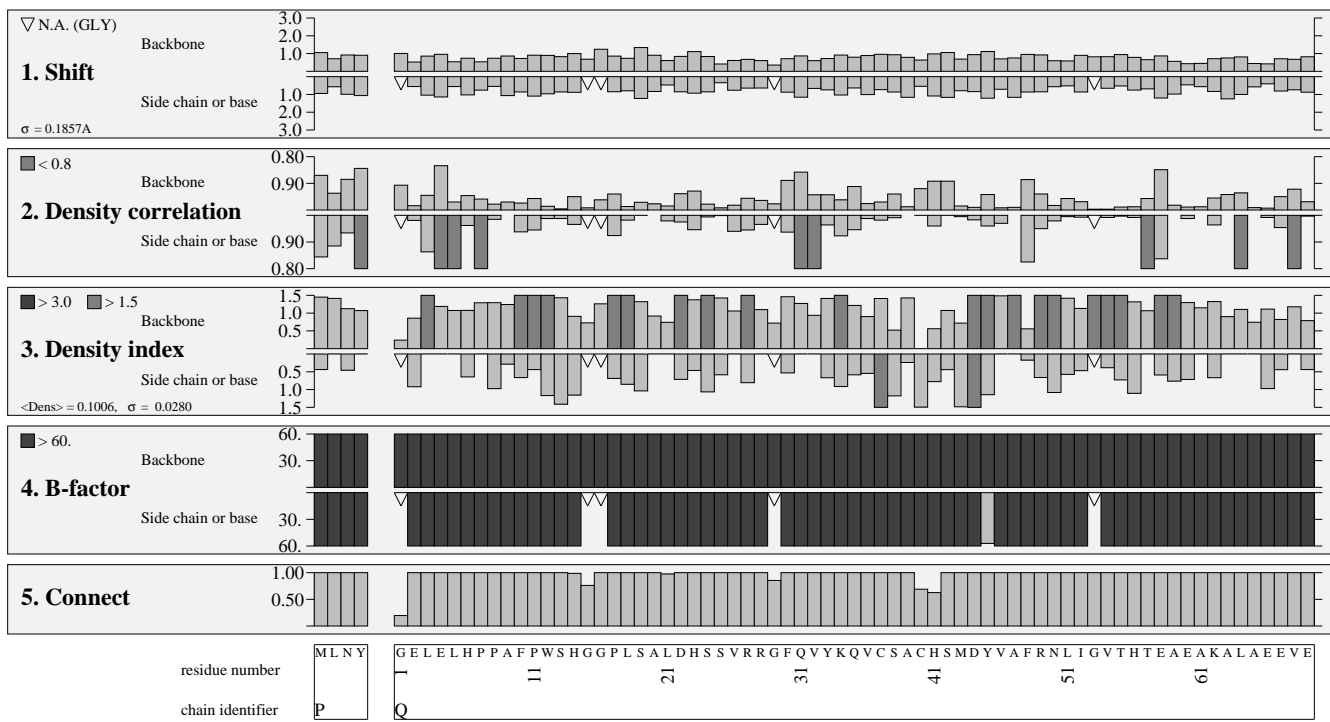




# Structure Factor Check

## 3H1I

