

# Structure Factor Check

## 1PP9

Title: BOVINE CYTOCHROME BC1 COMPLEX WITH STIGMATELLIN BOUND  
 Date: 16-JUN-03  
 PDB code: 1PP9

### Crystal

Cell parameters:  
 a: 139.12 A b: 171.05 A c: 227.20 A  
 $\alpha$ : 90.00  $\beta$ : 90.00  $\gamma$ : 90.00  
 Space group: P 21 21 21  
 Number of NCS-operators: 1  
 NC-symmetry only for information

### Model

33959 atoms (1437 water molecules)  
 Number of chains: 51  
 Volume not occupied by model: 46.2 %  
 $\langle B \rangle$  (for atomic model): 46.6 A<sup>2</sup>  
 $\sigma(B)$ : 15.40 A<sup>2</sup>  
 Matthews coefficient: 2.84  
 Corresponding solvent % : 56.40

### Refinement

Program: CNS 1.1  
 Nominal resolution range: 25.0 – 2.10 A  
 Reported R-factor: 0.250  
 Number of reflections used: 305496  
 Reported Rfree: 0.29  
 Sigma cut-off: N.A.

### Structure Factors

#### Input

Nominal resolution range: 40.0 – 2.08 A  
 Reflections in file: 308206  
 Unique reflections above 0: 308206  
 above 1 $\sigma$ : 294636  
 above 3 $\sigma$ : 173856

#### SFCHECK

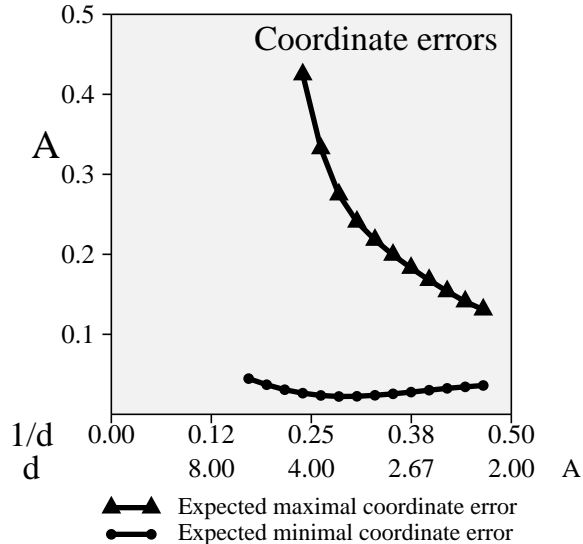
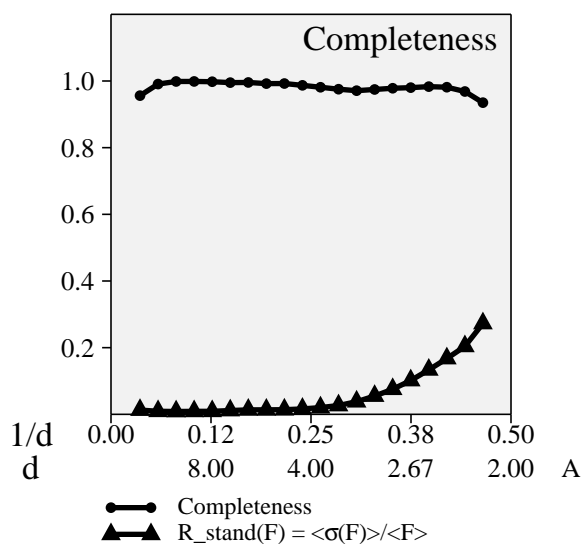
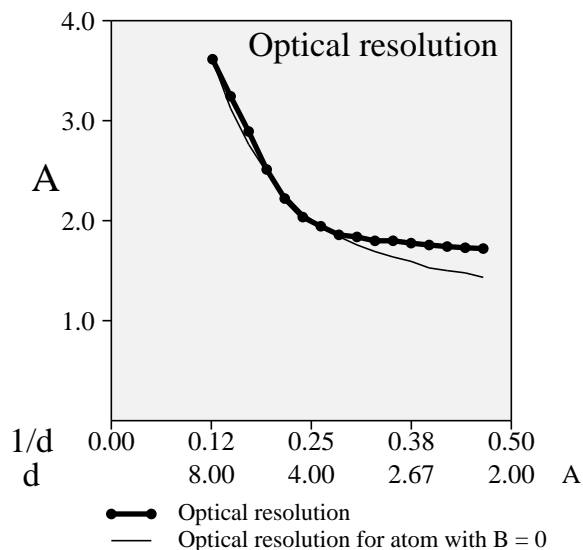
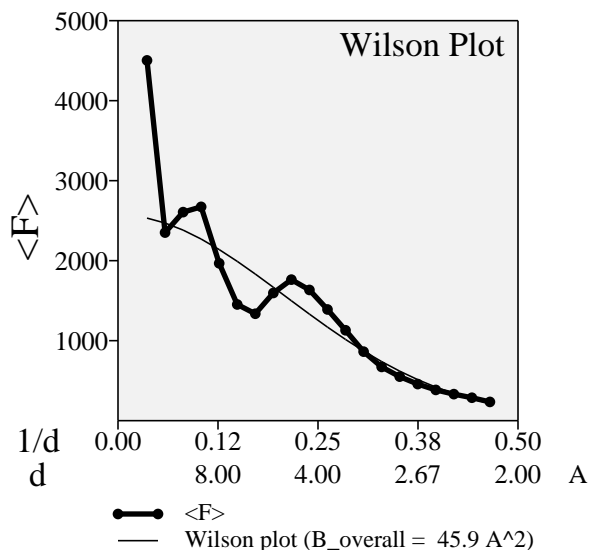
Nominal resolution range: 40.0 – 2.10 A  
\05max. from input data, min. from author\05  
 Used reflections: 305656  
 Reflections out of resolution: 2550  
 Completeness: 97.4 %  
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$  : 0.063  
 Anisotropic distribution of Structure Factors  
 ratio of eigen values: 1.0000 0.7621 0.5479  
 $B_{\text{overall}}$  (by Patterson): 36.A<sup>2</sup>  
 Optical resolution: 1.72 A  
 Expected opt. resol. for complete data set: 1.72 A  
 Estimated minimal error: 0.036 A

### Model vs. Structure Factors

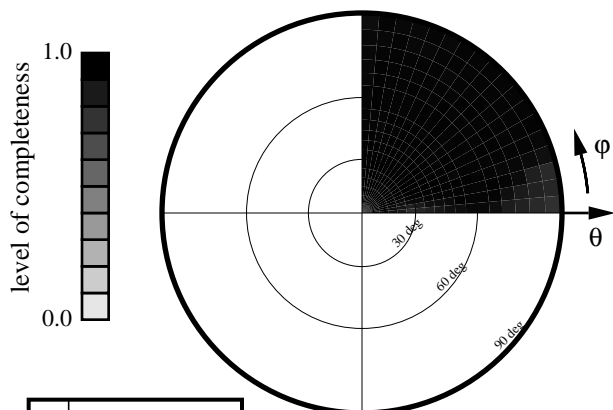
R-factor for all reflections: 0.273  
 Correlation factor: 0.923  
 R-factor: 0.271  
 for  $F > 2.0\sigma$   
 nom. resolution range: 24.98 – 2.10A  
 reflections used: 292442  
 Rfree: 0.290  
 Nfree: 14590  
 R-factor without free-refl.: 0.270  
 Non free-reflections: 277852  
 $\langle u \rangle$  (error in coords by Luzzati plot): 0.355 A  
 Estimated maximal error: 0.131 A  
 DPI: 0.200 A  
**Scaling**  
 Scale: 1.092  
 Bdiff: -5.07  
 Anisothermal Scaling (Beta):  
 5.0663 1.0855 -2.4833 0.0000 0.0000 0.0000  
 Solvent correction – Ks,Bs: 0.778 317.459

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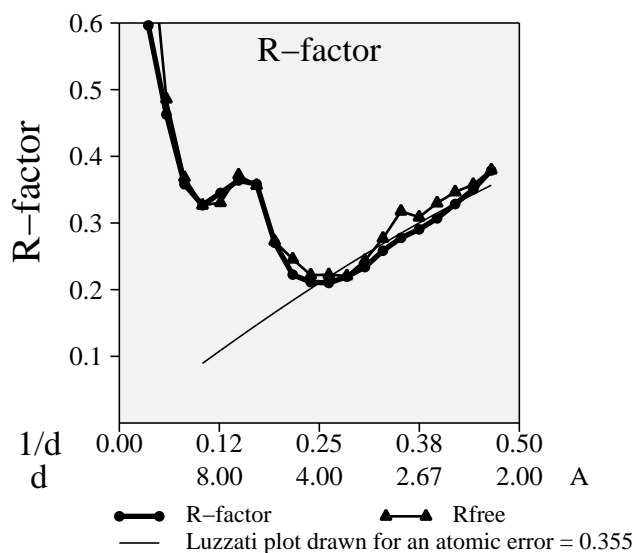


Stereographic projection of the averaged radial completeness



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

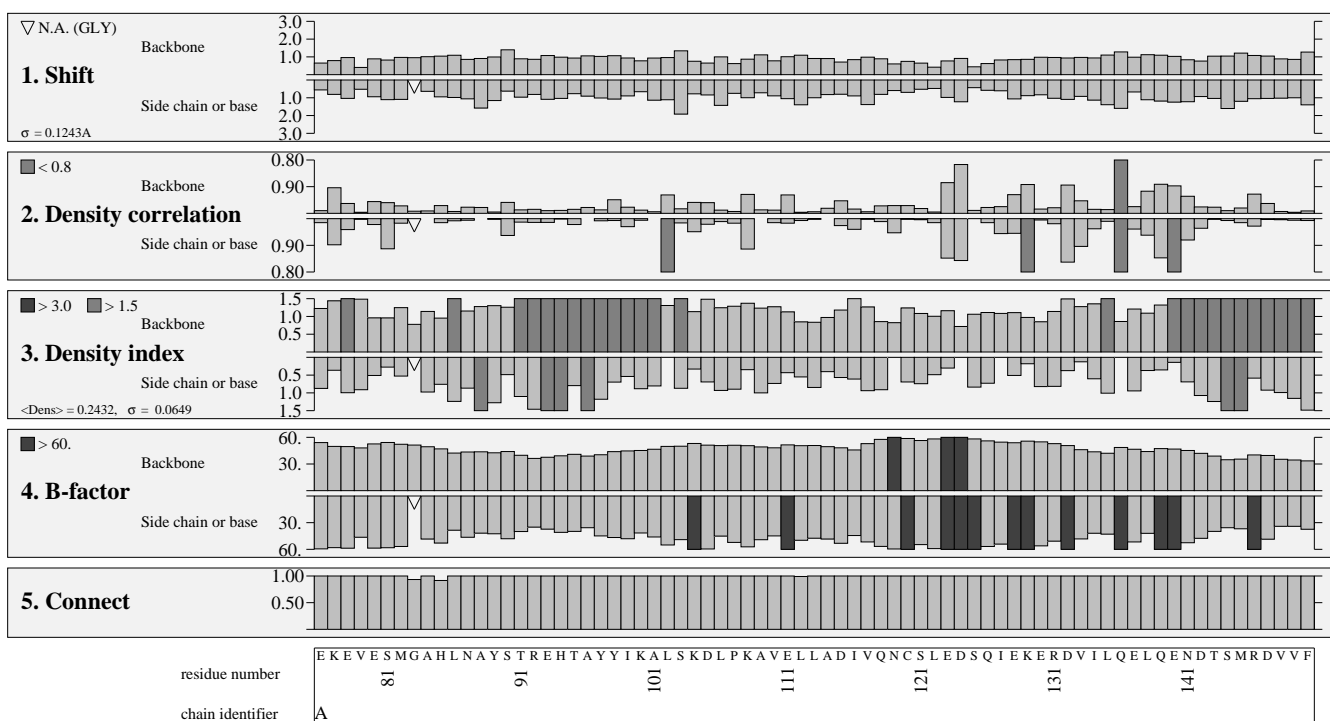
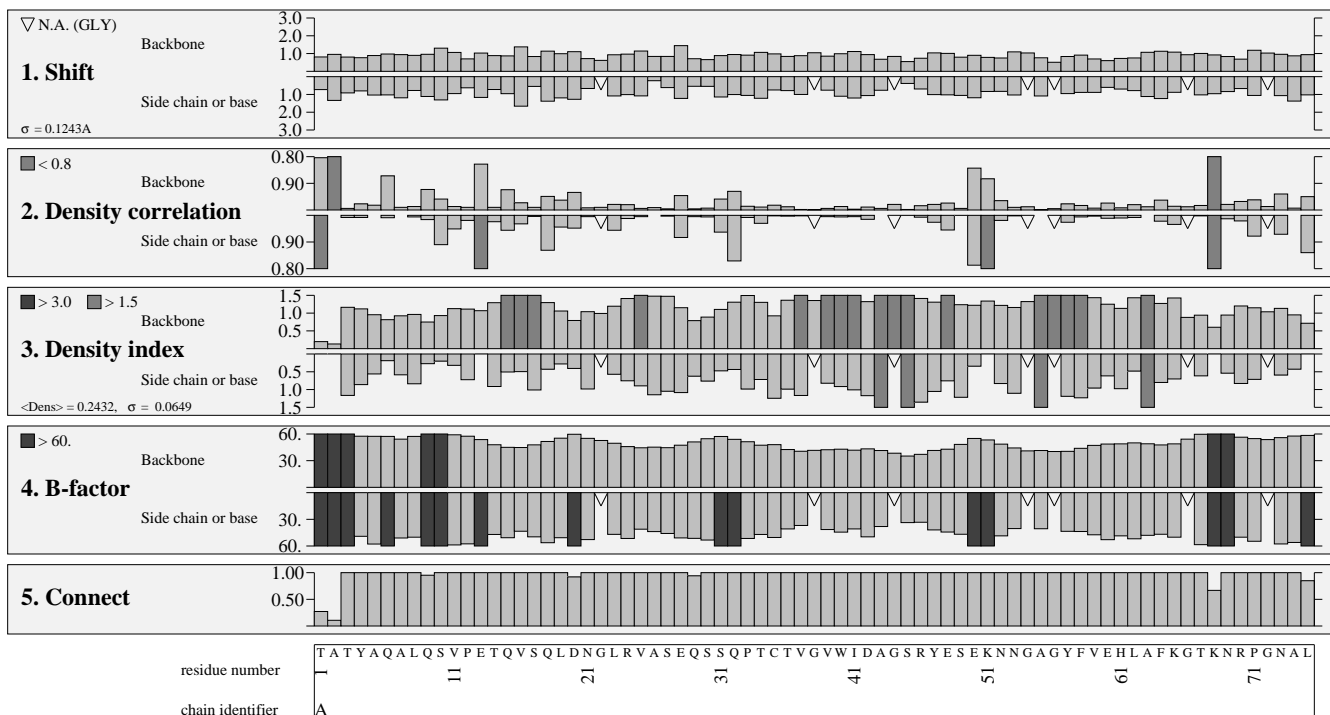
polar coordinates of the crystallographical axes



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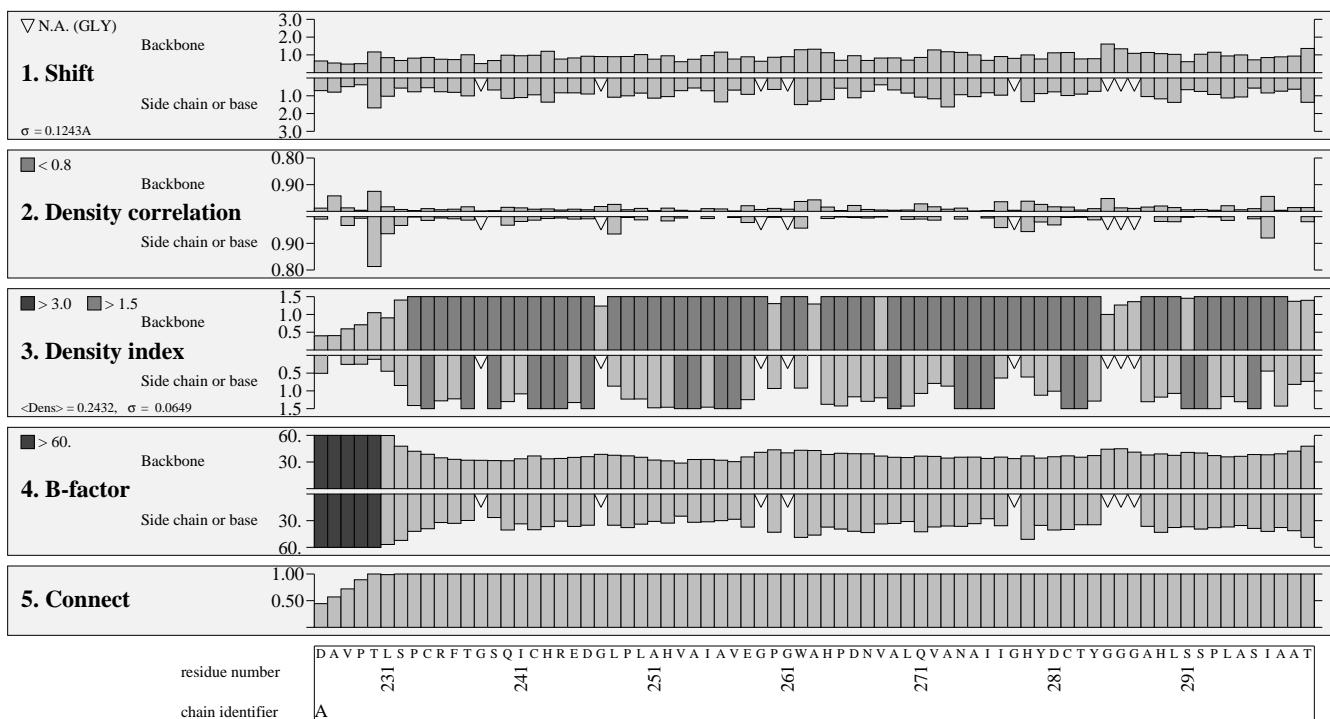
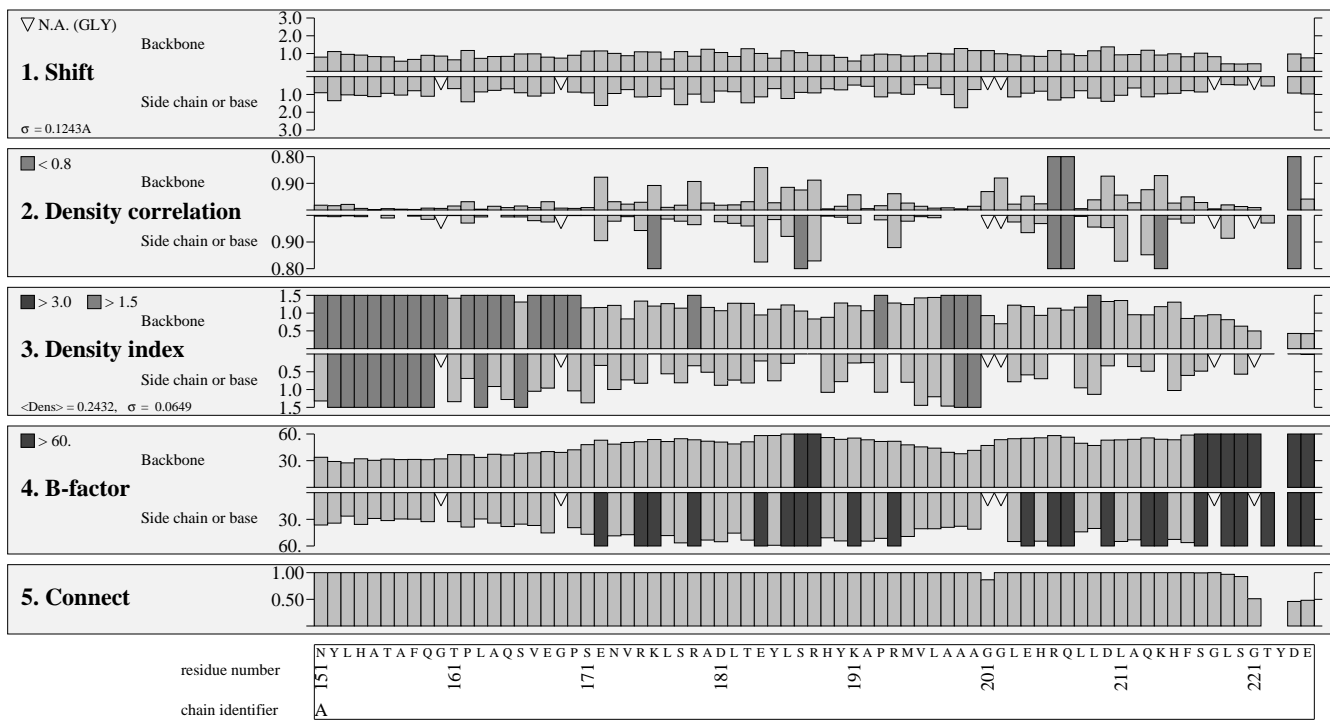
### Local estimation



