"Judge not, that you be not judged" Bible, Matthew, ch.7

Structure Factor Check

1YQ4

Title: AVIAN RESPIRATORY COMPLEX II WITH 3−NITROPROPIONATE AND UBIQ
Date: 01−FEB−05
PDB code: 1YQ4

Crystal

Cell parameters:

a: 69.59 A b: 83.49 A c: 288.59 A
α: 90.00 β: 90.00 γ: 90.00

Space group: P 21 21 21

Model

9291 atoms (575 water molecules)

Number of chains:	19
Volume not occupied by model:	52.5 %
<B> (for atomic model):	49.2 A^2
σ(B):	15.31 A^2
Matthews coefficient:	3.22
Corresponding solvent % :	61.53

Refinement

Program:	CNS 1.1
Nominal resolution range:	56.4 − 2.33 A
Reported R−factor:	0.202
Number of reflections used:	68868
Reported Rfree:	0.25
Sigma cut−off:	N.A.

Structure Factors

Input

Nominal resolution range:		47.5 − 2.20 A
Reflections in file:		77928
Unique reflections	above 0:	77928
	above 1σ:	77181
	above 3σ:	58844

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Nominal resolution range: 47.5 − 2.33 A
\05max. from input data, min. from author\05

Used reflections:	68868
Reflections out of resolution:	9060
Completeness:	94.4 %
R_stand(F) = <σ(F)>/<F> :	0.043

Anisotropic distribution of Structure Factors
ratio of eigen values: 0.8632 1.0000 0.6245

B_overall (by Patterson):	39.A^2
Optical resolution:	1.83 A
Expected opt. resol. for complete data set:	1.83 A
Estimated minimal error:	0.026 A

Model vs. Structure Factors

R−factor for all reflections:	0.220
Correlation factor:	0.928
R−factor:	0.227

for F > 2.0 σ
nom. resolution range: 56.38 − 2.33A
reflections used: 68397

Rfree:	0.274
Nfree:	3313
R−factor without free−refl.:	0.224
Non free−reflections:	65084
<u> (error in coords by Luzzati plot):	0.290 A
Estimated maximal error:	0.102 A
DPI:	0.195 A

Scaling

Scale:	0.905
Bdiff:	−4.09

Anisothermal Scaling (Beta):
2.8026 4.0289 −1.9500 0.0000 0.0000 0.0000

Solvent correction − Ks,Bs: 0.673 250.046

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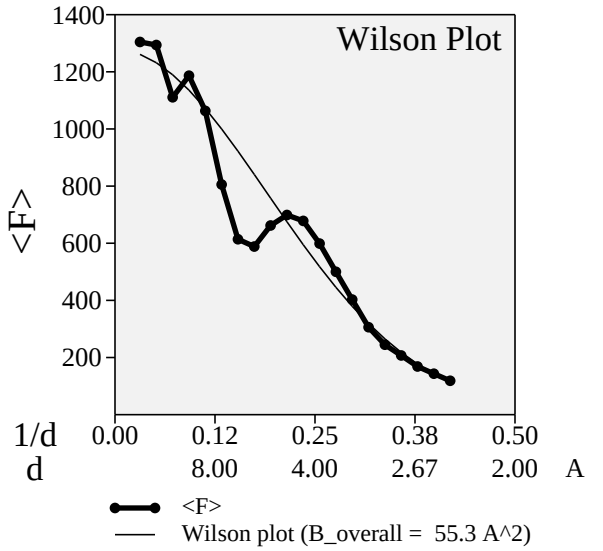
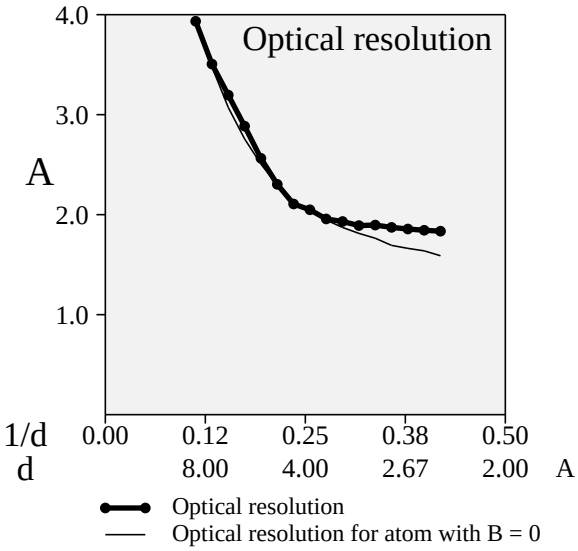
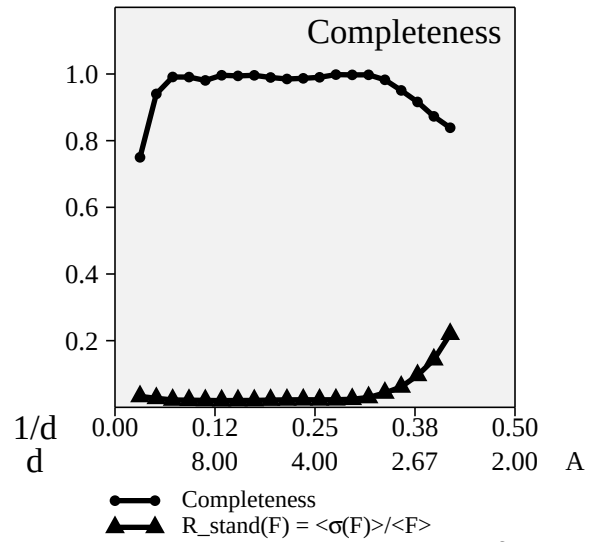
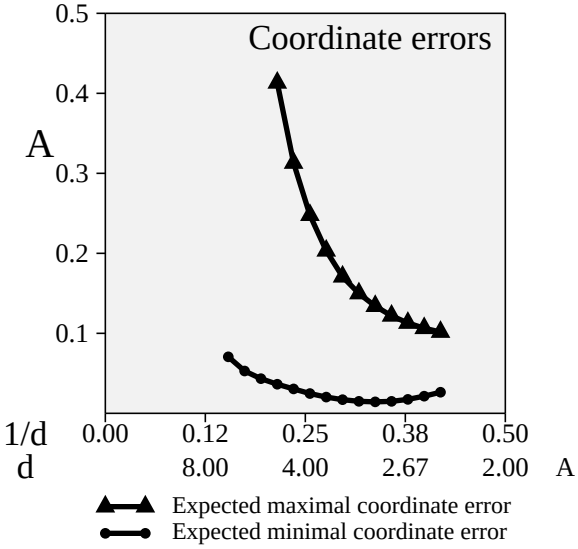
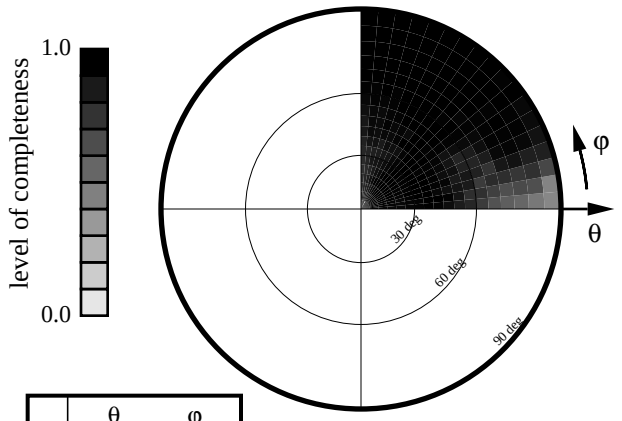






