

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 Å b: 182.36 Å c: 241.63 Å
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 Å
Reflections in file: 125230
Unique reflections above 0: 125230
above 1σ: 122444
above 3σ: 83686

SFCHECK

Nominal resolution range: 40.0 – 3.21 Å
05max. from input data, min. from author05
Used reflections: 125071
Reflections out of resolution: 159
Completeness: 99.4 %
R_{stand}(F) = <σ(F)>/<F> : 0.067
Anisotropic distribution of Structure Factors
ratio of eigen values: 1.0000 0.4647 0.5420
B_{overall} (by Patterson): 59.Å²
Optical resolution: 2.38 Å
Expected opt. resol. for complete data set: 2.38 Å
Estimated minimal error: 0.110 Å

Model

32657 atoms (14 water molecules)

Number of chains: 51

Volume not occupied by model: 62.9 %

 (for atomic model): 89.5 Å²

σ(B): 14.75 Å²

Matthews coefficient: 4.20

Corresponding solvent % : 70.45

Model vs. Structure Factors

R-factor for all reflections: 0.338
Correlation factor: 0.810
R-factor: 0.338
for F > 2.0 σ
nom. resolution range: 29.99 – 3.21 Å
reflections used: 122210

Rfree: 0.356
Nfree: 2436
R-factor without free-refl.: 0.338
Non free-reflections: 119774
<u> (error in coords by Luzzati plot): 0.707 Å
Estimated maximal error: 0.490 Å
DPI: 0.484 Å

Scaling

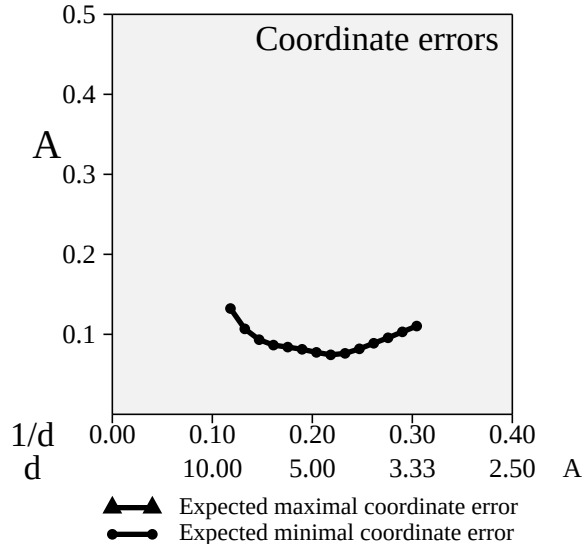
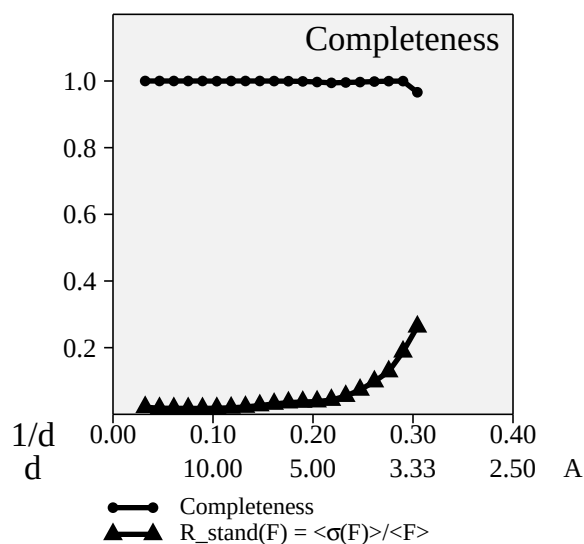
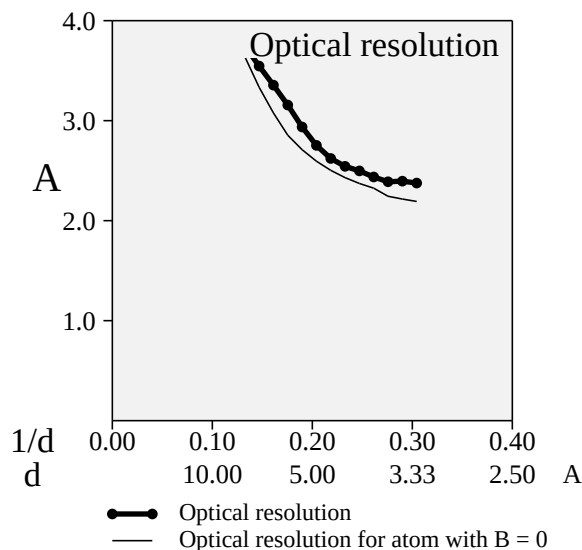
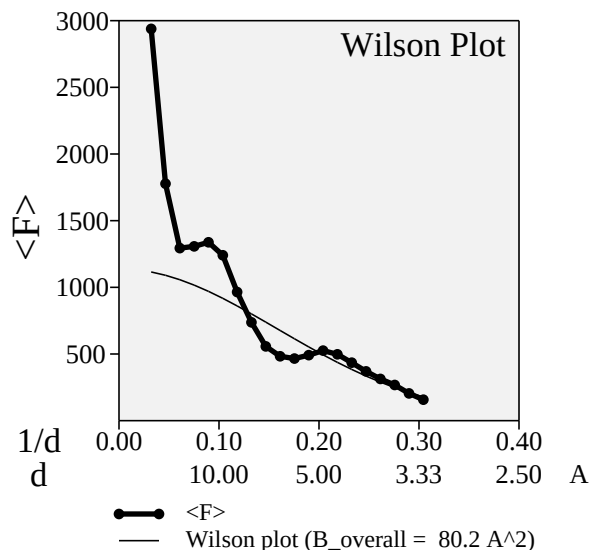
Scale: 0.458
Bdiff: -7.31
Anisothermal Scaling (Beta):
12.8885 -4.5093 -0.1496 0.0000 0.0000 0.0000
Solvent correction – Ks,Bs: 0.510 250.205

Refinement

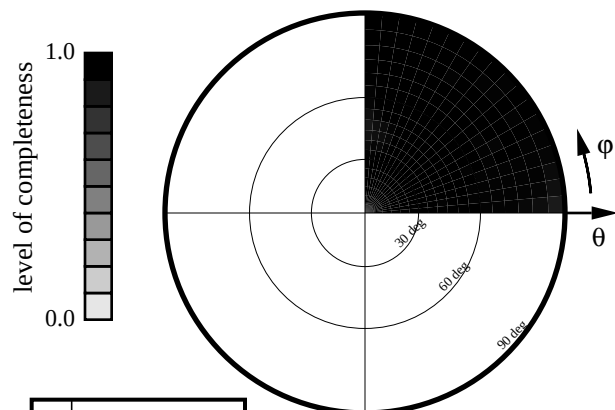
Program: CNS 1.1
Nominal resolution range: 30.0 – 3.21 Å
Reported R-factor: 0.267
Number of reflections used: 125125
Reported Rfree: 0.29
Sigma cut-off: N.A.

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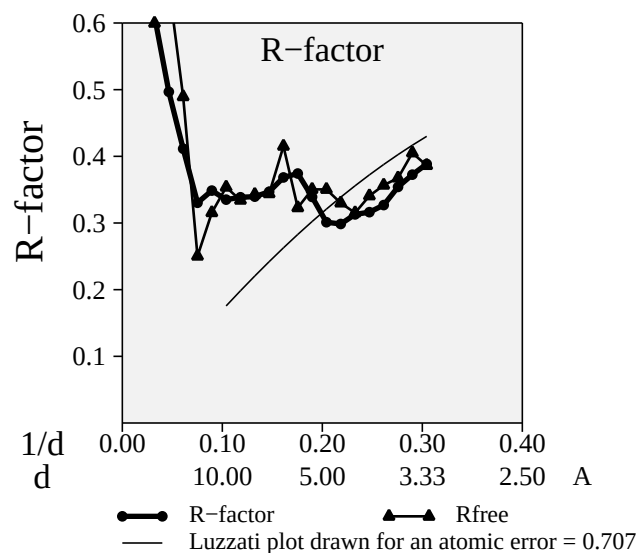


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

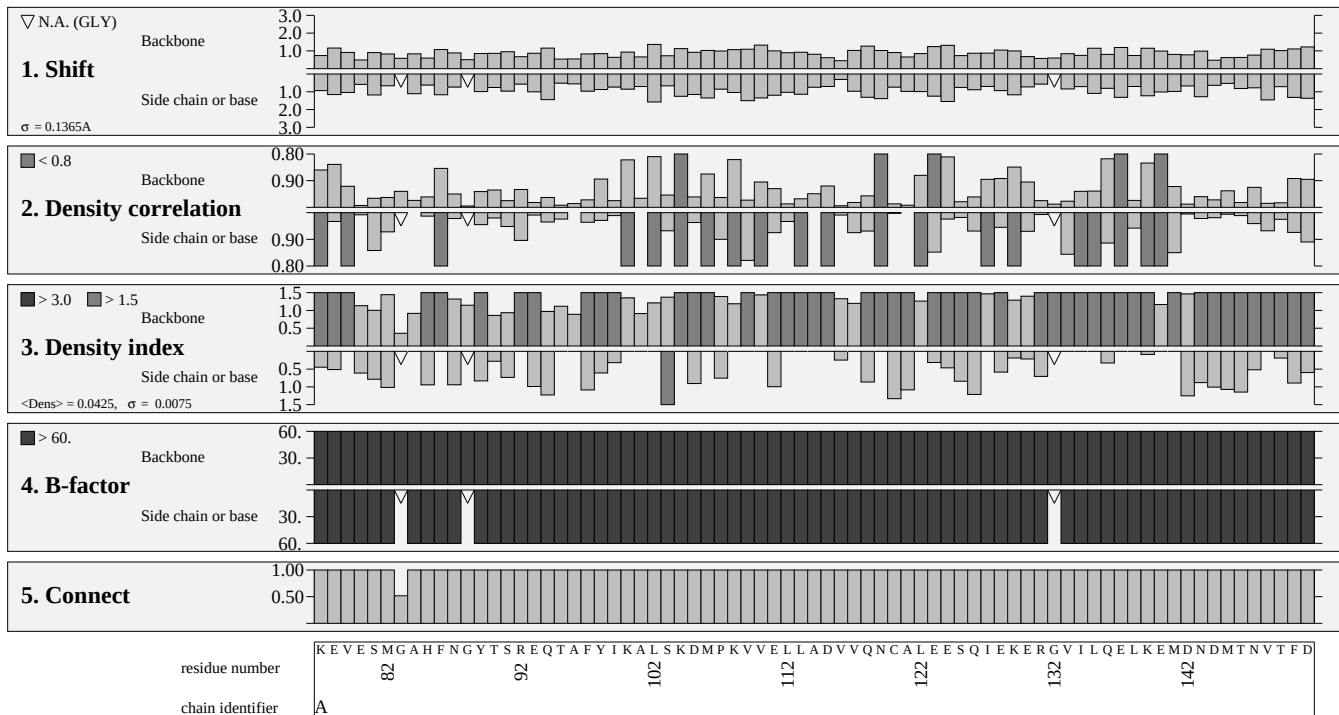
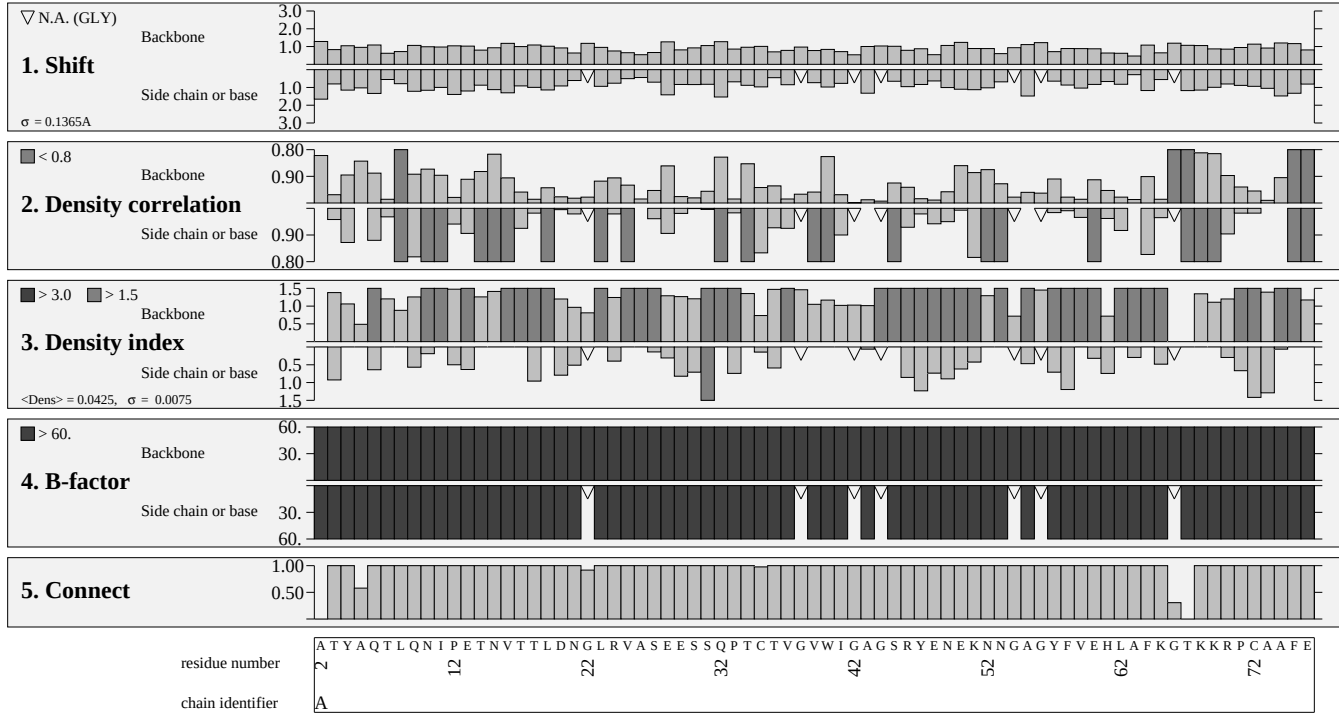
polar coordinates of the crystallographical axes



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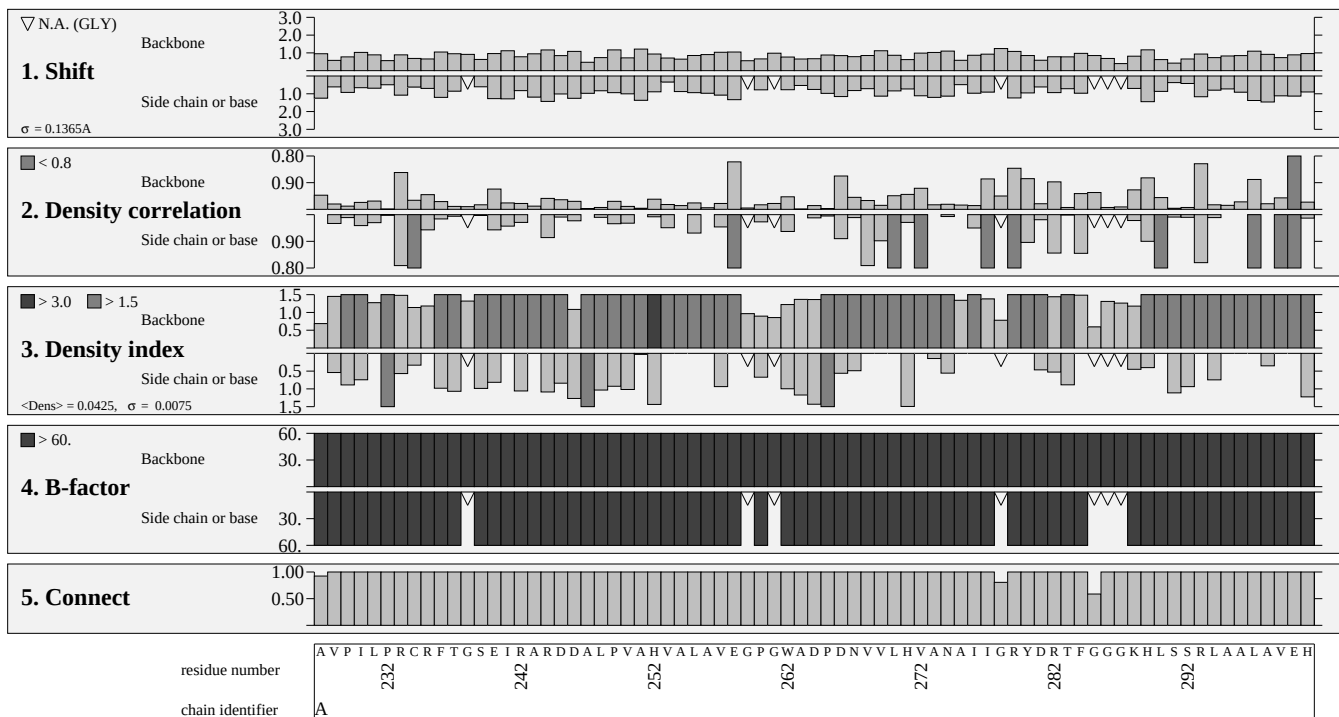
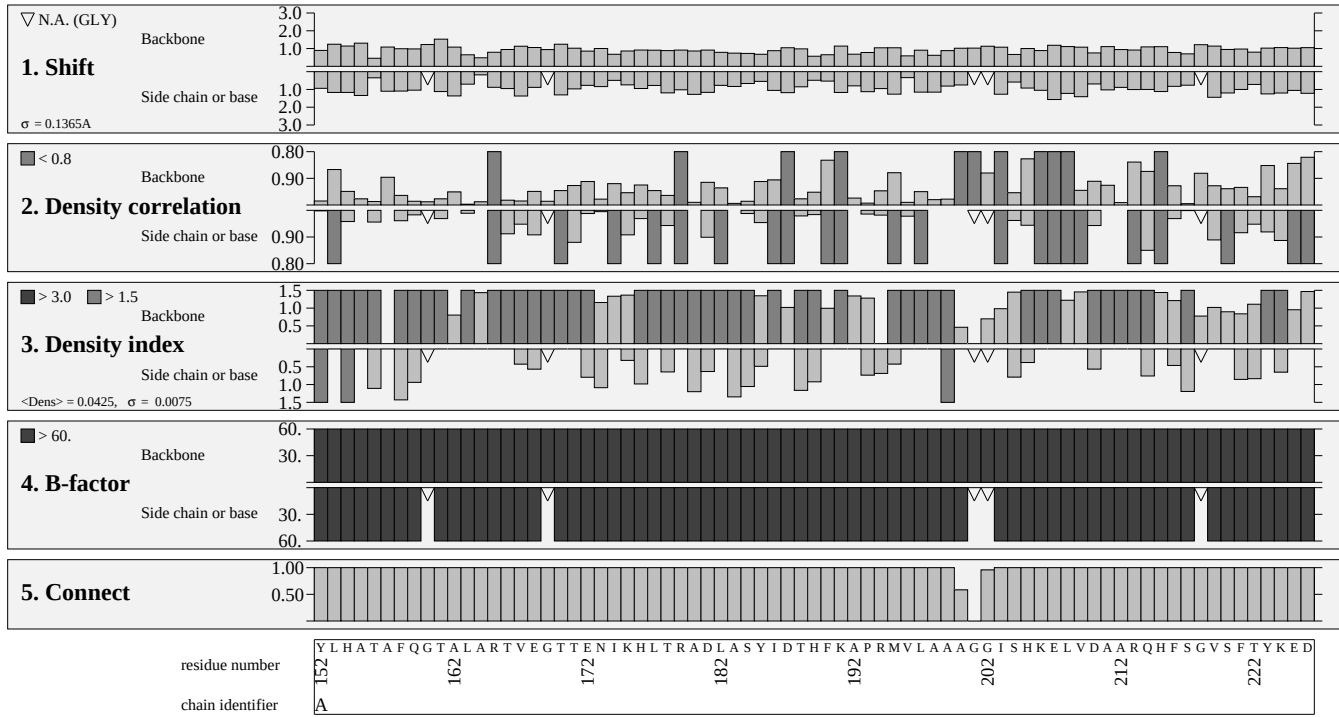
Local estimation