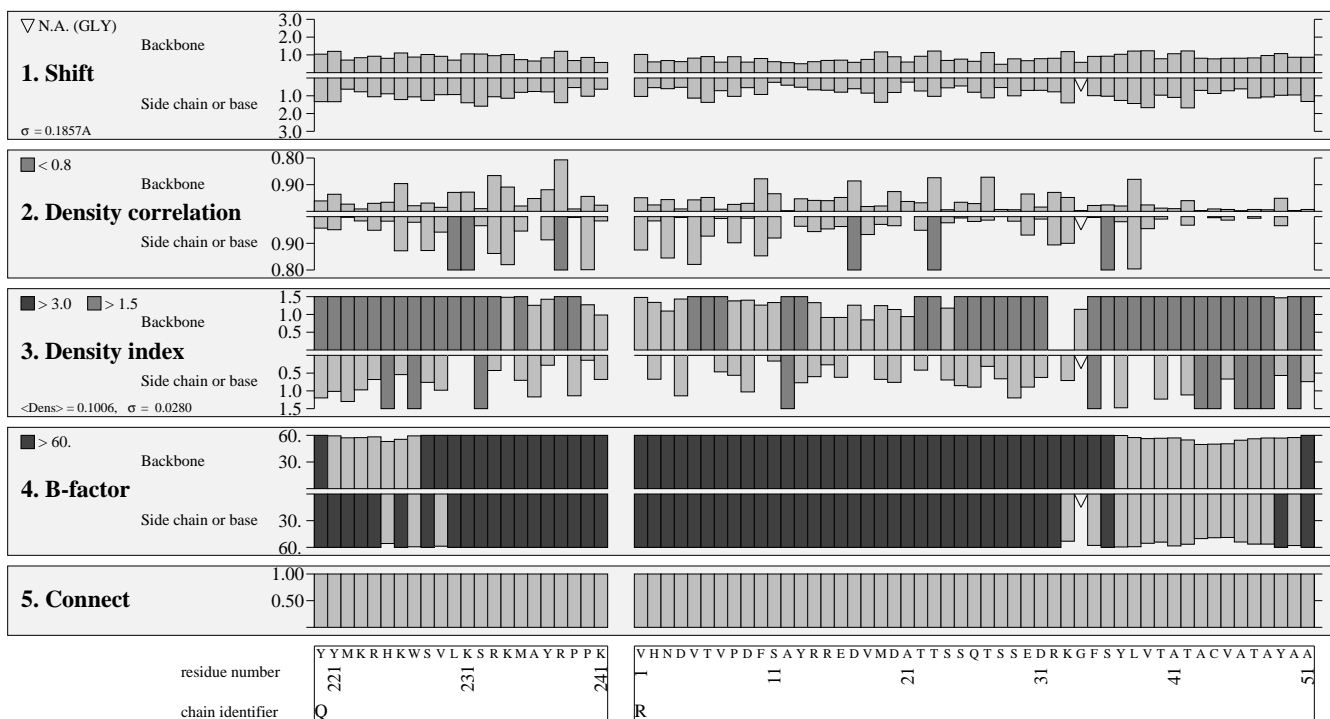
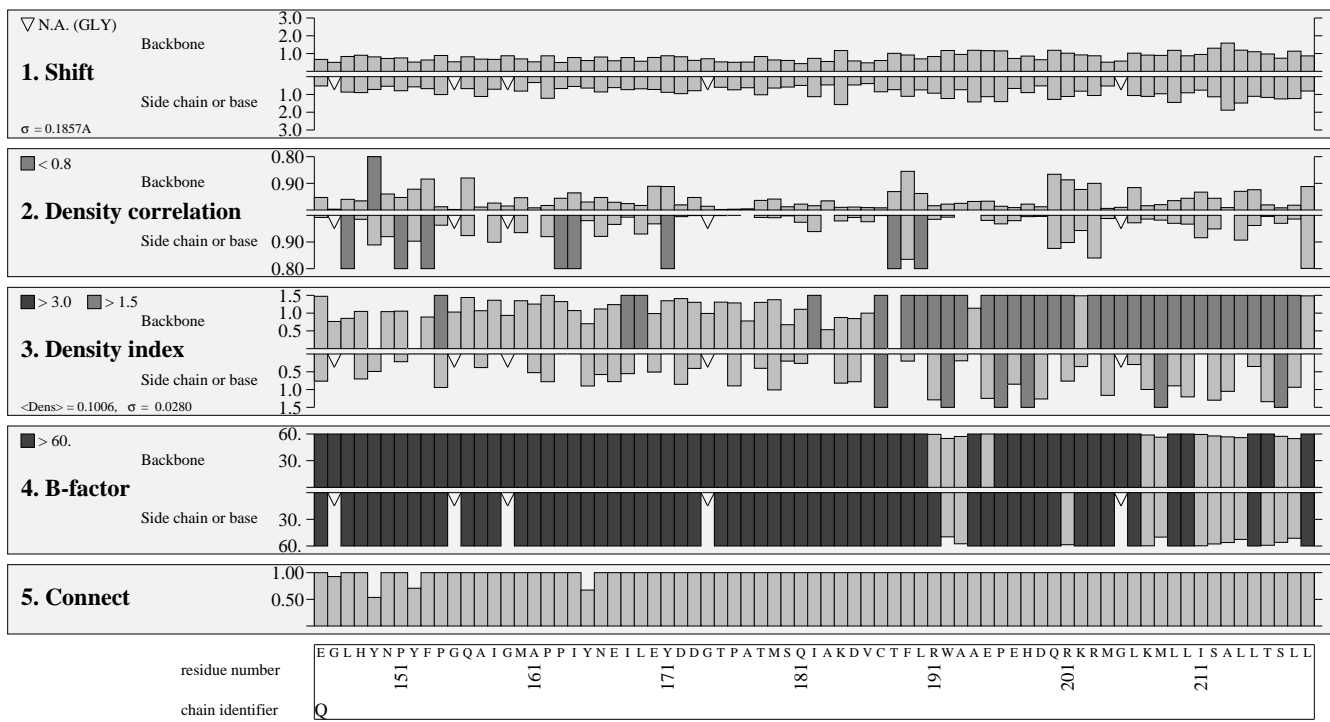
### Local estimation (23)