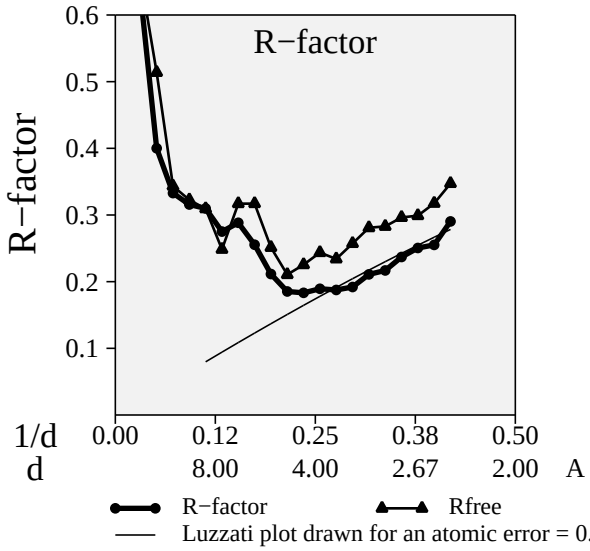


Stereographic projection of
the averaged radial completeness



	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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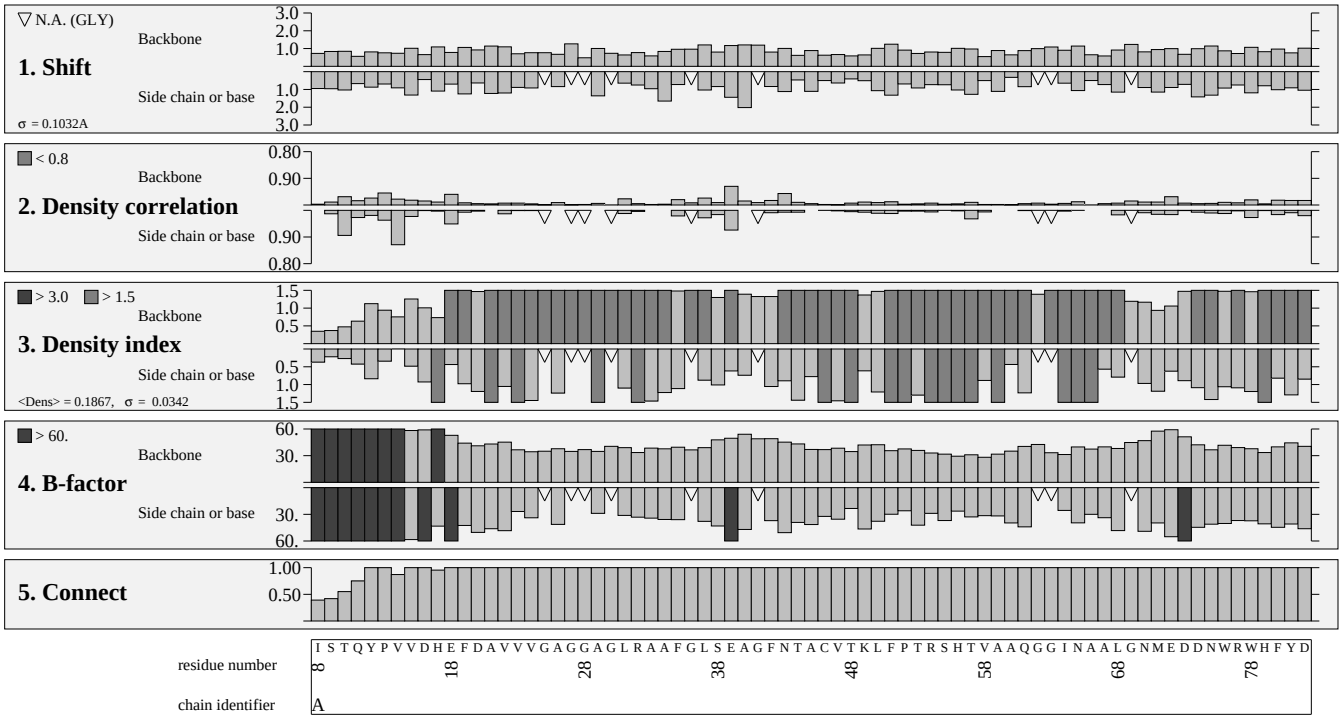
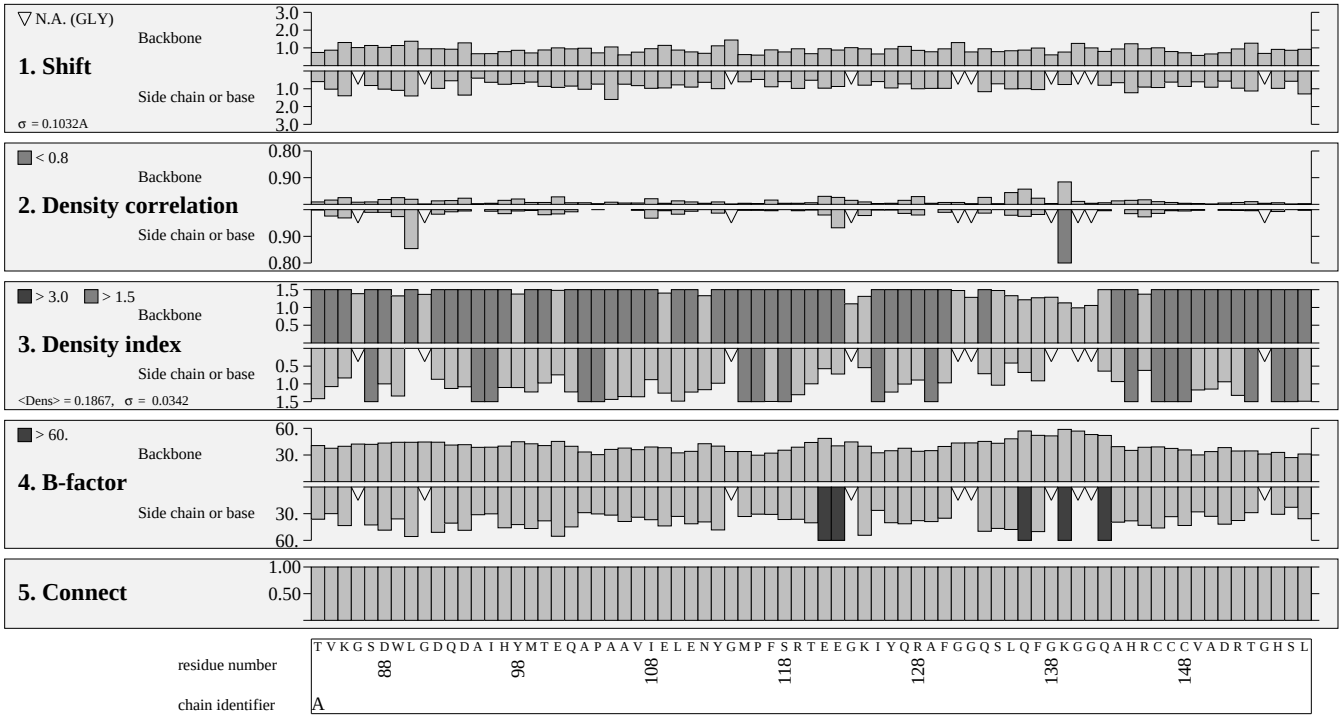
Local estimation





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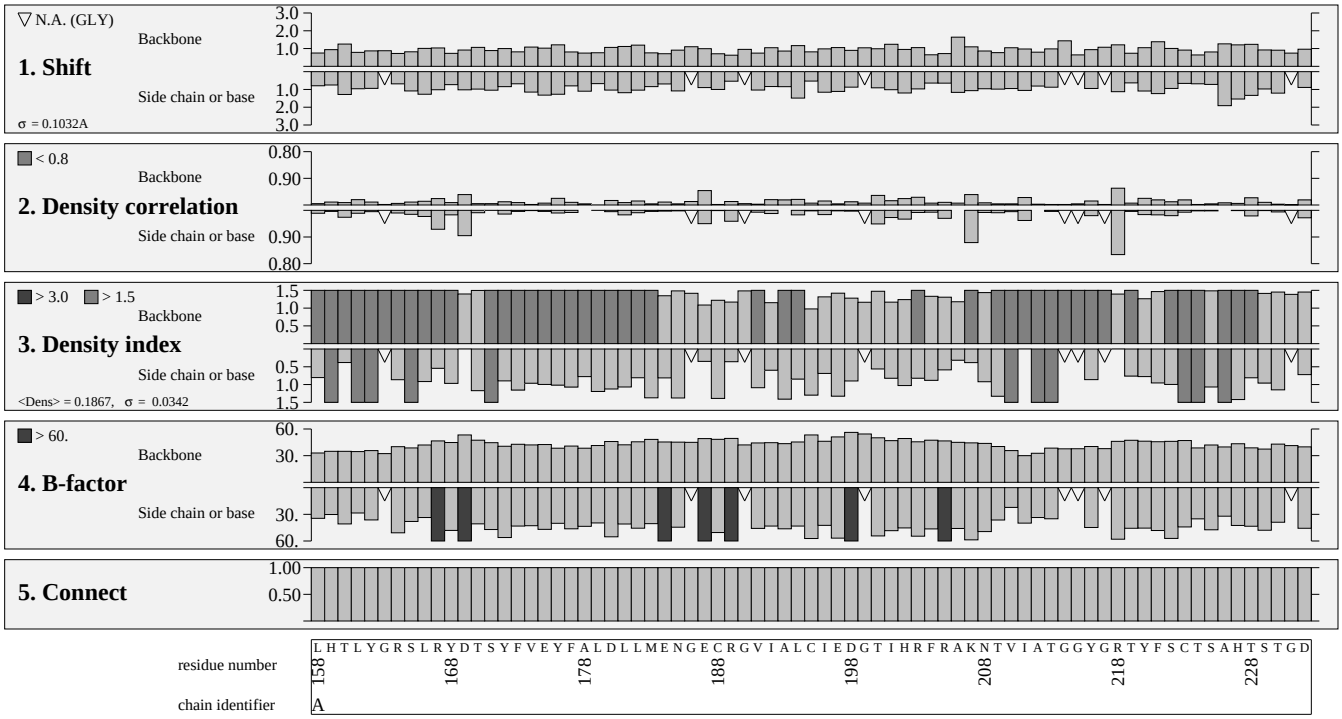
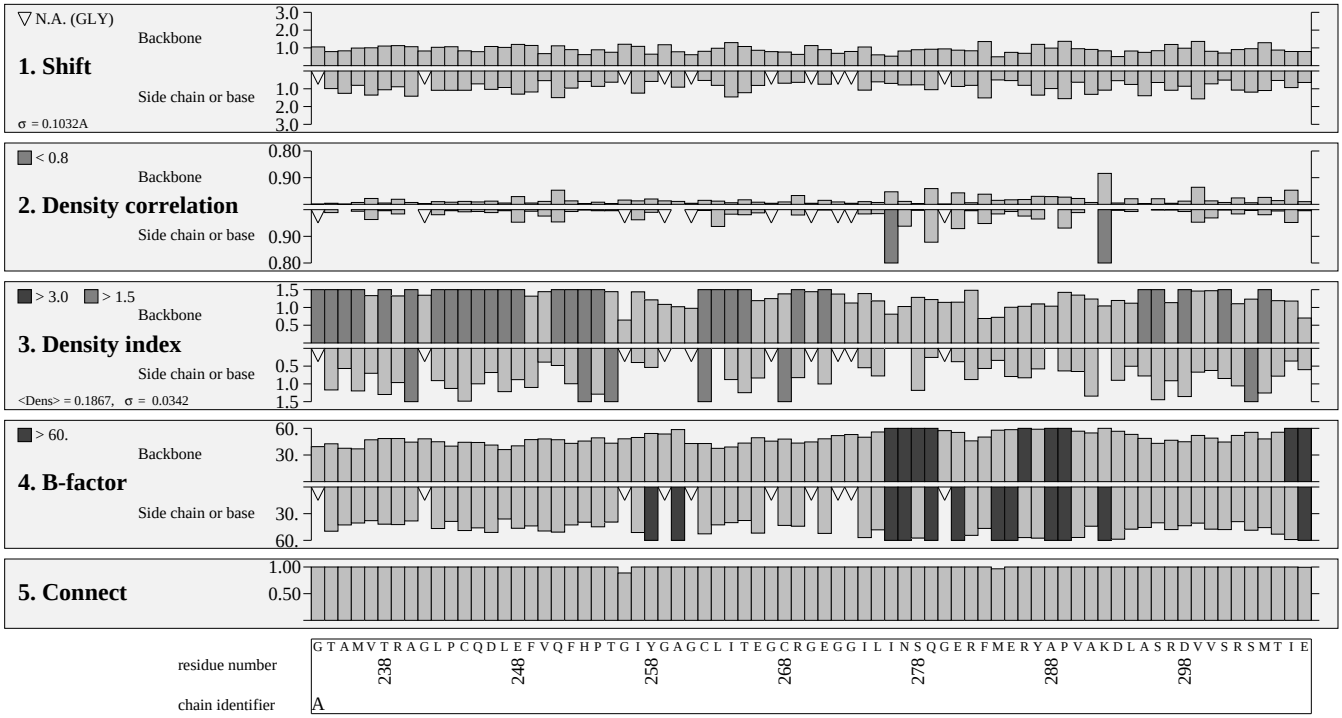
Structure Factor Check

