

Structure Factor Check

3H1L

Title: CHICKEN CYTOCHROME BC1 COMPLEX WITH ASCOCHLORIN BOUND AT QO
AND QI SITES
Date: 12-APR-09
PDB code: 3H1L

Crystal

Cell parameters:

a: 174.14 A b: 182.36 A c: 241.63 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 40.0 – 3.20 A
 Reflections in file: 125230
 Unique reflections above 0: 125230
 above 1 σ : 122444
 above 3 σ : 83686

SFCHECK

Nominal resolution range: 40.0 – 3.21 A
\05max. from input data, min. from author\05
 Used reflections: 125071
 Reflections out of resolution: 159
 Completeness: 99.4 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.067
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.4647 0.5420
 B_{overall} (by Patterson): 59. A²
 Optical resolution: 2.38 A
 Expected opt. resol. for complete data set: 2.38 A
 Estimated minimal error: 0.110 A

Model

32657 atoms (14 water molecules)

Number of chains: 51
 Volume not occupied by model: 62.9 %
 $\langle B \rangle$ (for atomic model): 89.5 A²
 $\sigma(B)$: 14.75 A²
 Matthews coefficient: 4.20
 Corresponding solvent % : 70.45

Model vs. Structure Factors

R-factor for all reflections: 0.337
 Correlation factor: 0.810
 R-factor: 0.338
 for $F > 2.0\sigma$
 nom. resolution range: 29.99 – 3.21A
 reflections used: 122213

Rfree: 0.357
 Nfree: 2437
 R-factor without free-refl.: 0.338
 Non free-reflections: 119776
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.707 A
 Estimated maximal error: 0.490 A
 DPI: 0.484 A

Scaling

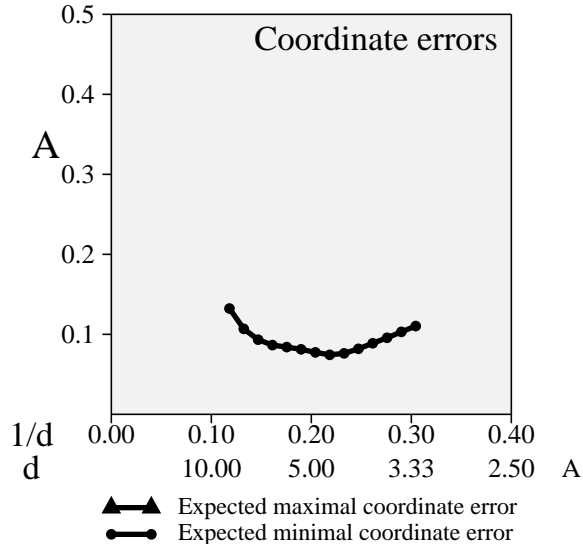
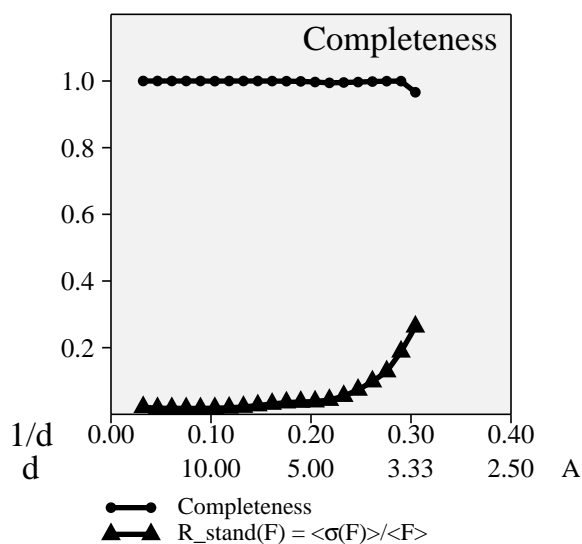
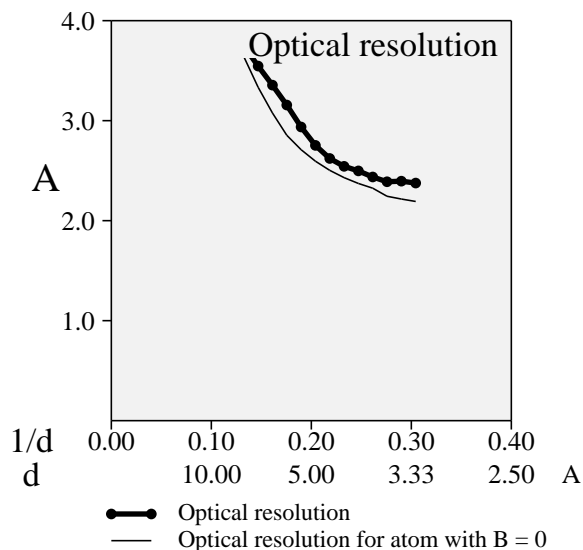
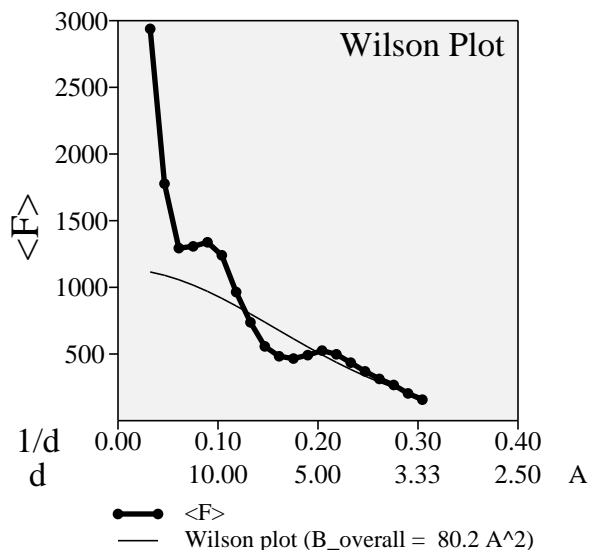
Scale: 0.458
 Bdiff: -7.31
 Anisothermal Scaling (Beta):
 12.8887 -4.5126 -0.1529 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.510 250.205

Refinement

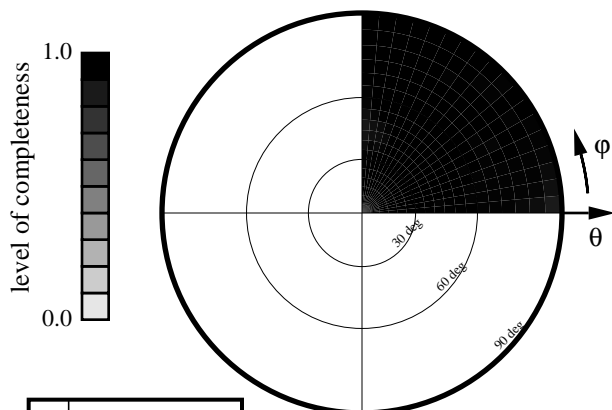
Program: CNS 1.1
 Nominal resolution range: 30.0 – 3.21 A
 Reported nominal resolution: 3.00 A
 Reported R-factor: 0.267
 Number of reflections used: 125125
 Reported Rfree: 0.29
 Sigma cut-off: N.A.

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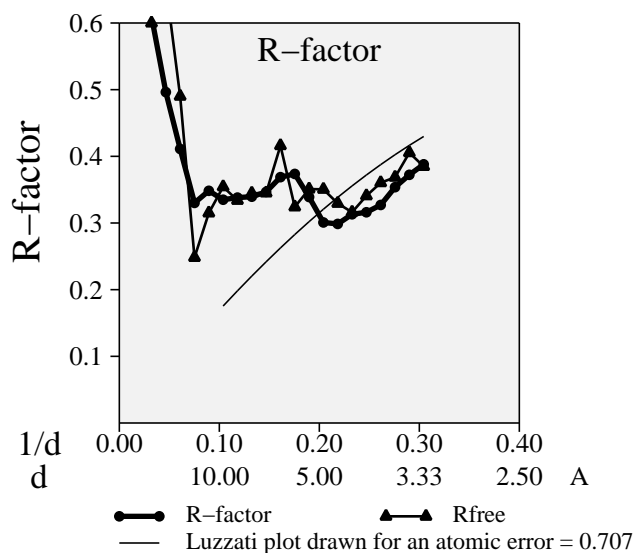


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

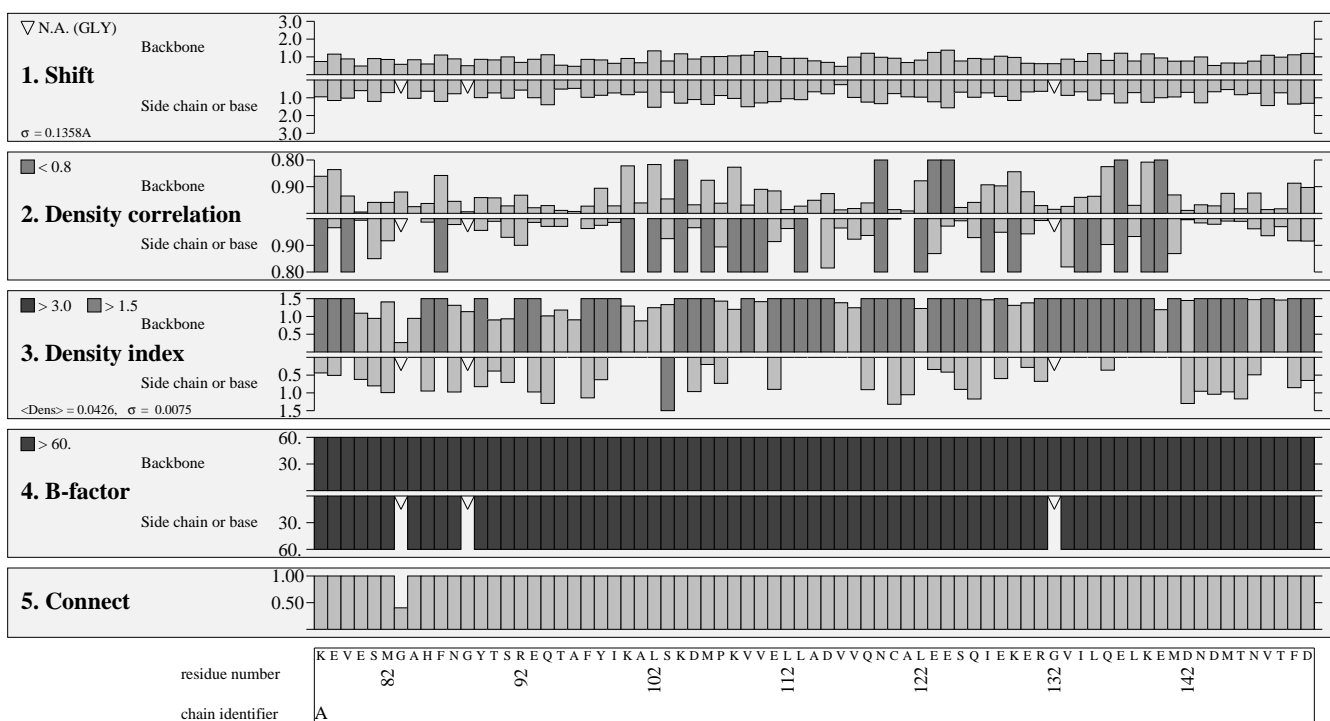
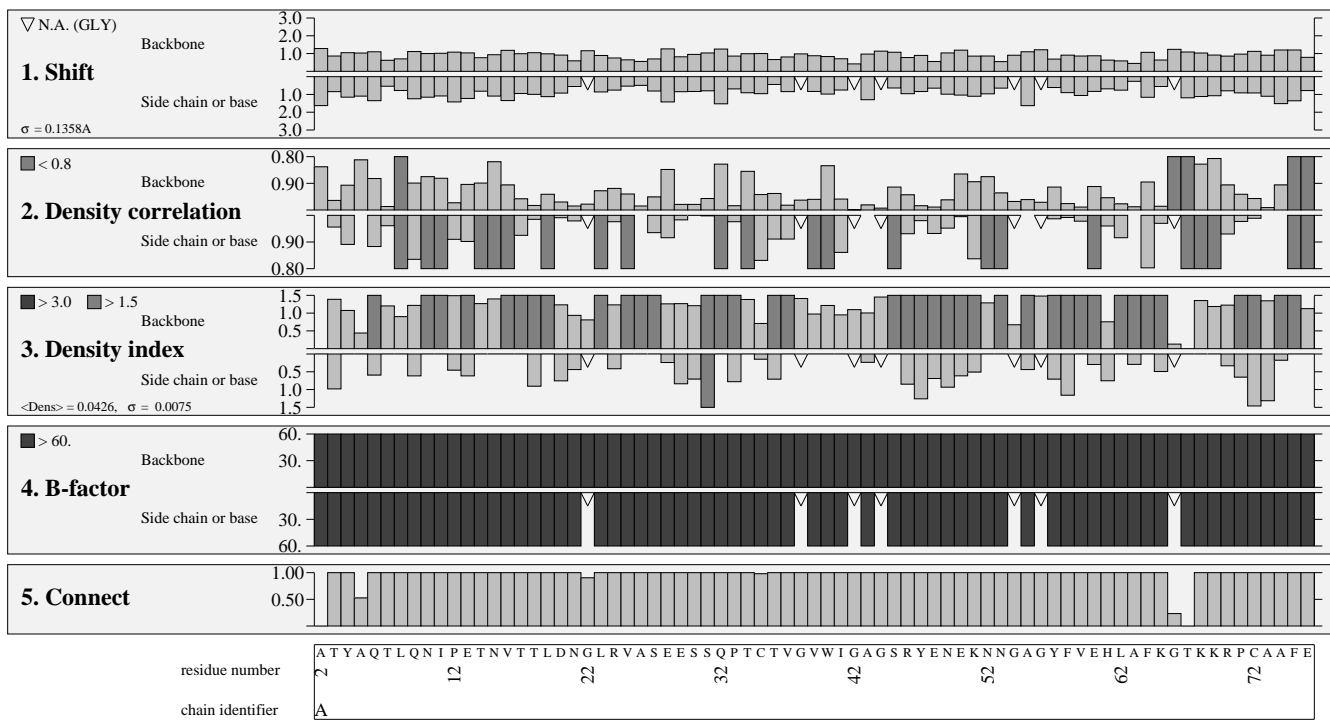
polar coordinates of the crystallographical axes



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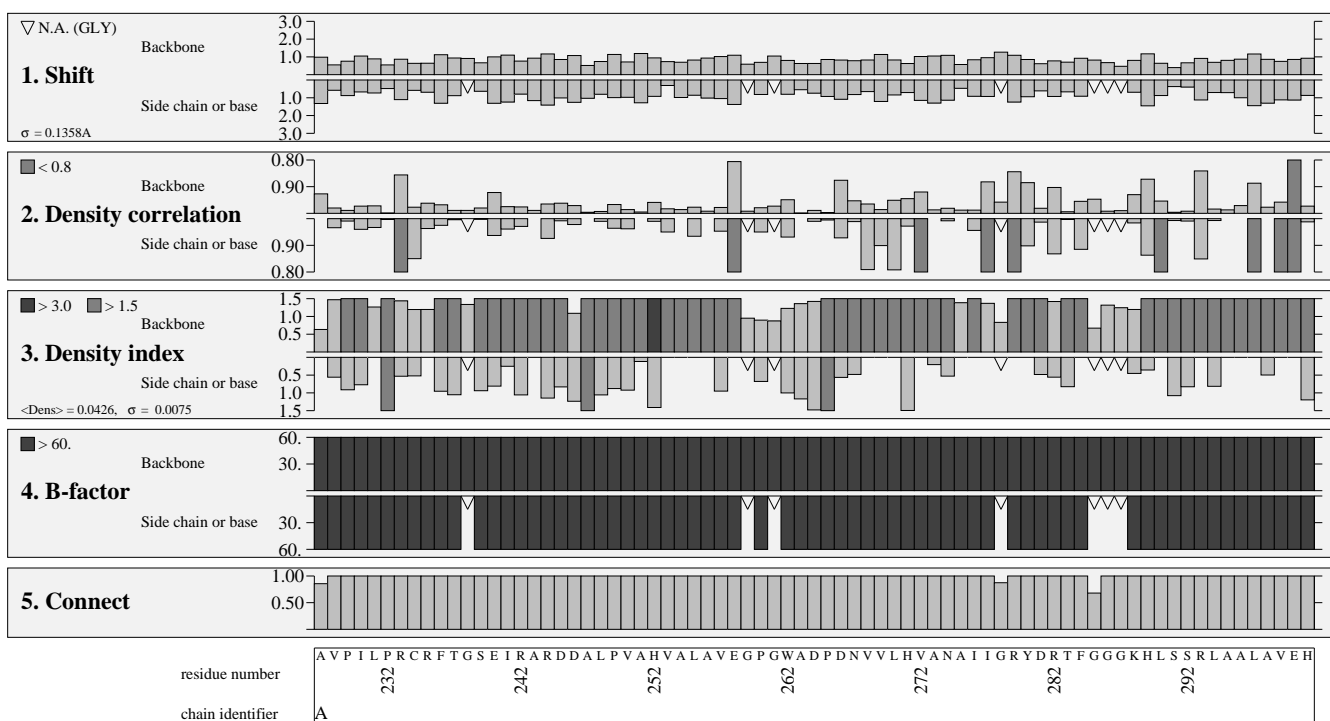
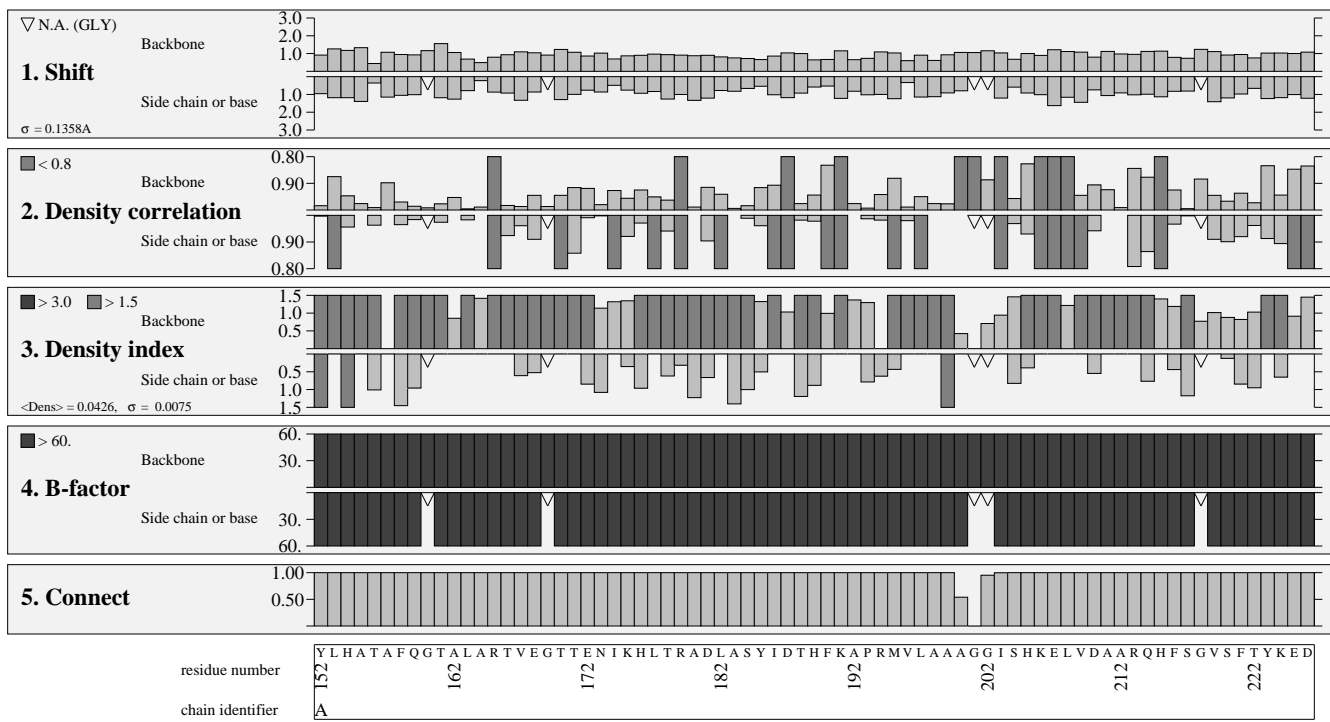
Local estimation



