

Structure Factor Check

1YQ3

Title: AVIAN RESPIRATORY COMPLEX II WITH OXALOACETATE AND UBIQUINON
Date: 01-FEB-05
PDB code: 1YQ3

Crystal

Cell parameters:

a: 70.01 Å b: 84.40 Å c: 289.50 Å
α: 90.00 β: 90.00 γ: 90.00

Space group: P 21 21 21

Model

9576 atoms (834 water molecules)

Number of chains: 49

Volume not occupied by model: 51.7 %

 (for atomic model): 44.9 Å²

σ(B): 12.74 Å²

Matthews coefficient: 3.19

Corresponding solvent % : 61.14

Refinement

Program: CNS 1.1

Nominal resolution range: 38.7 – 2.20 Å

Reported R-factor: 0.175

Number of reflections used: 78719

Reported Rfree: 0.22

Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 38.7 – 2.20 Å

Reflections in file: 78719

Unique reflections above 0: 78719

above 1σ: 78184

above 3σ: 67042

SFCHECK

Nominal resolution range: 38.7 – 2.20 Å
05max. from input data, min. from author\05

Used reflections: 78719

Completeness: 89.5 %

R_{stand}(F) = <σ(F)>/<F> : 0.046

Anisotropic distribution of Structure Factors

ratio of eigen values: 0.7915 1.0000 0.4959

B_{overall} (by Patterson): 37.Å²

Optical resolution: 1.76 Å

Expected opt. resol. for complete data set: 1.76 Å

Estimated minimal error: 0.018 Å

Model vs. Structure Factors

R-factor for all reflections: 0.187

Correlation factor: 0.951

R-factor: 0.196

for F > 2.0σ

nom. resolution range: 38.66 – 2.20Å

reflections used: 78182

Rfree: 0.242

Nfree: 3815

R-factor without free-refl.: 0.193

Non free-reflections: 74367

<u> (error in coords by Luzzati plot): 0.229 Å

Estimated maximal error: 0.080 Å

DPI: 0.178 Å

Scaling

Scale: 0.849

Bdiff: -1.64

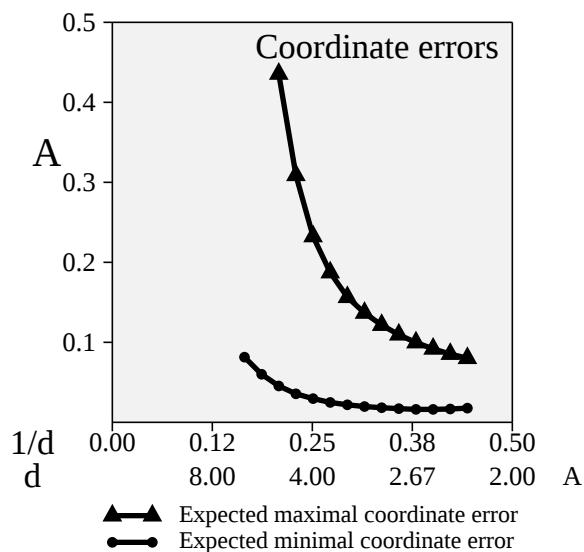
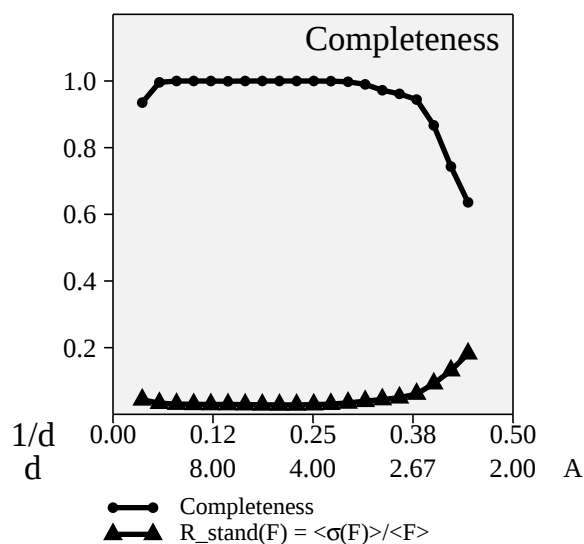
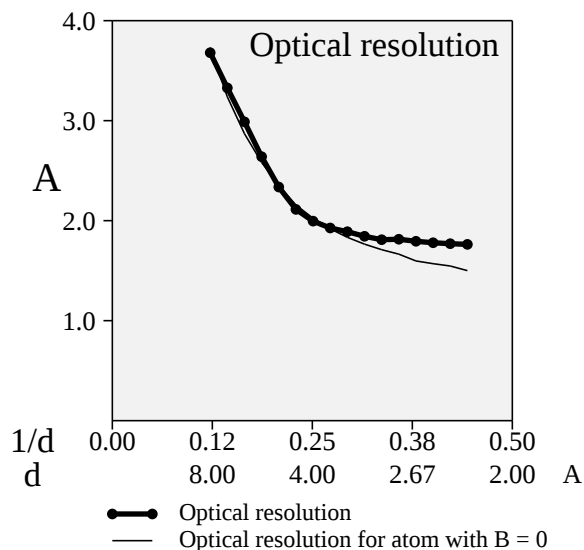
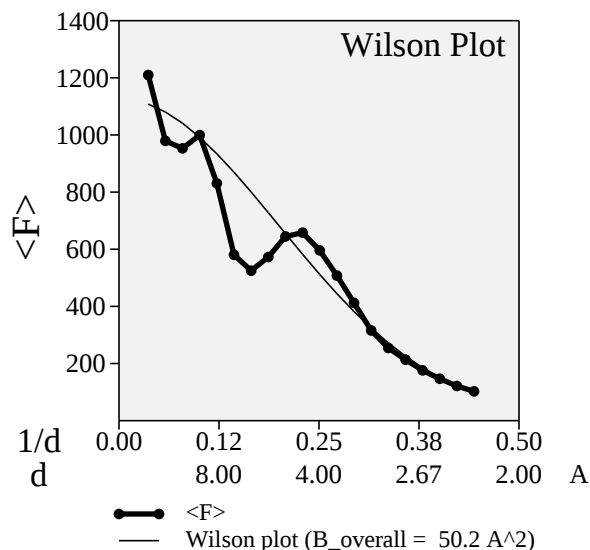
Anisothermal Scaling (Beta):

2.1332 5.3680 -3.1932 0.0000 0.0000 0.0000

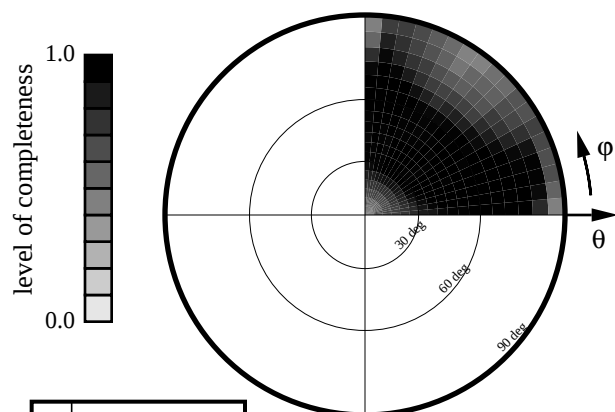
Solvent correction – Ks,Bs: 0.753 250.038

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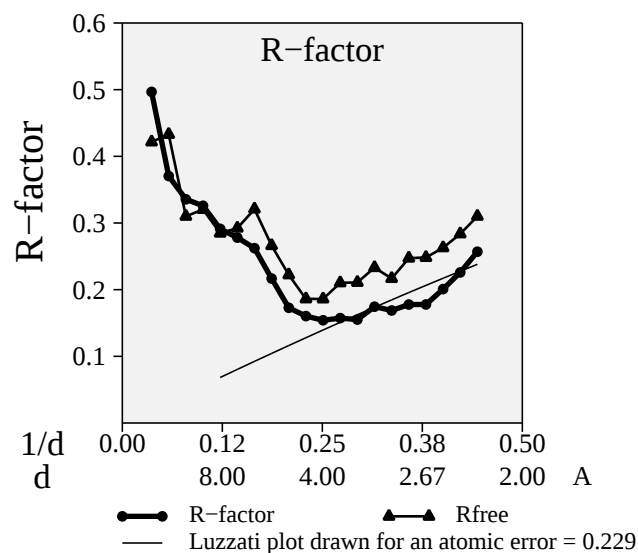