Structure Factor Check

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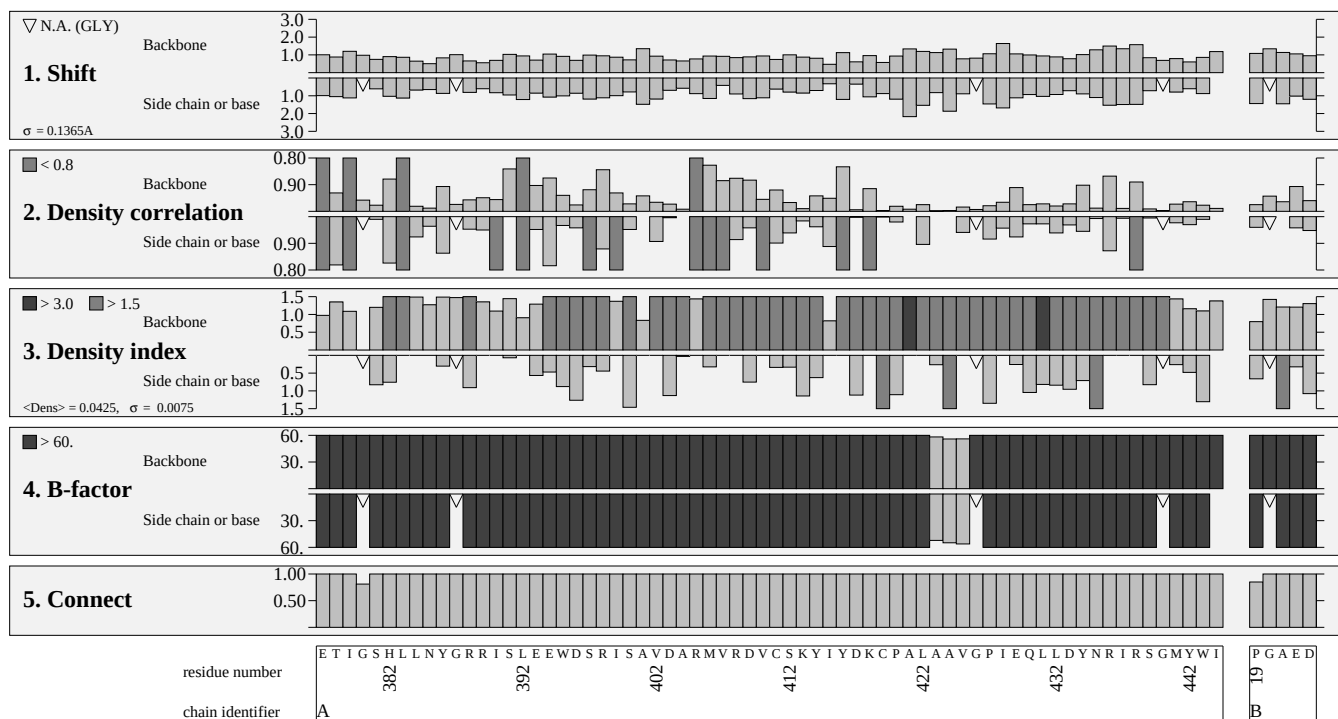
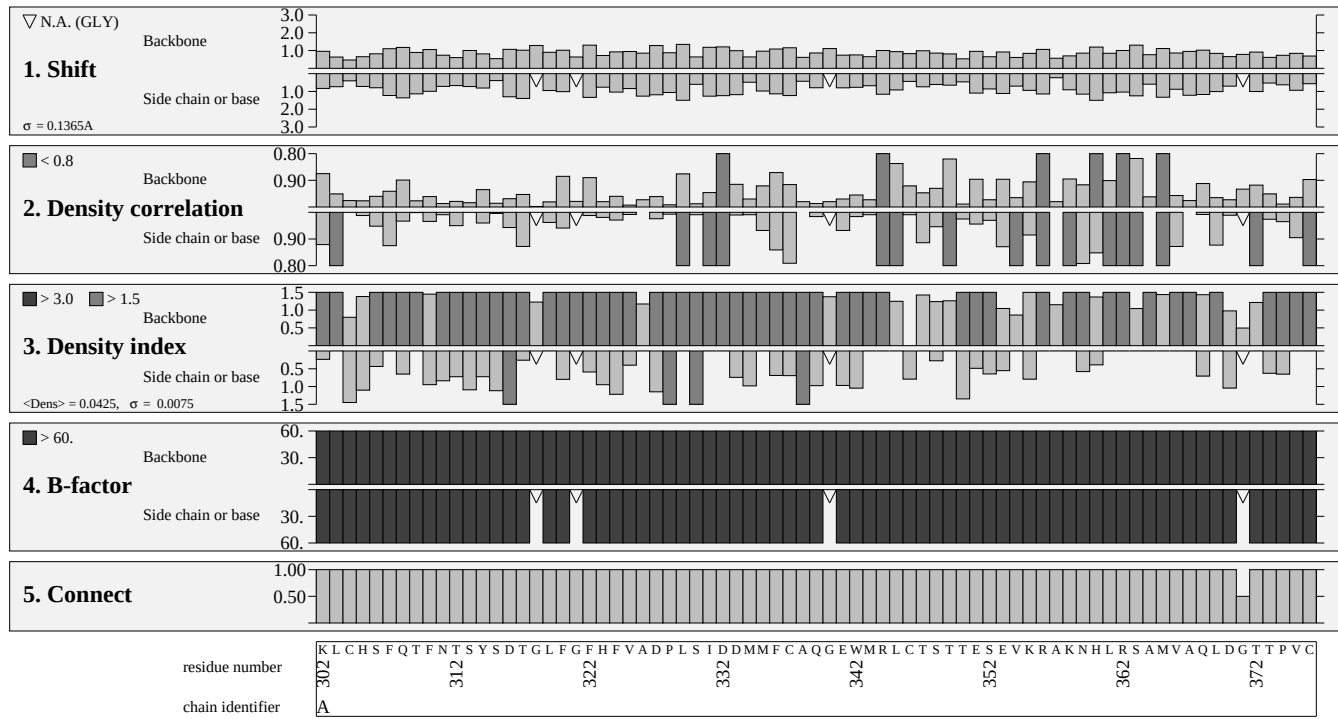
Local estimation (2)



Structure Factor Check

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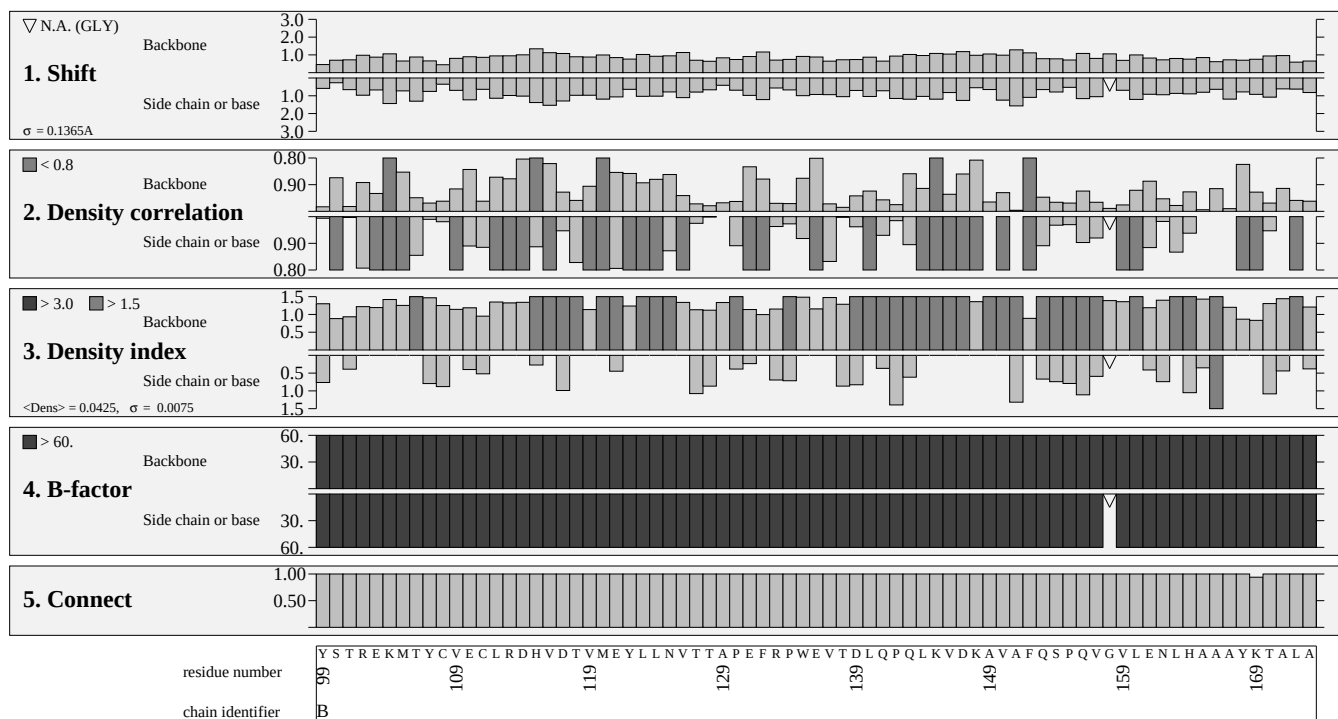
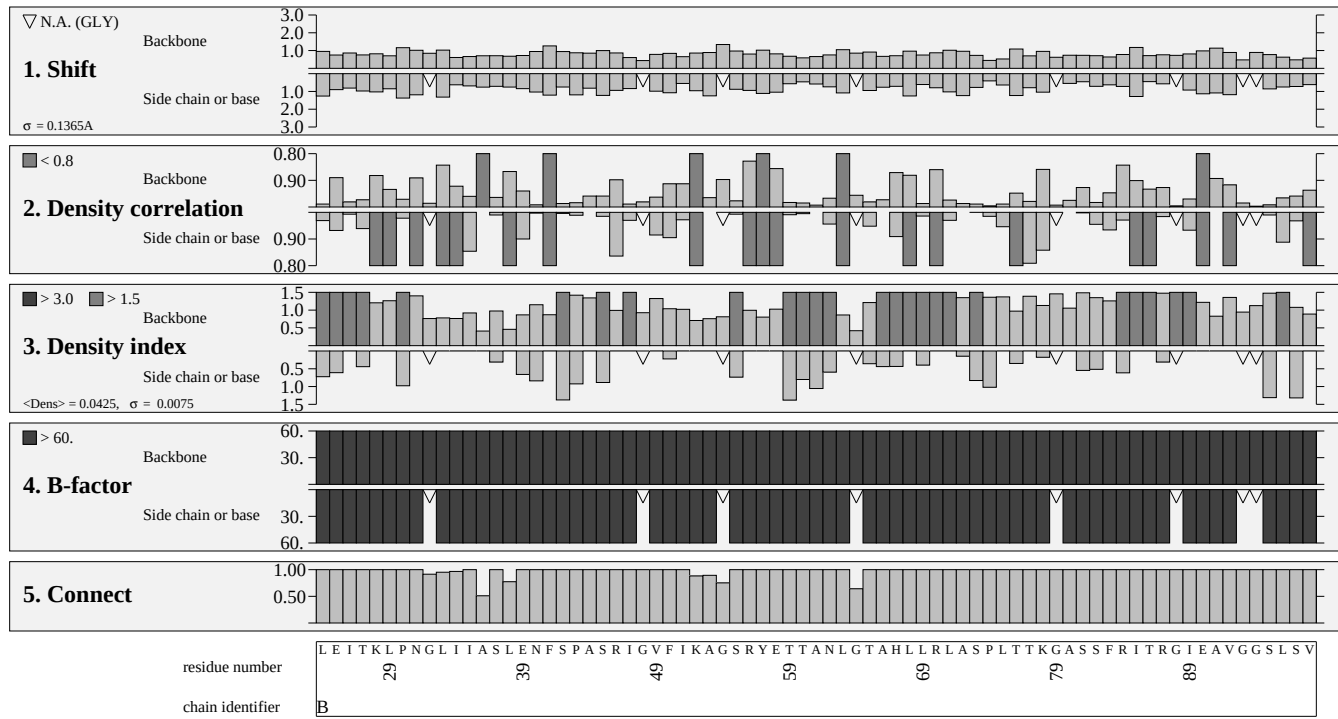
Local estimation (3)



Structure Factor Check

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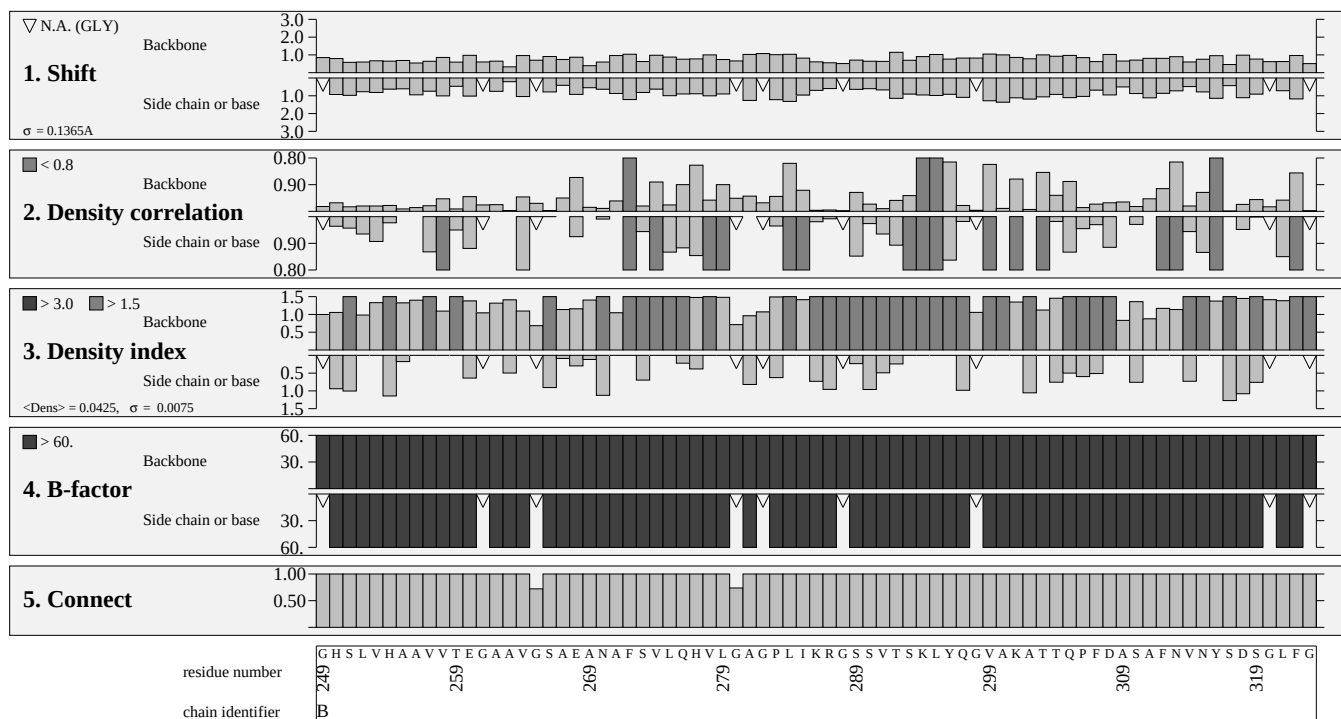
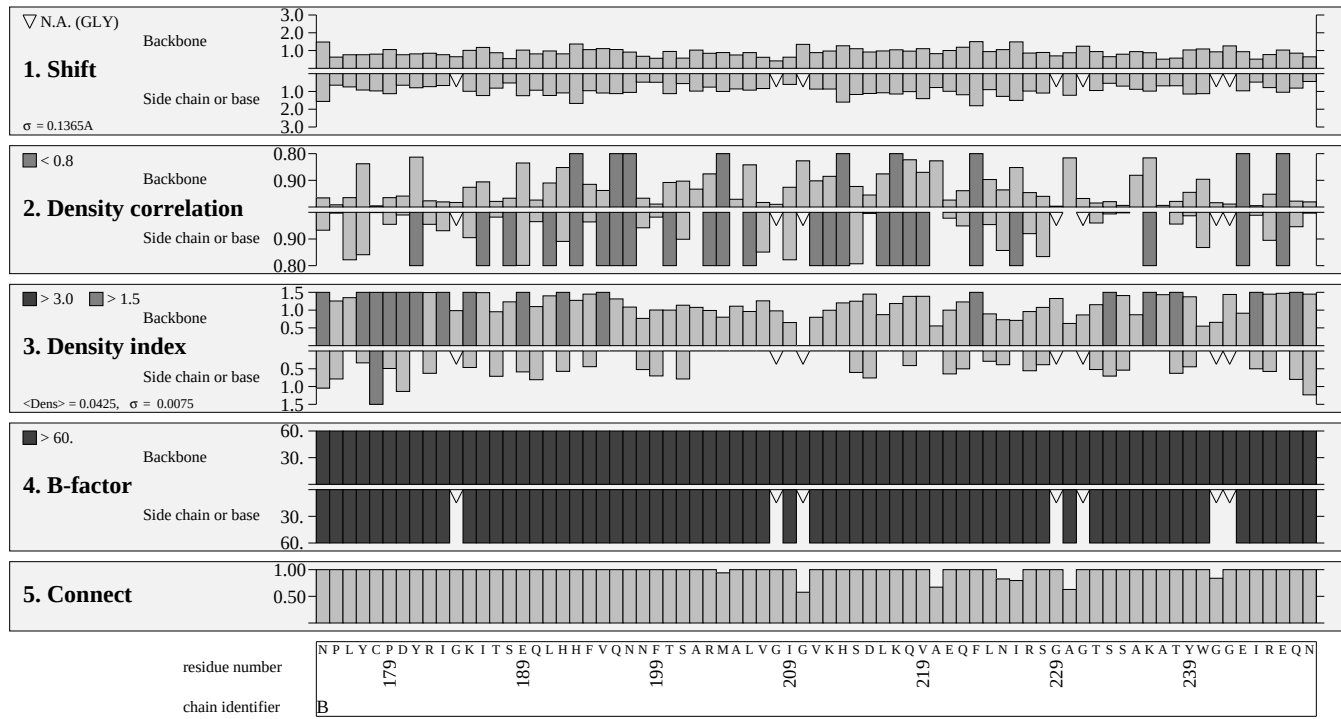
Local estimation (4)



Structure Factor Check

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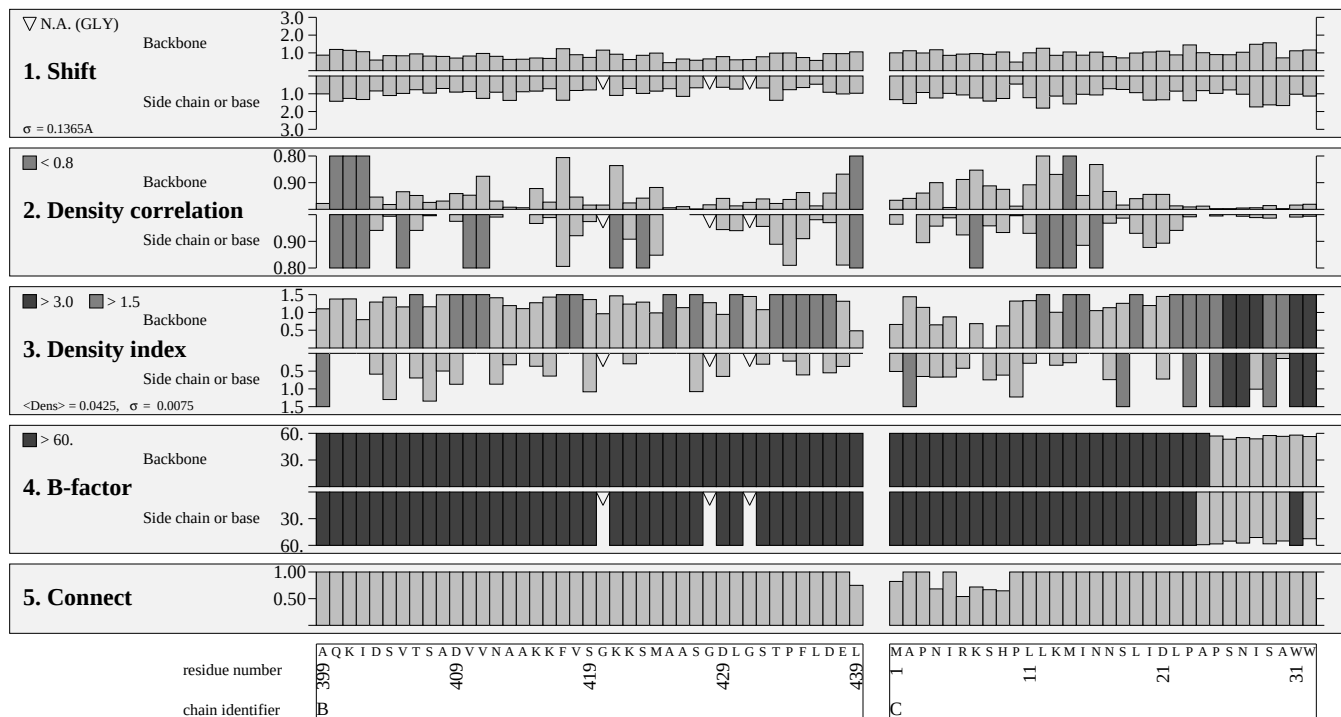
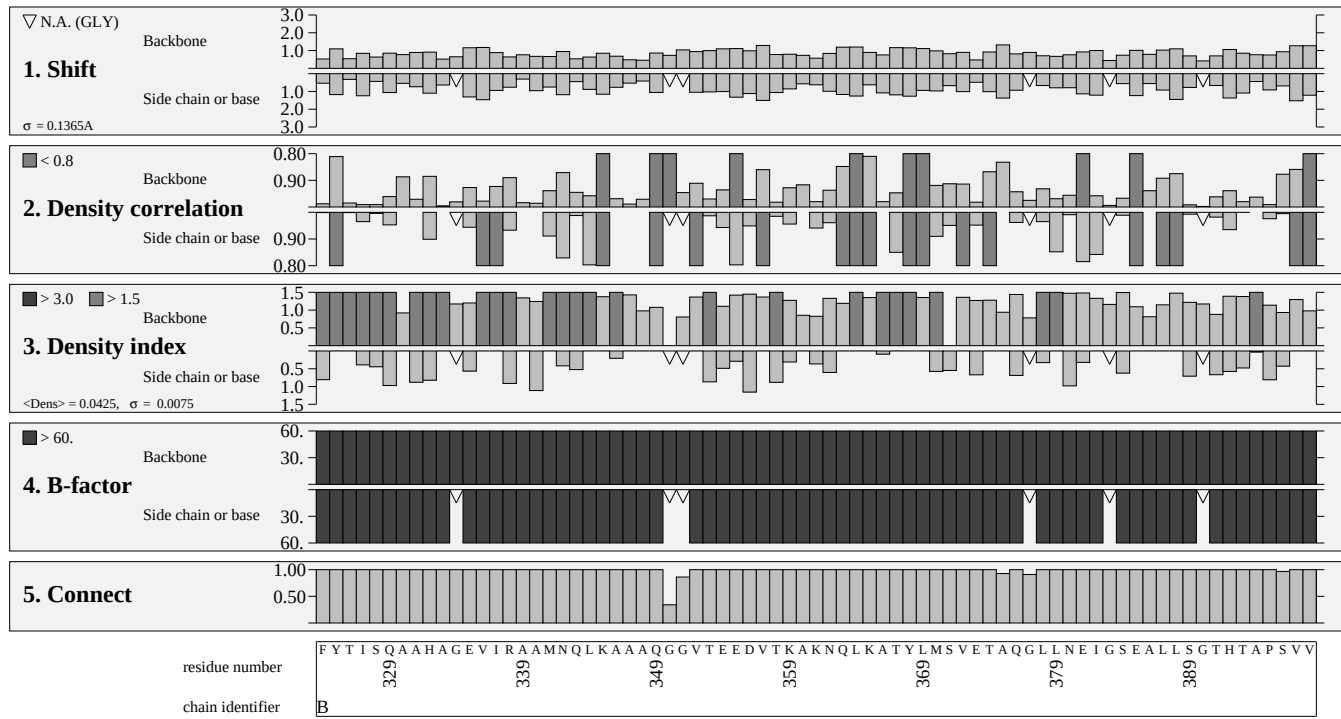
Local estimation (5)