1YQ4

Local estimation (2)





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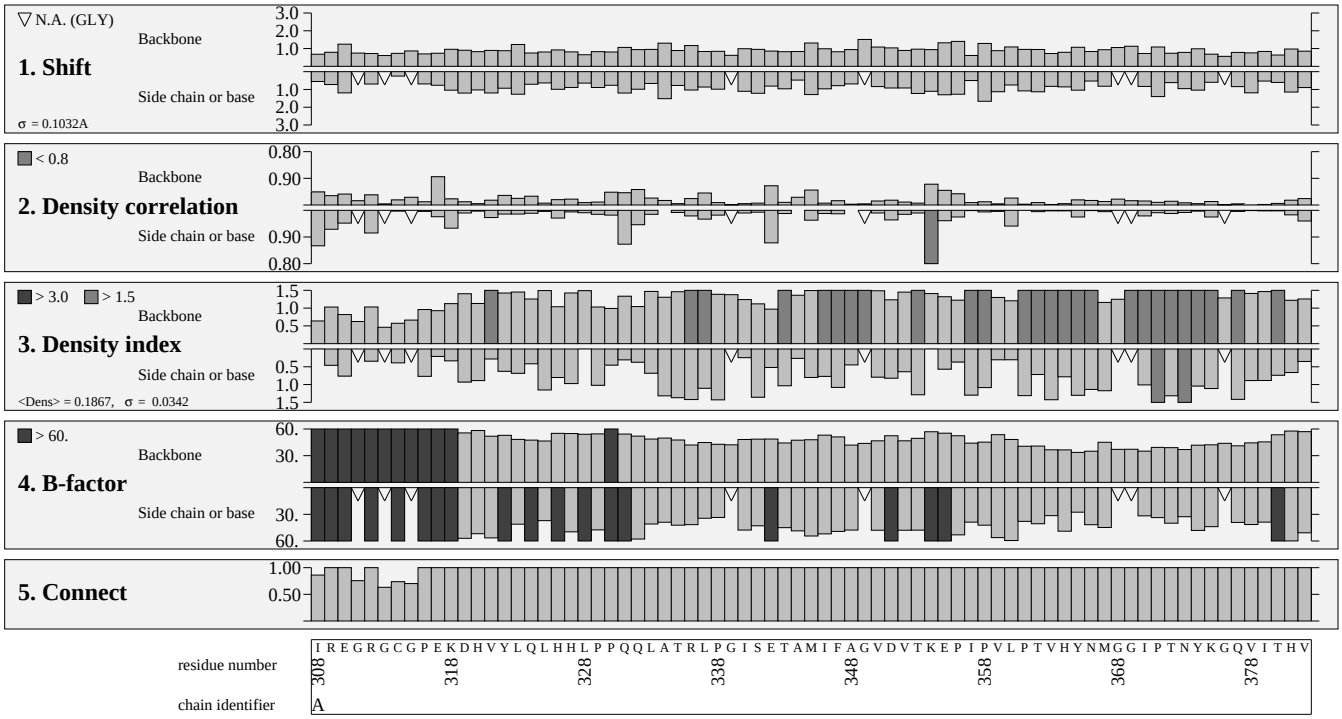
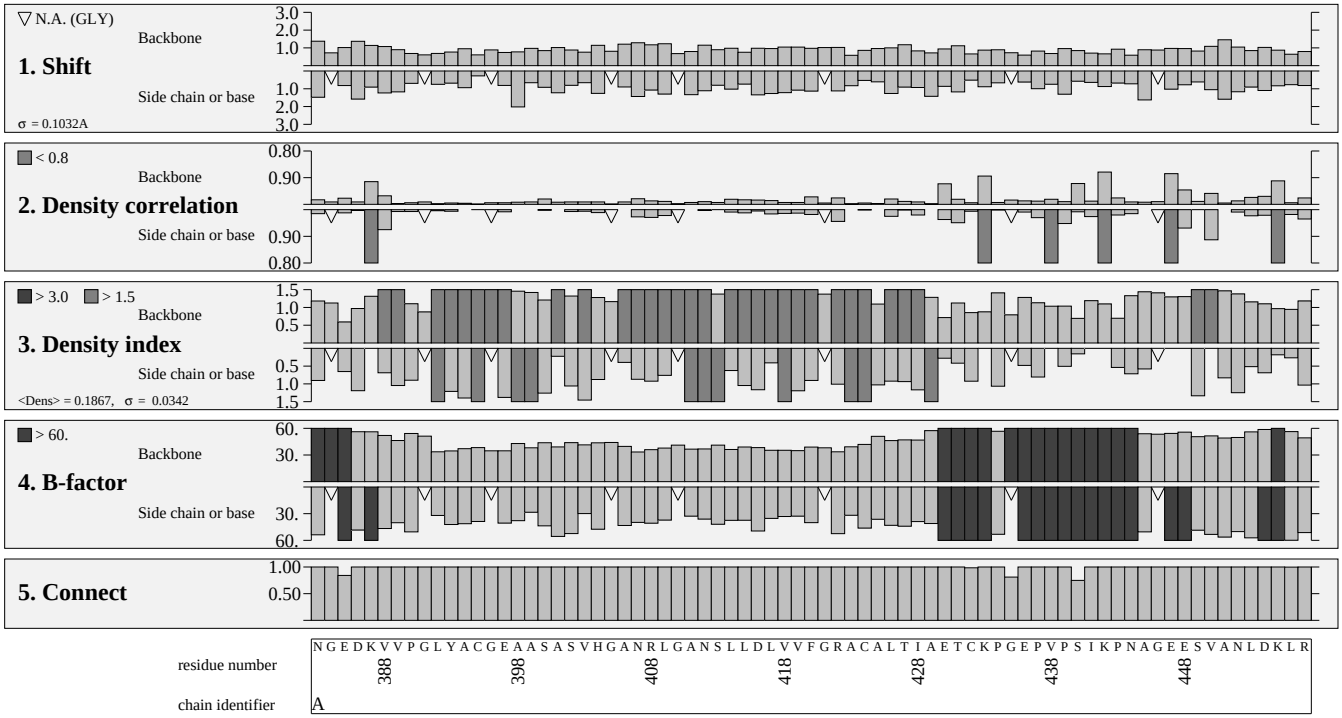
Local estimation (3)





