

Structure Factor Check

3H1H

Title: CYTOCHROME BC1 COMPLEX FROM CHICKEN
Date: 12-APR-09
PDB code: 3H1H

Crystal

Cell parameters:

a: 169.59 Å b: 182.52 Å c: 240.57 Å
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Model

32608 atoms (19 water molecules)

Number of chains: 51

Volume not occupied by model: 61.7 %

 (for atomic model): 75.7 Å²

σ (B): 19.83 Å²

Matthews coefficient: 4.08

Corresponding solvent % : 69.60

Refinement

Program: CNS 1.1

Nominal resolution range: 20.0 – 3.16 Å

Reported R-factor: 0.253

Number of reflections used: 123634

Reported Rfree: 0.29

Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 69.3 – 3.16 Å

Reflections in file: 123804

Unique reflections above 0: 123804

above 1 σ : 122044

above 3 σ : 92275

SF CHECK

Nominal resolution range: 69.3 – 3.16 Å
\\05max. from input data, min. from author\\05

Used reflections: 123804

Completeness: 96.8 %

R_{stand}(F) = $\langle \sigma(F) \rangle / \langle F \rangle$: 0.064

Anisotropic distribution of Structure Factors

ratio of eigen values: 1.0000 0.3725 0.3752

B_{overall} (by Patterson): 52.Å²

Optical resolution: 2.28 Å

Expected opt. resol. for complete data set: 2.28 Å

Estimated minimal error: 0.090 Å

Model vs. Structure Factors

R-factor for all reflections: 0.296

Correlation factor: 0.848

R-factor: 0.301

for $F > 2.0\sigma$

nom. resolution range: 20.00 – 3.16Å

reflections used: 121876

Rfree: 0.331

Nfree: 2419

R-factor without free-refl.: 0.301

Non free-reflections: 119457

<u> (error in coords by Luzzati plot): 0.594 Å

Estimated maximal error: 0.476 Å

DPI: 0.477 Å

Scaling

Scale: 0.685

Bdiff: -7.62

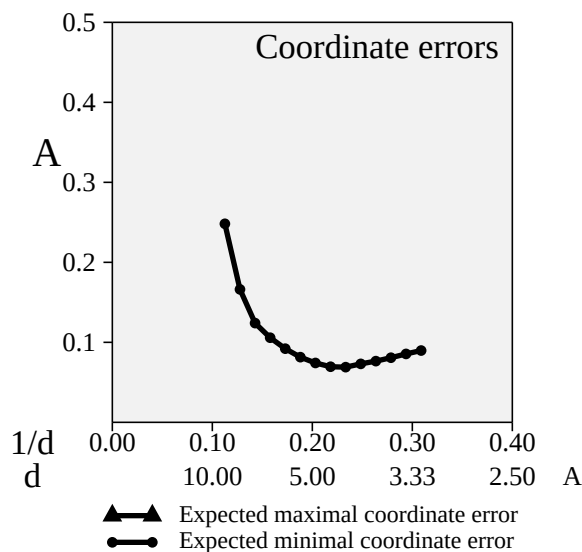
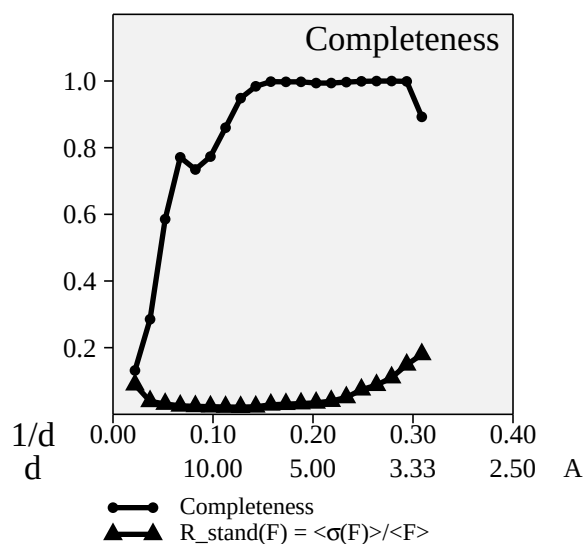
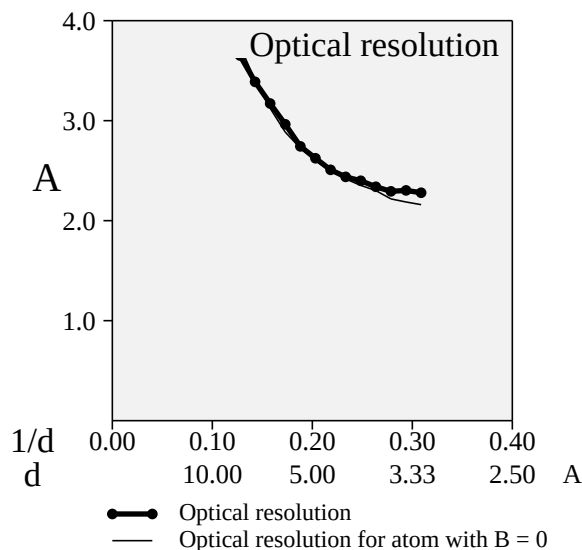
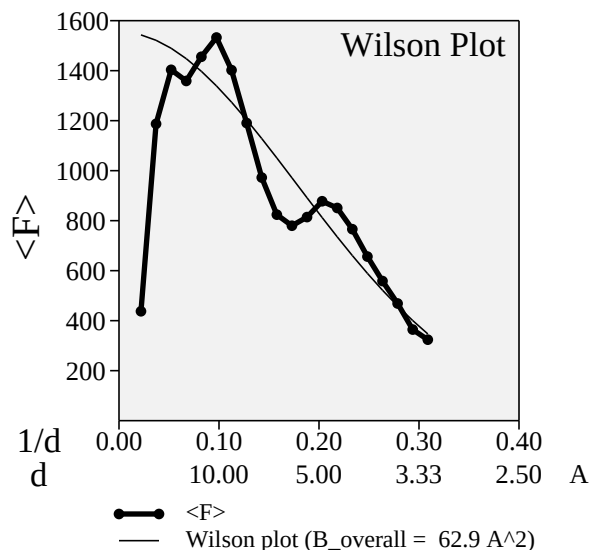
Anisothermal Scaling (Beta):

17.8193 -1.4625 -1.0966 0.0000 0.0000 0.0000

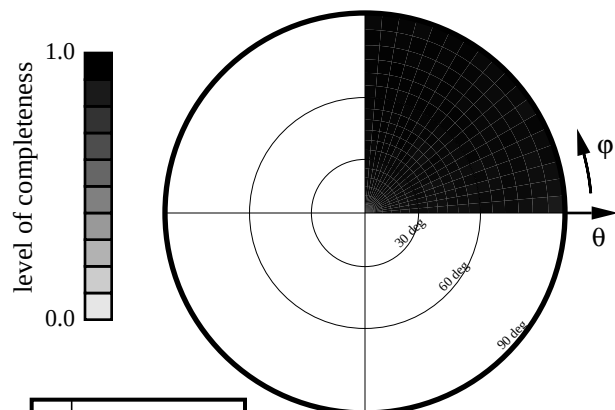
Solvent correction – Ks,Bs: 0.844 250.356

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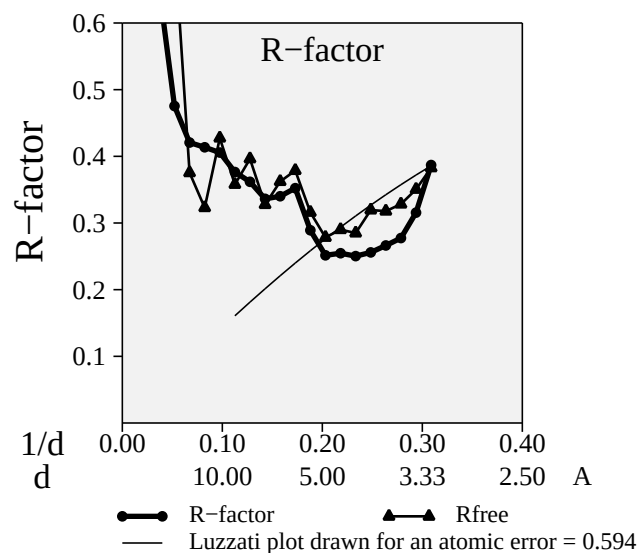


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

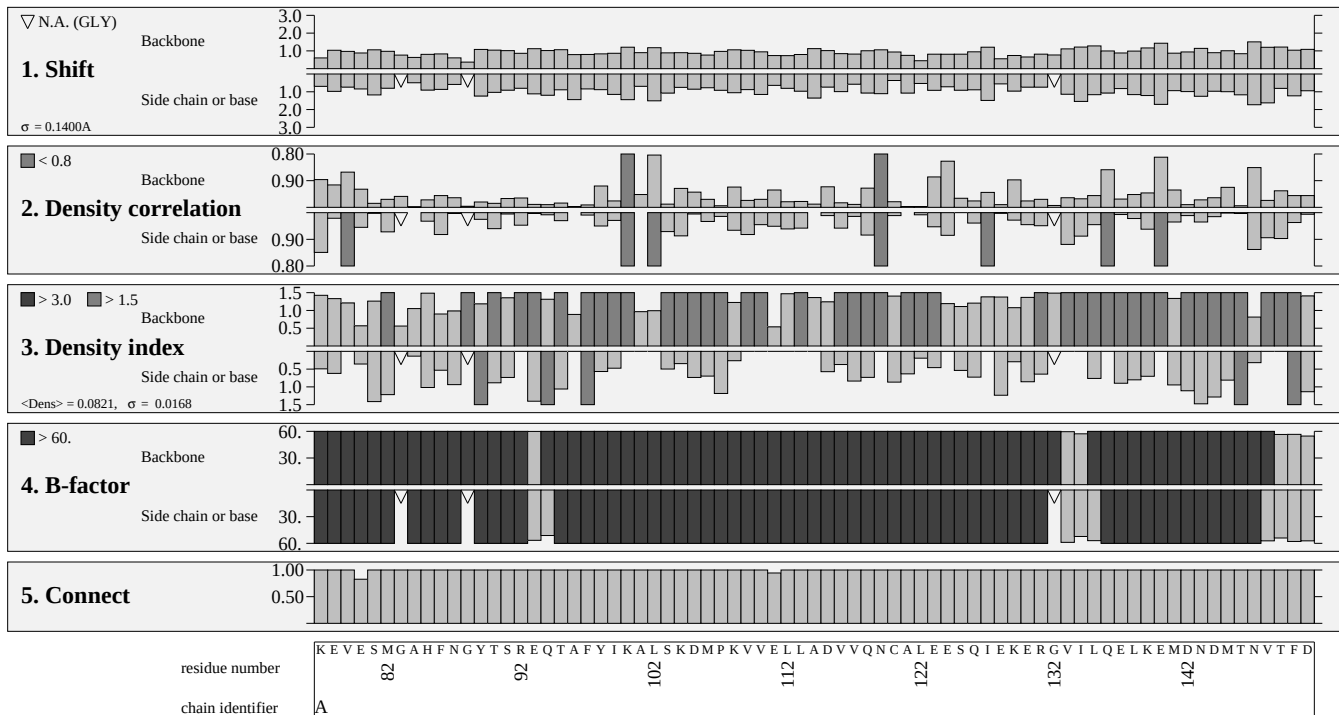
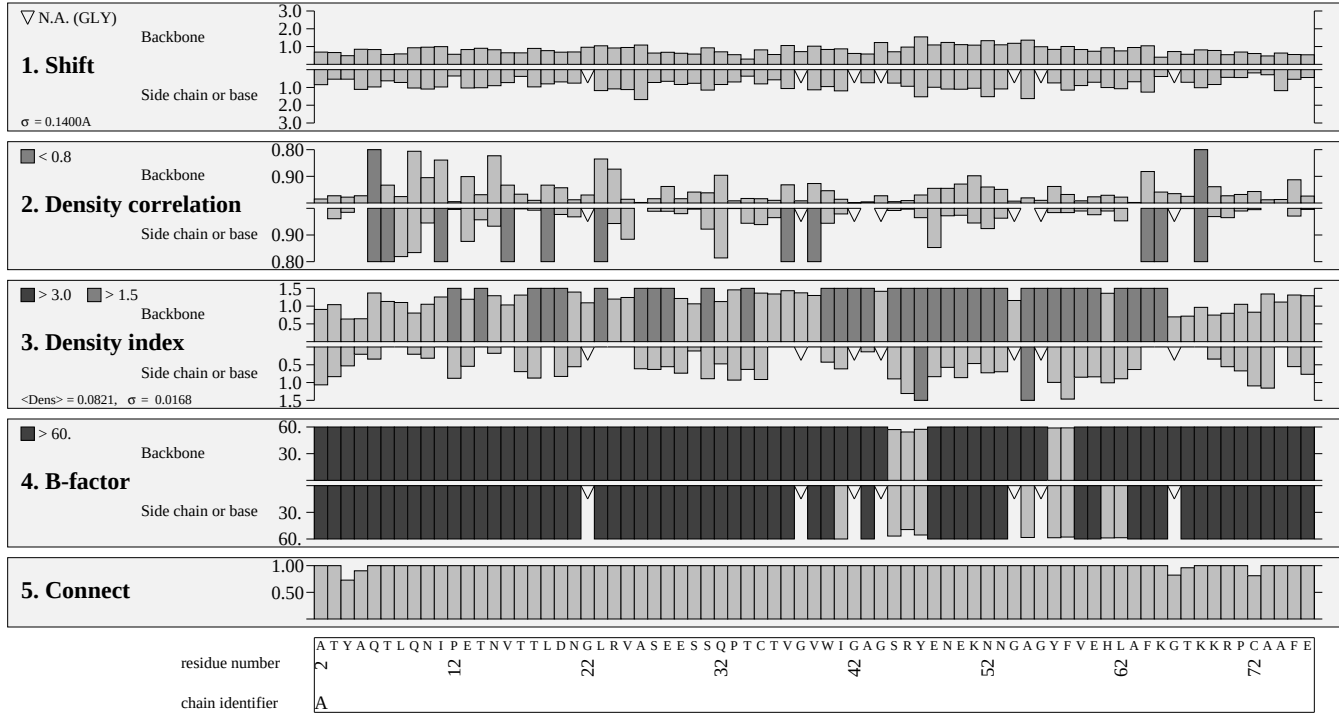
polar coordinates of the crystallographical axes



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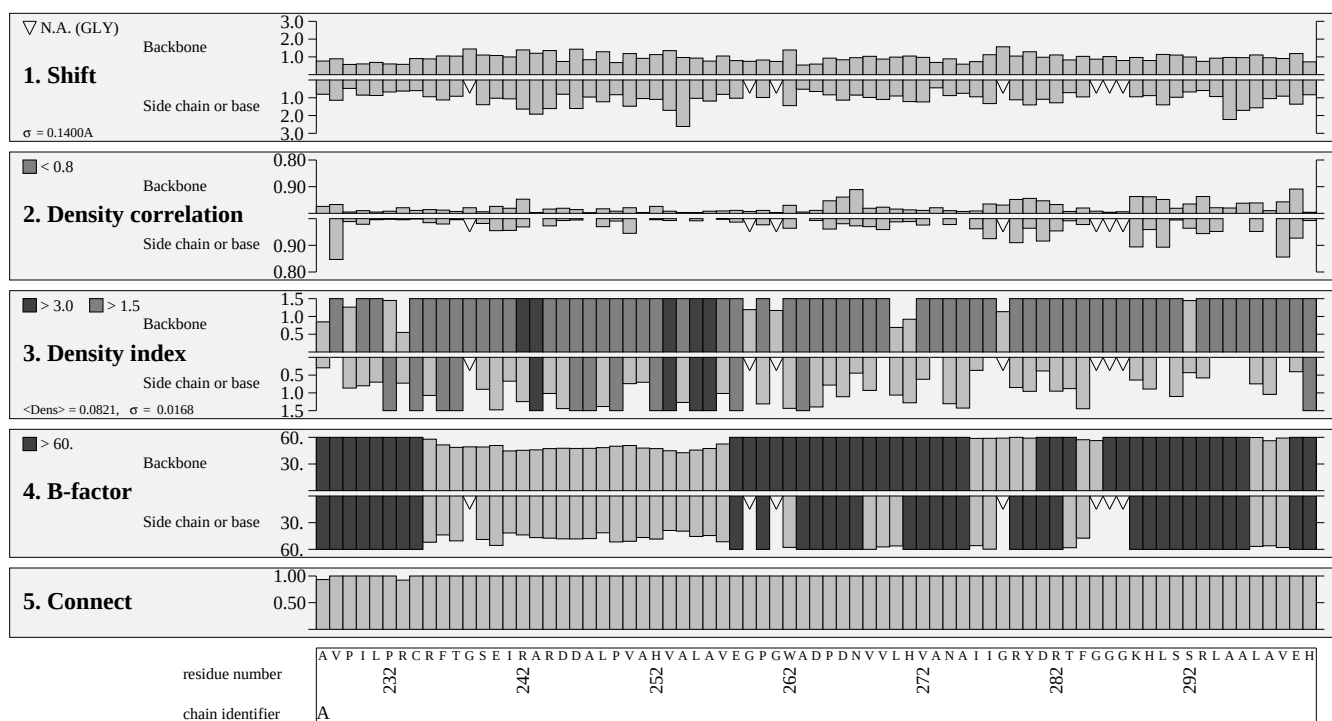
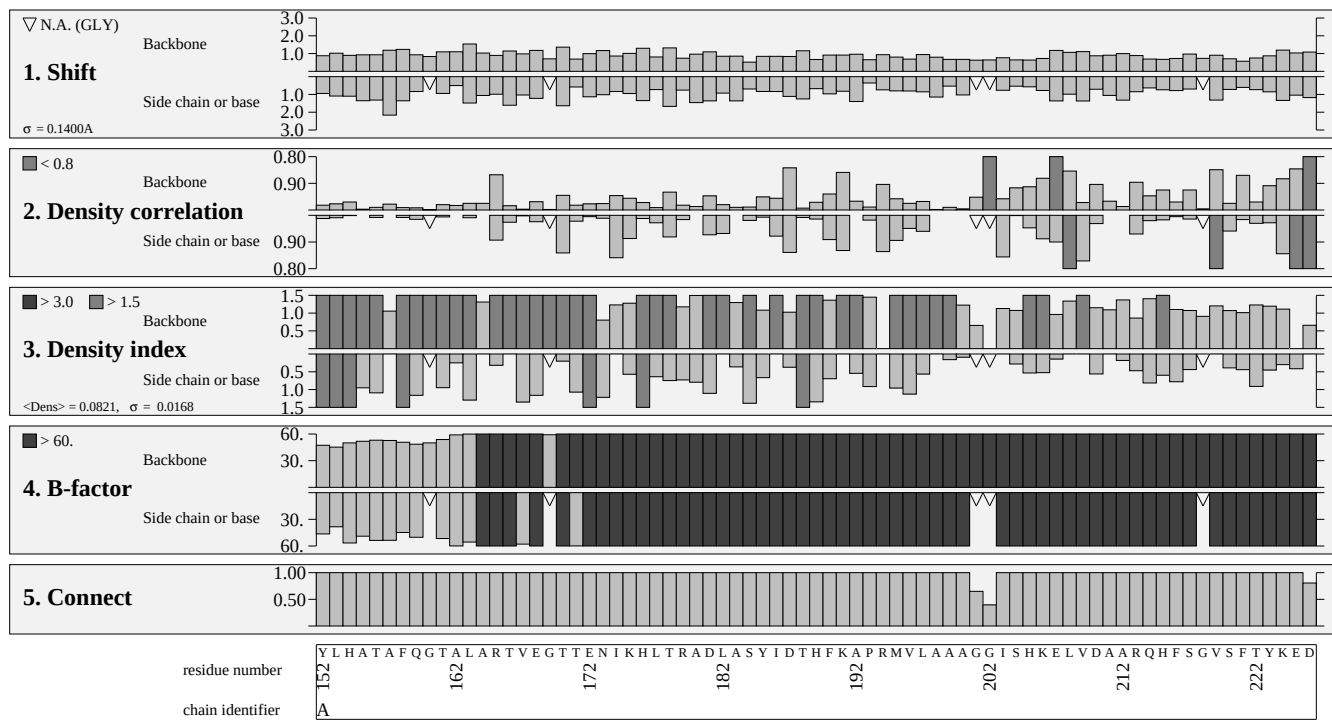
Local estimation