Structure Factor Check

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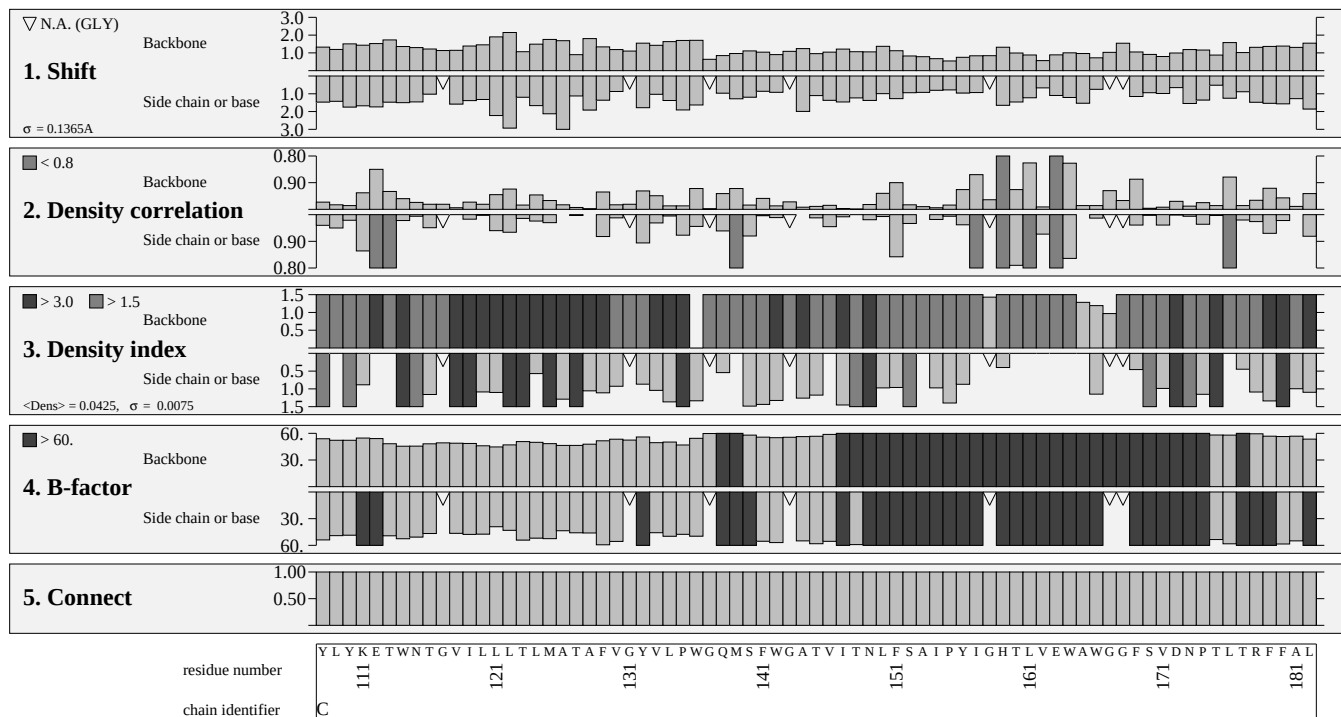
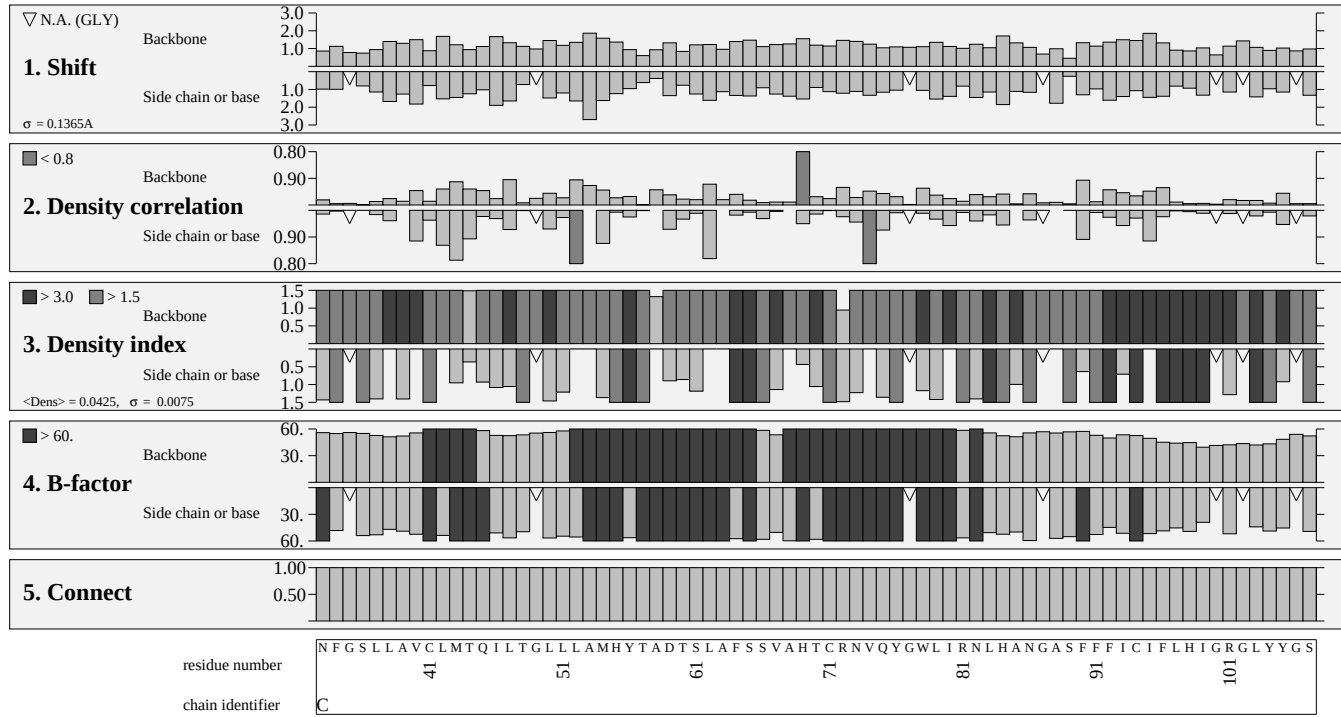
Local estimation (6)



Structure Factor Check

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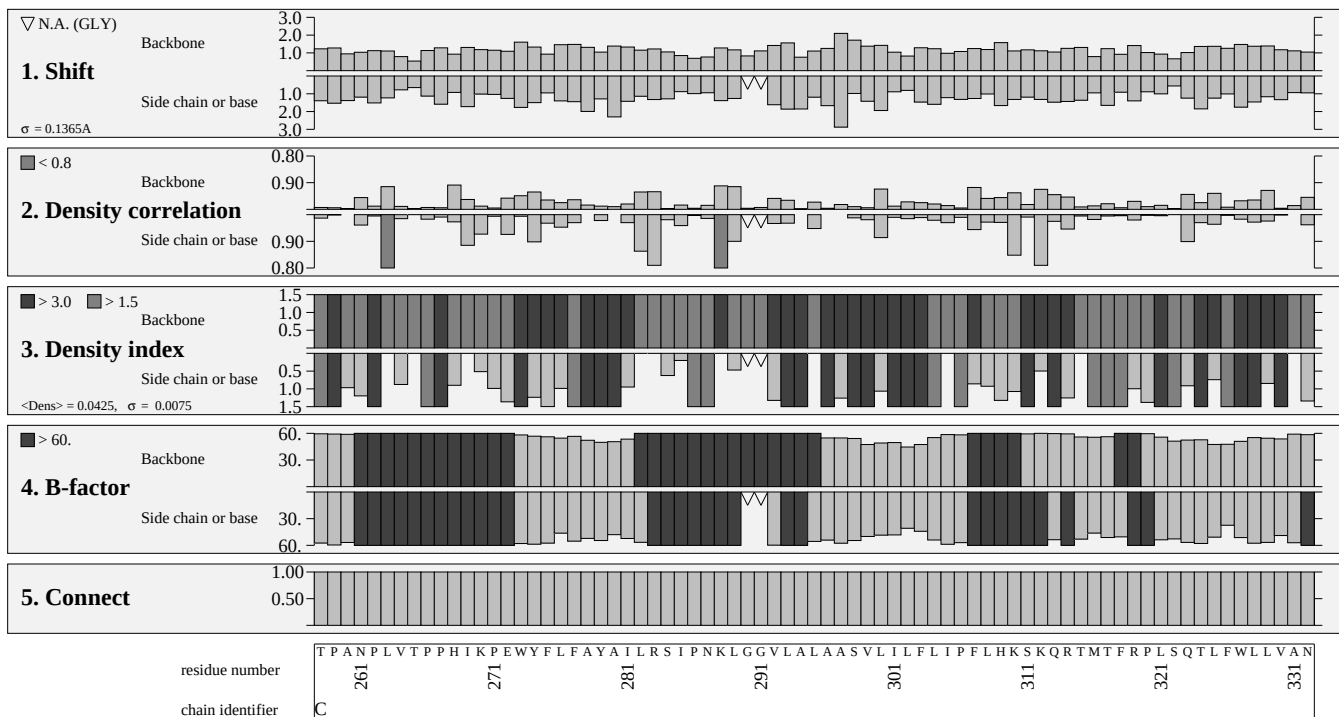
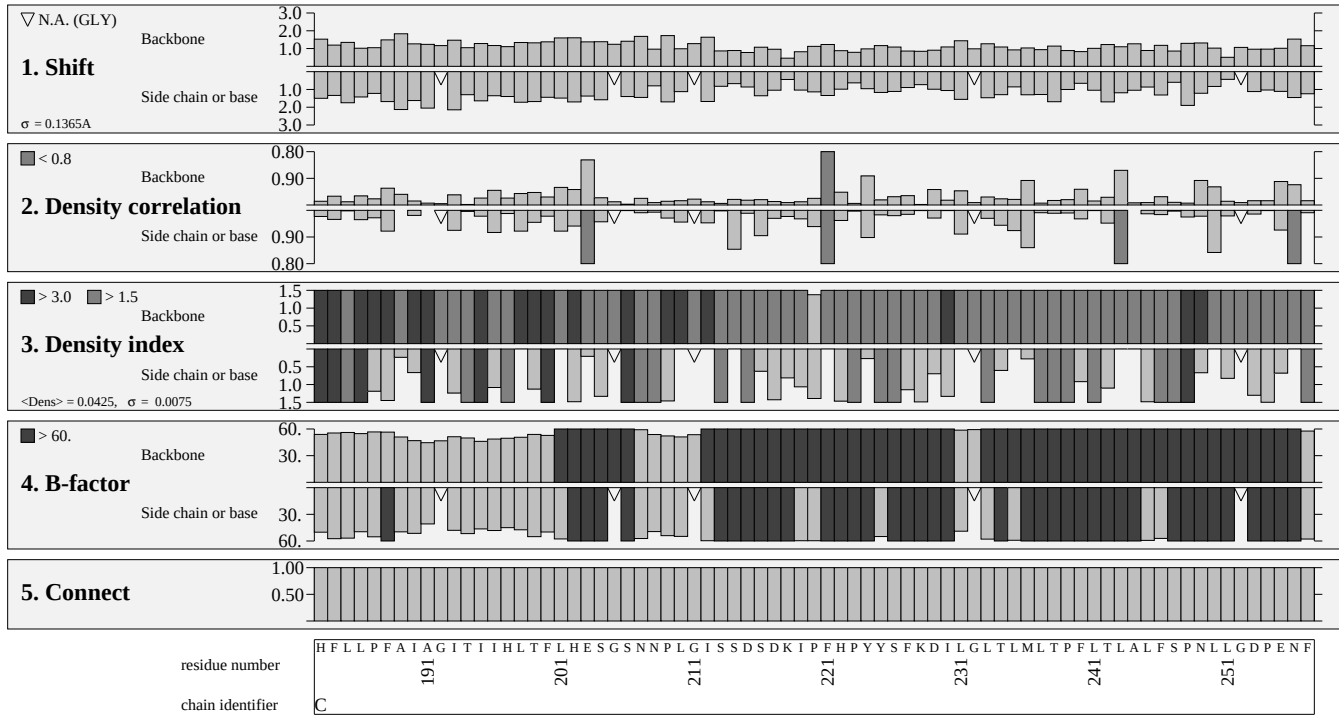
Local estimation (7)



Structure Factor Check

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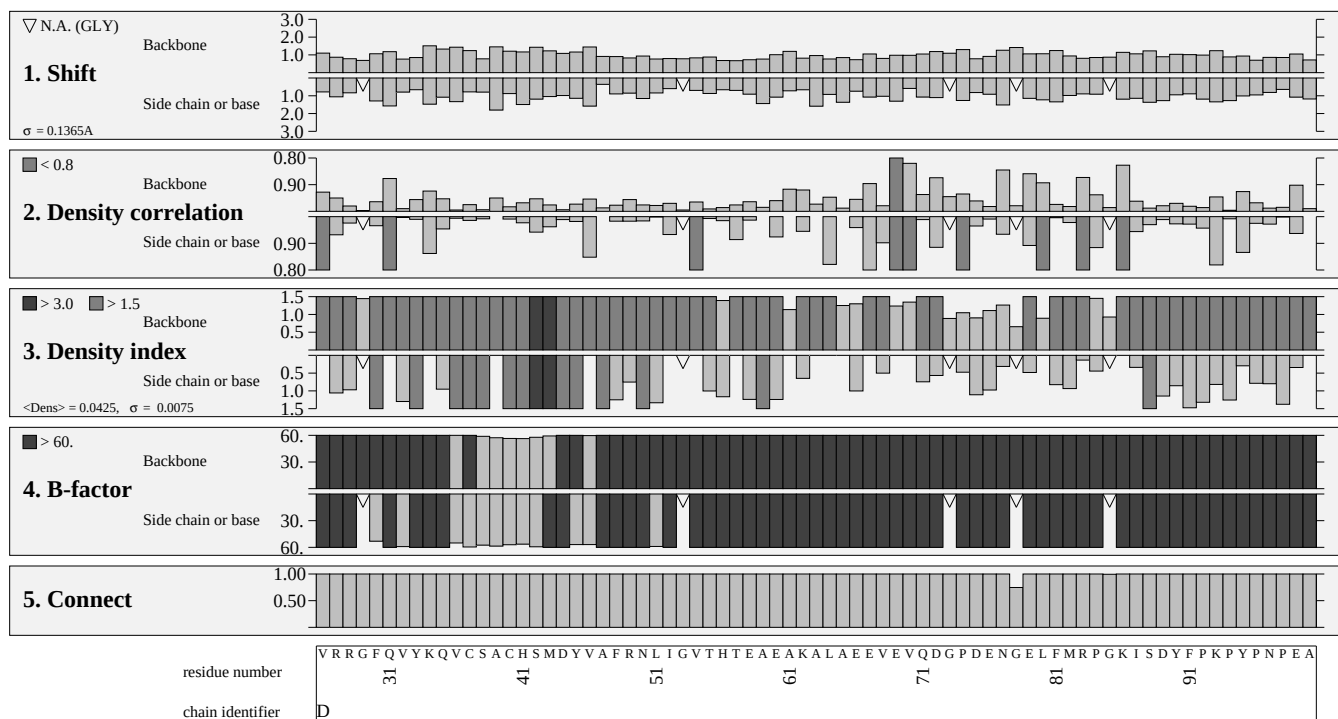
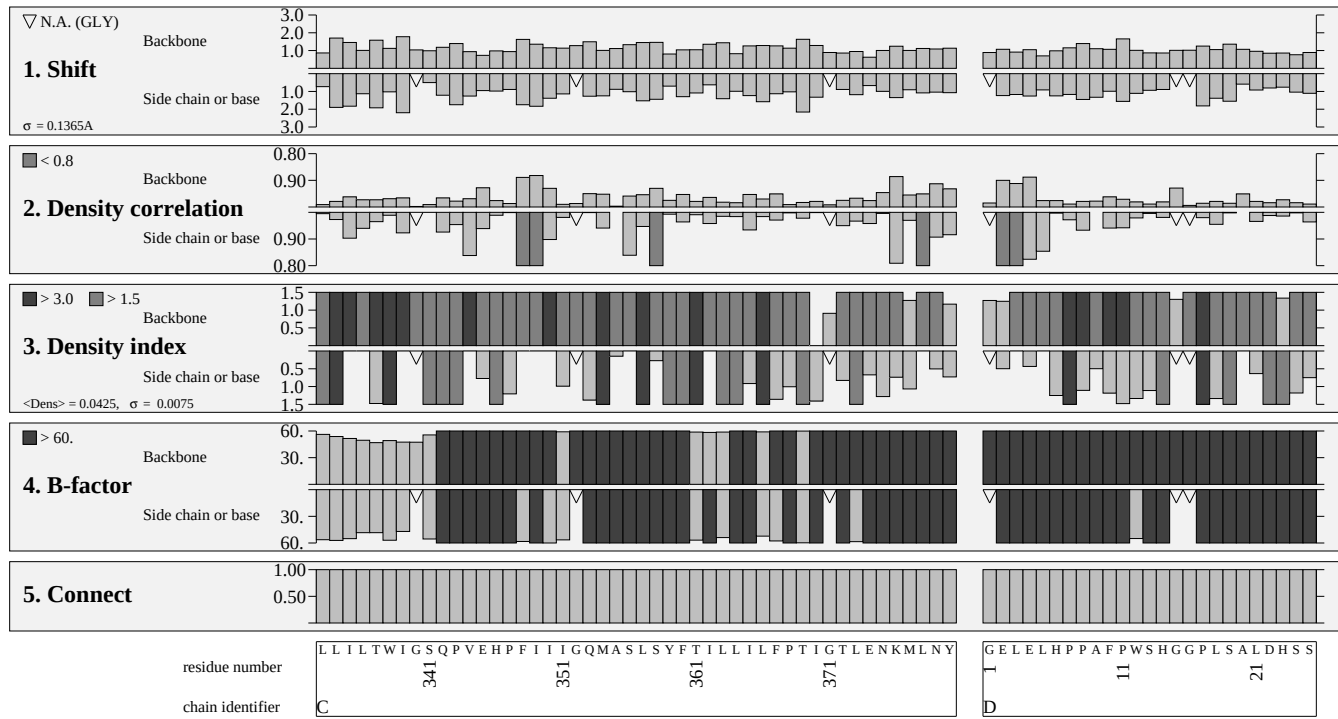
Local estimation (8)



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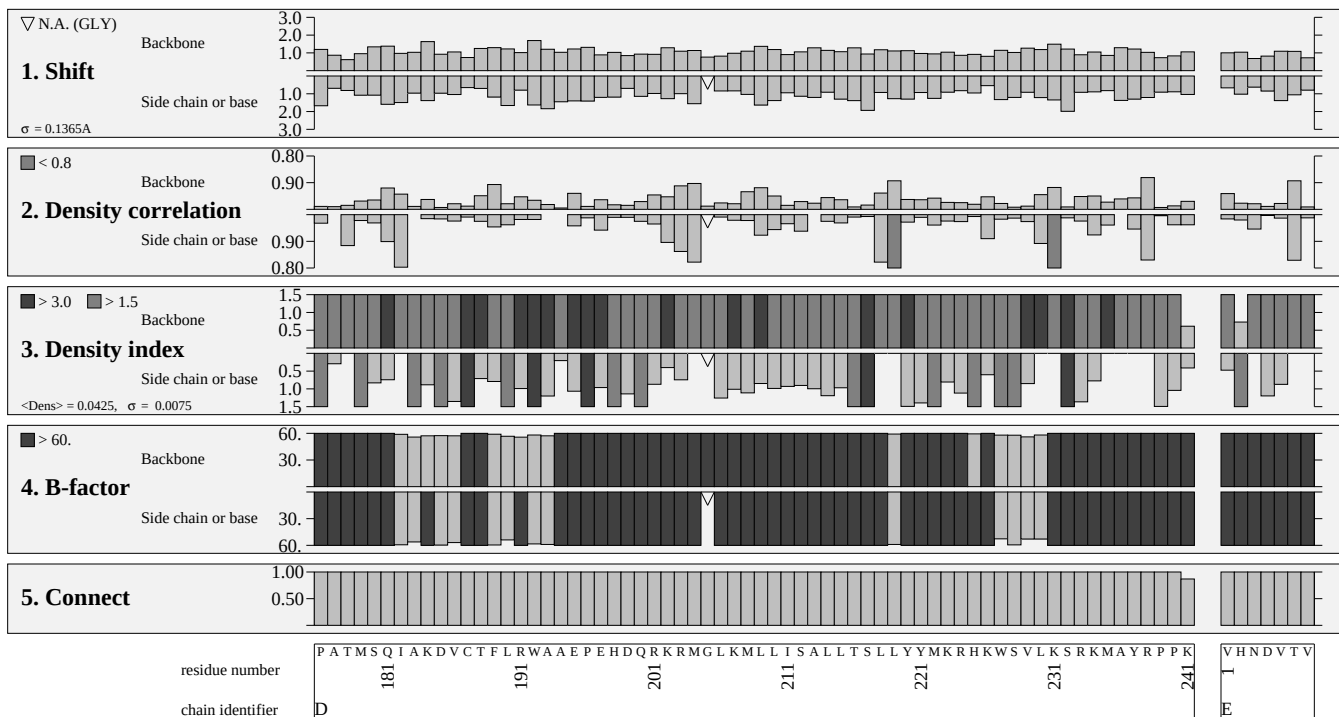
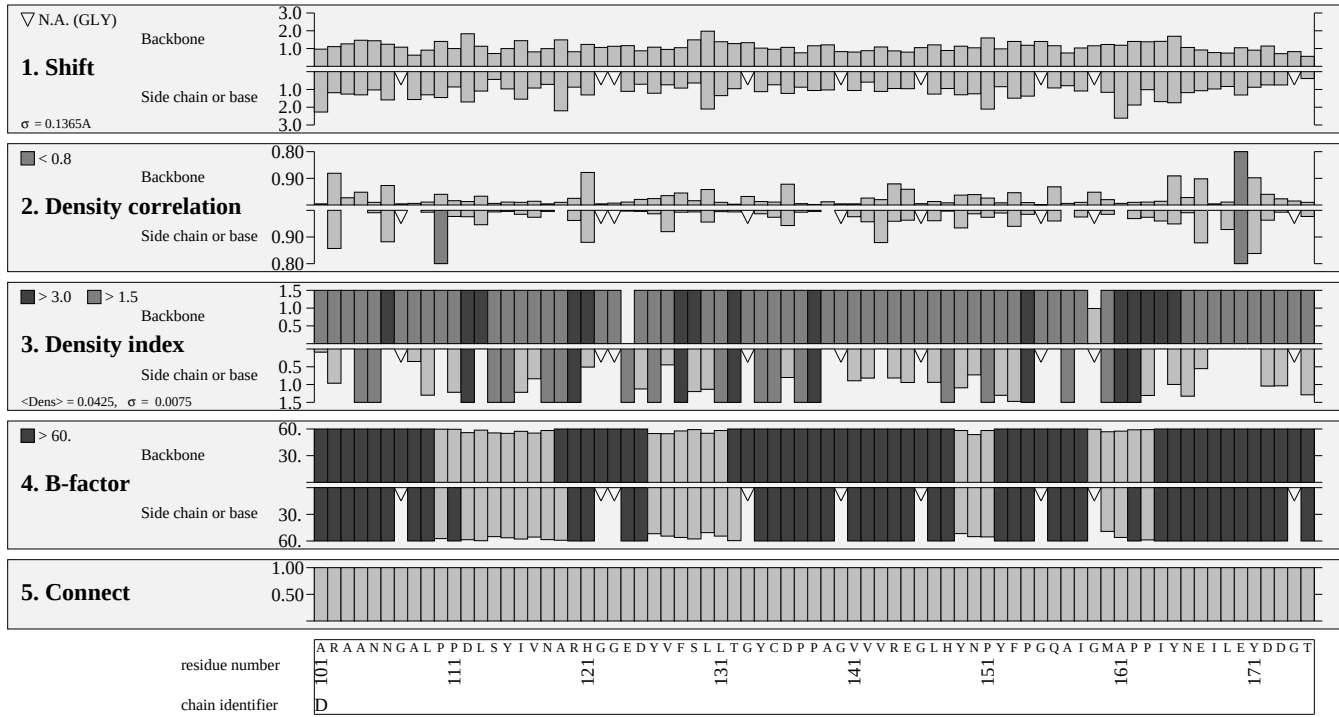
Local estimation (9)