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

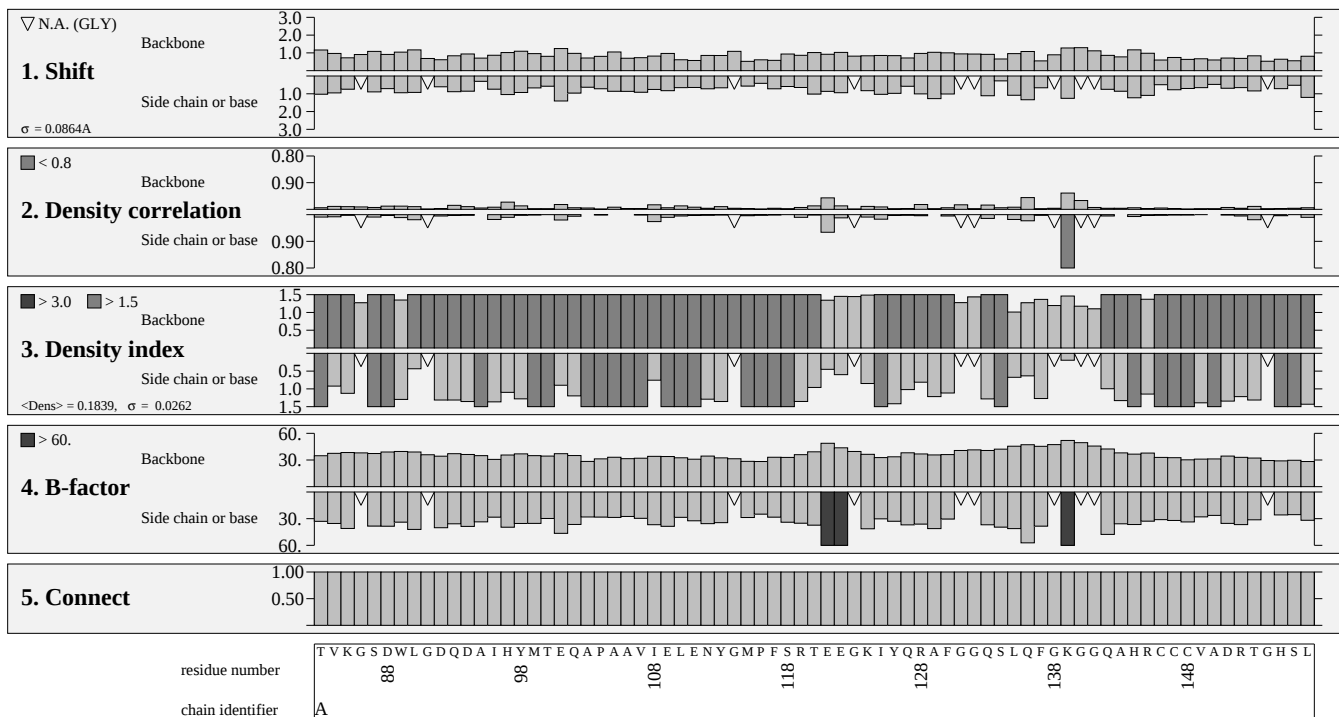
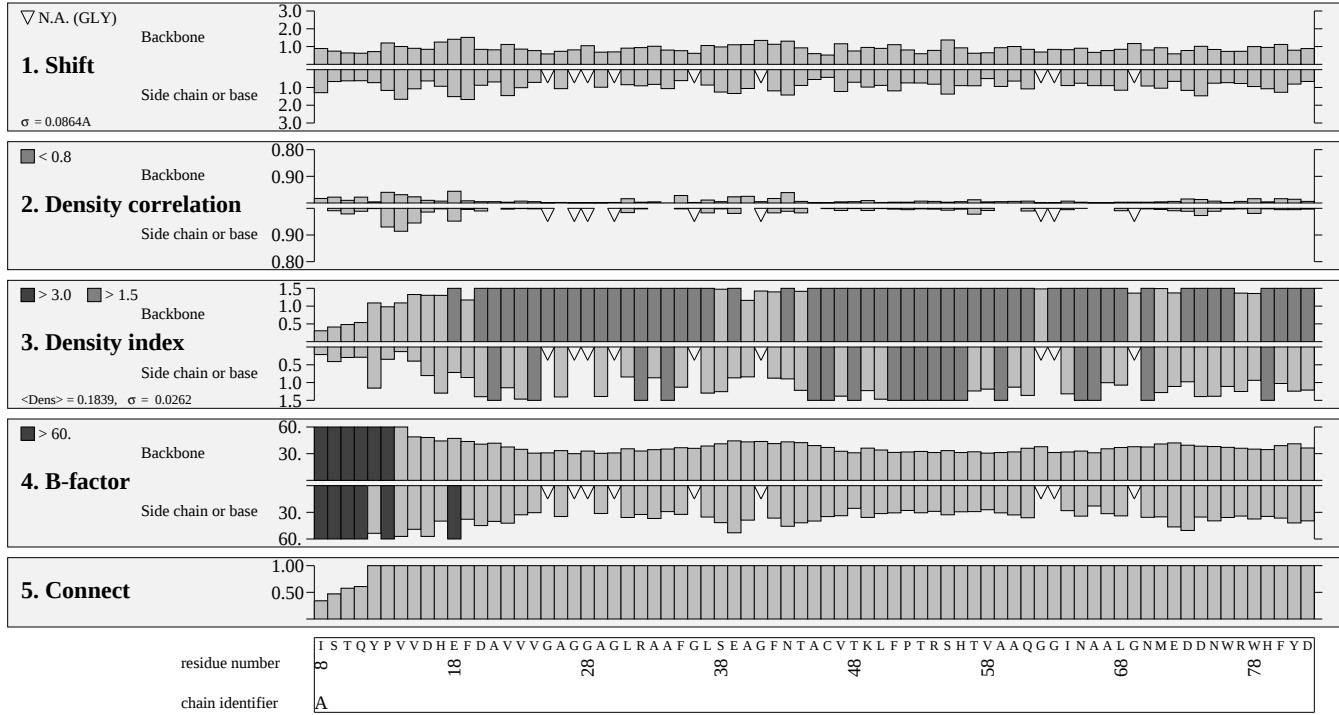
polar coordinates of the crystallographical axes



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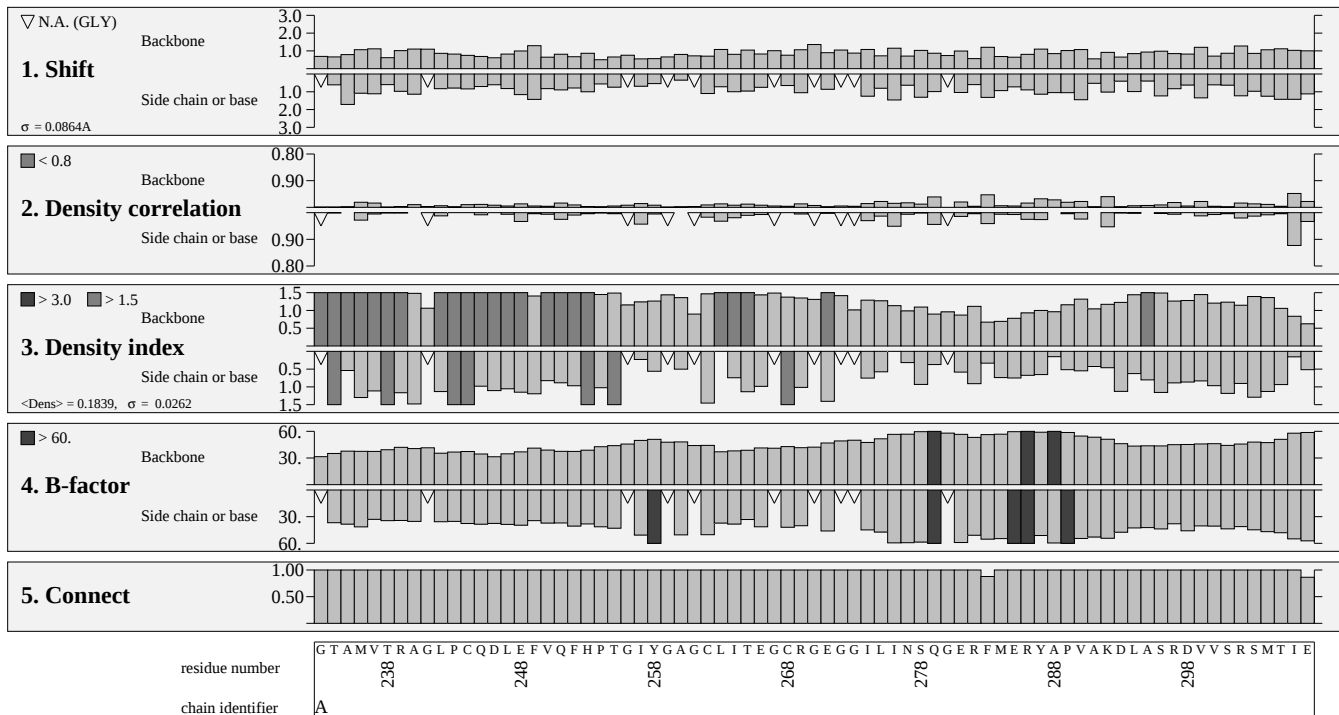
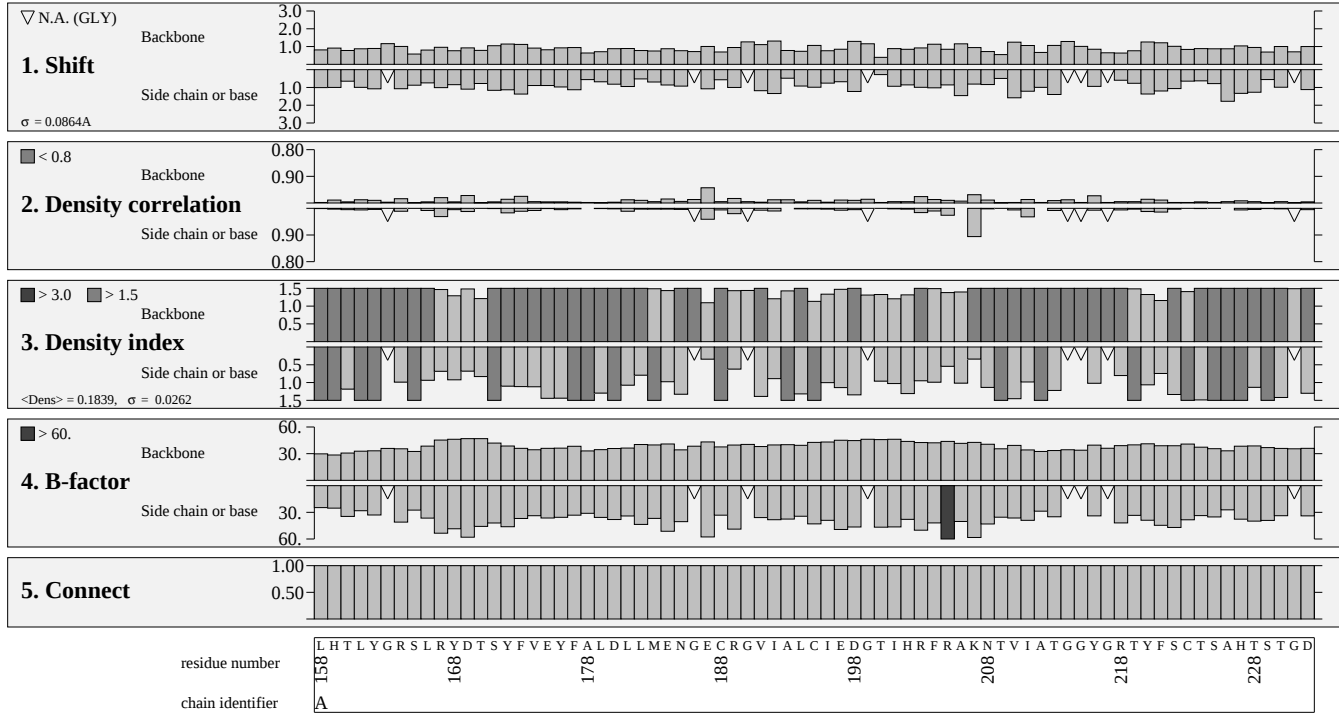
Local estimation