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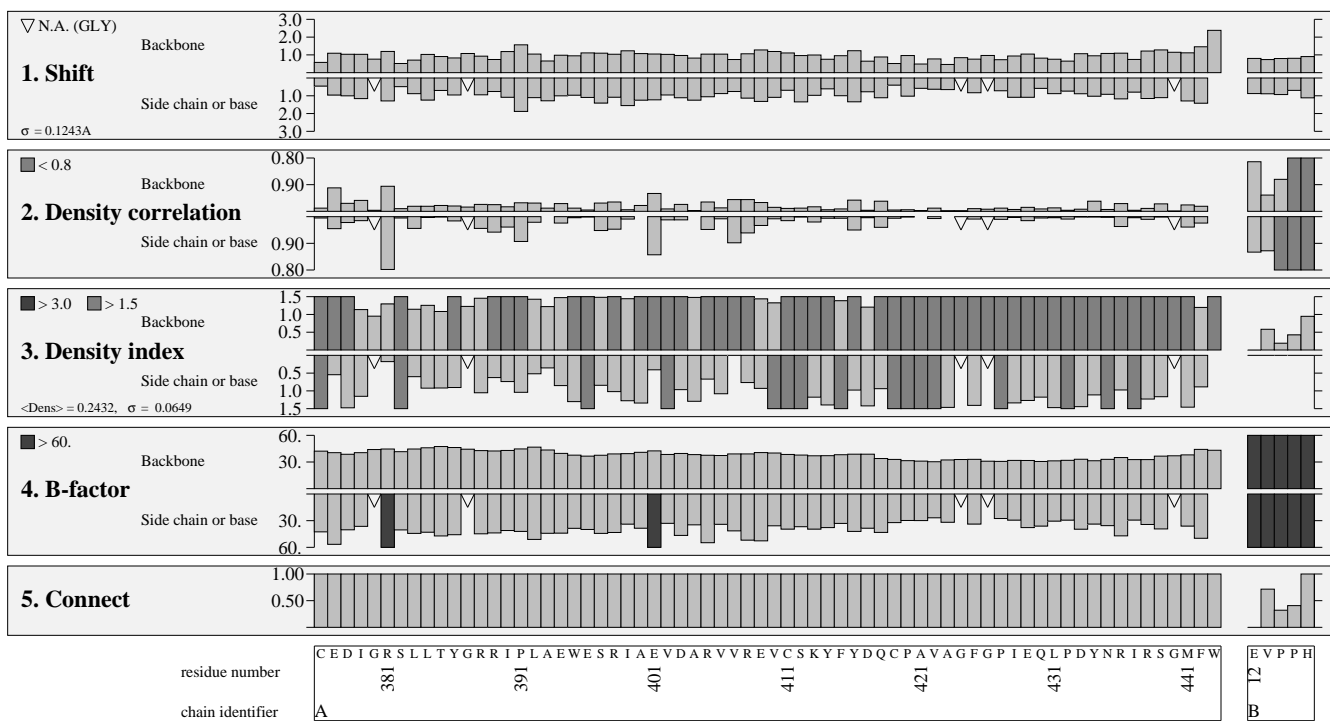
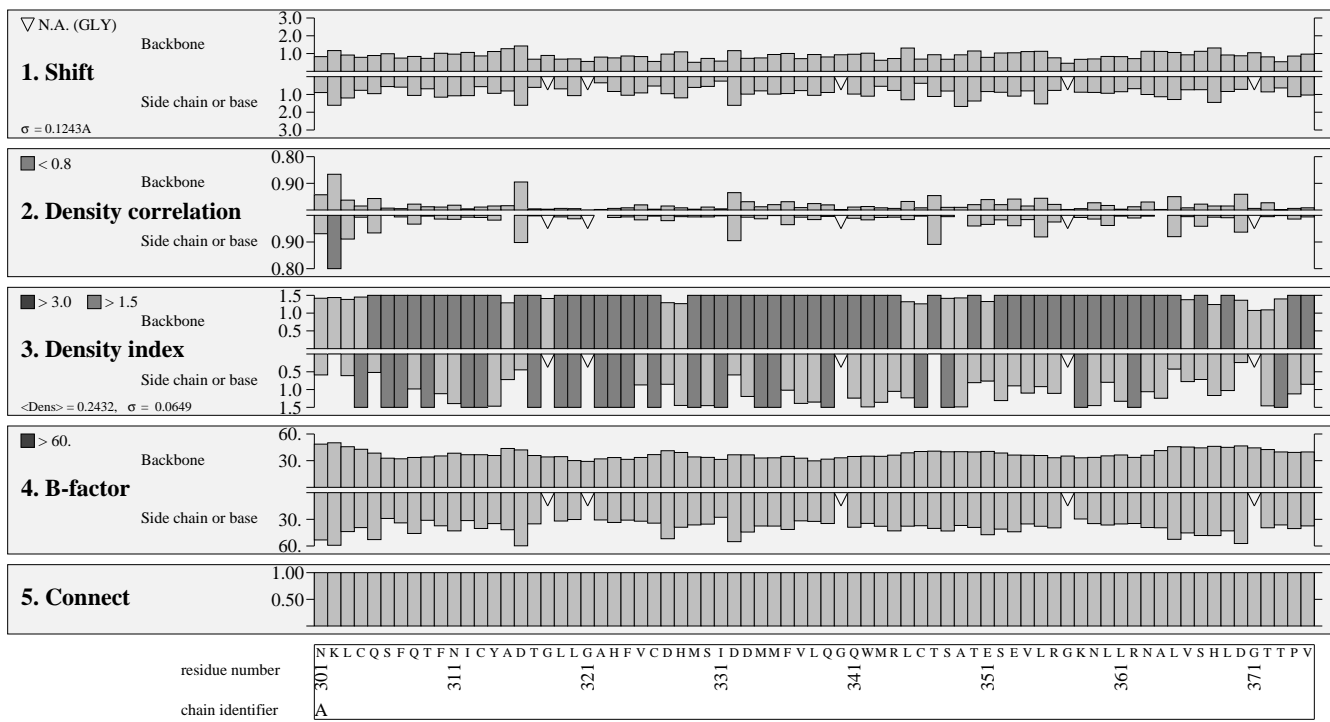
### Local estimation (2)



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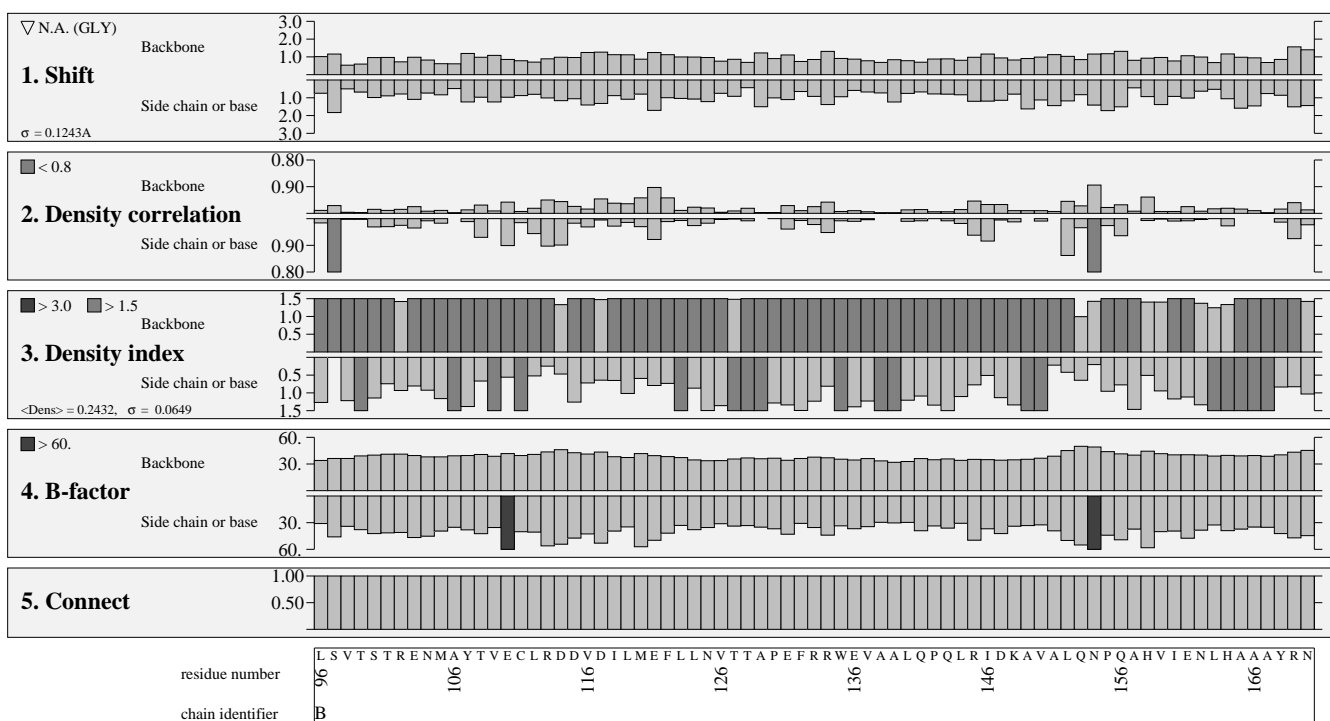
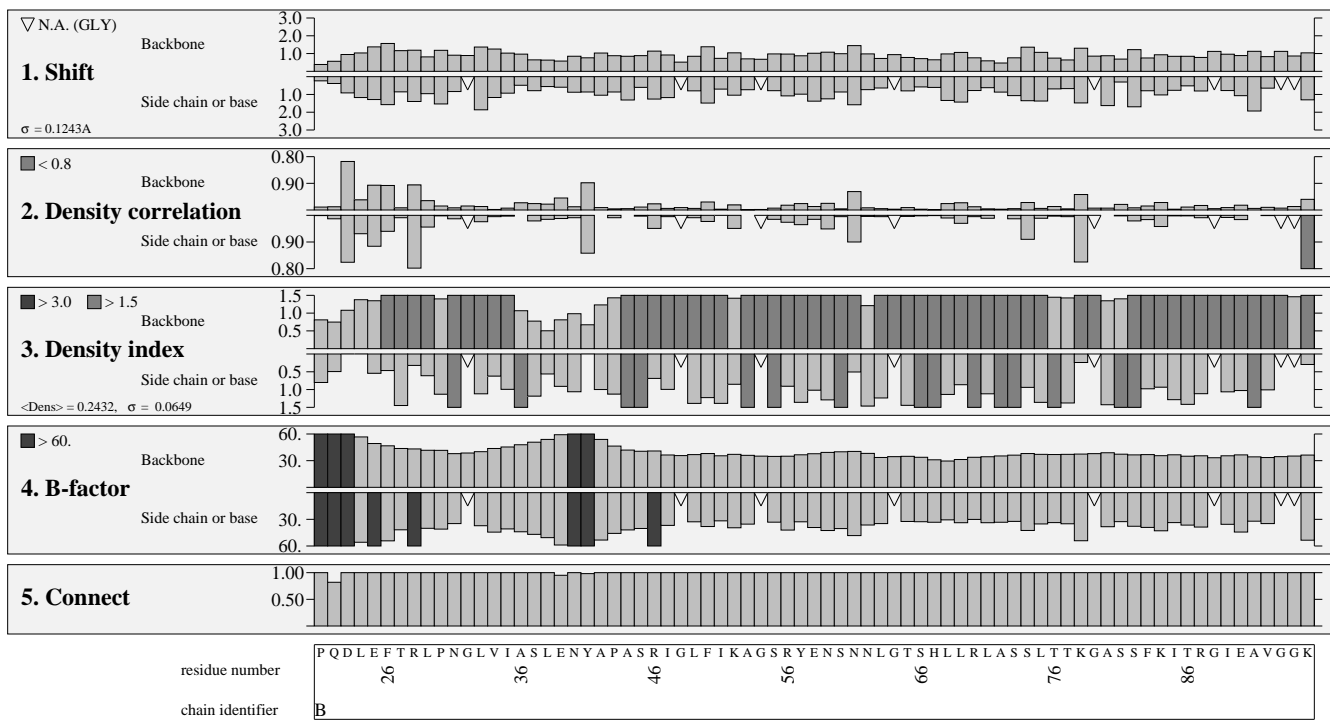
### Local estimation (3)



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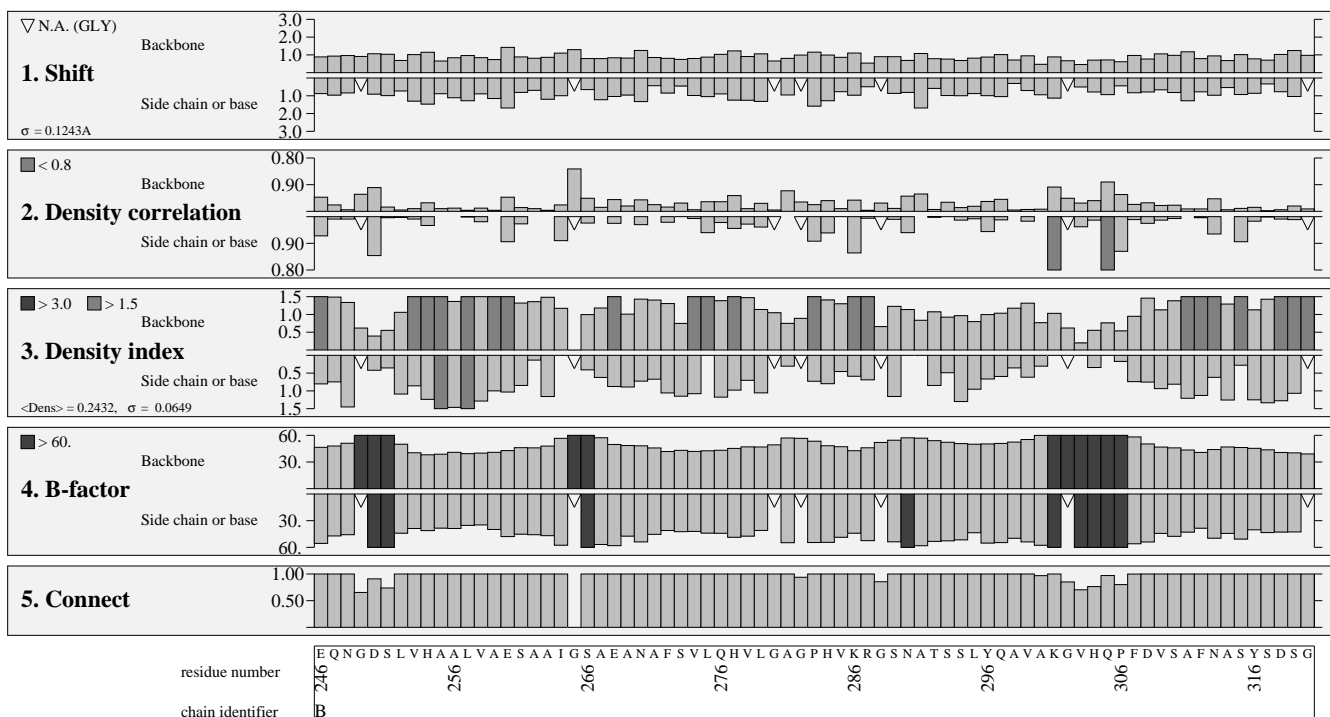
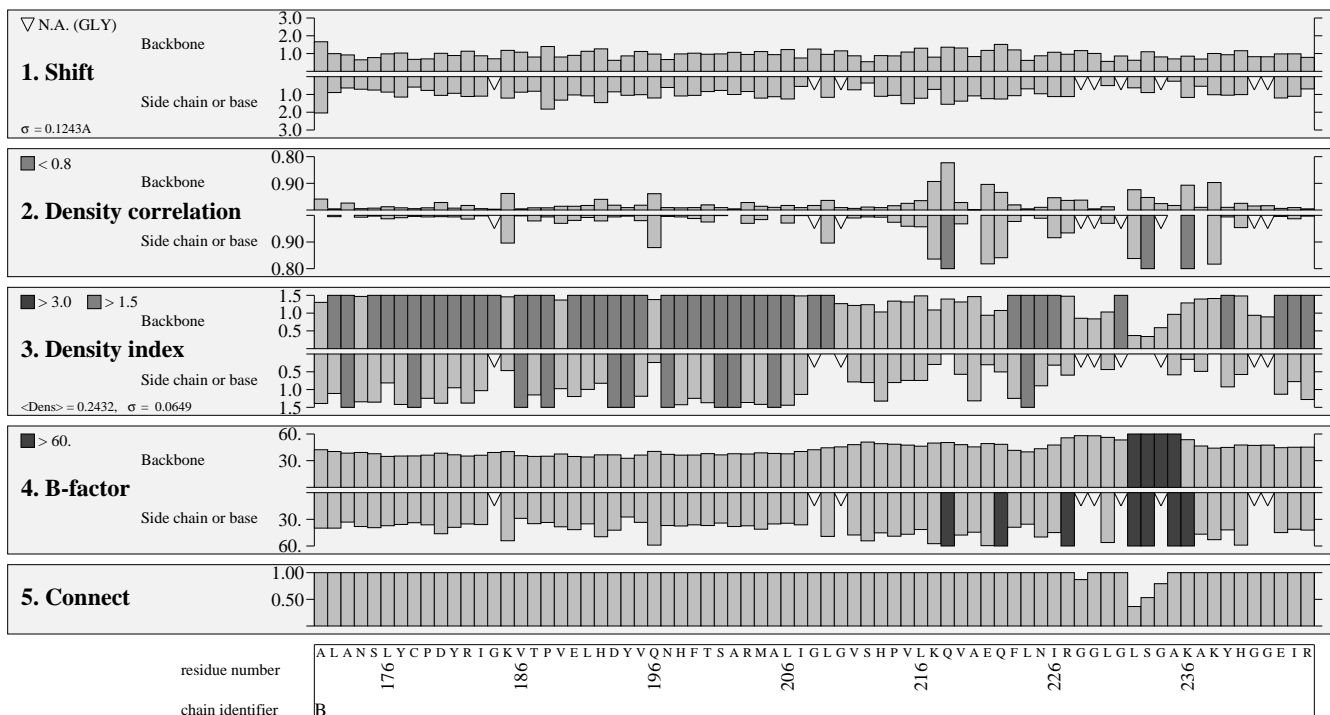
### Local estimation (4)



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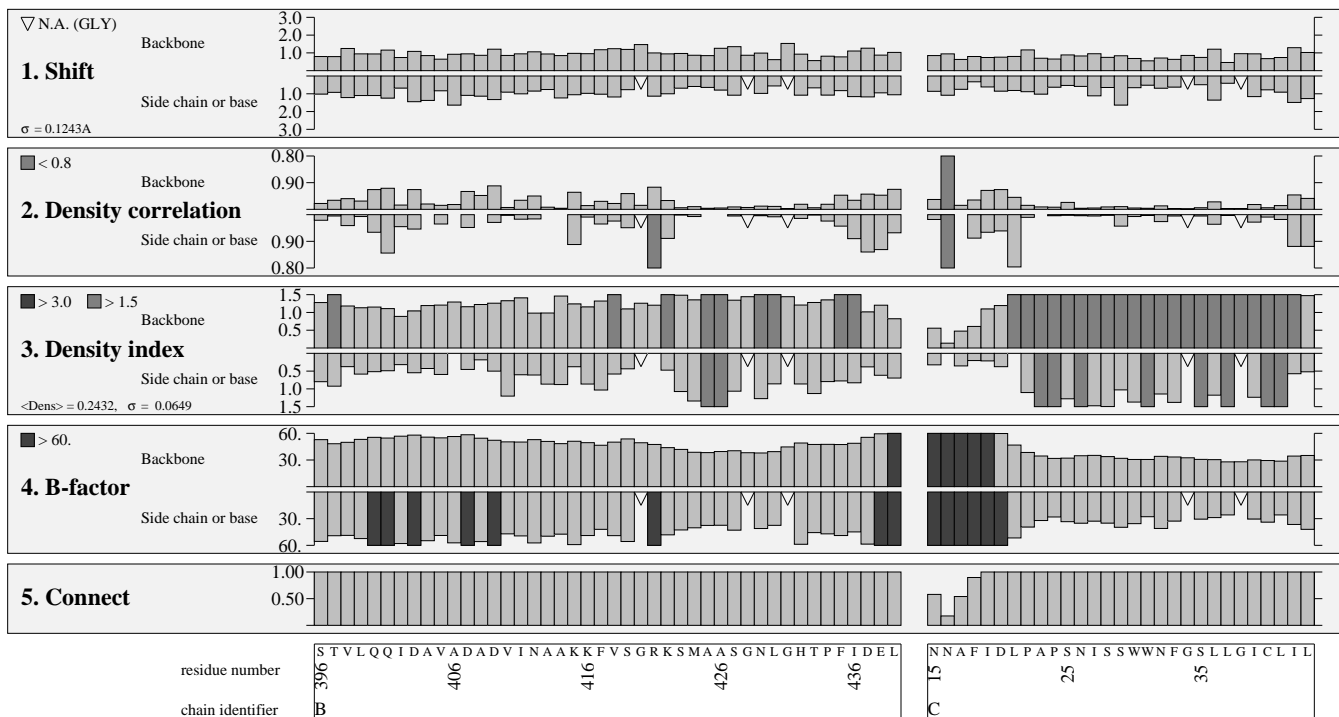
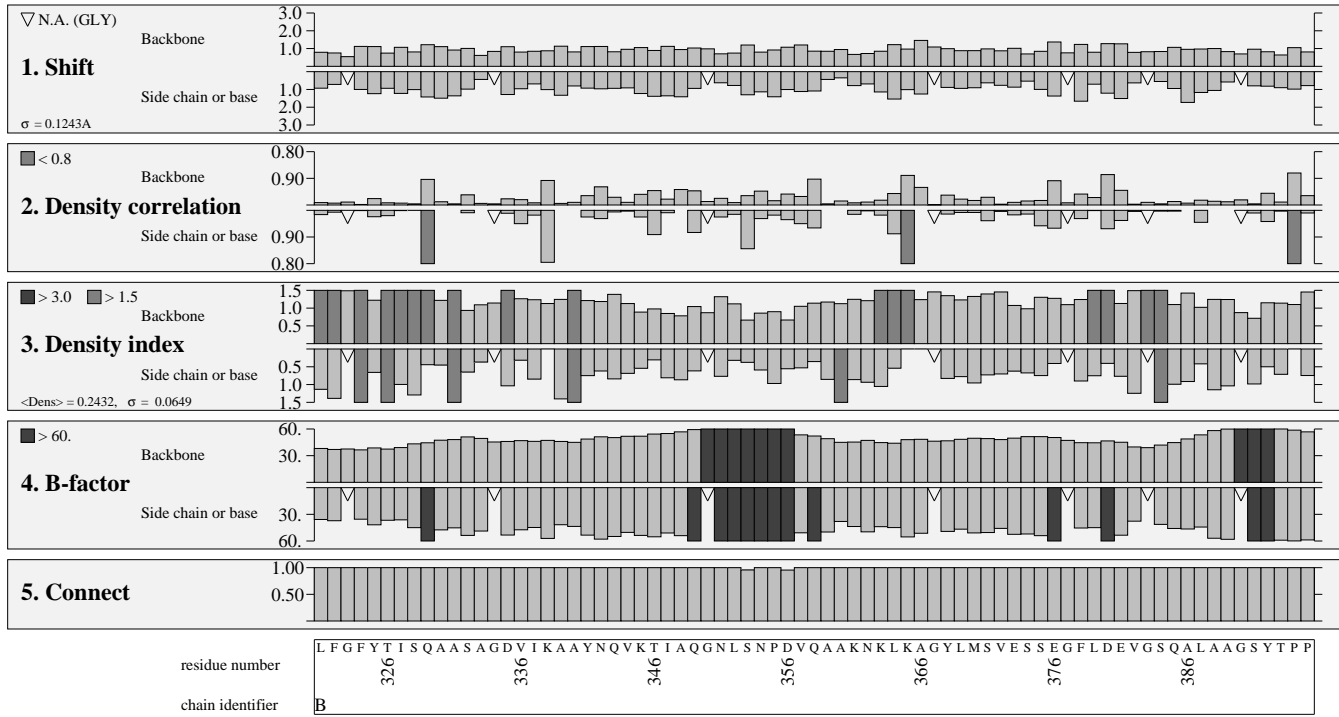
### Local estimation (5)