Structure Factor Check

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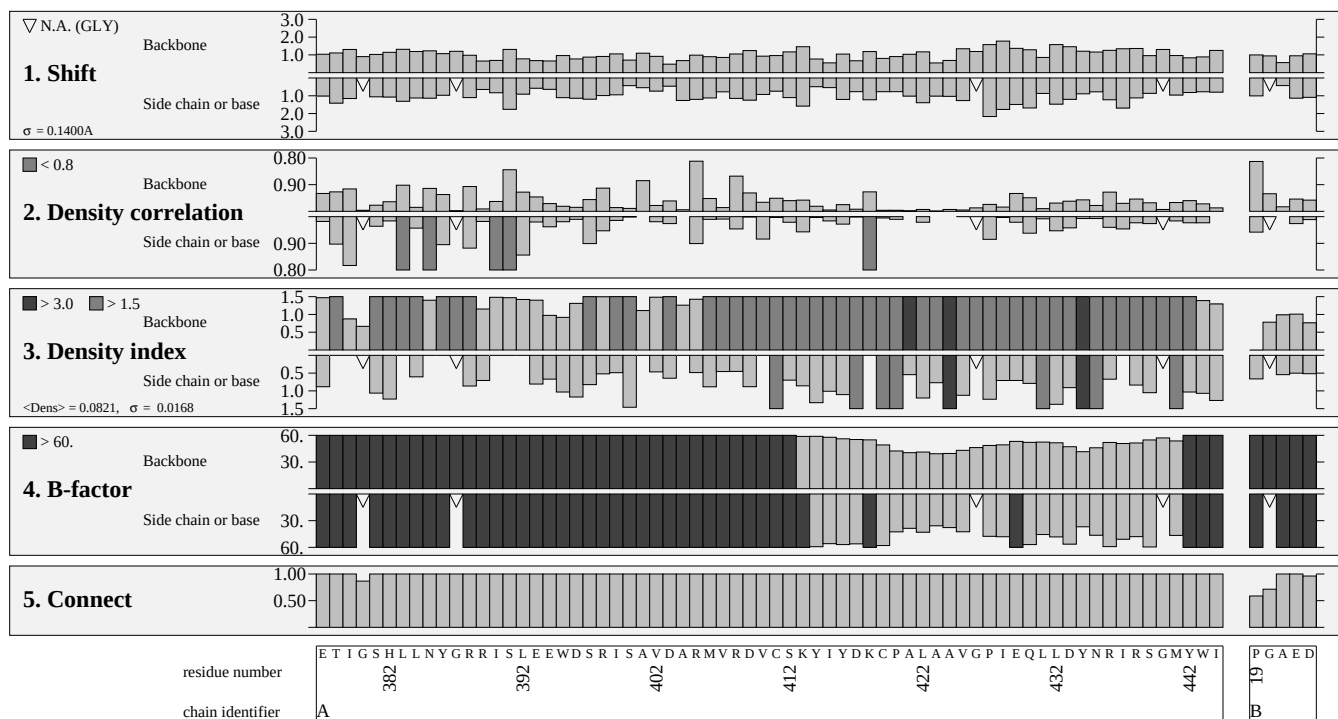
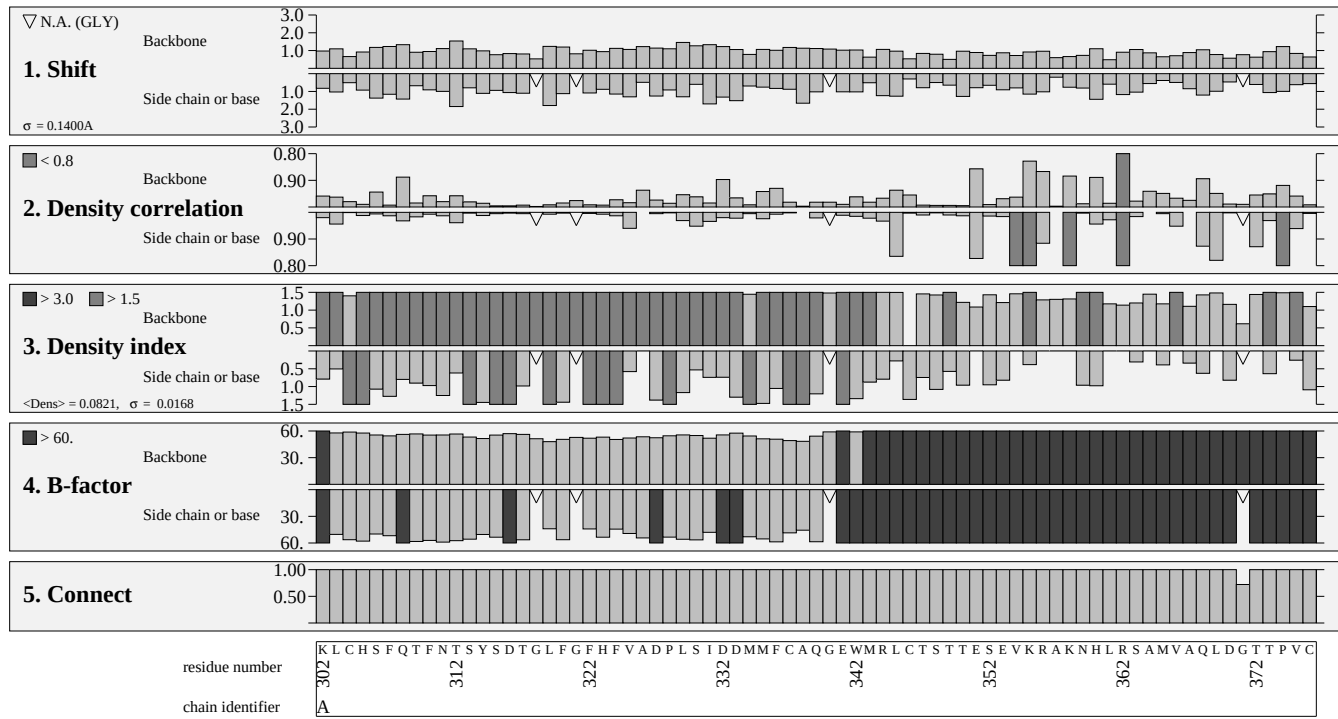
Local estimation (2)



Structure Factor Check

3H1H

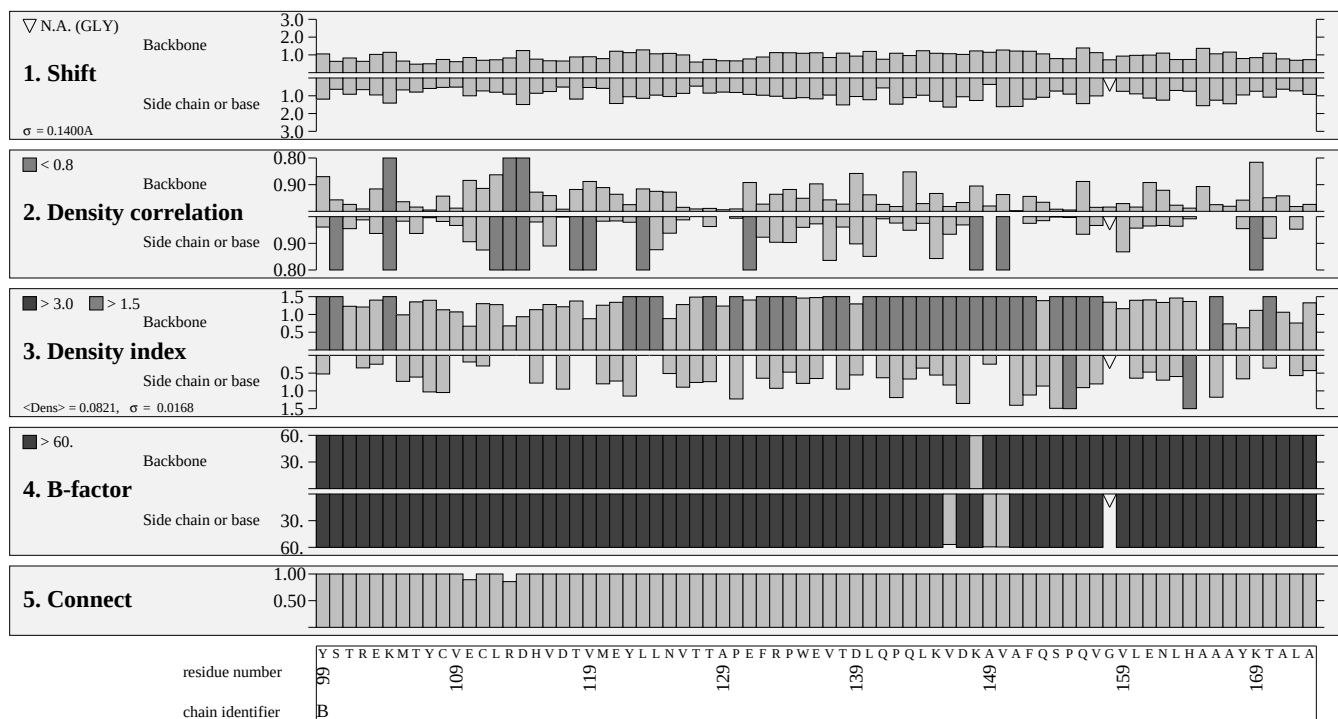
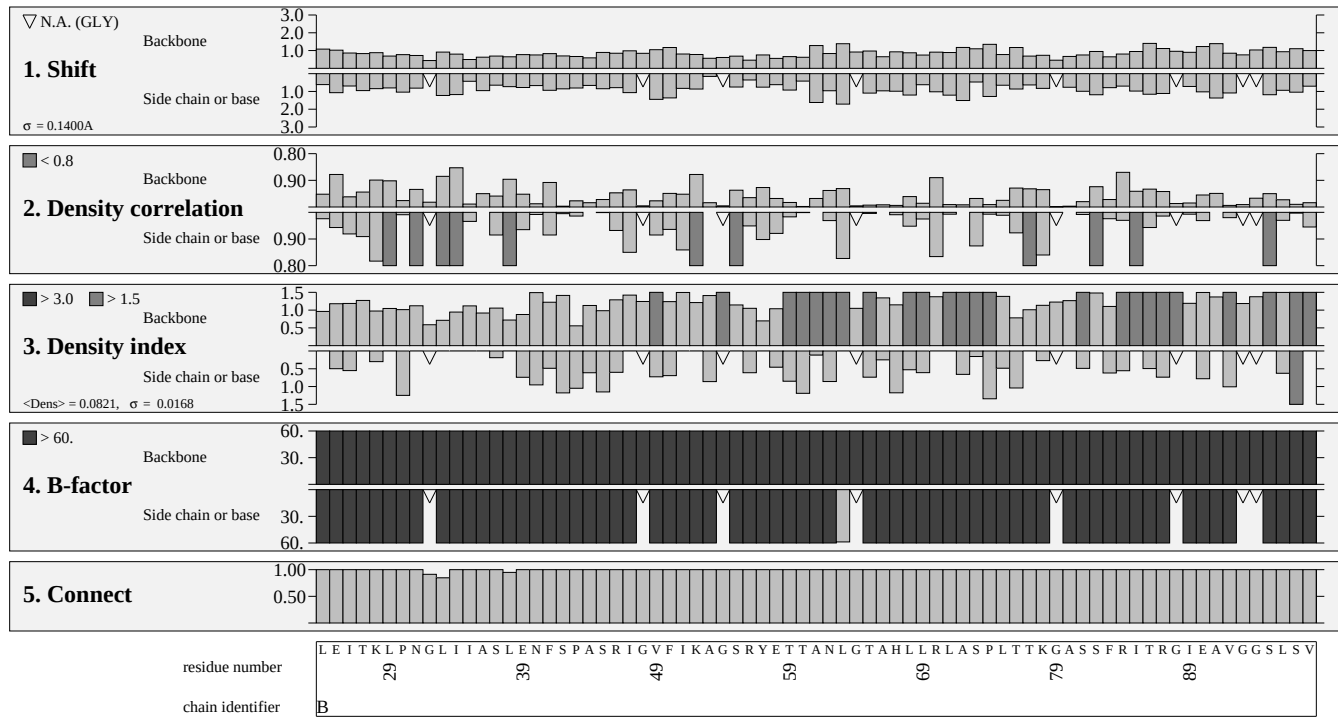
Local estimation (3)



Structure Factor Check

3H1H

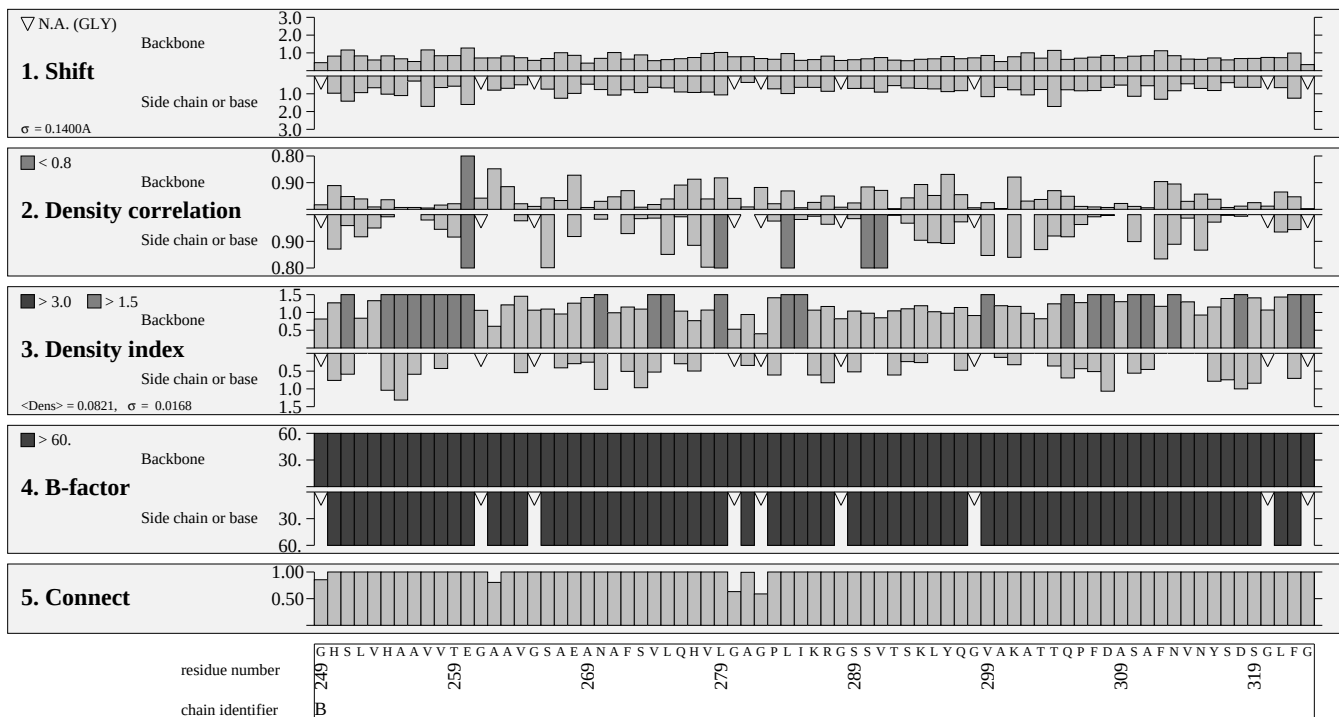
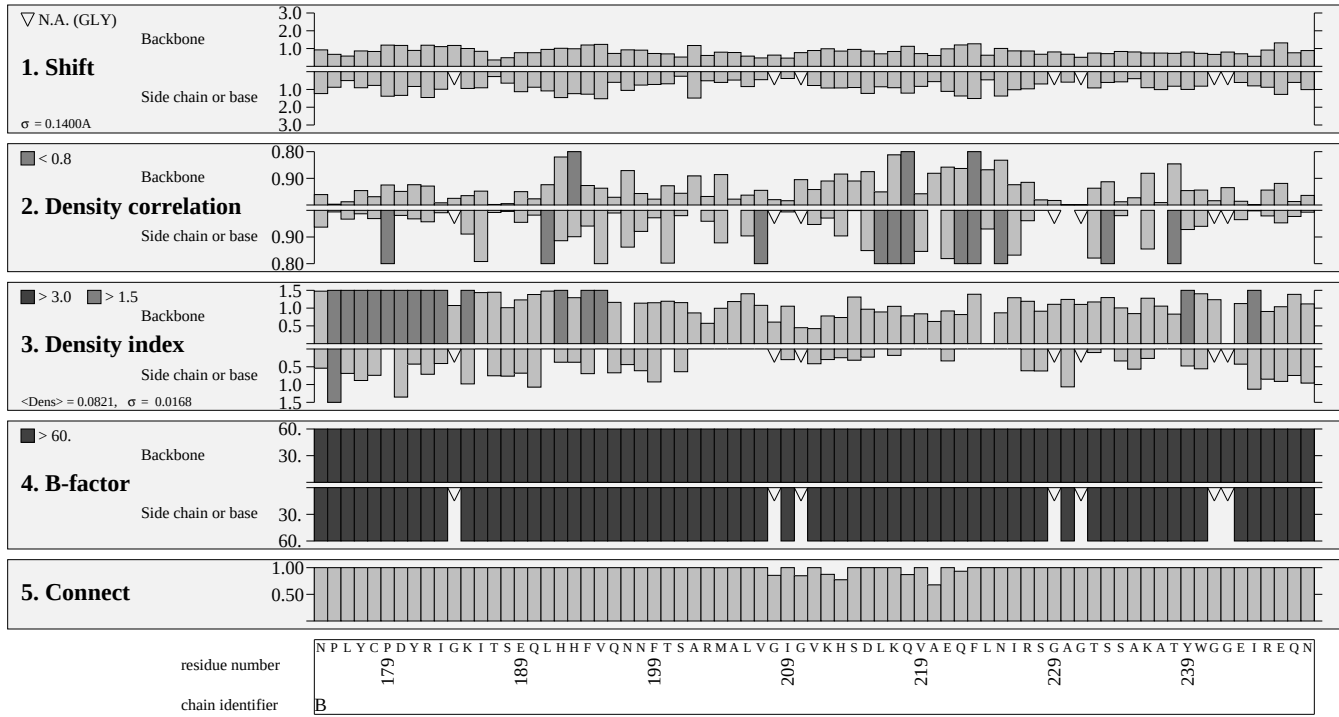
Local estimation (4)