Structure Factor Check

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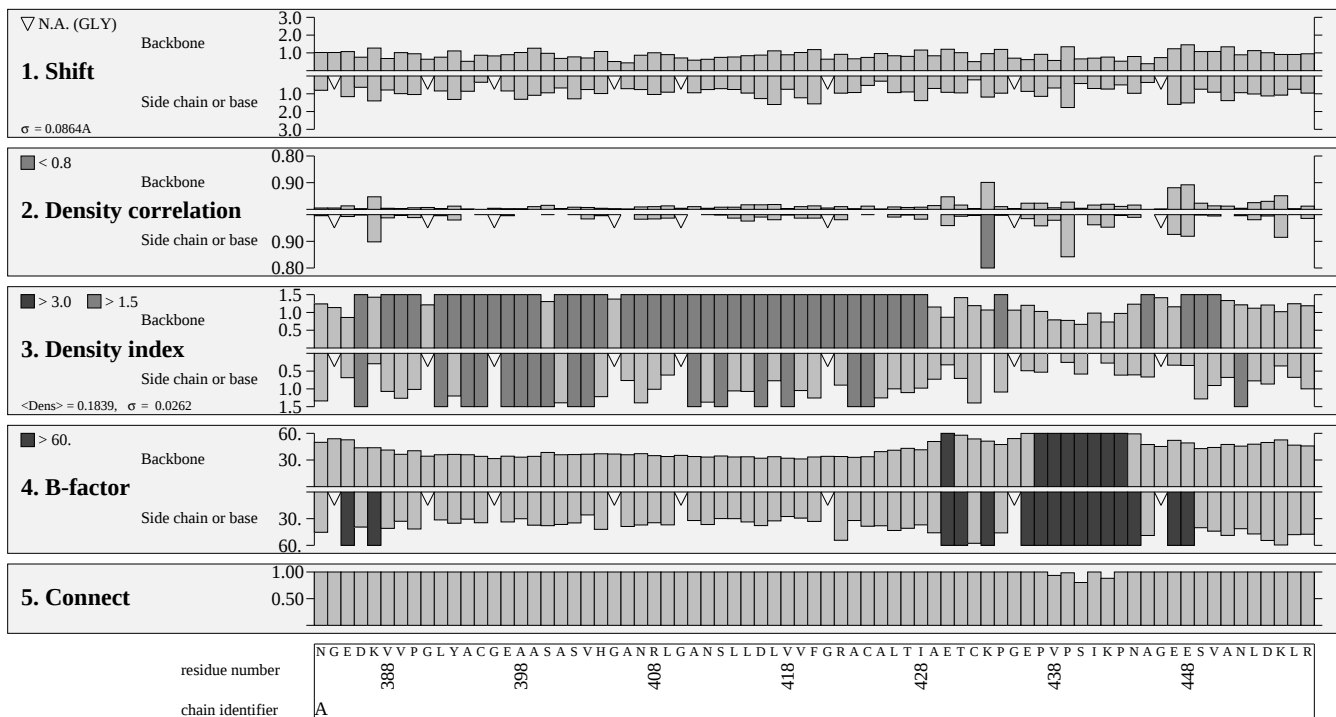
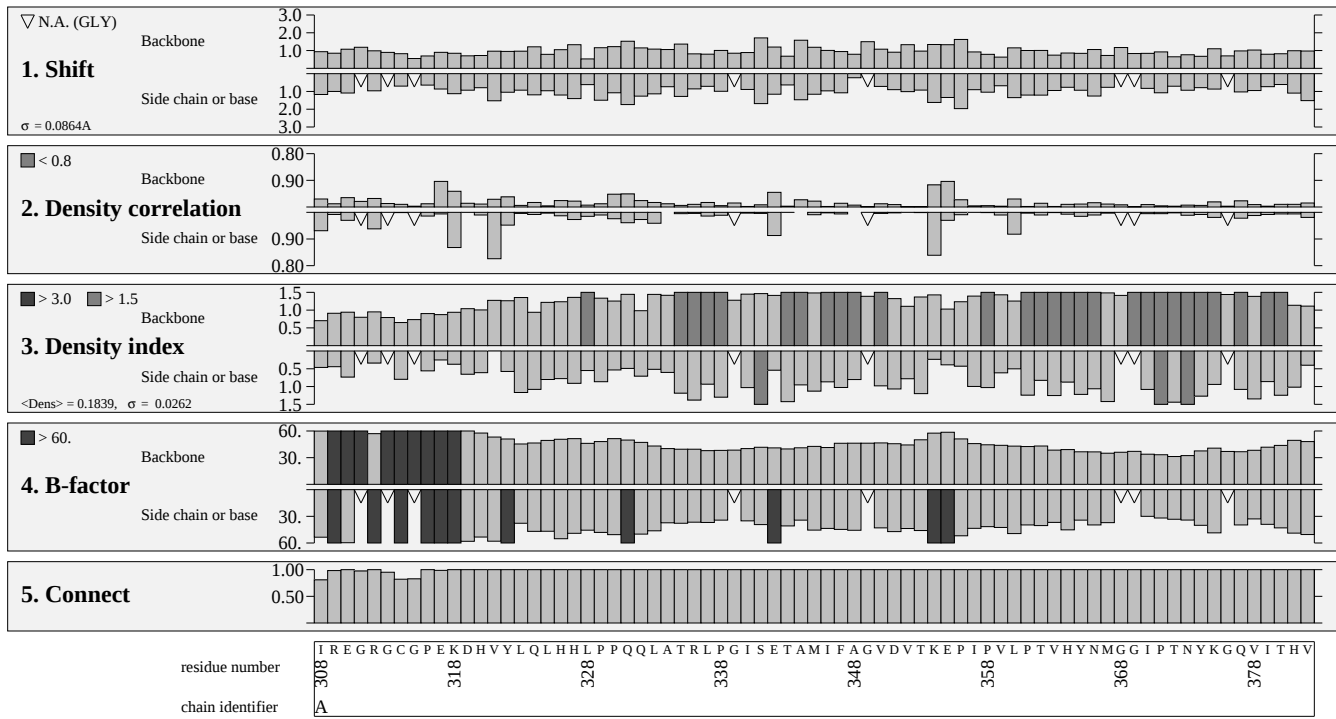
Local estimation (2)