Structure Factor Check

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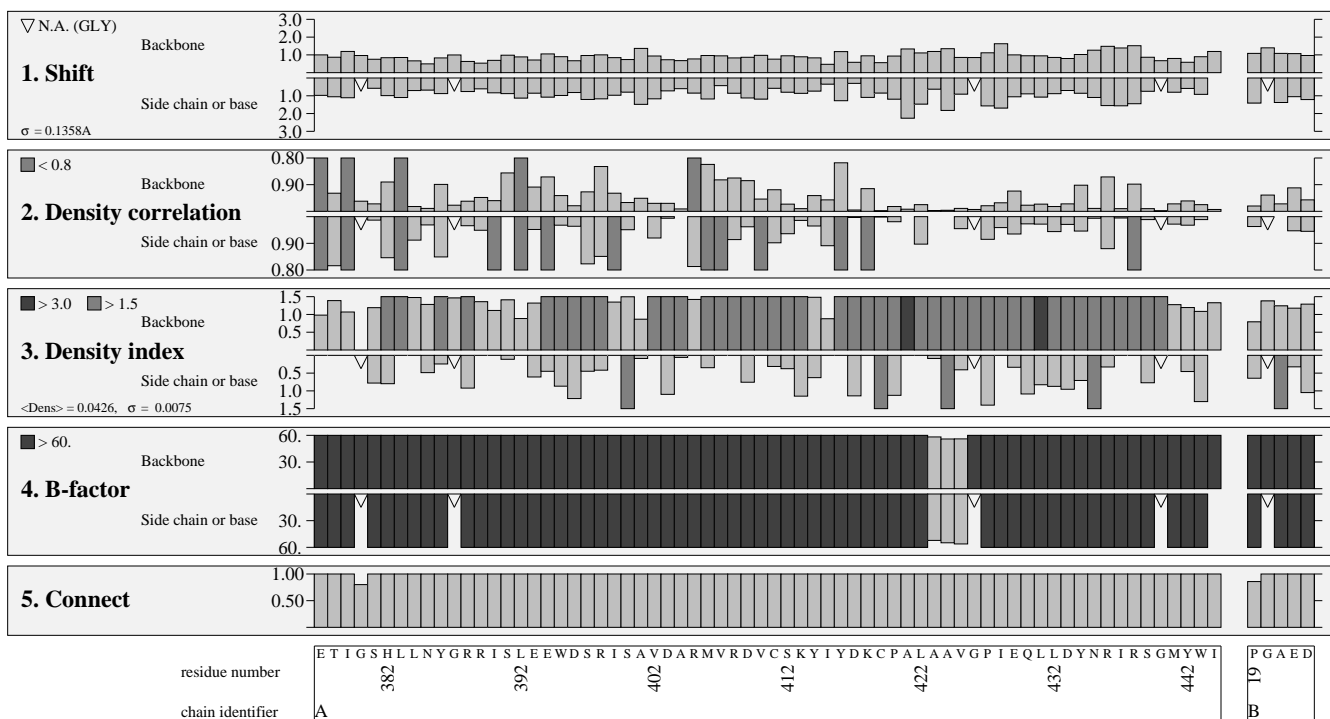
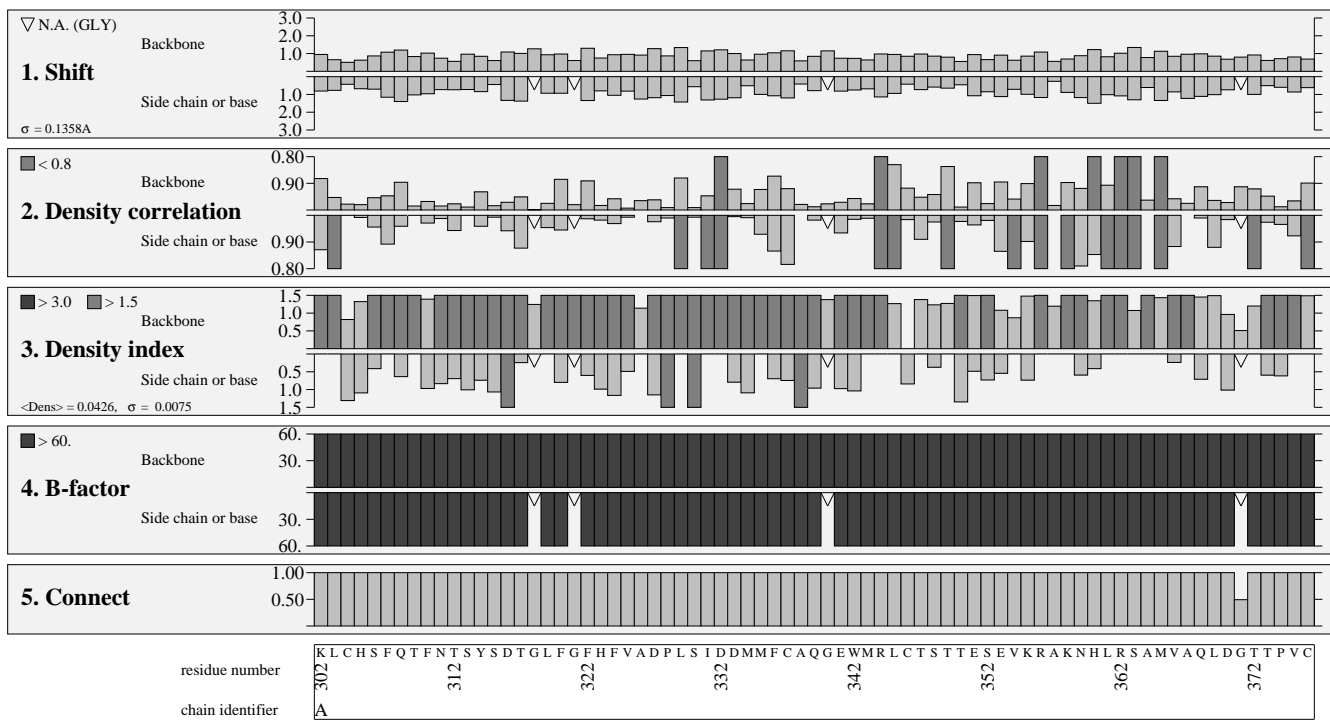
Local estimation (2)



Structure Factor Check

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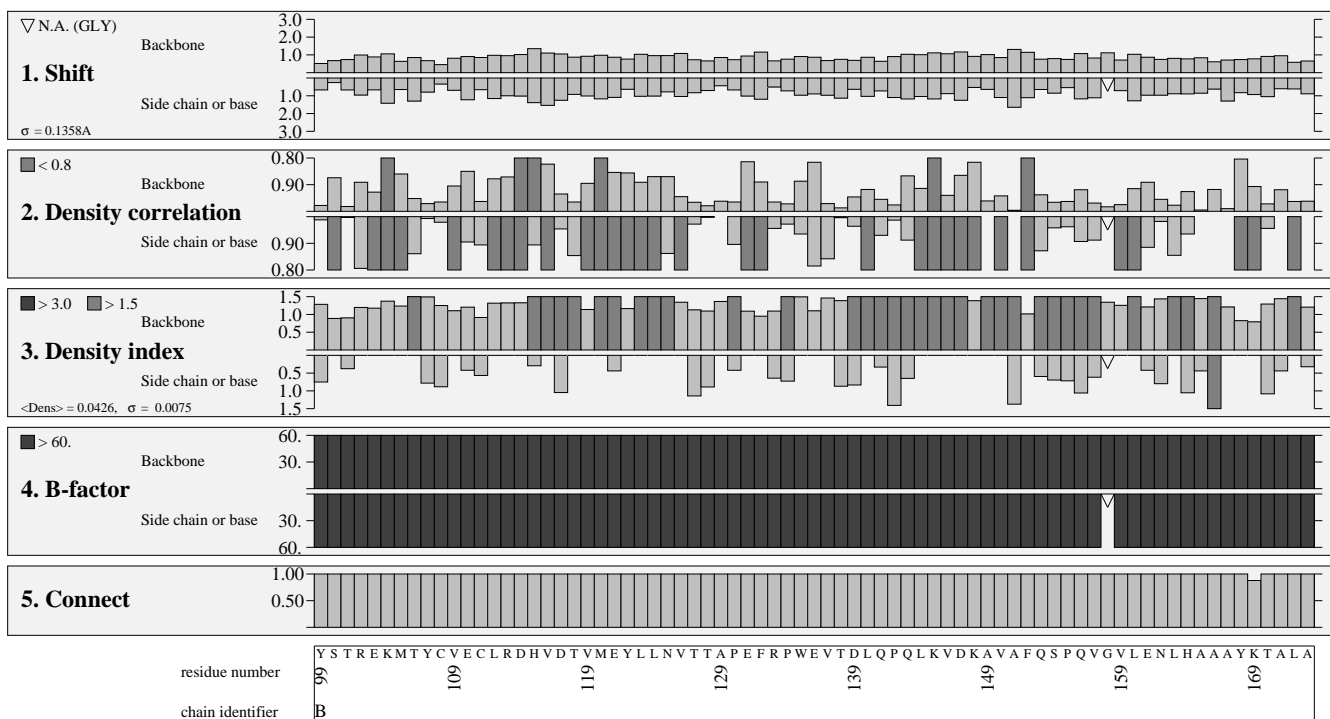
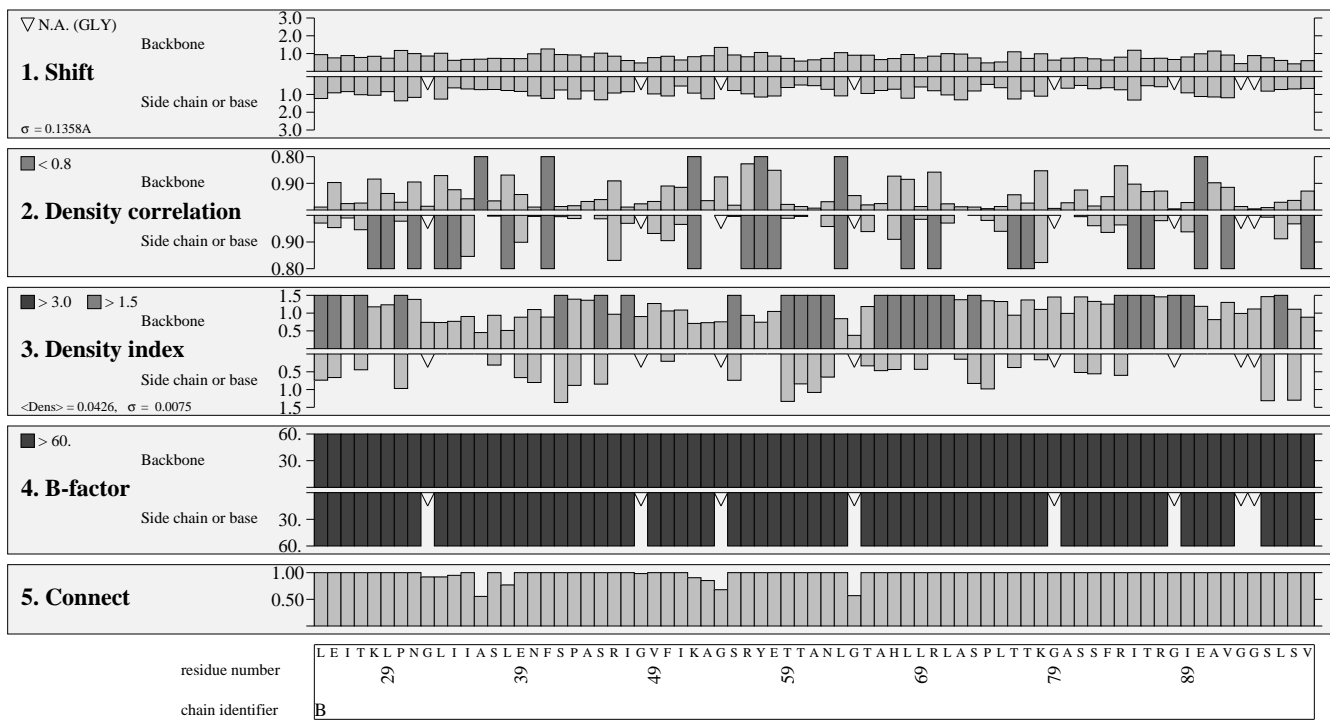
Local estimation (3)



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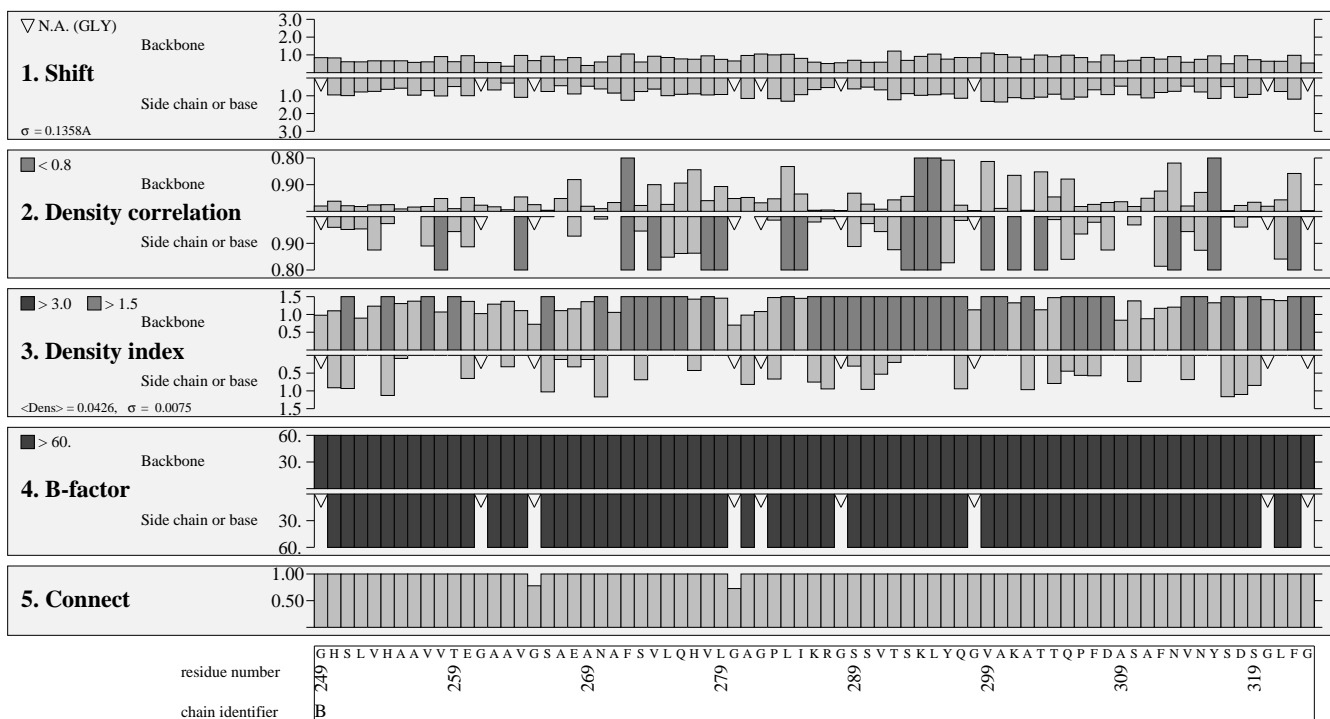
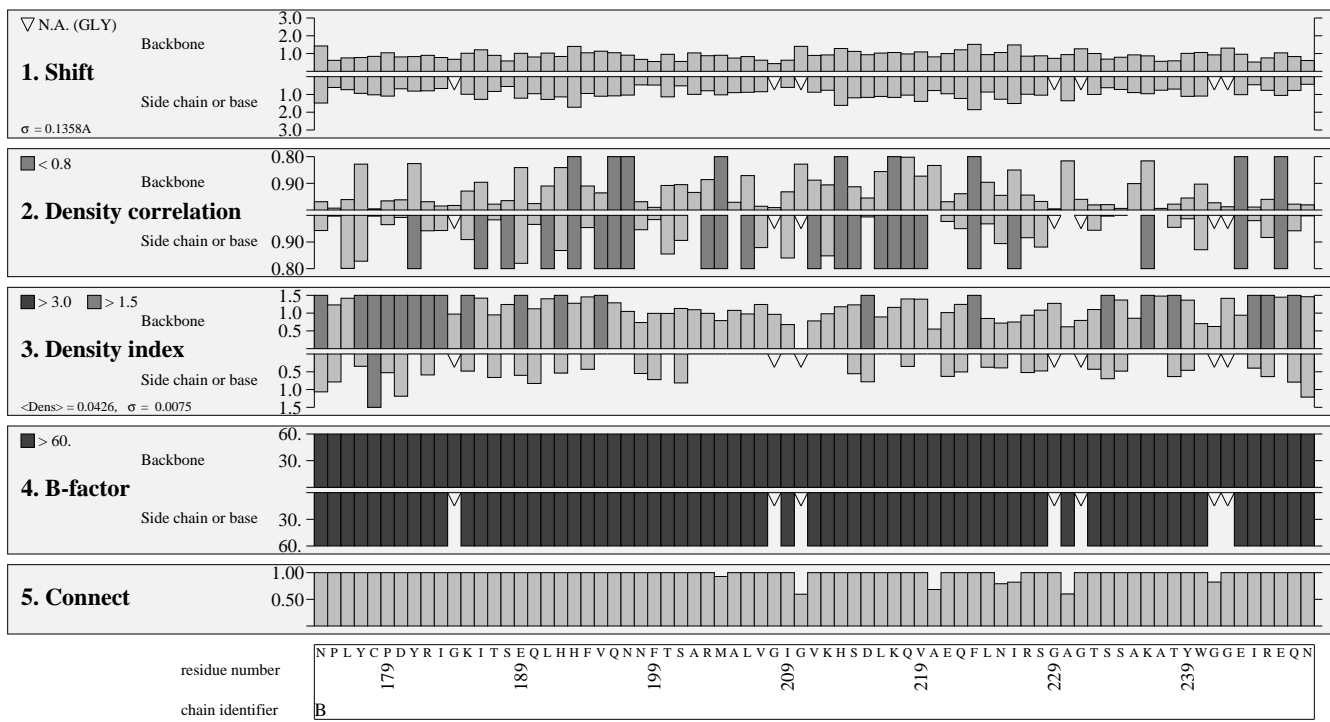
Local estimation (4)