# Structure Factor Check

## 3H1I

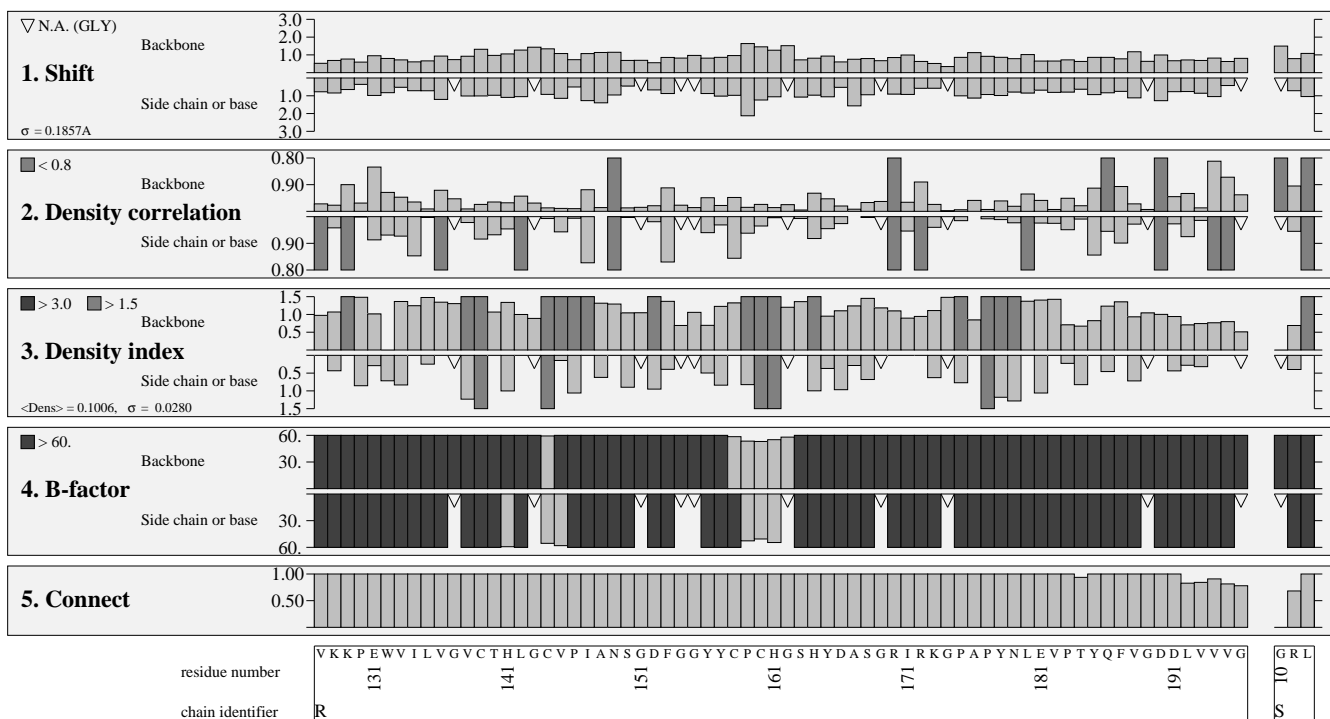