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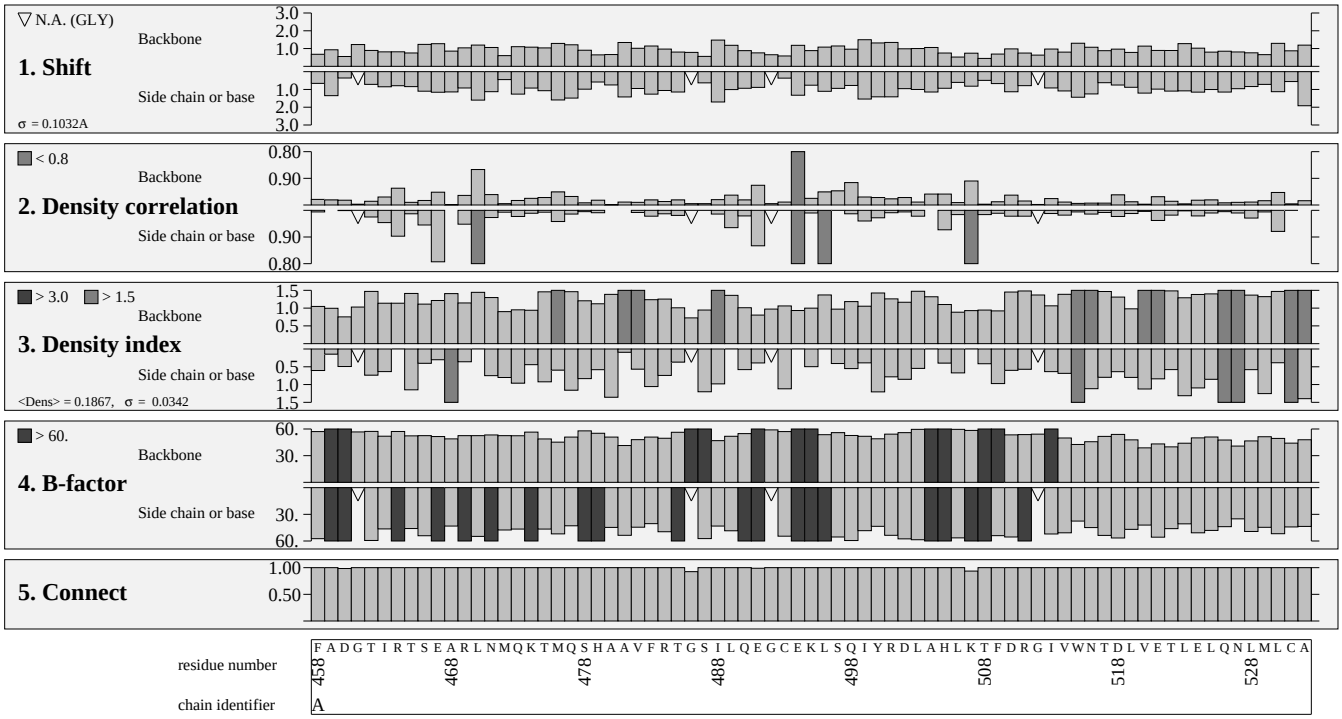
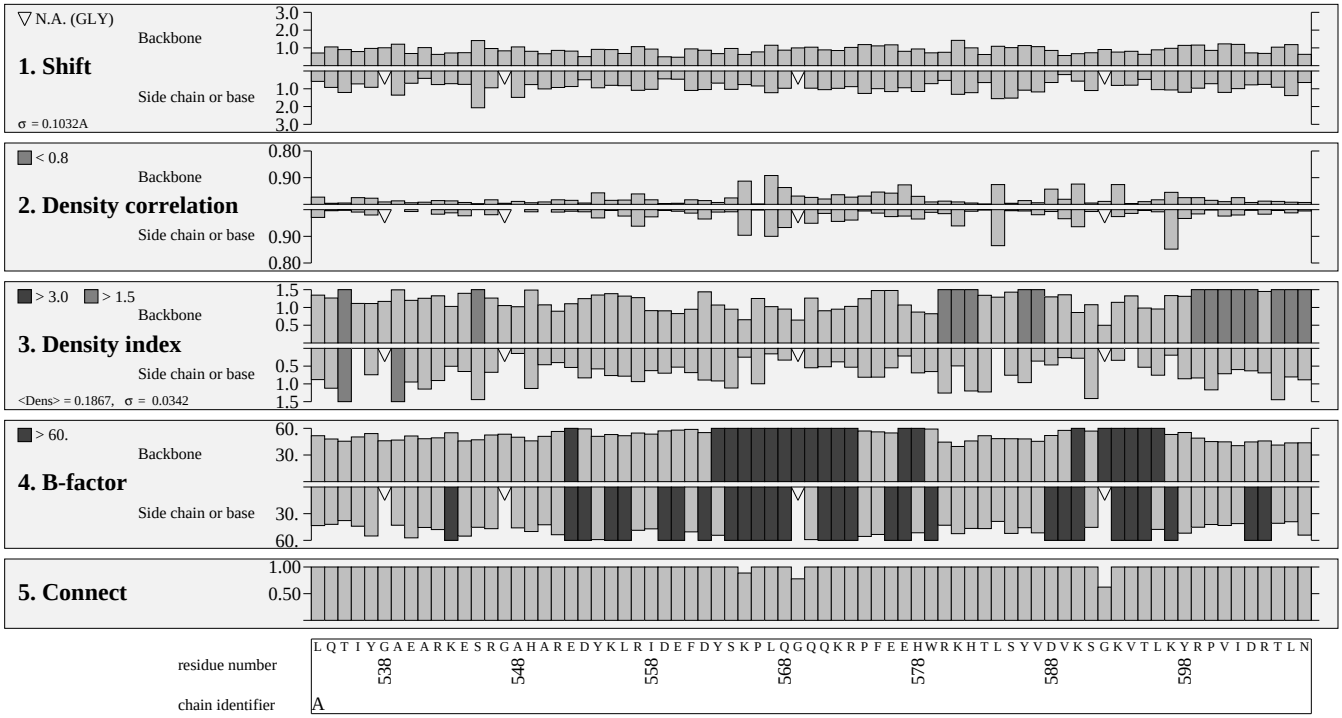
Local estimation (4)





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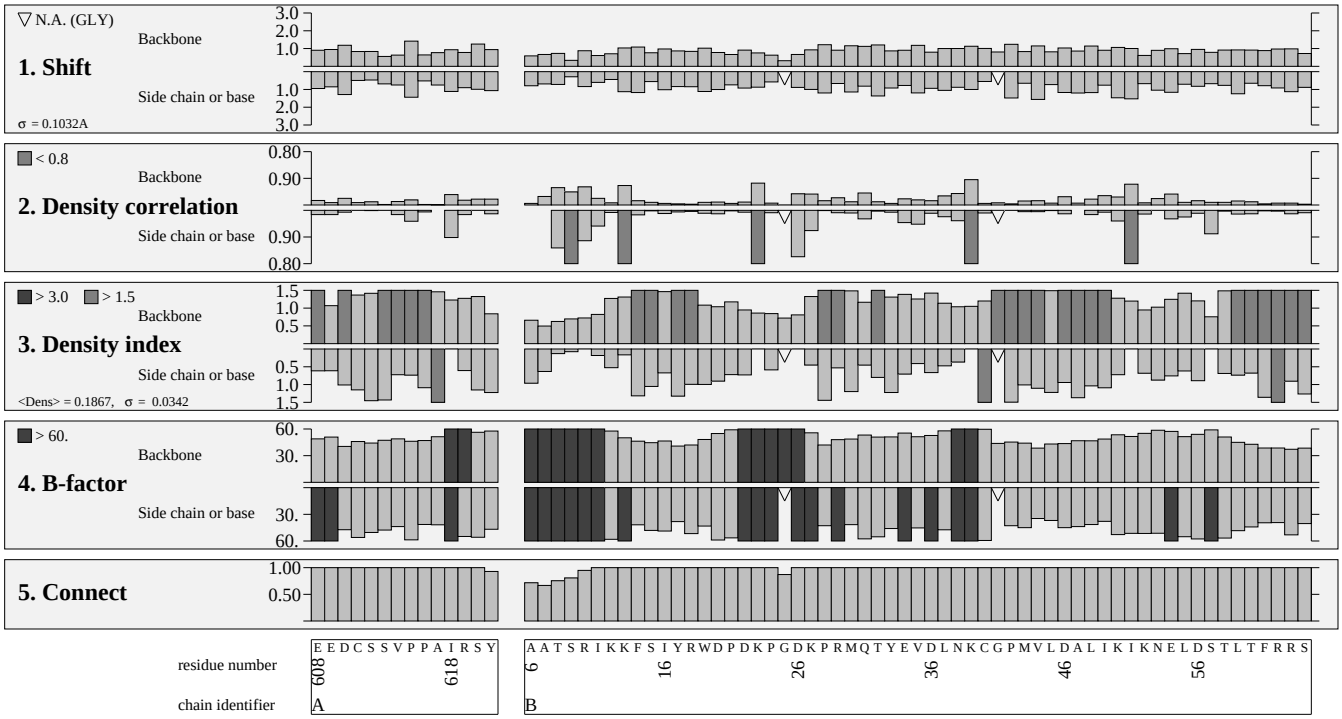
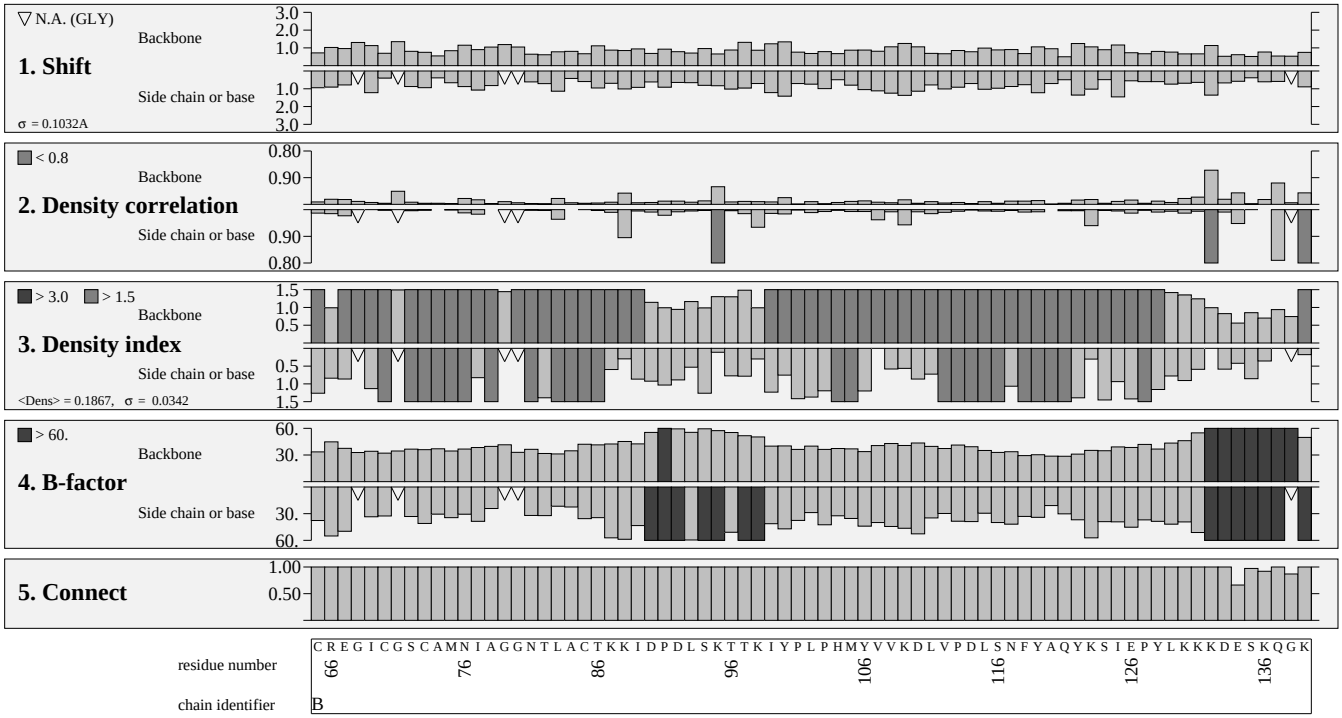
Local estimation (5)