Structure Factor Check

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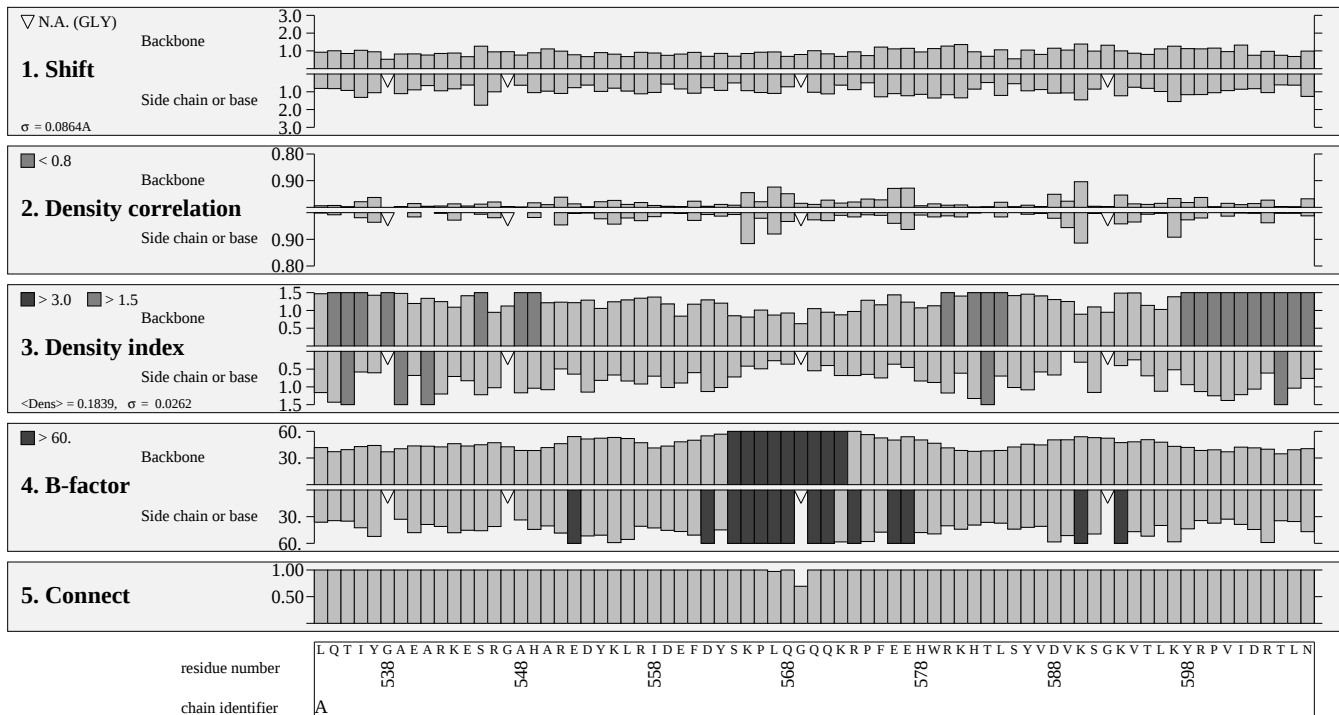
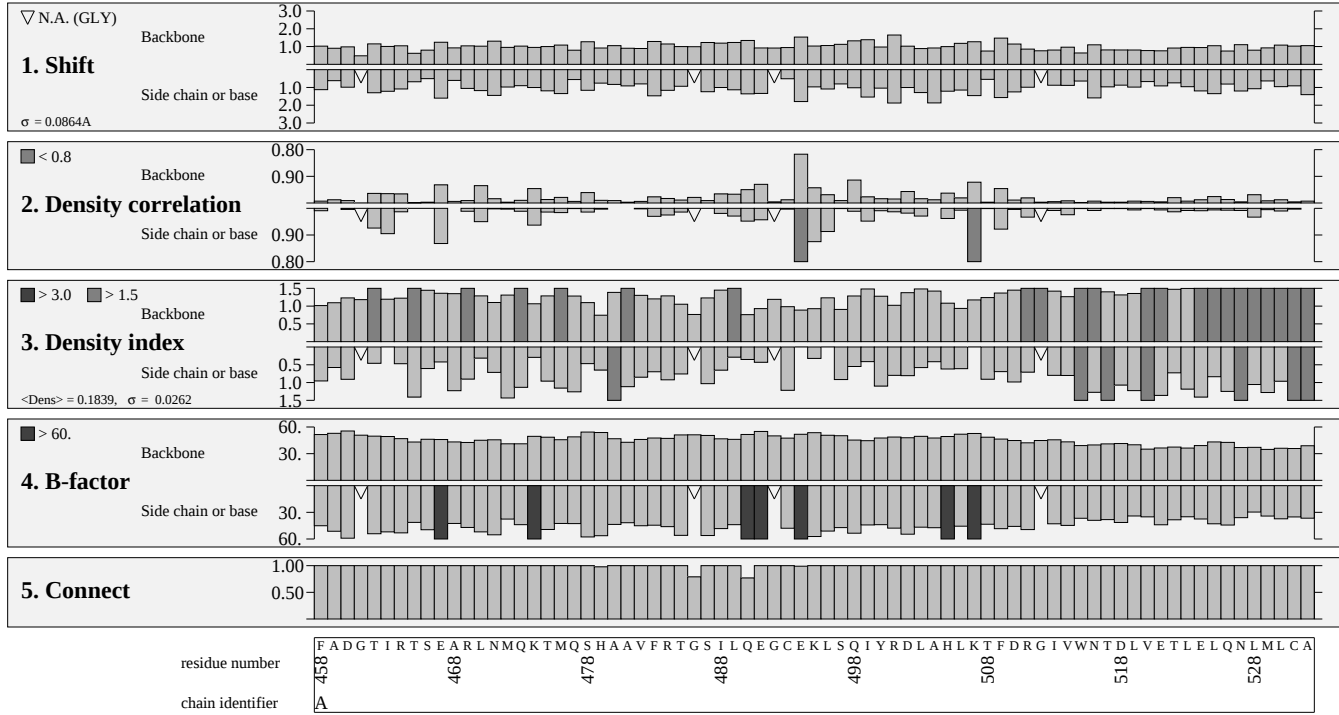
Local estimation (3)



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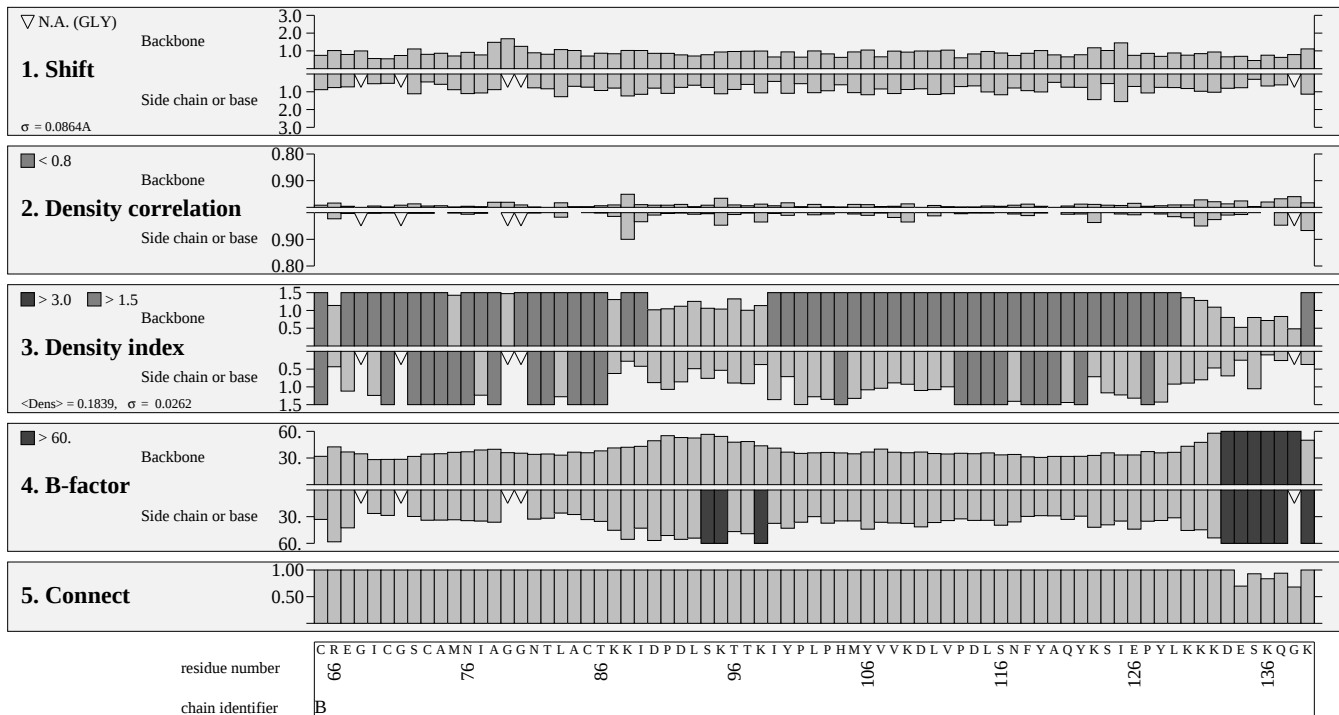
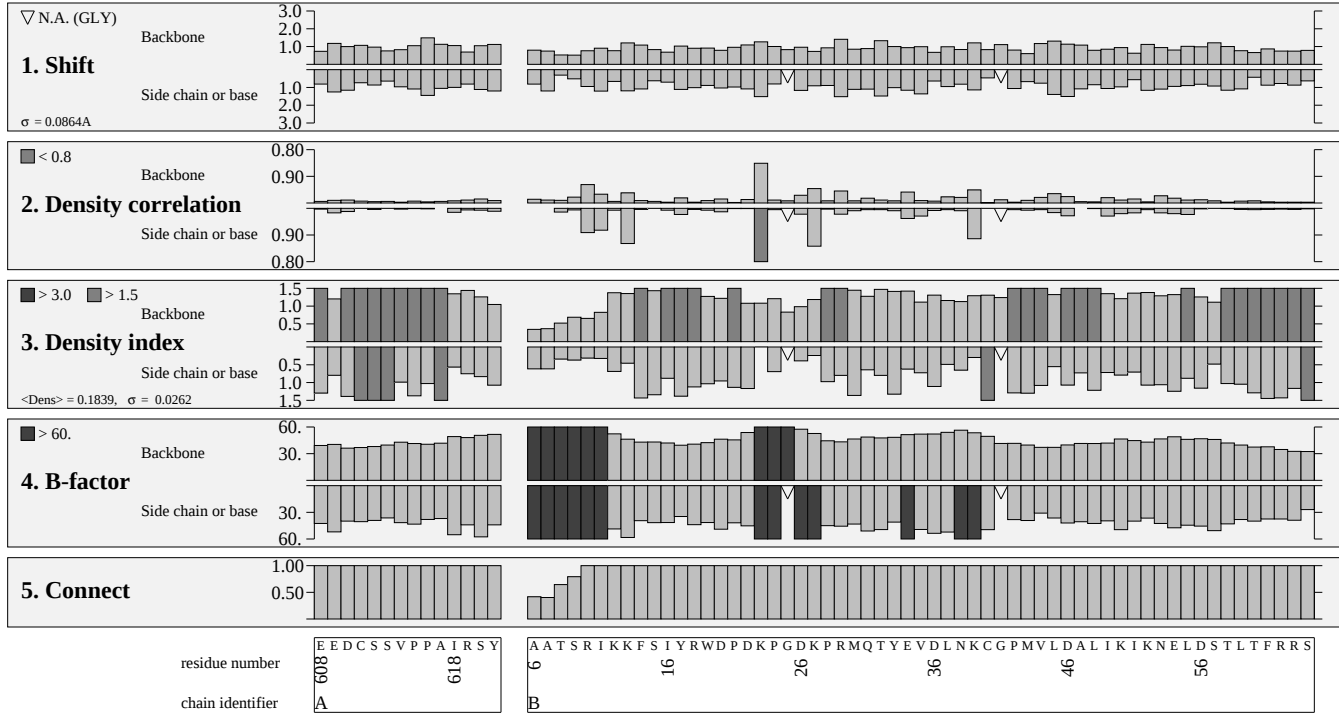
Local estimation (4)