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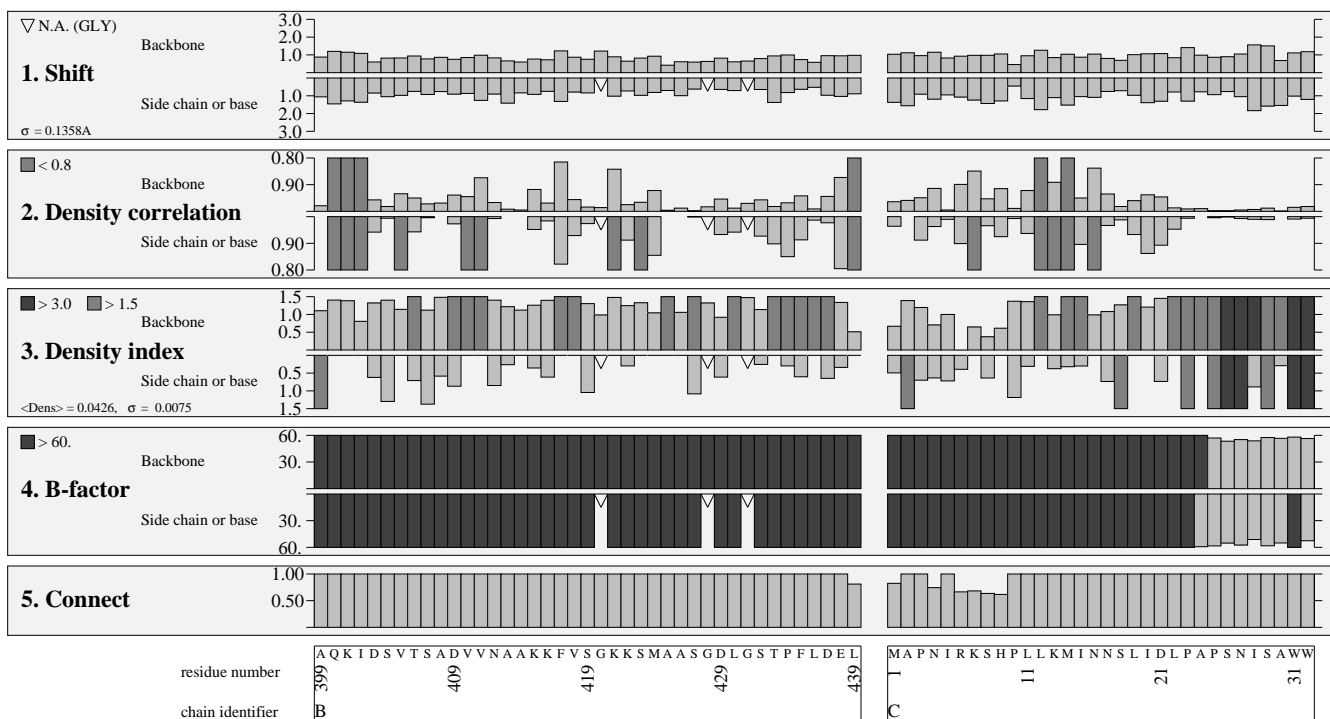
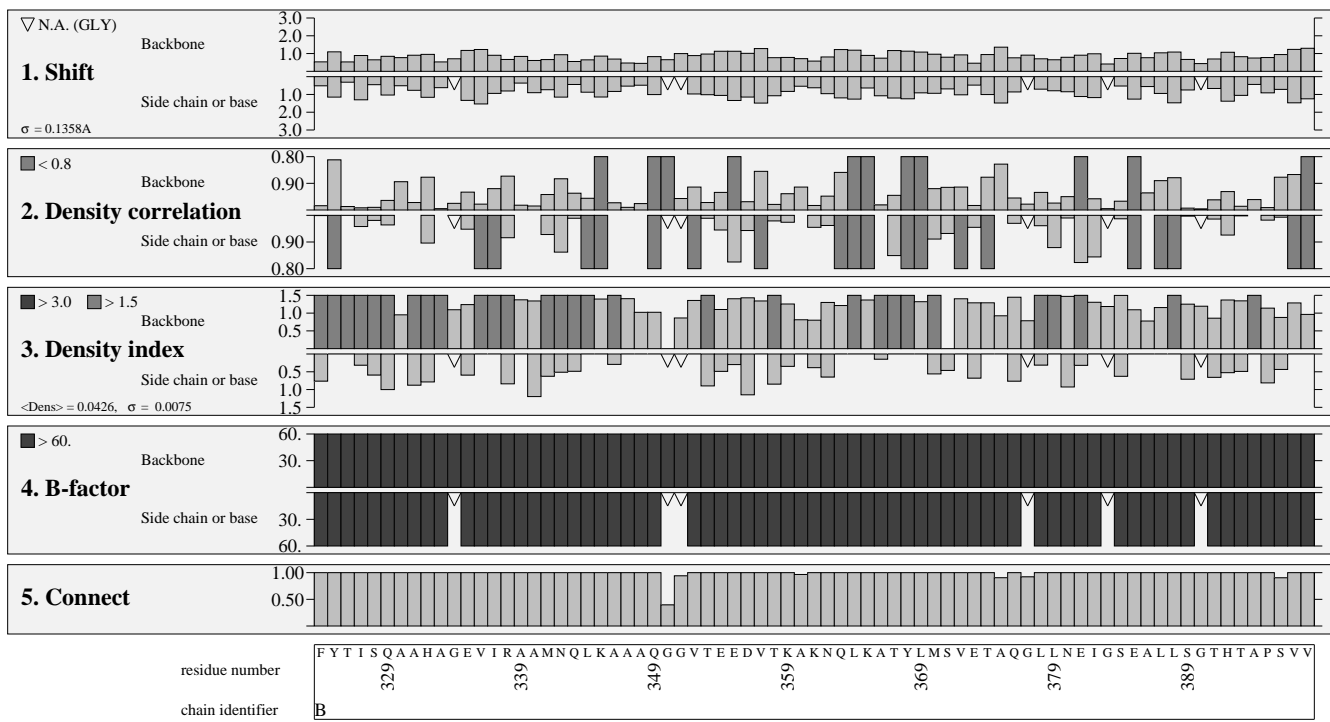
Local estimation (5)



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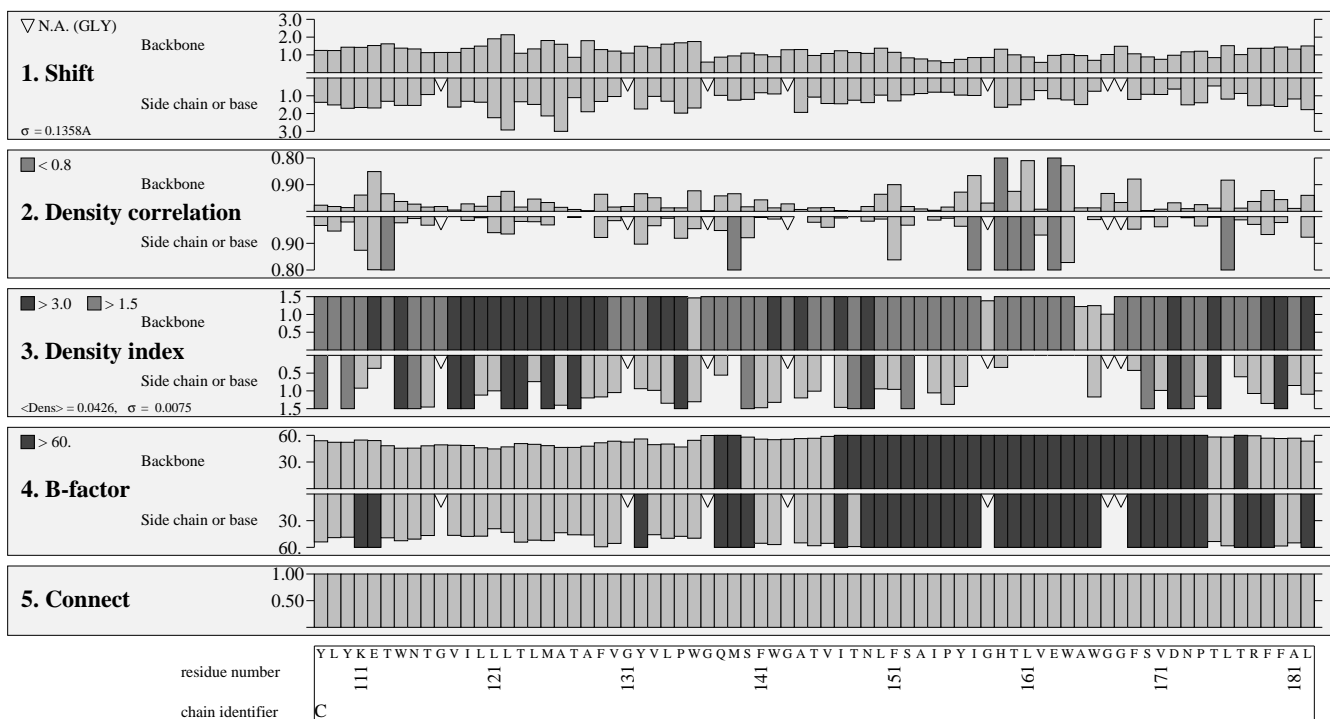
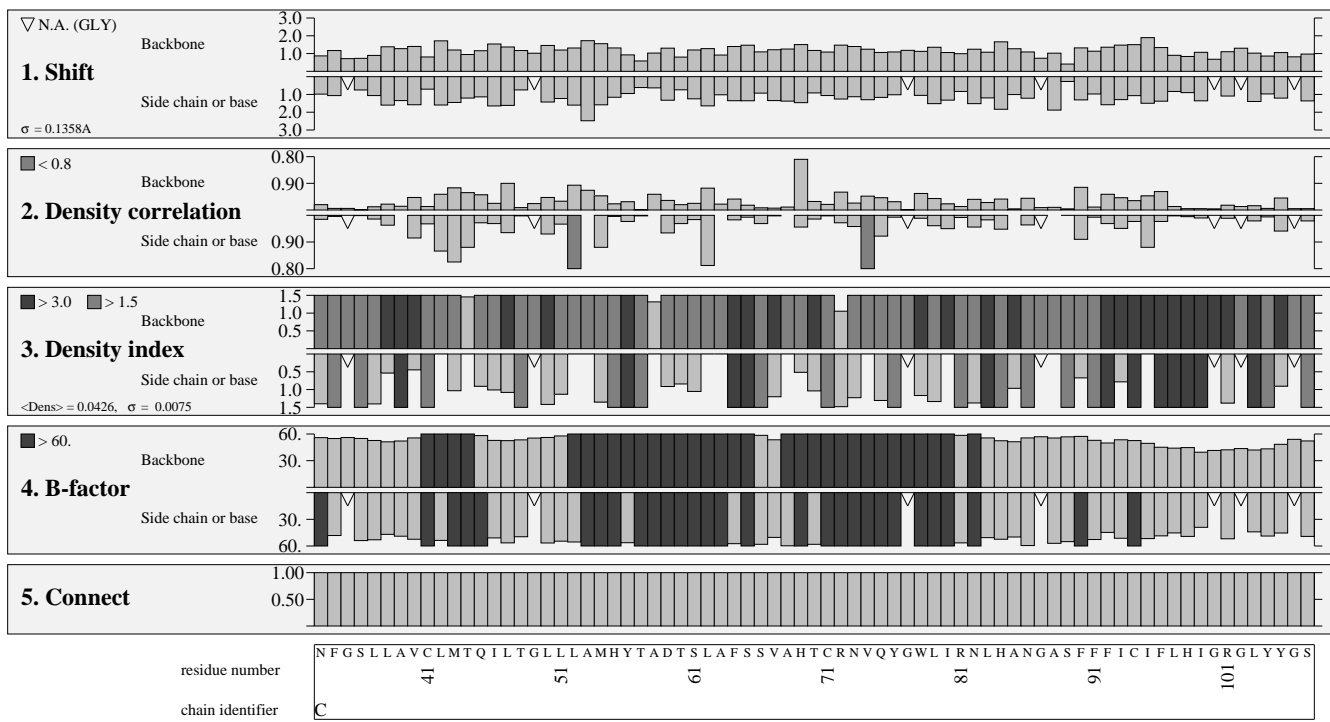
Local estimation (6)



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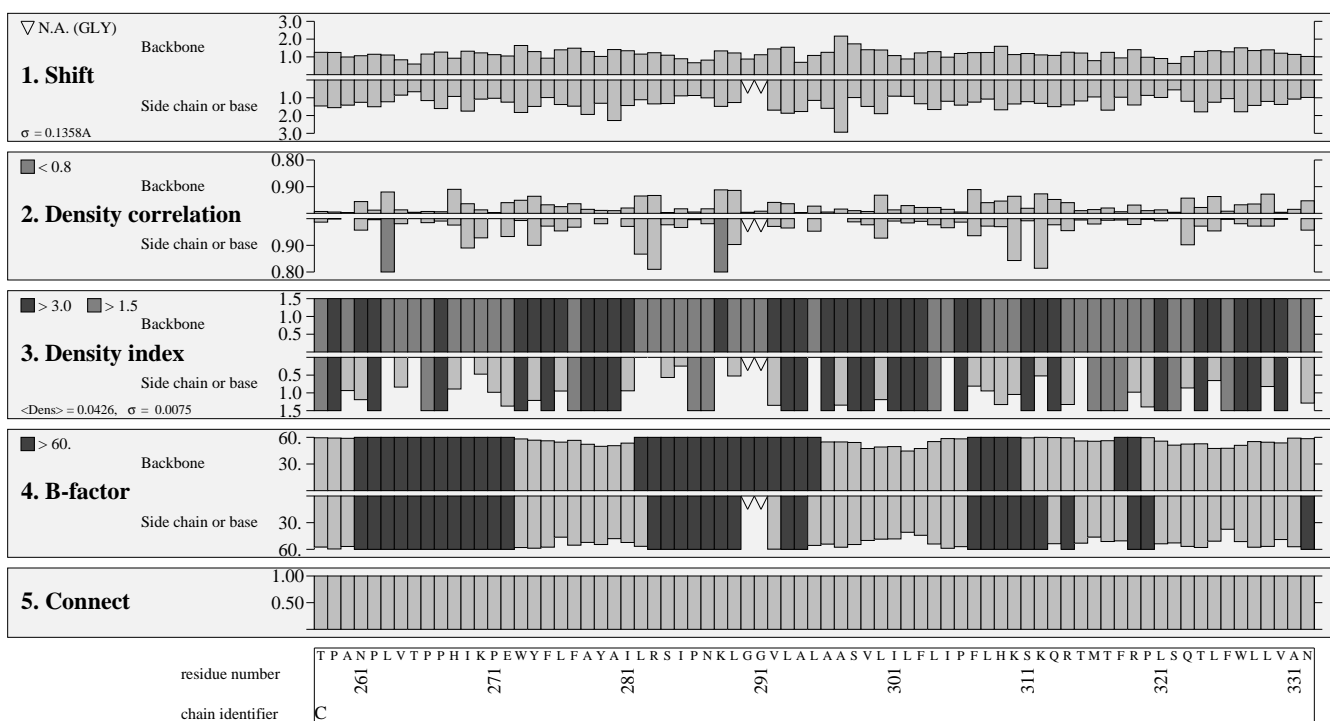
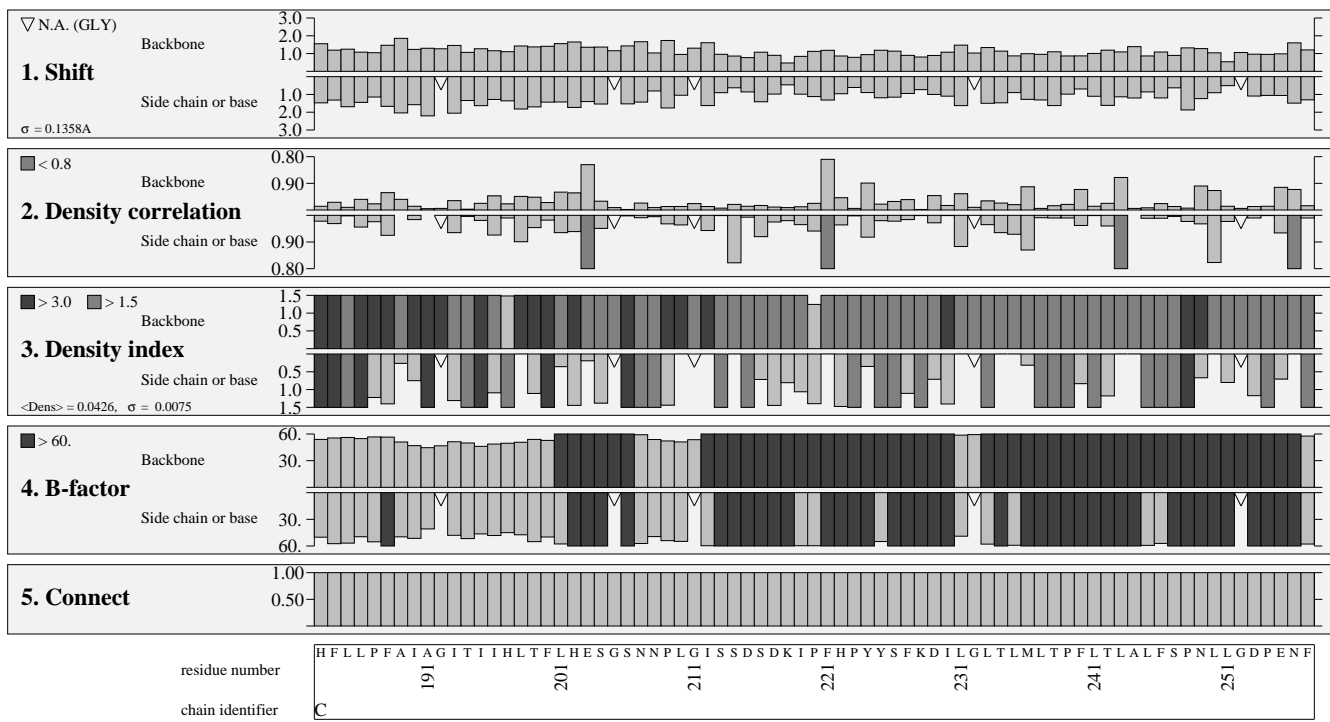
Local estimation (7)



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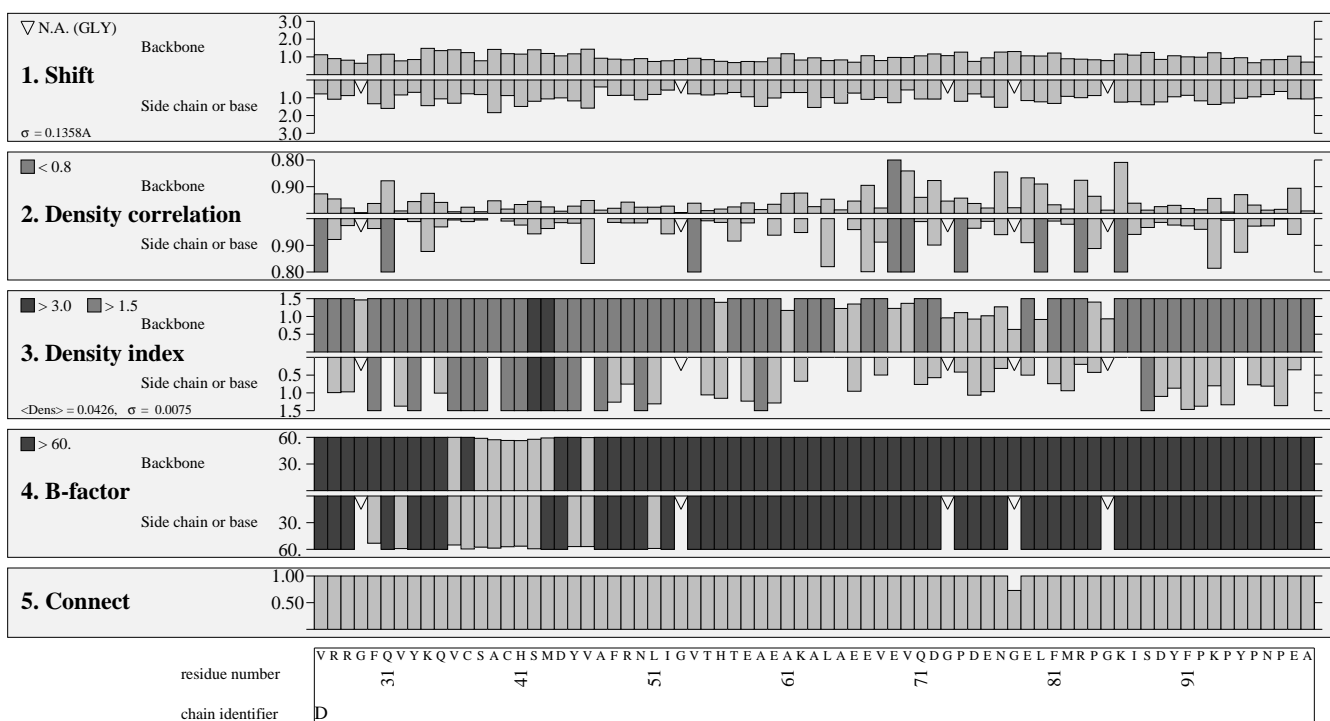
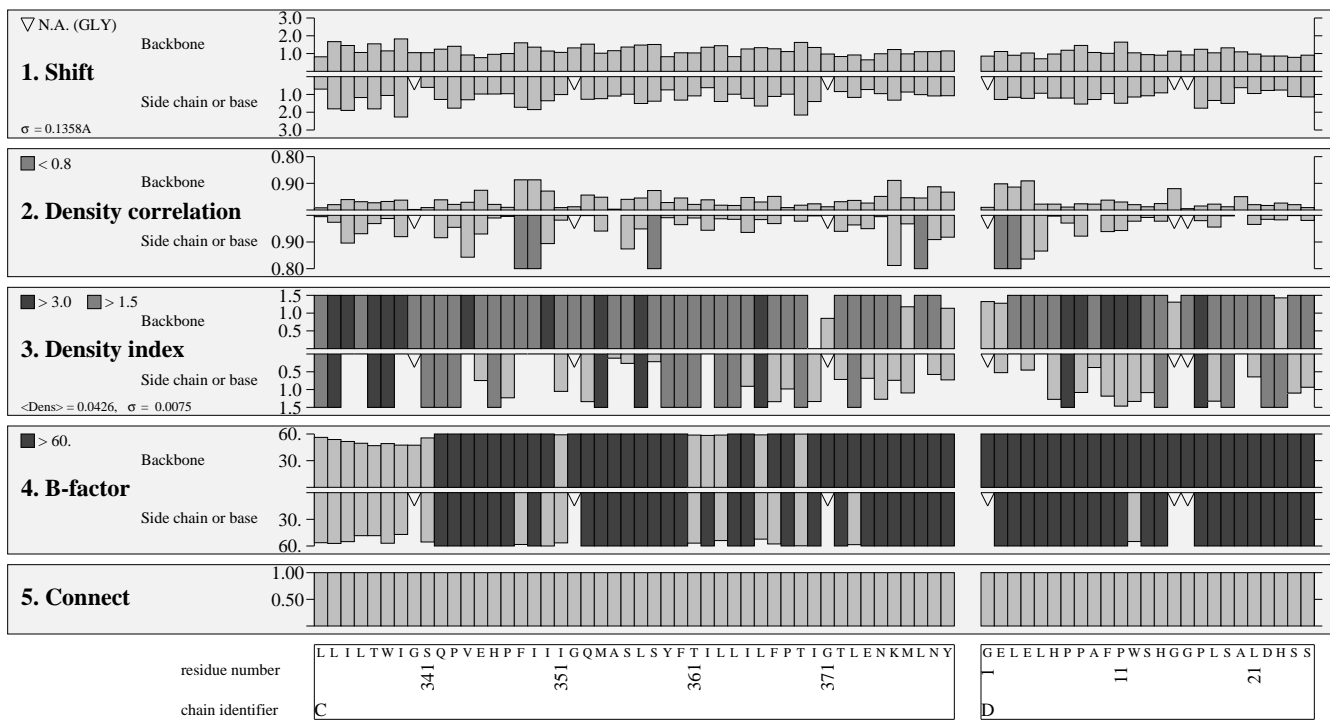
Local estimation (8)