Structure Factor Check

3H1H

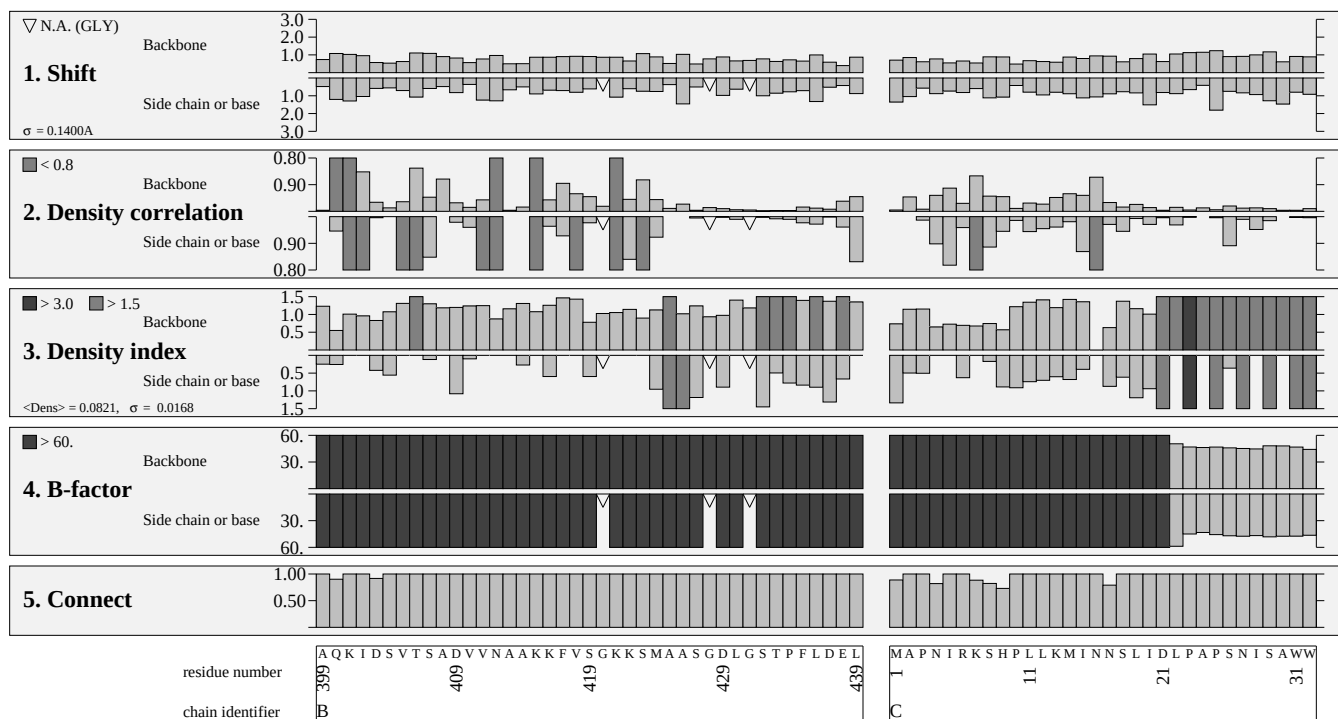
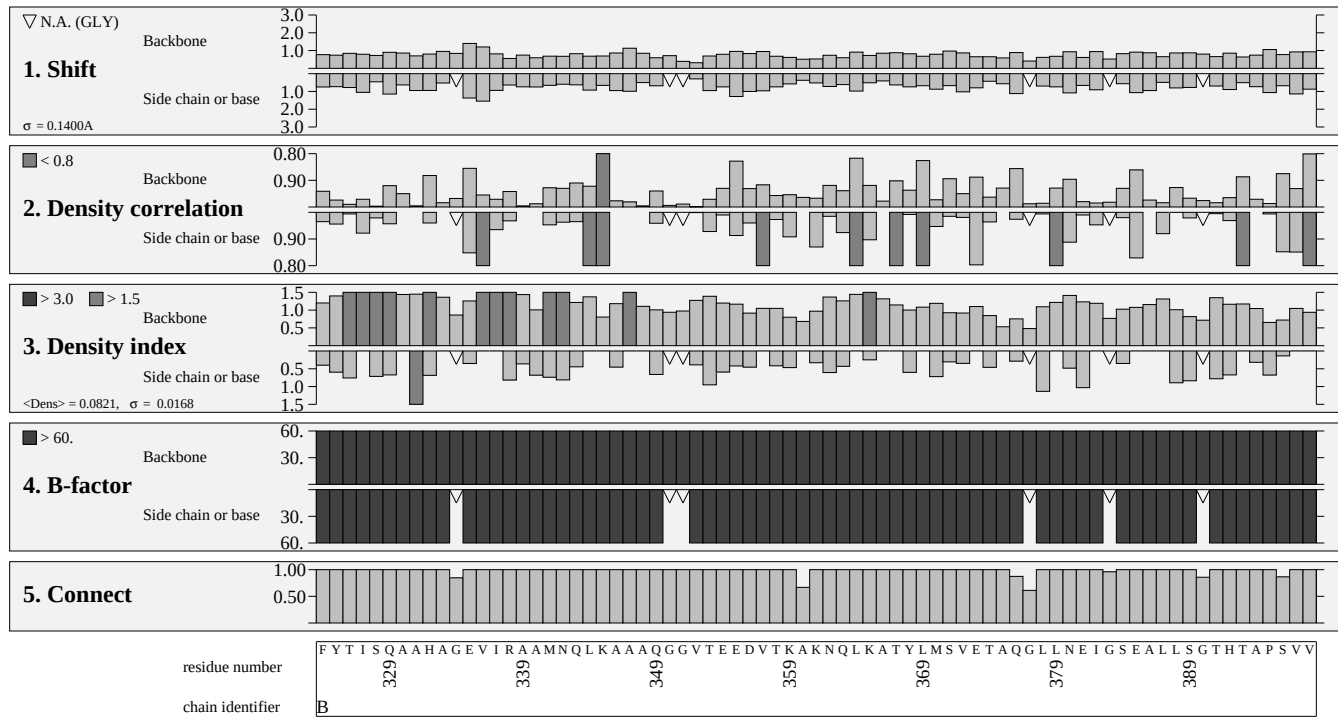
Local estimation (5)



Structure Factor Check

3H1H

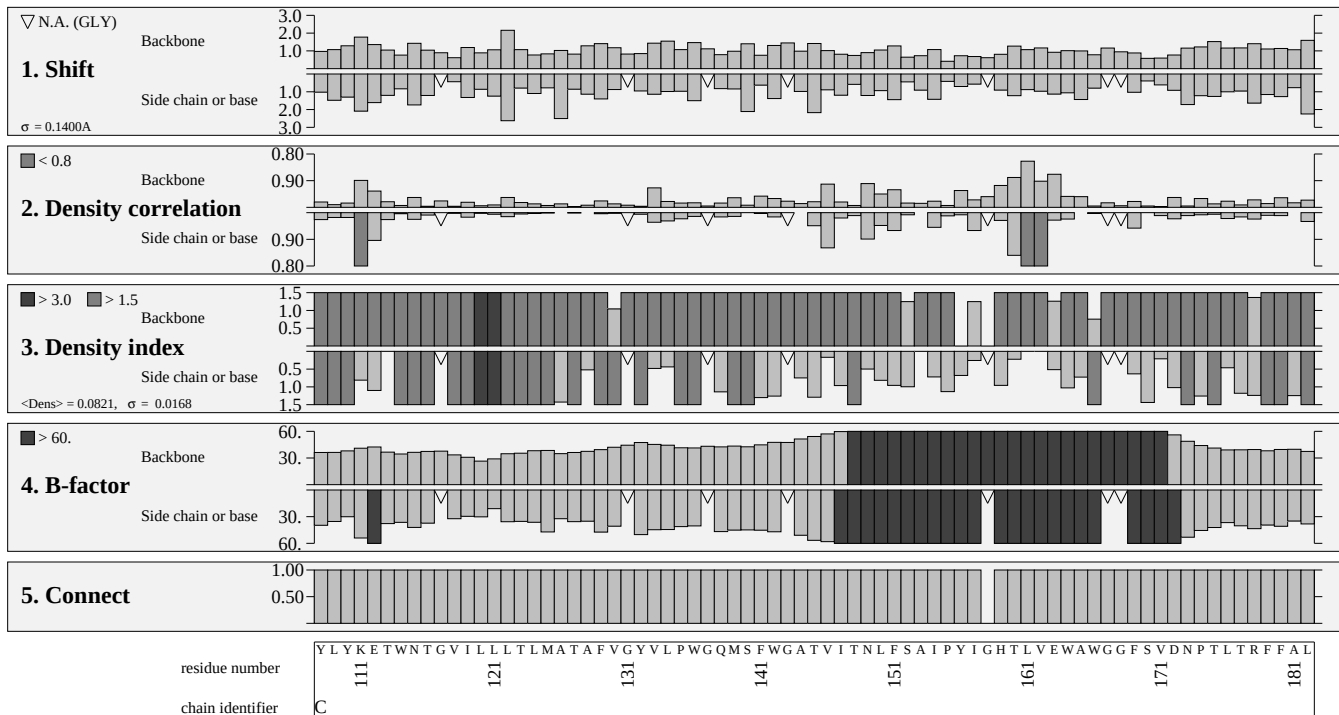
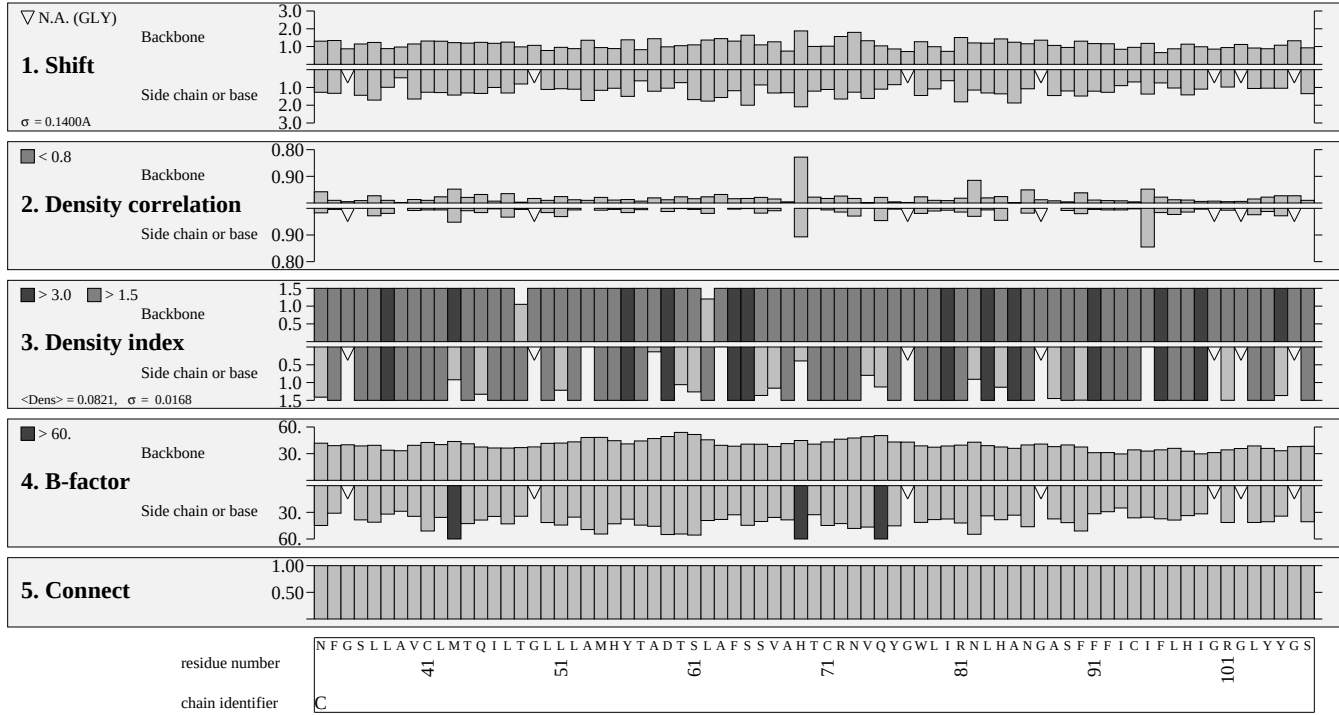
Local estimation (6)



Structure Factor Check

3H1H

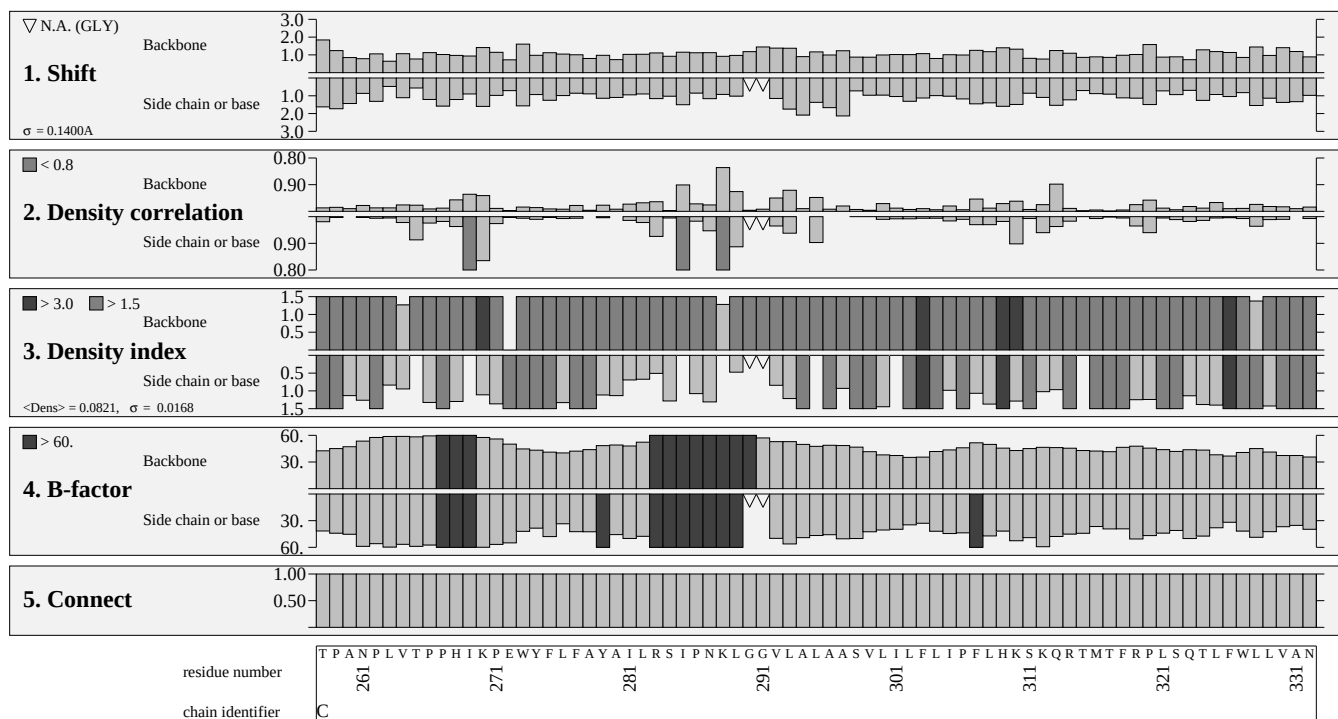
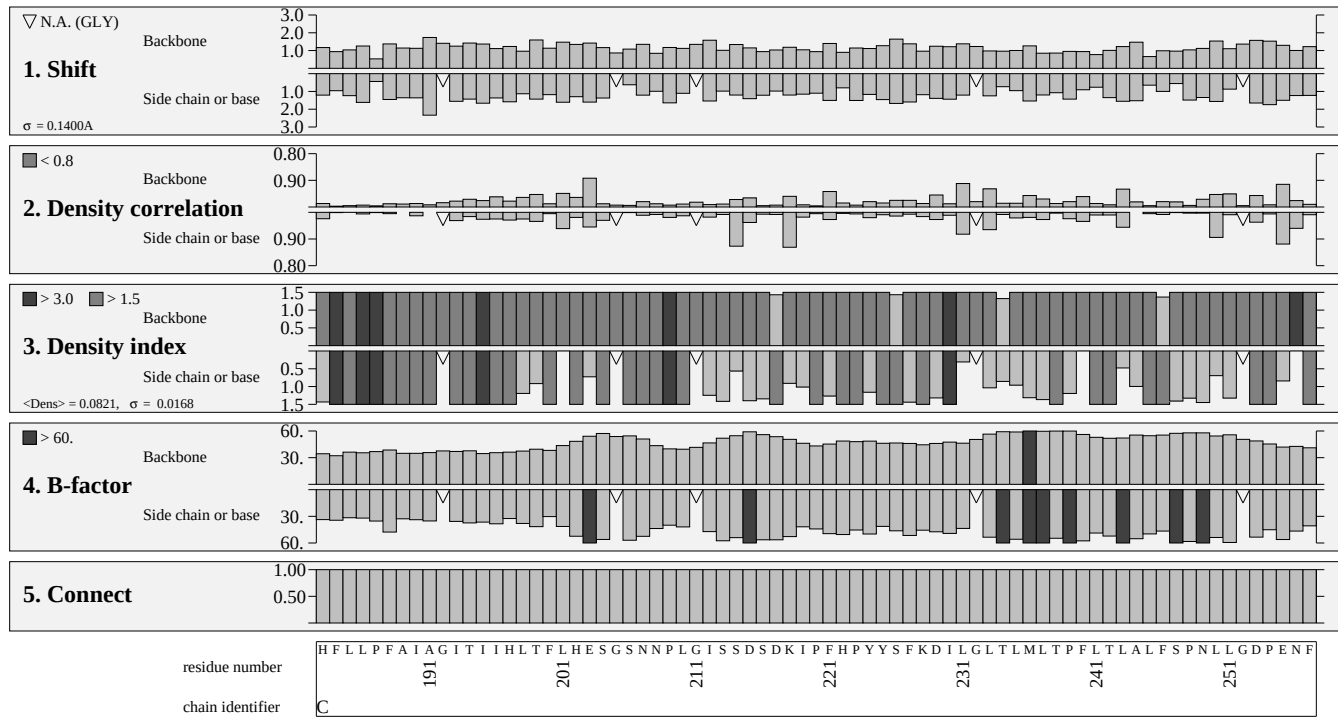
Local estimation (7)



Structure Factor Check

3H1H

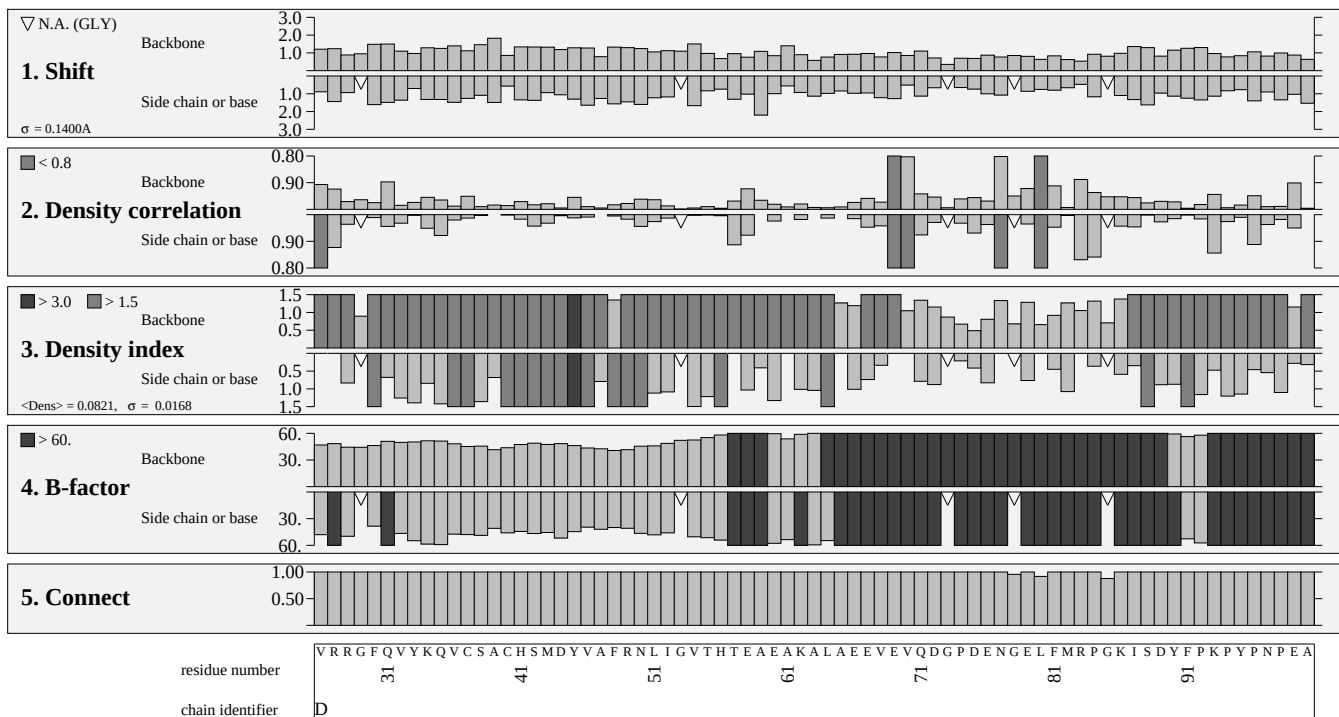
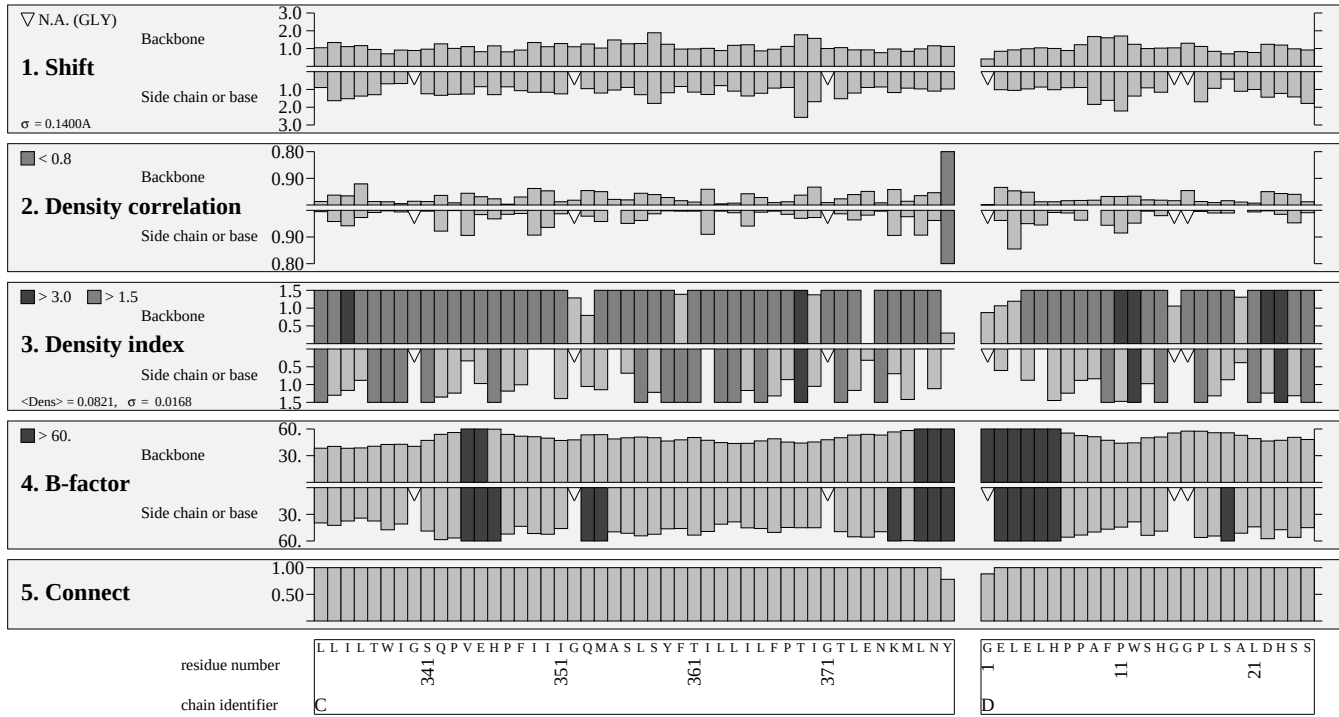
Local estimation (8)