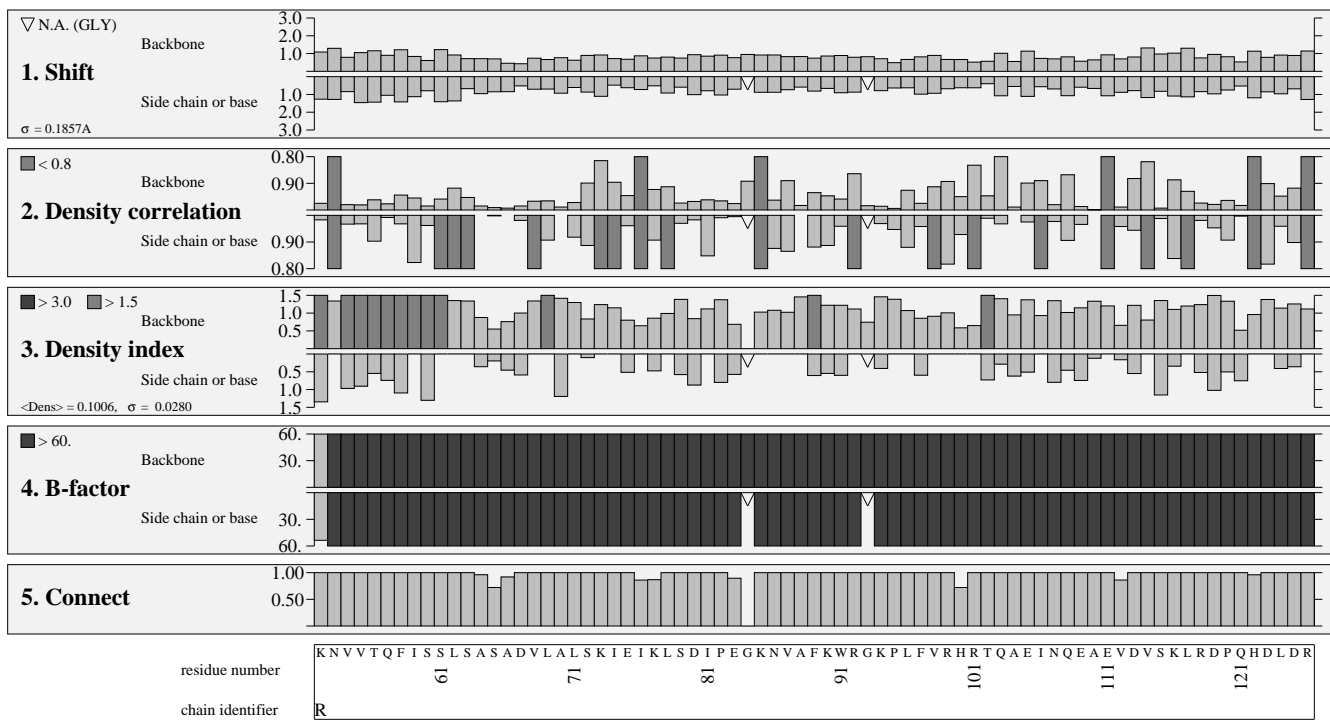
### Local estimation (24)