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### Local estimation (6)

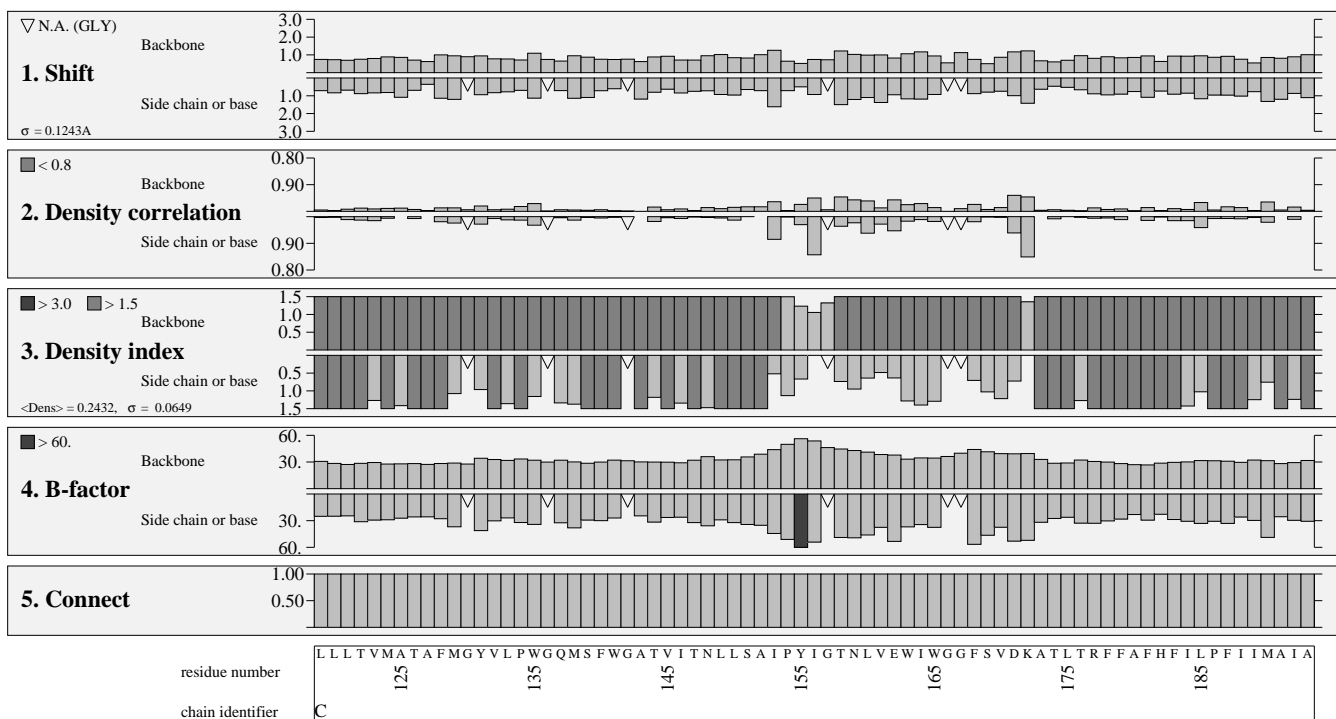
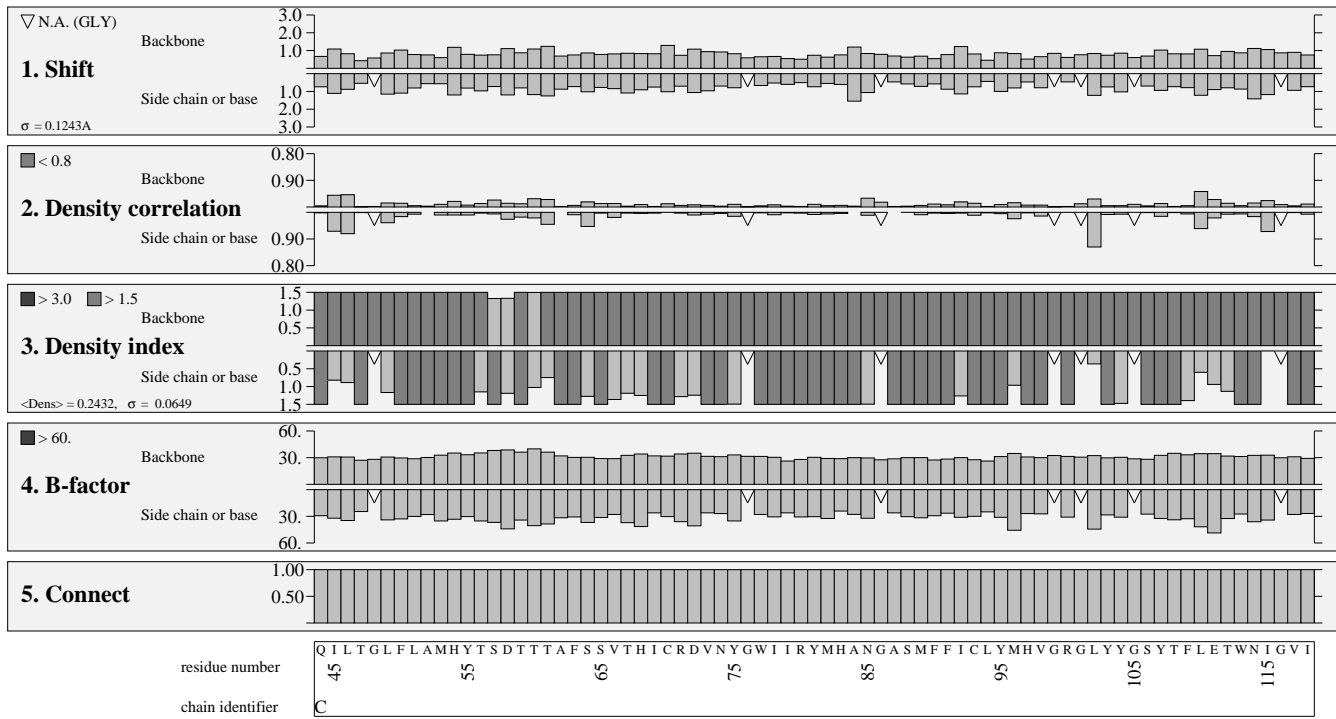




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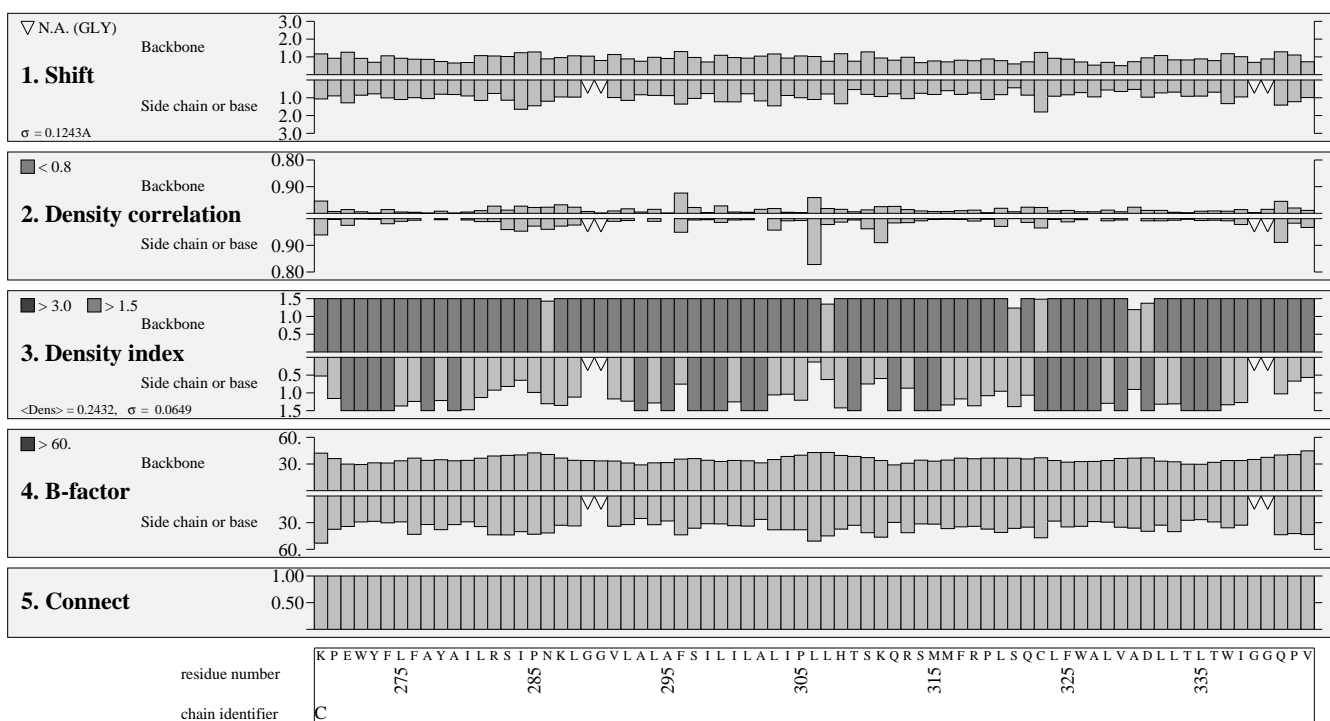
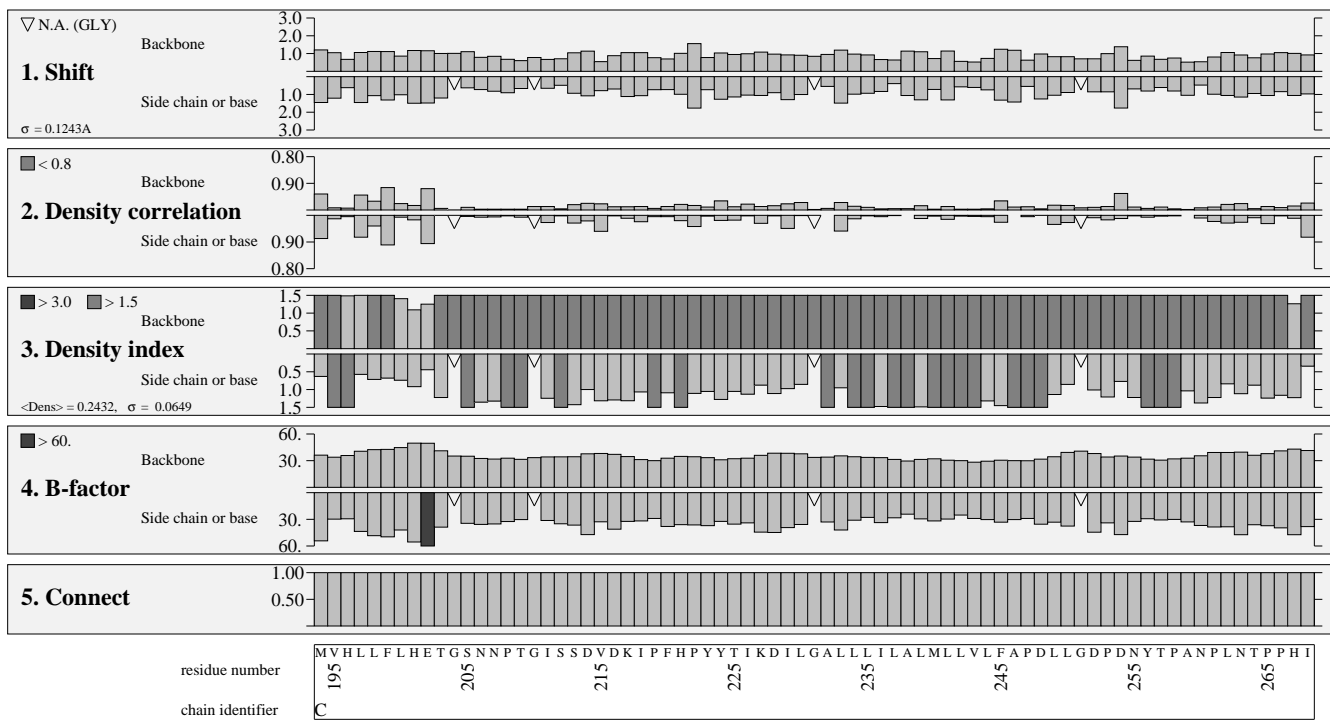
### Local estimation (7)



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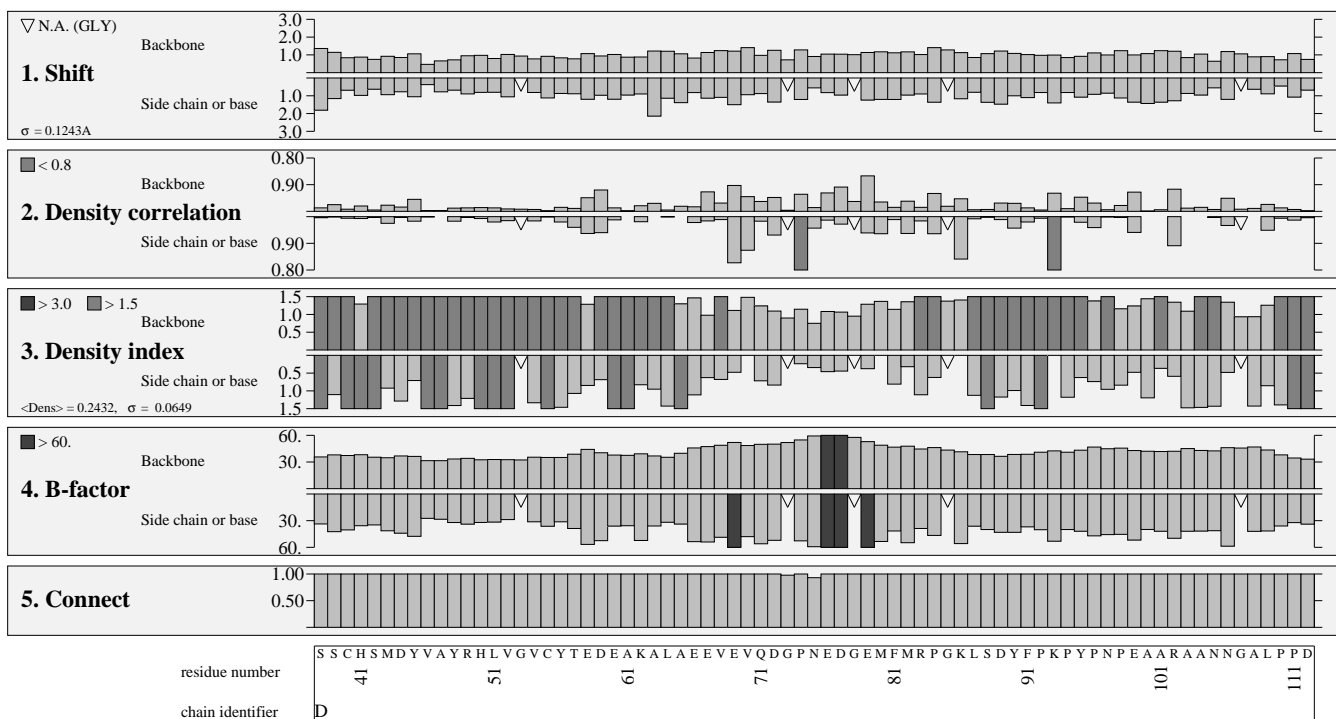
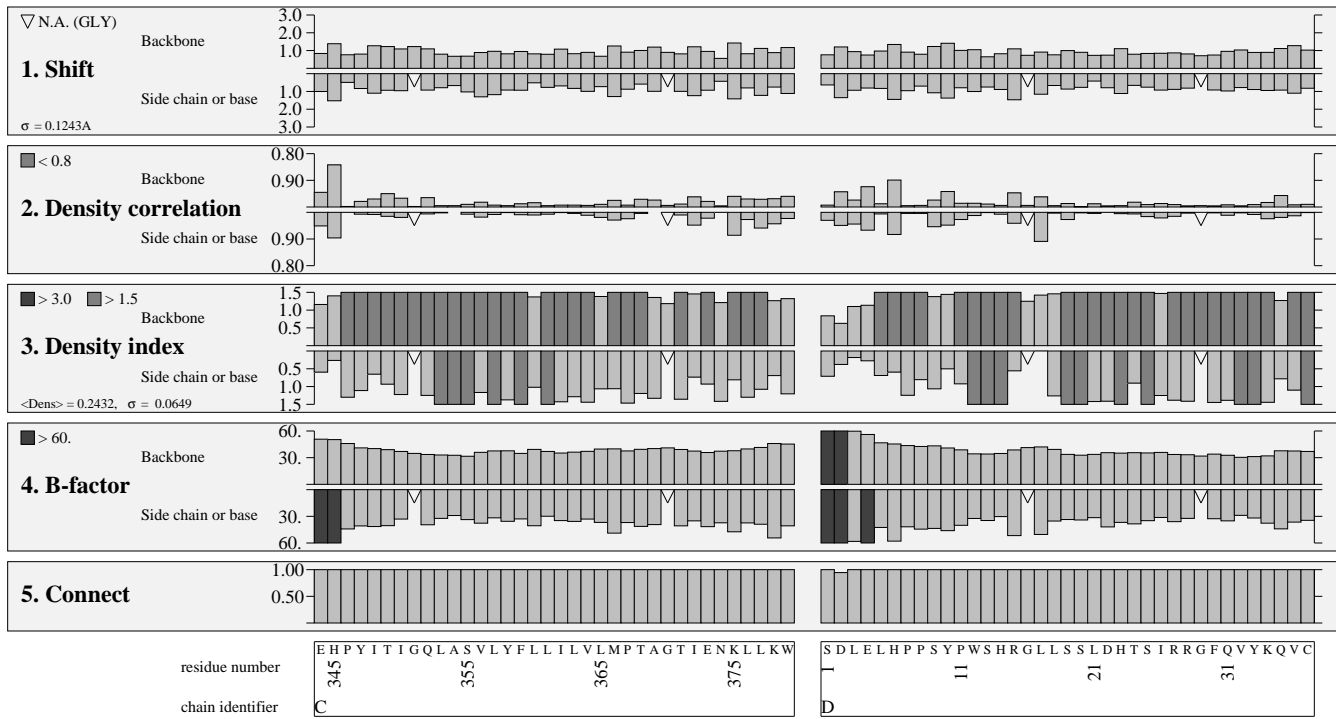
### Local estimation (8)



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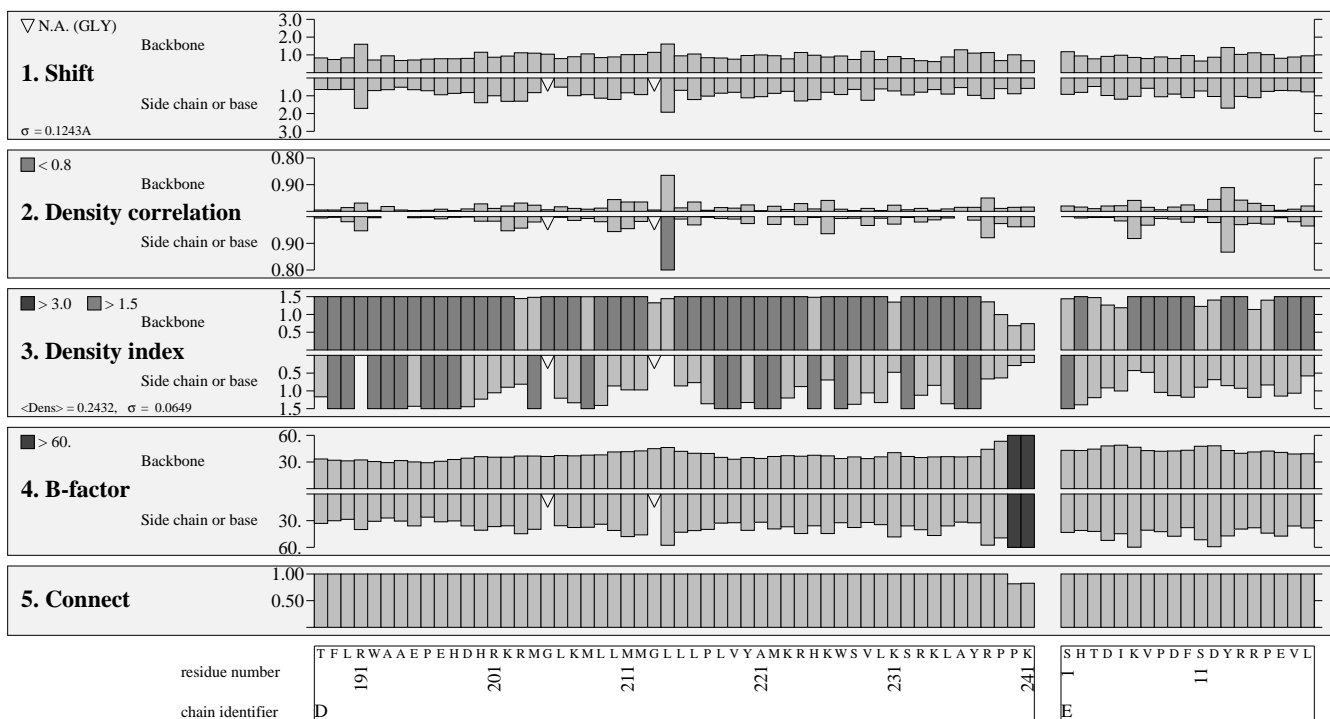
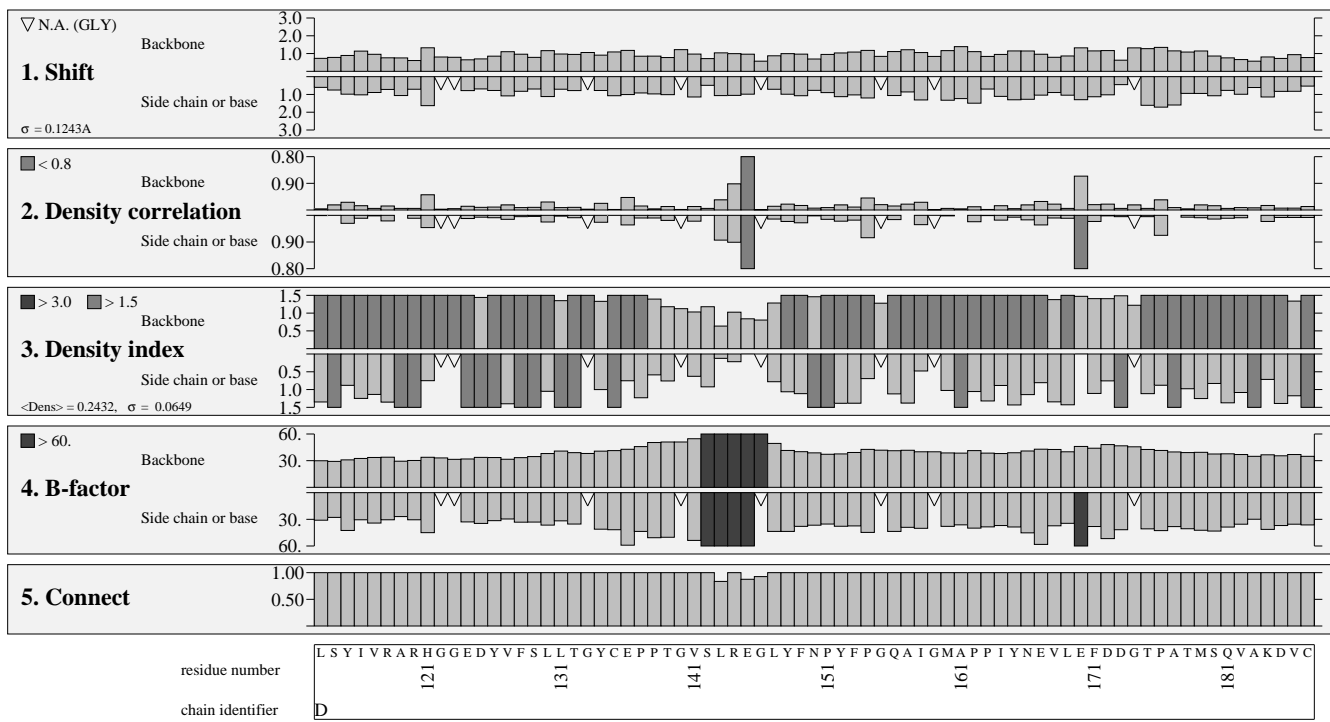
### Local estimation (9)