Structure Factor Check

3H1H

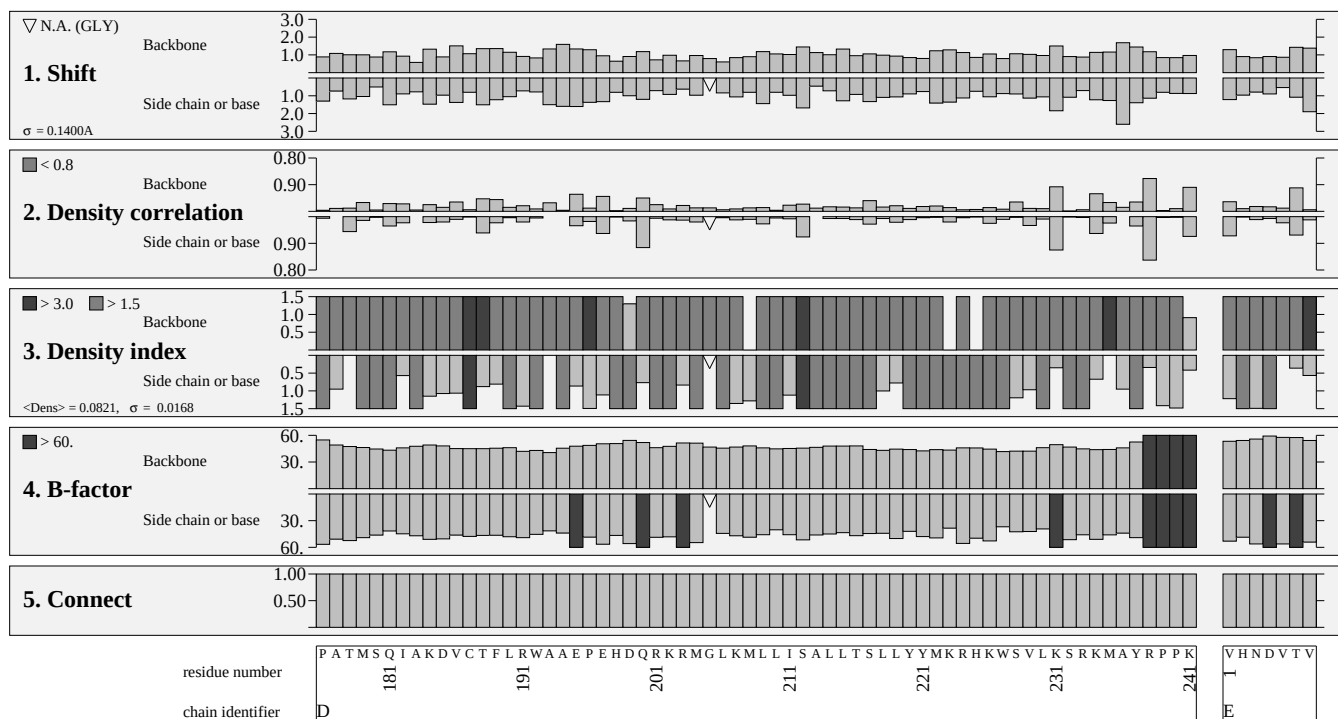
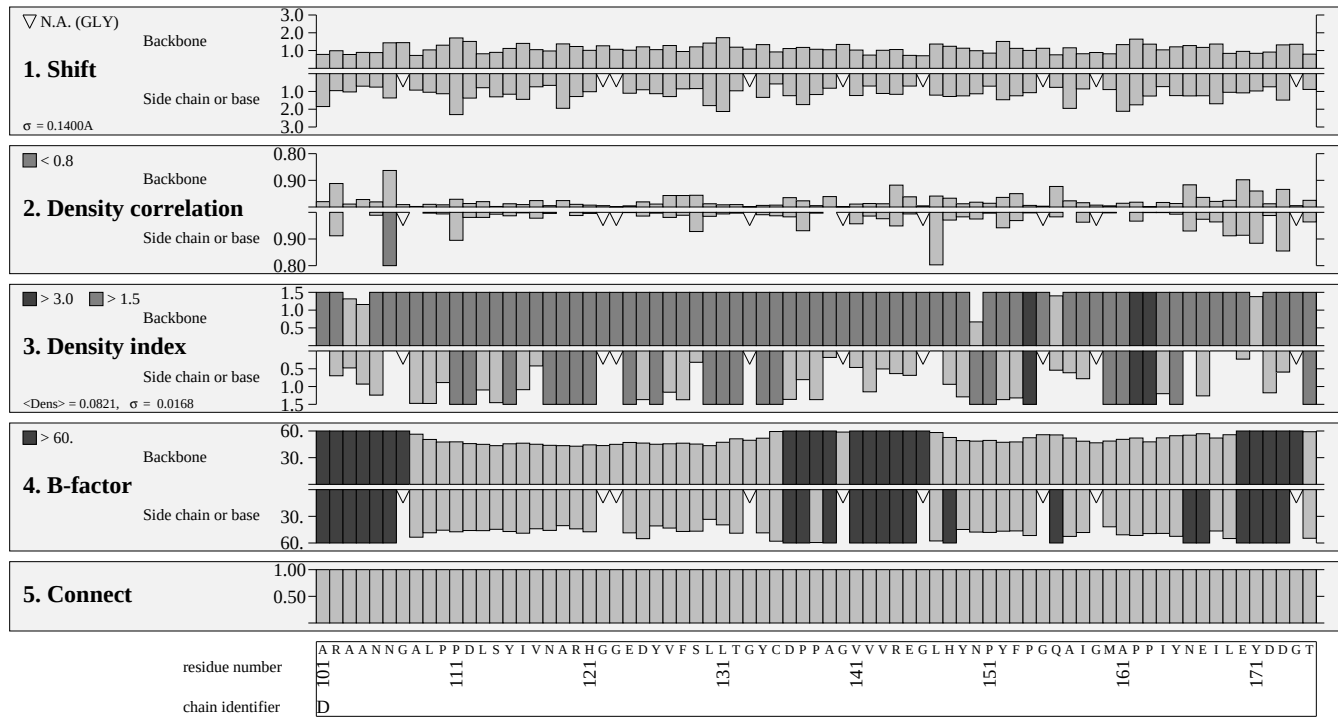
Local estimation (9)



Structure Factor Check

3H1H

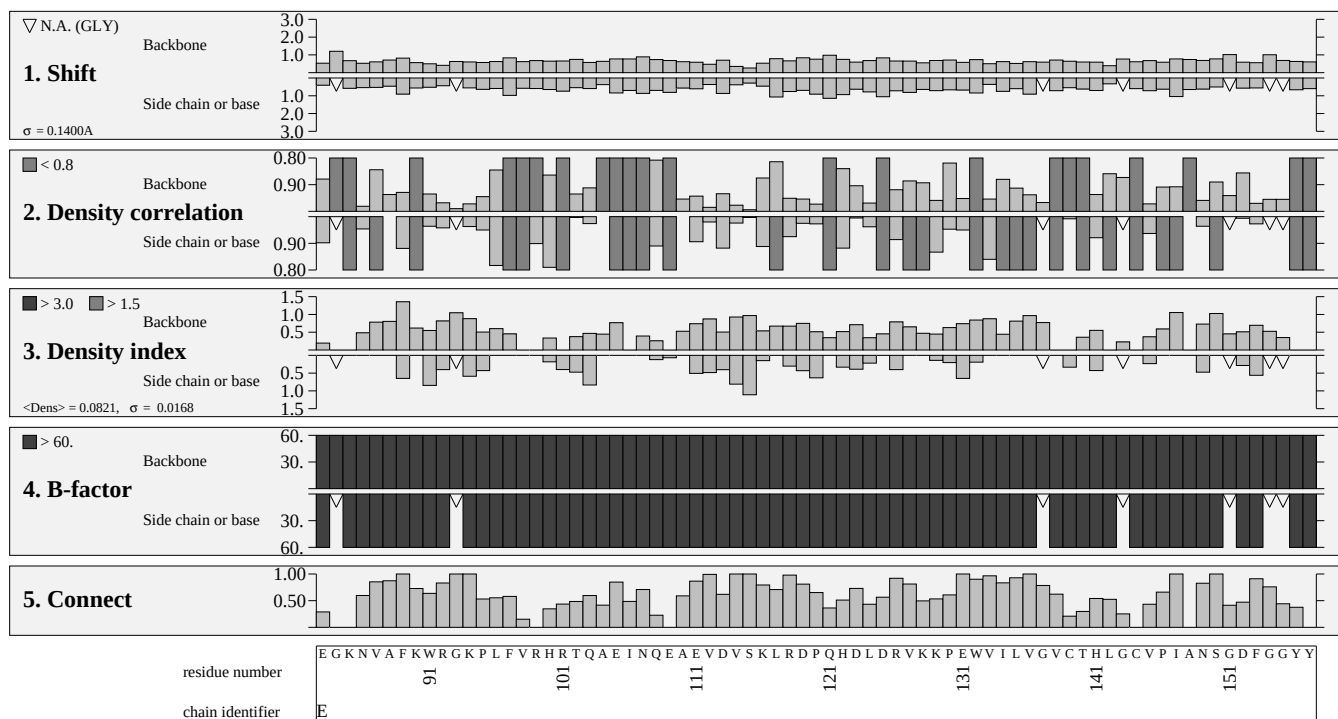
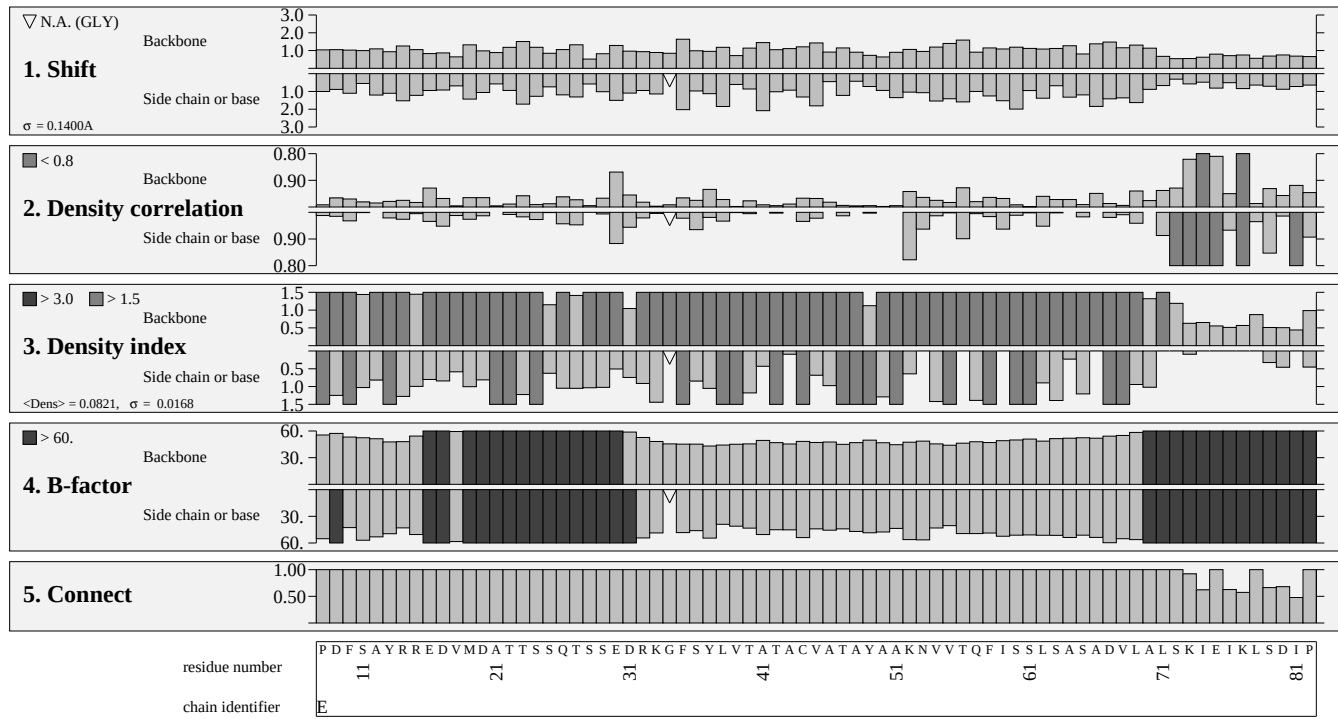
Local estimation (10)



Structure Factor Check

3H1H

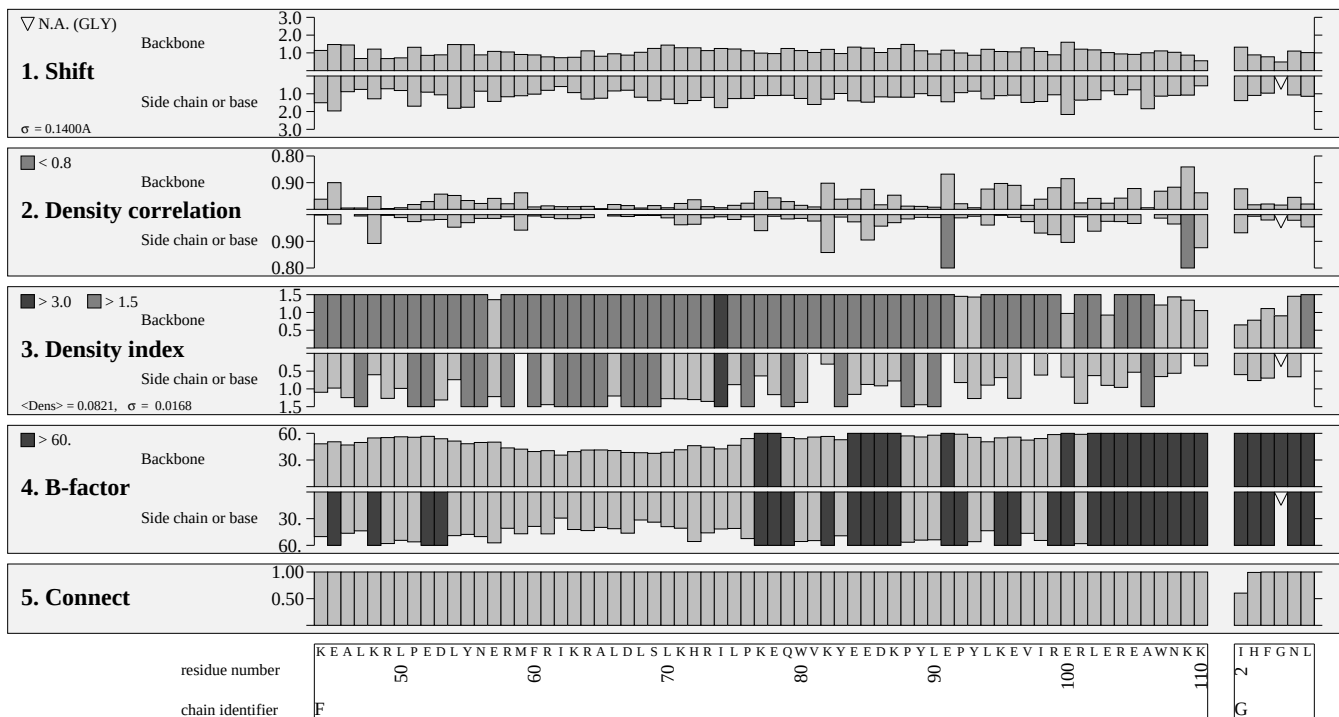
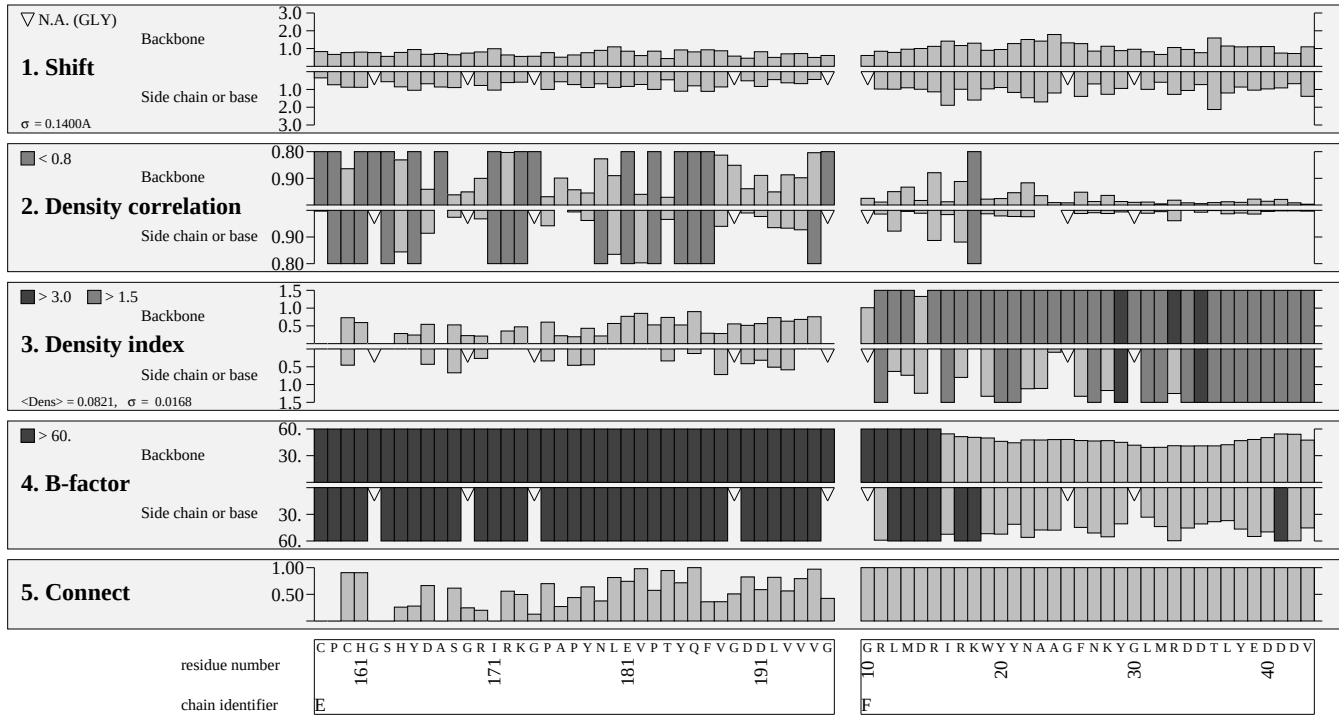
Local estimation (11)