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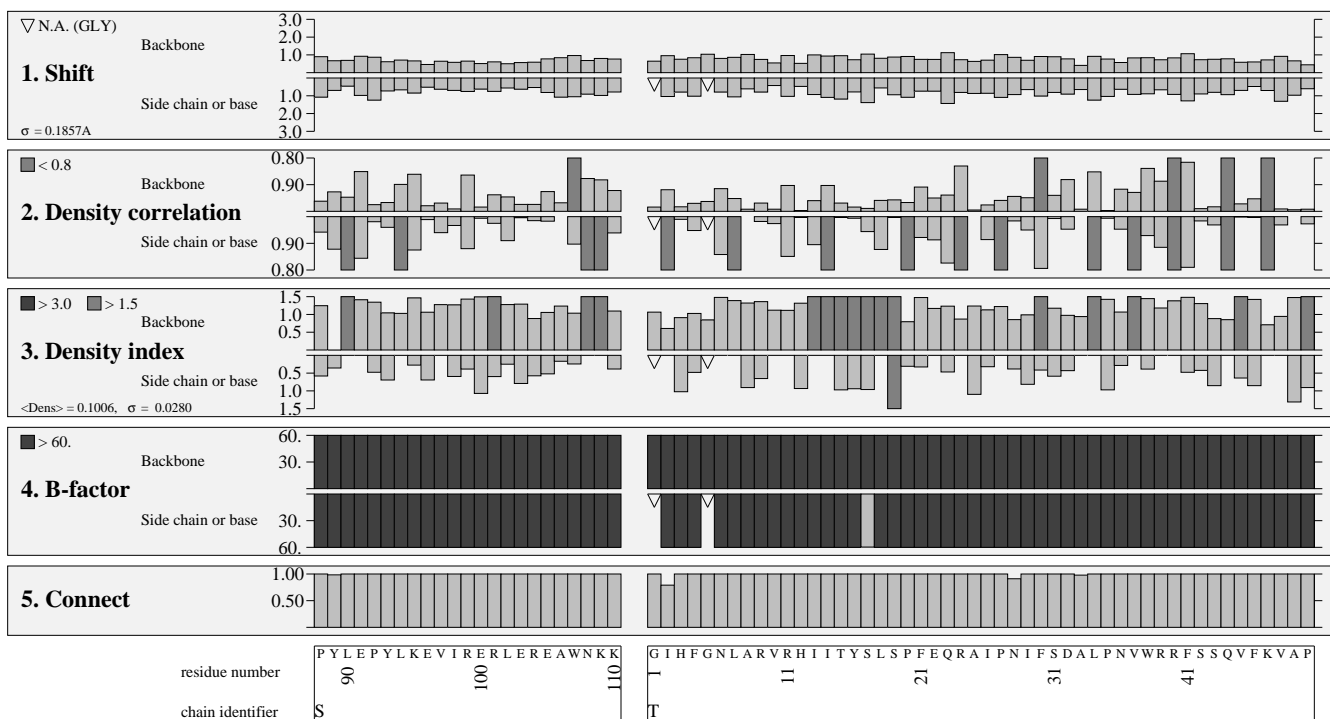
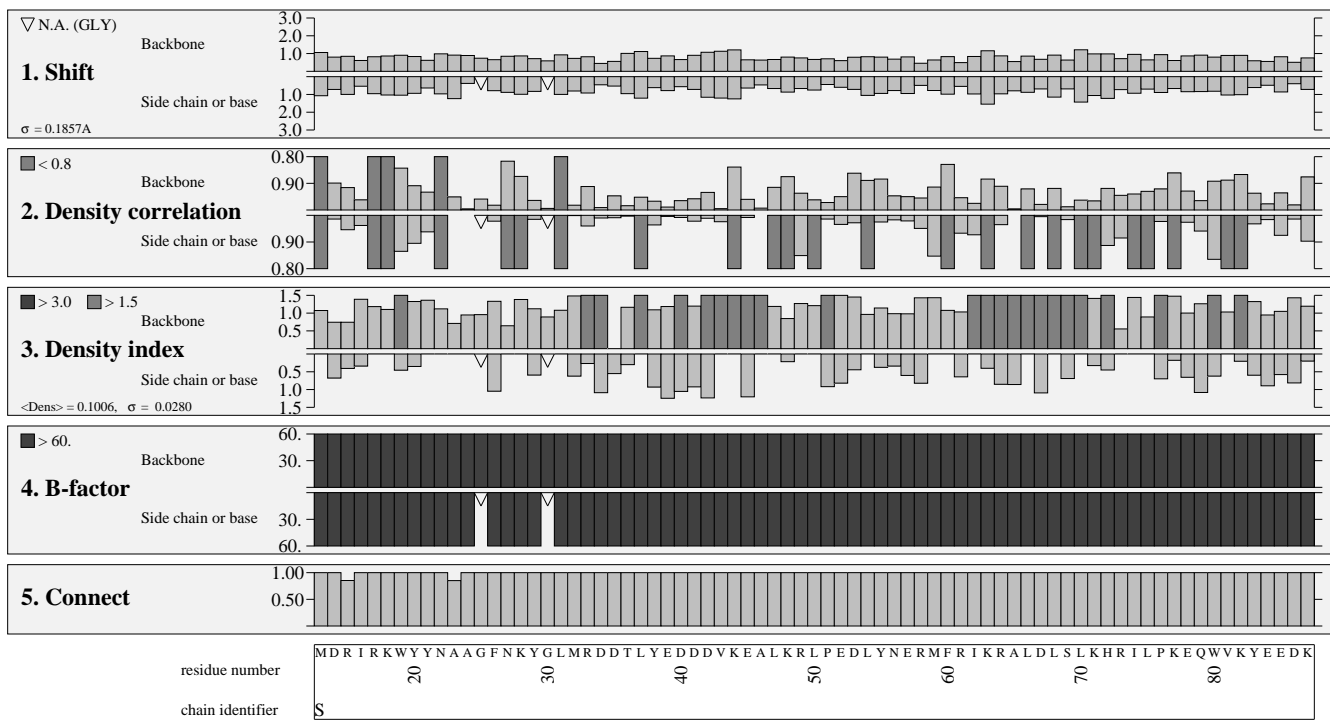
### Local estimation (25)