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### Local estimation (10)





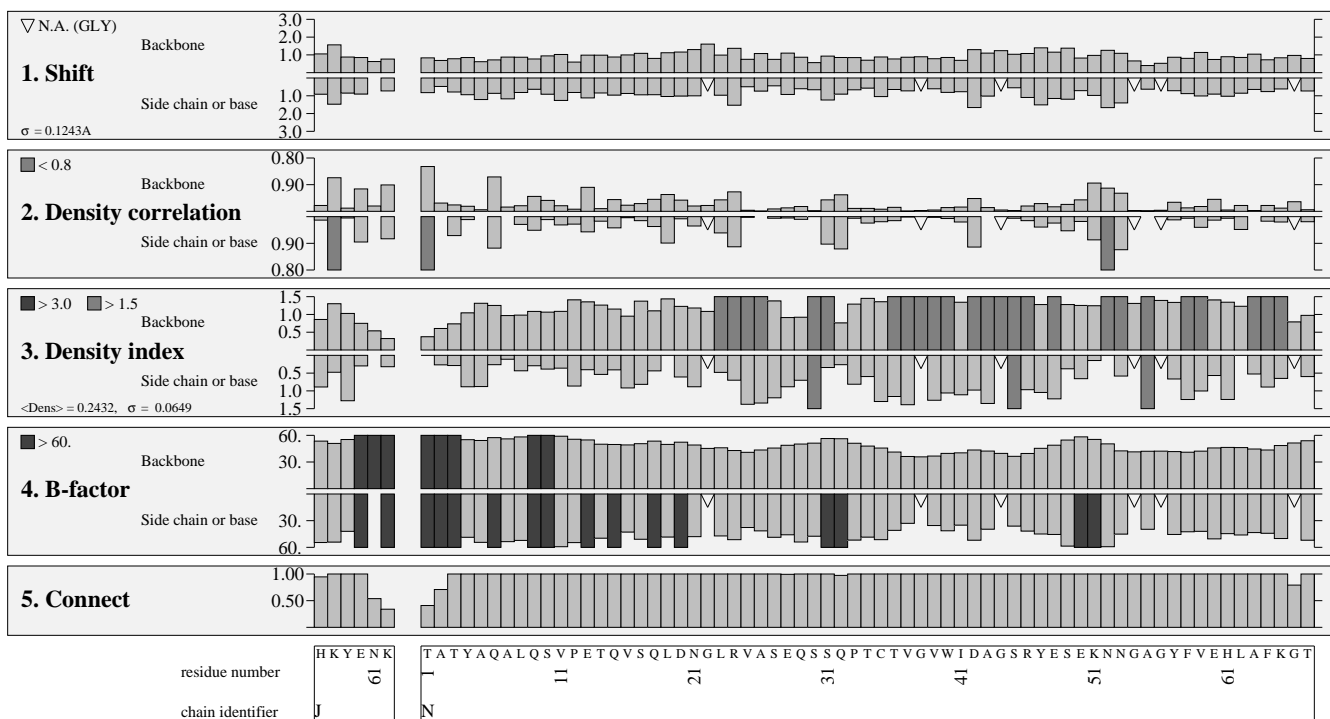
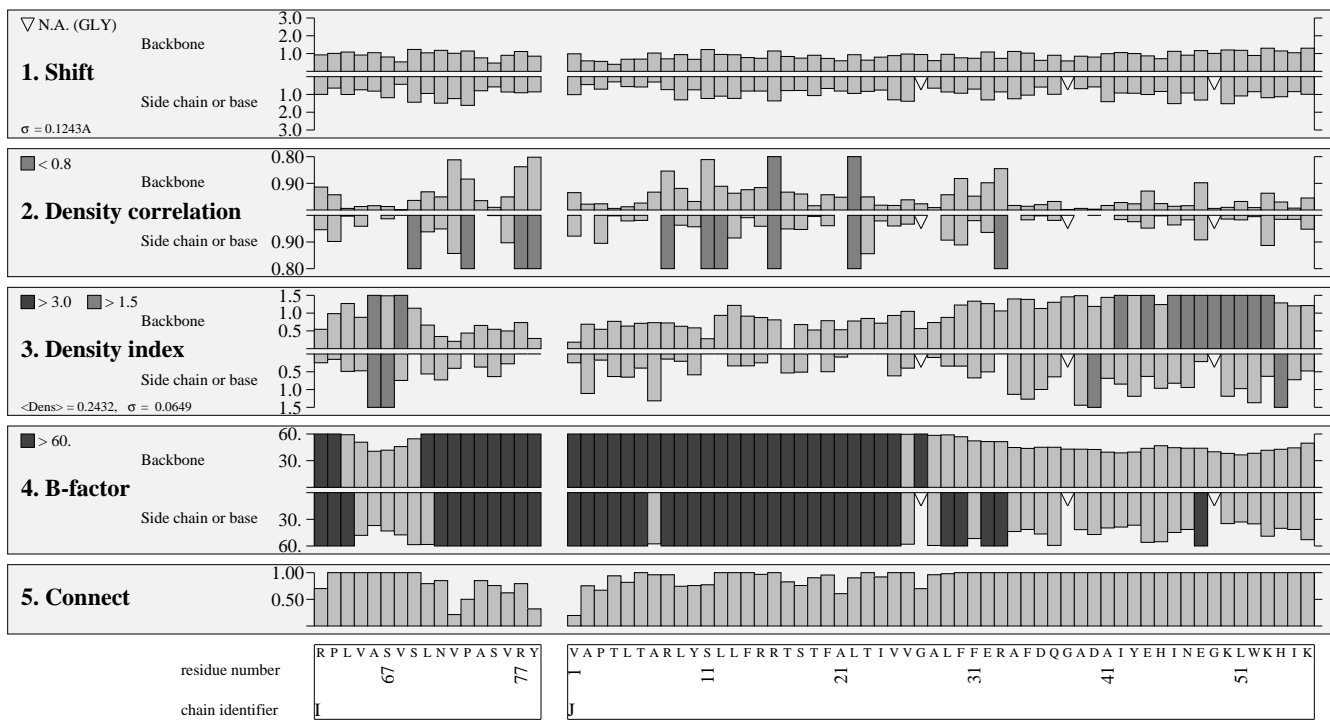




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### Local estimation (14)

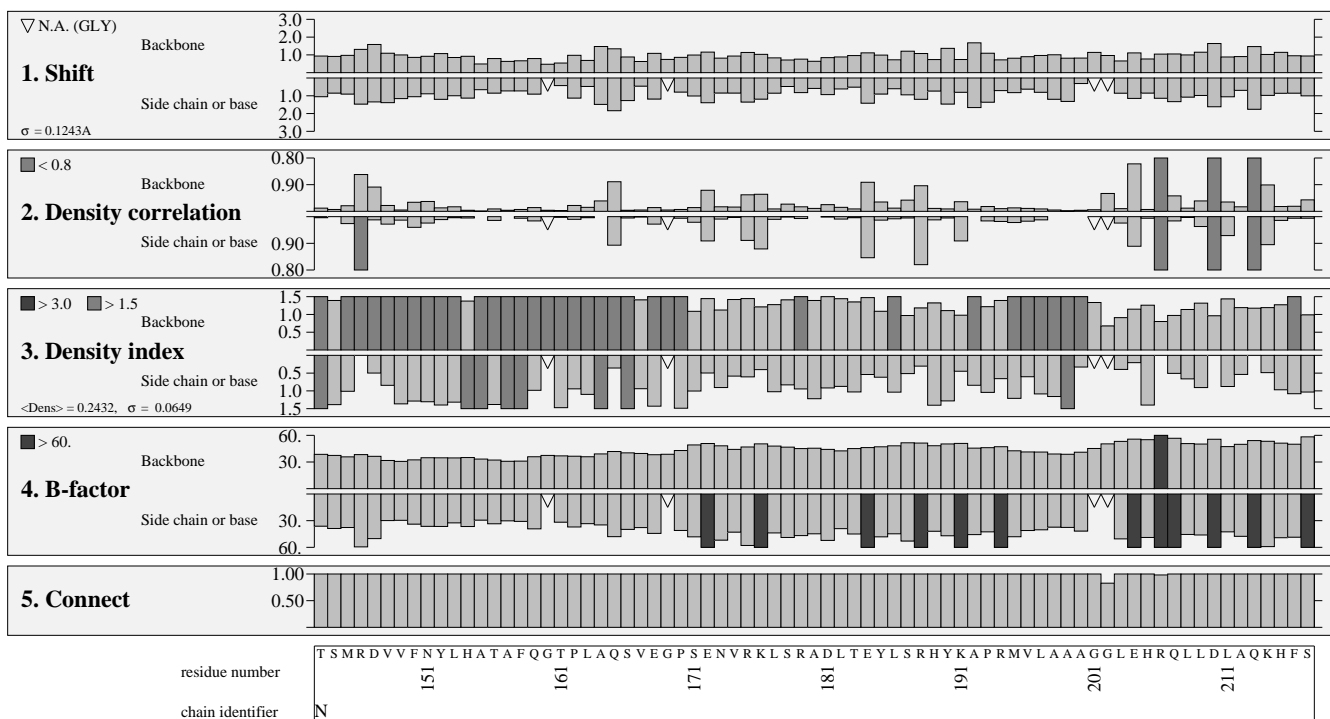
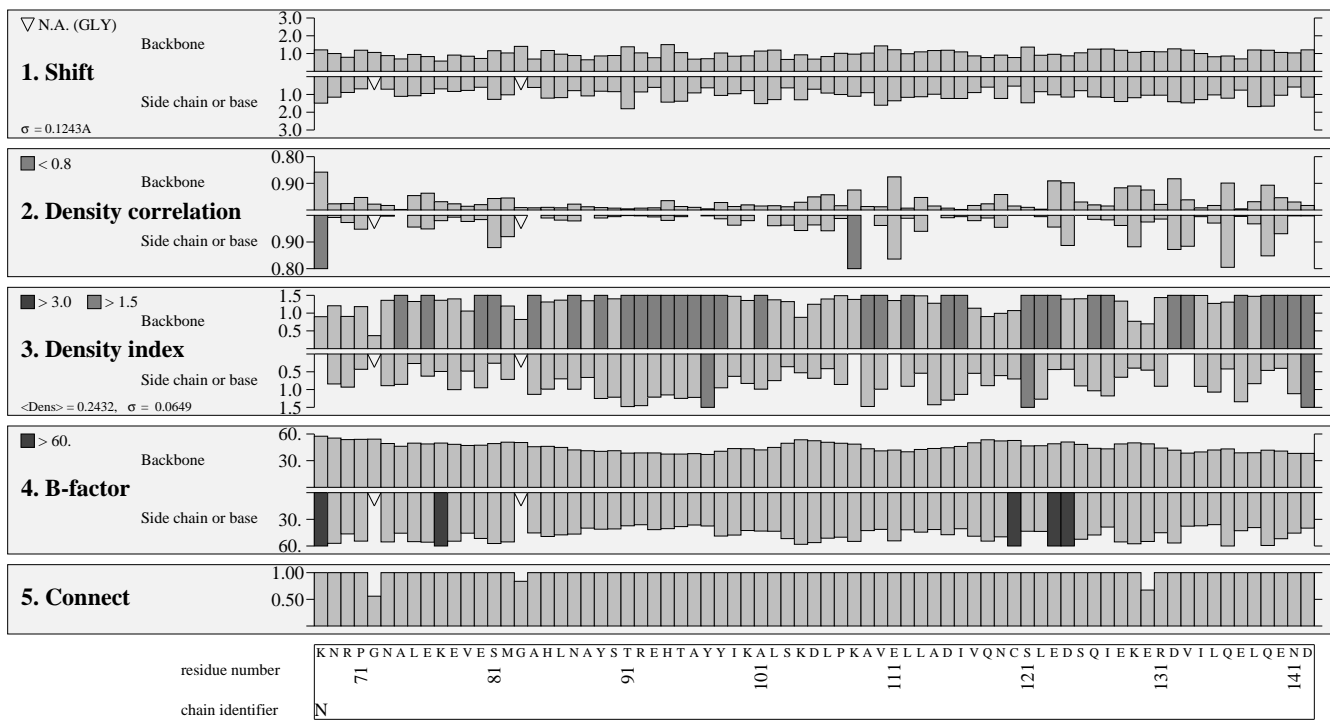




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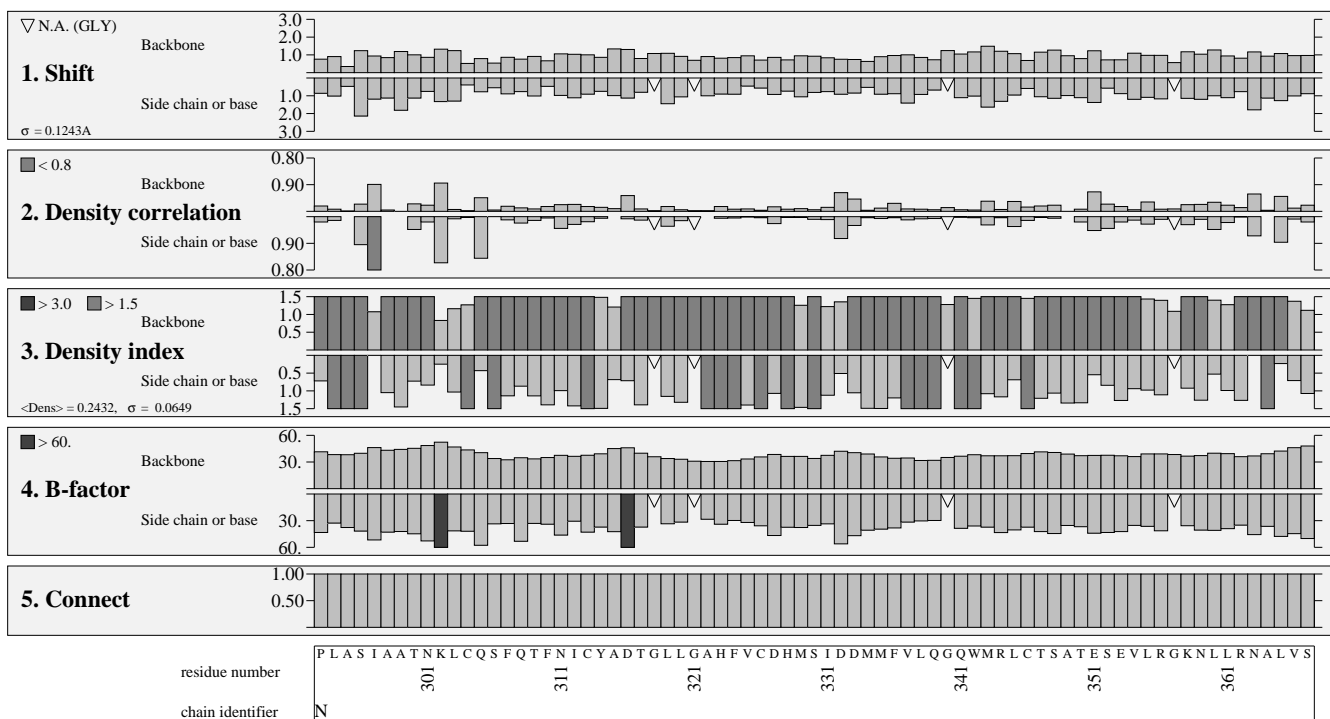
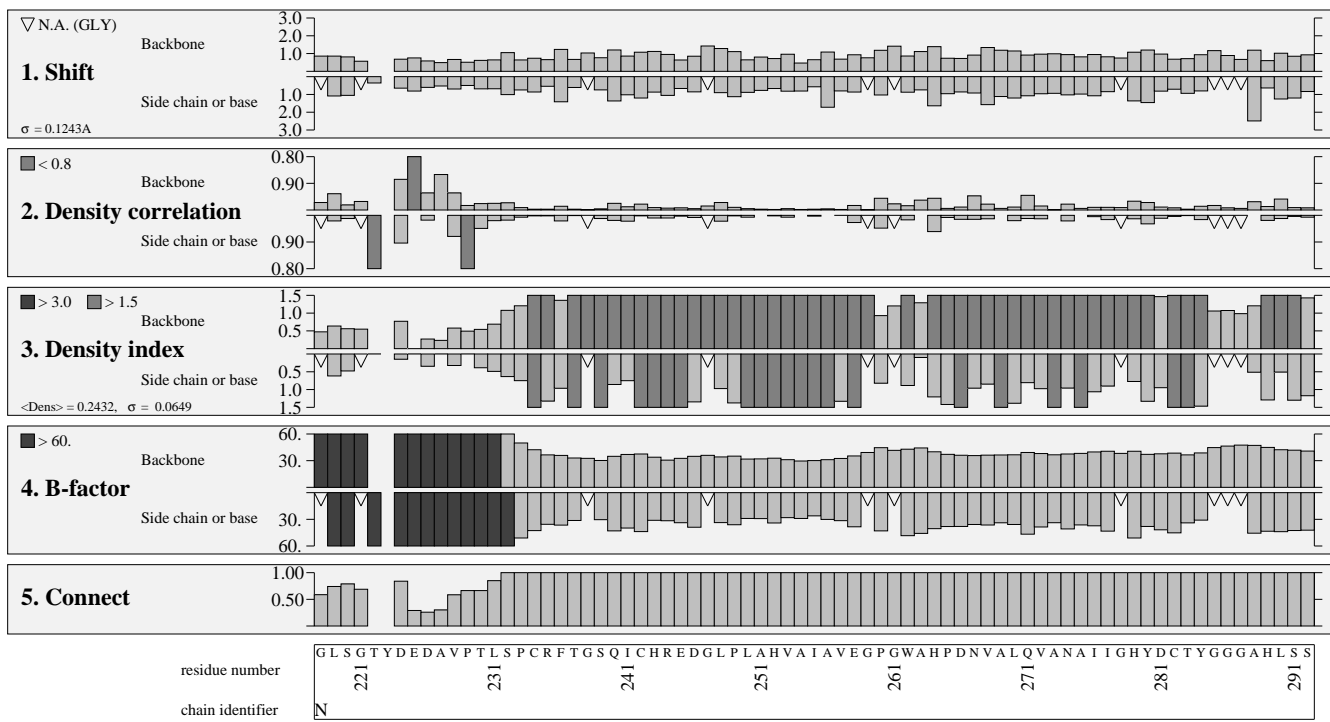
### Local estimation (15)