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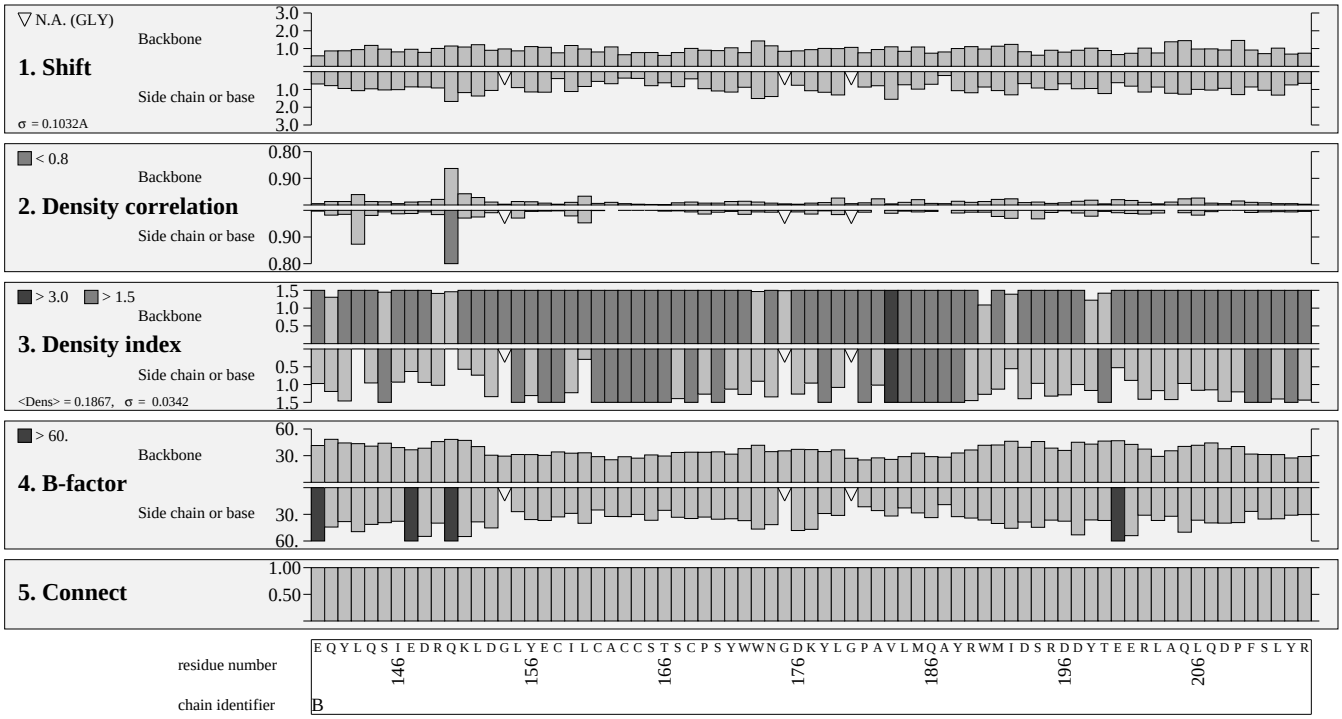
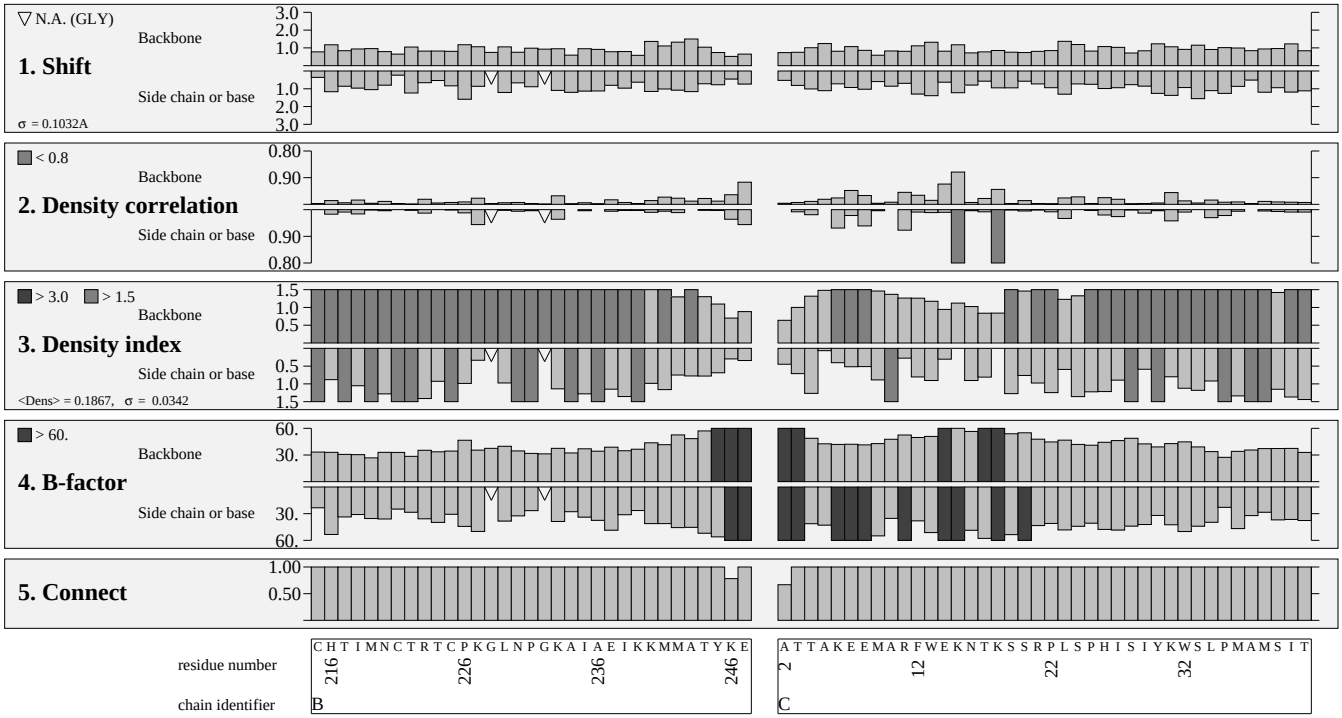
Local estimation (6)





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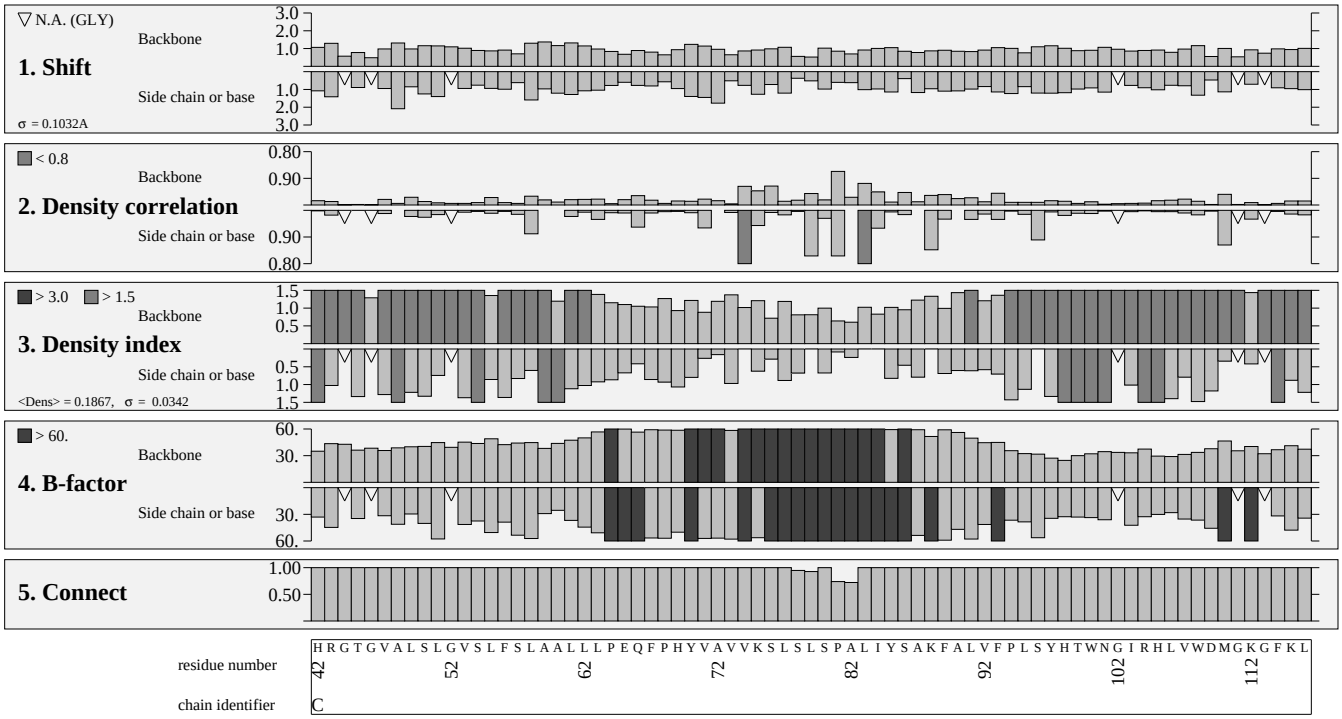
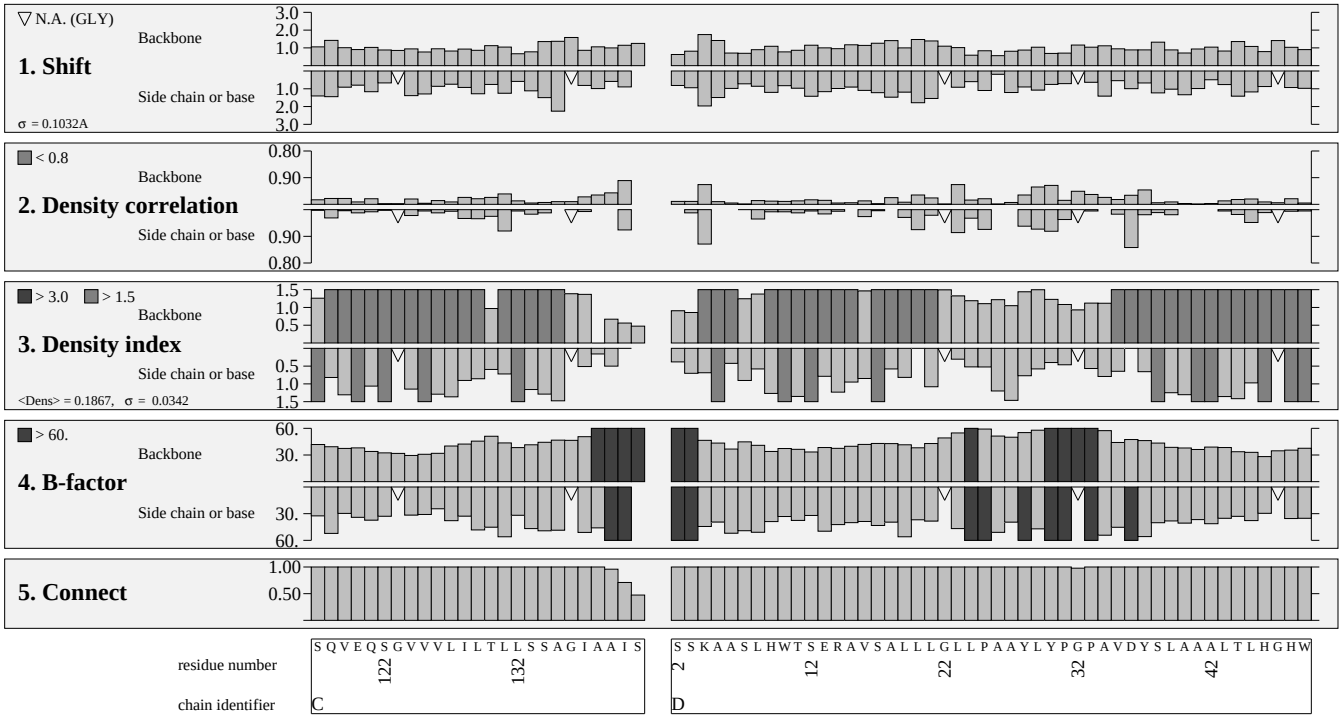
Local estimation (7)