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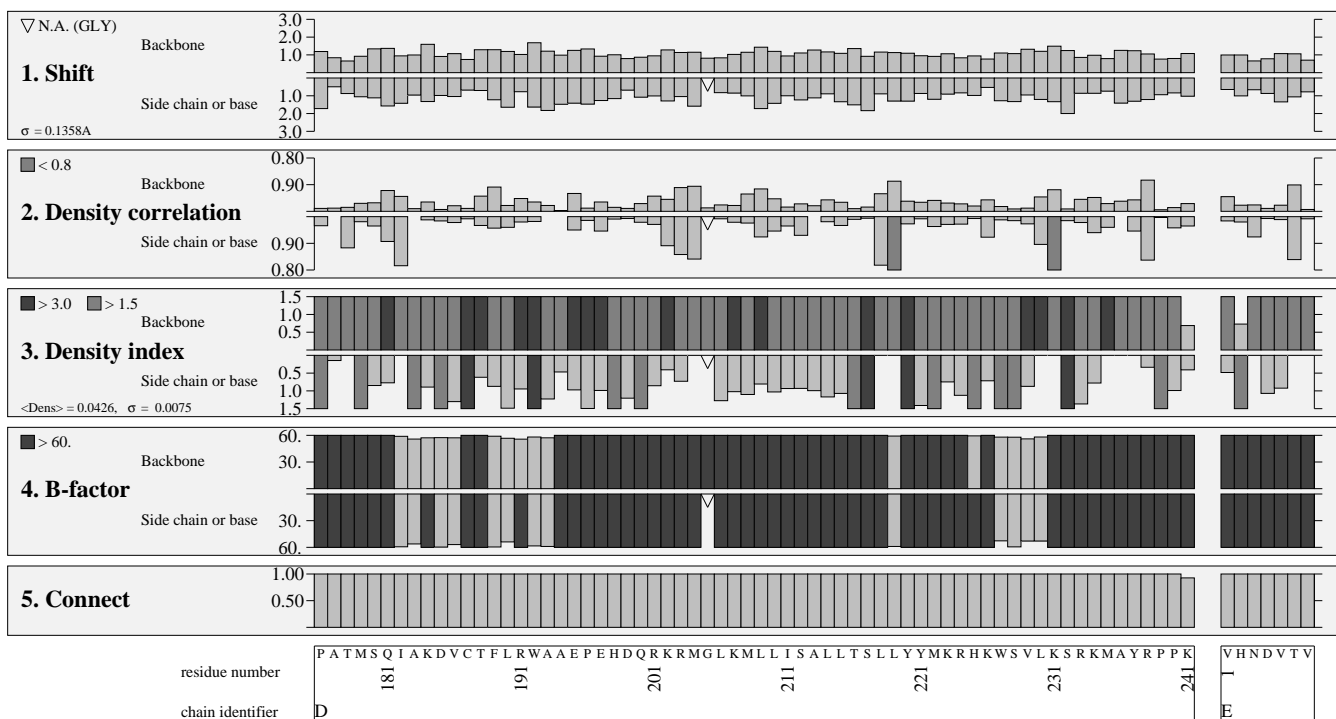
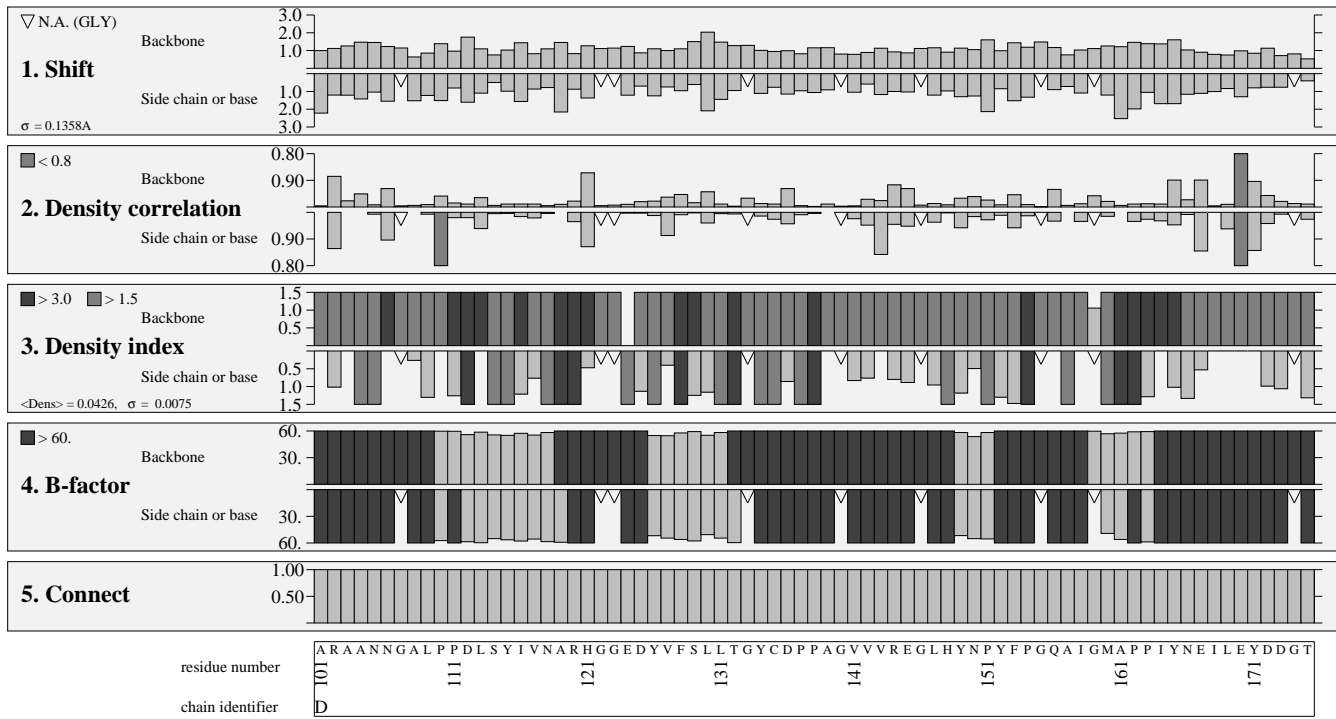
Local estimation (9)



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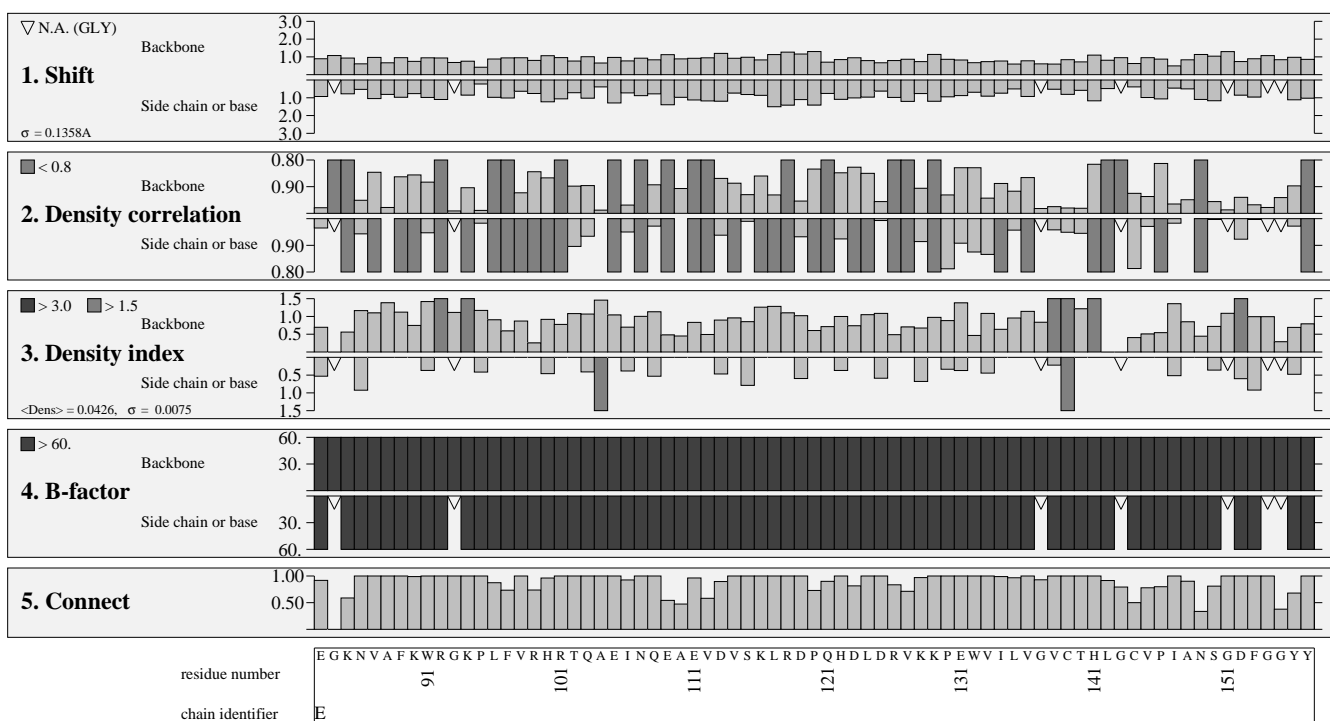
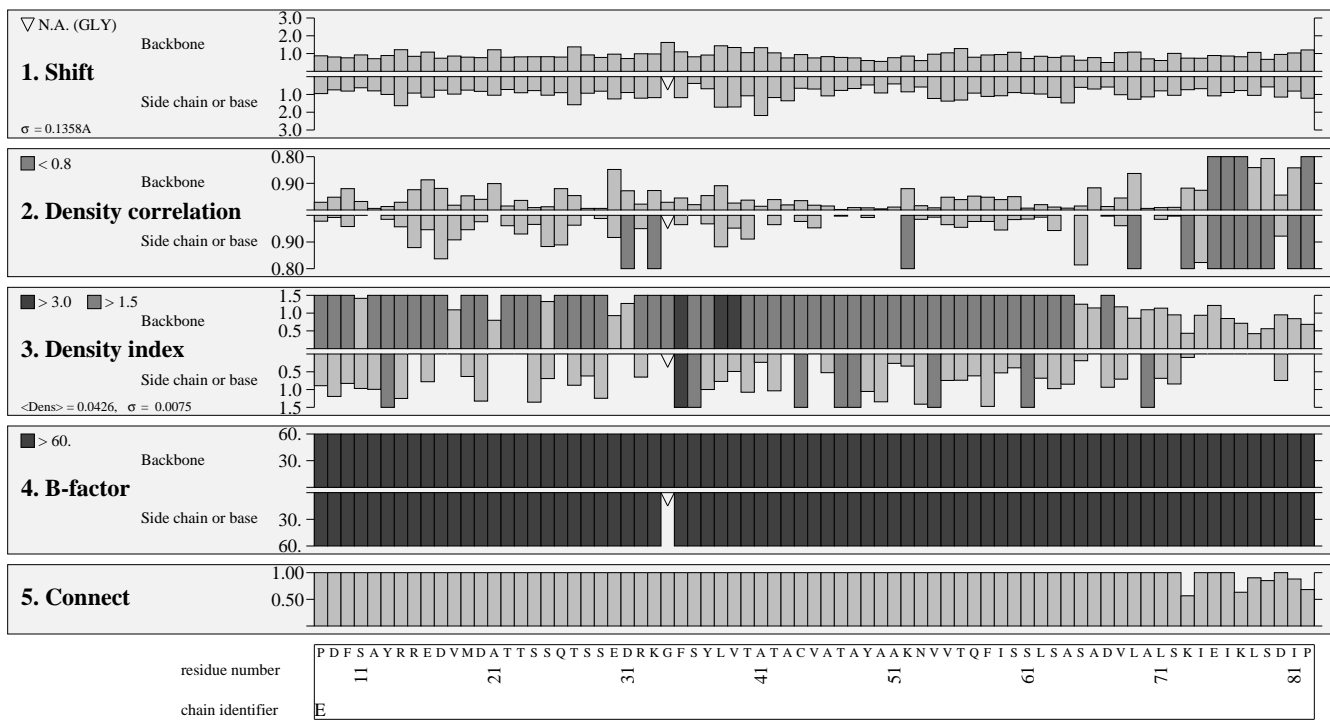
Local estimation (10)



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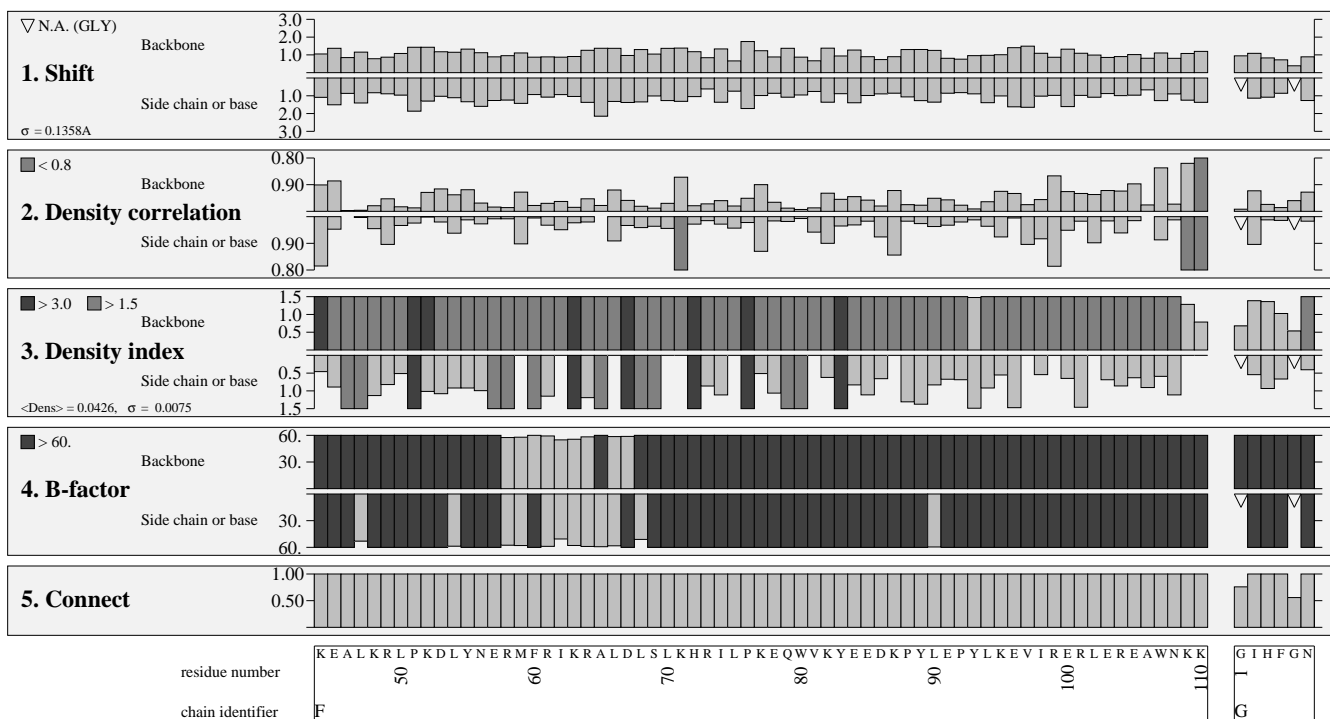
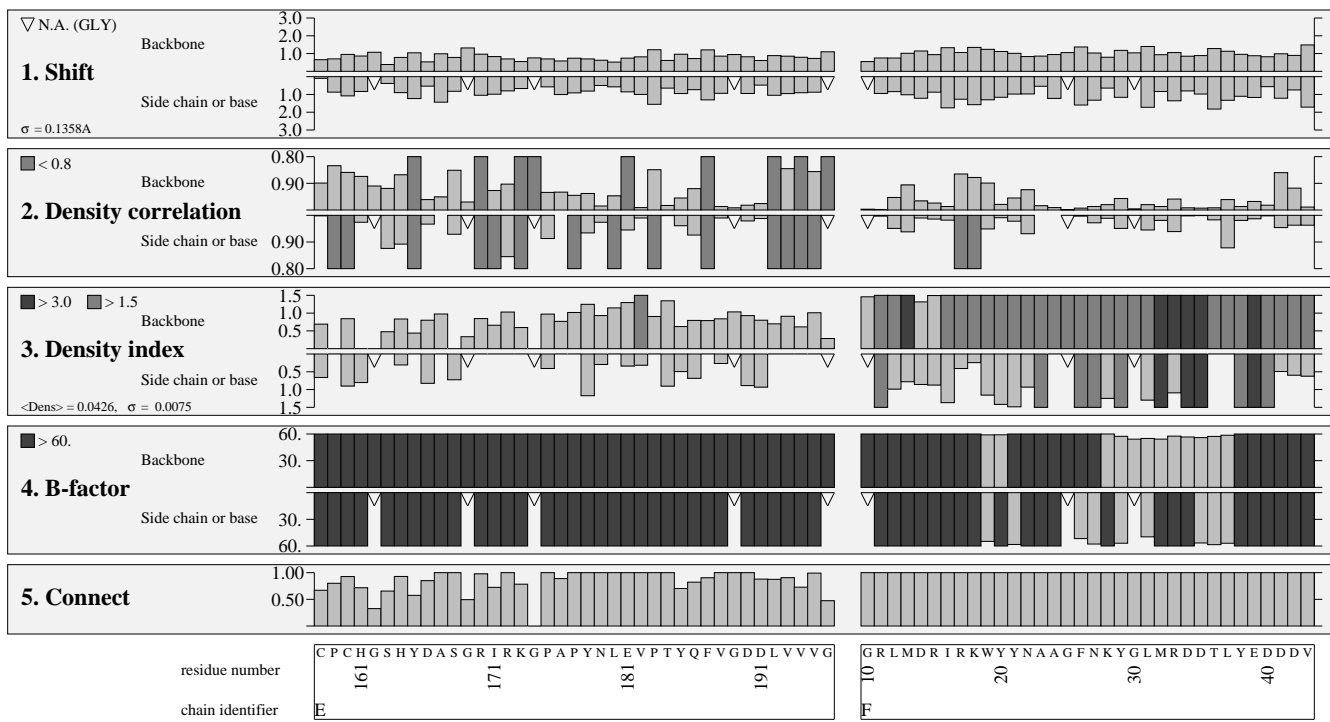
Local estimation (11)