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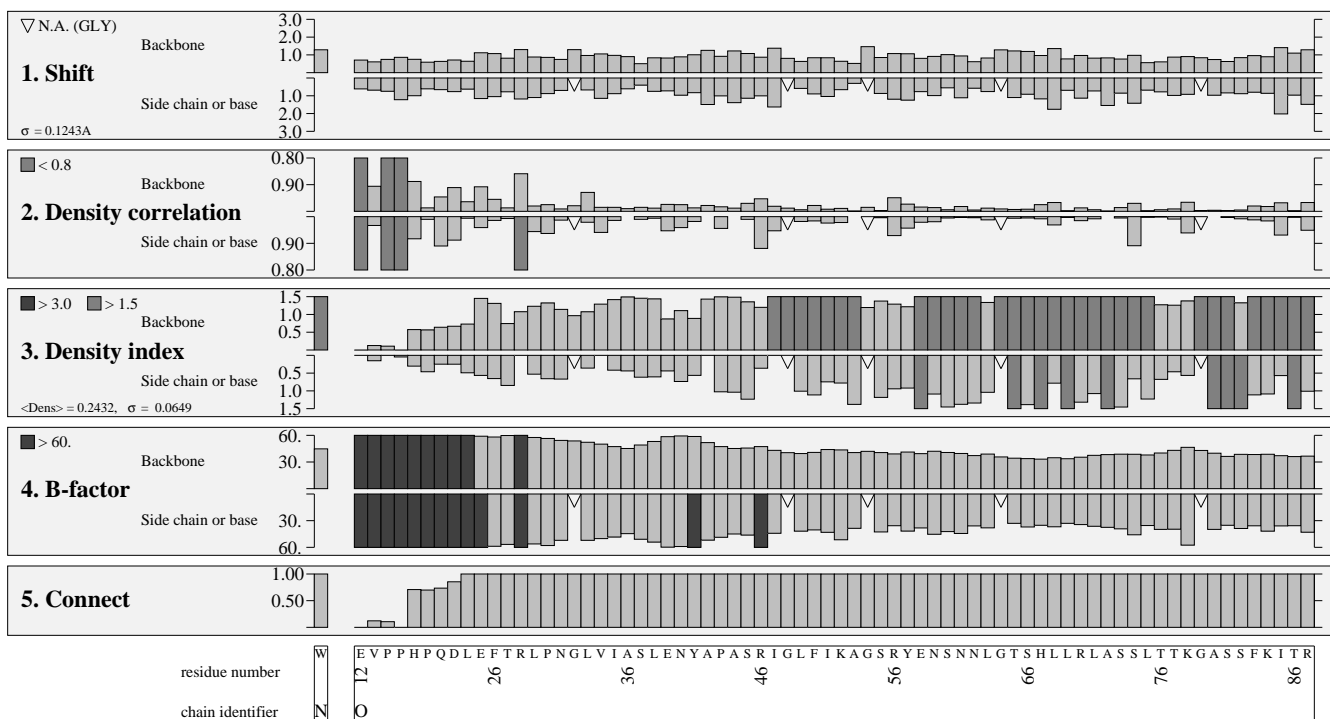
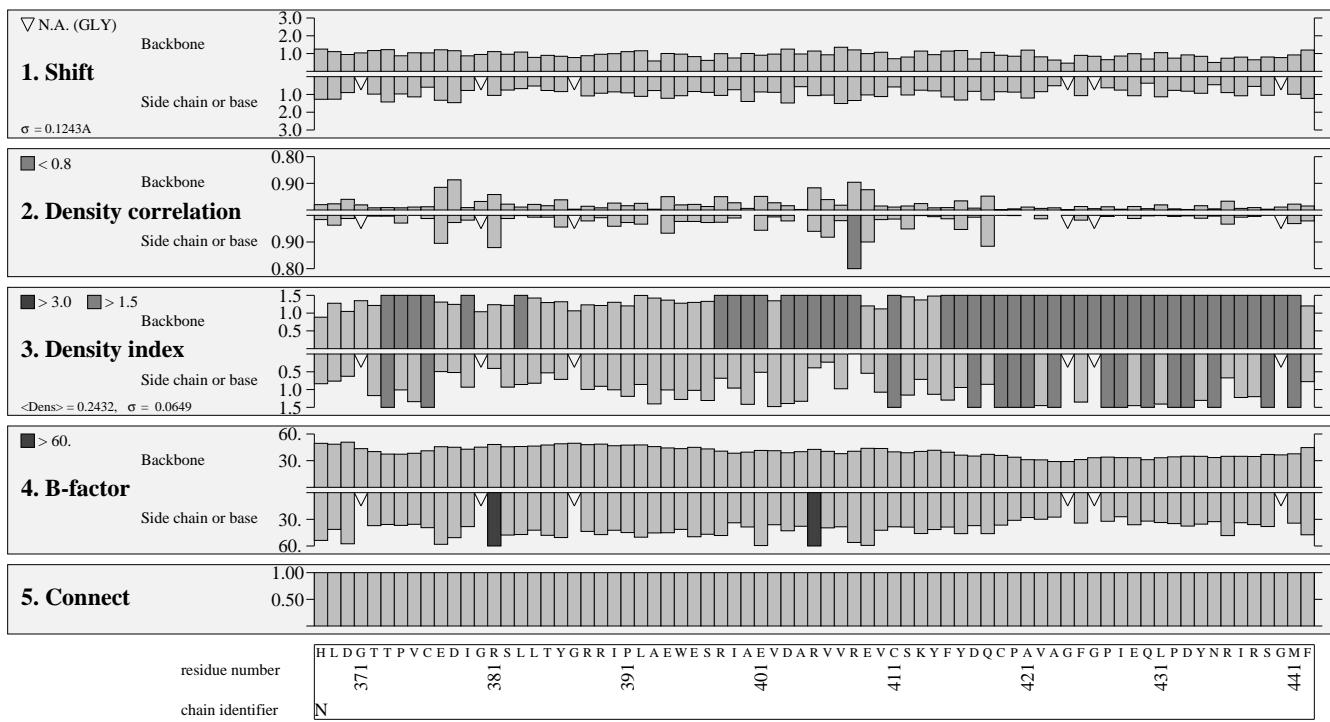
### Local estimation (16)



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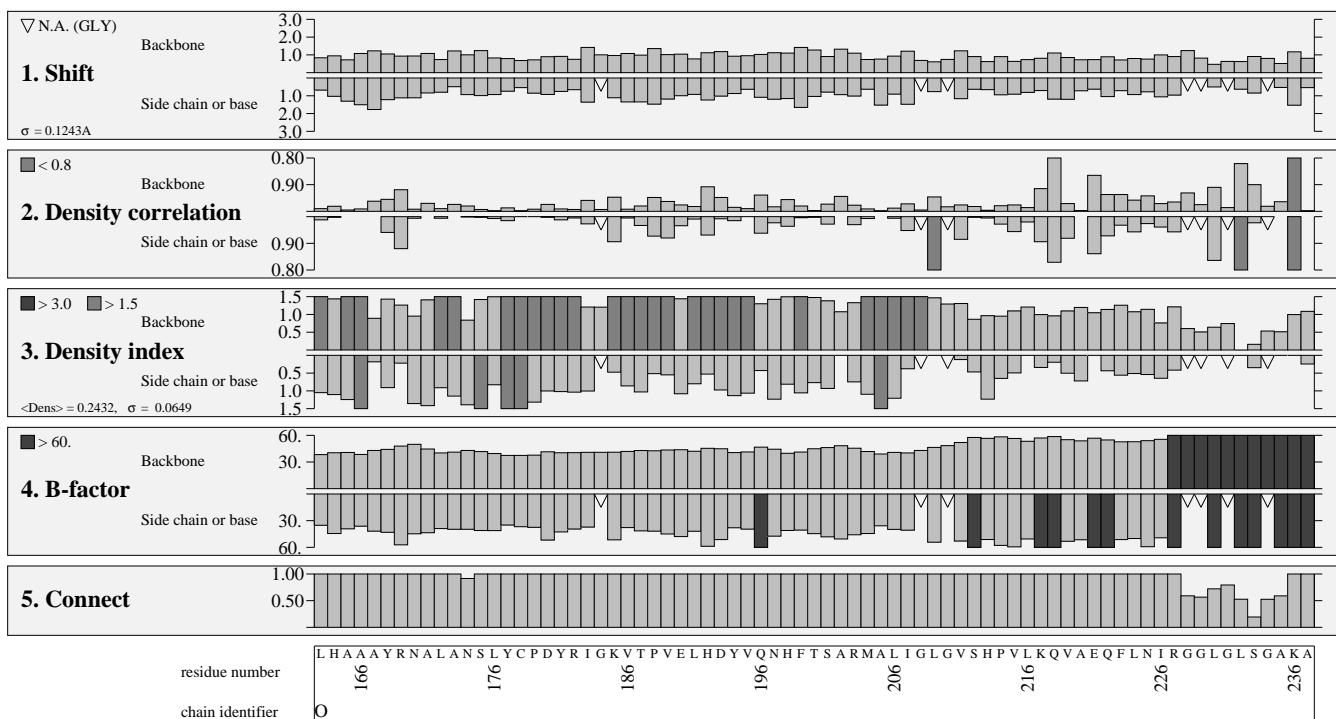
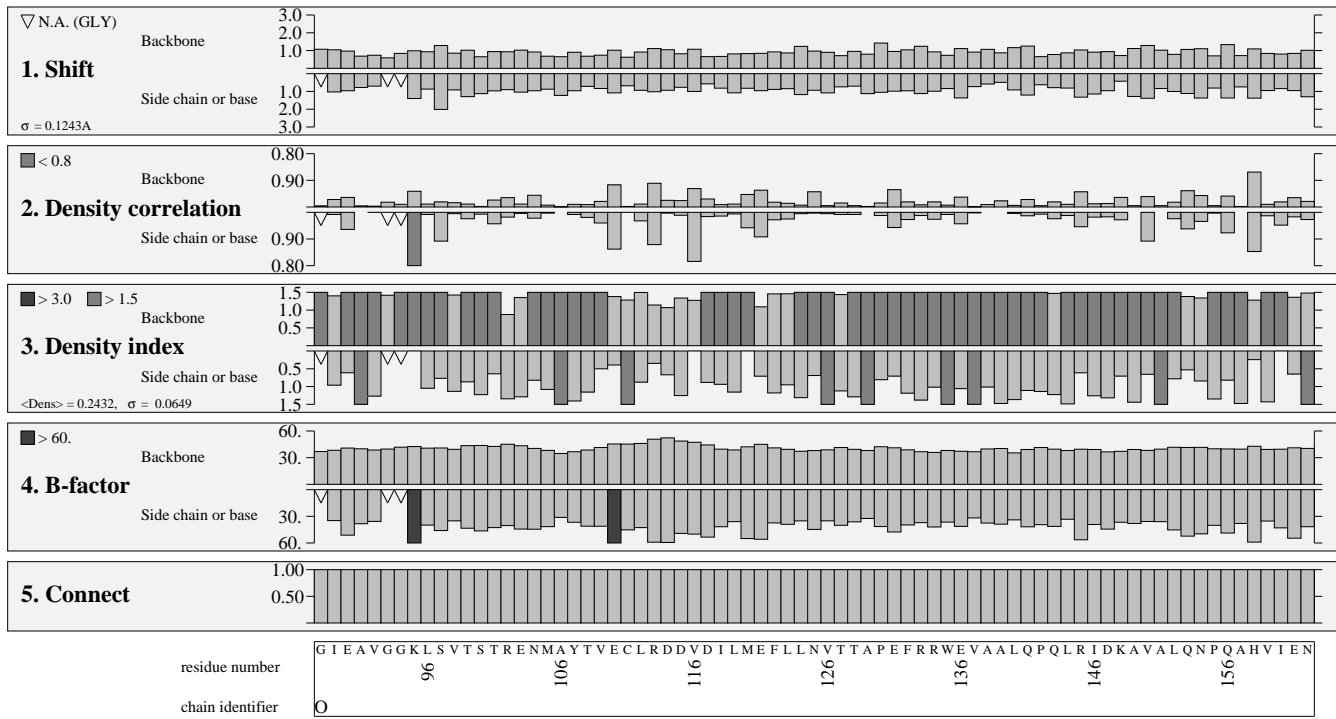
### Local estimation (17)



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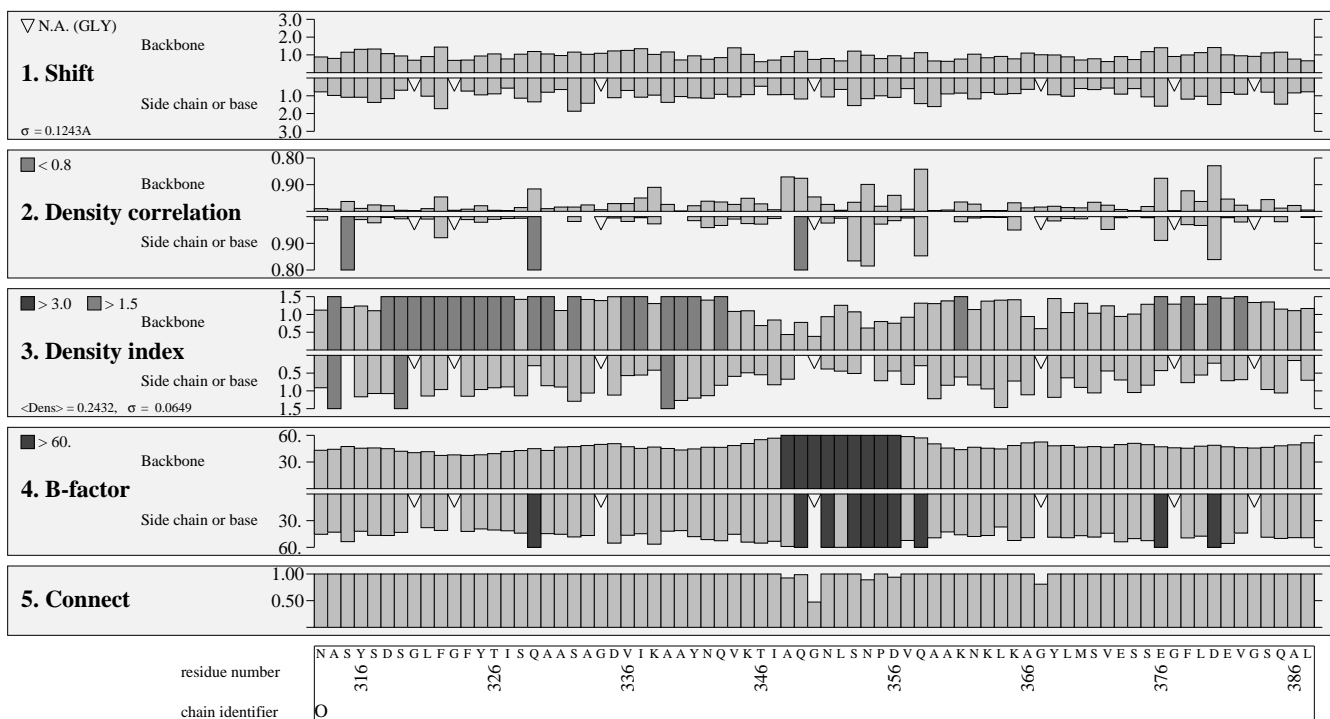
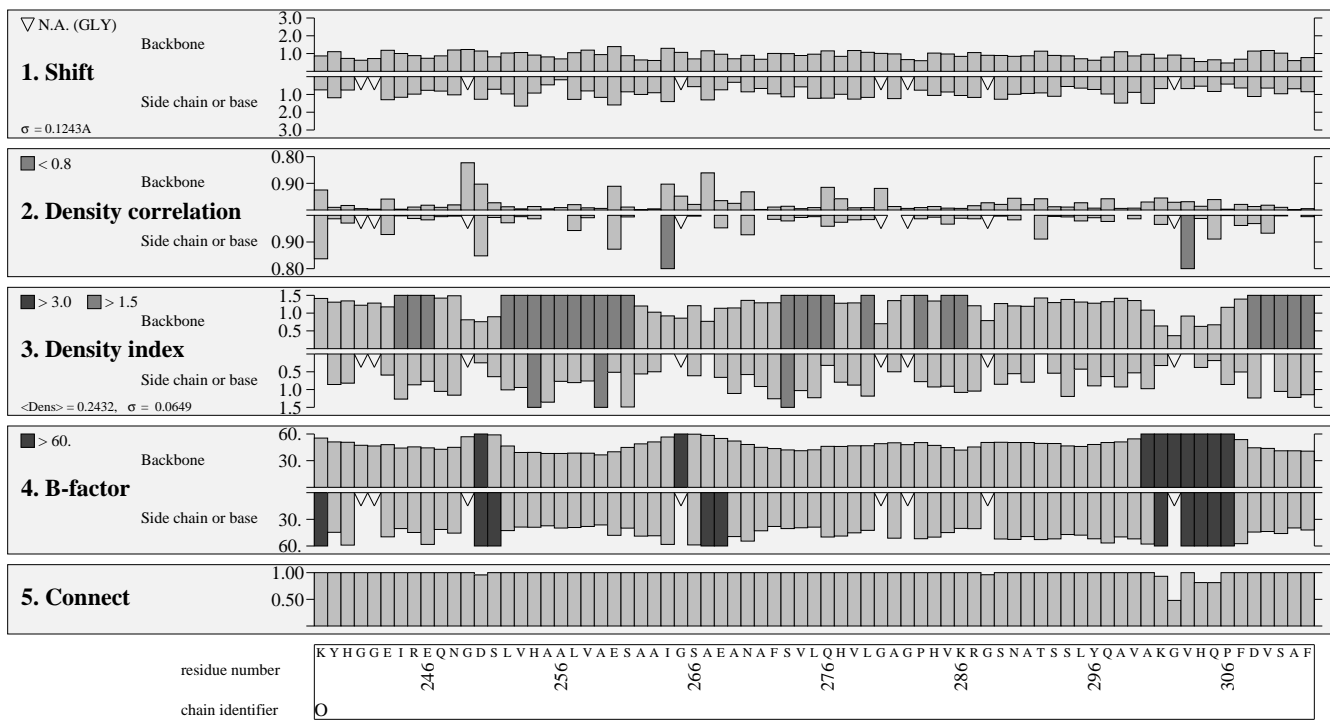
### Local estimation (18)



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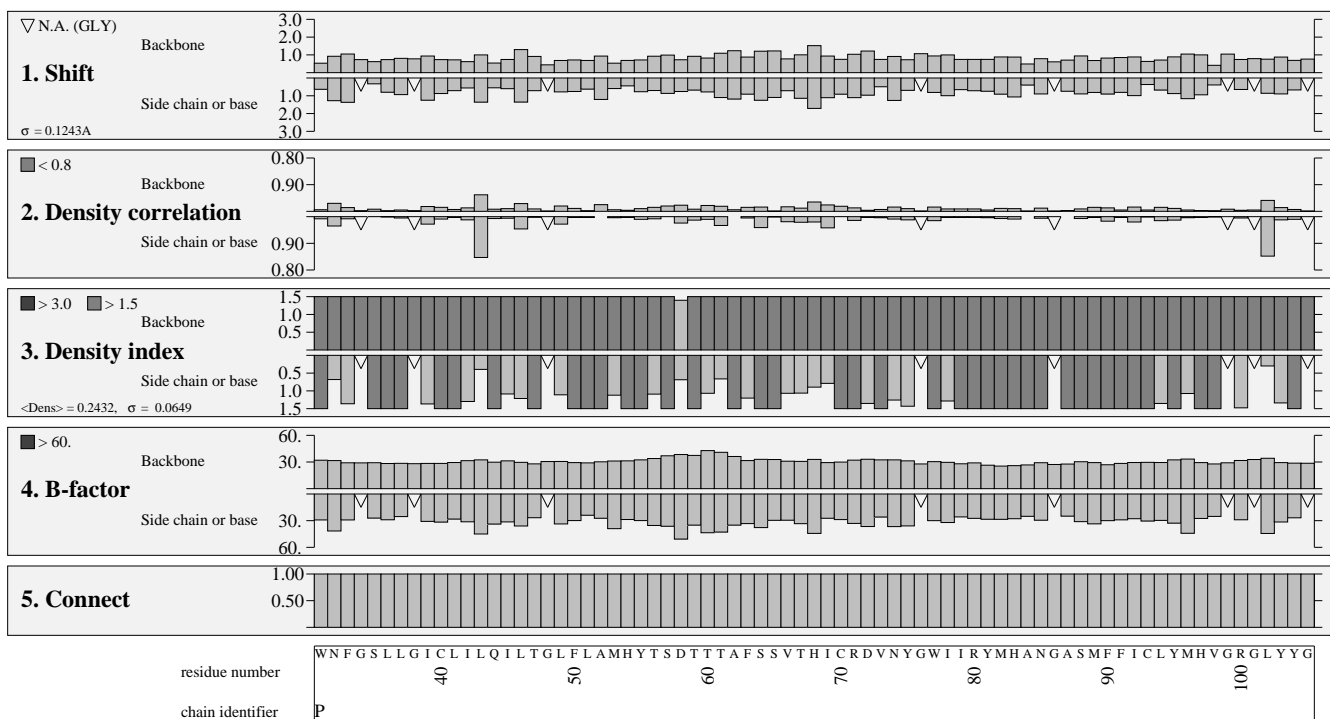
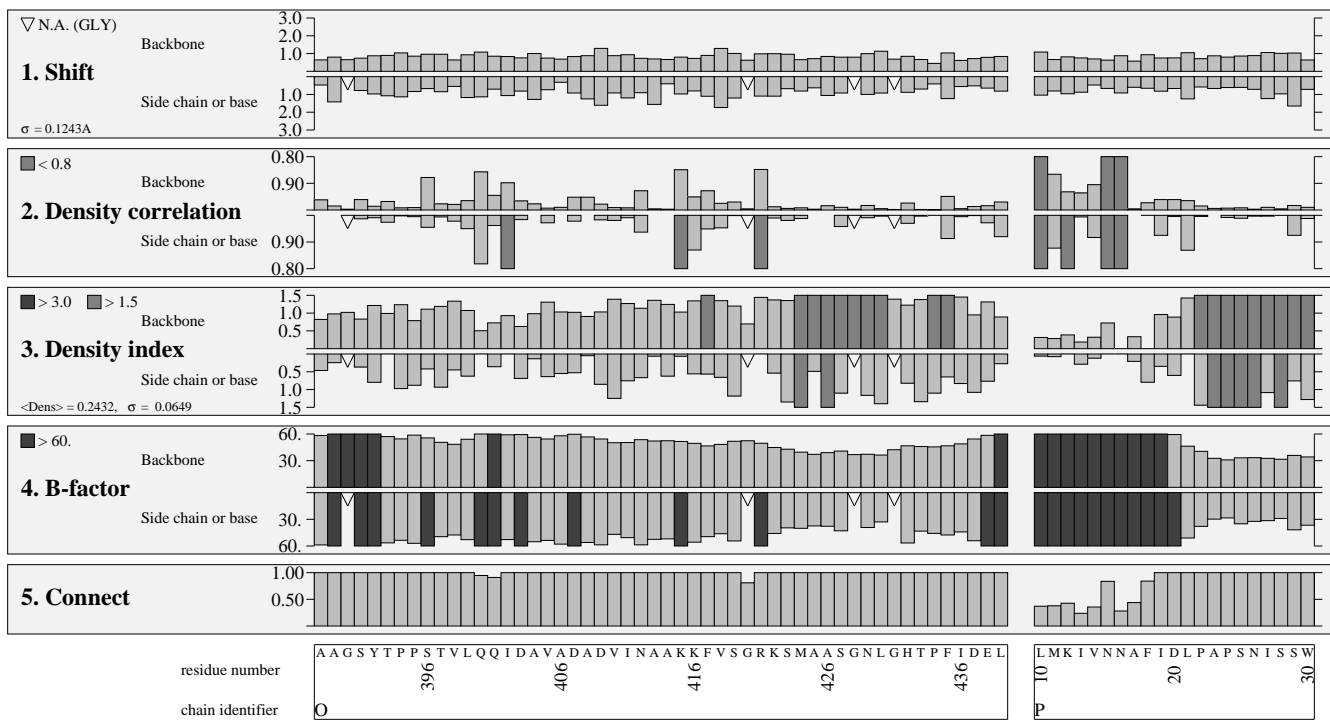
### Local estimation (19)