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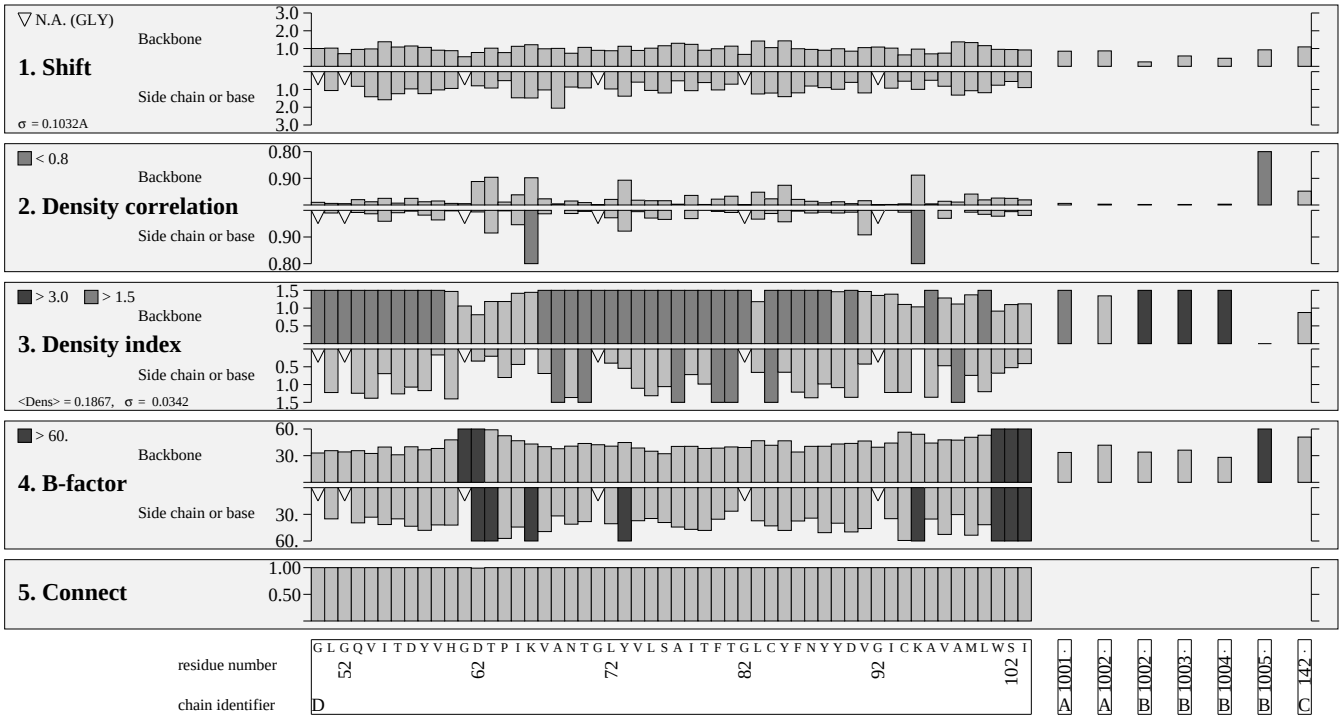
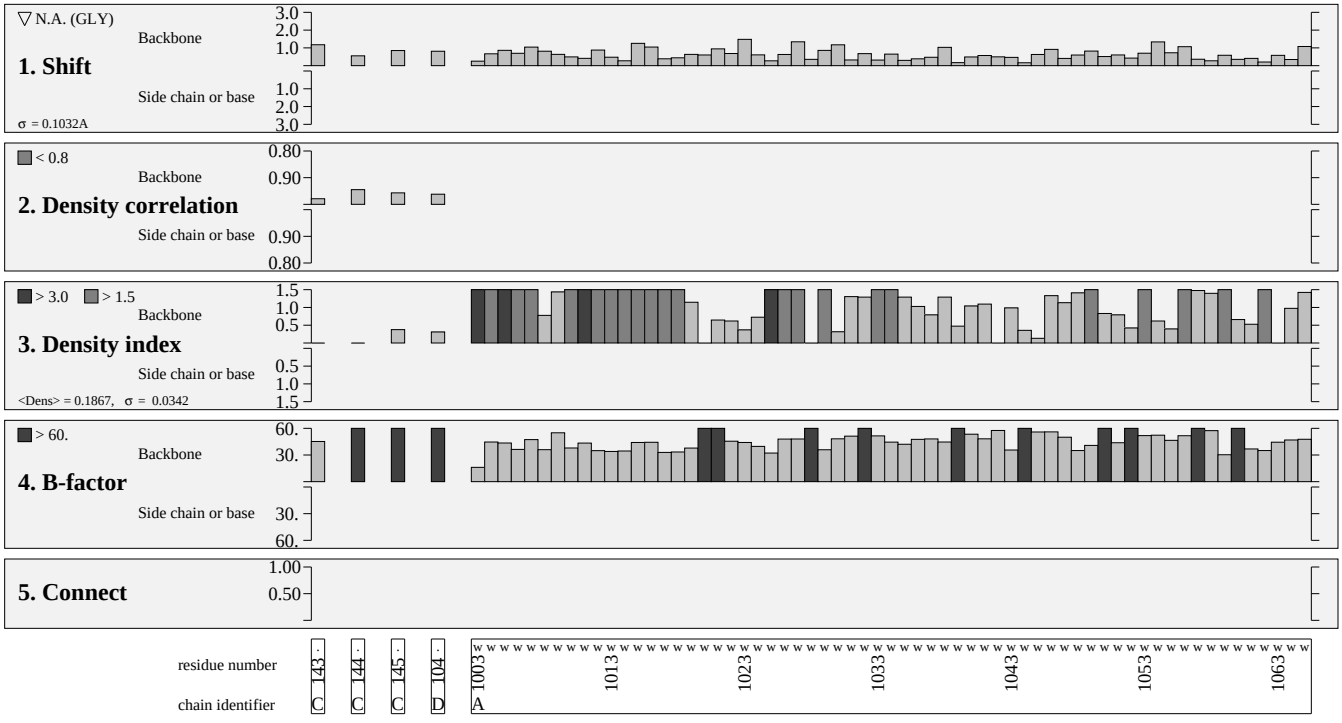
Local estimation (8)