# Structure Factor Check

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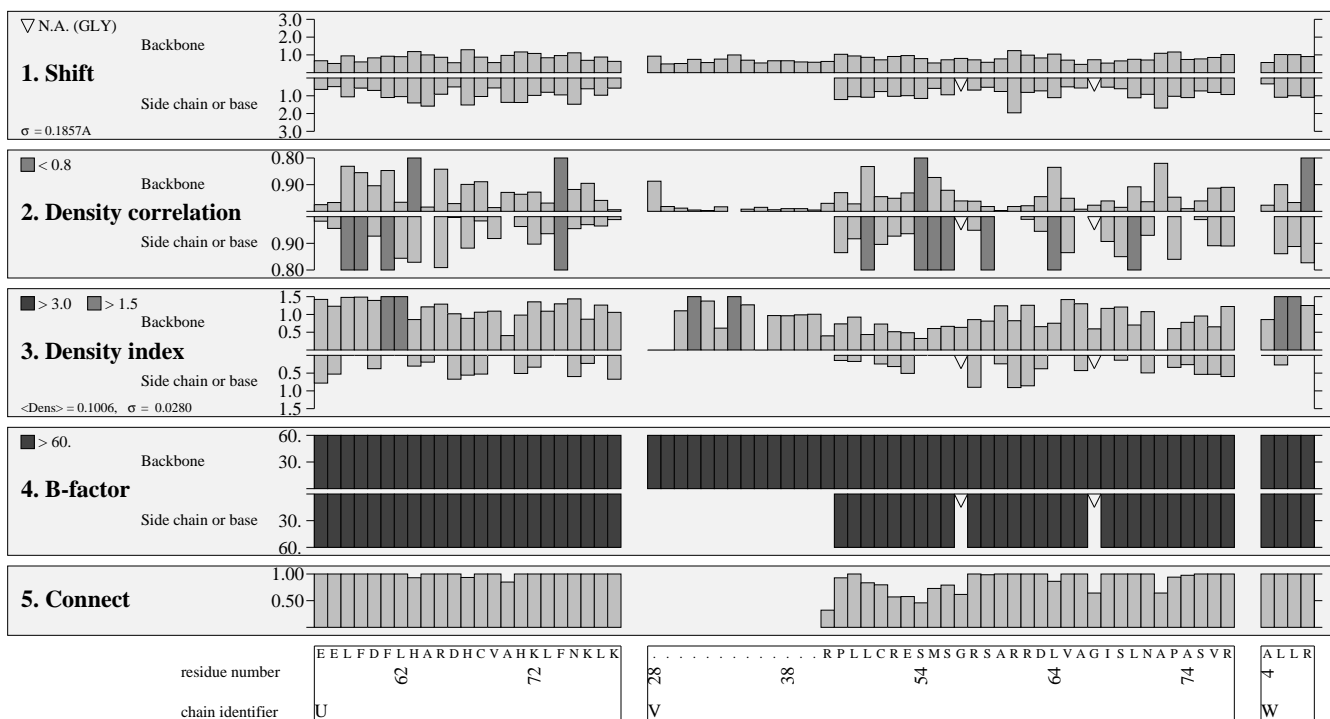
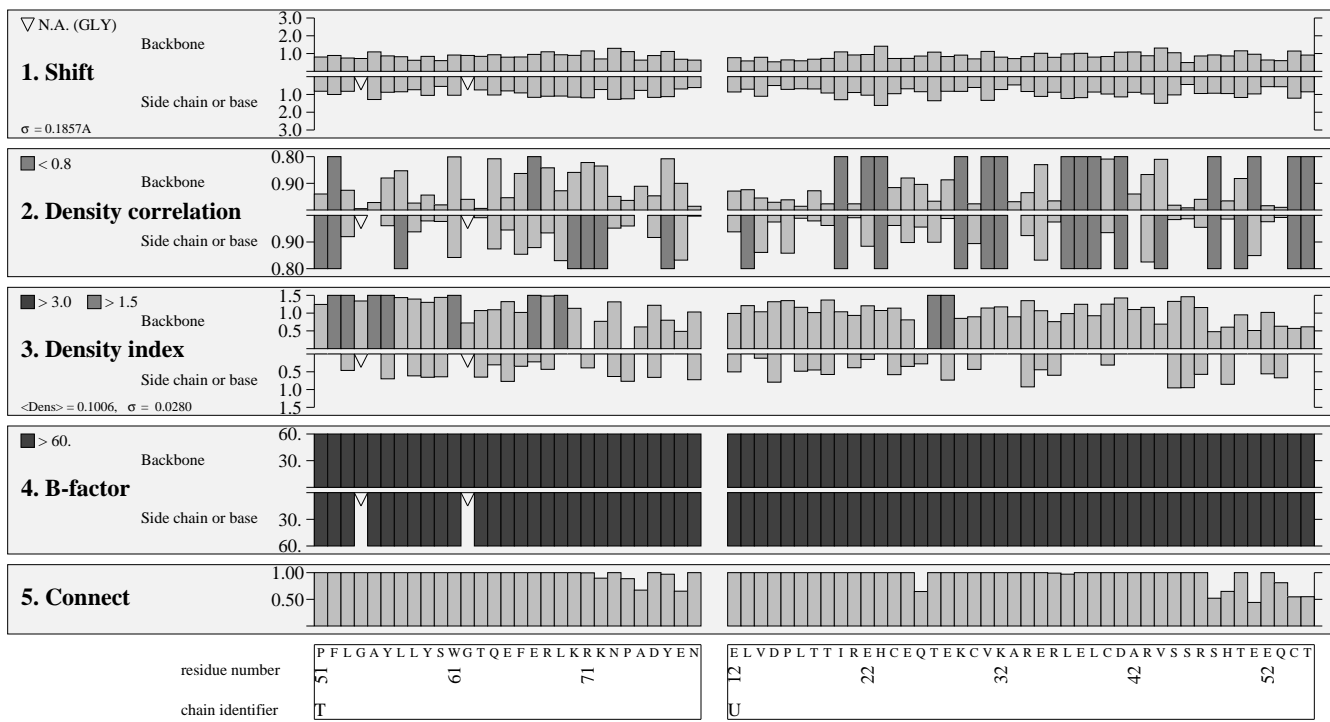
### Local estimation (26)