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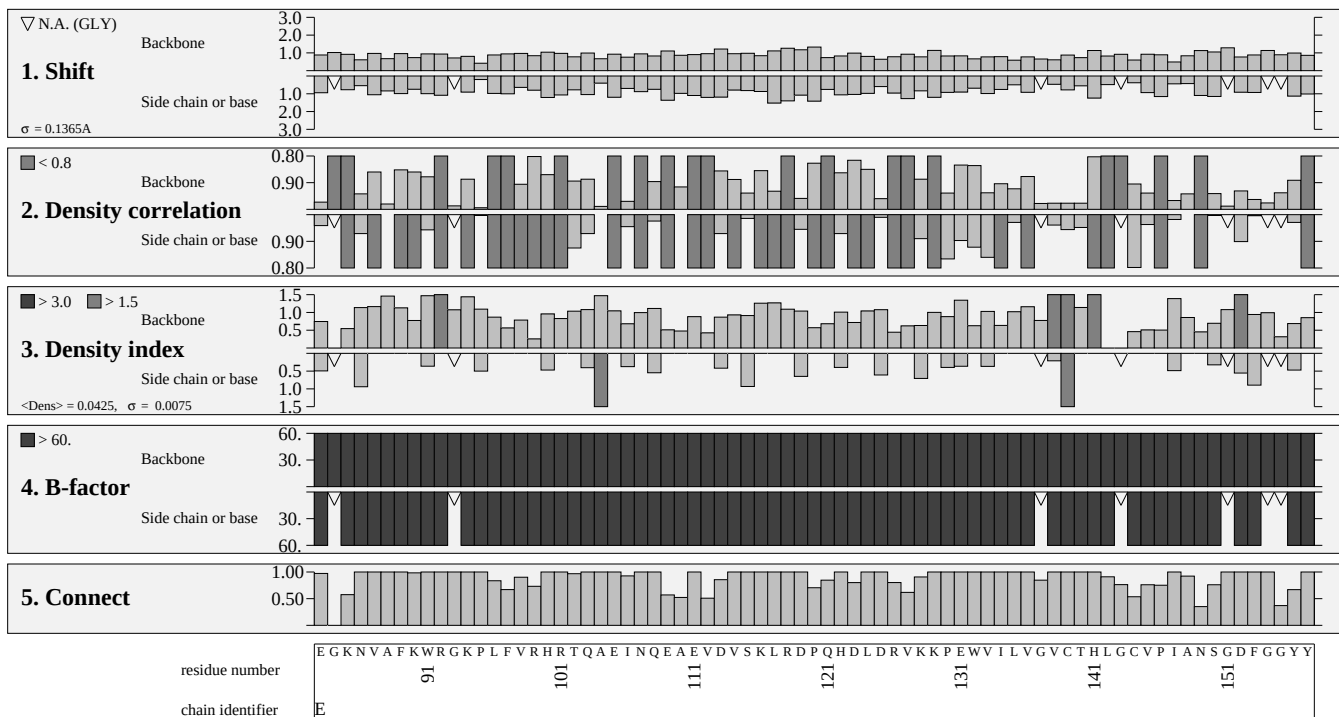
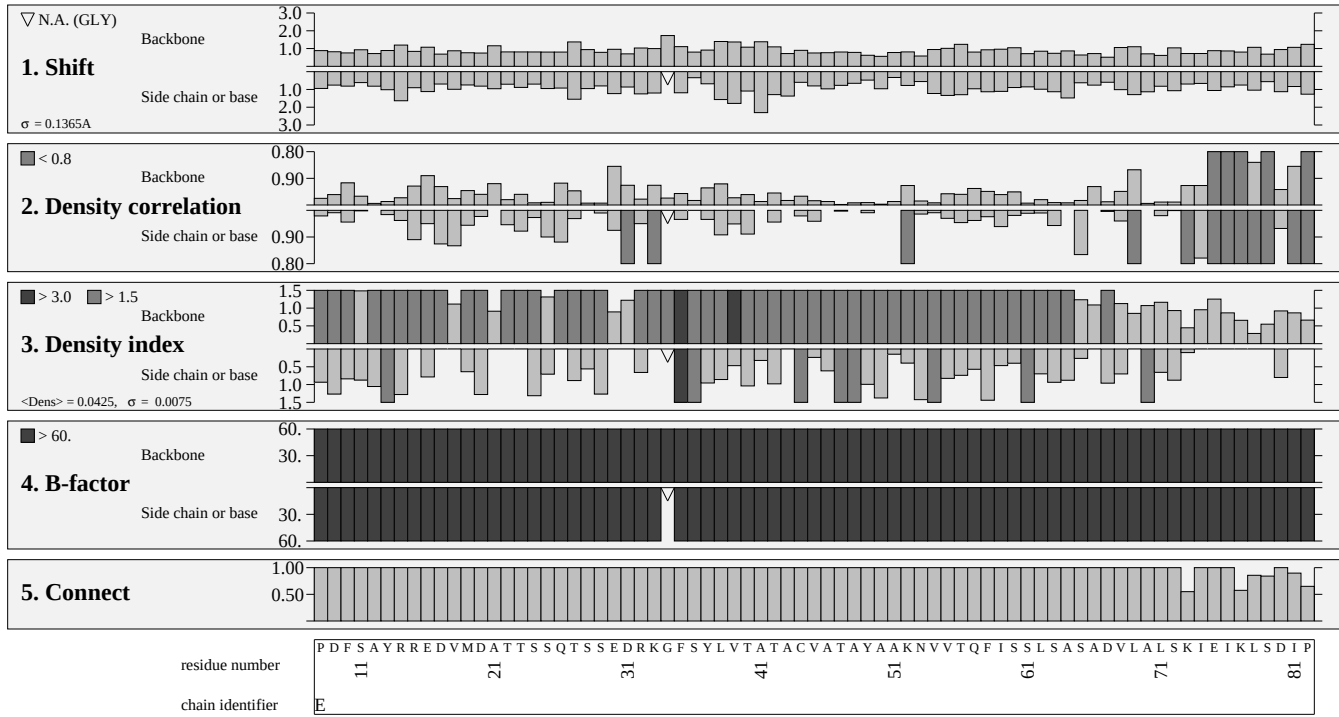
Local estimation (10)



Structure Factor Check

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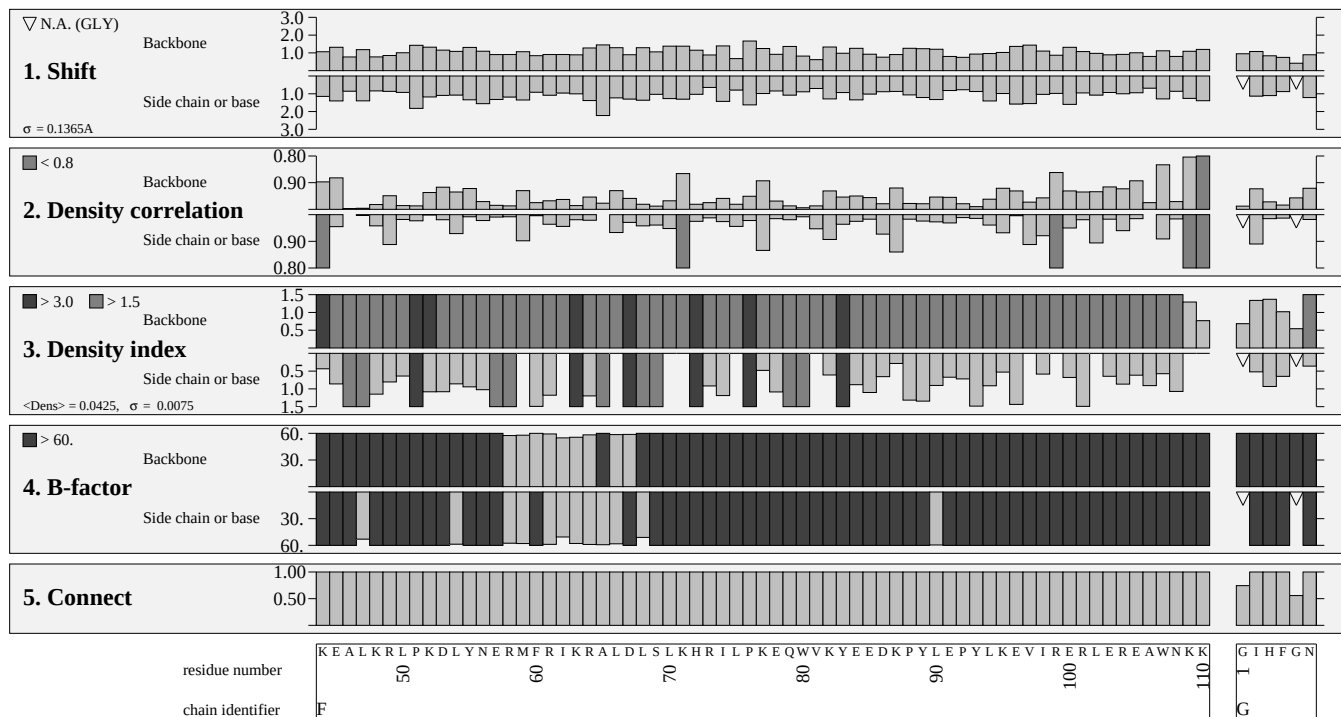
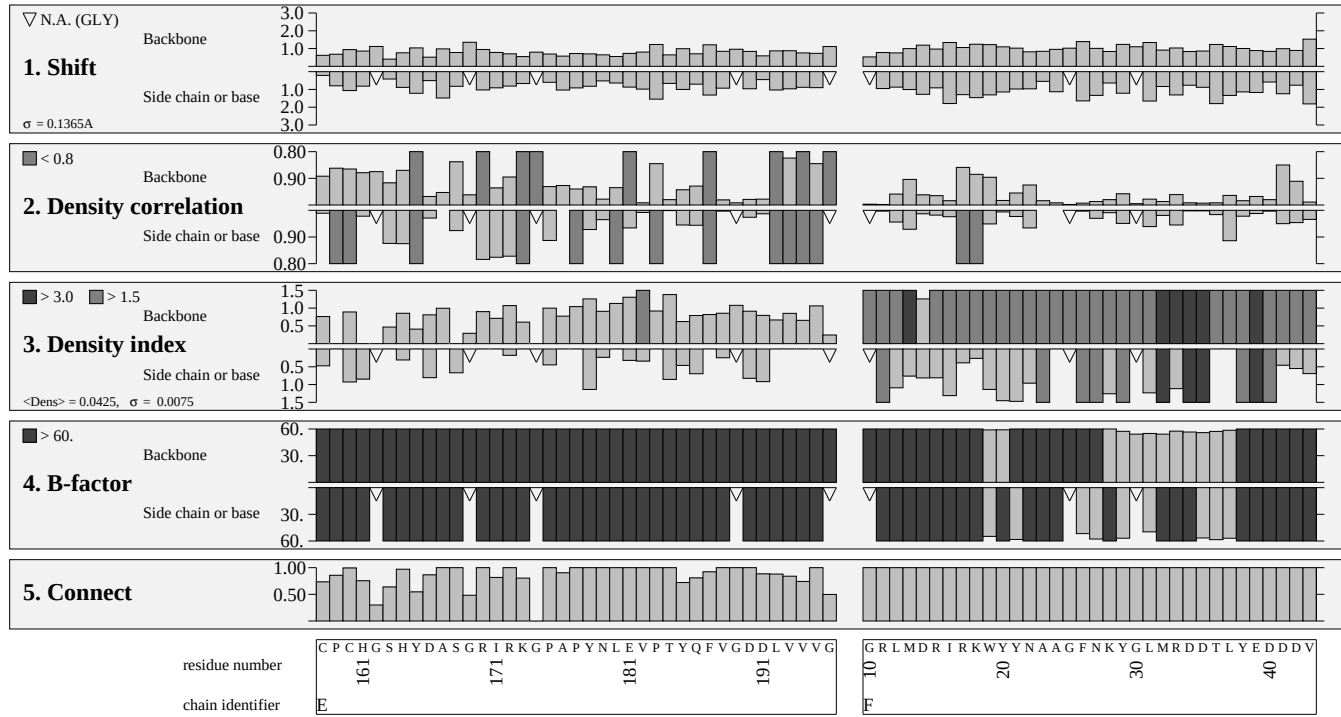
Local estimation (11)



Structure Factor Check

3H1L

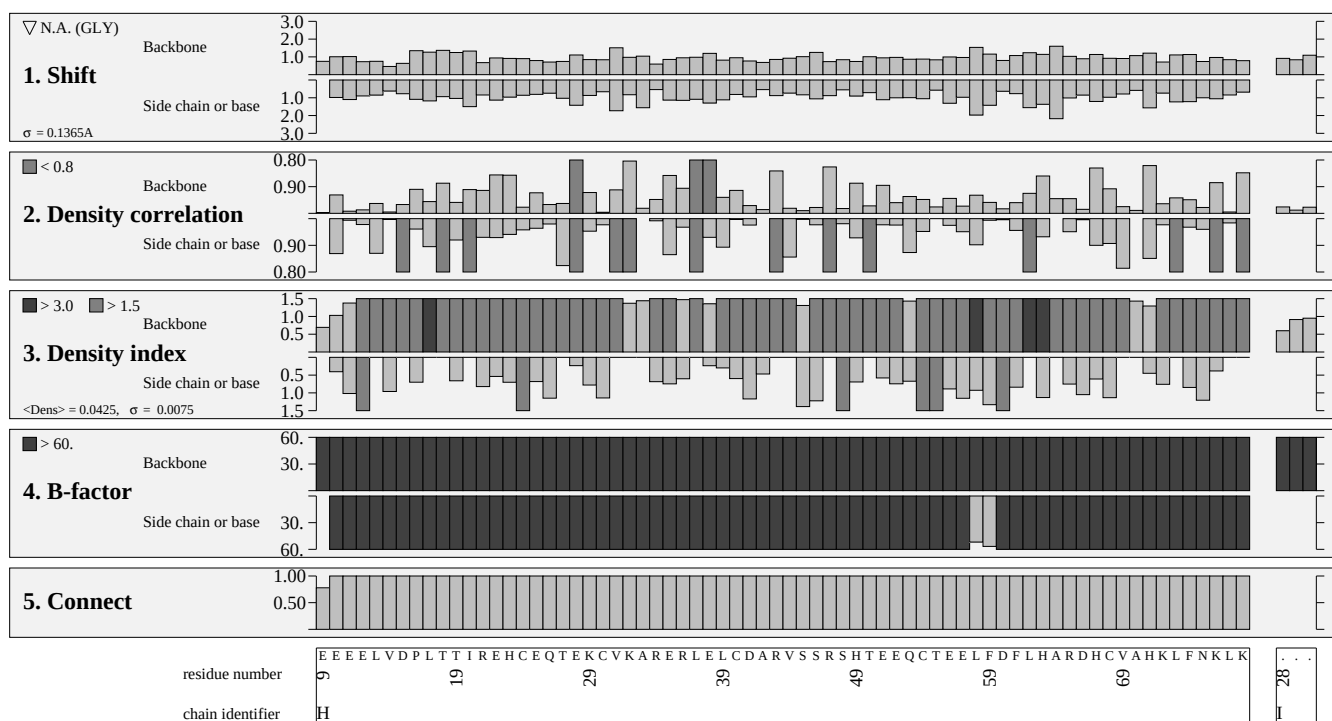
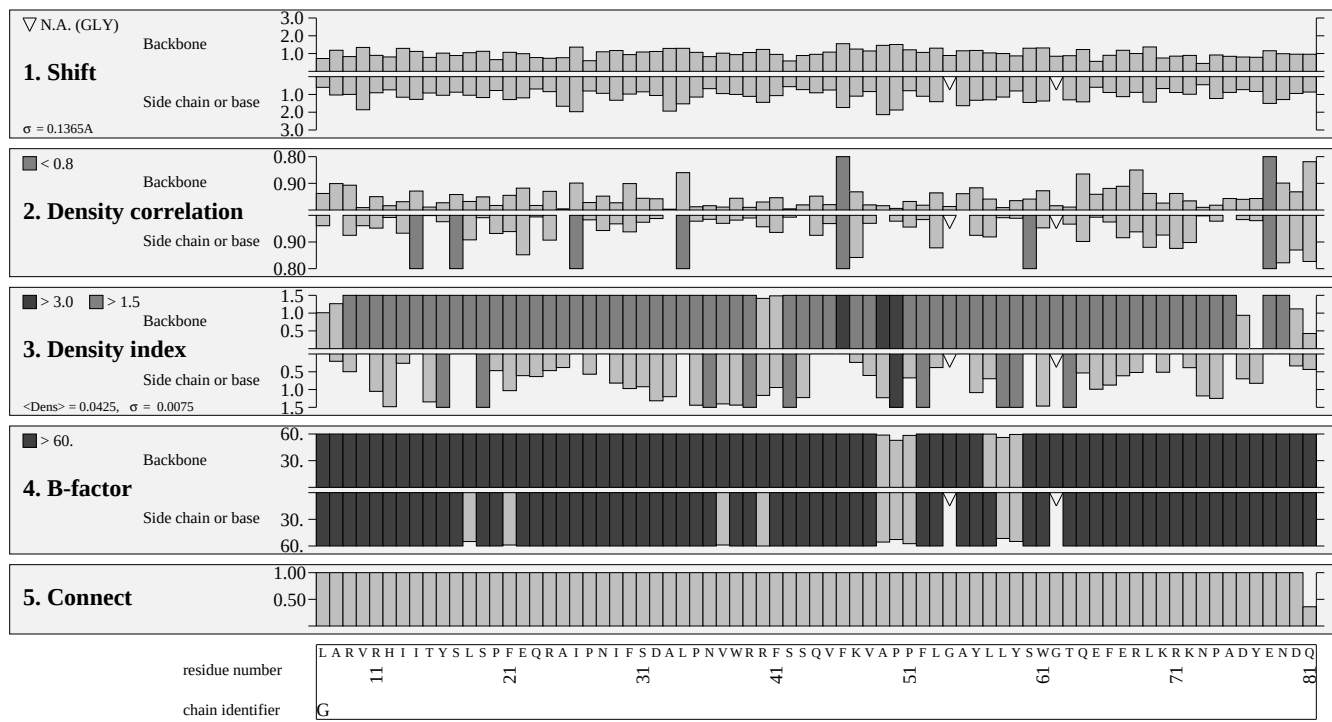
Local estimation (12)