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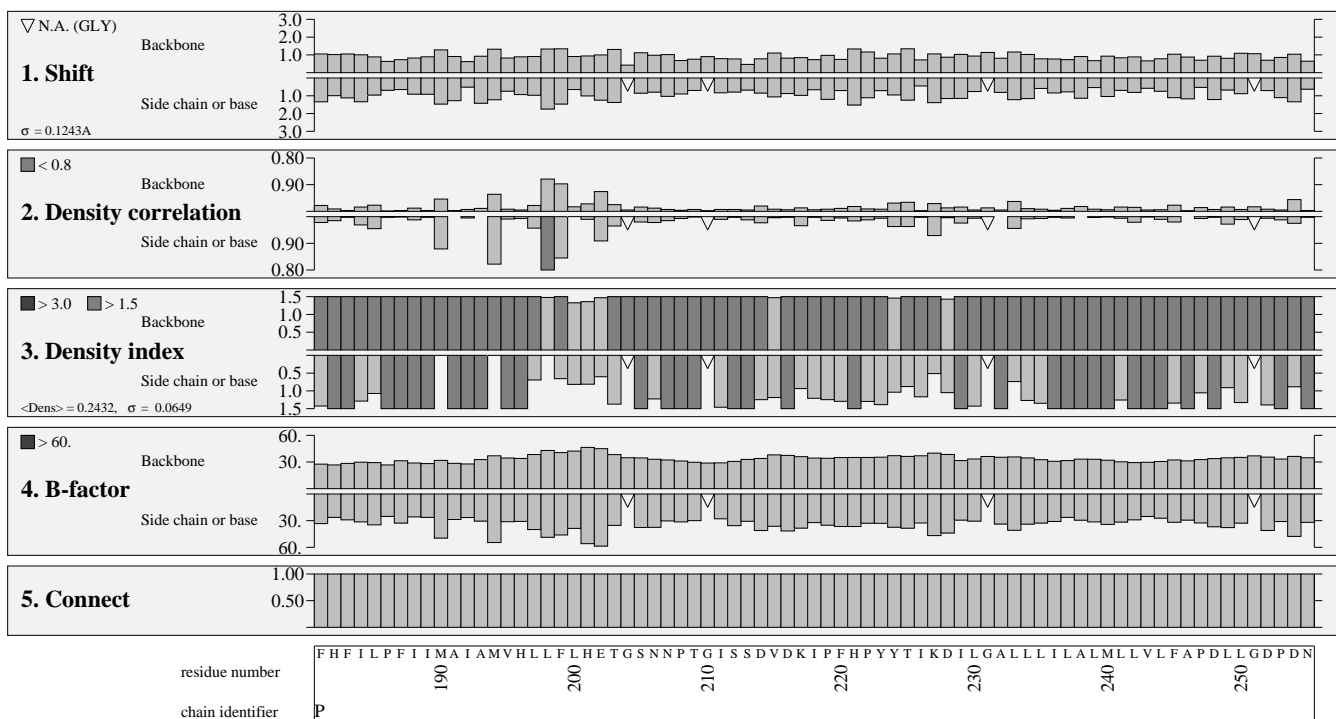
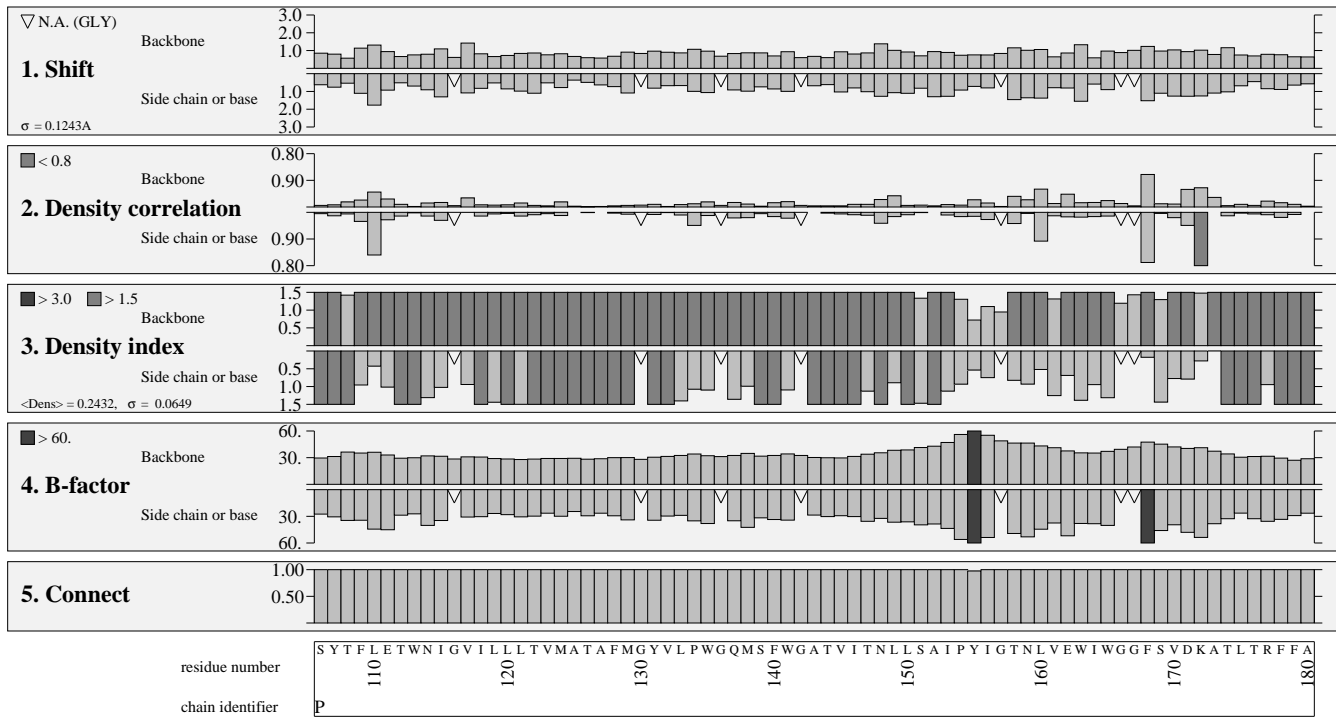
### Local estimation (20)



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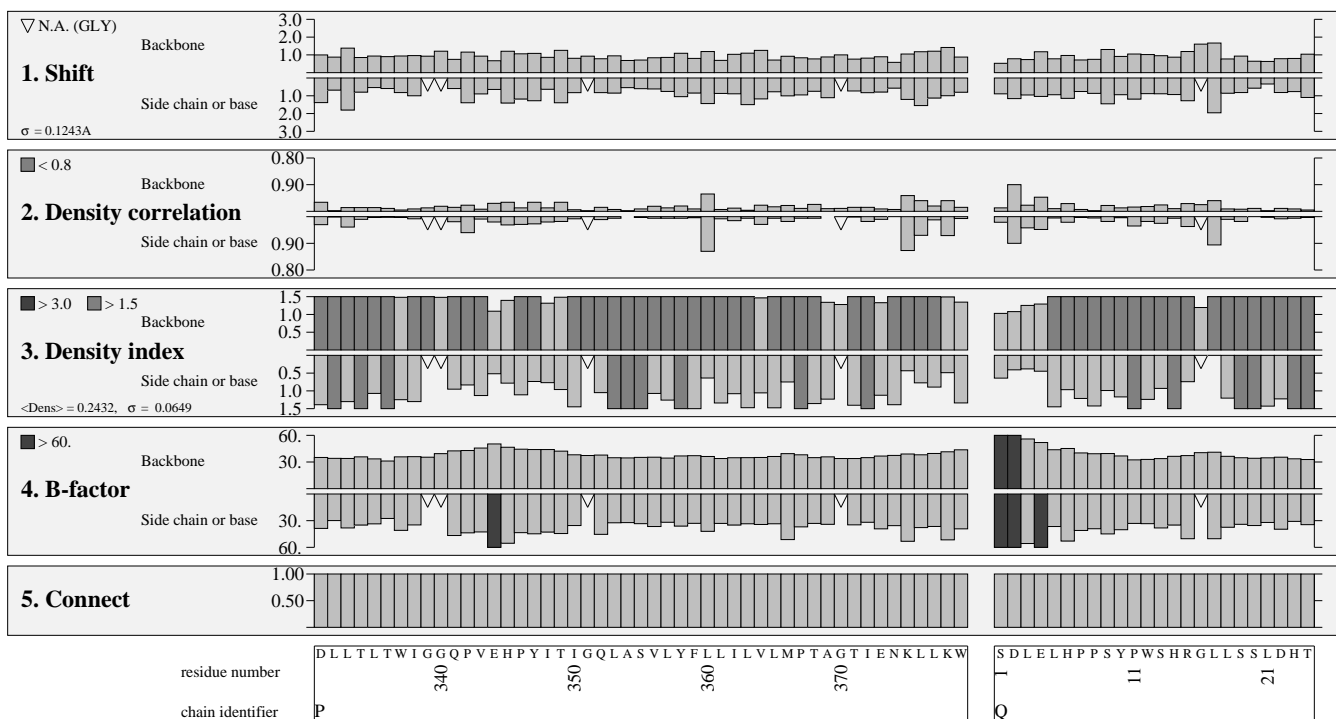
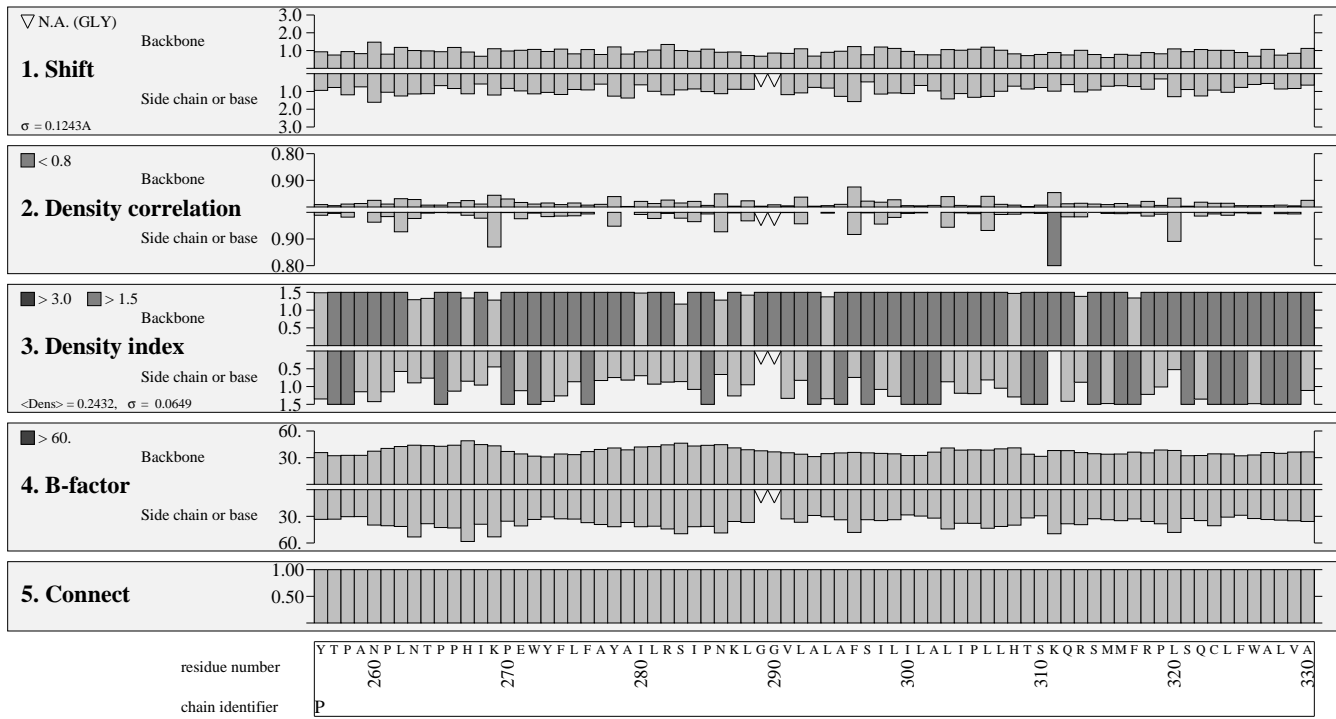
### Local estimation (21)



# Structure Factor Check

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### Local estimation (22)

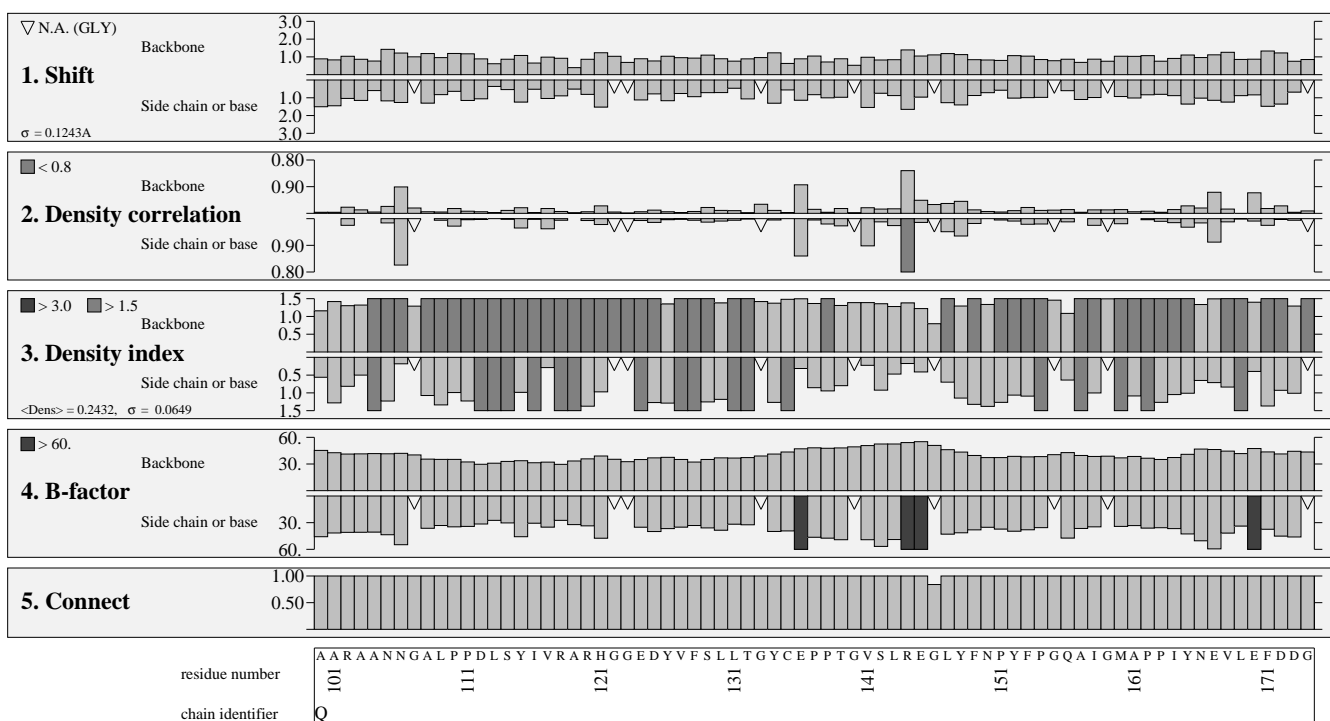
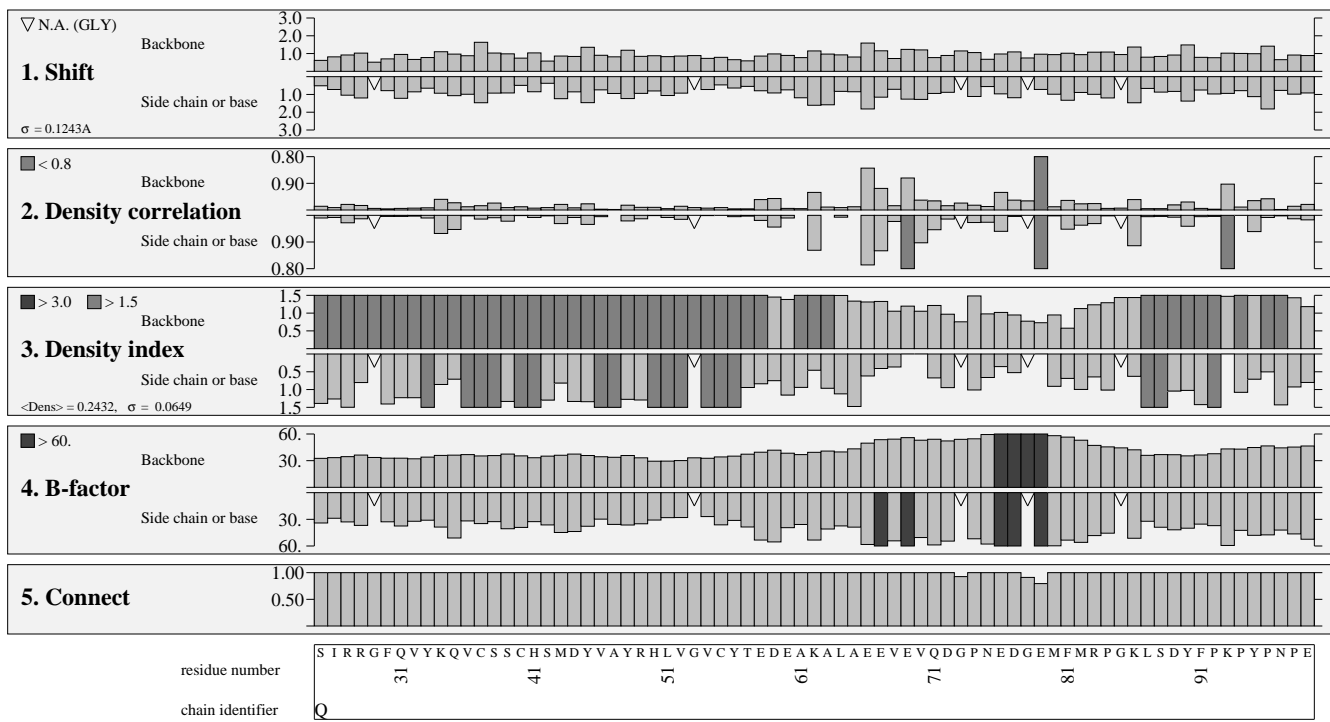




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### Local estimation (23)

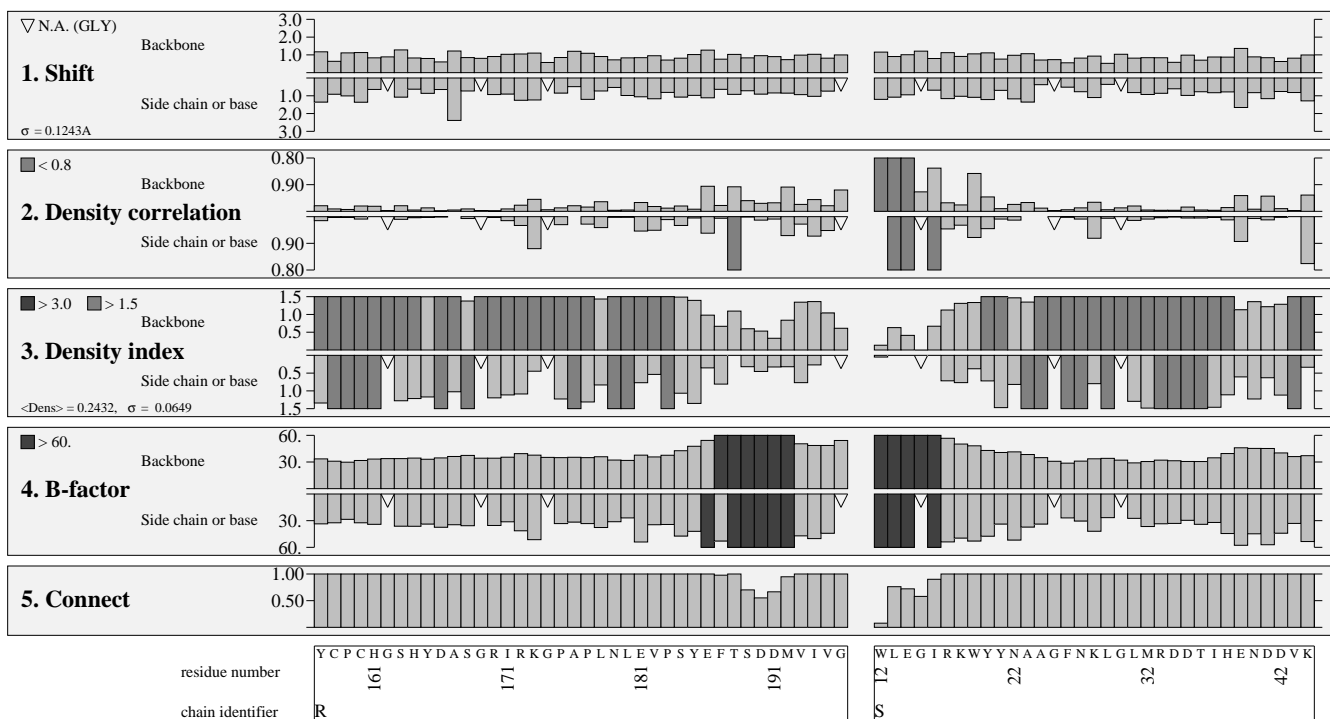
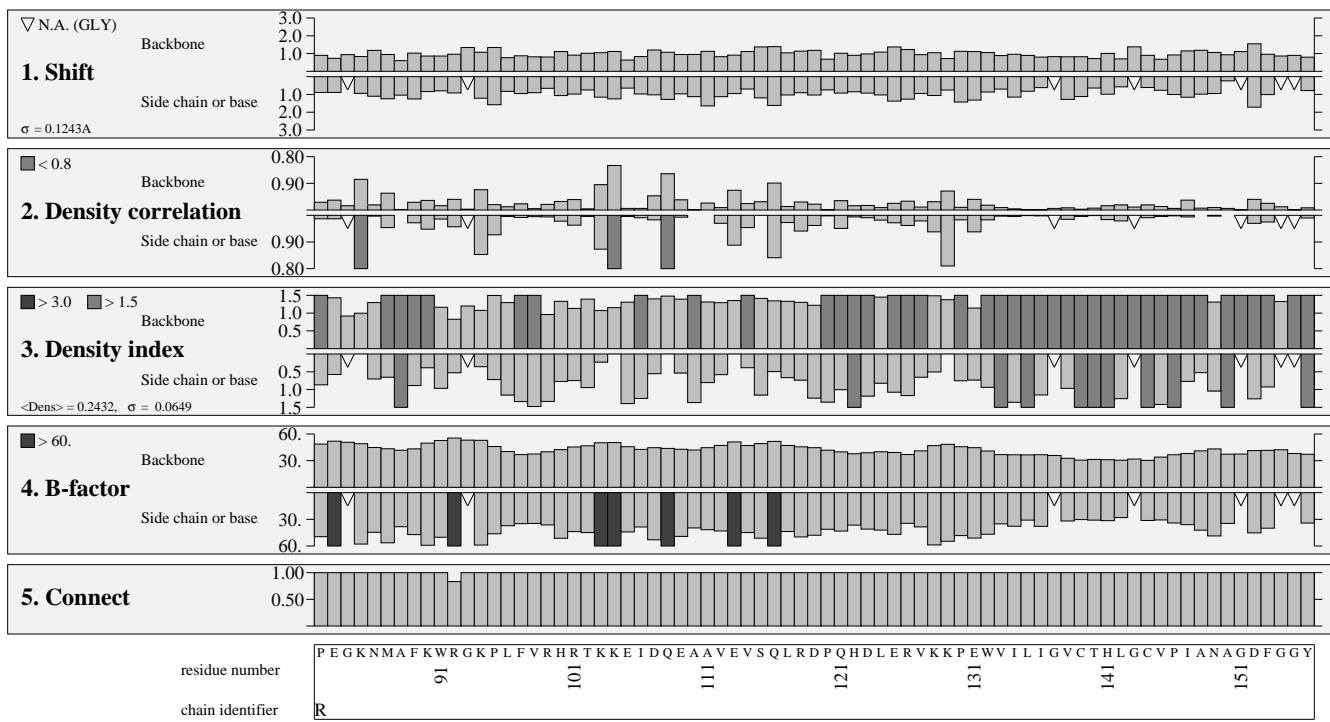