Structure Factor Check

3H1H

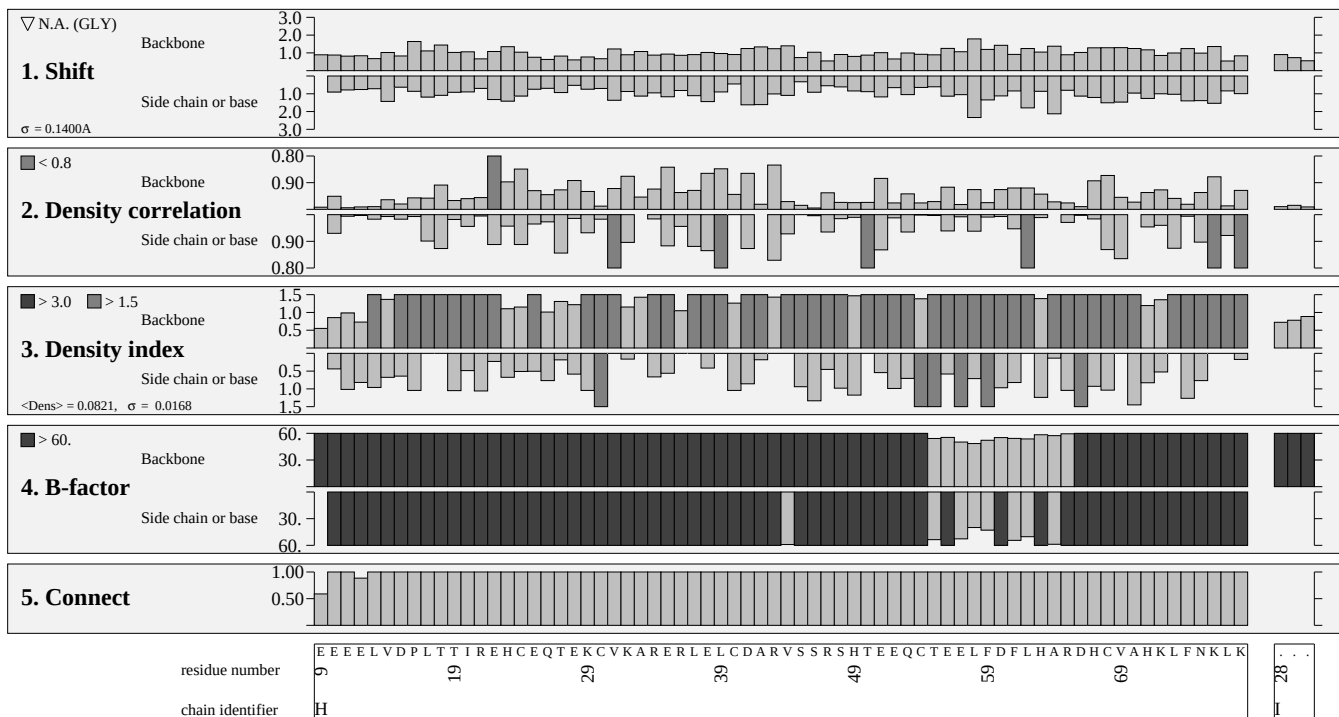
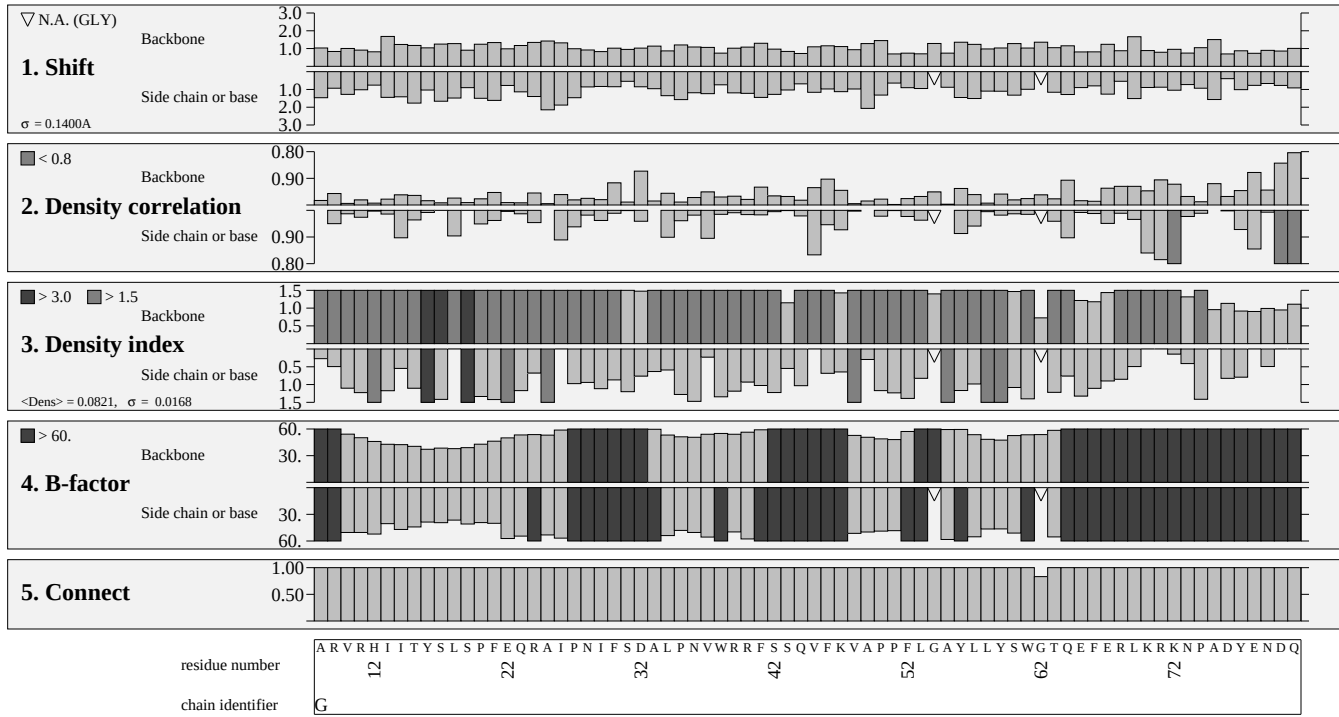
Local estimation (12)



Structure Factor Check

3H1H

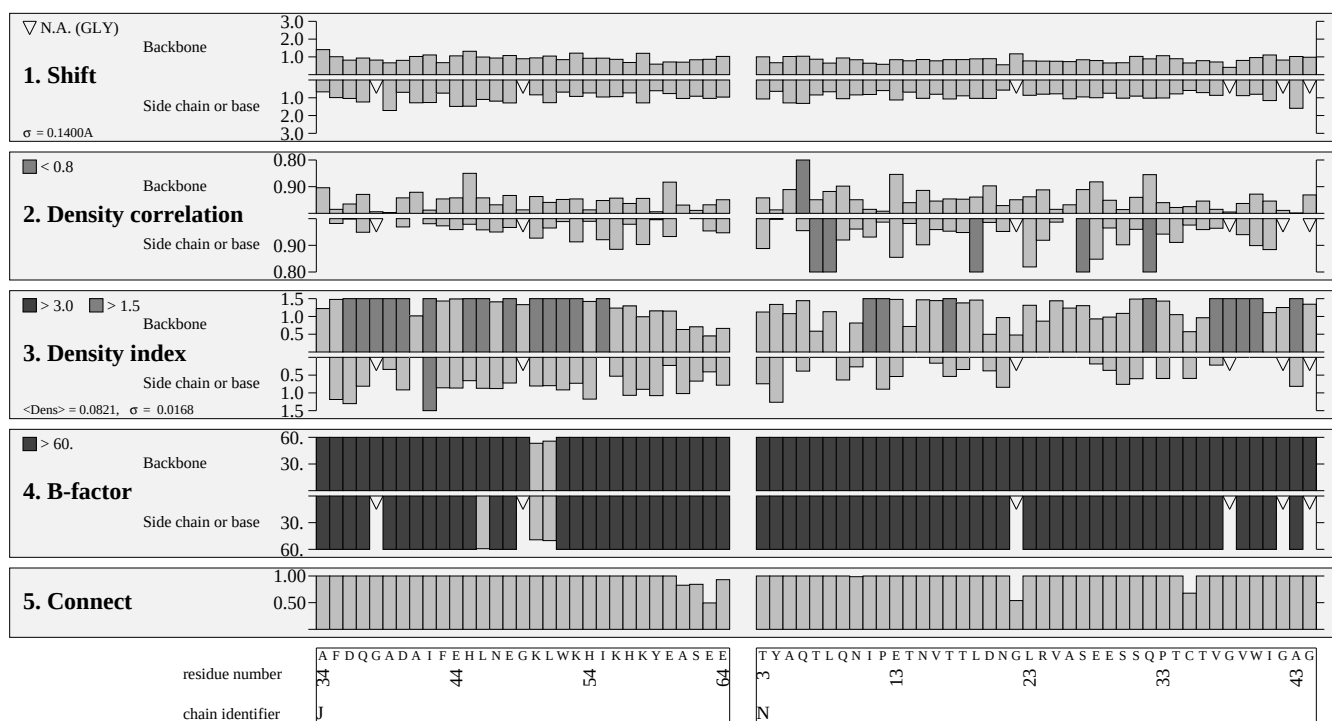
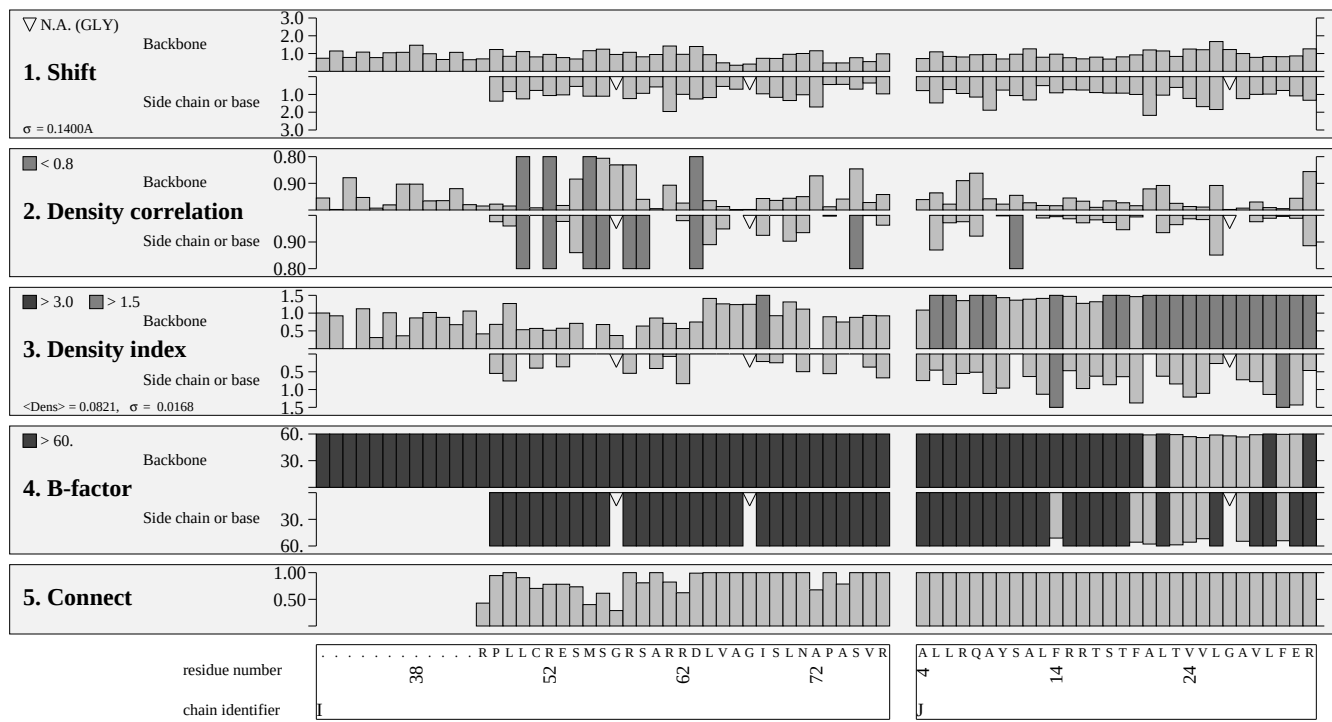
Local estimation (13)



Structure Factor Check

3H1H

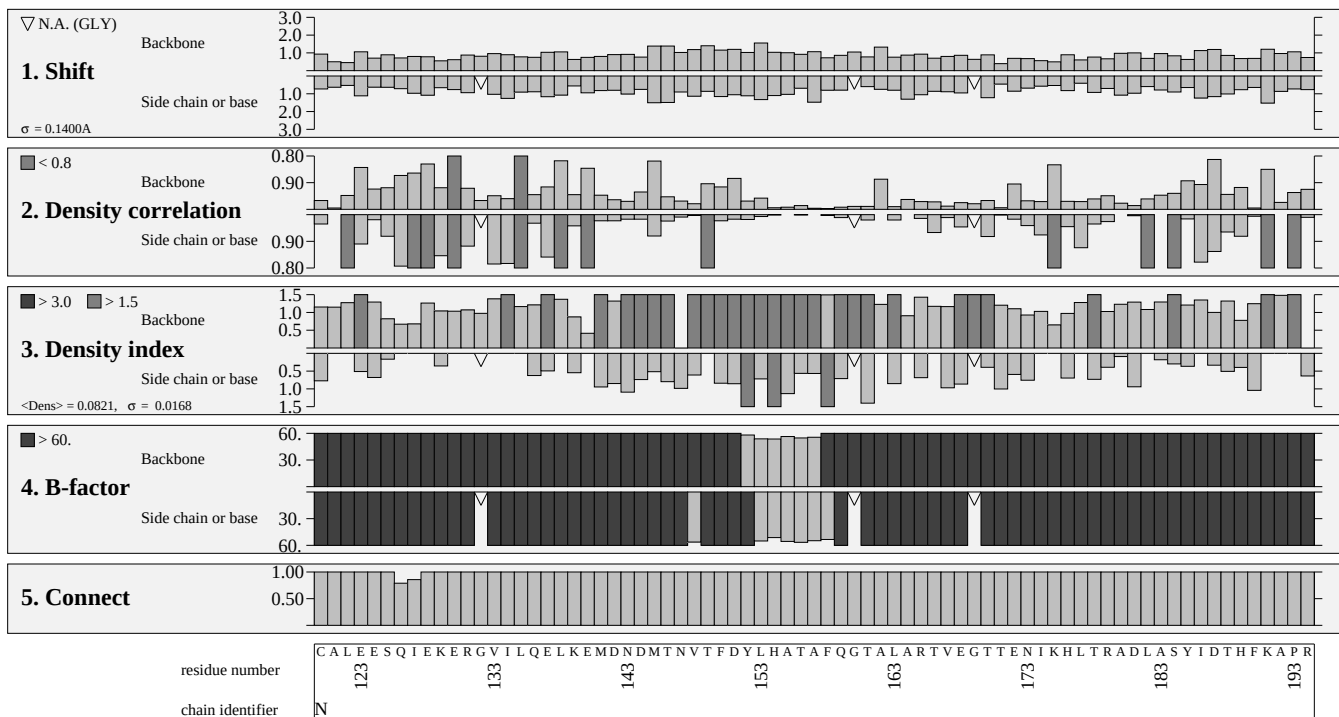
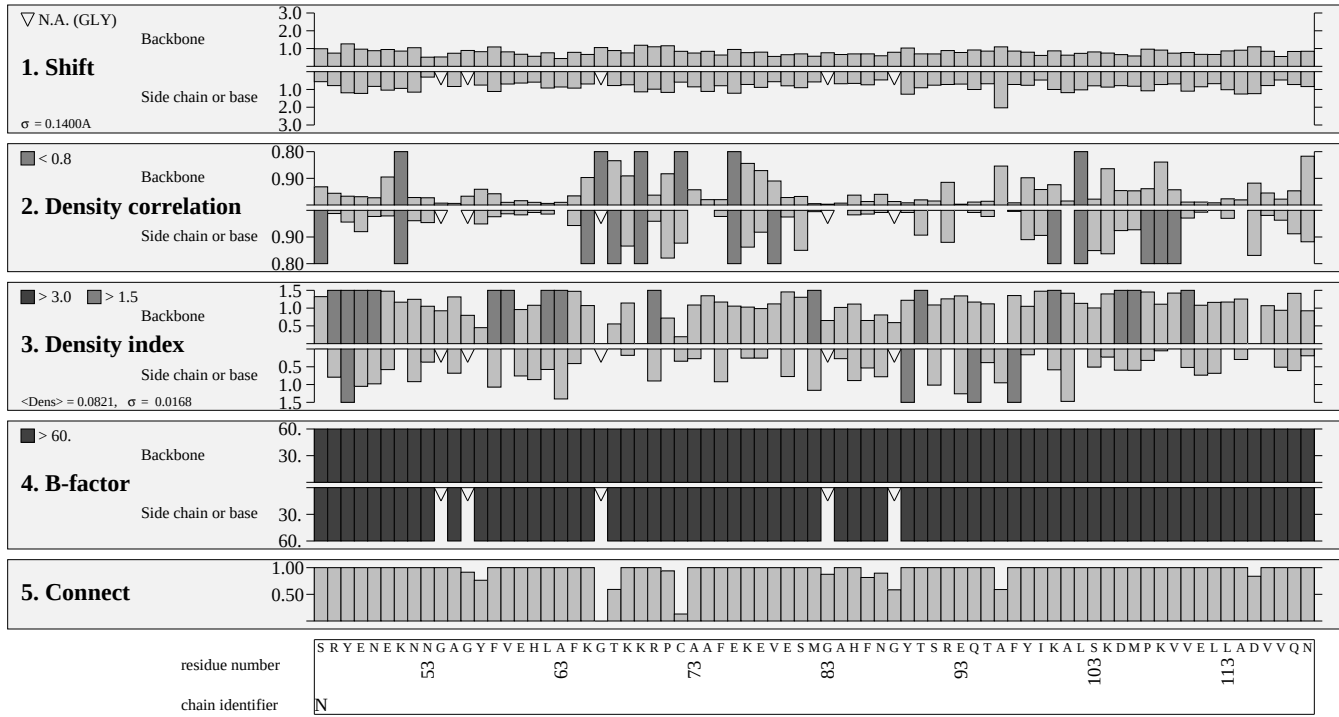
Local estimation (14)