Structure Factor Check

3H1L

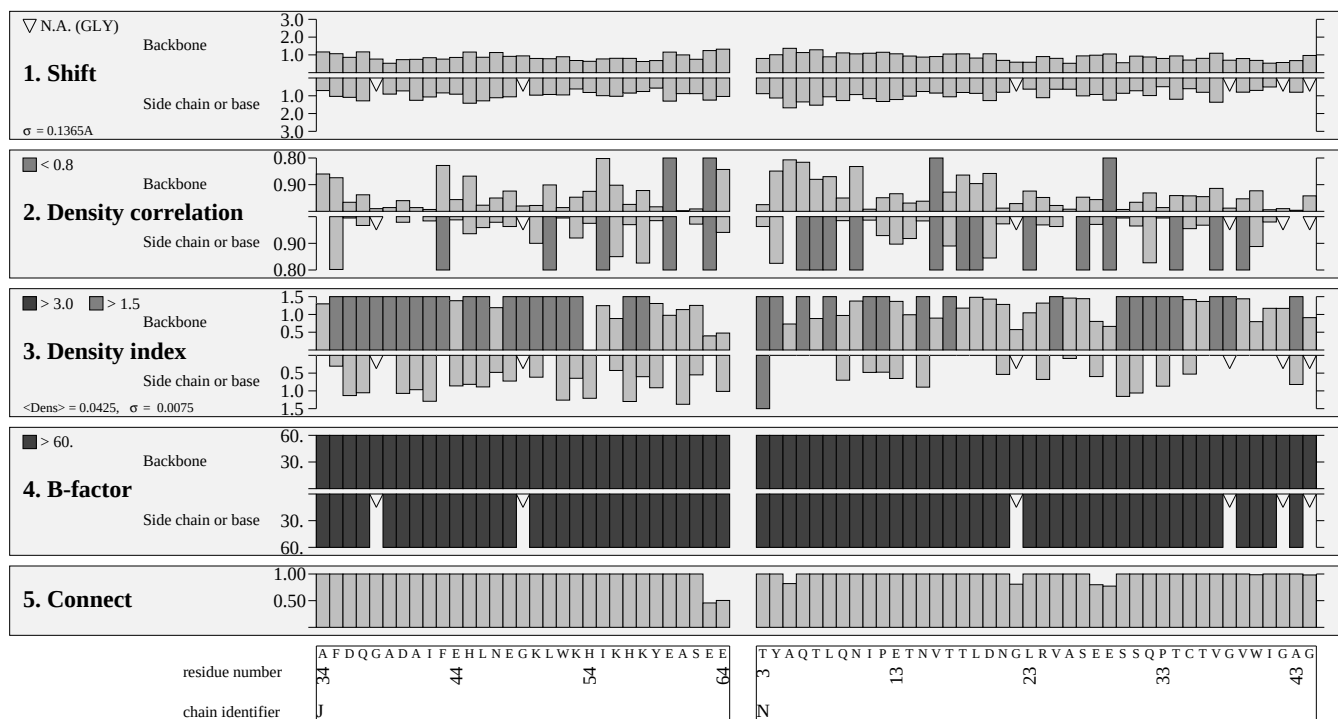
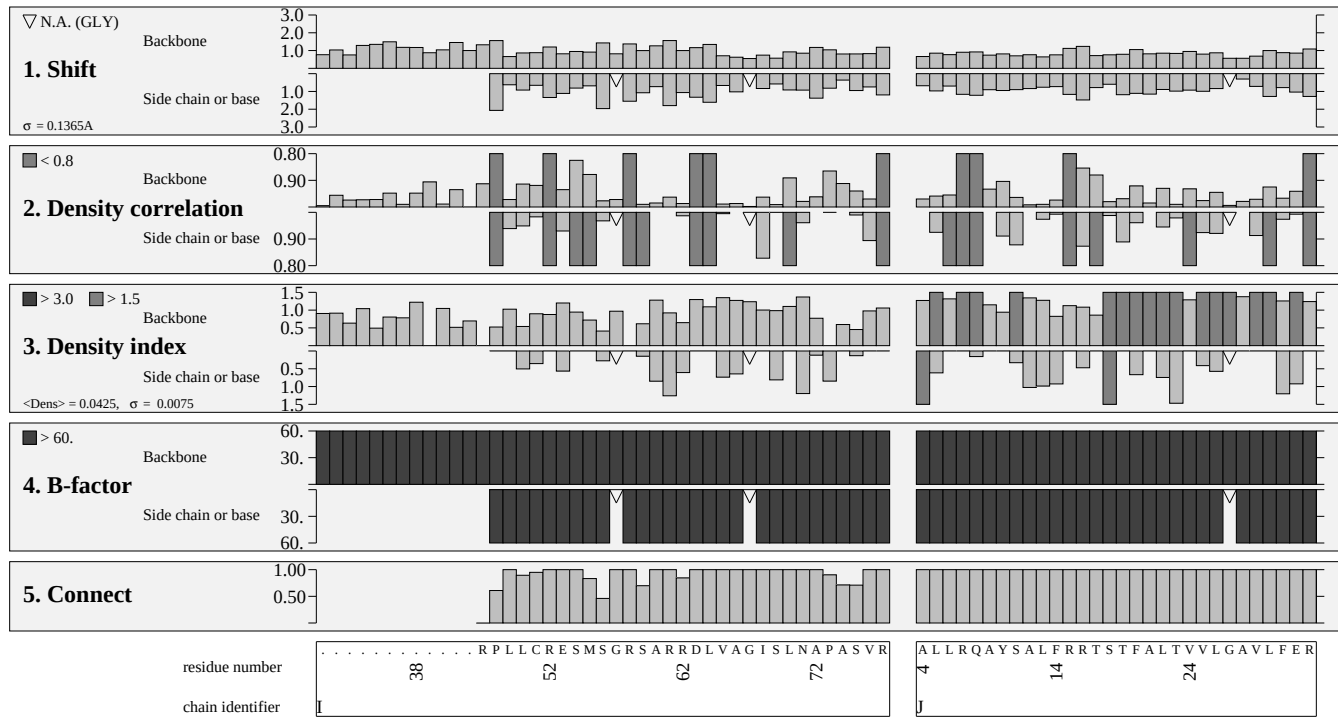
Local estimation (13)



Structure Factor Check

3H1L

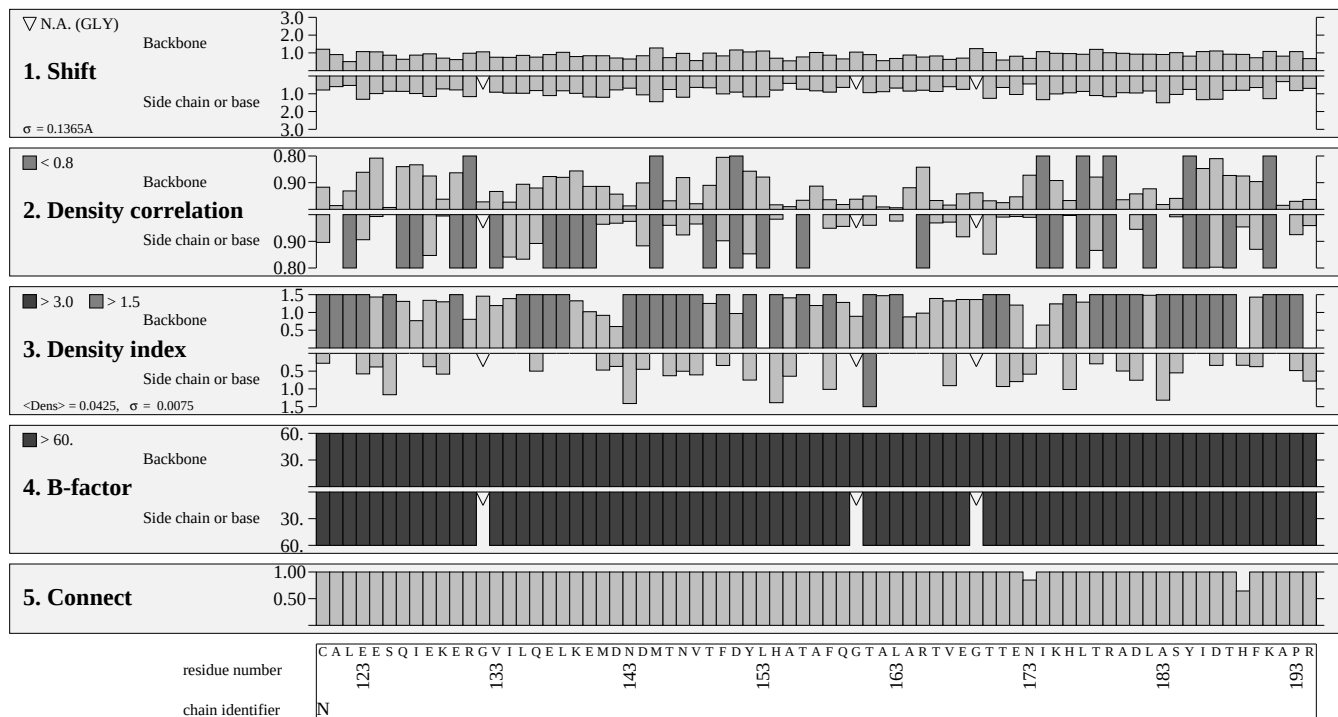
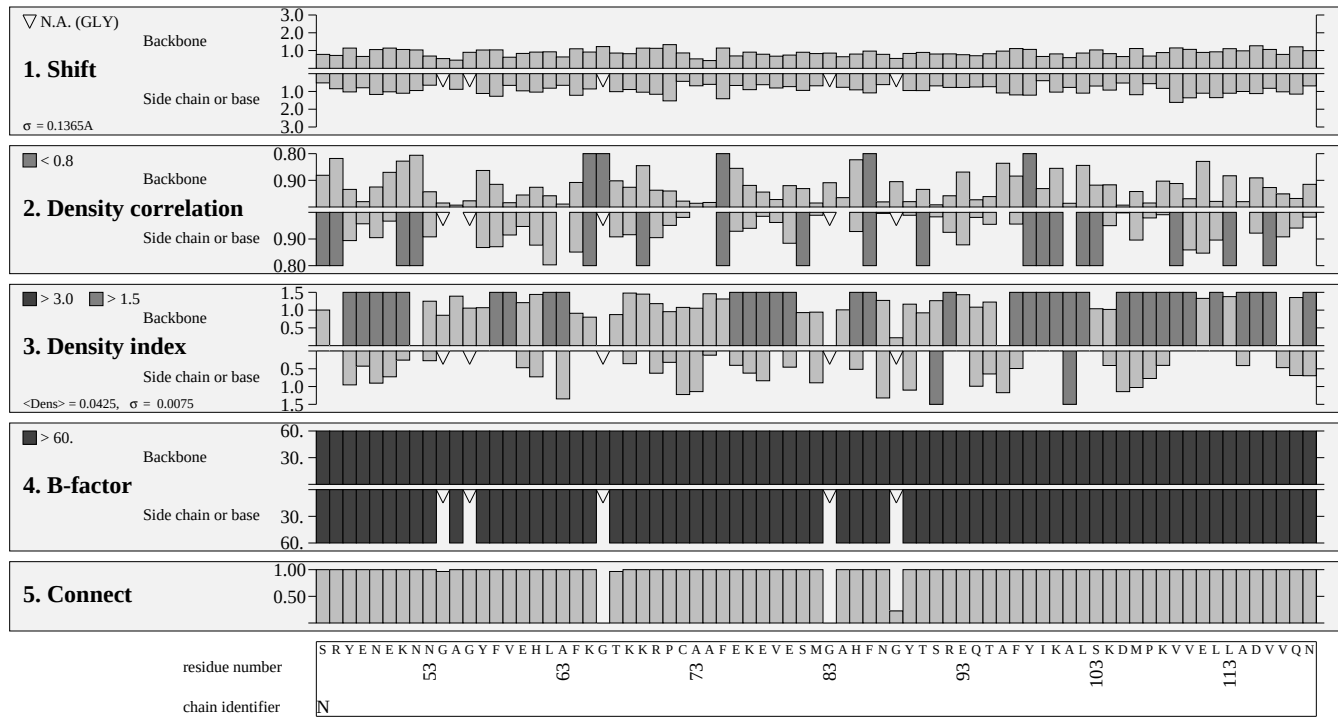
Local estimation (14)



Structure Factor Check

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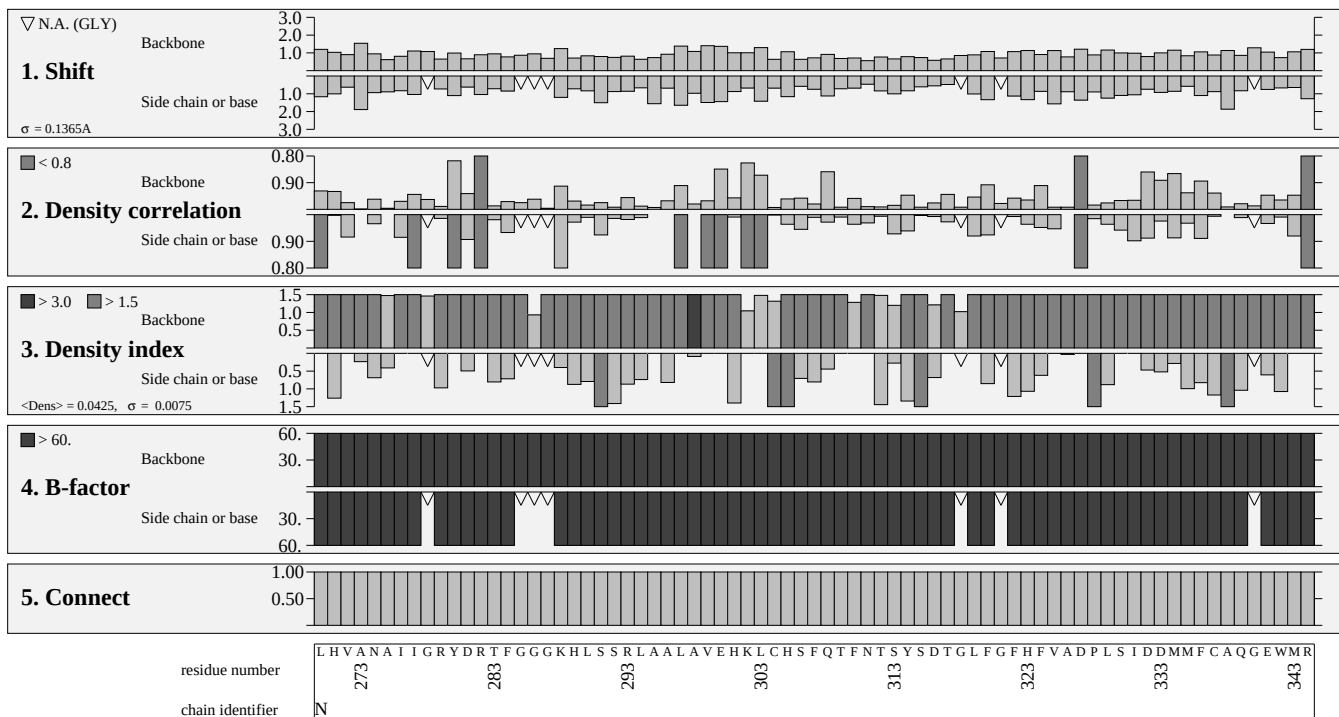
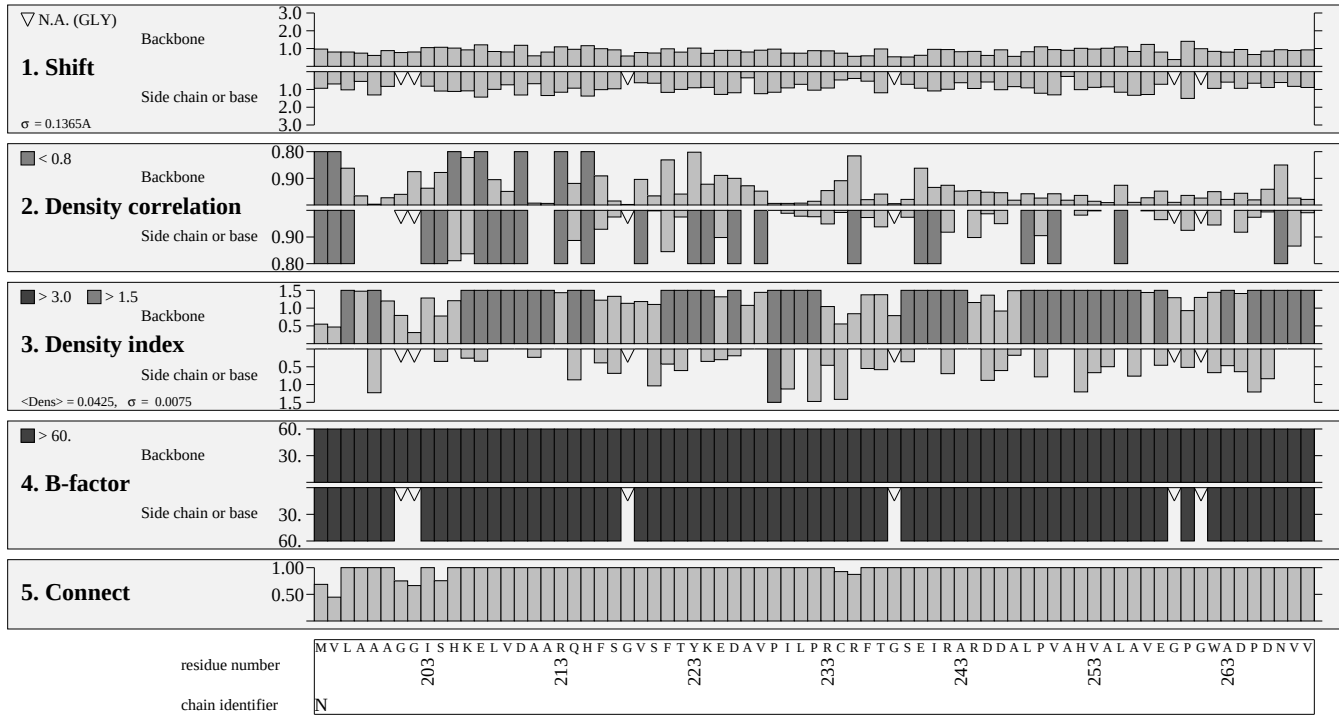
Local estimation (15)



Structure Factor Check

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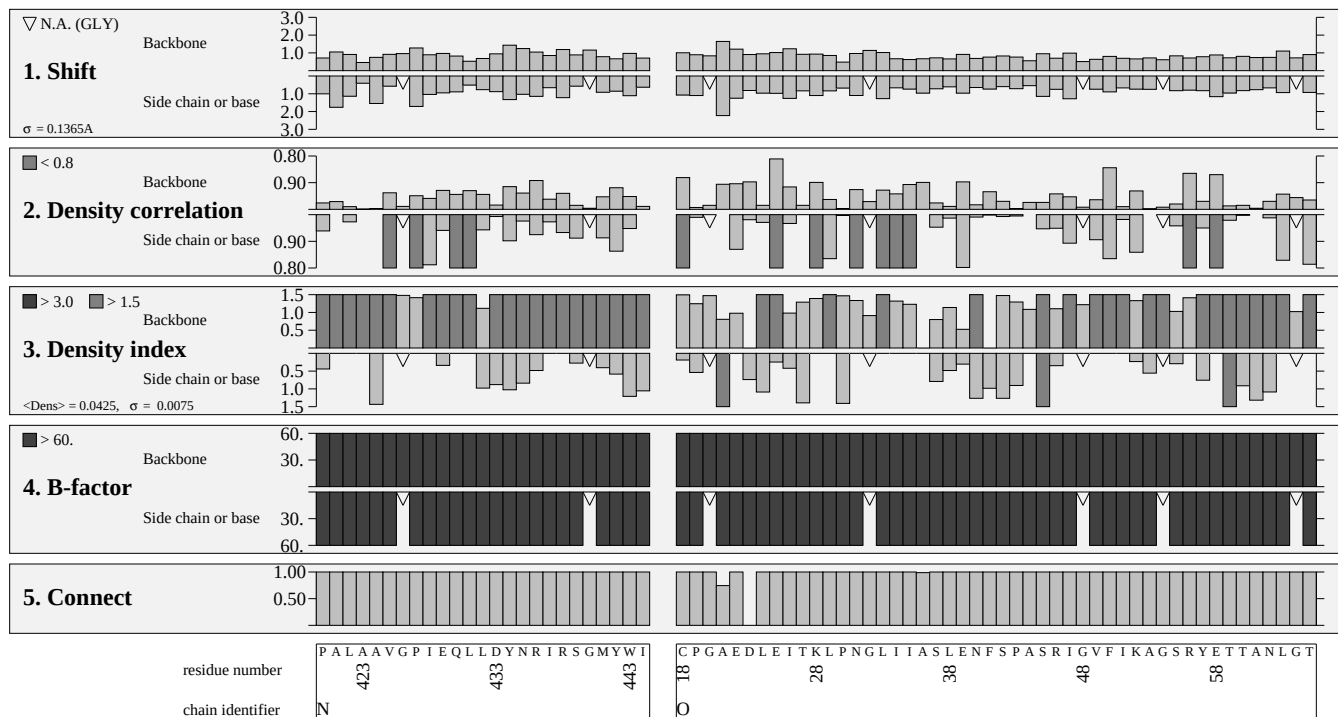
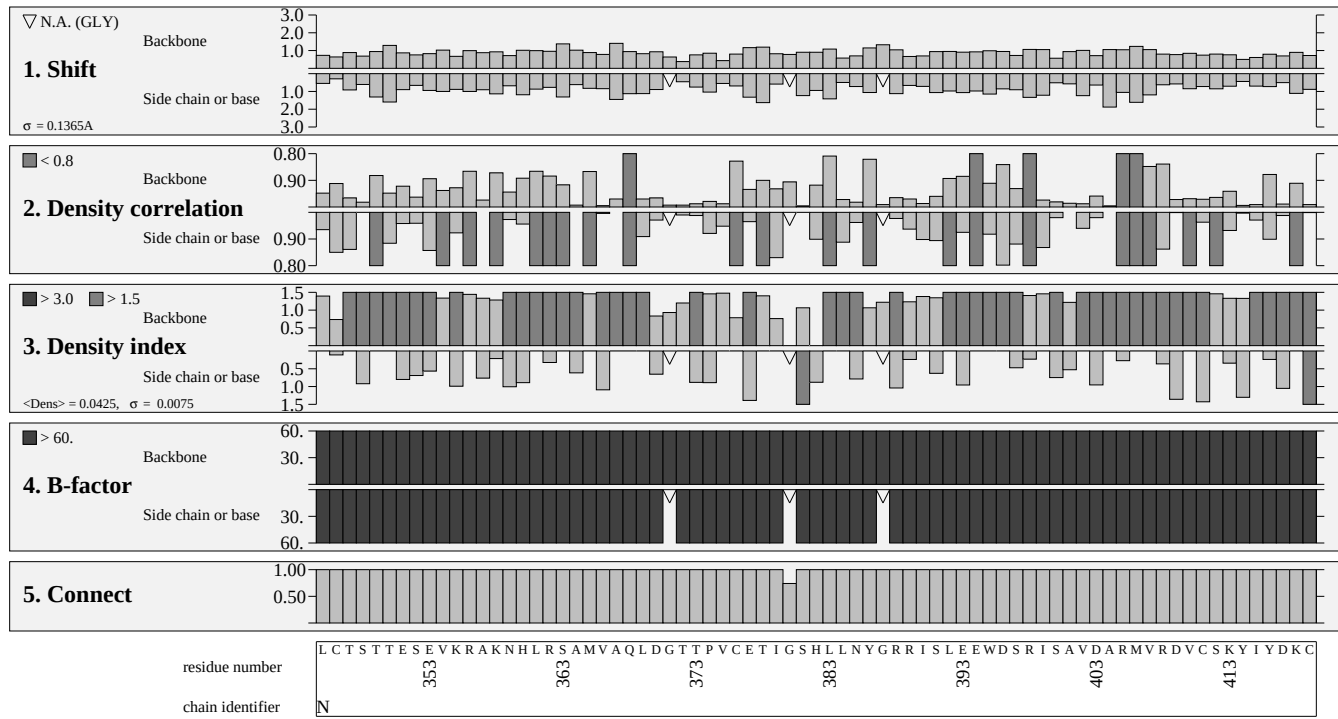
Local estimation (16)