Structure Factor Check

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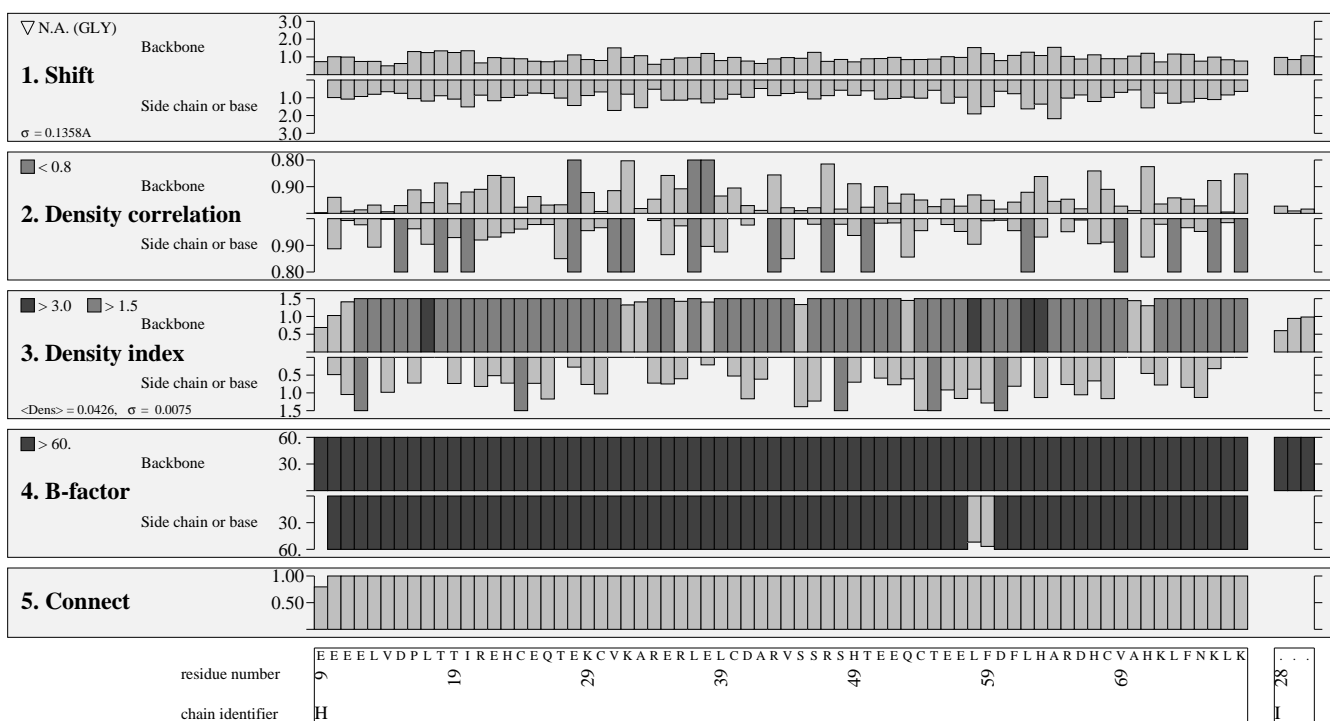
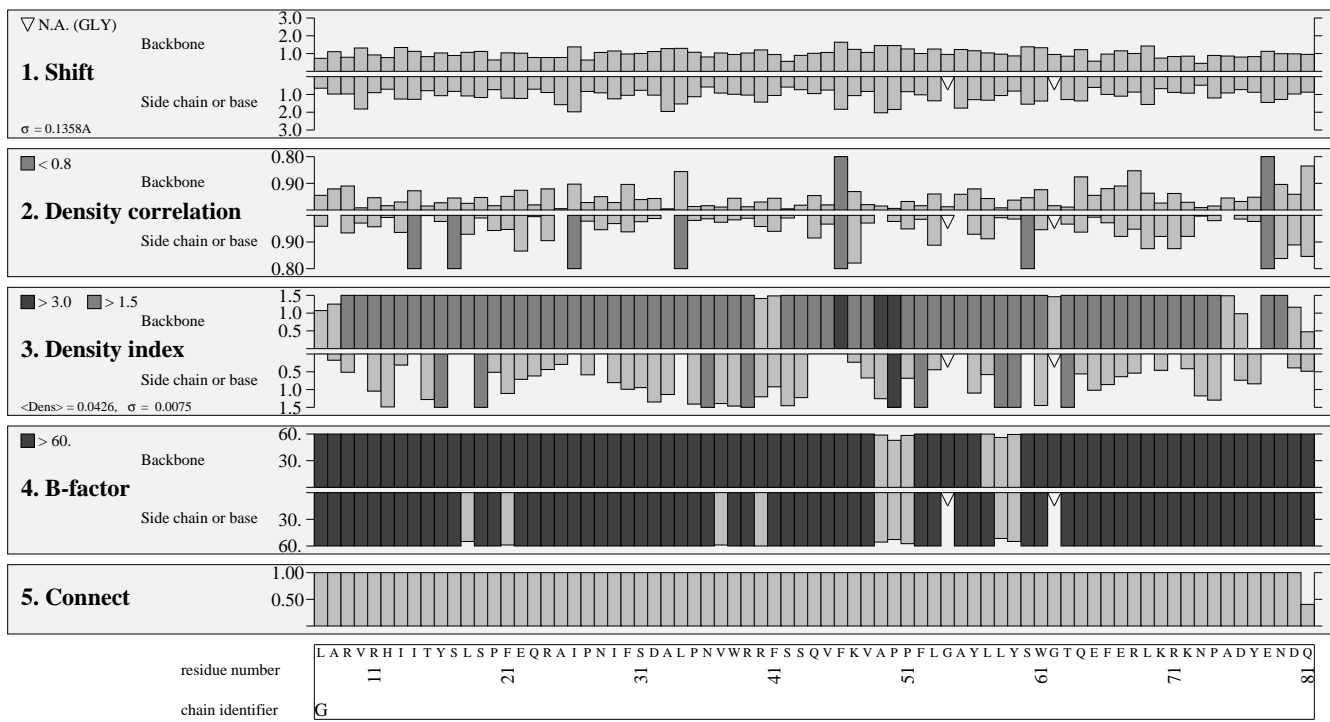
Local estimation (12)



Structure Factor Check

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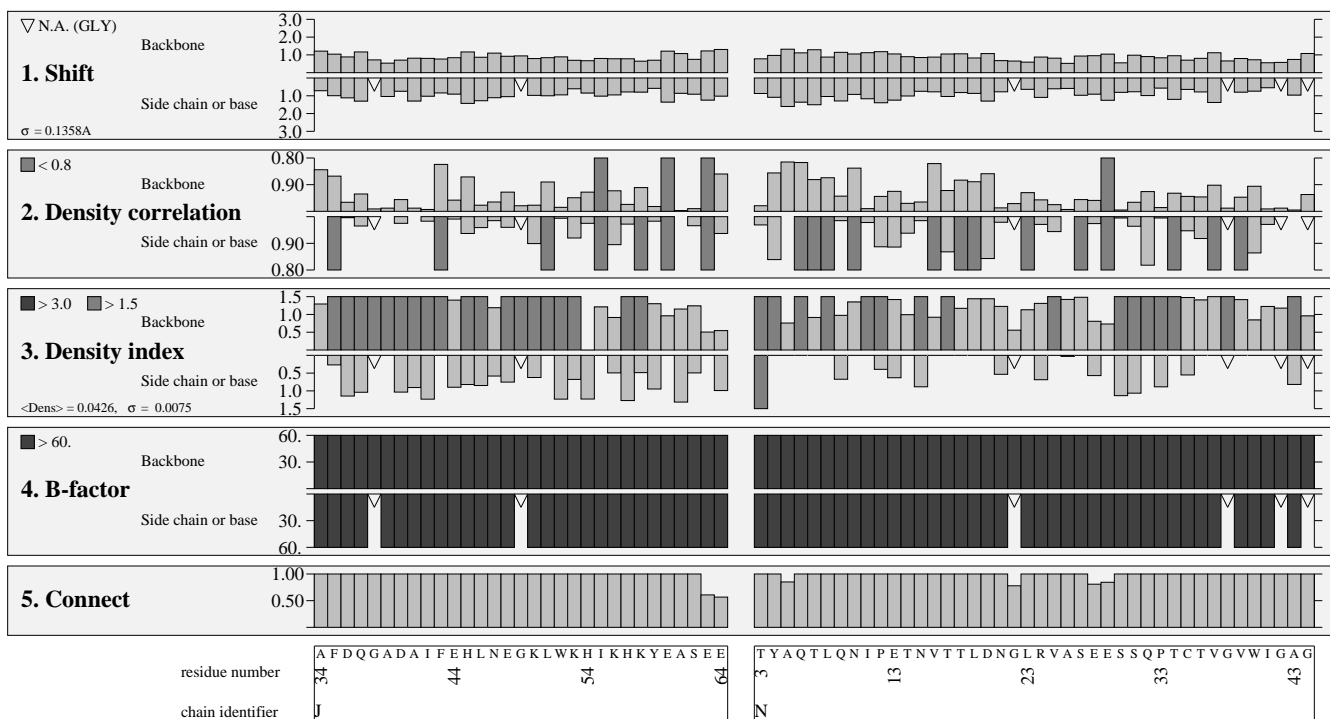
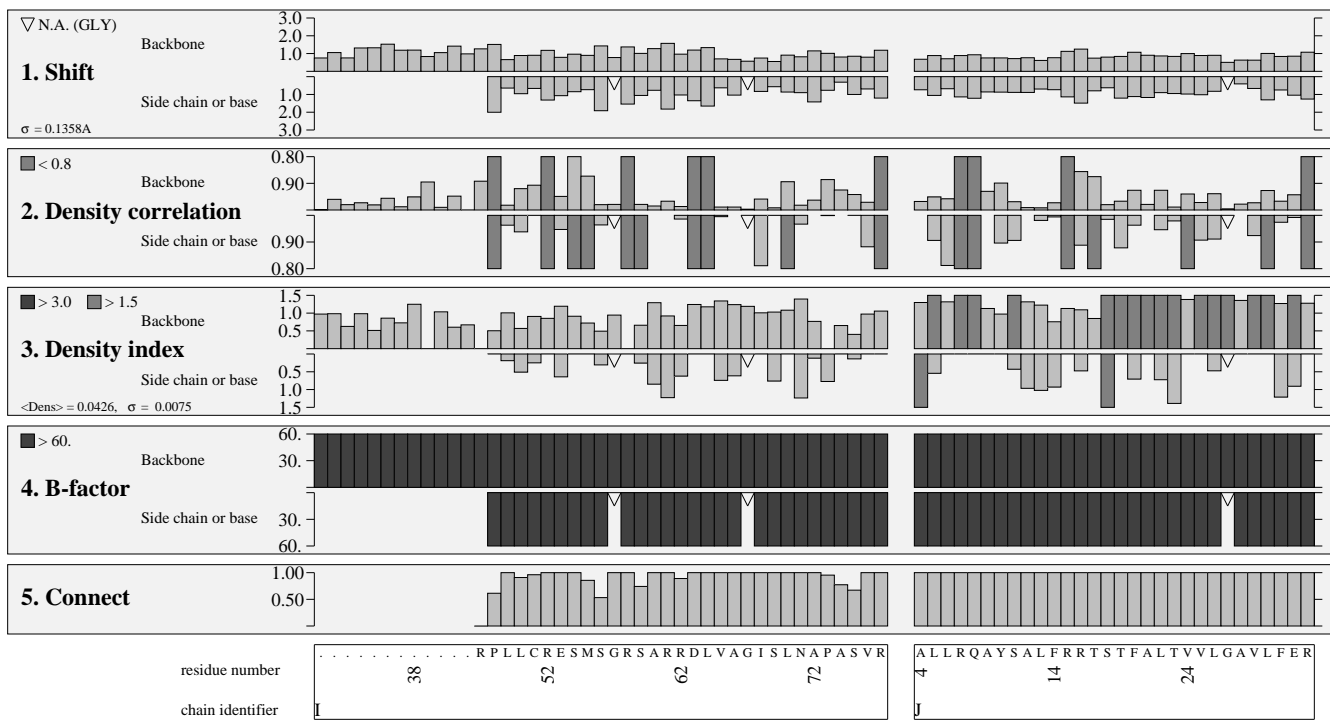
Local estimation (13)



Structure Factor Check

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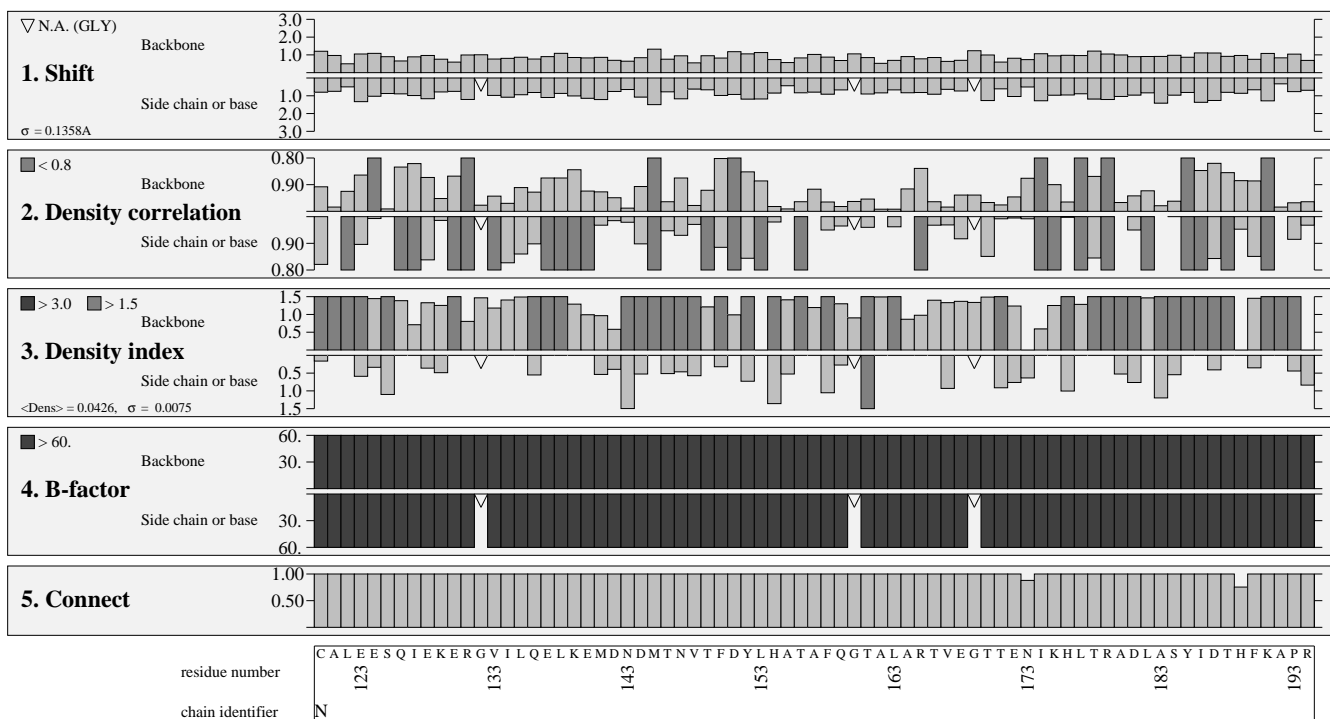
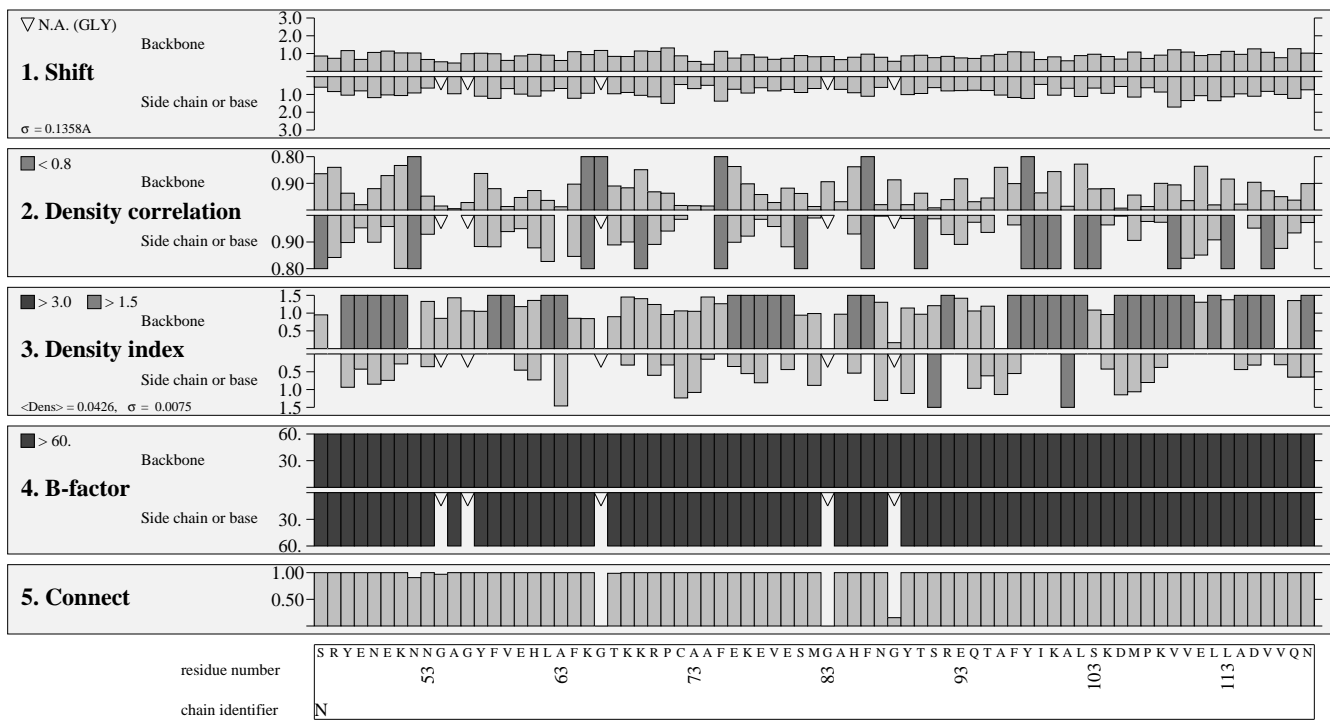
Local estimation (14)