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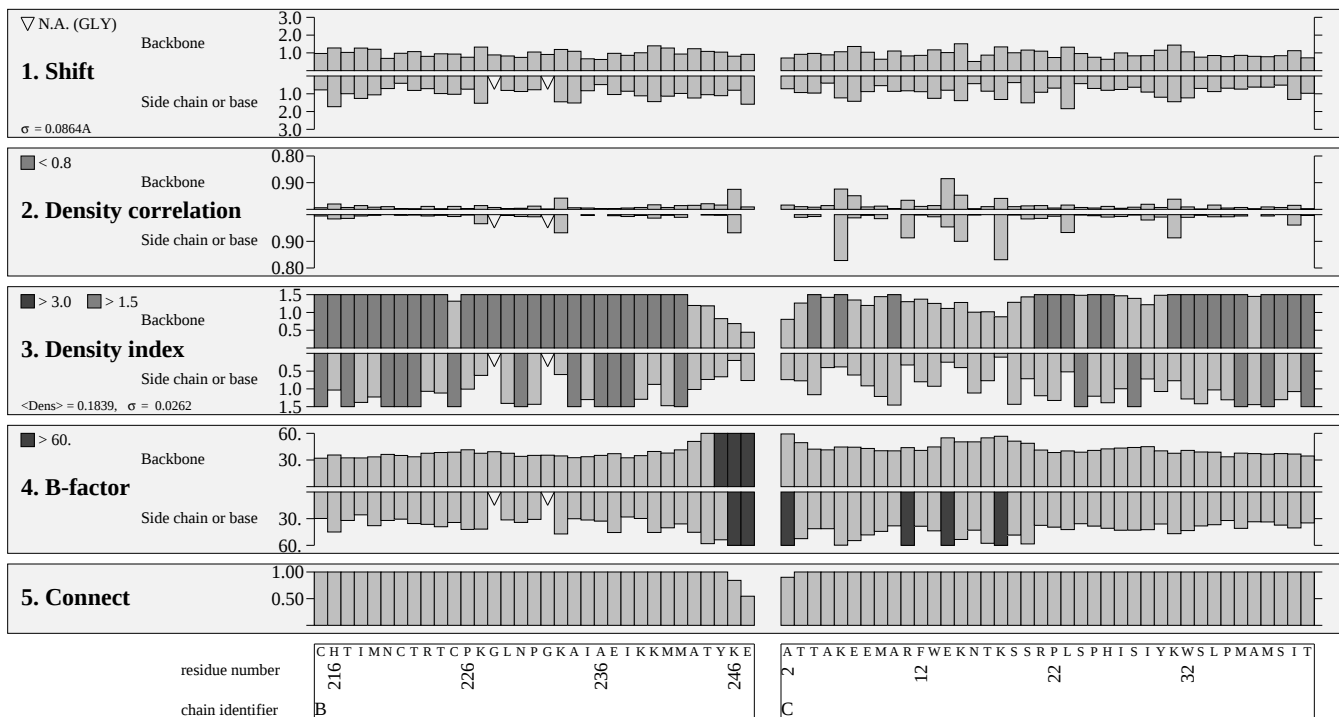
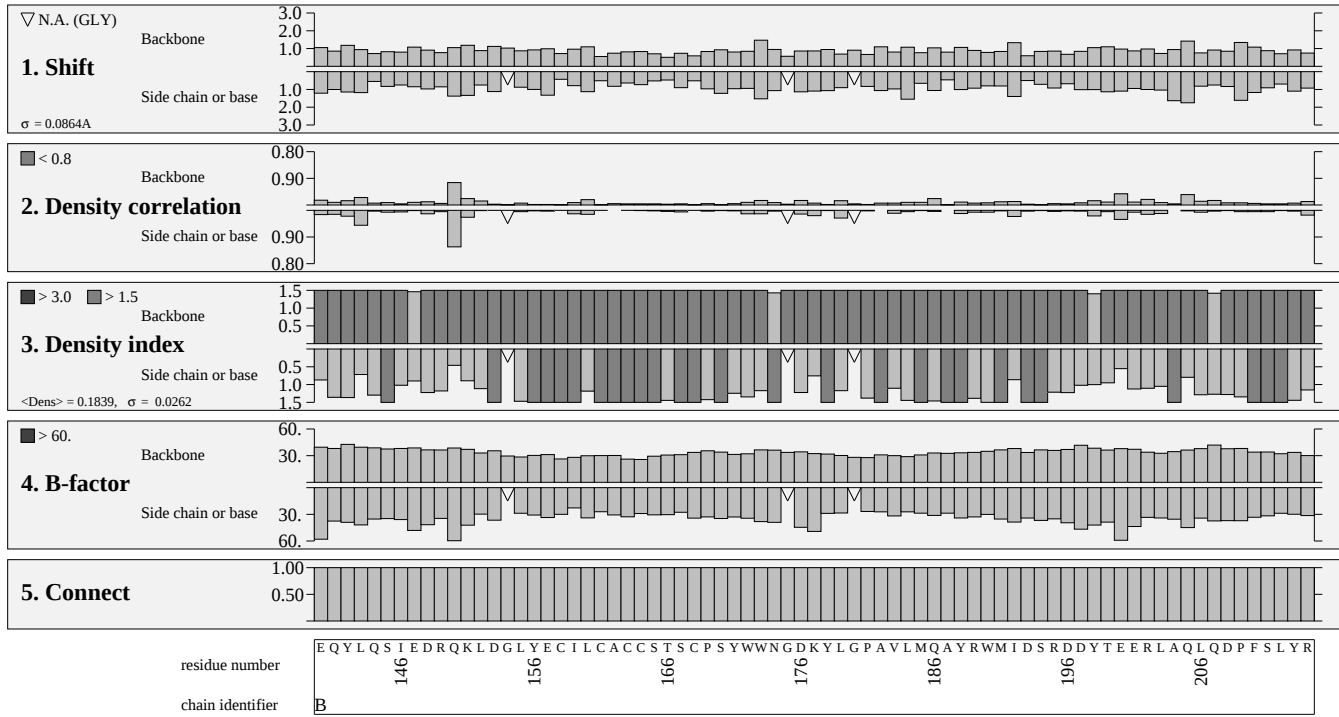
Local estimation (5)