Structure Factor Check

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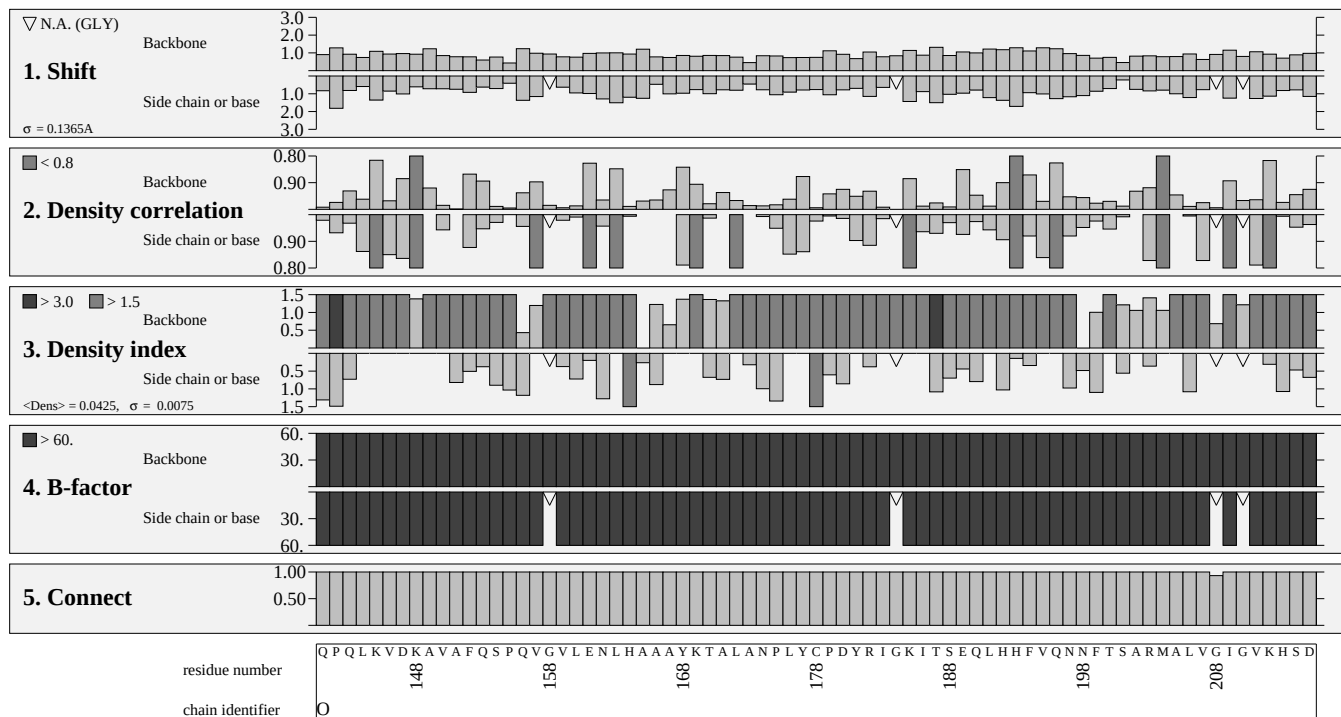
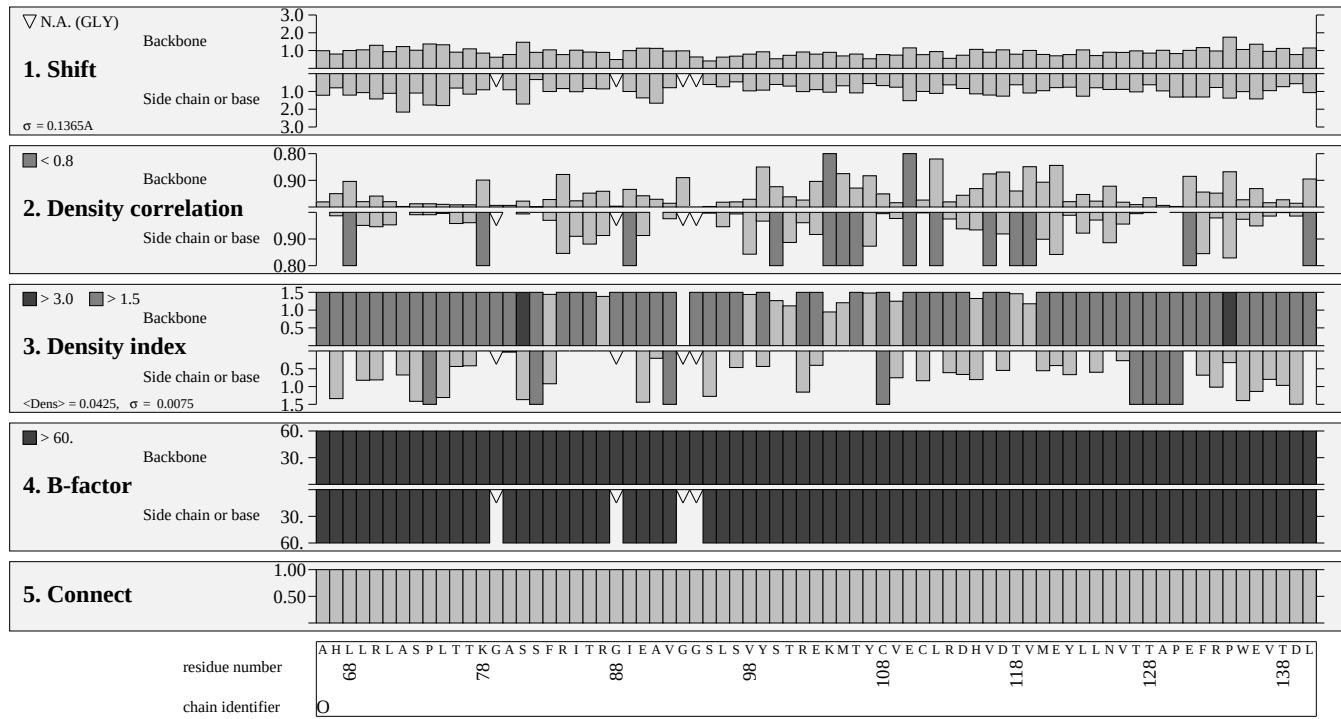
Local estimation (17)



Structure Factor Check

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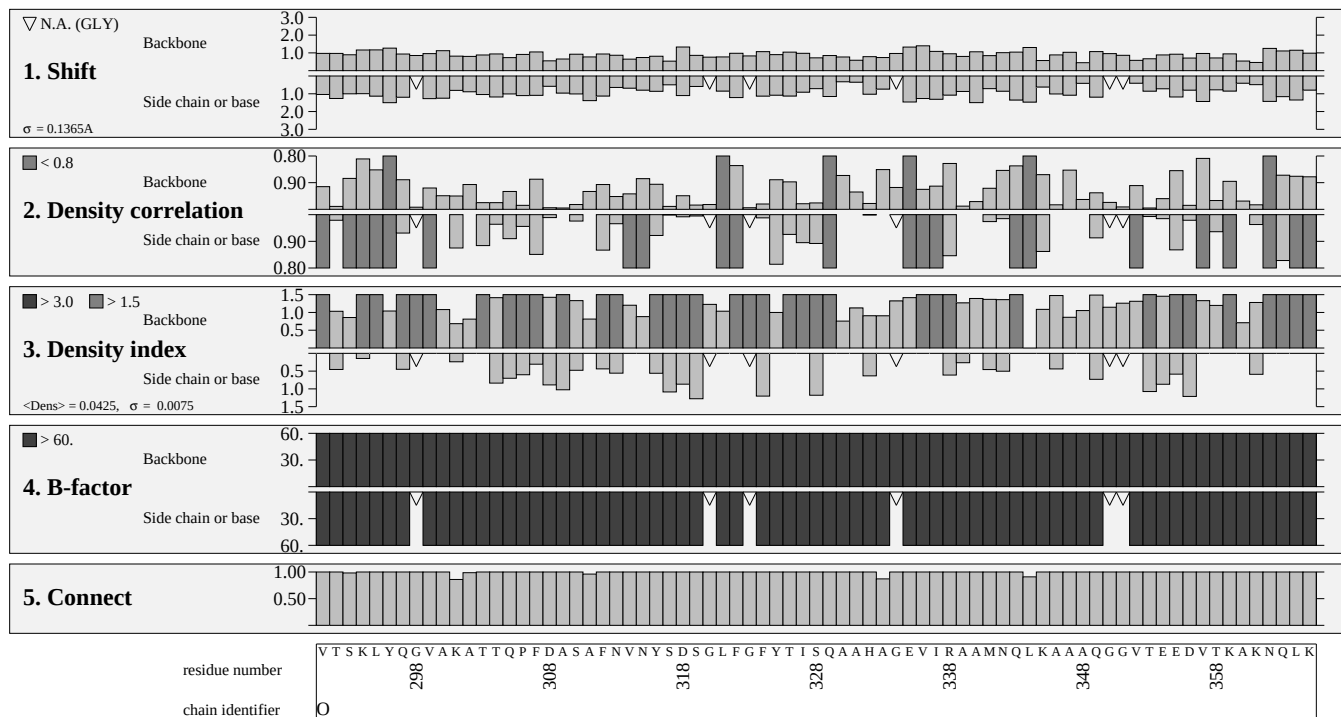
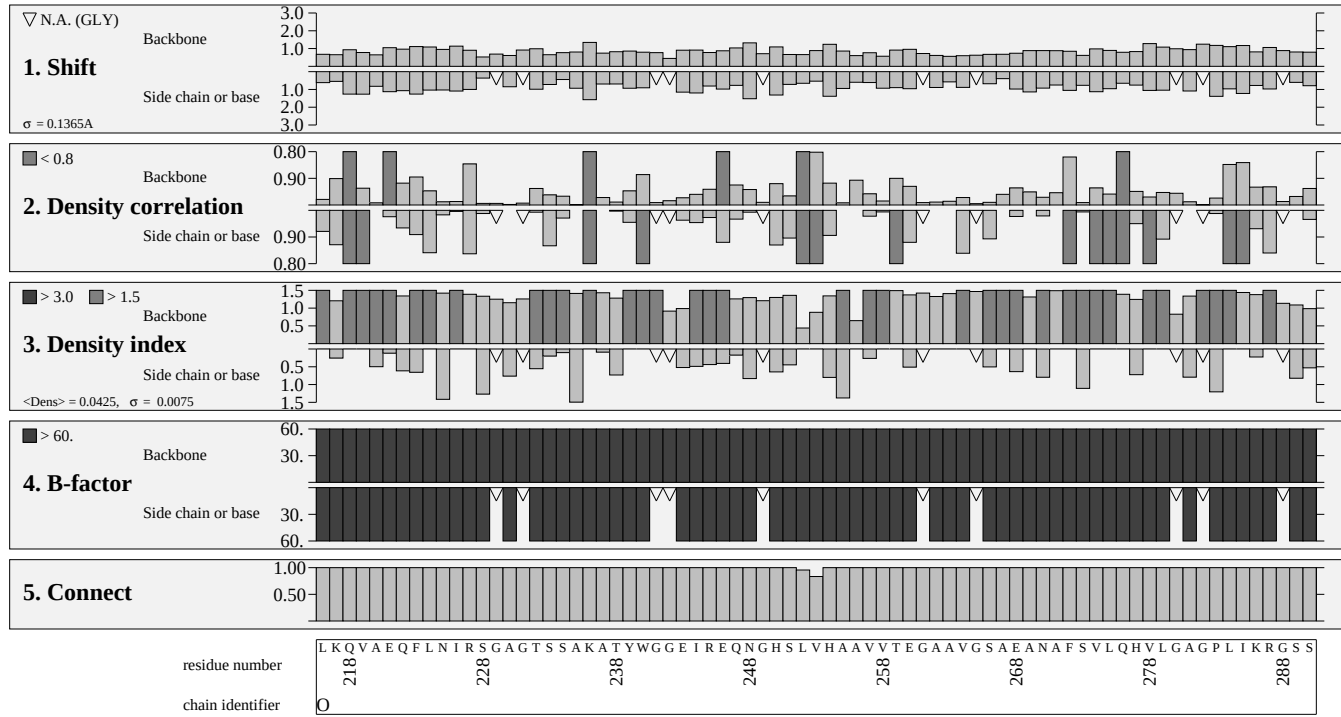
Local estimation (18)



Structure Factor Check

3H1L

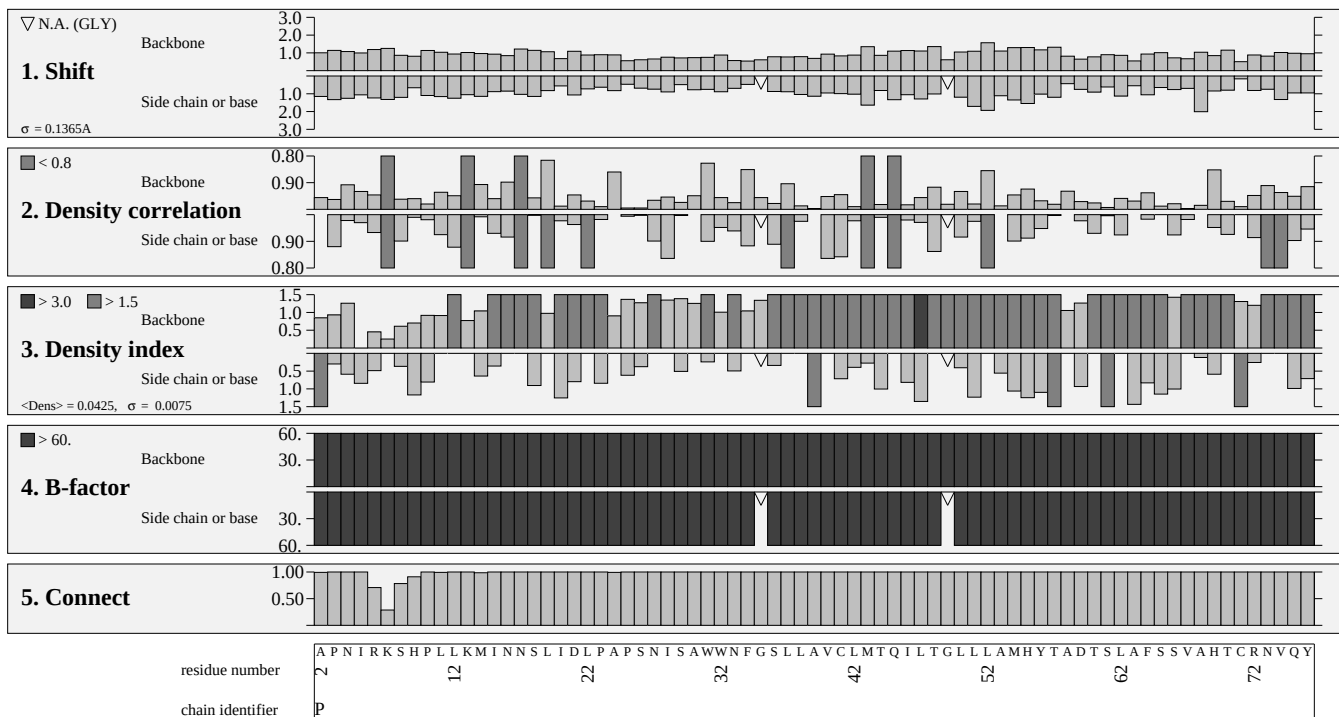
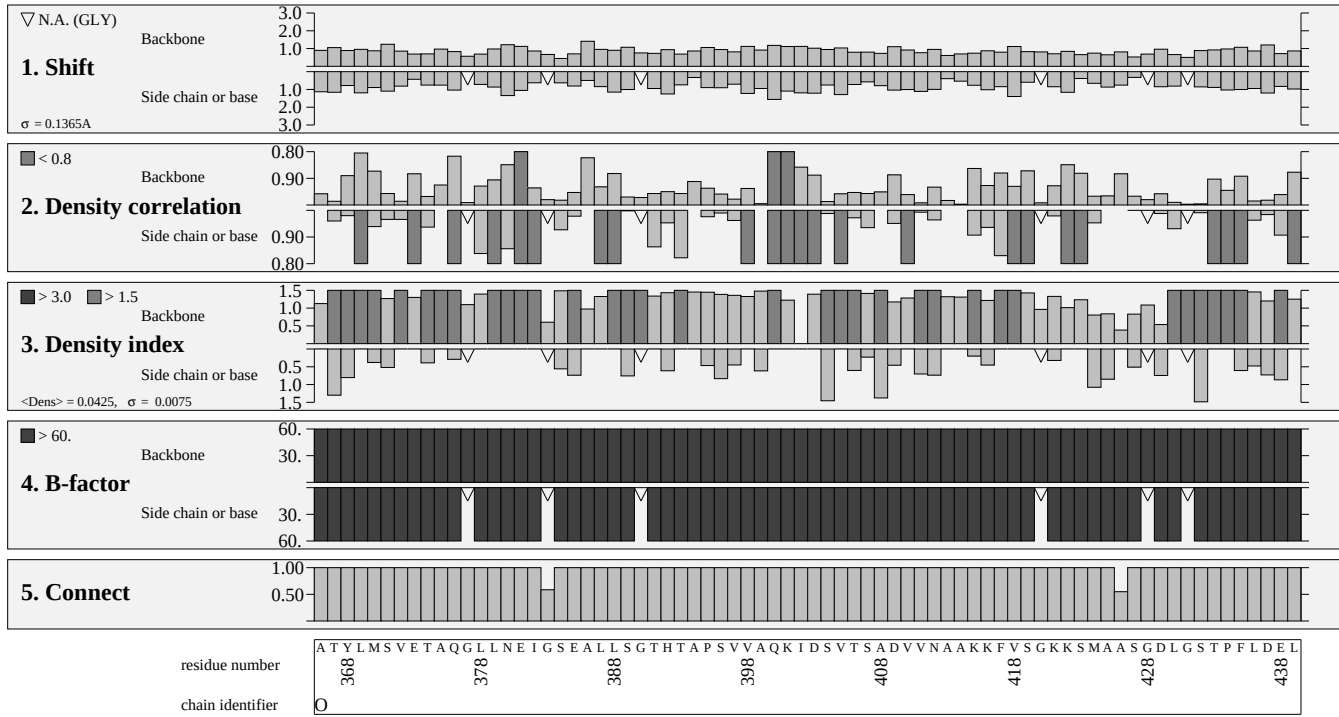
Local estimation (19)



Structure Factor Check

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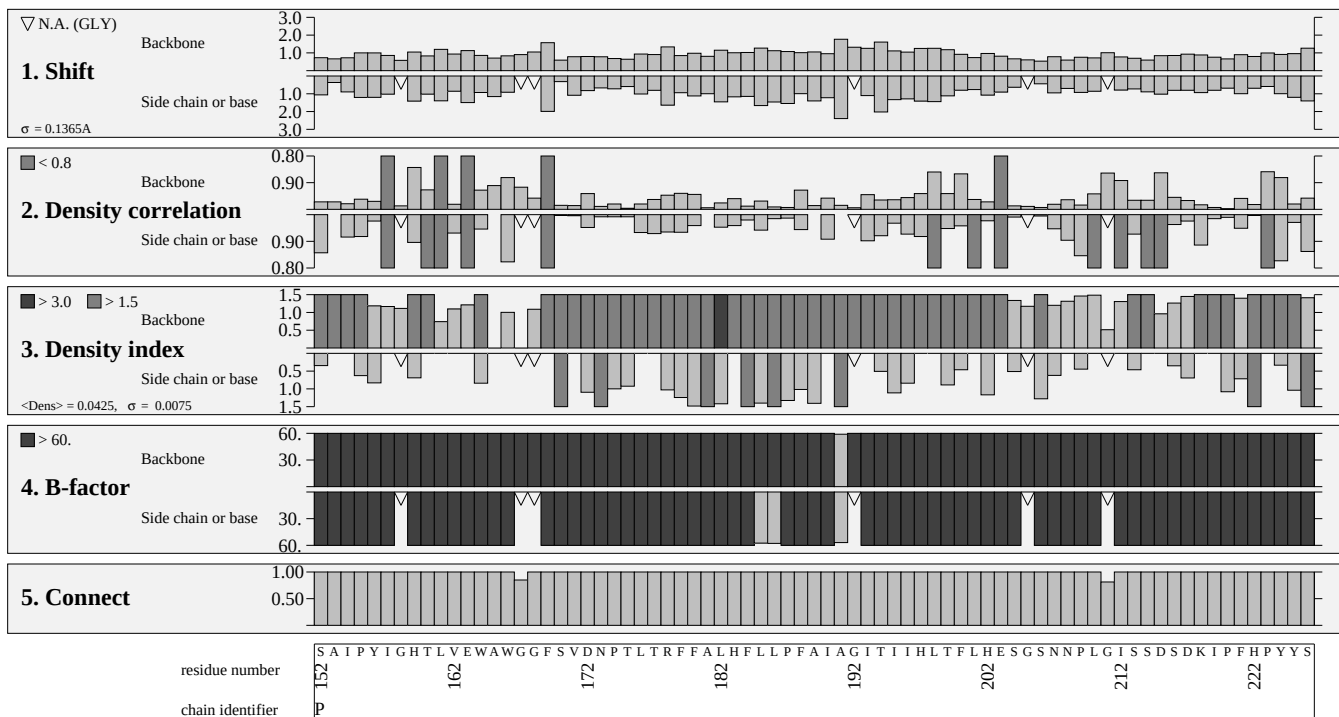
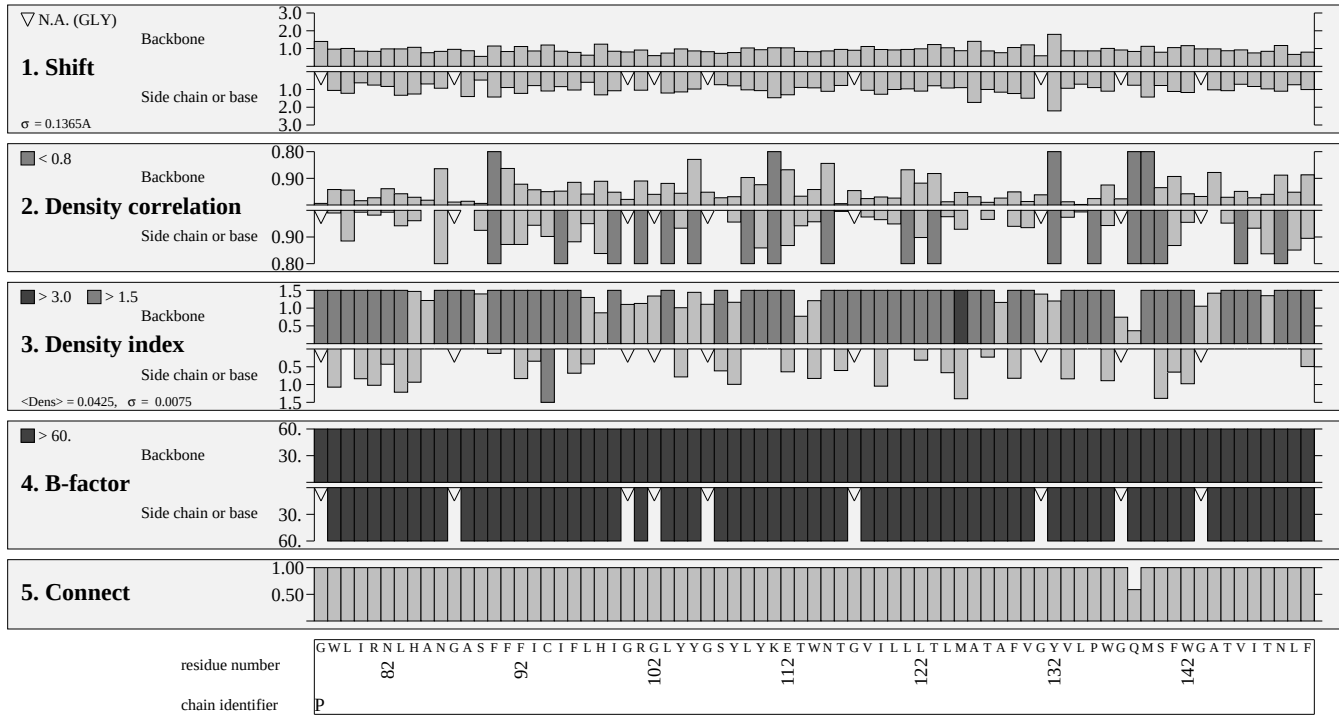
Local estimation (20)