Structure Factor Check

3H1H

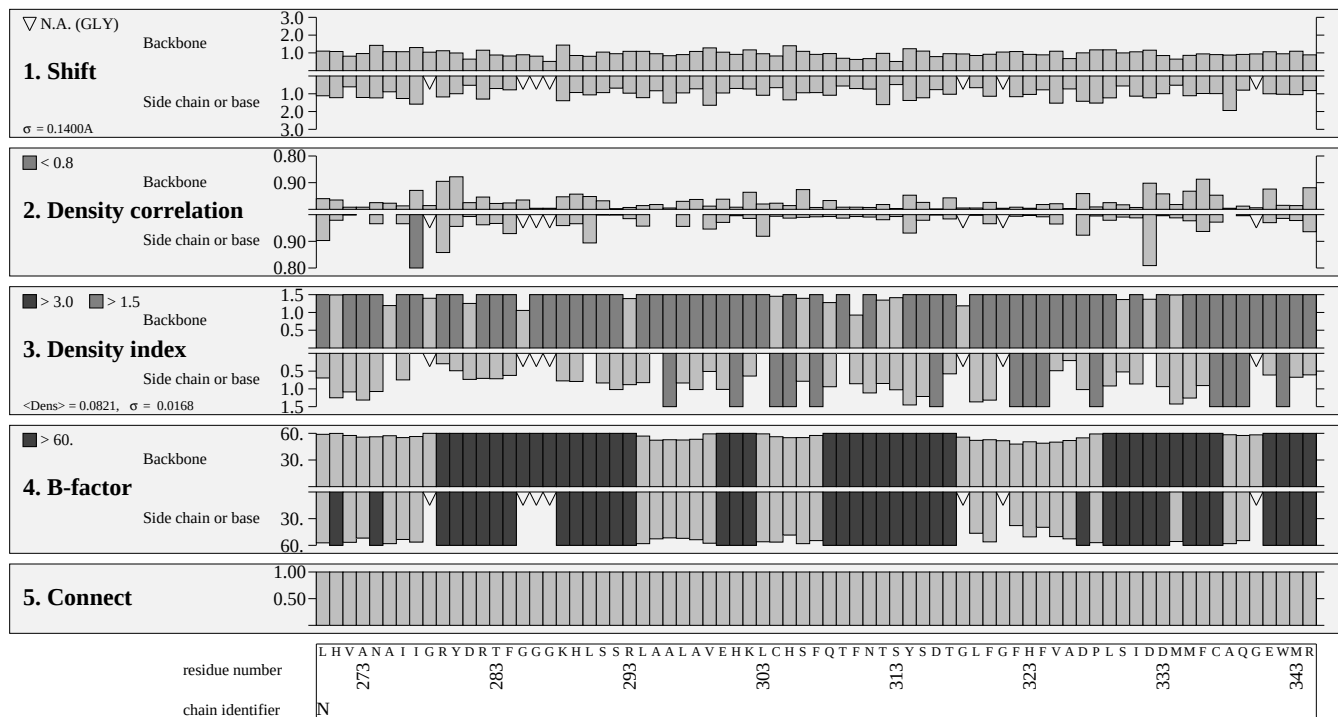
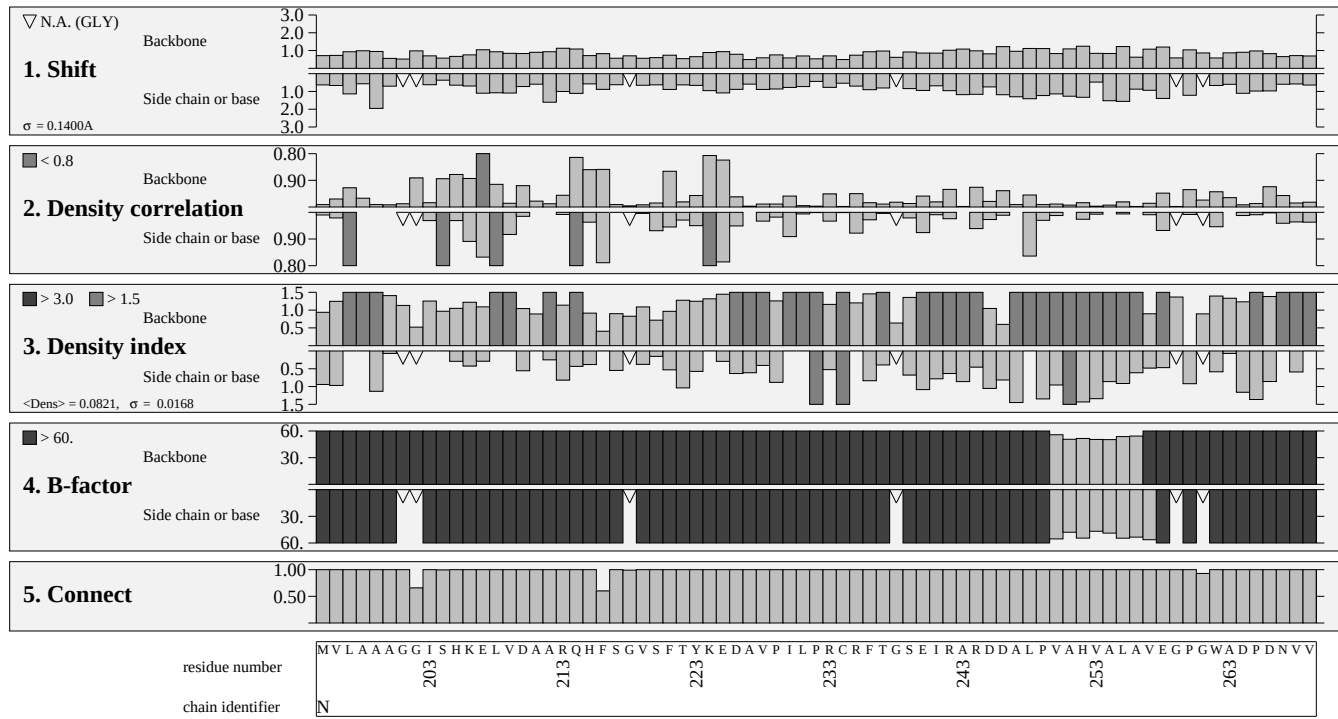
Local estimation (15)



Structure Factor Check

3H1H

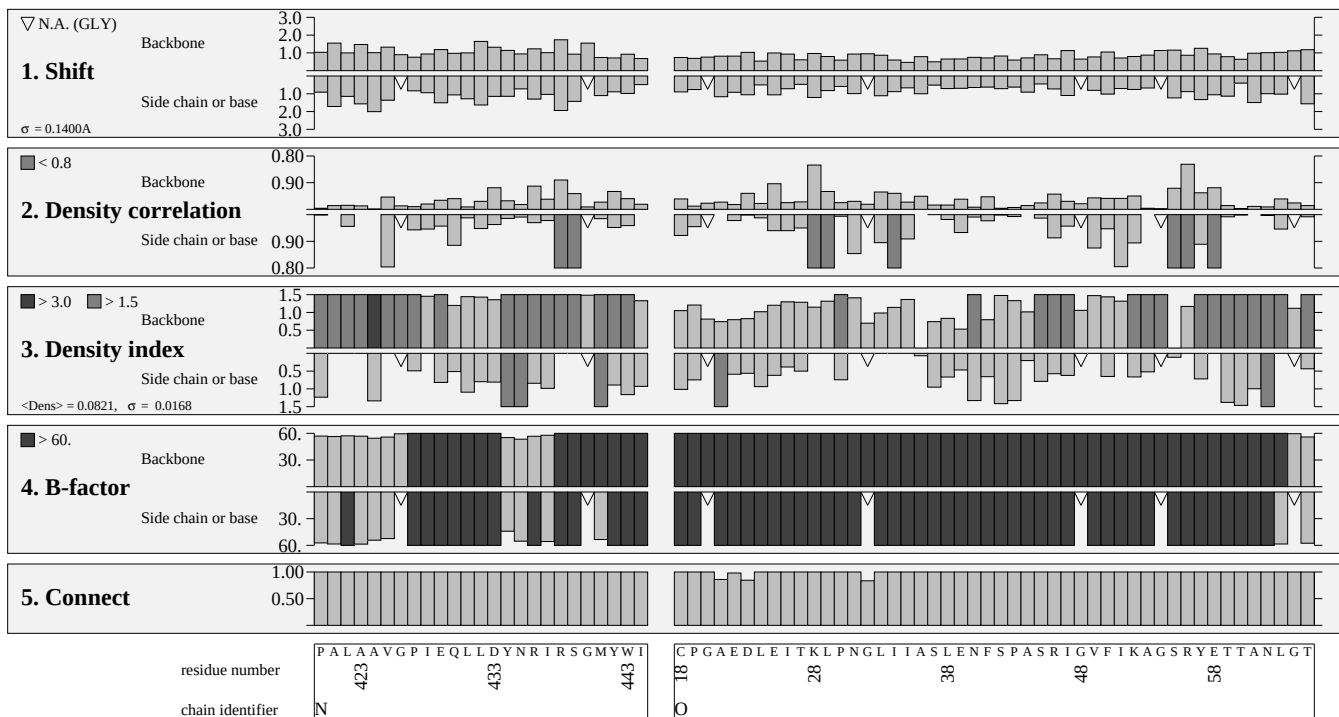
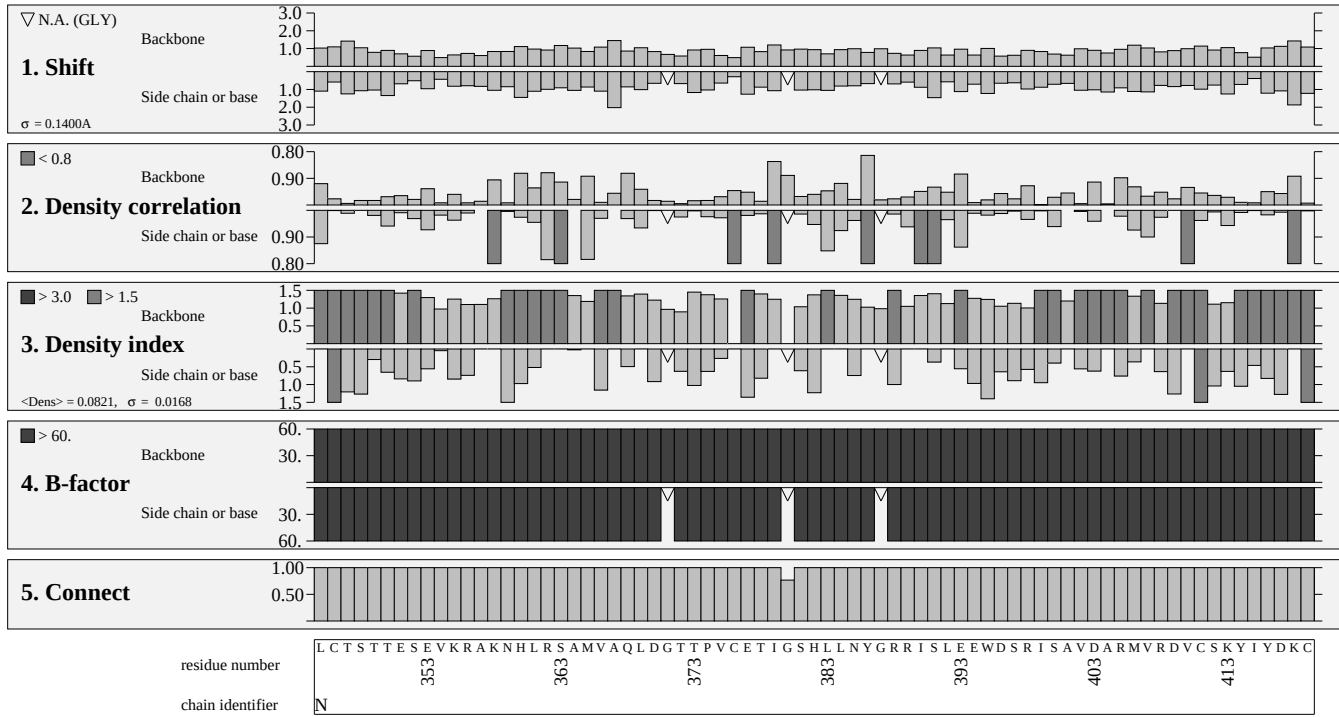
Local estimation (16)



Structure Factor Check

3H1H

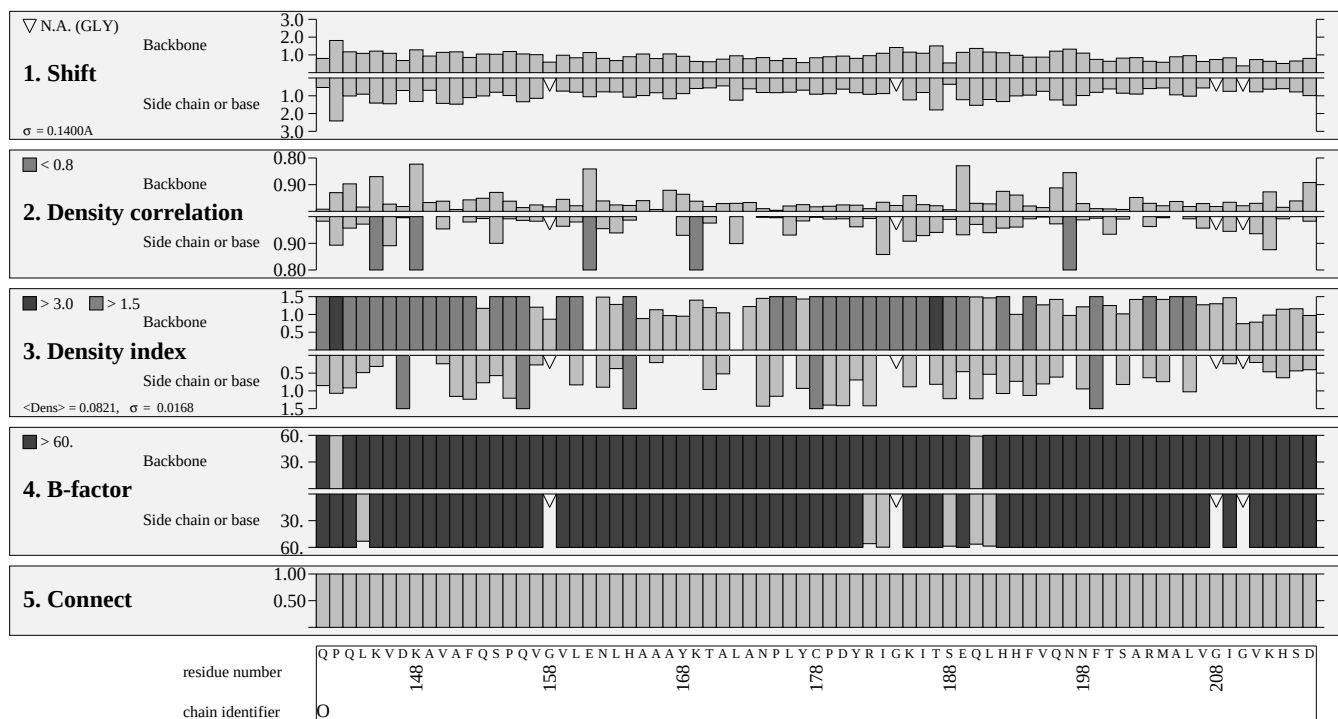
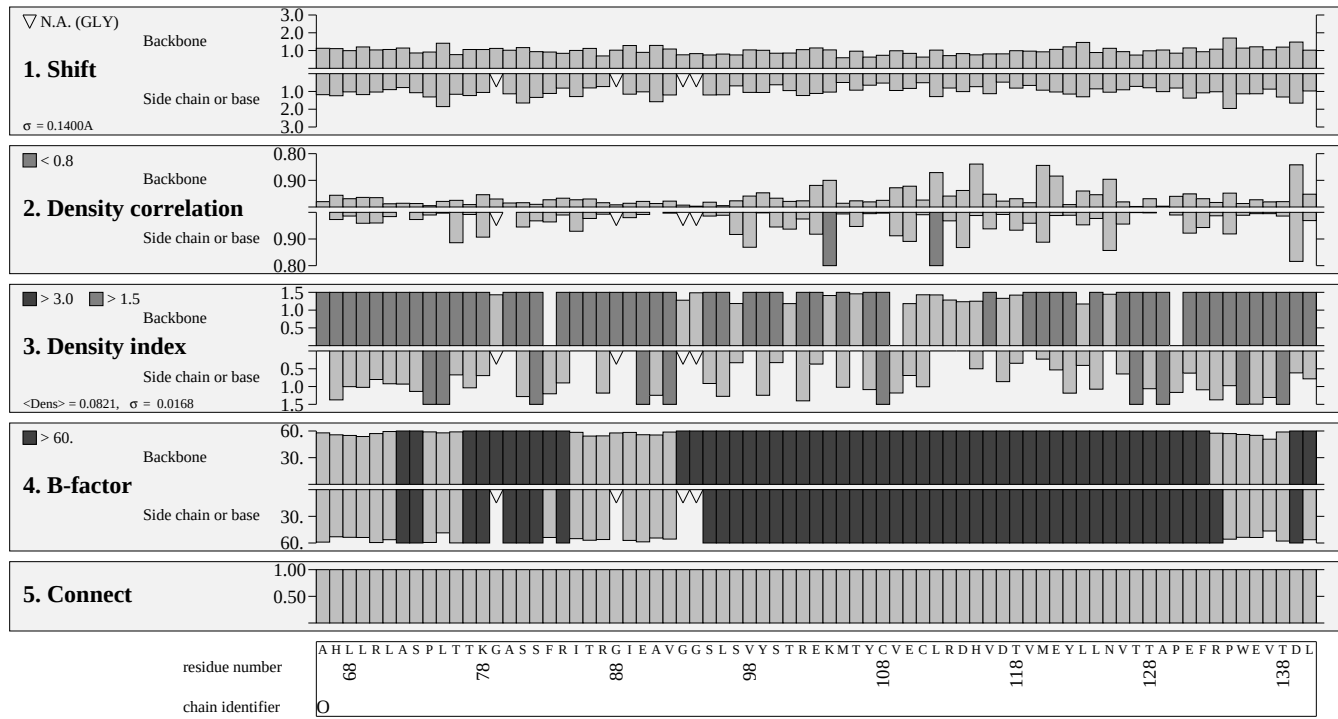
Local estimation (17)



Structure Factor Check

3H1H

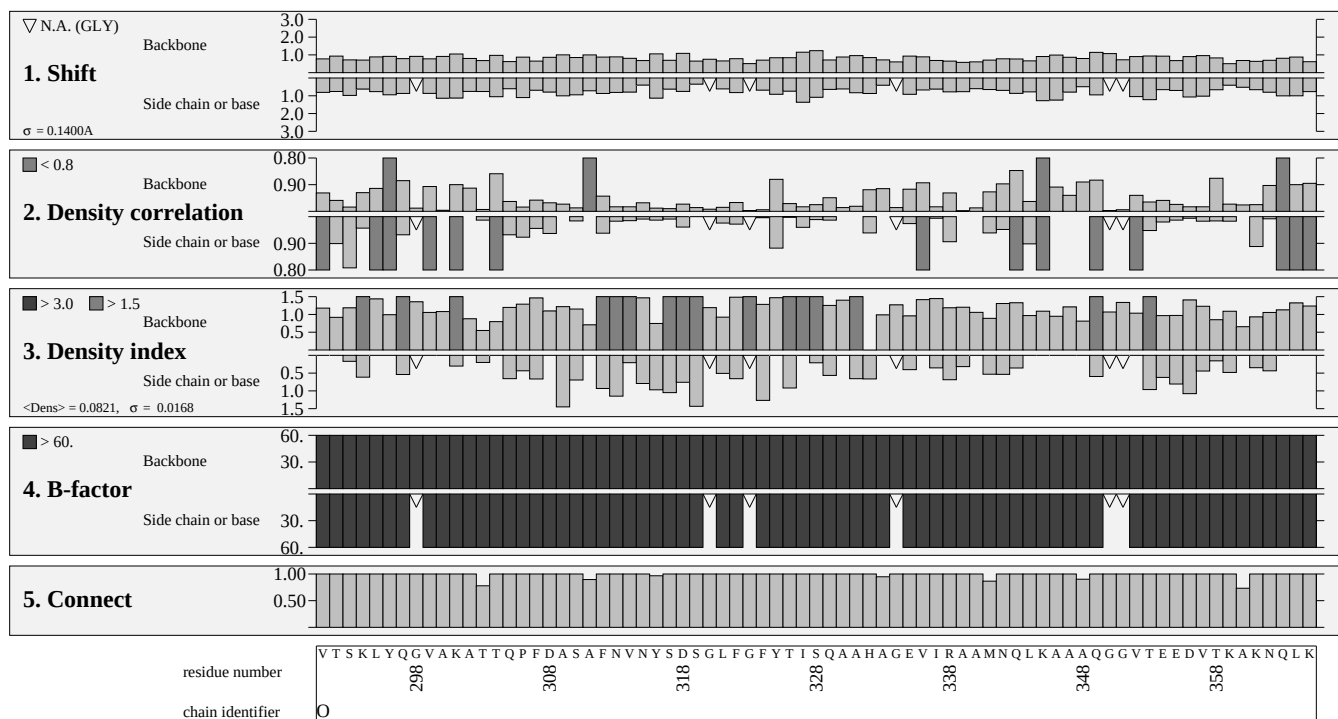
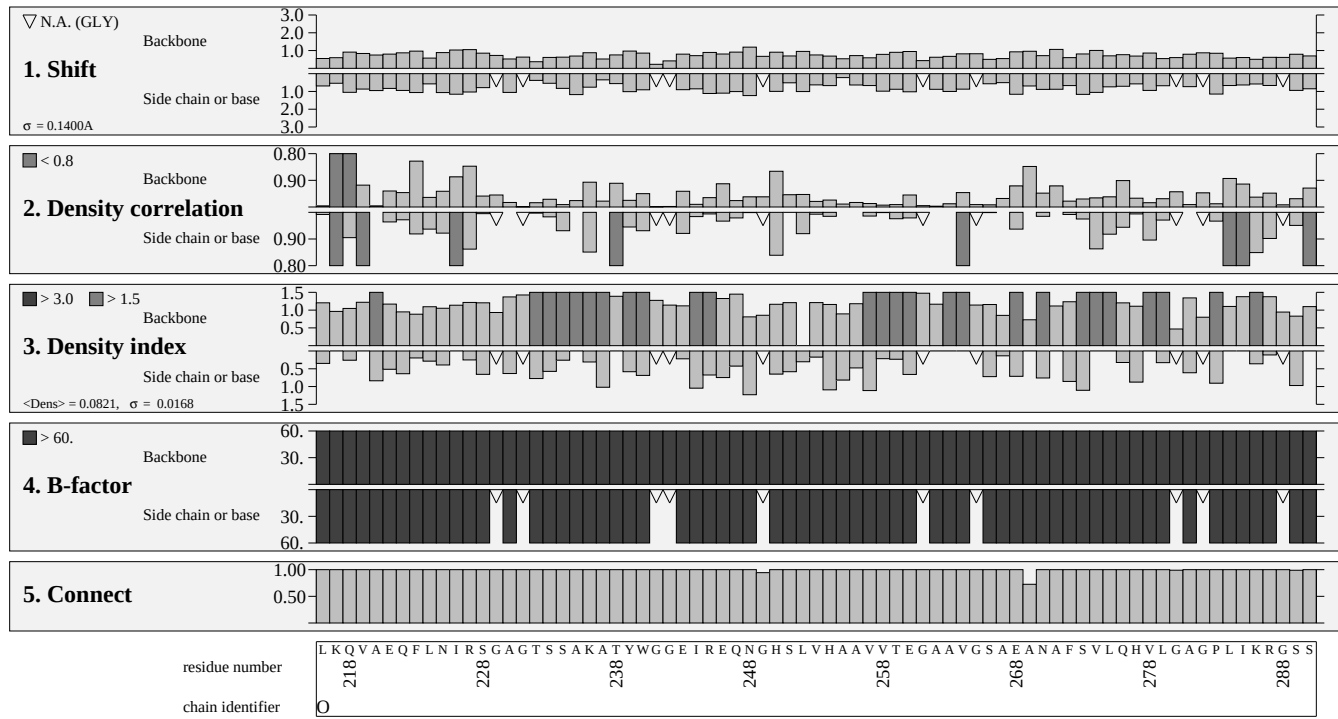
Local estimation (18)