Structure Factor Check

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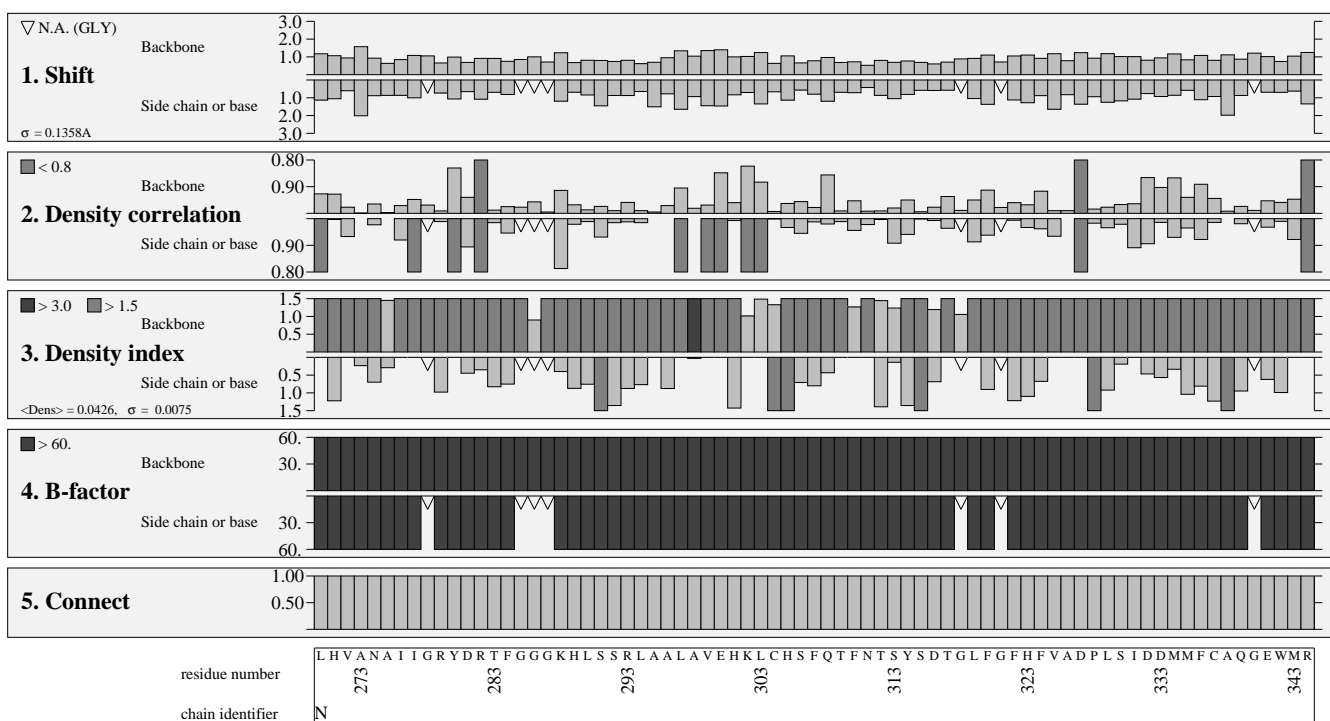
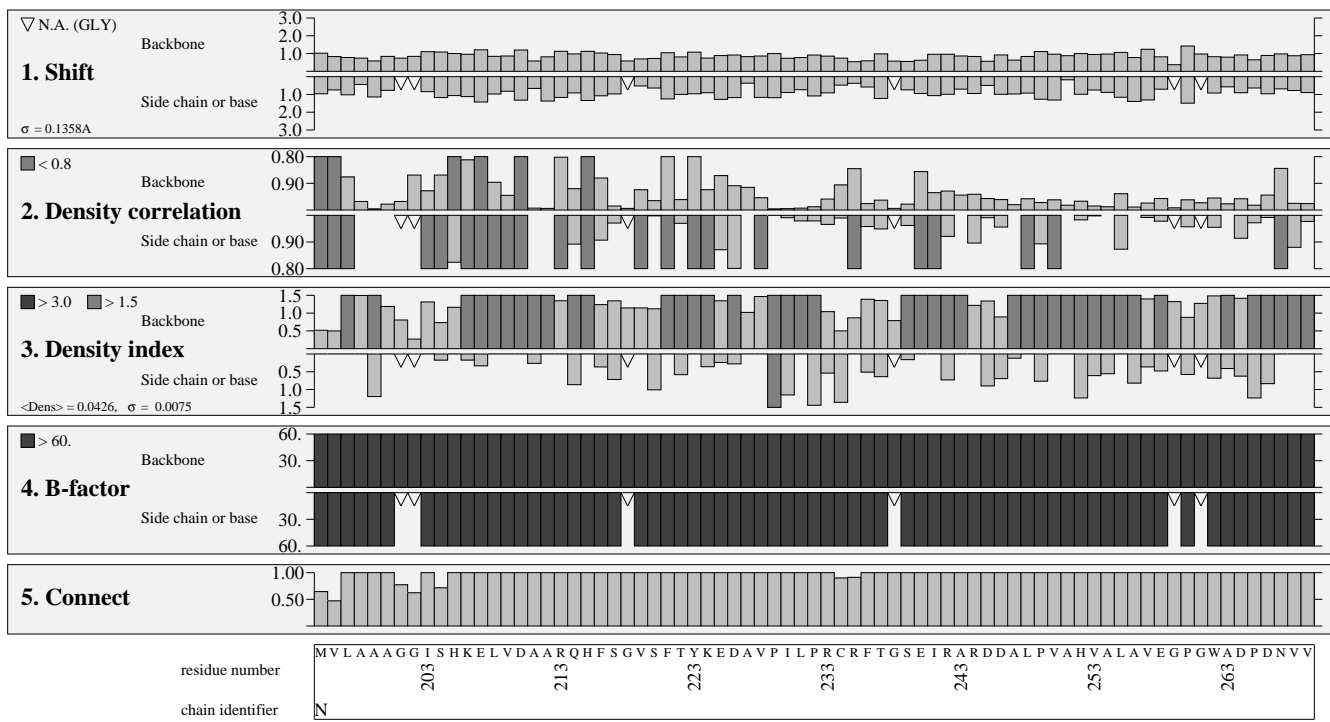
Local estimation (15)



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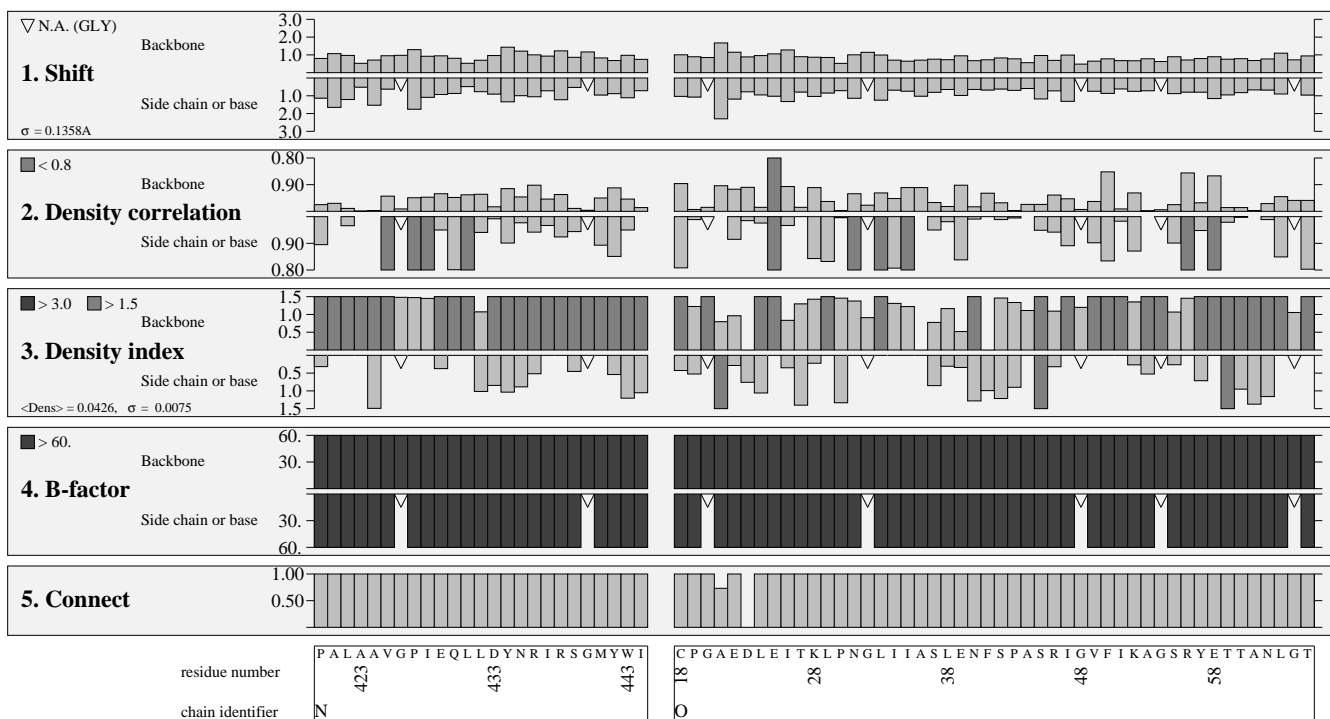
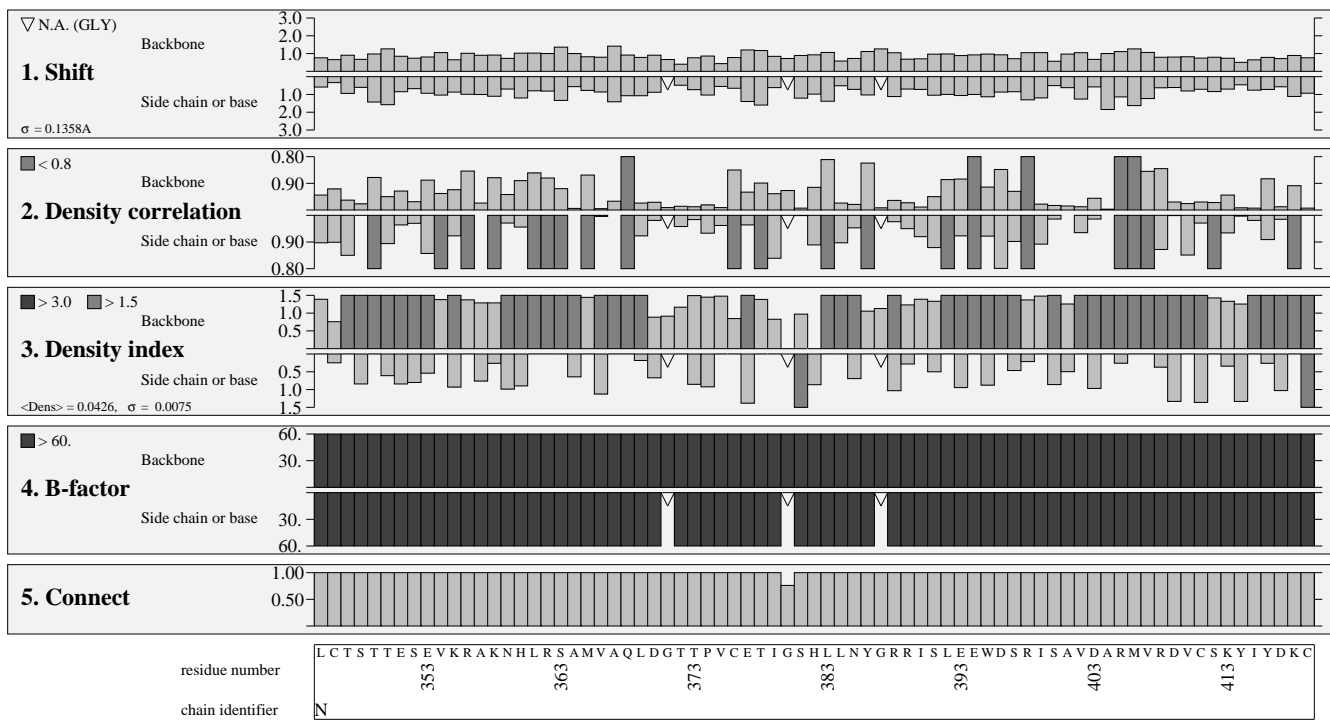
Local estimation (16)



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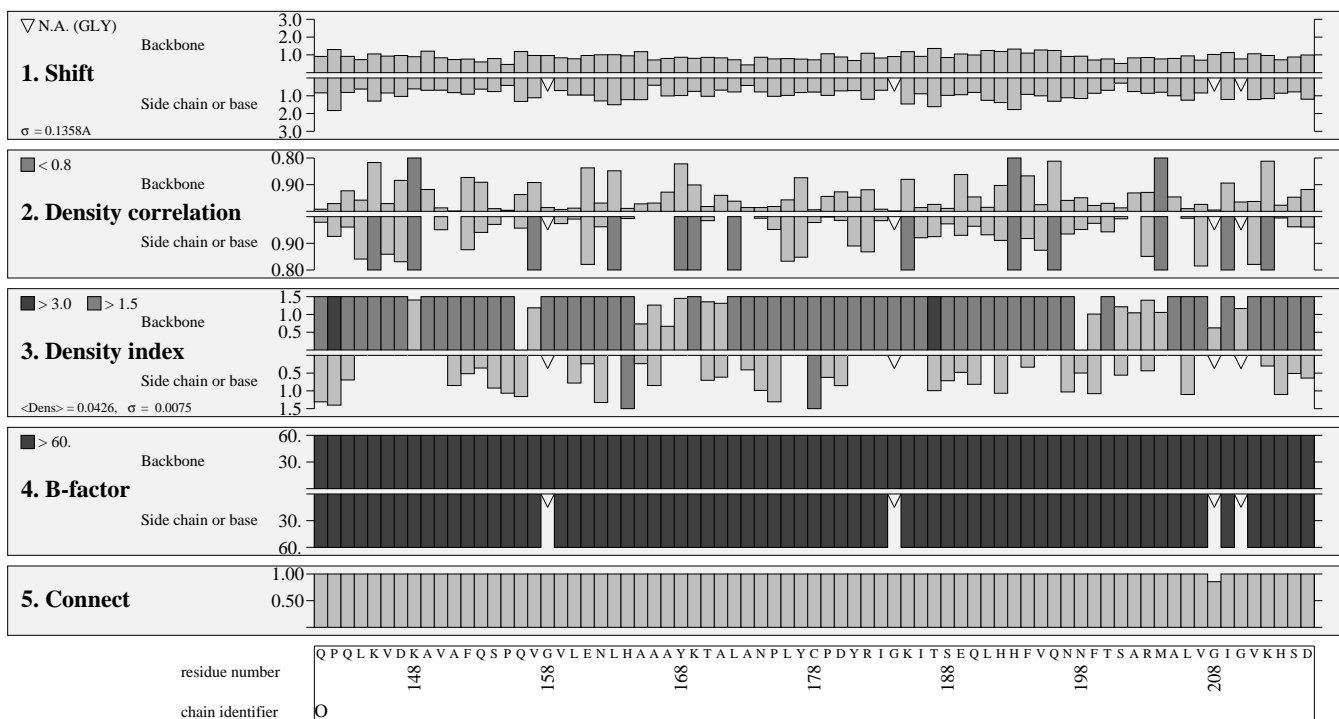
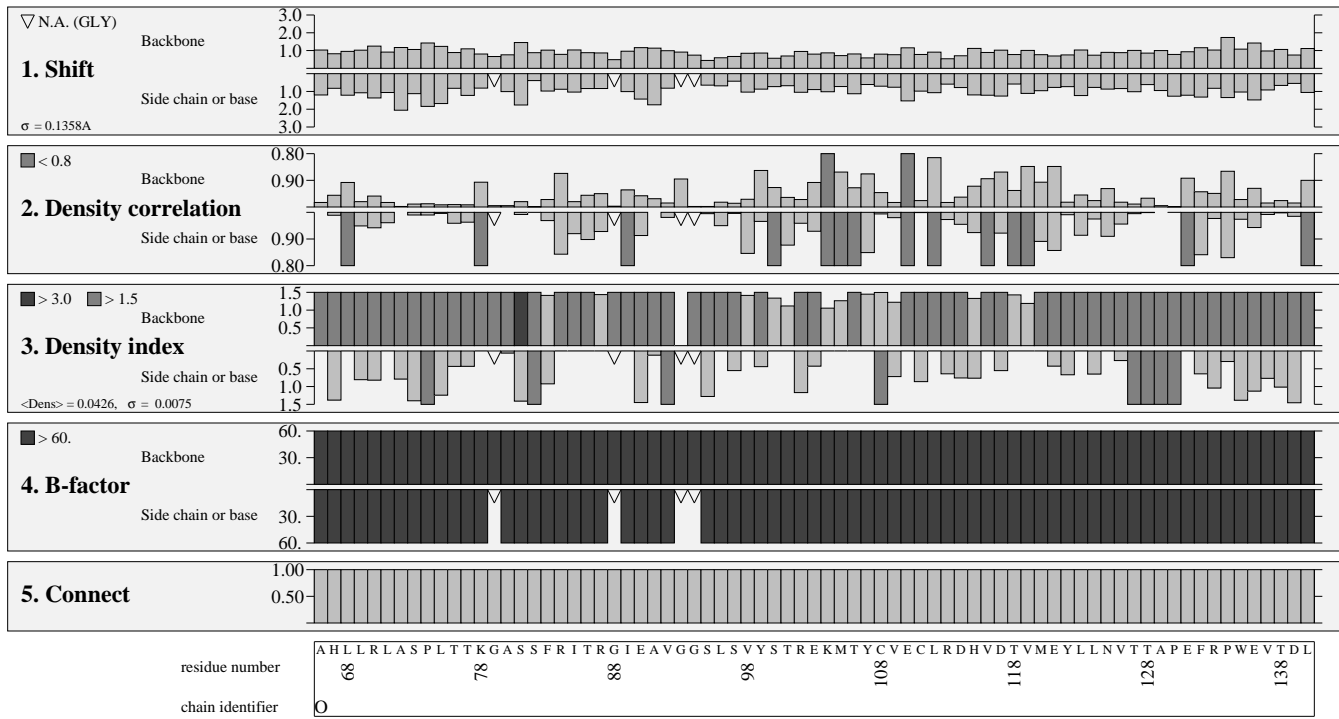
Local estimation (17)