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### Local estimation (25)

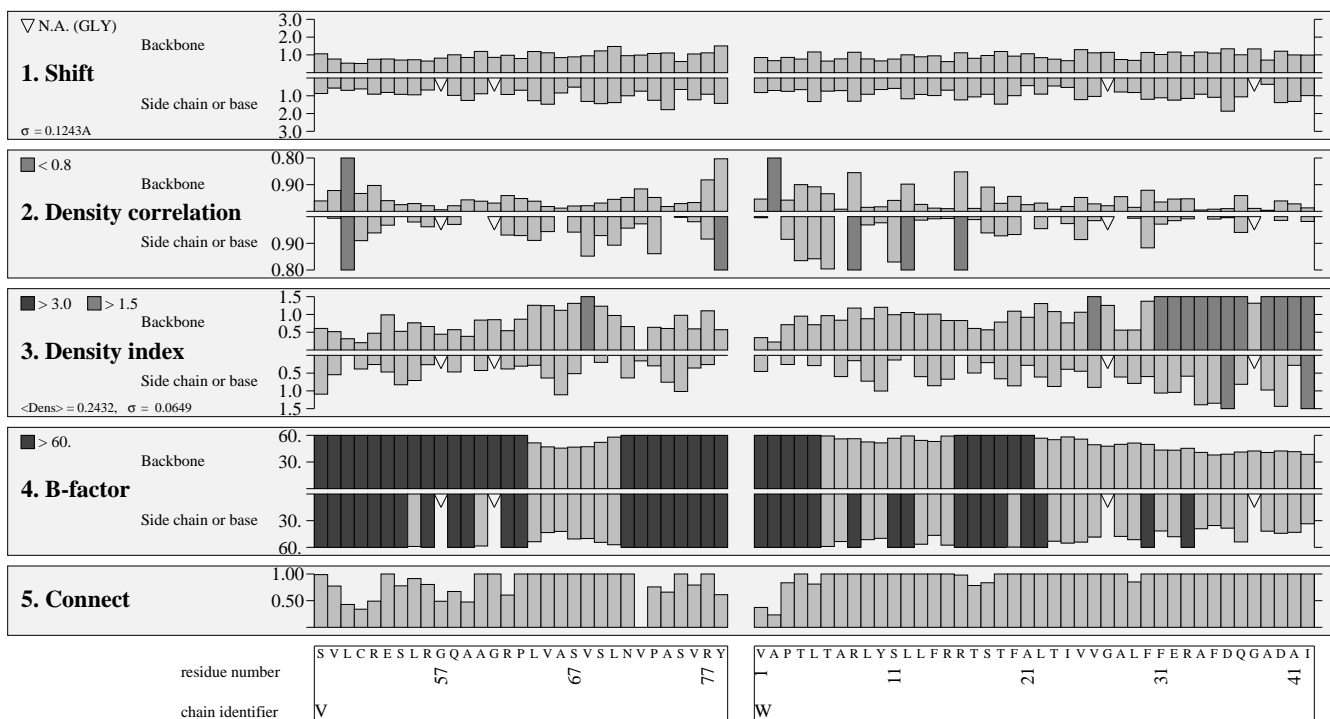
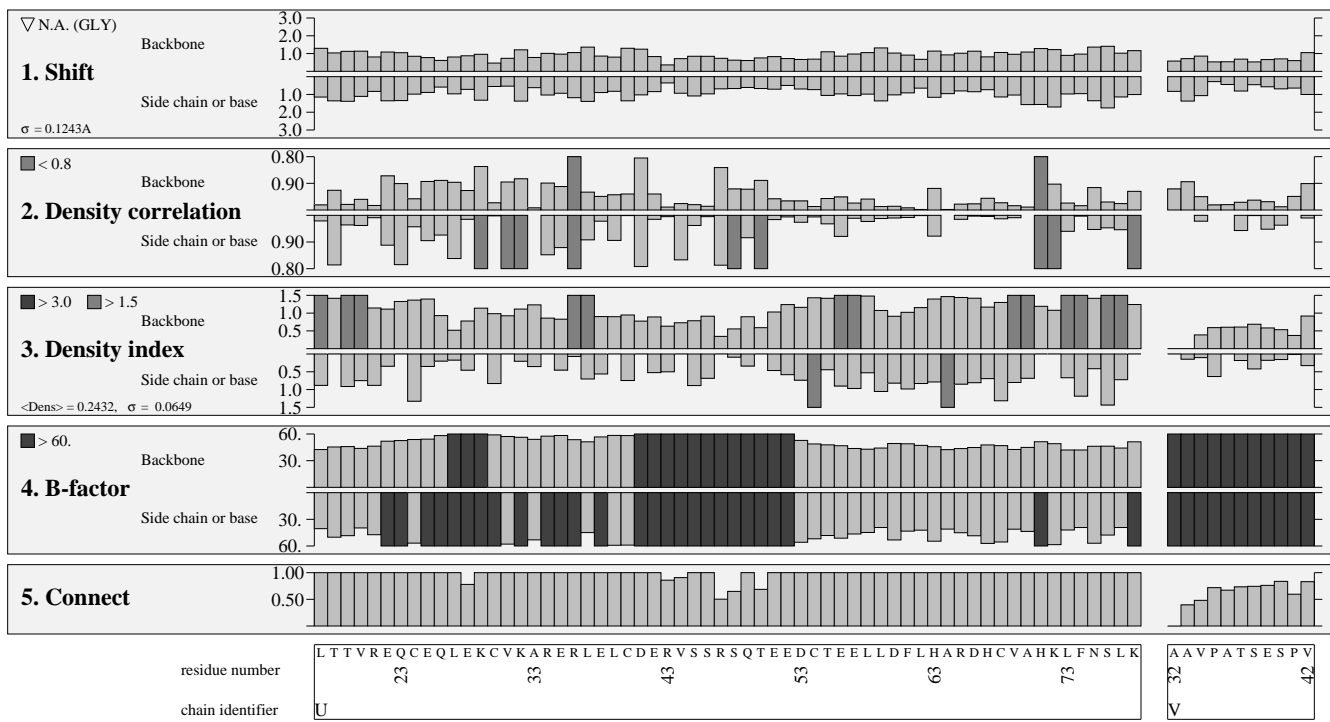




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### Local estimation (27)







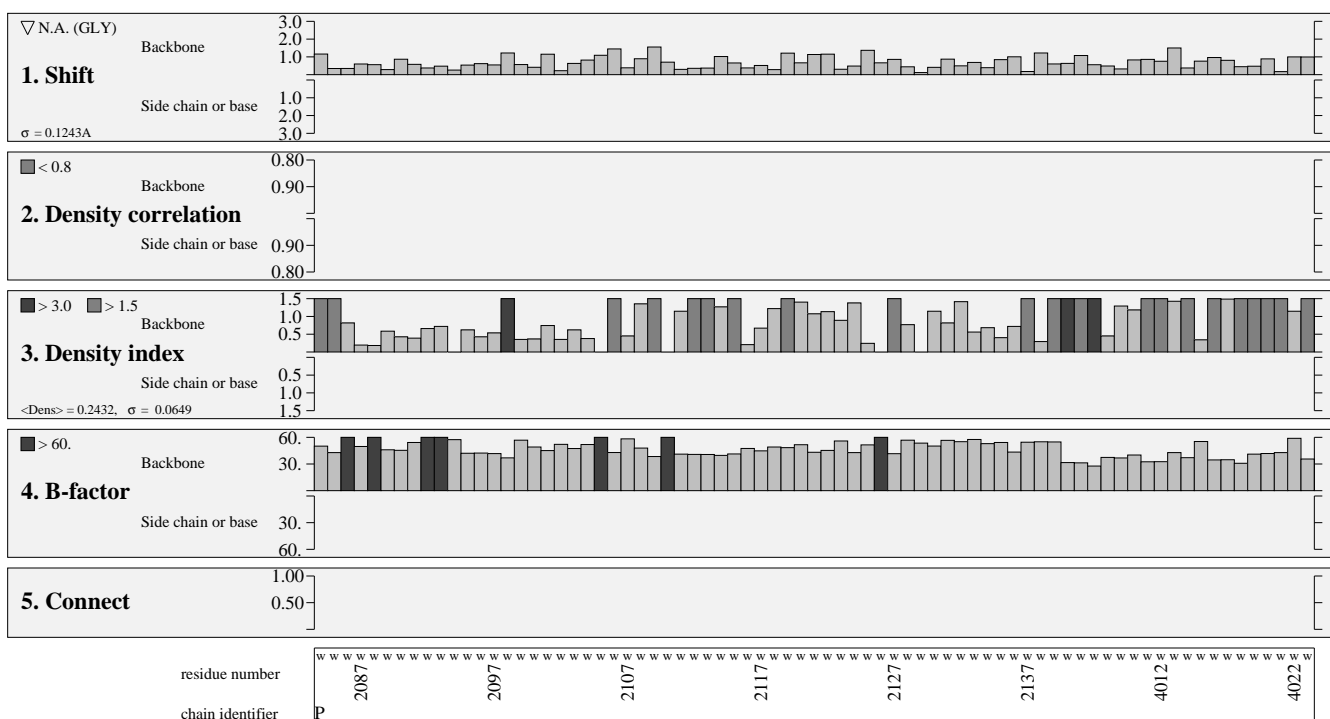
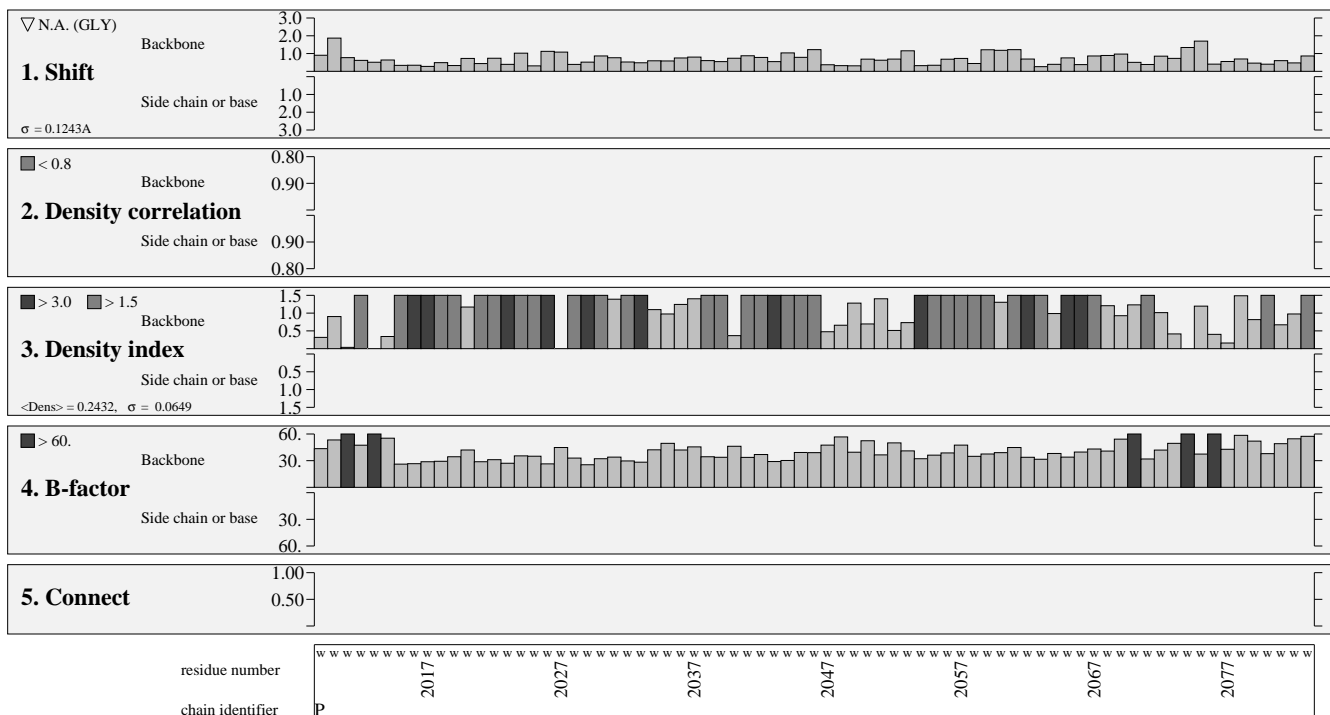




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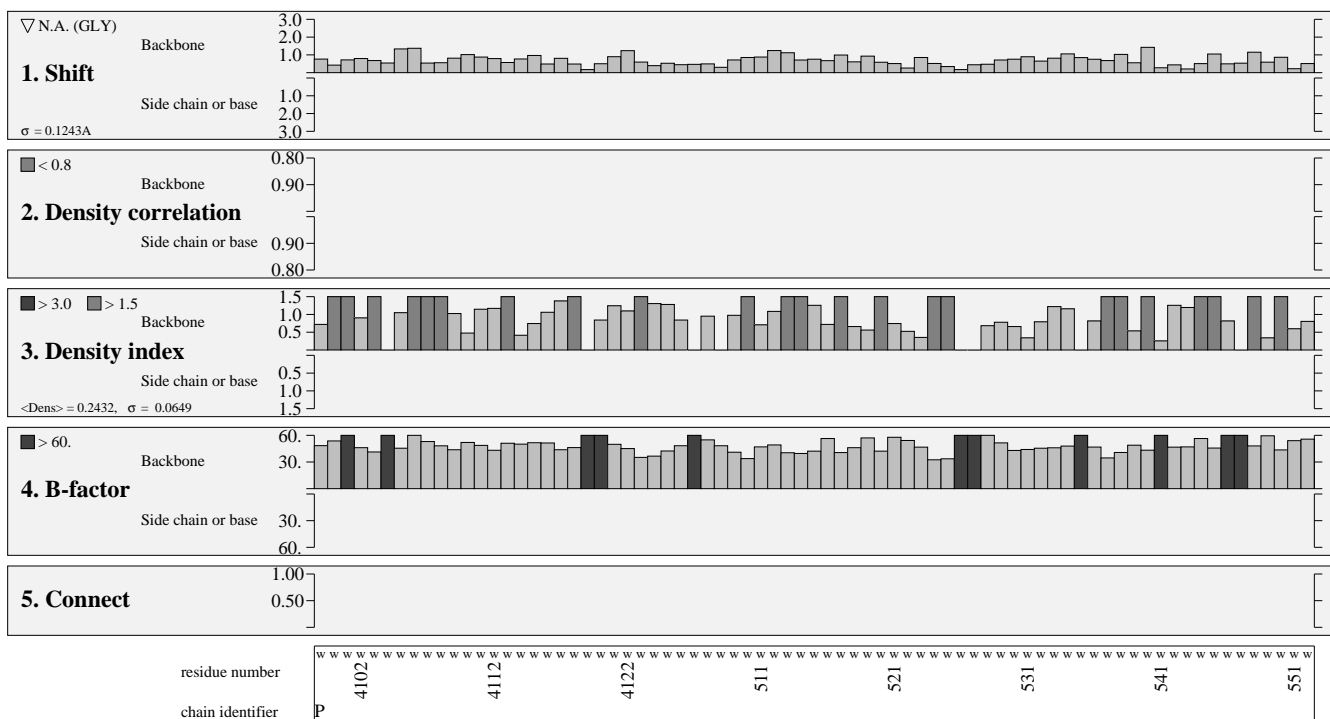
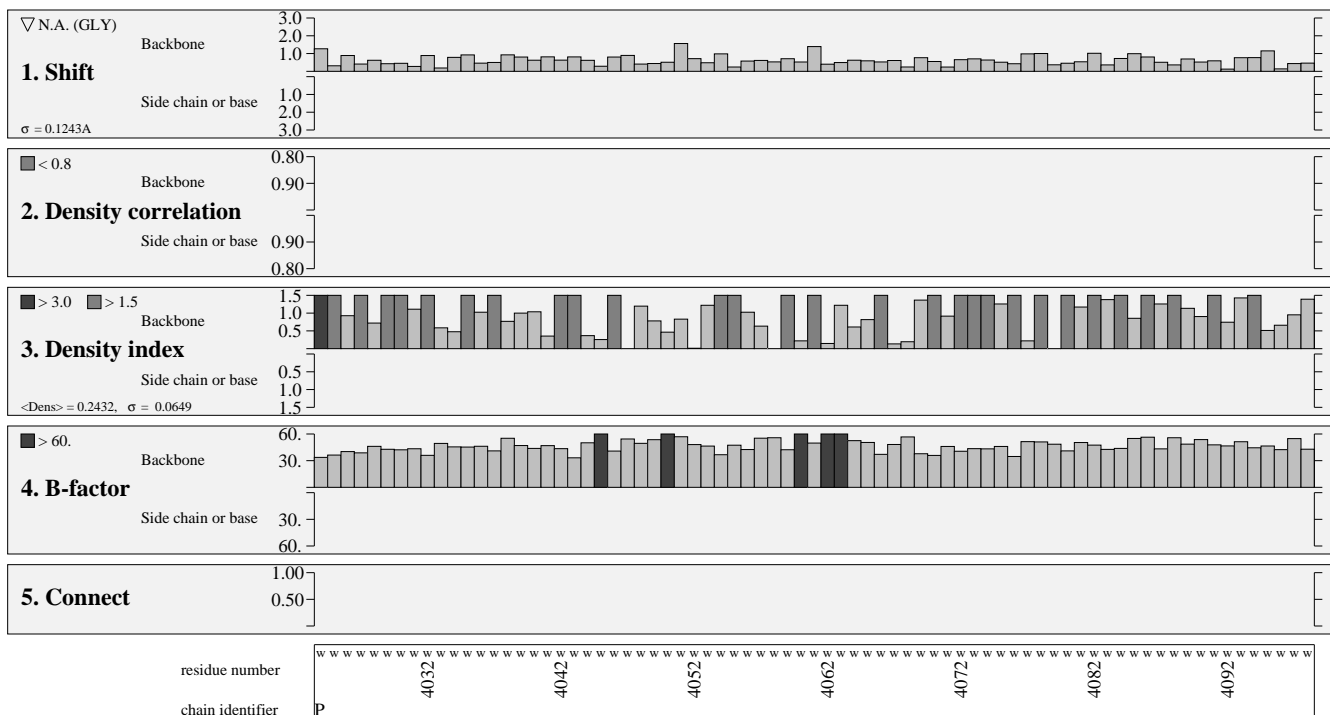
### Local estimation (31)



# Structure Factor Check

## 1PP9

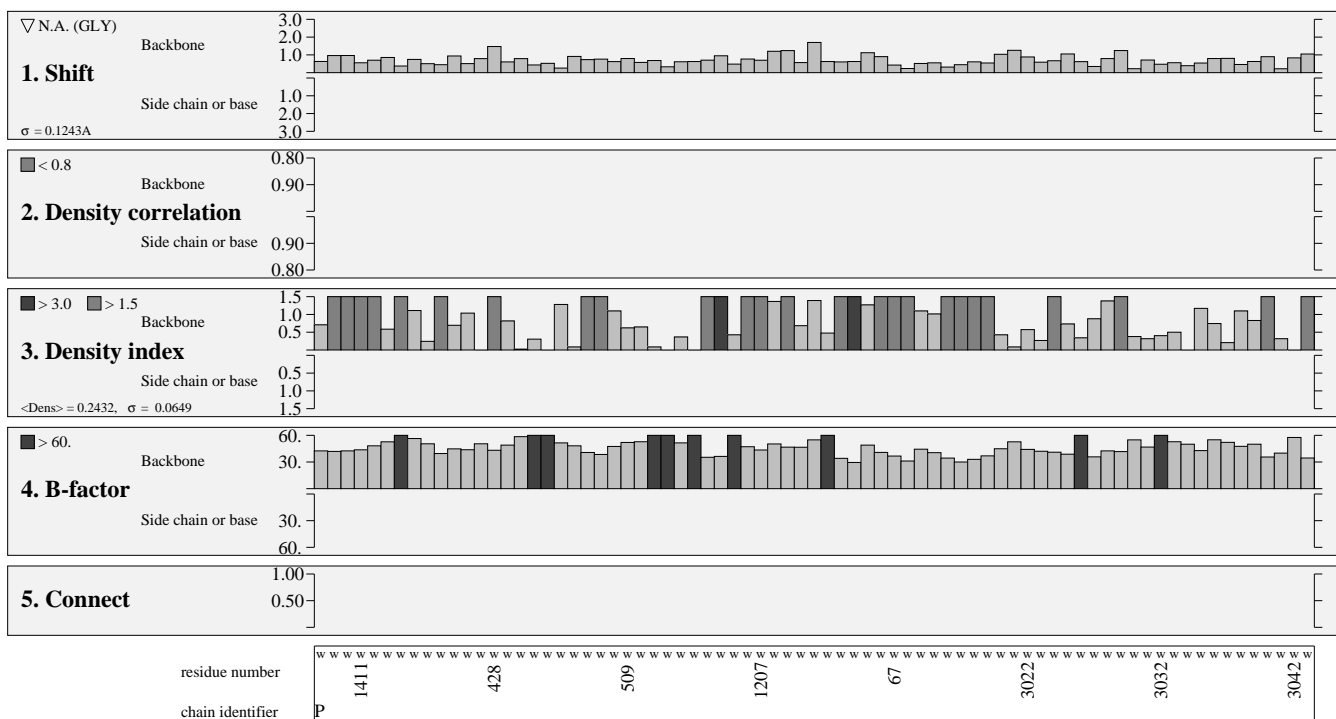
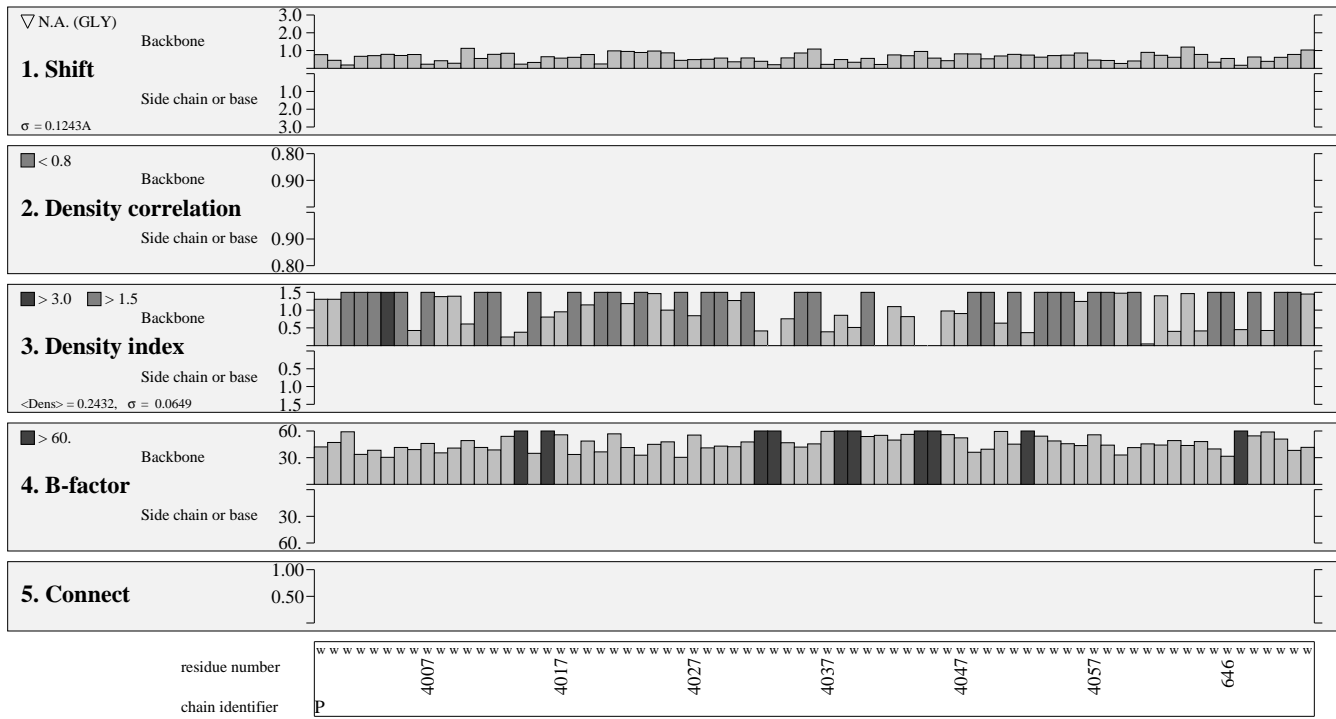
### Local estimation (32)