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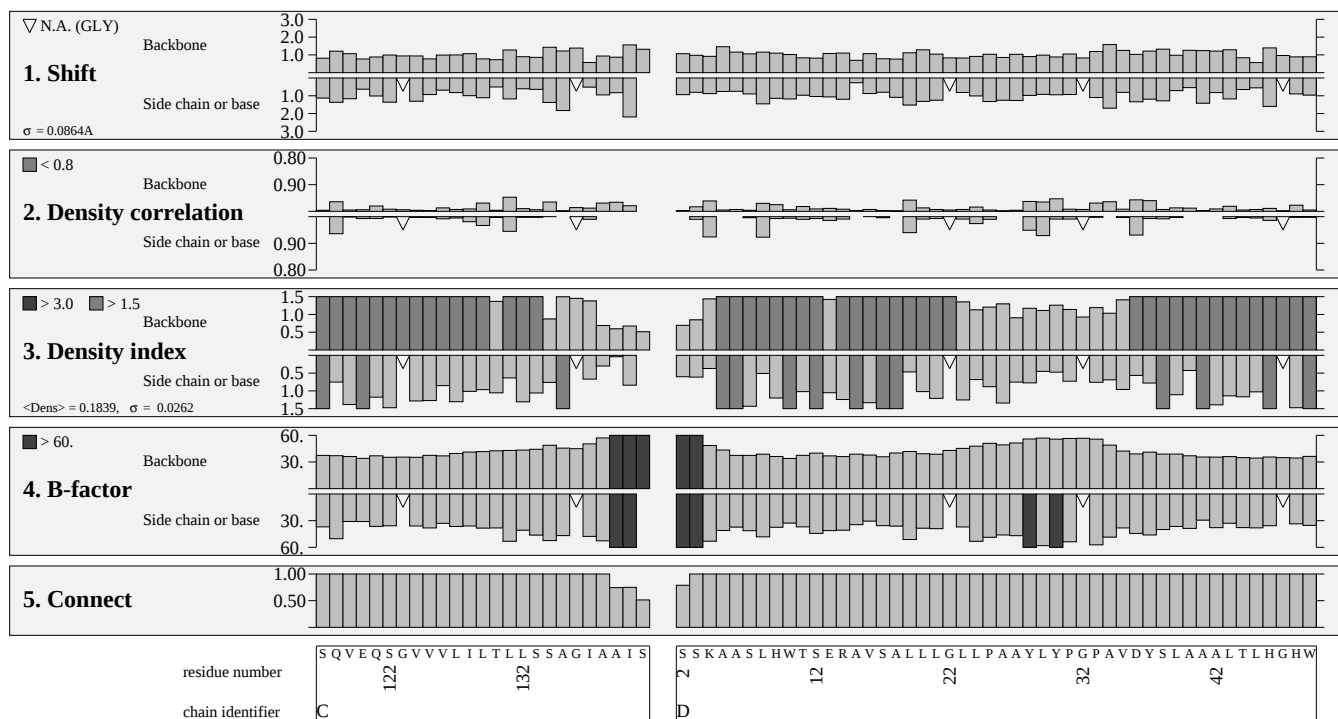
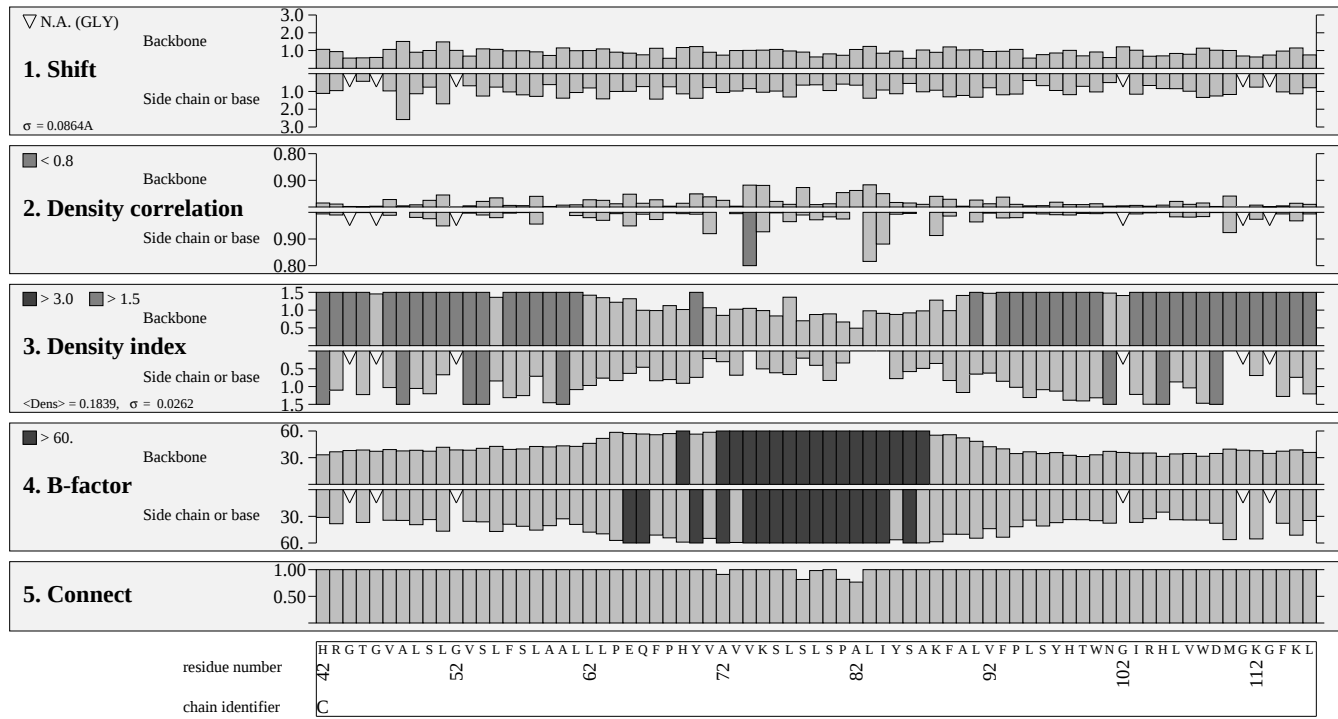
Local estimation (6)



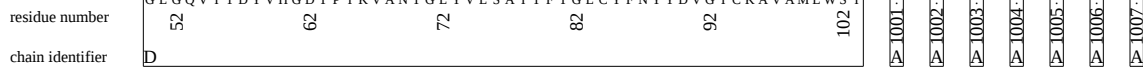
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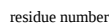
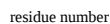
Local estimation (7)



Local estimation (8)



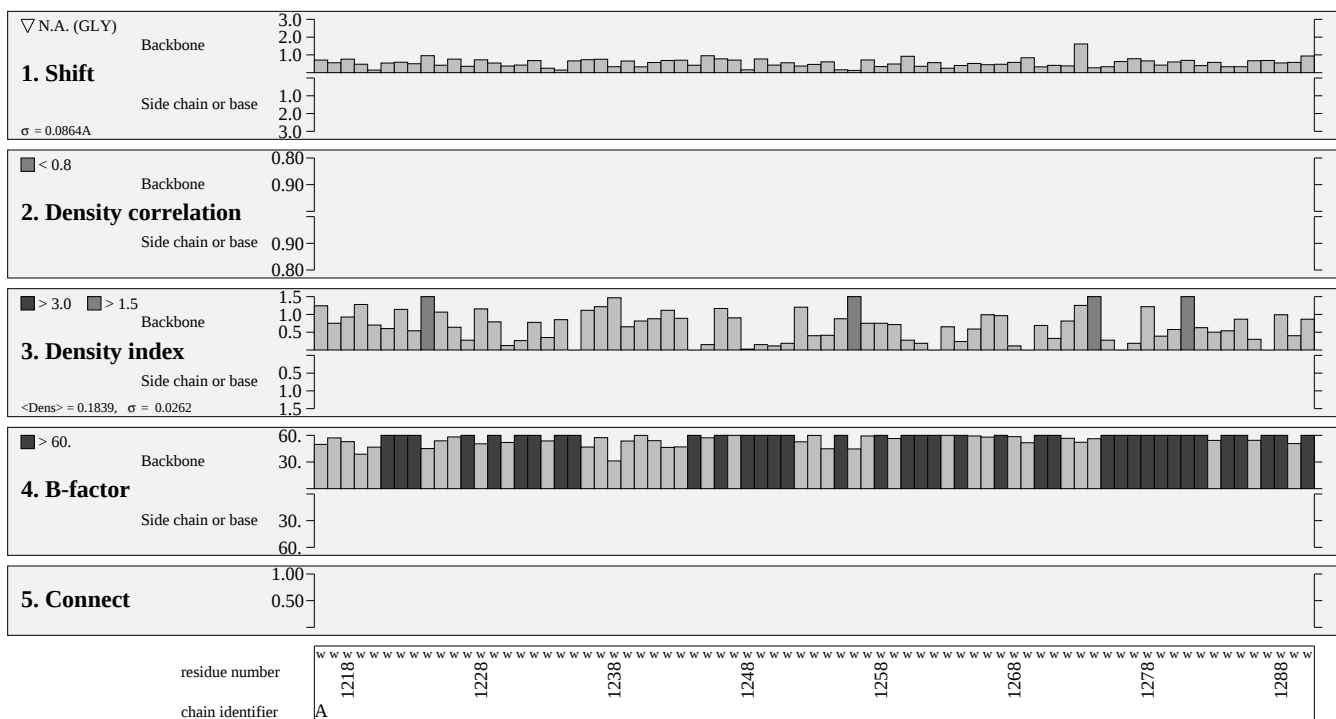
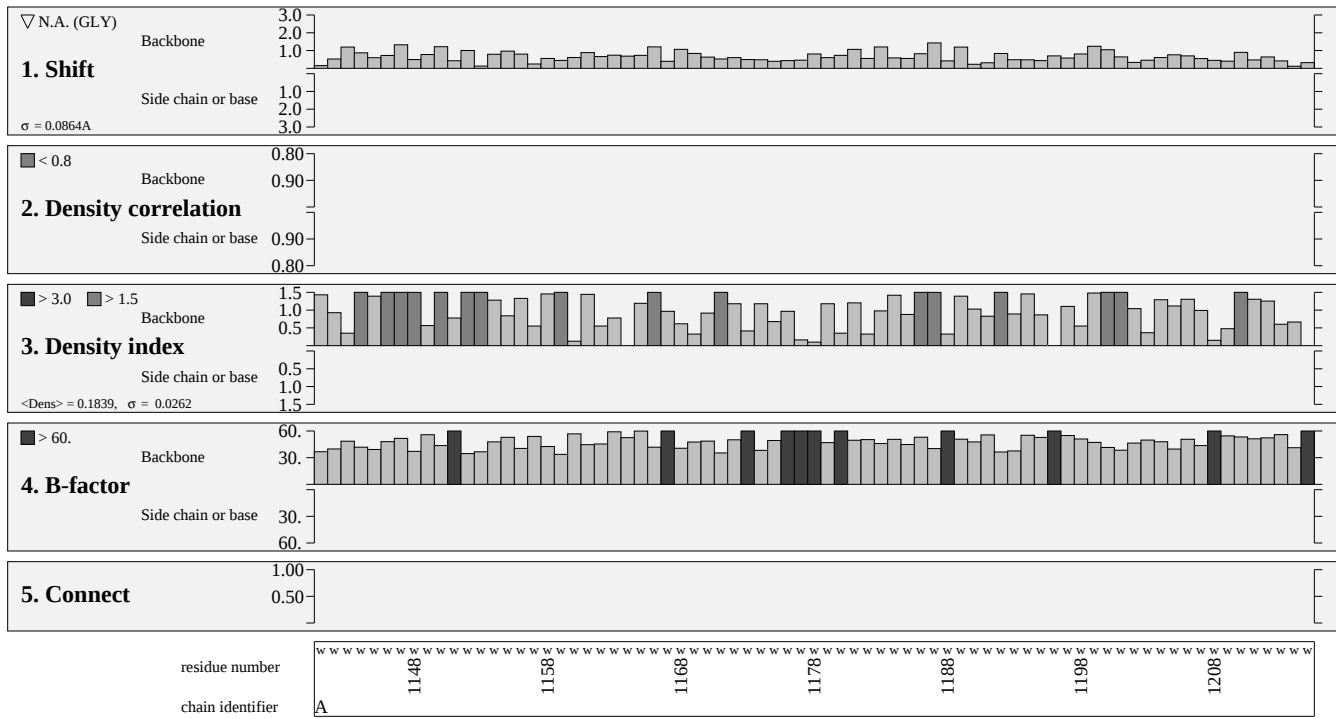
Local estimation (9)