Structure Factor Check

3H1L

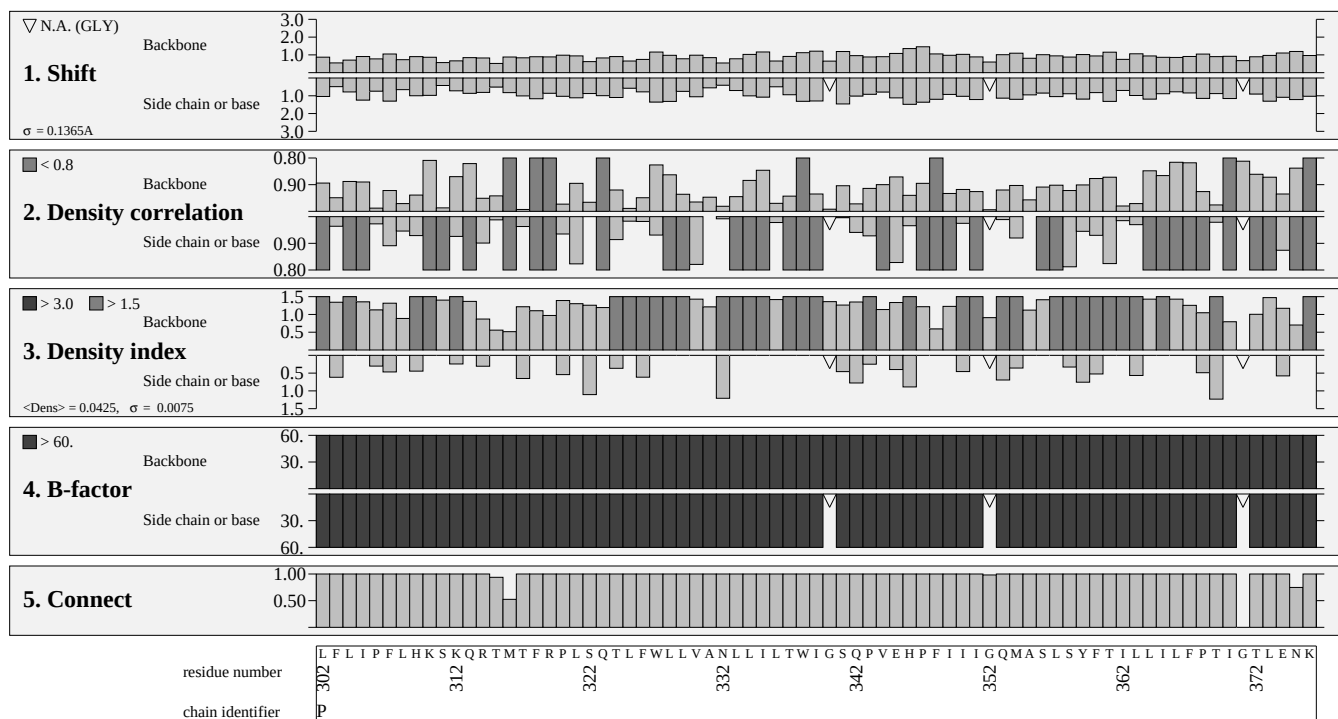
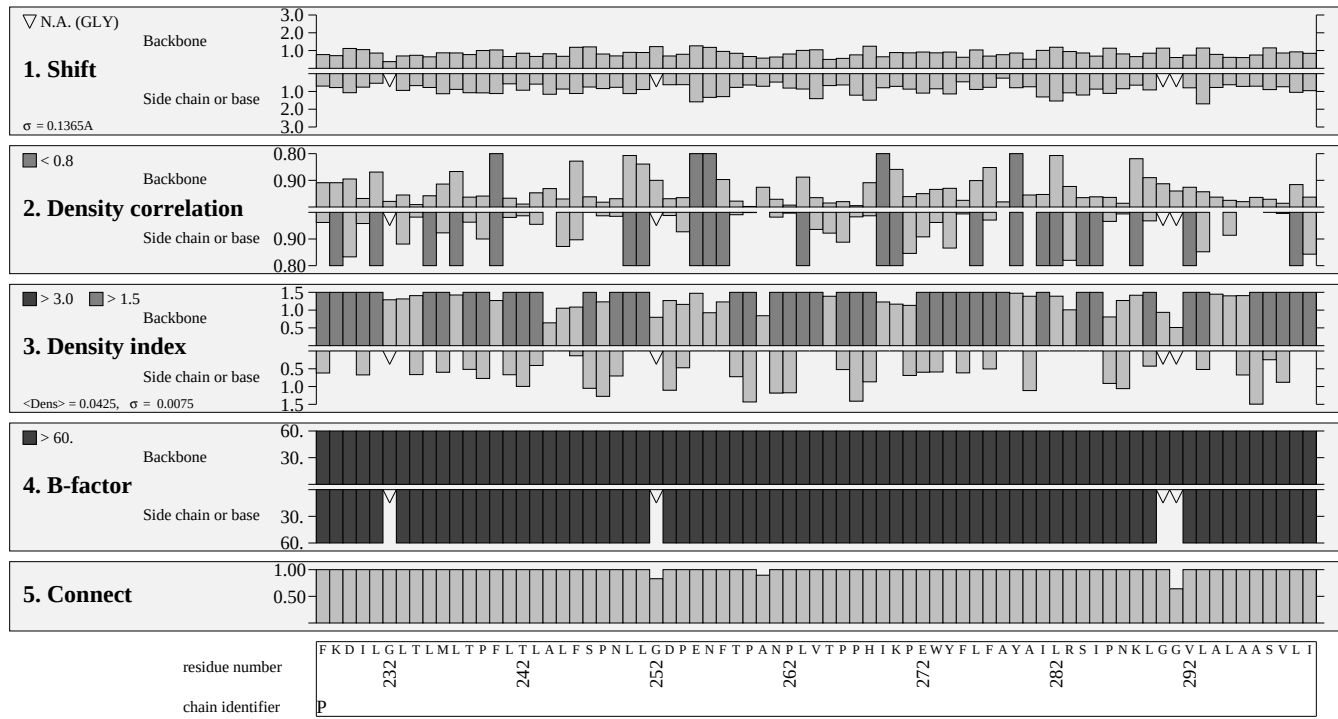
Local estimation (21)



Structure Factor Check

3H1L

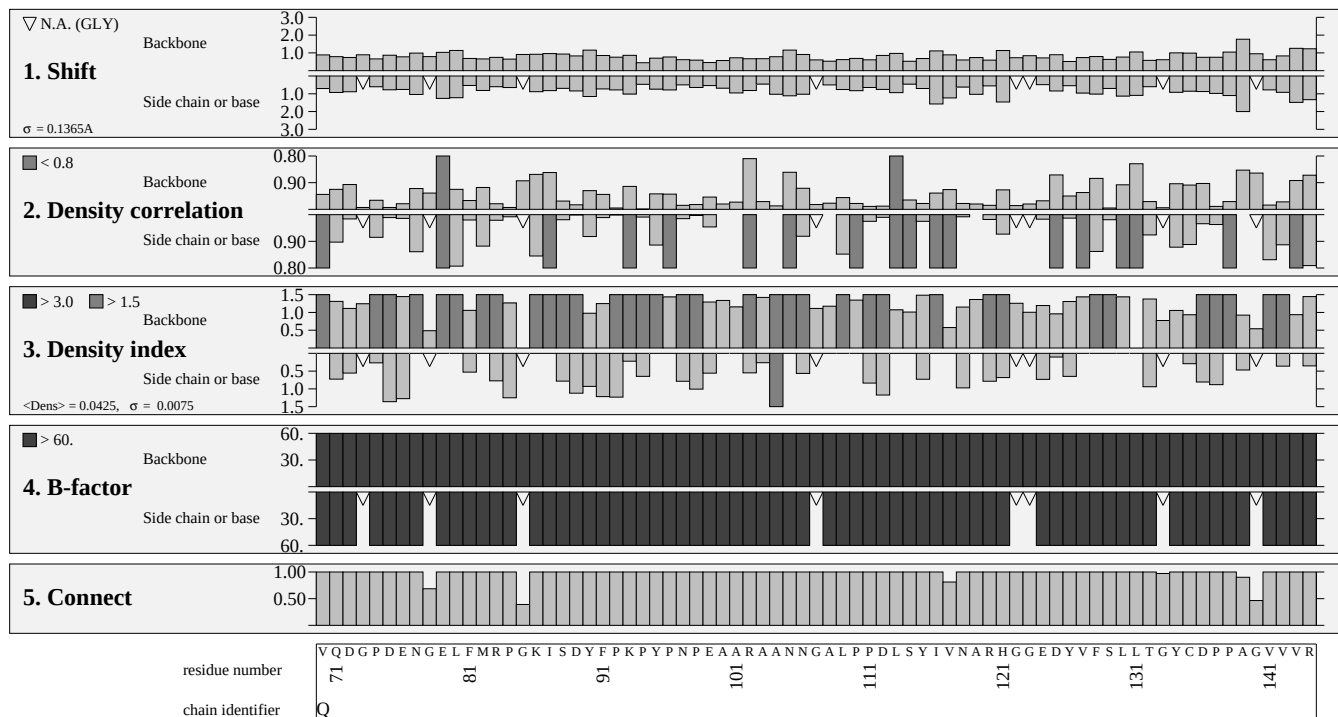
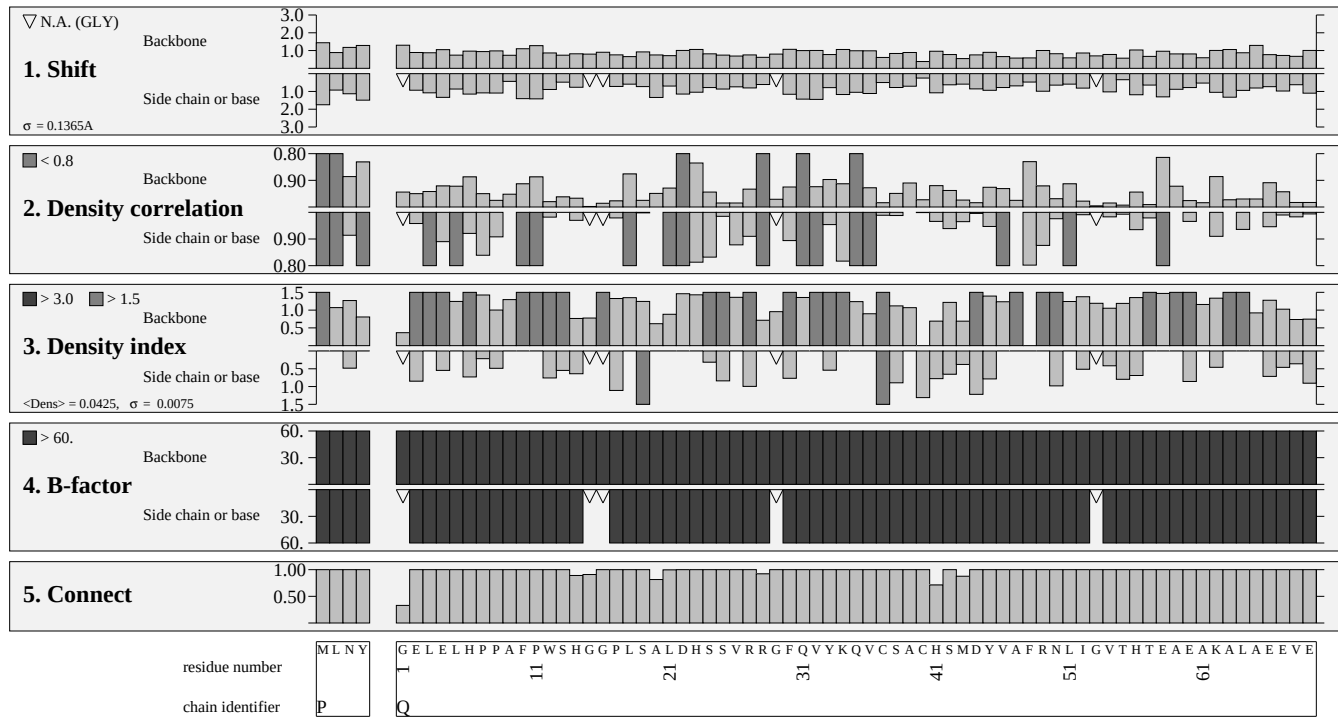
Local estimation (22)



Structure Factor Check

3H1L

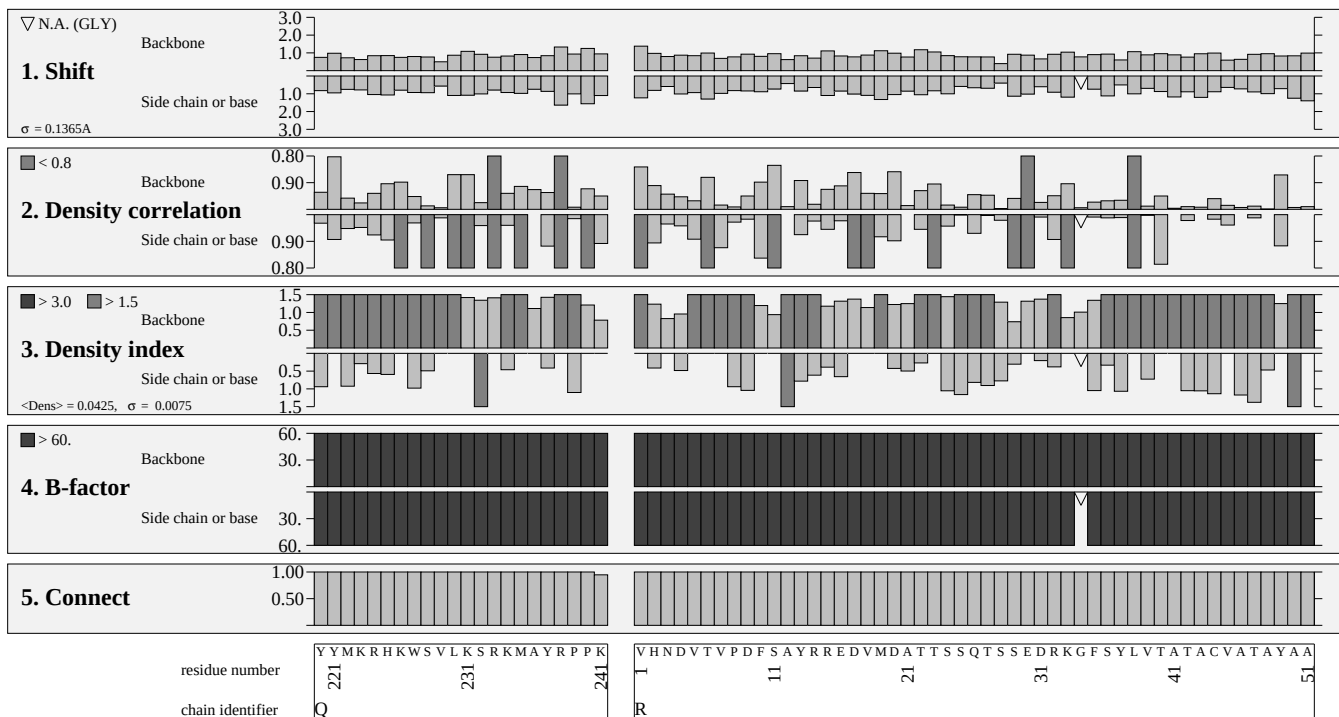
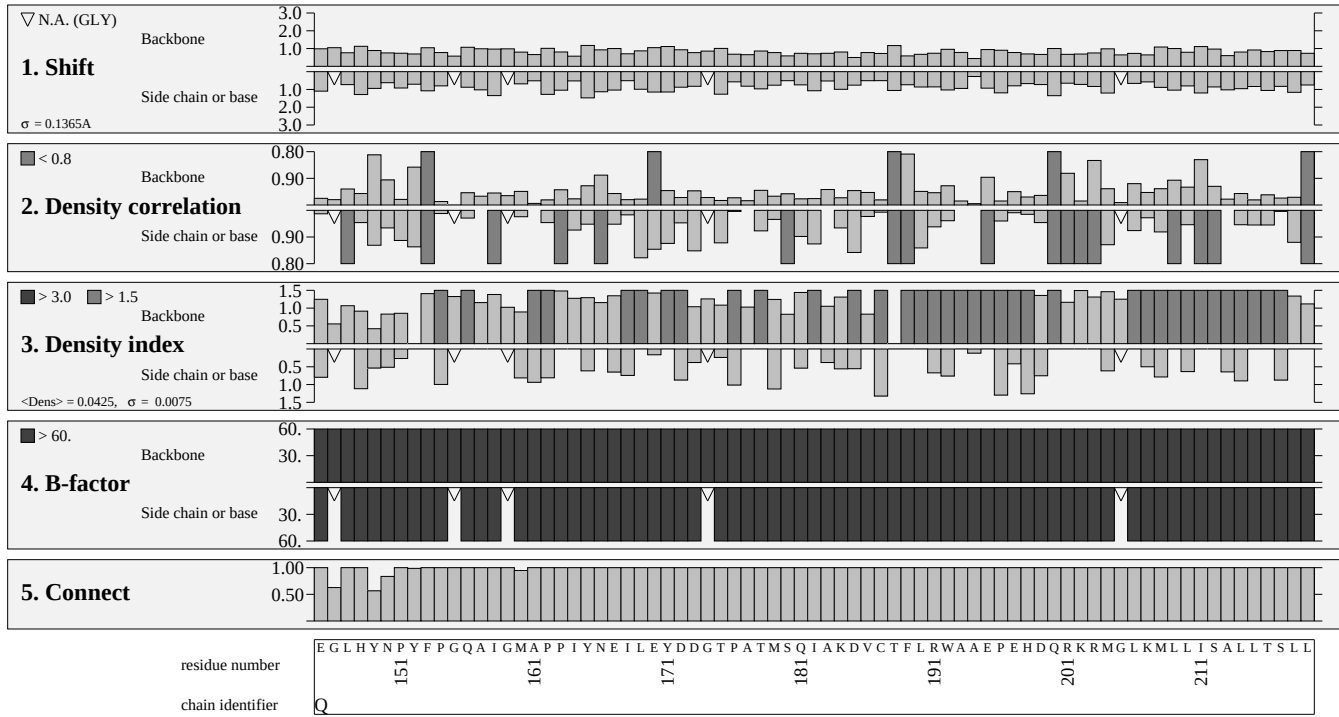
Local estimation (23)