Structure Factor Check

3H1H

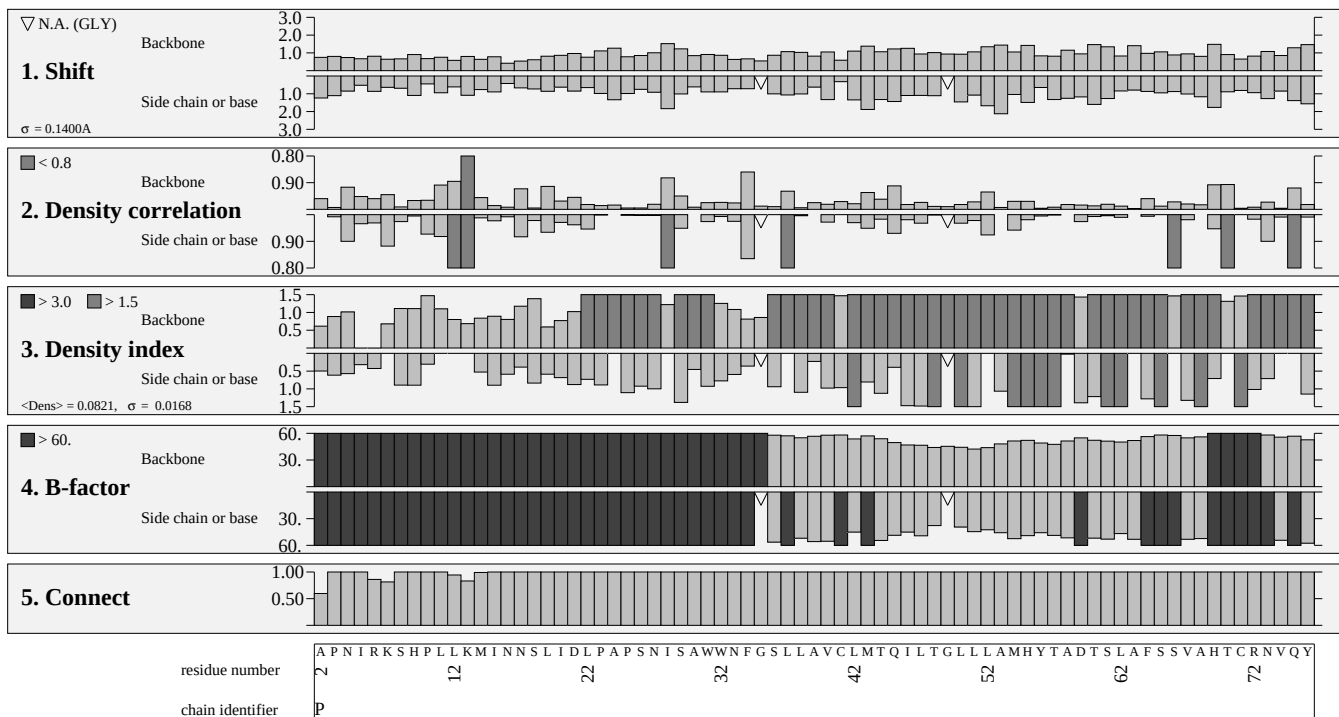
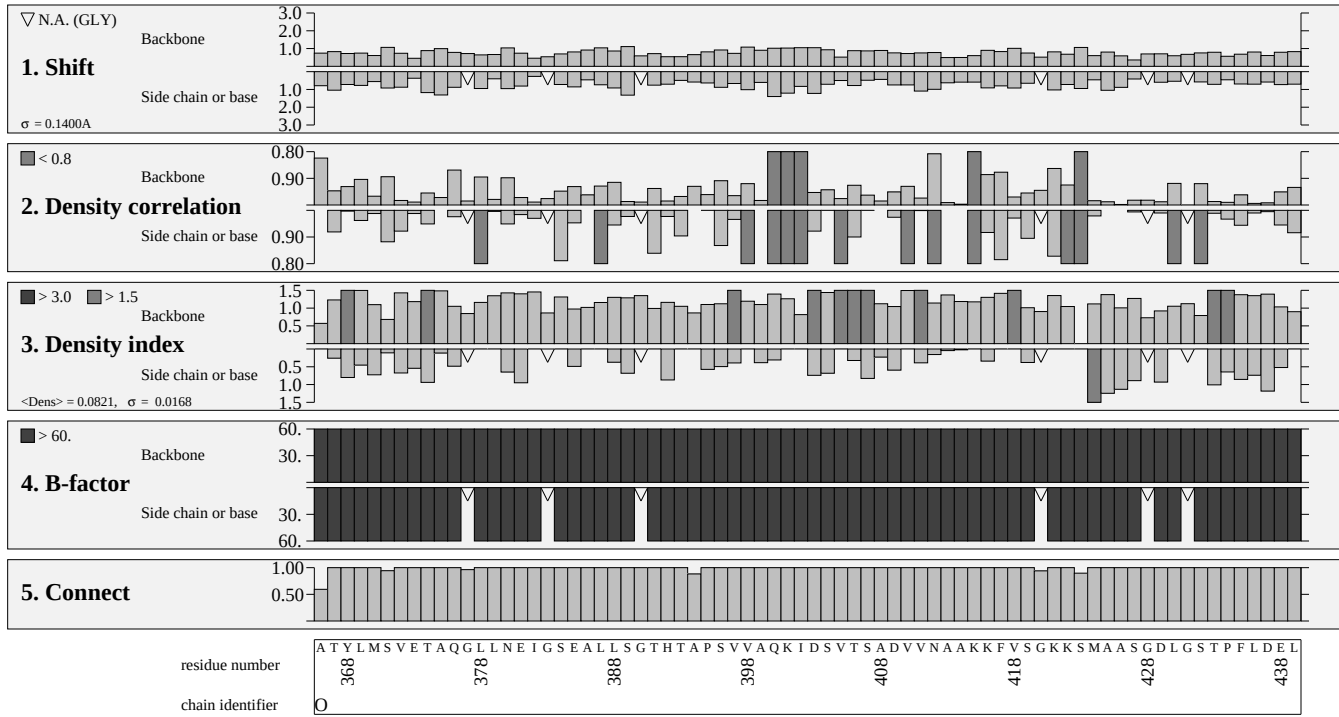
Local estimation (19)



Structure Factor Check

3H1H

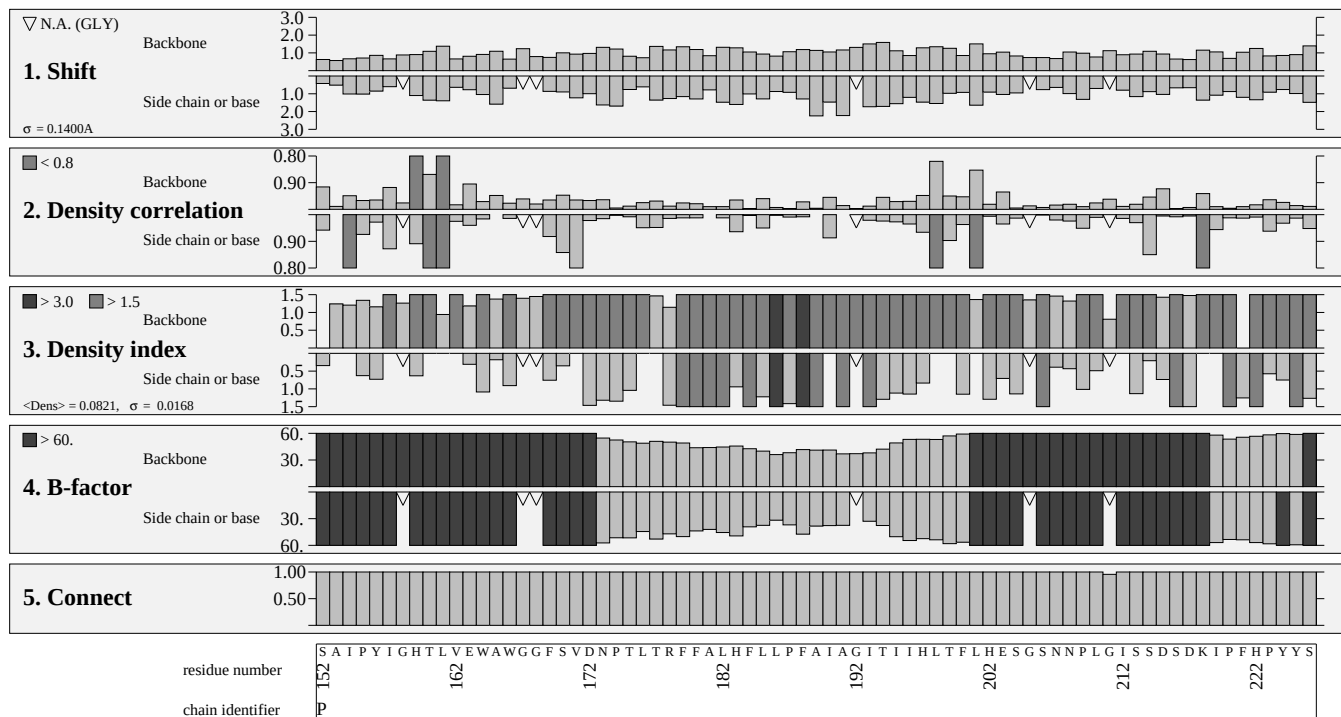
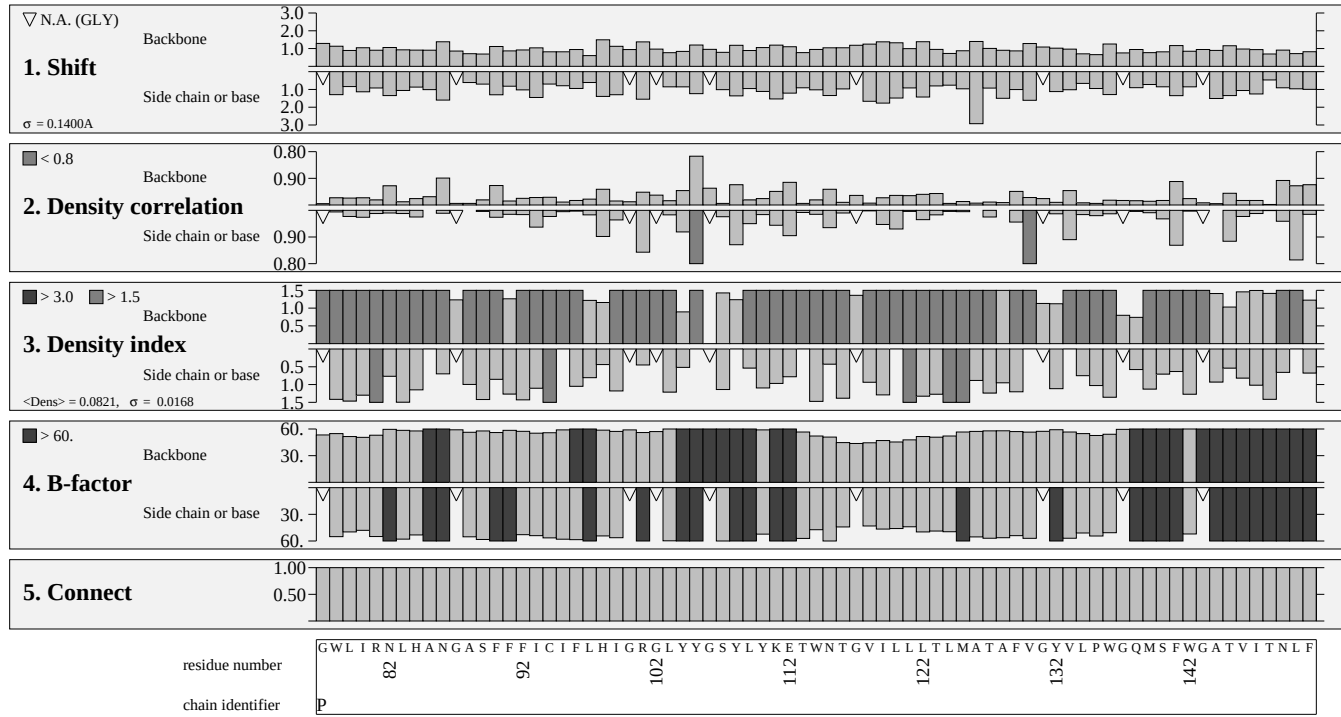
Local estimation (20)



Structure Factor Check

3H1H

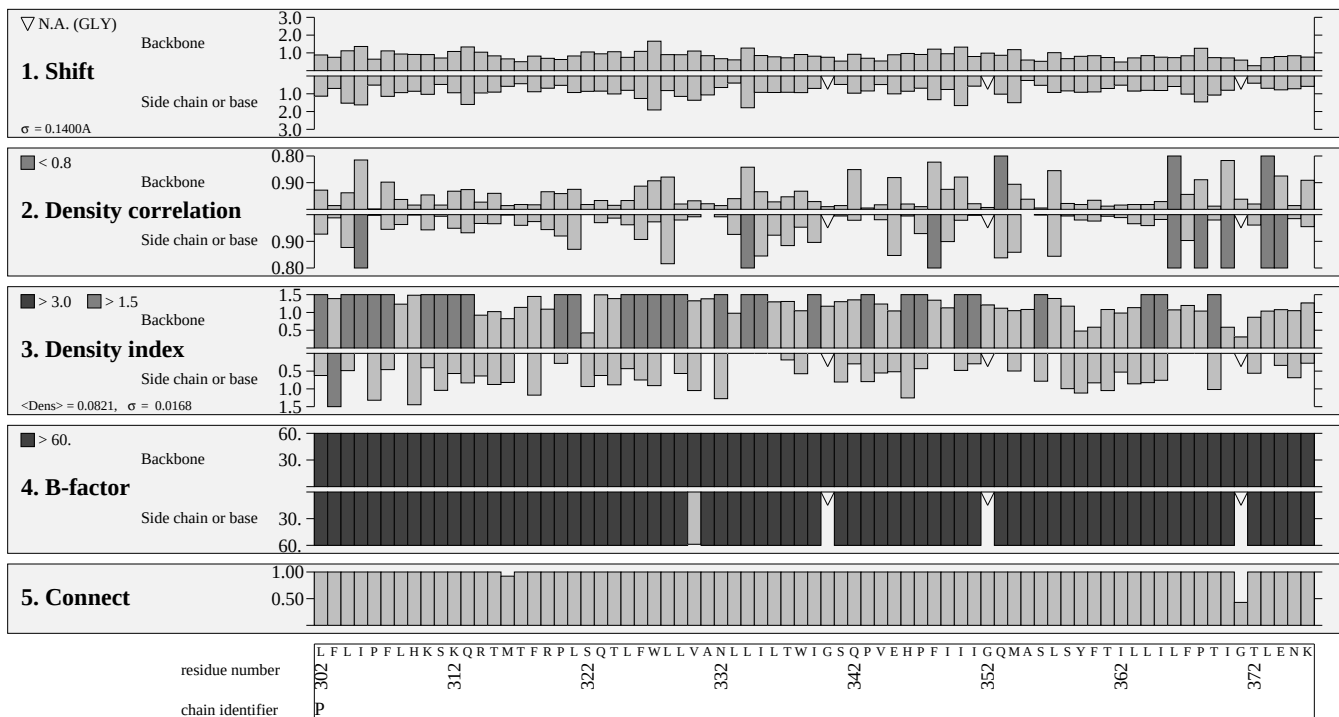
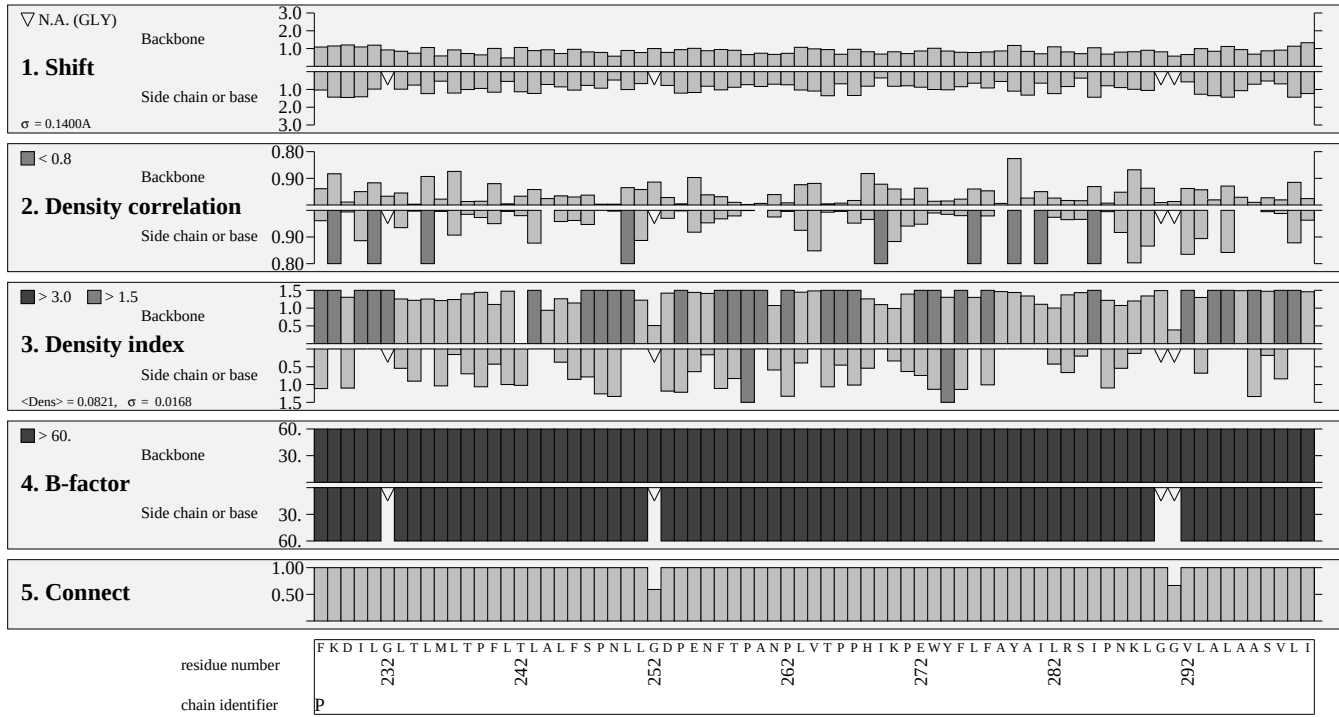
Local estimation (21)