# Structure Factor Check

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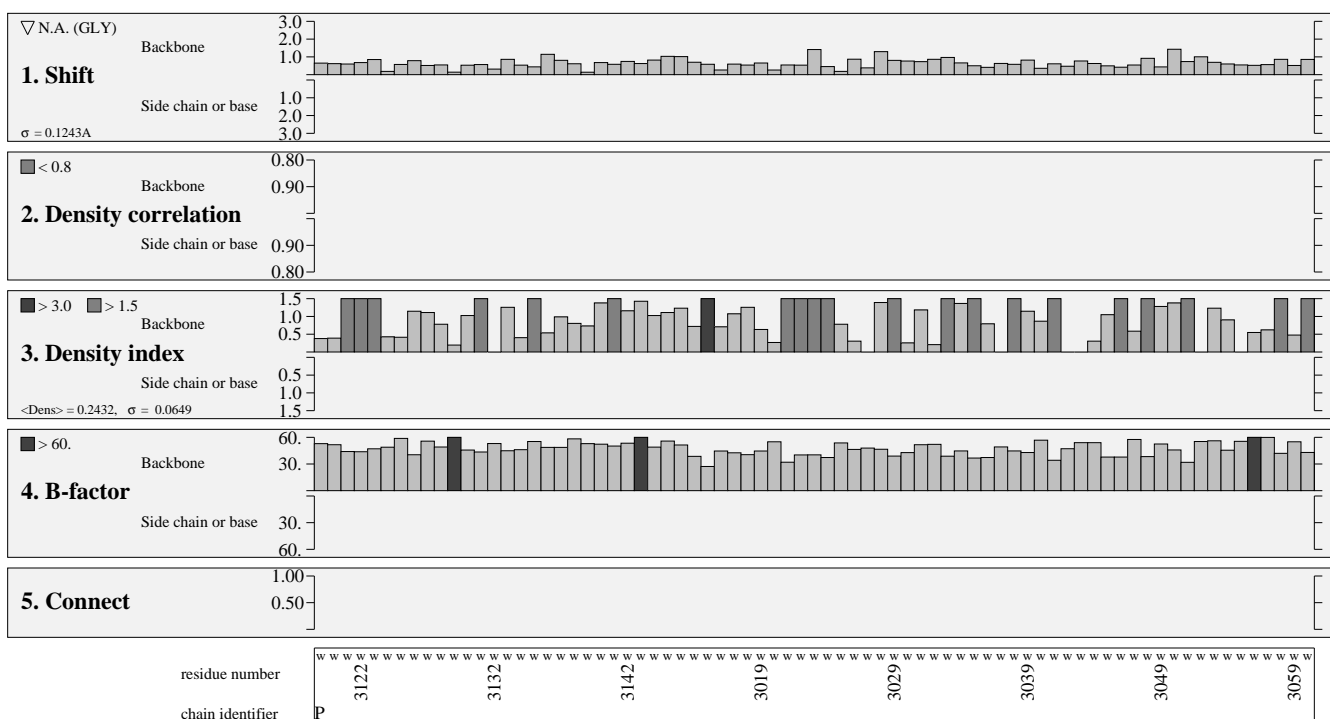
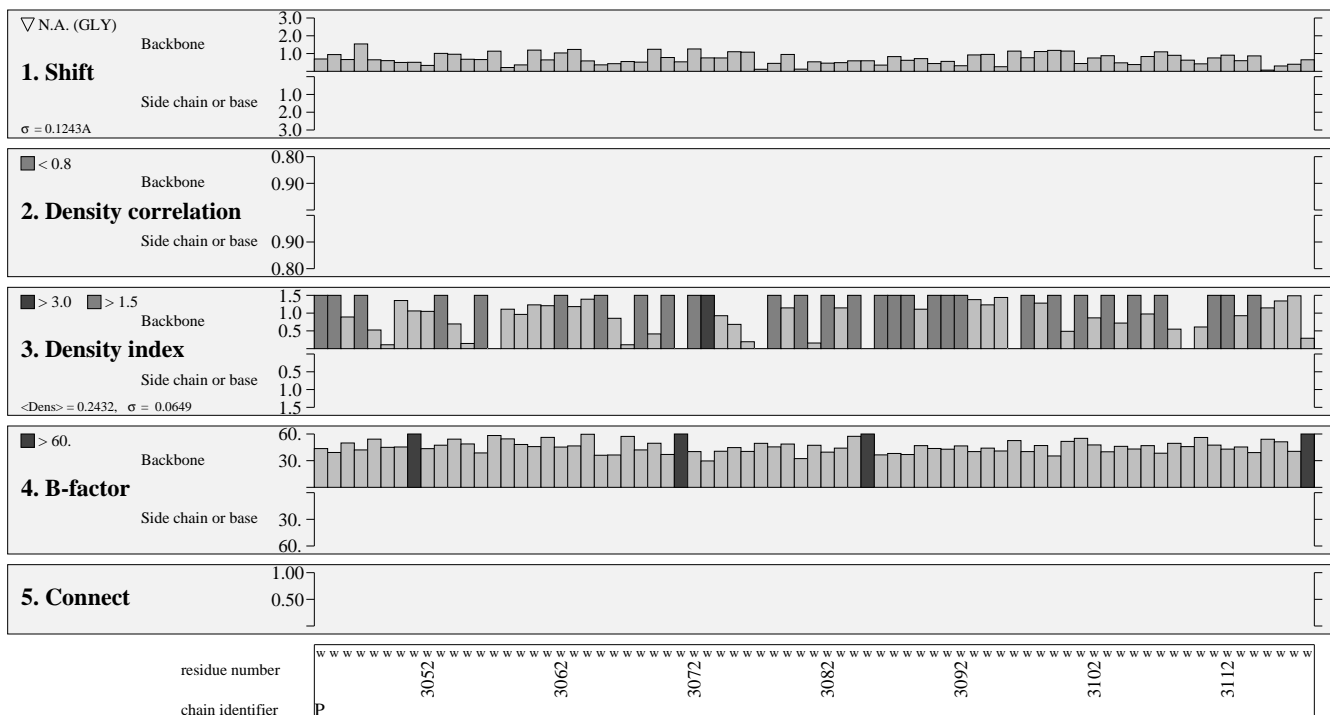
### Local estimation (33)



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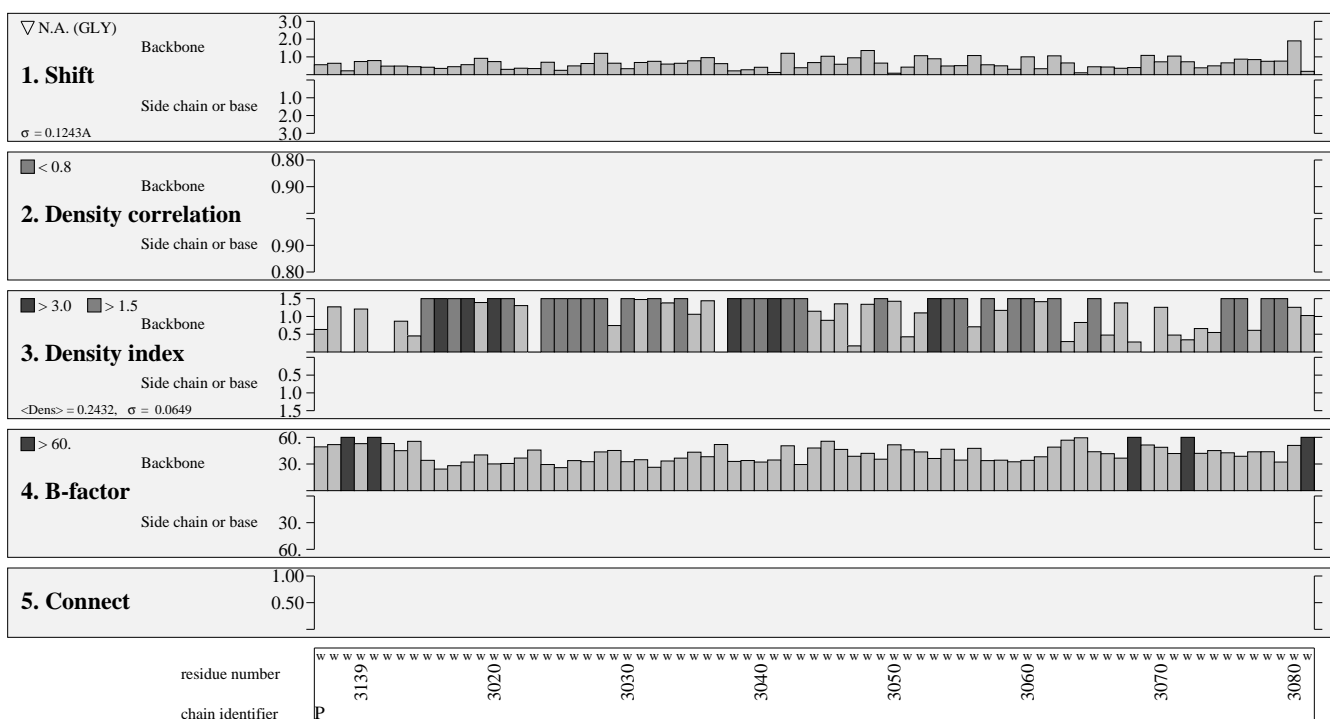
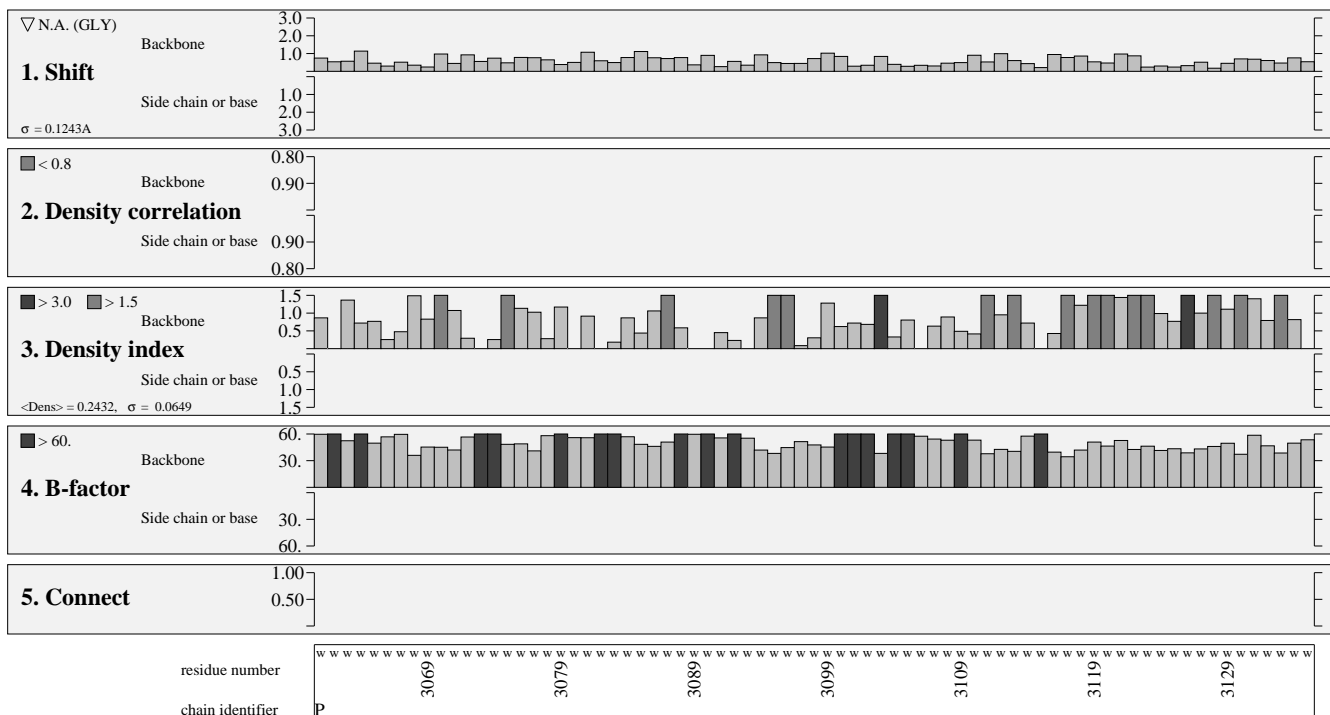
### Local estimation (34)



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### Local estimation (35)

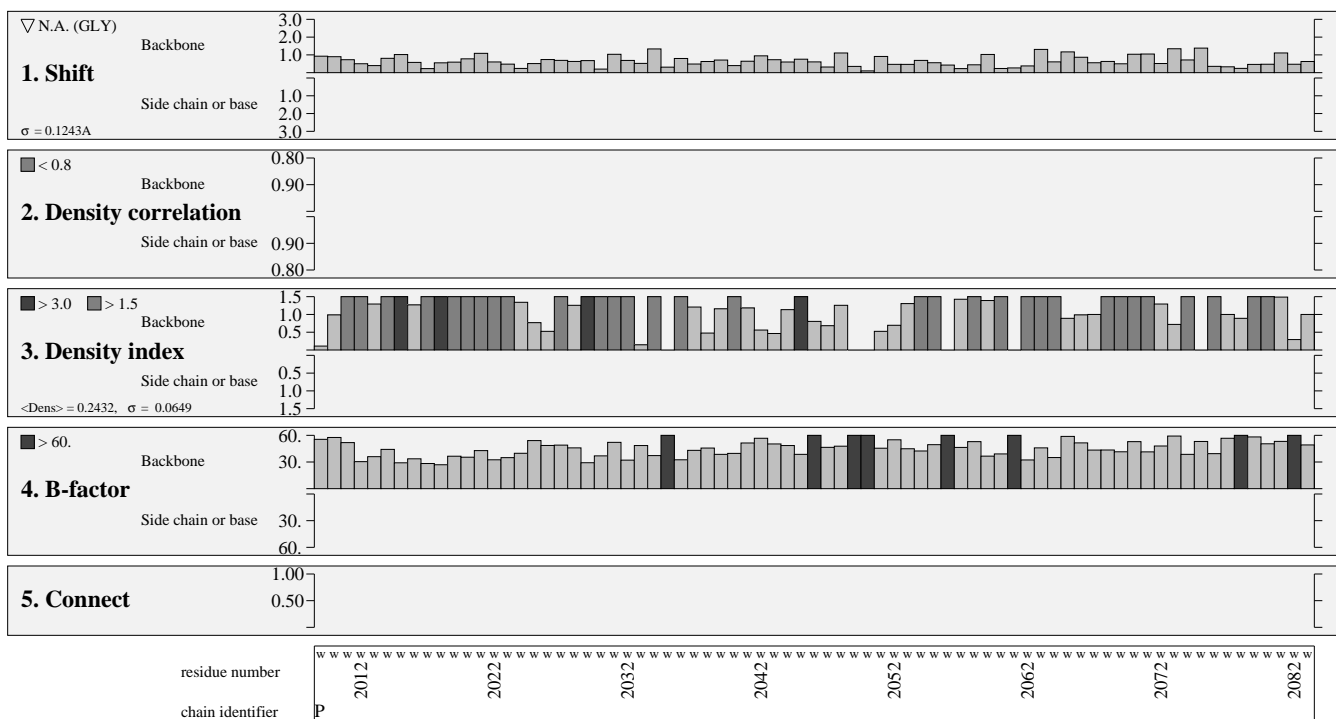
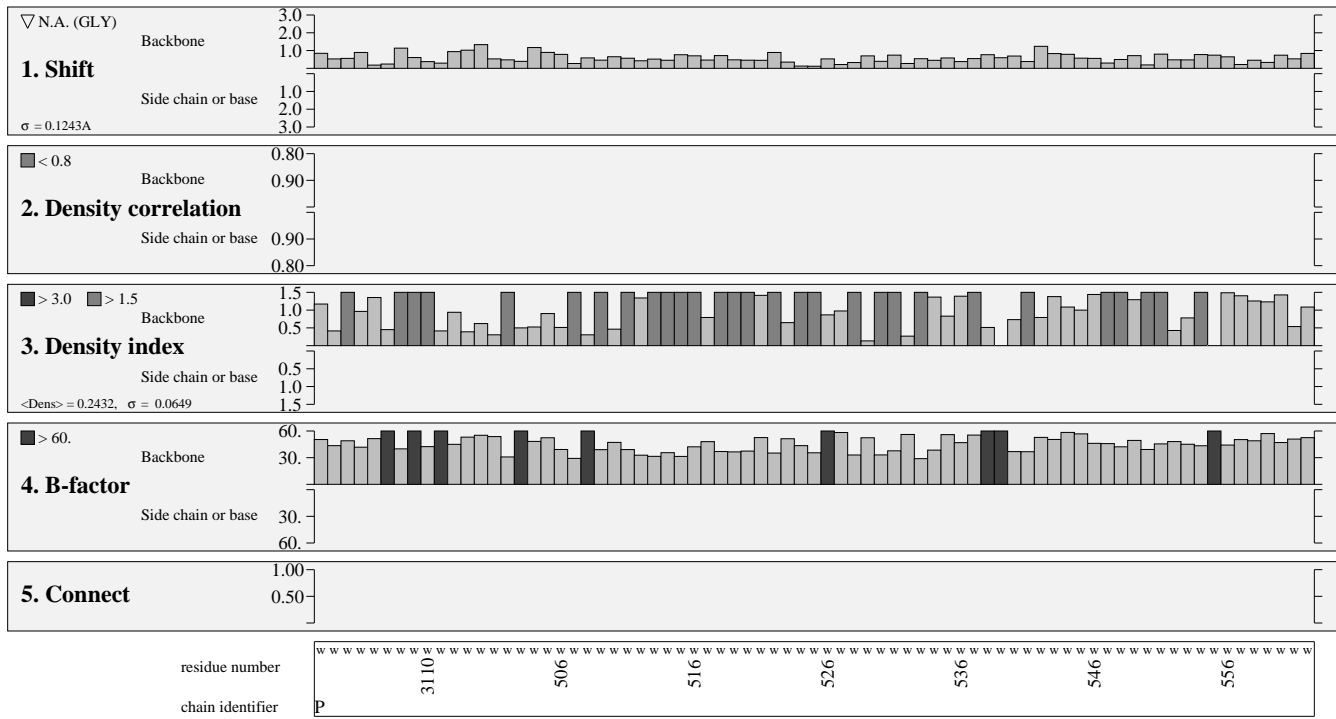




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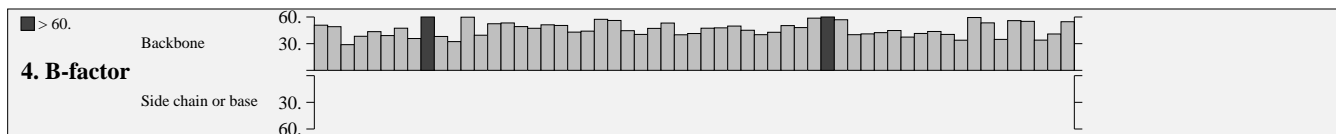
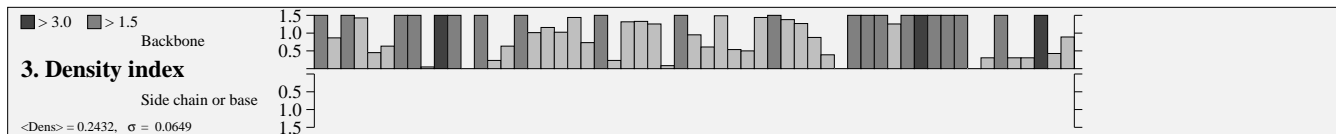
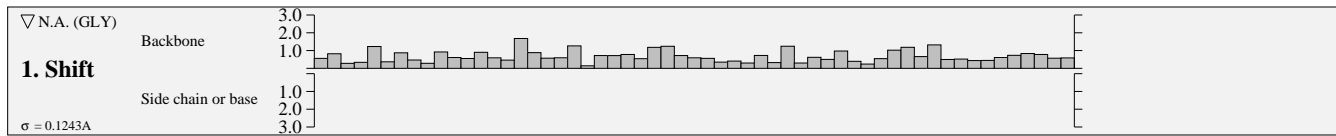
### Local estimation (37)



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### Local estimation (38)



residue number	chain identifier
3013	P
3023	P
1290	P
508	P
173	P