Structure Factor Check

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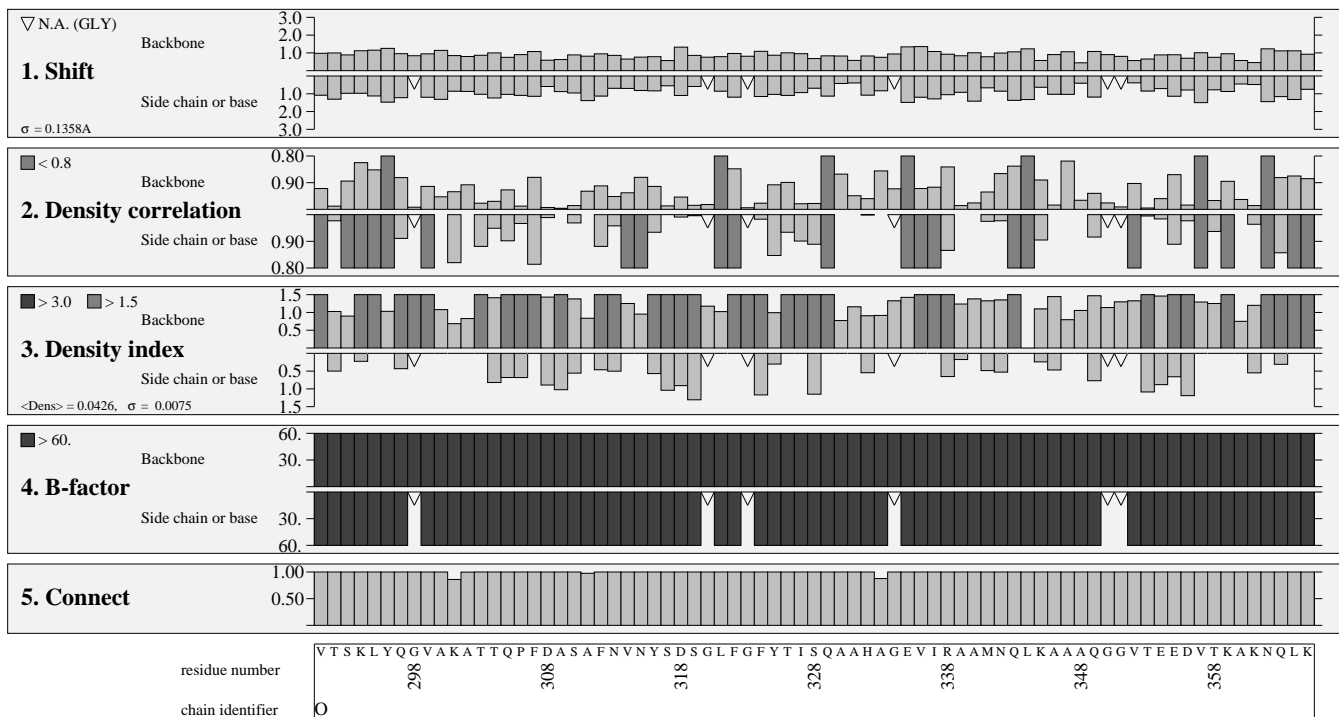
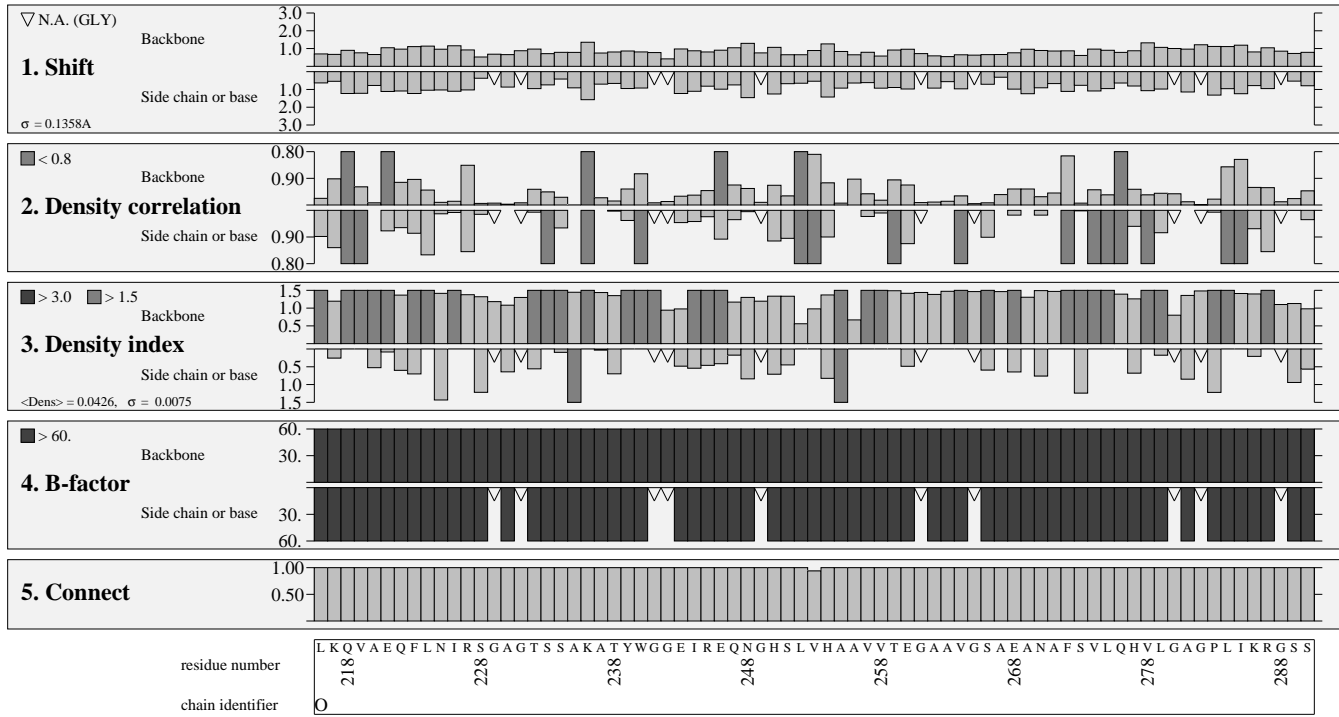
Local estimation (18)



Structure Factor Check

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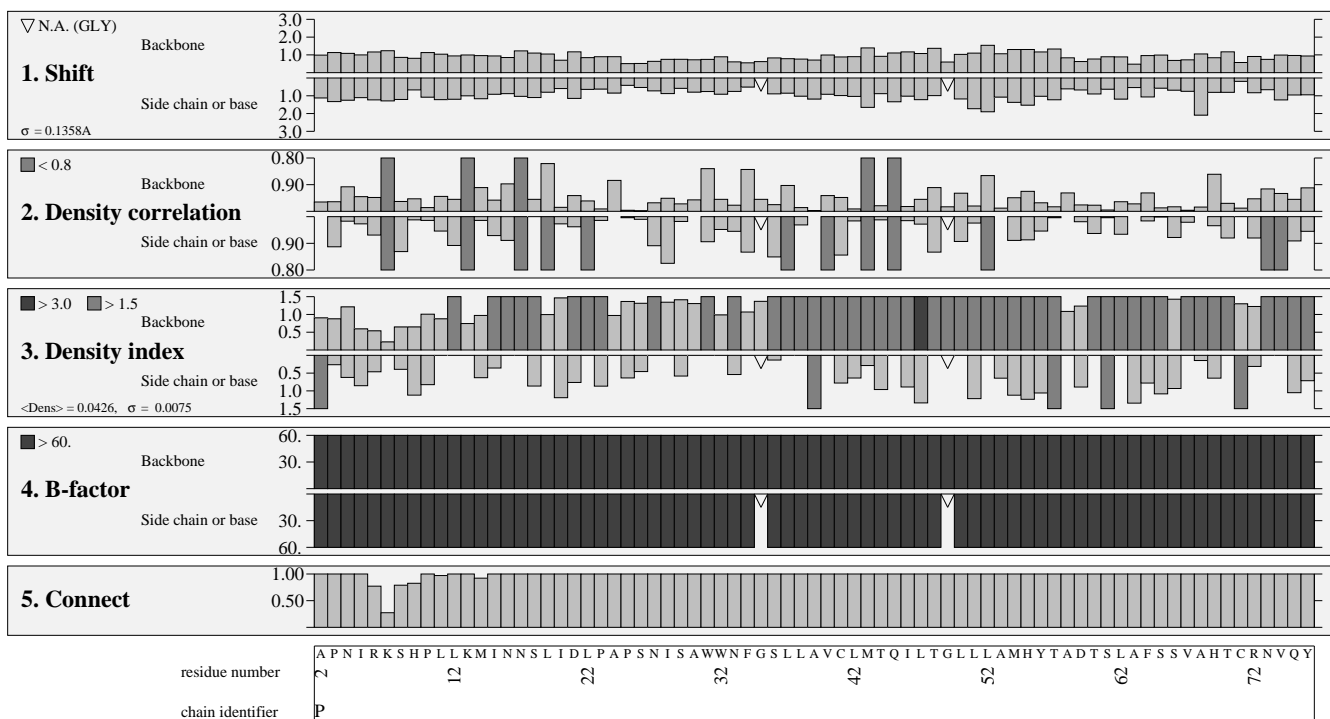
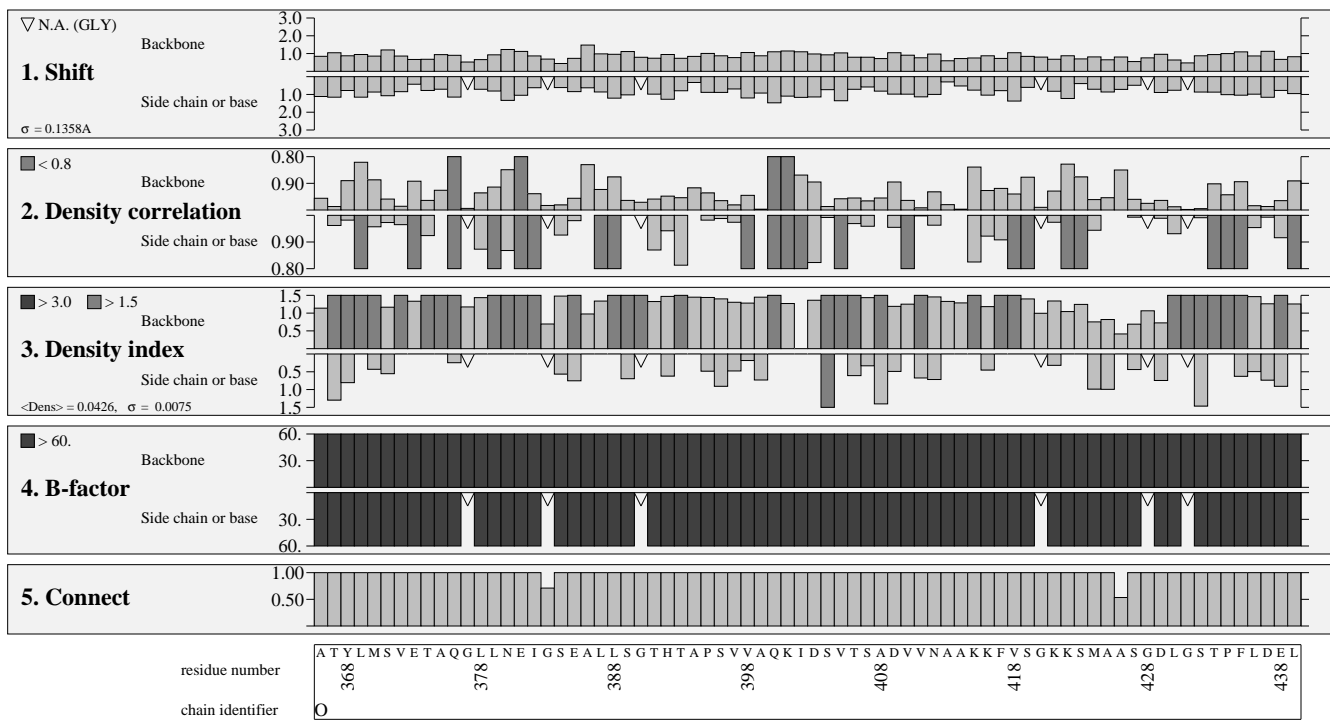
Local estimation (19)



Structure Factor Check

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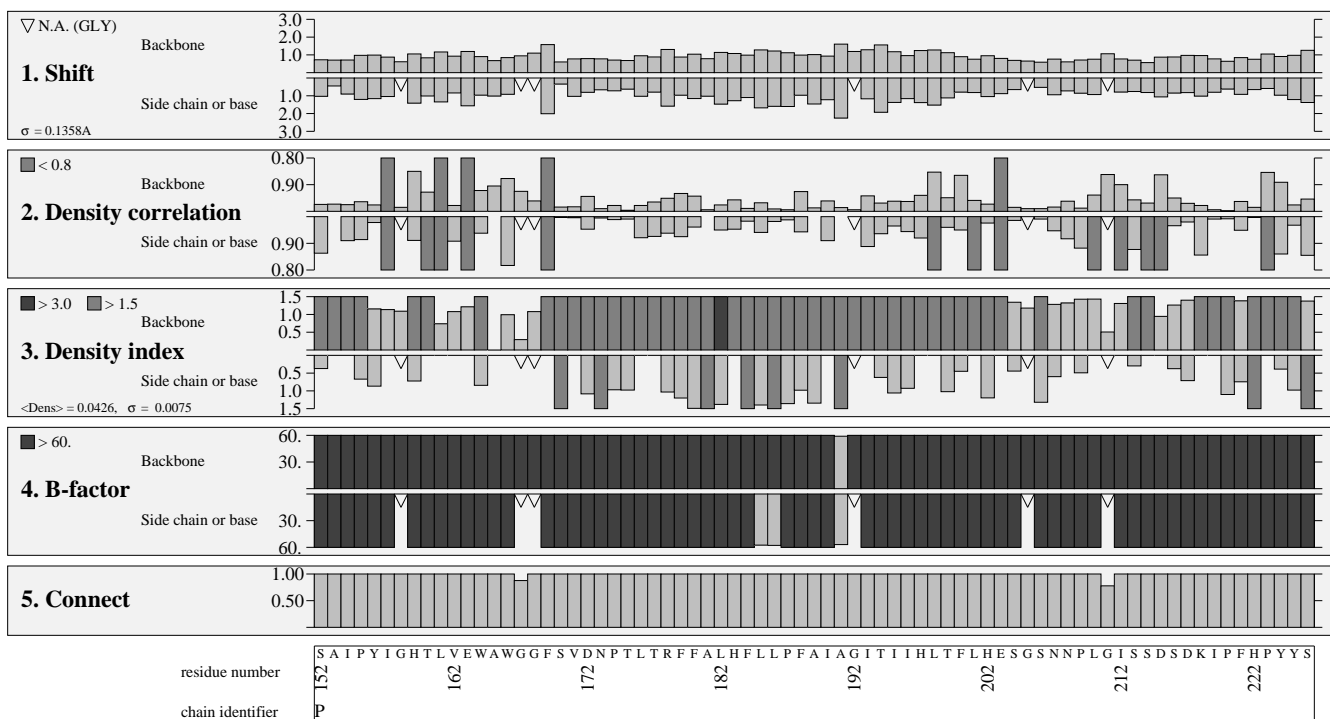
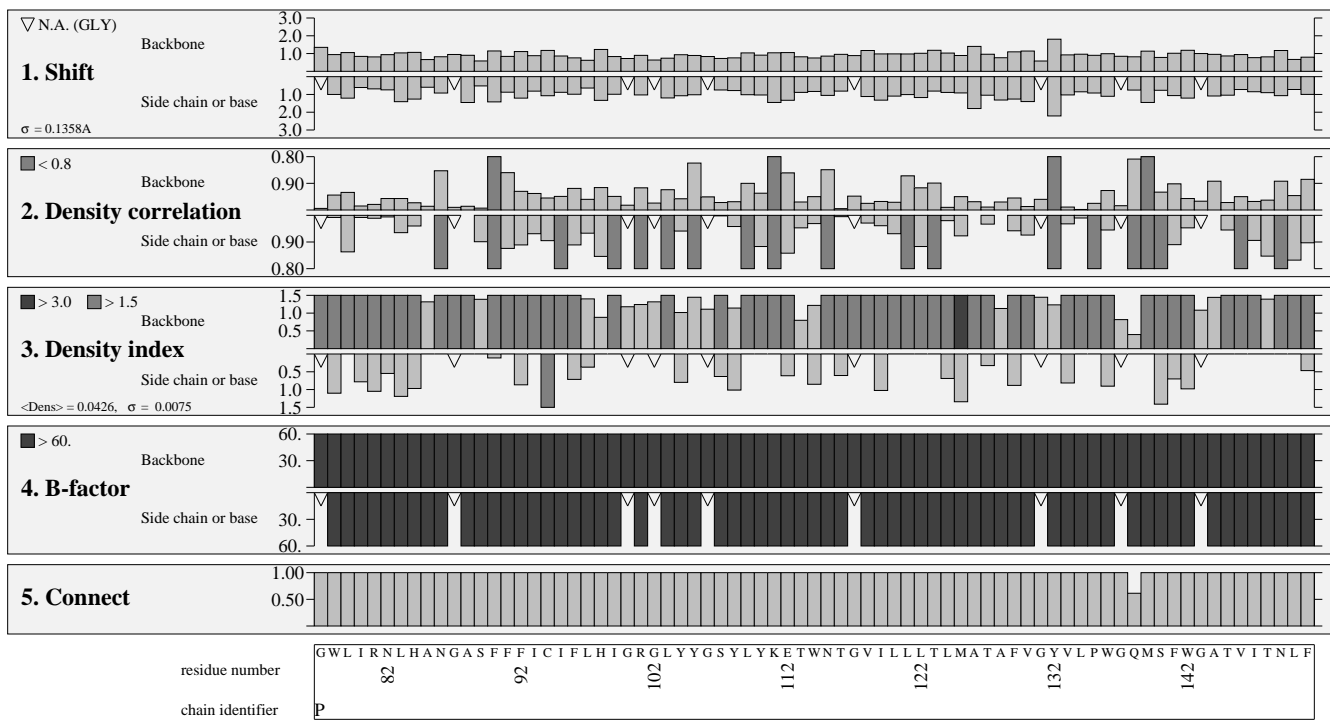
Local estimation (20)



Structure Factor Check

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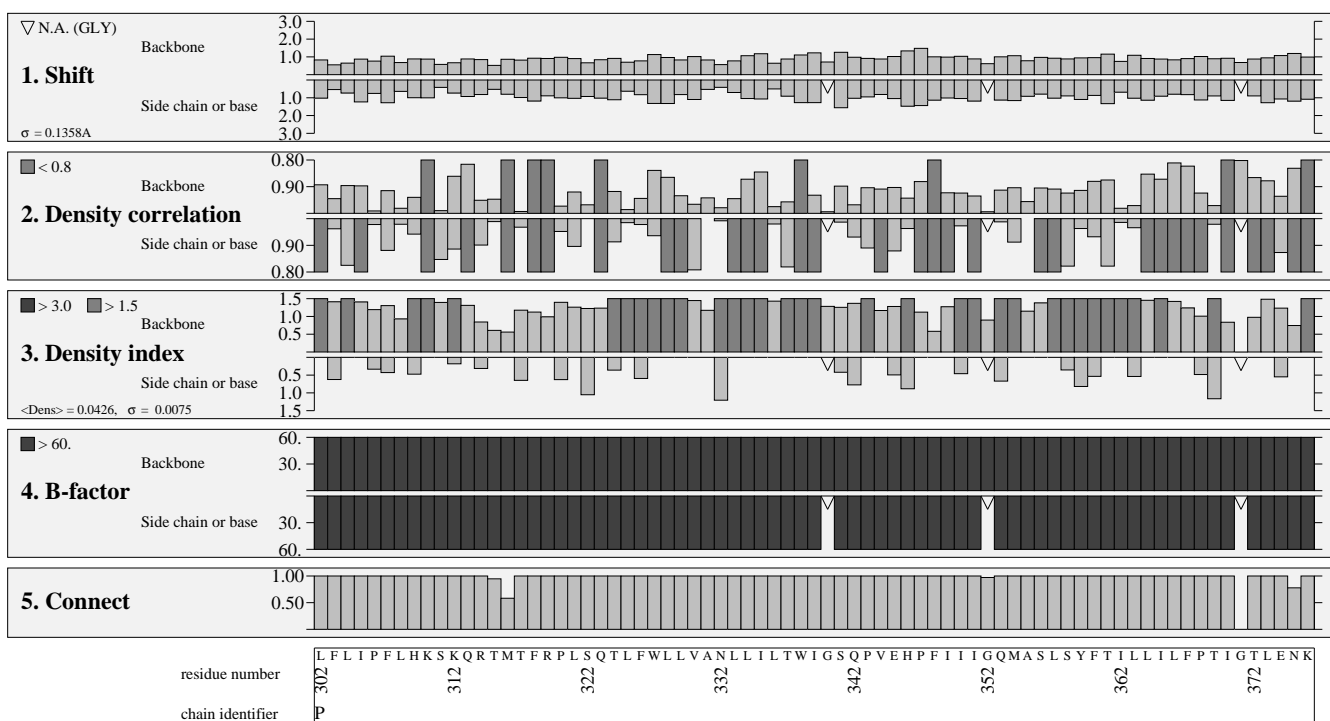
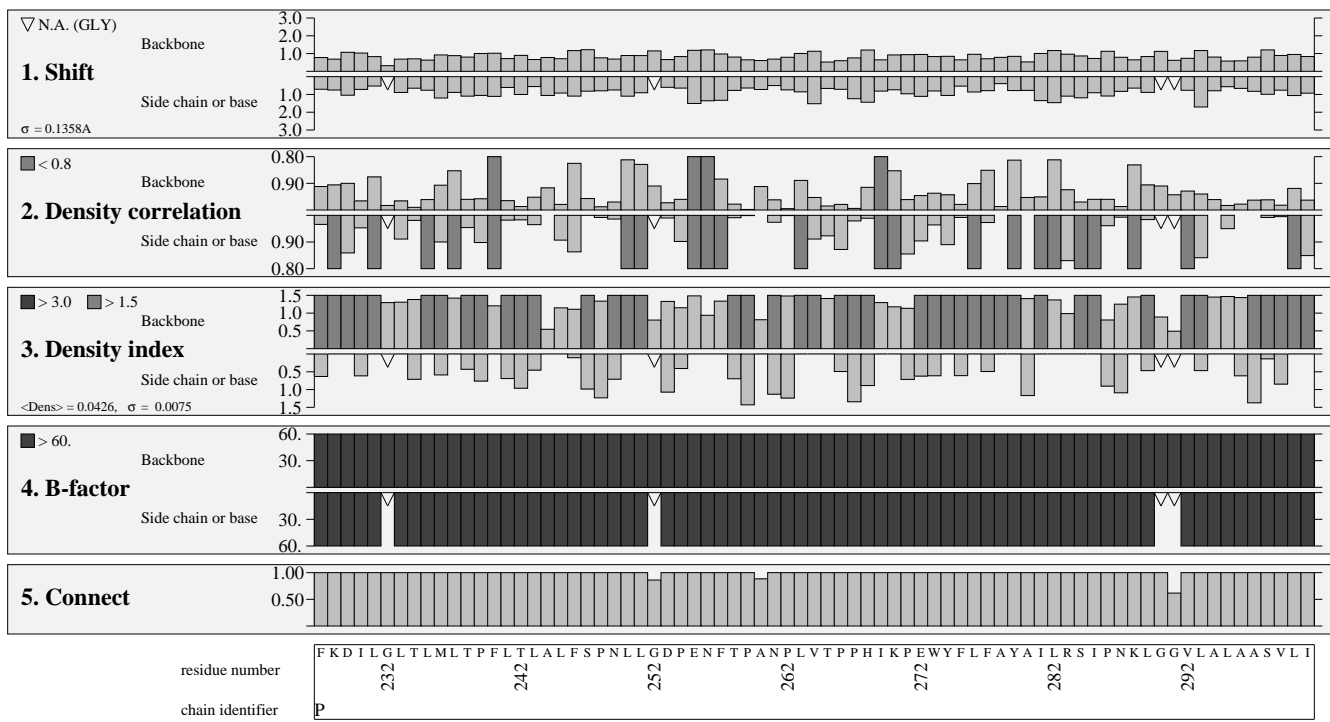
Local estimation (21)