Structure Factor Check

3H1L

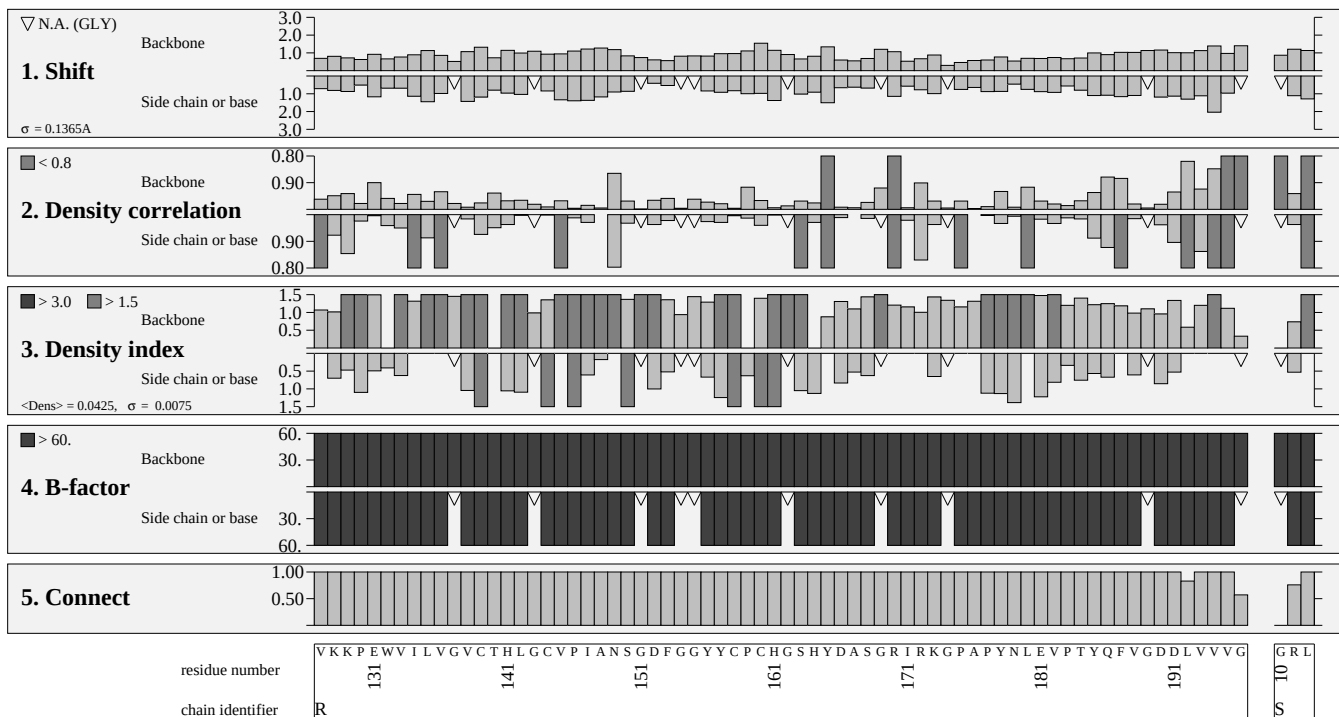
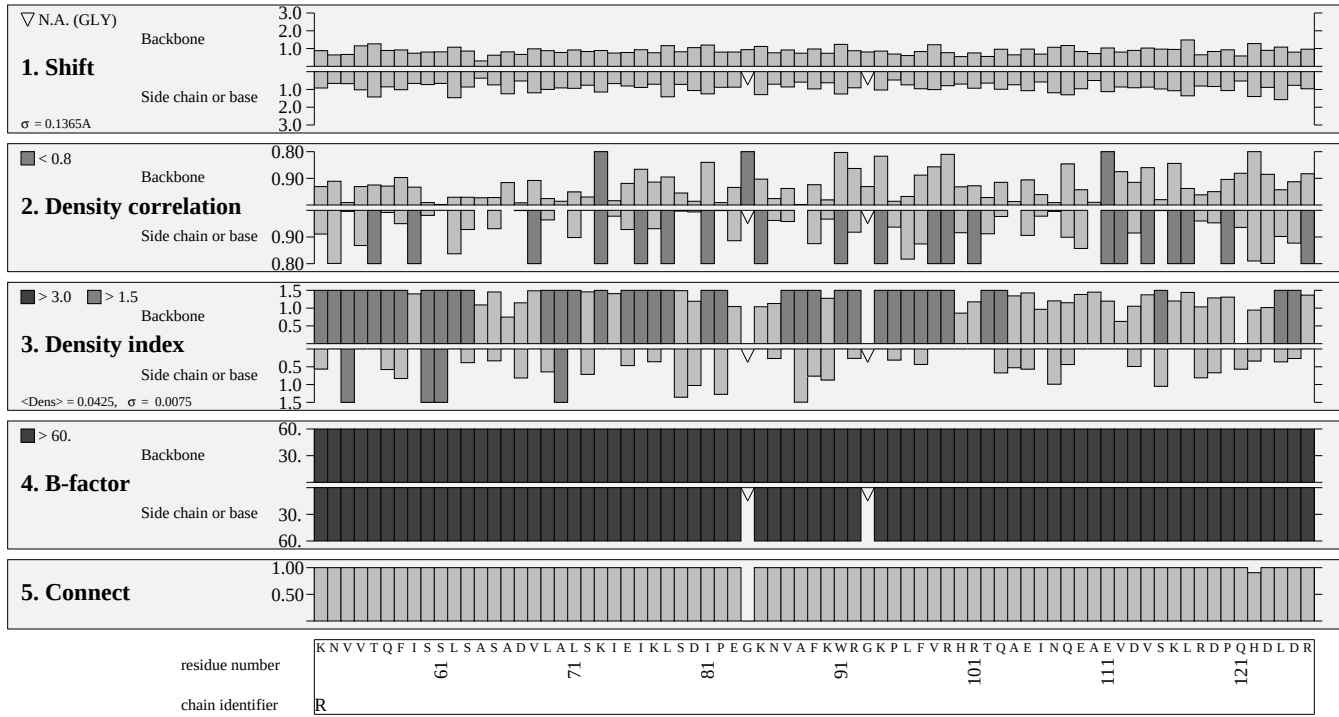
Local estimation (24)



Structure Factor Check

3H1L

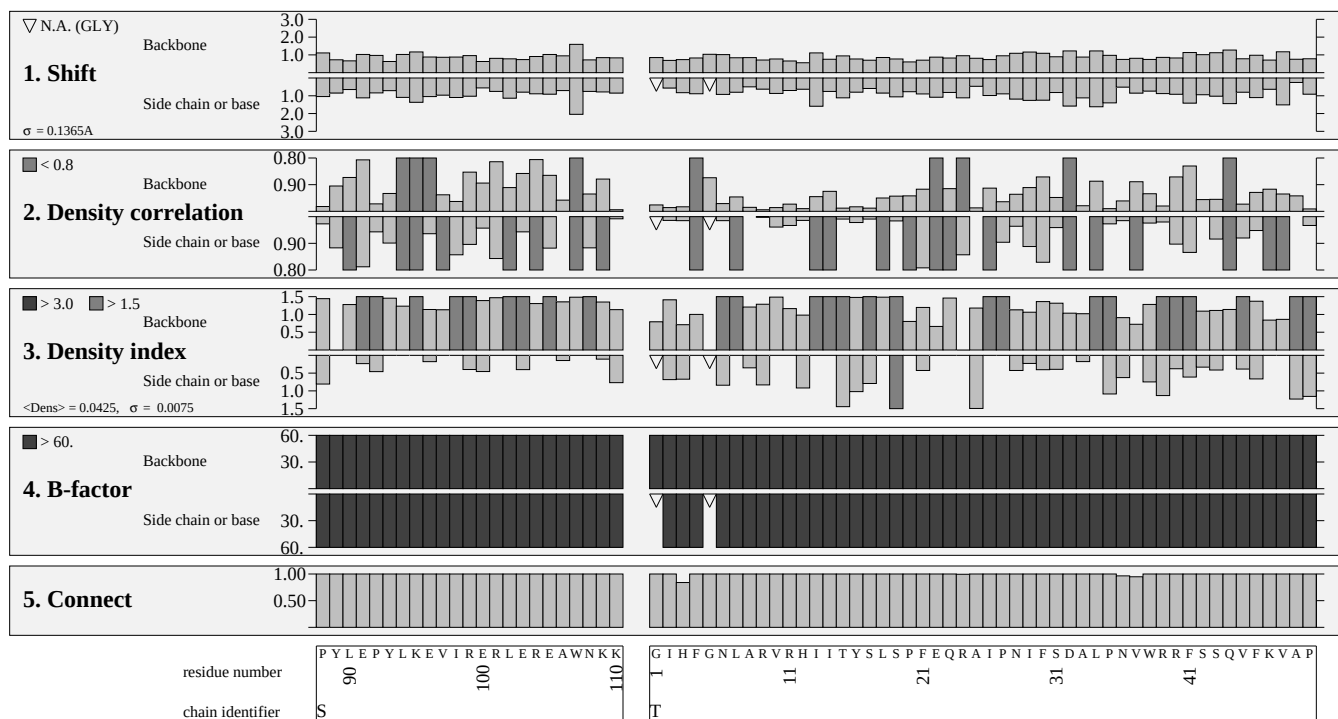
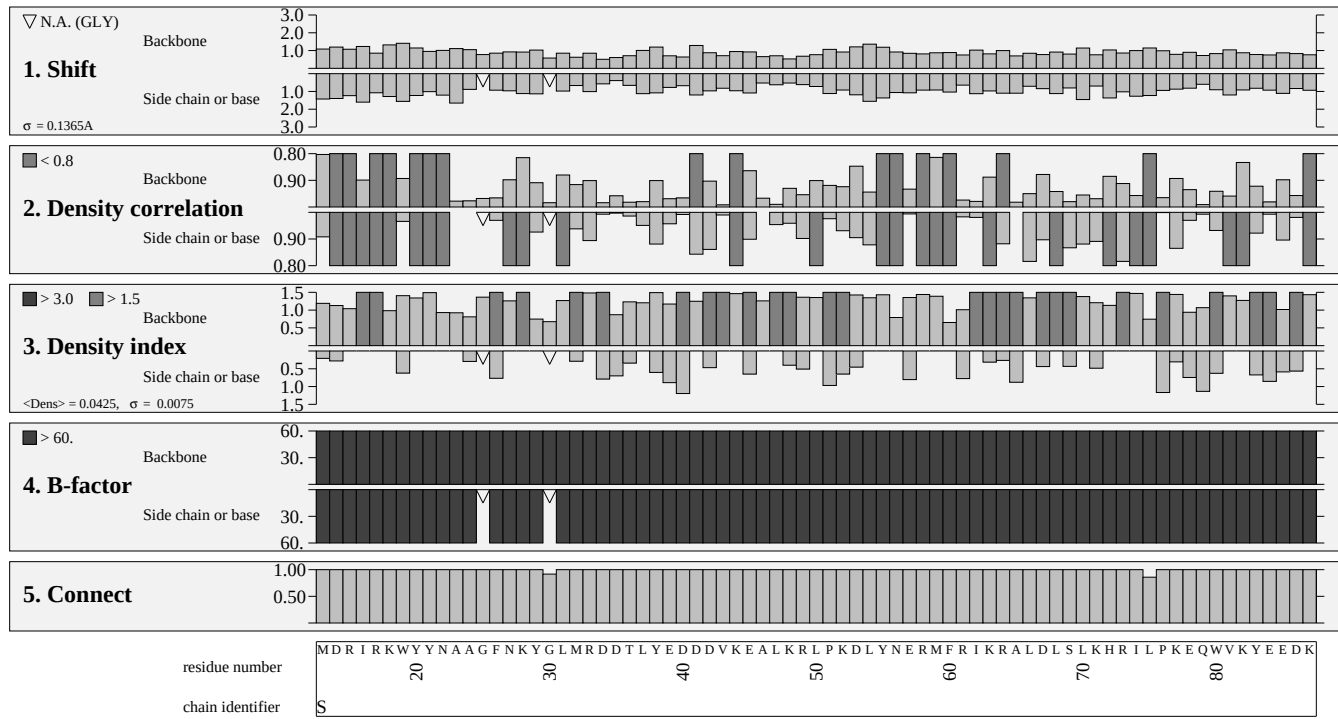
Local estimation (25)



Structure Factor Check

3H1L

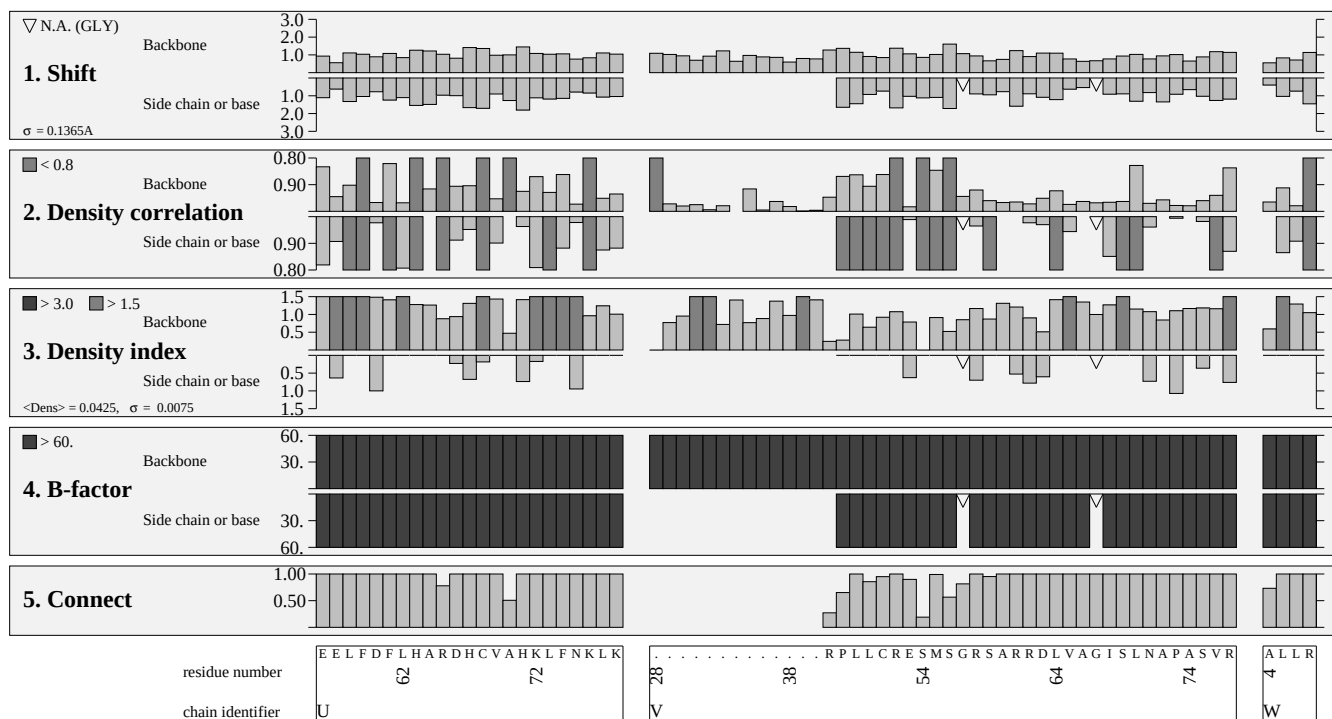
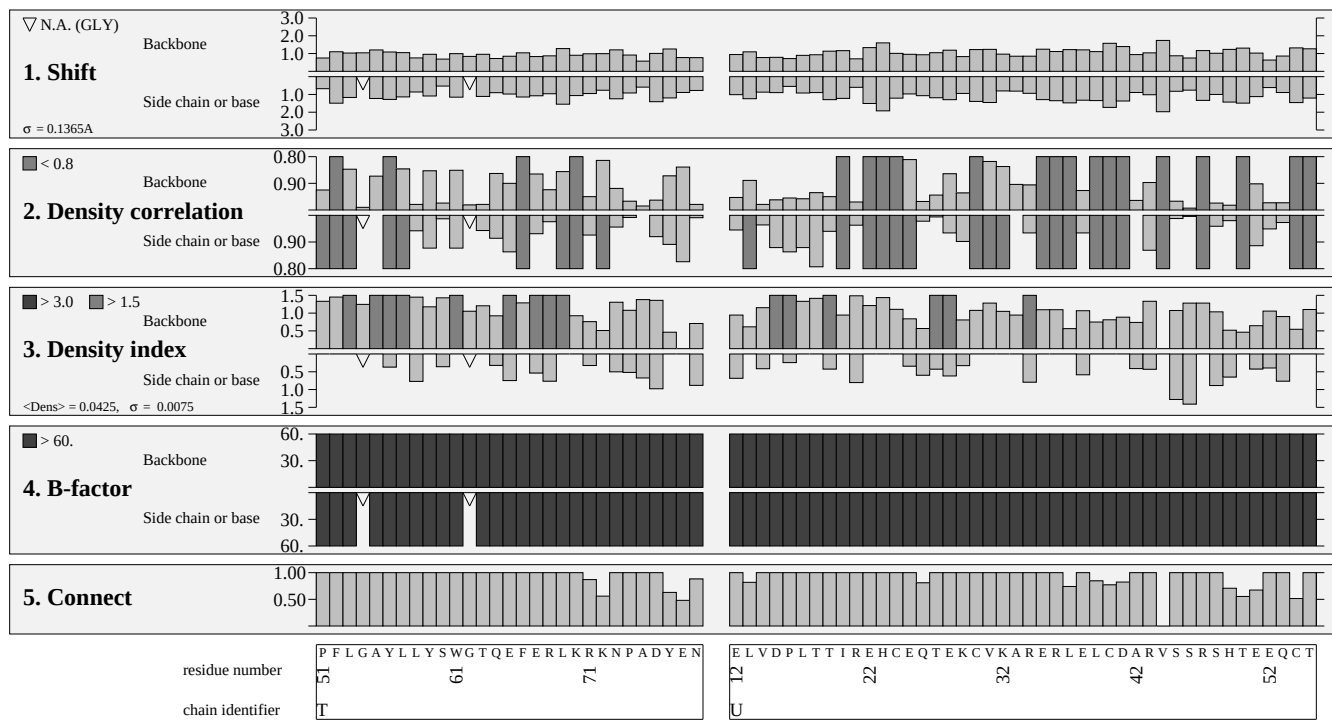
Local estimation (26)



Structure Factor Check

3H1L

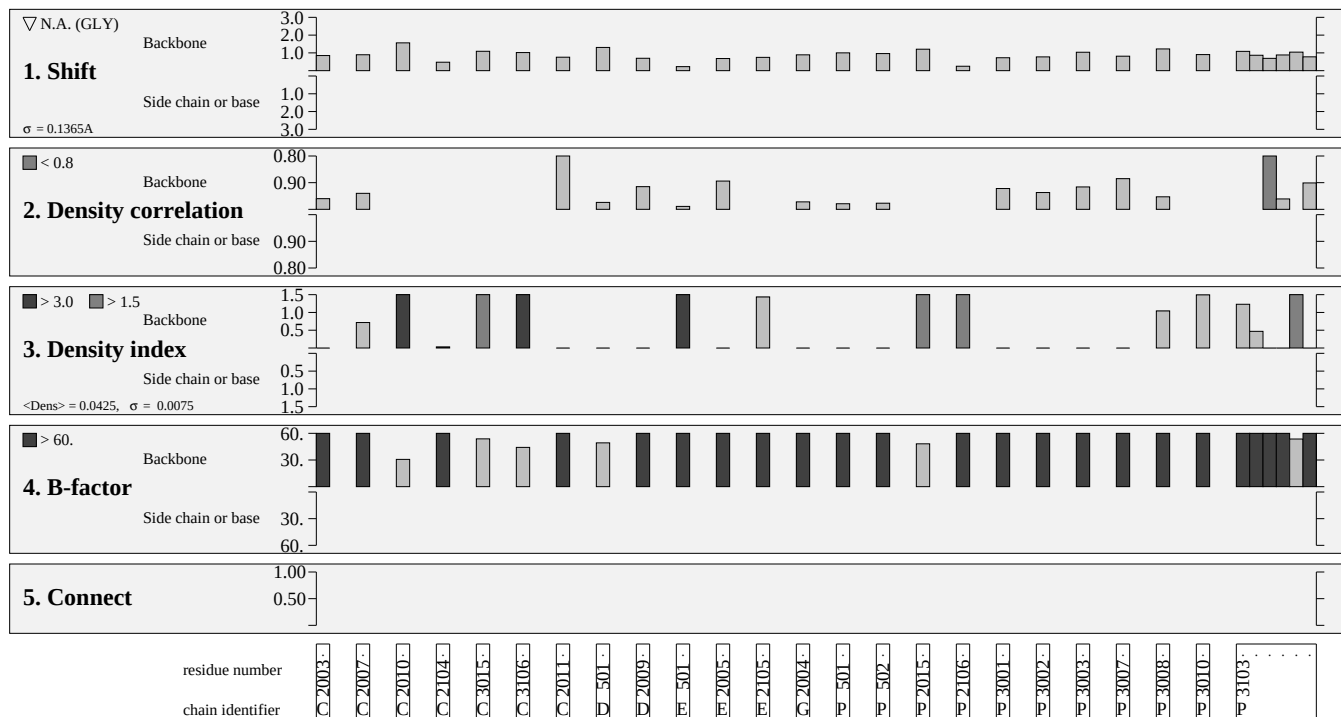
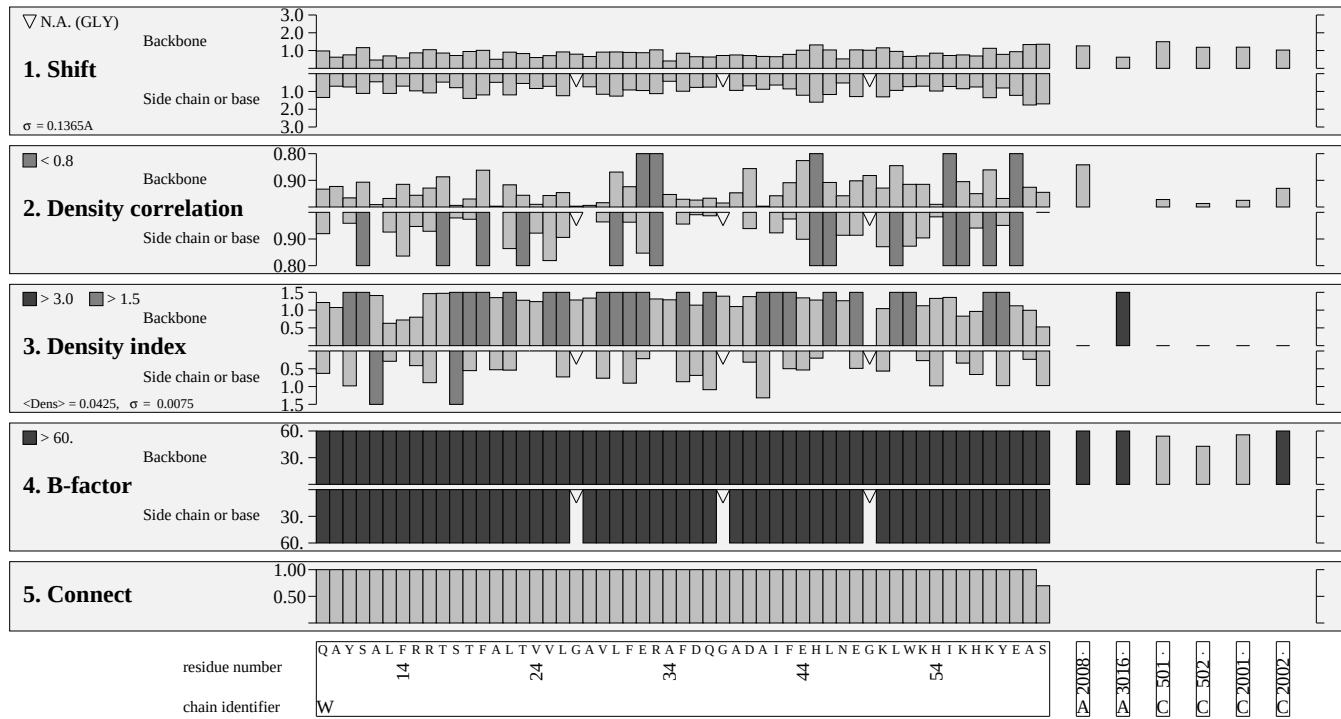
Local estimation (27)



Structure Factor Check

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Local estimation (28)



Local estimation (29)



chain identifier

382 959