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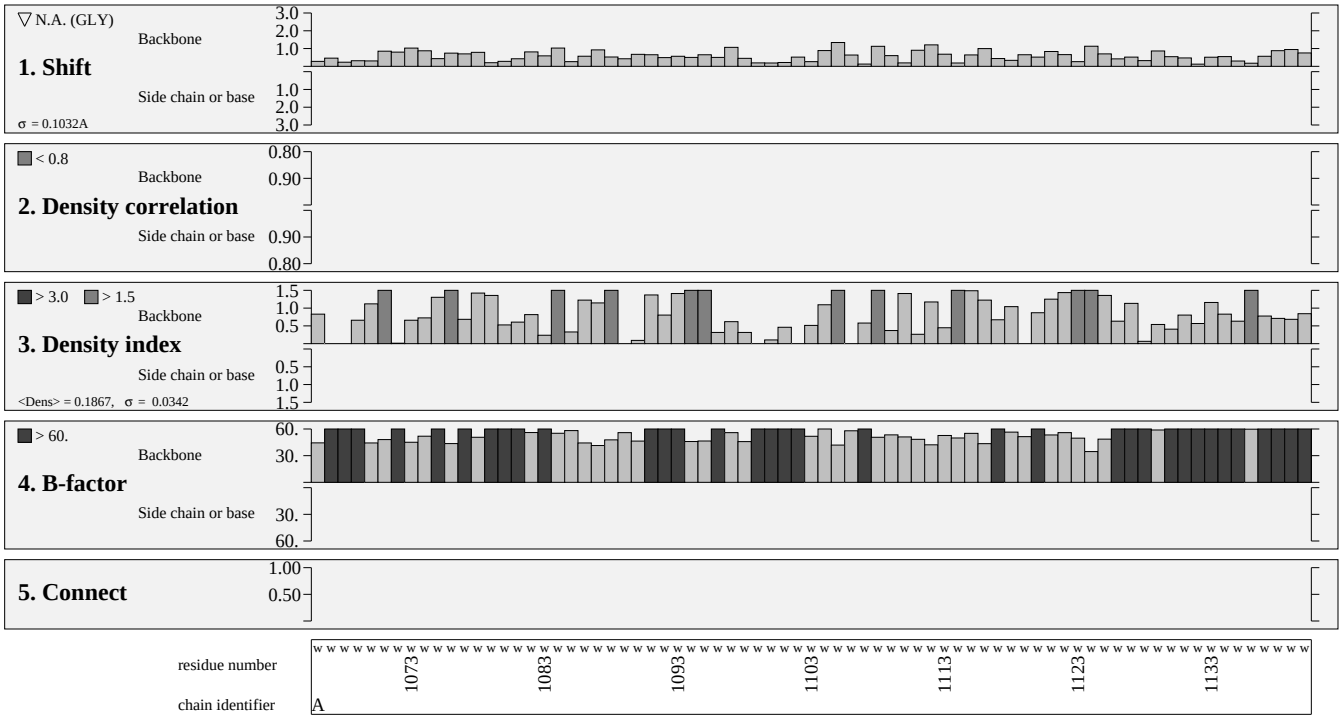
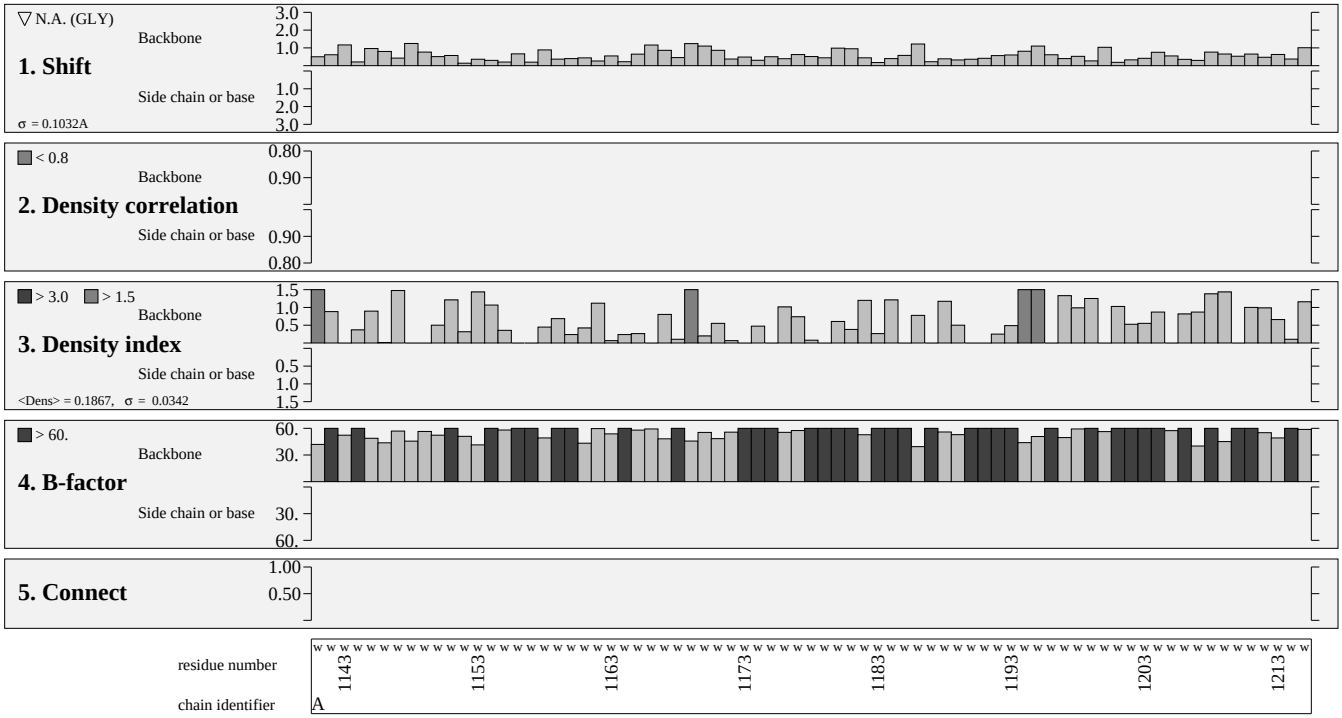
Local estimation (9)





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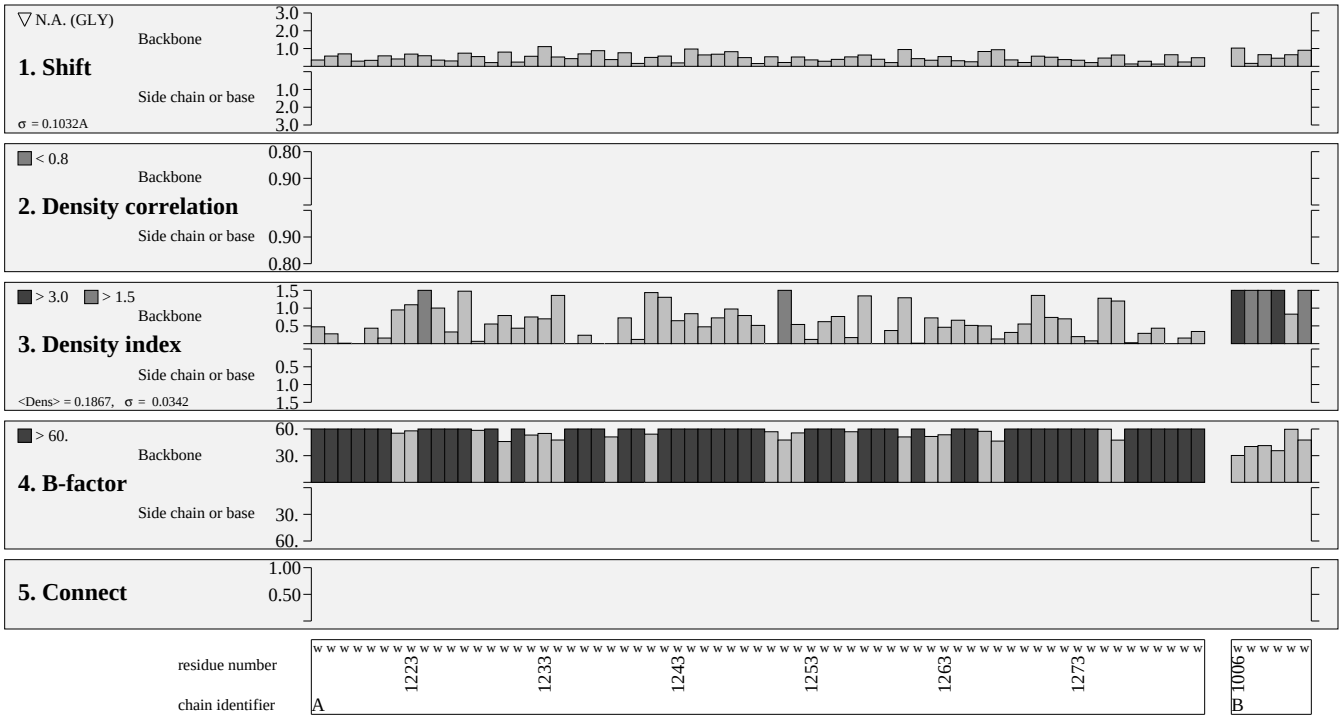
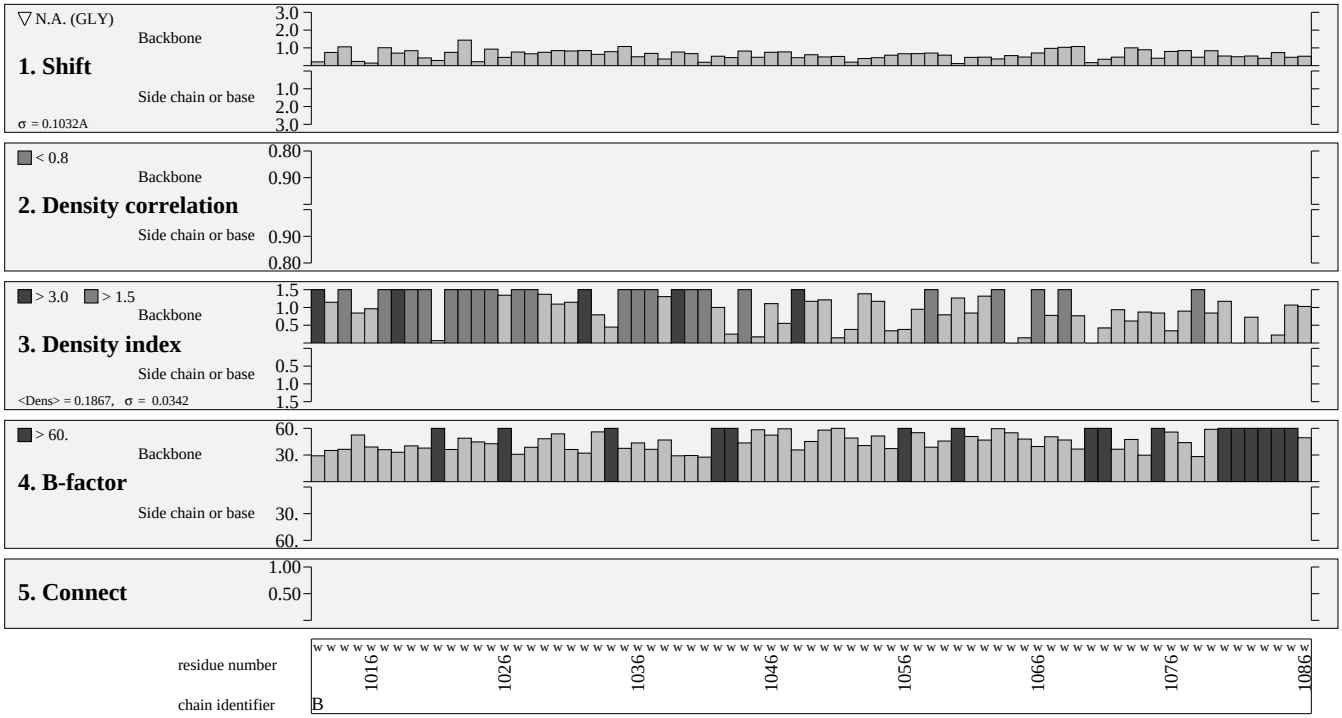
Local estimation (10)