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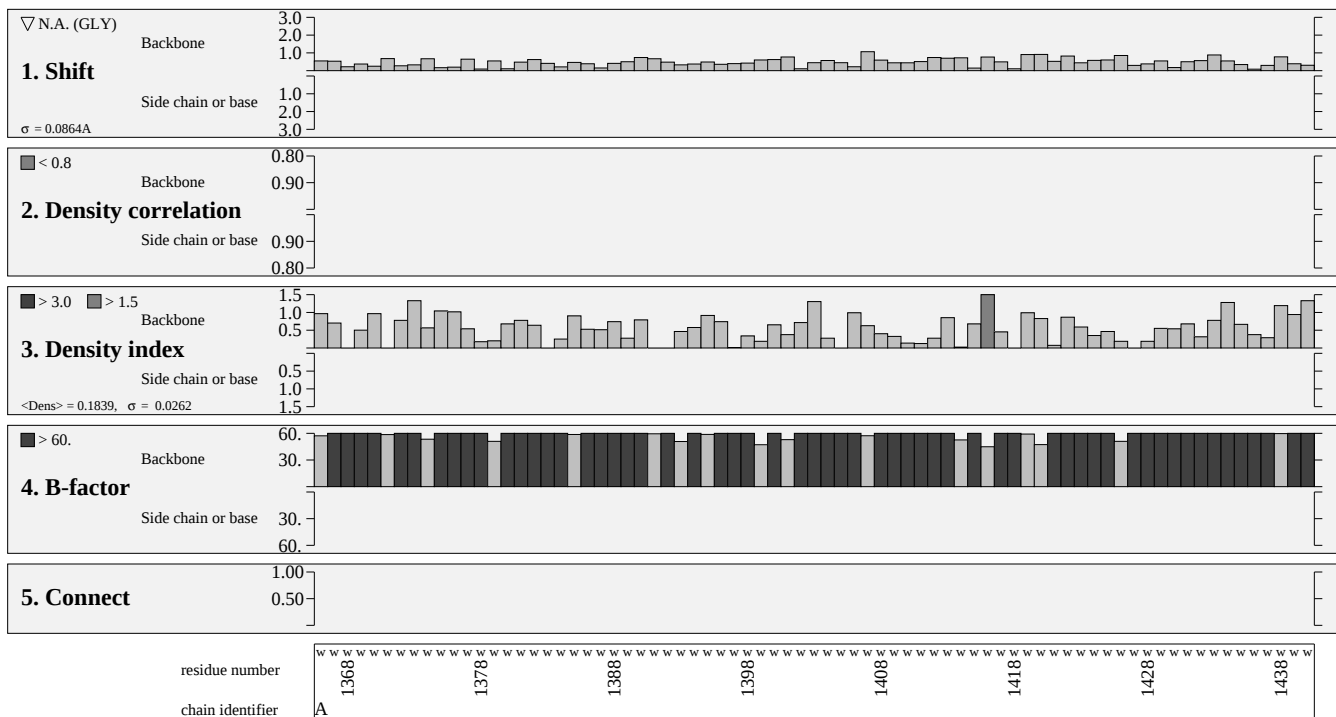
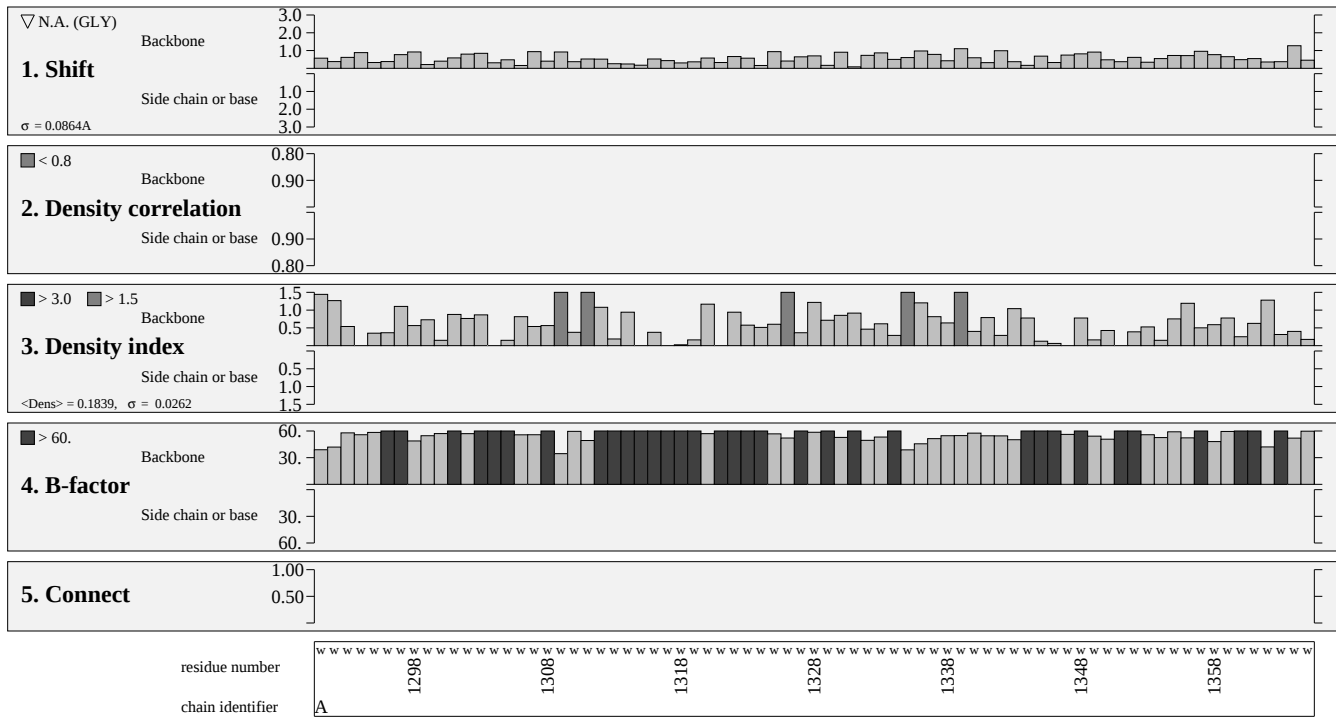
Local estimation (10)