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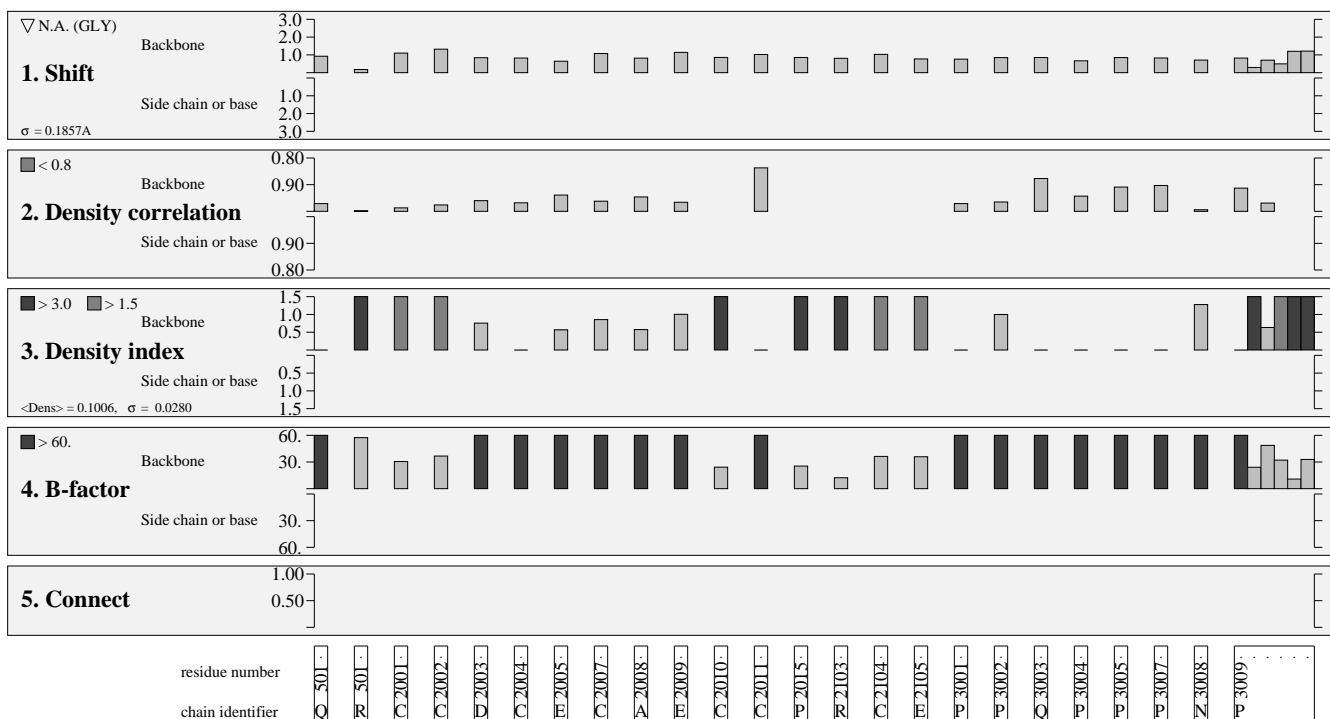
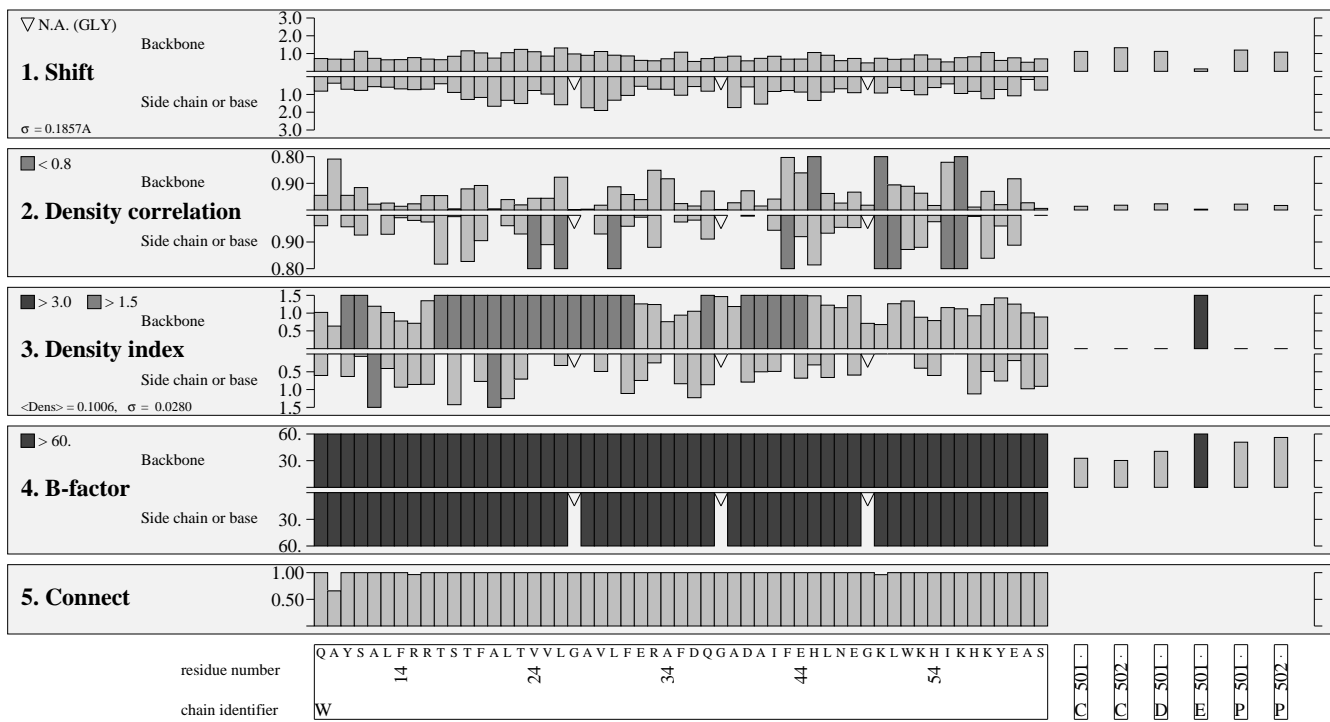
### Local estimation (27)



# Structure Factor Check

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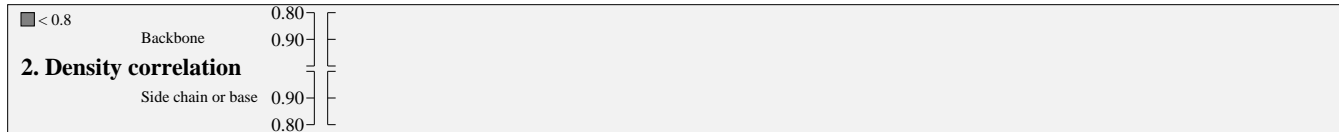
### Local estimation (28)



# Structure Factor Check

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### Local estimation (29)



residue number

chain identifier