Structure Factor Check

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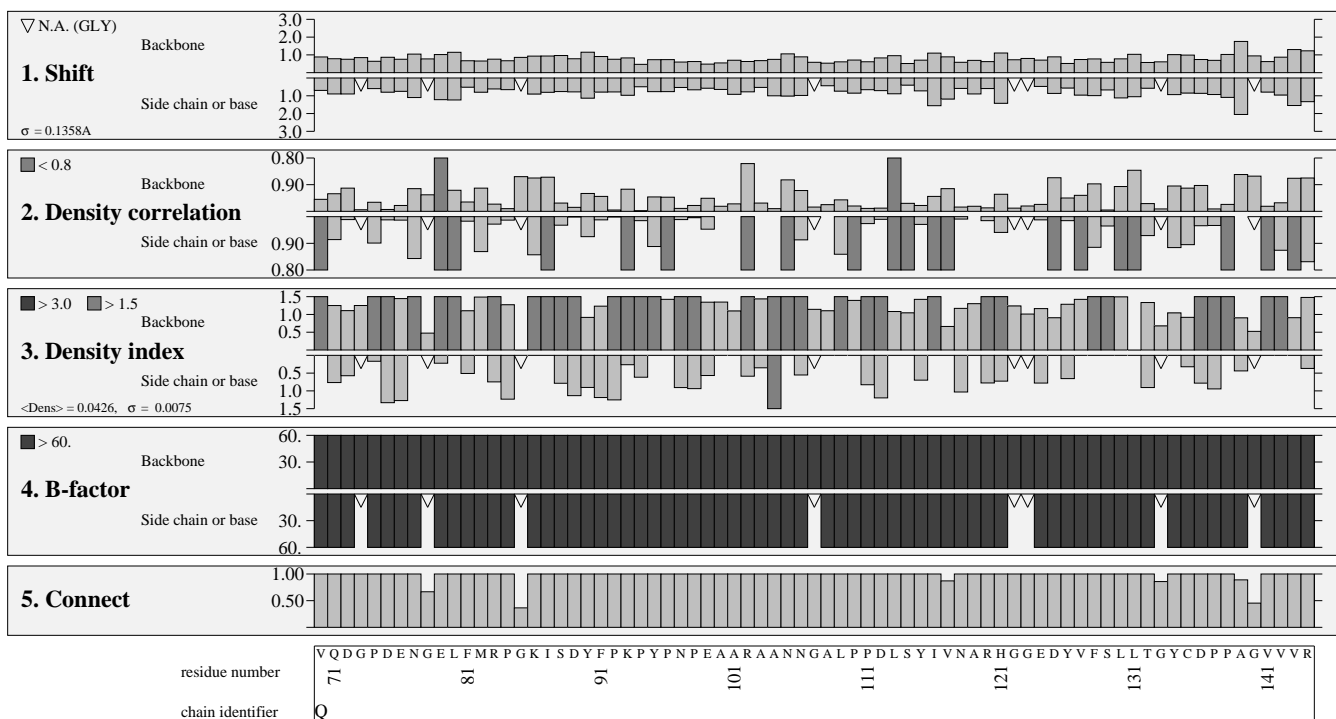
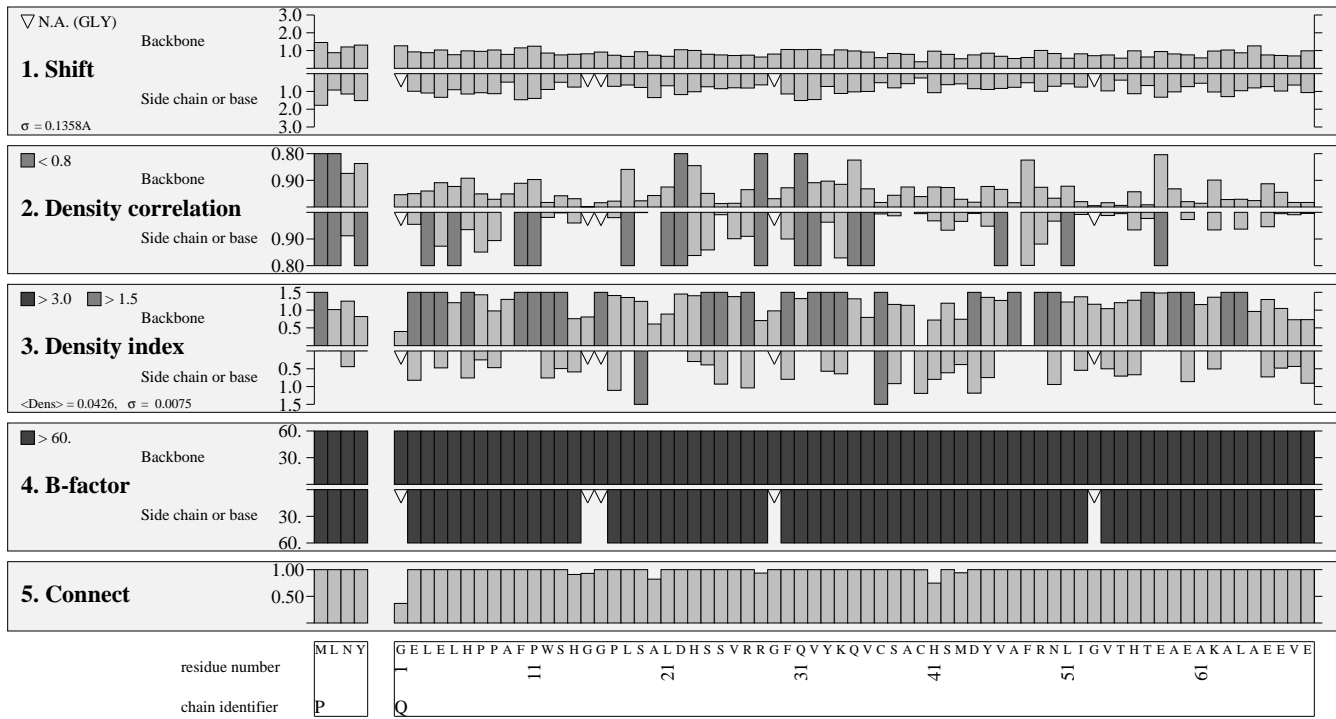
Local estimation (22)



Structure Factor Check

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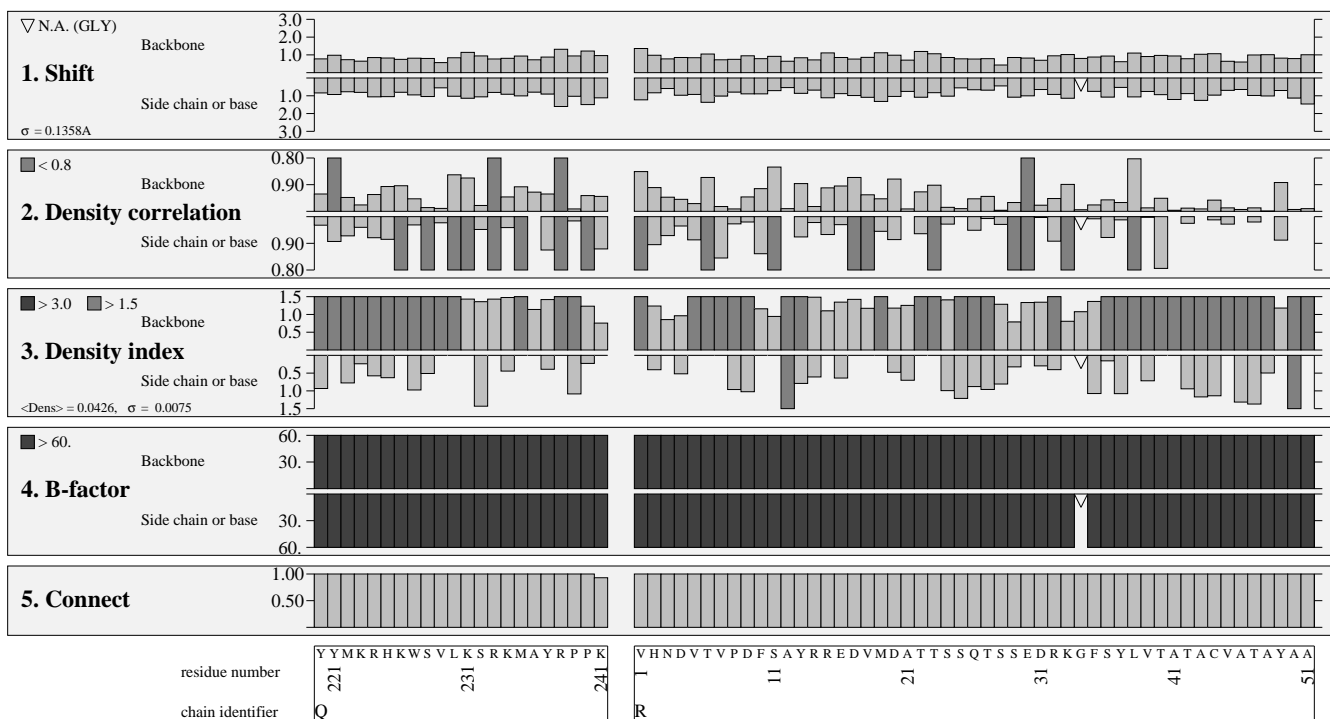
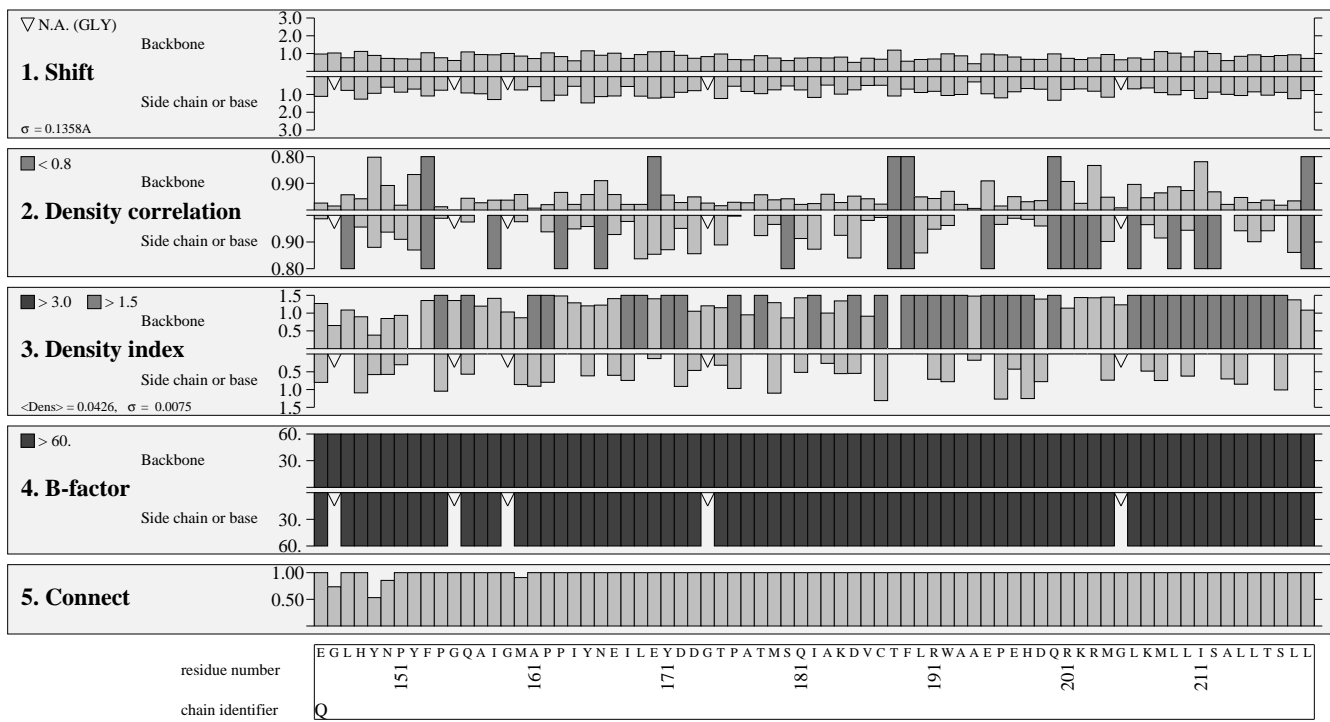
Local estimation (23)



Structure Factor Check

3H1L

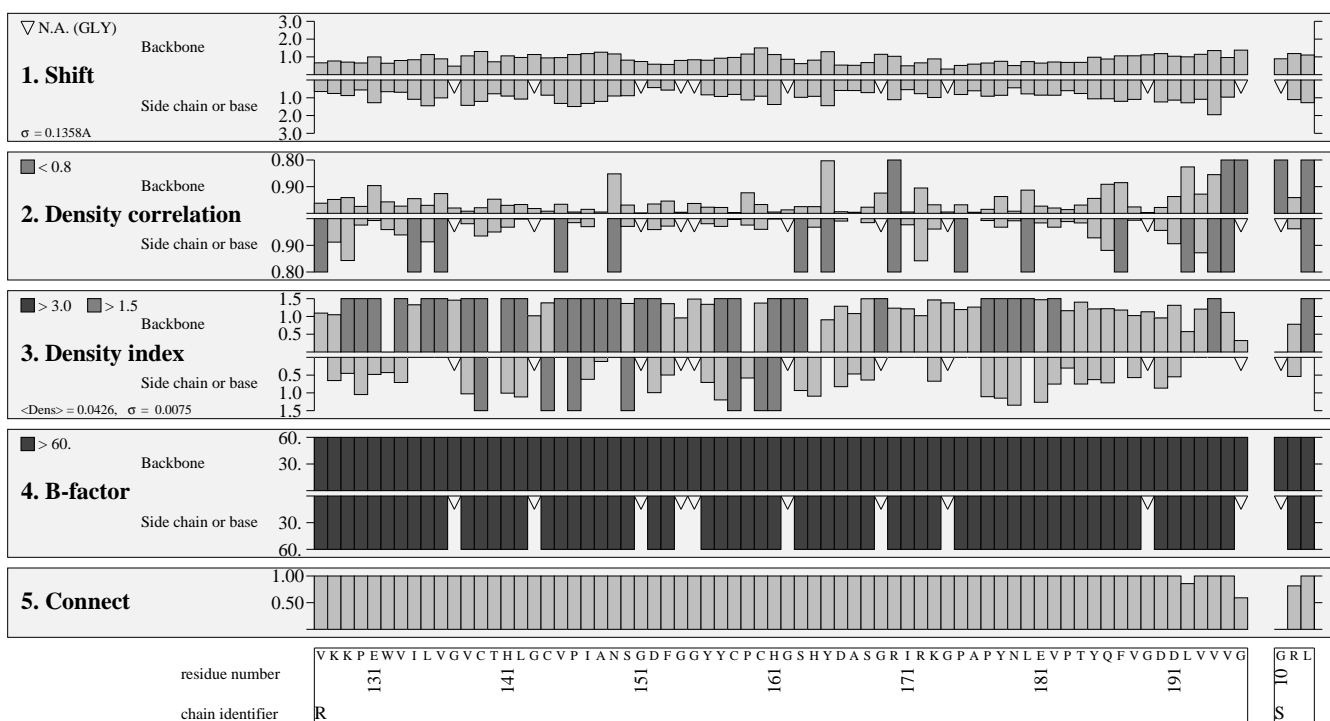
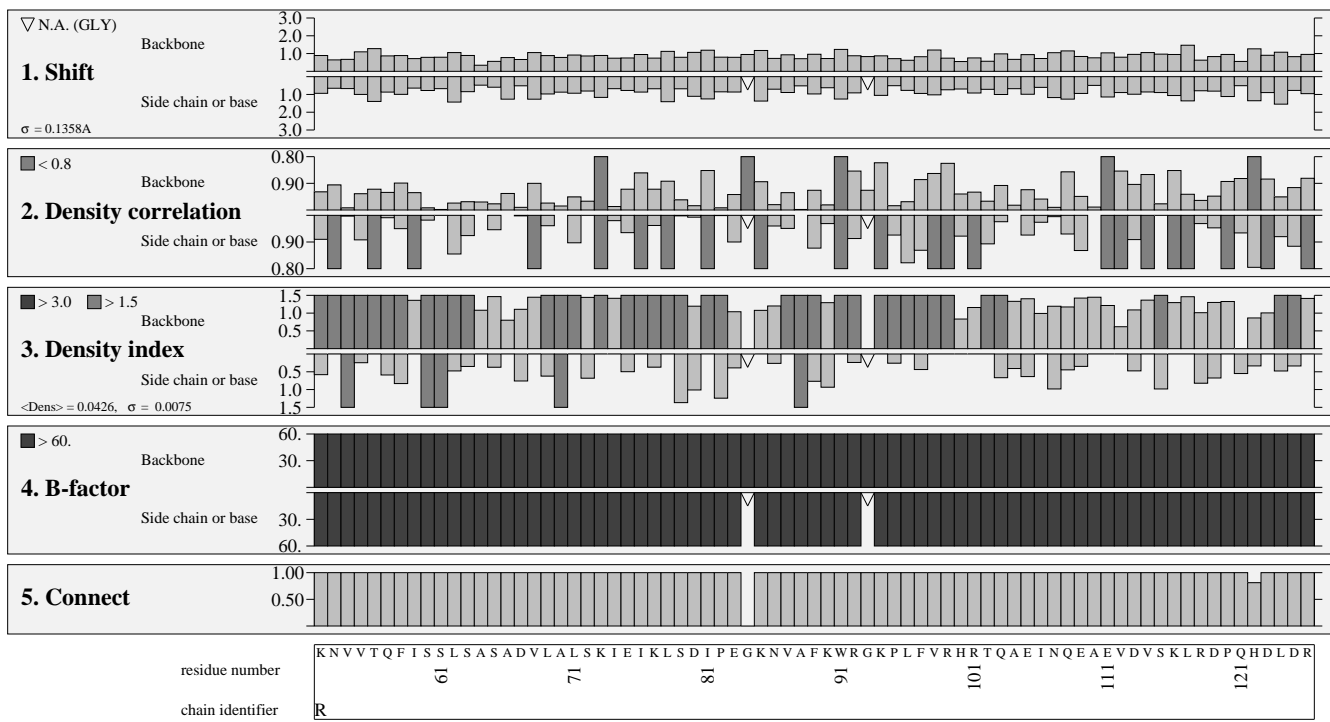
Local estimation (24)



Structure Factor Check

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Local estimation (25)



Structure Factor Check

3H1L

Local estimation (26)