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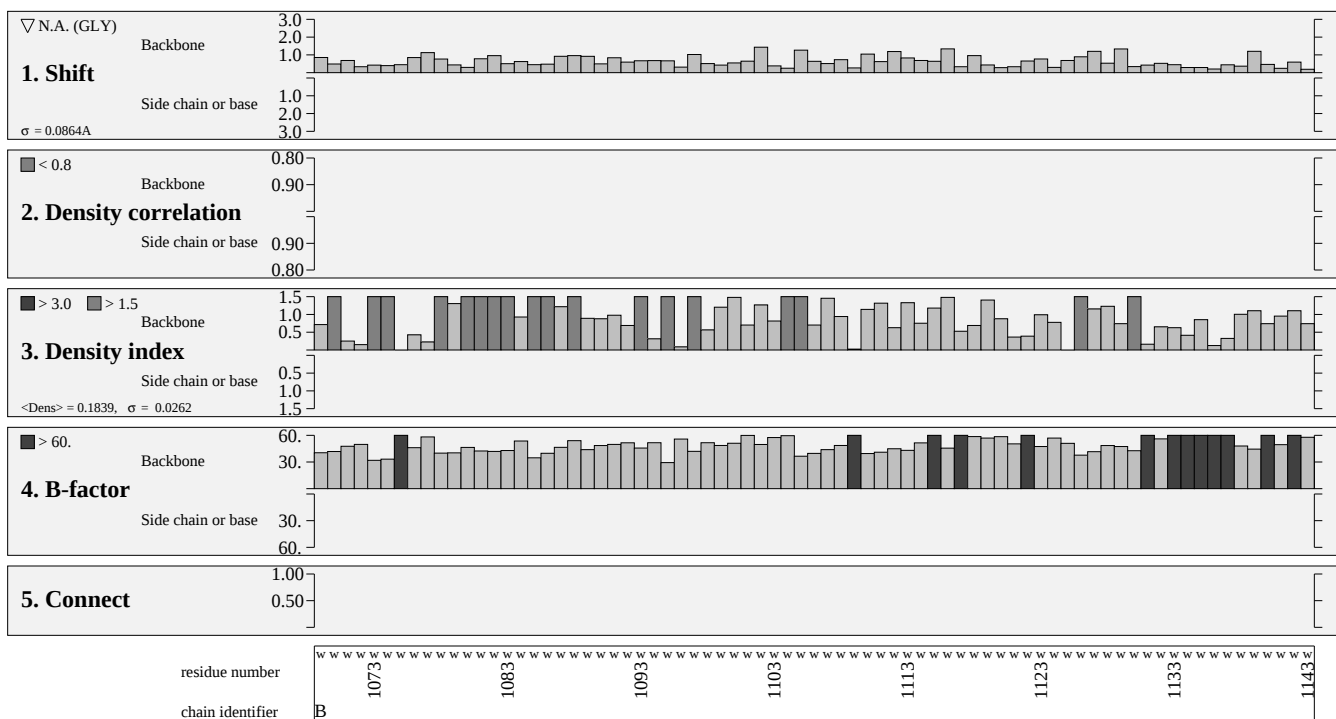
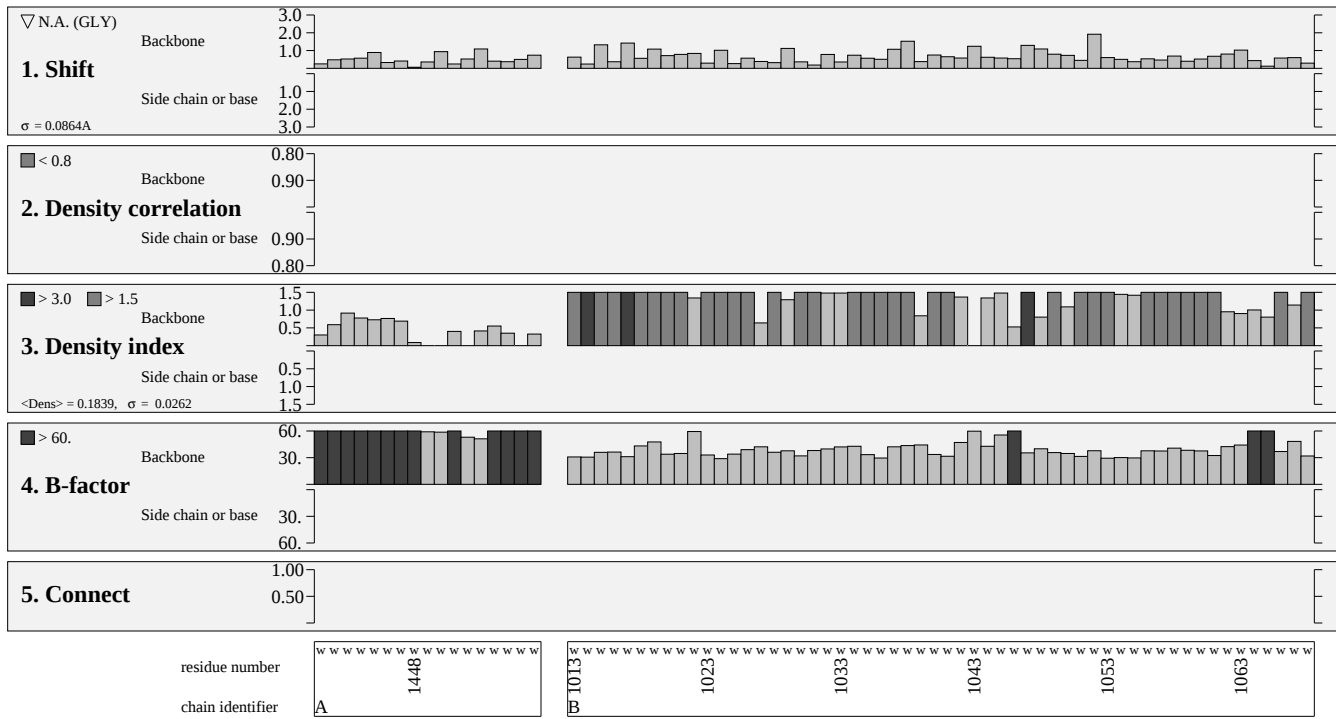
Local estimation (11)



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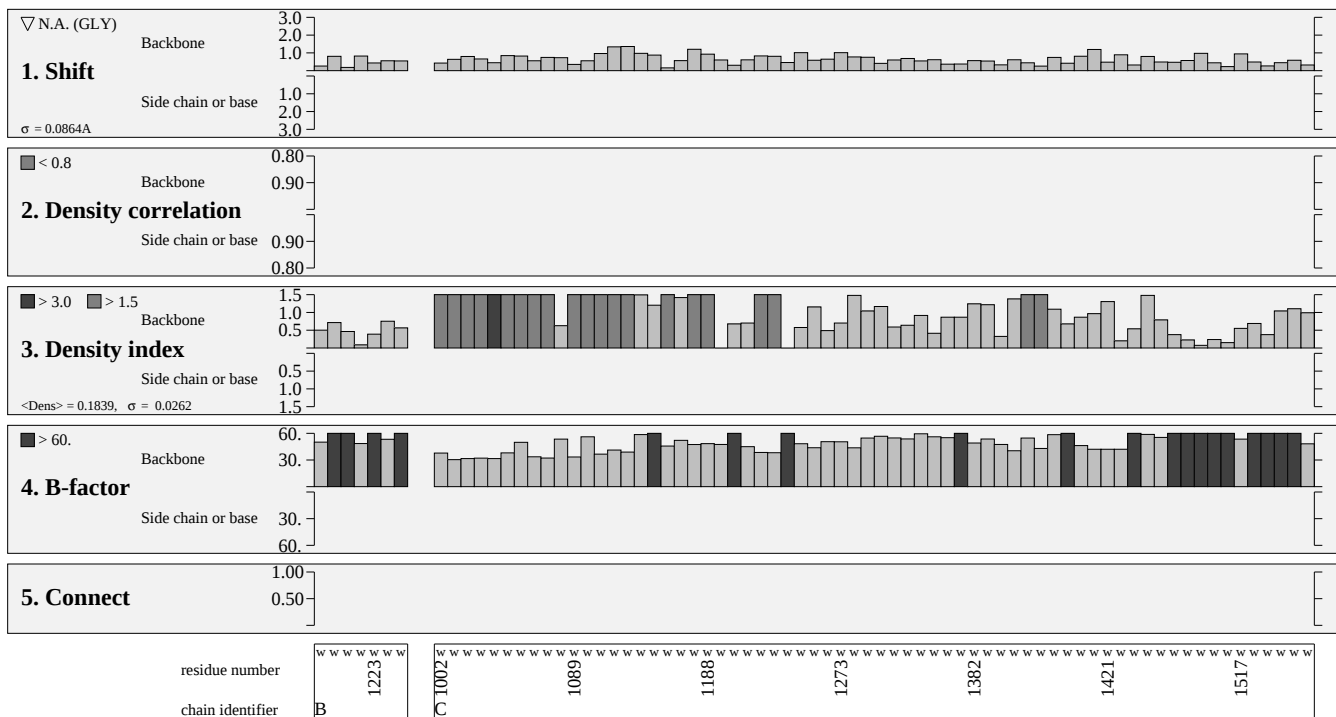
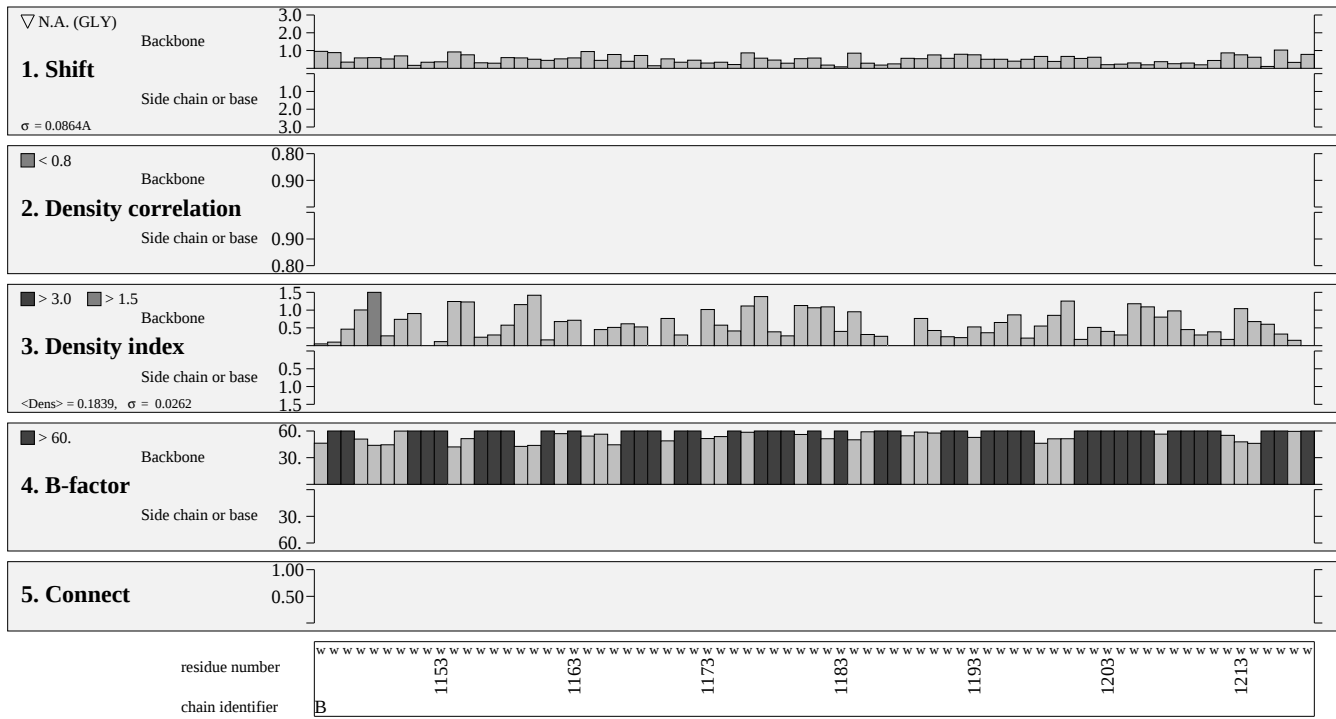
Local estimation (12)



Structure Factor Check

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Local estimation (13)



Structure Factor Check

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Local estimation (14)