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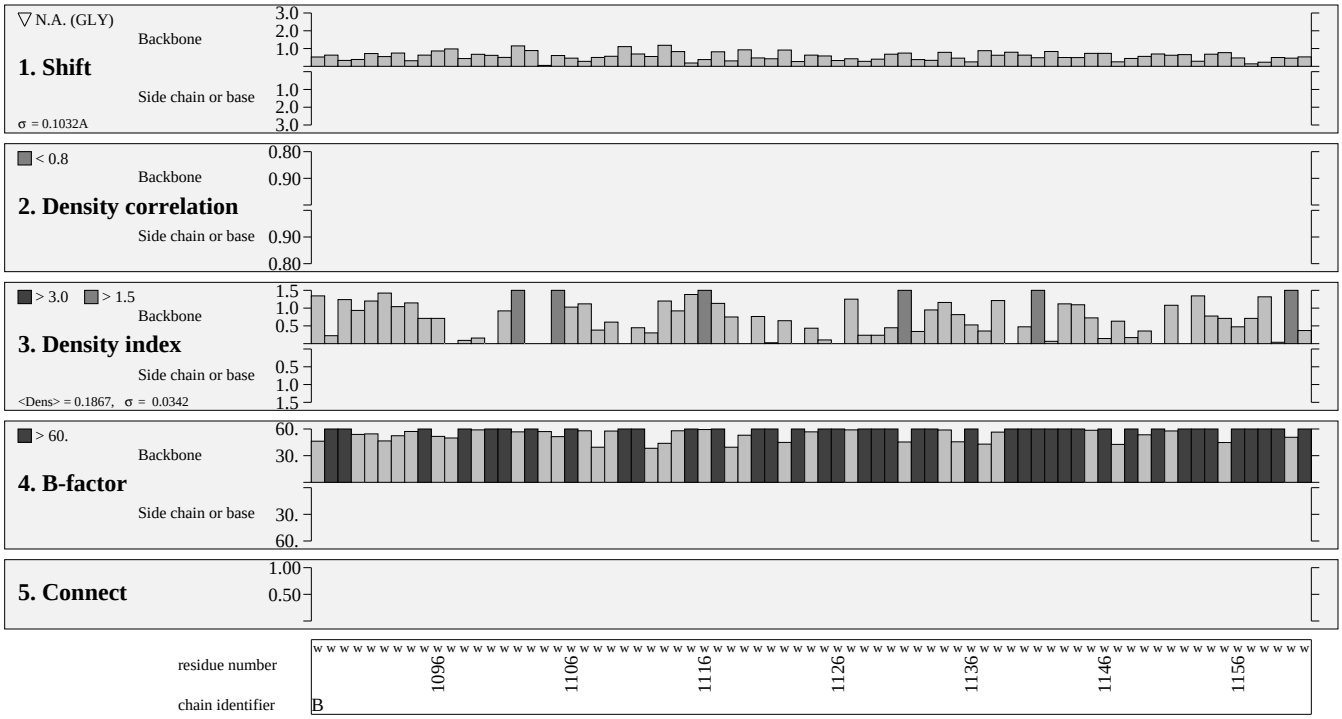
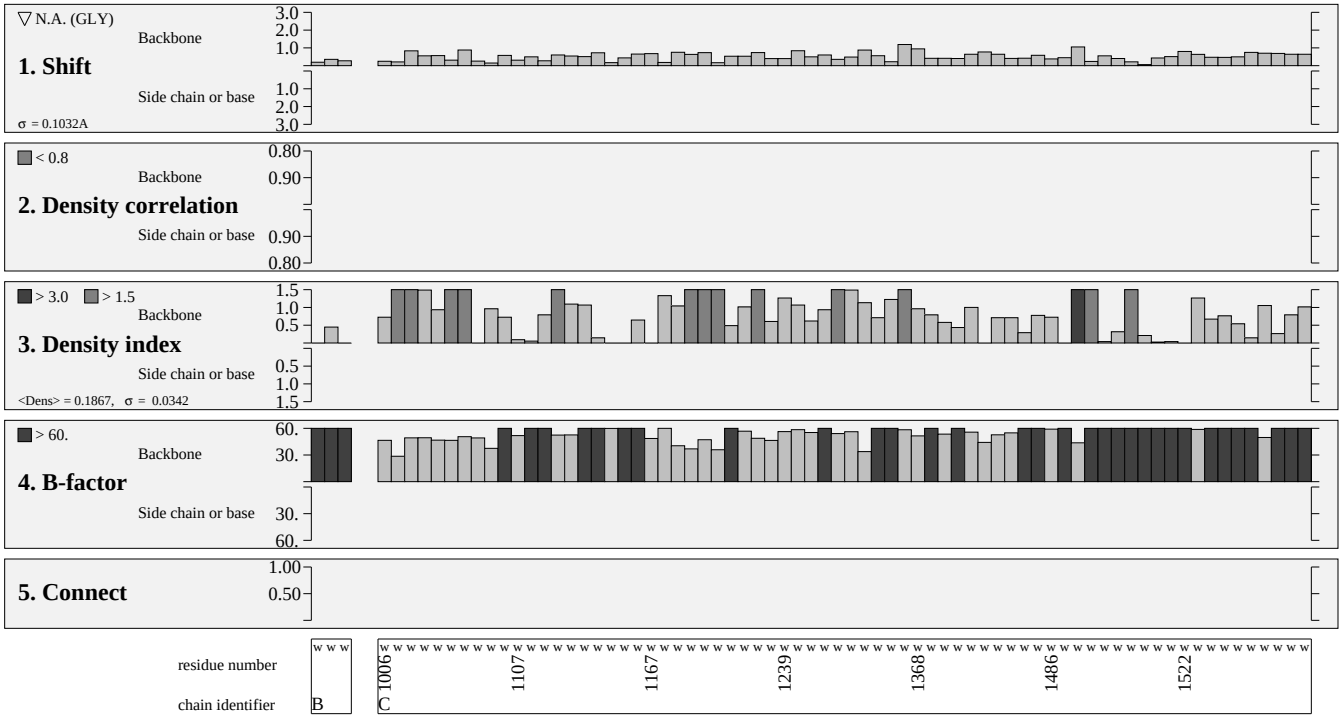
Local estimation (11)





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Structure Factor Check

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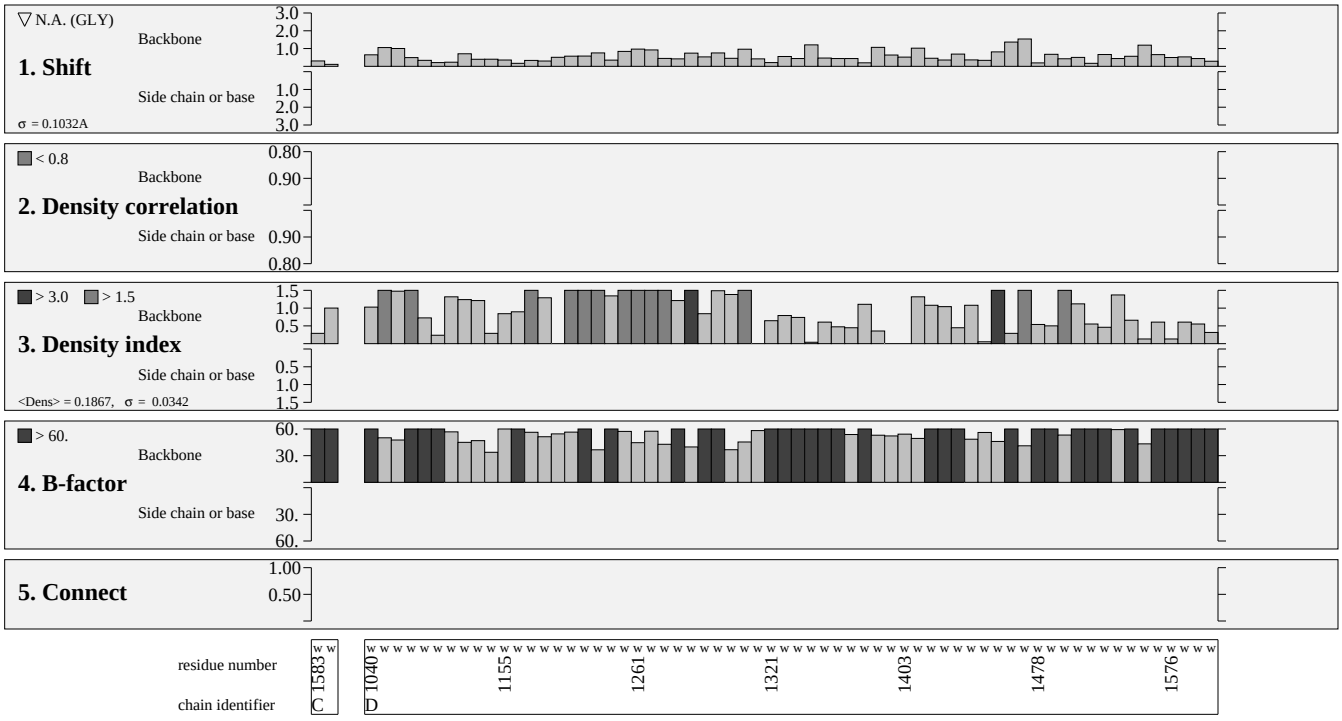
Local estimation (12)



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