Structure Factor Check

3H1H

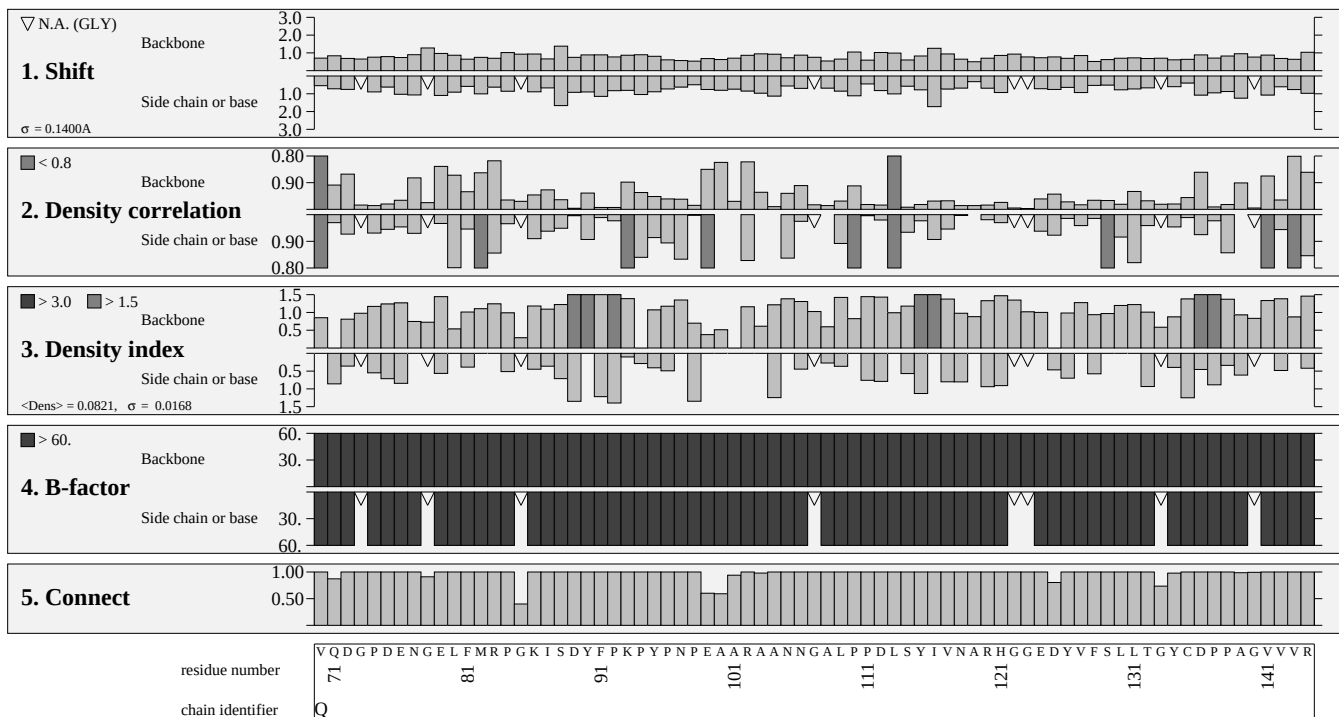
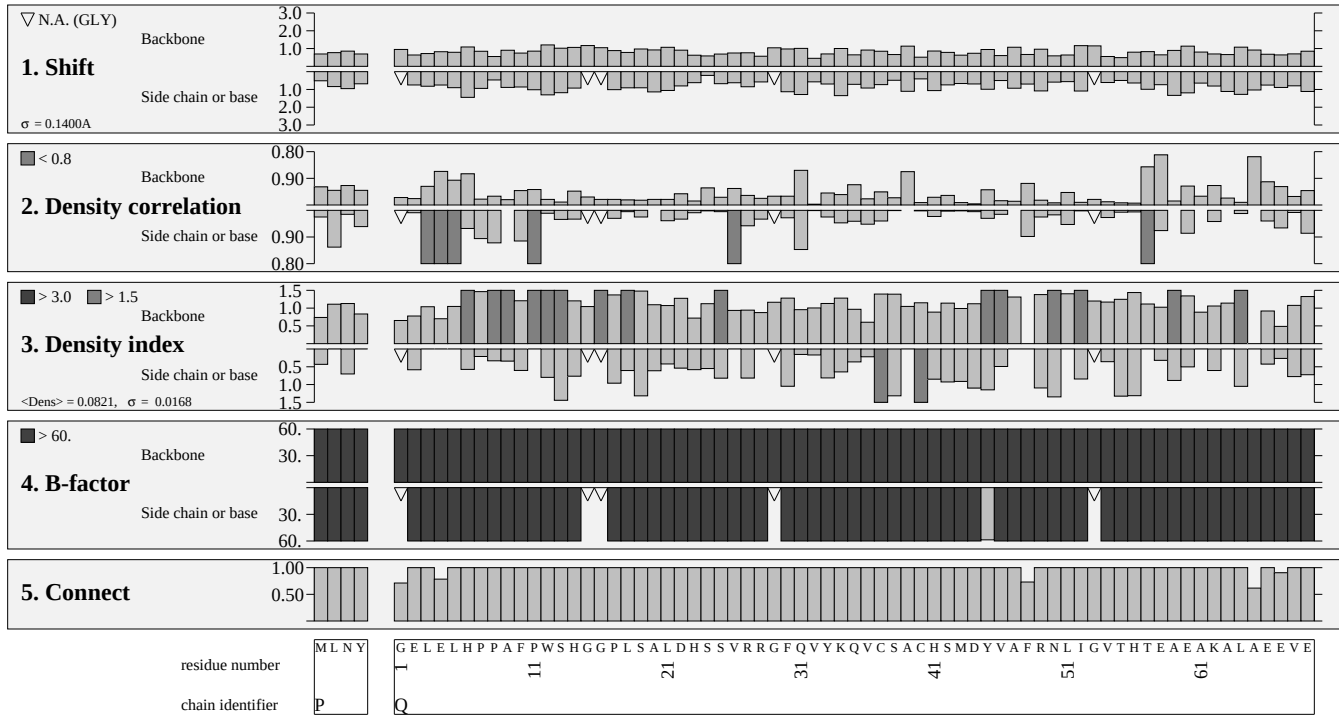
Local estimation (22)



Structure Factor Check

3H1H

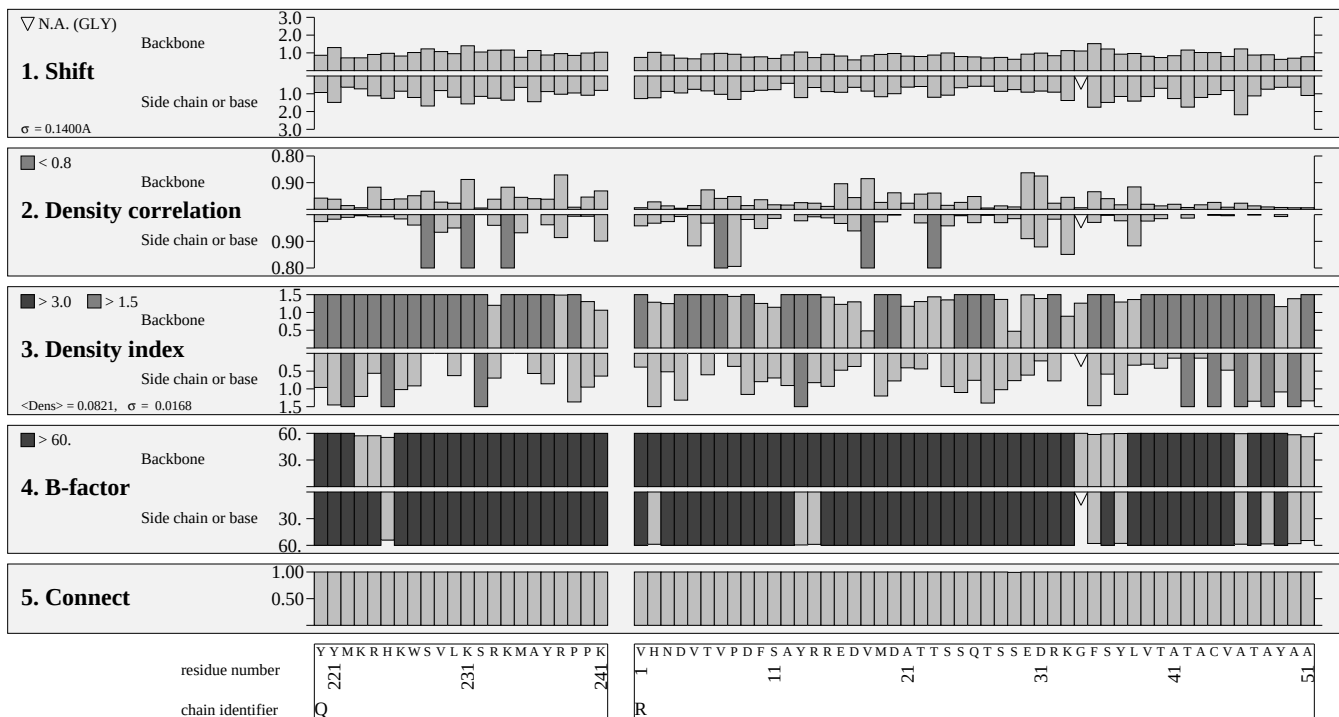
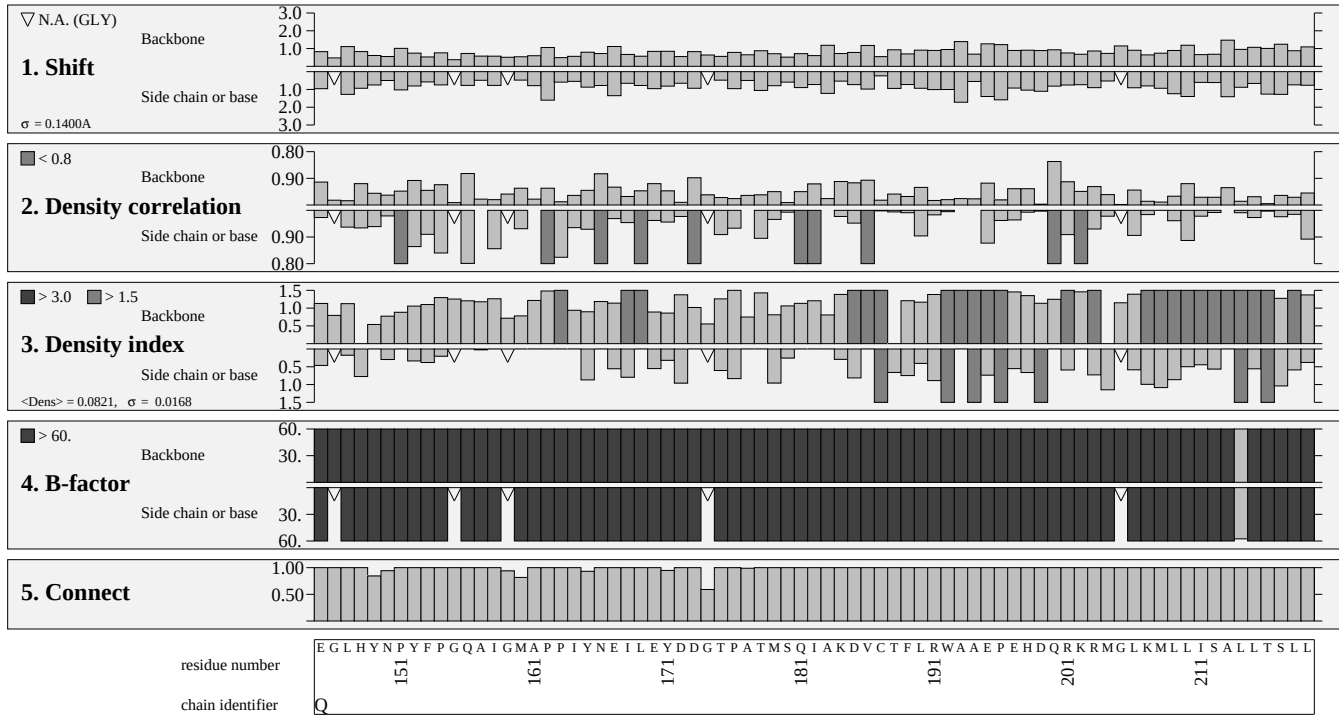
Local estimation (23)



Structure Factor Check

3H1H

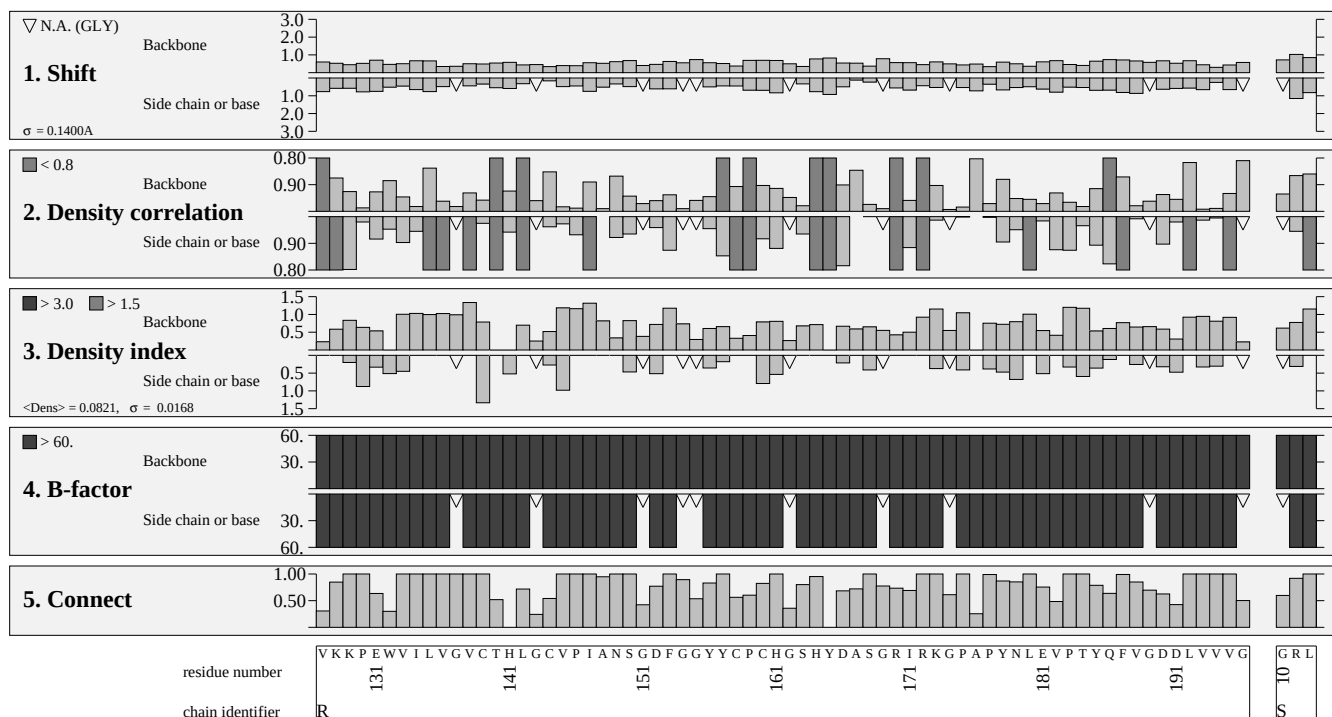
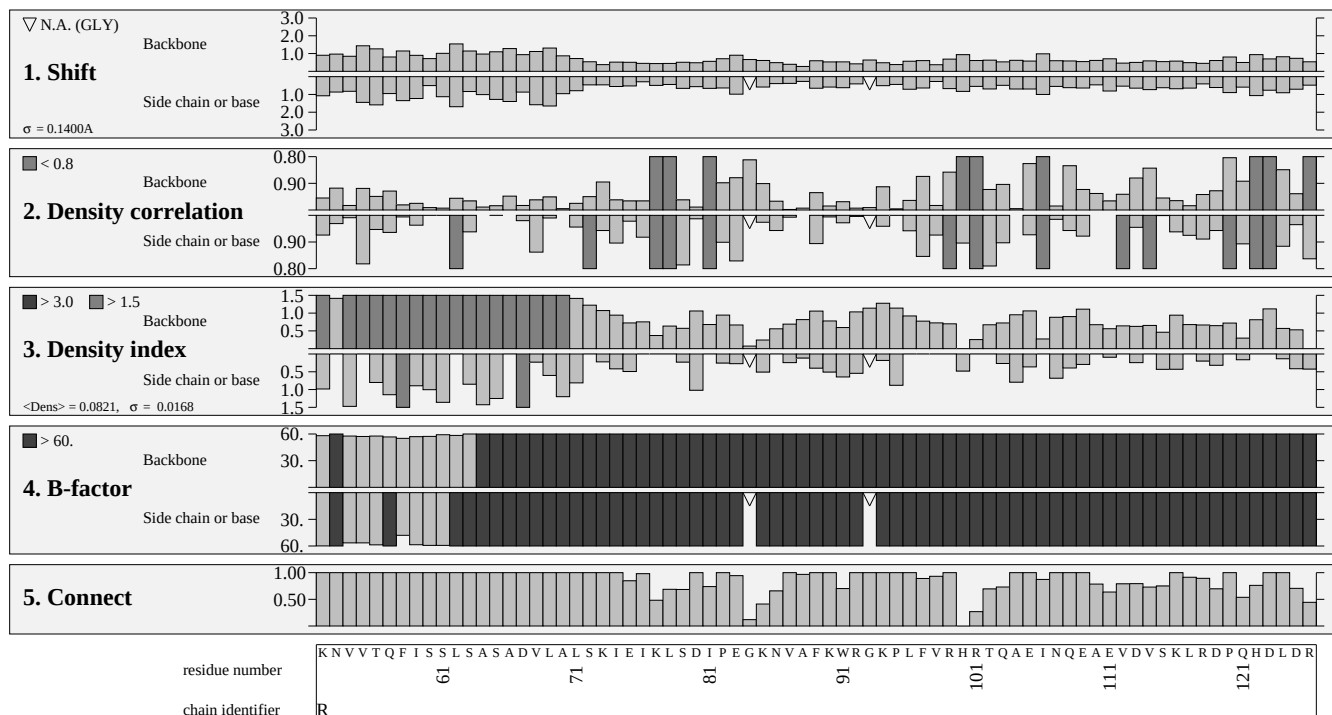
Local estimation (24)



Structure Factor Check

3H1H

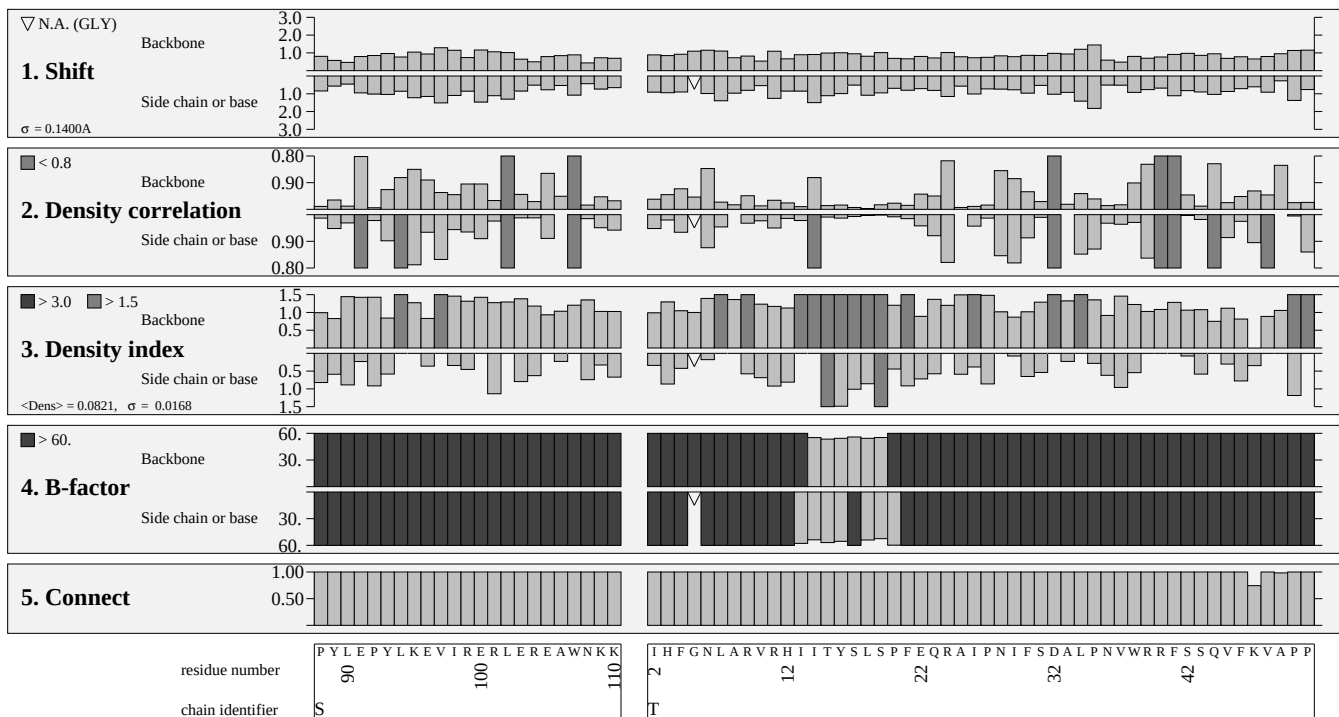
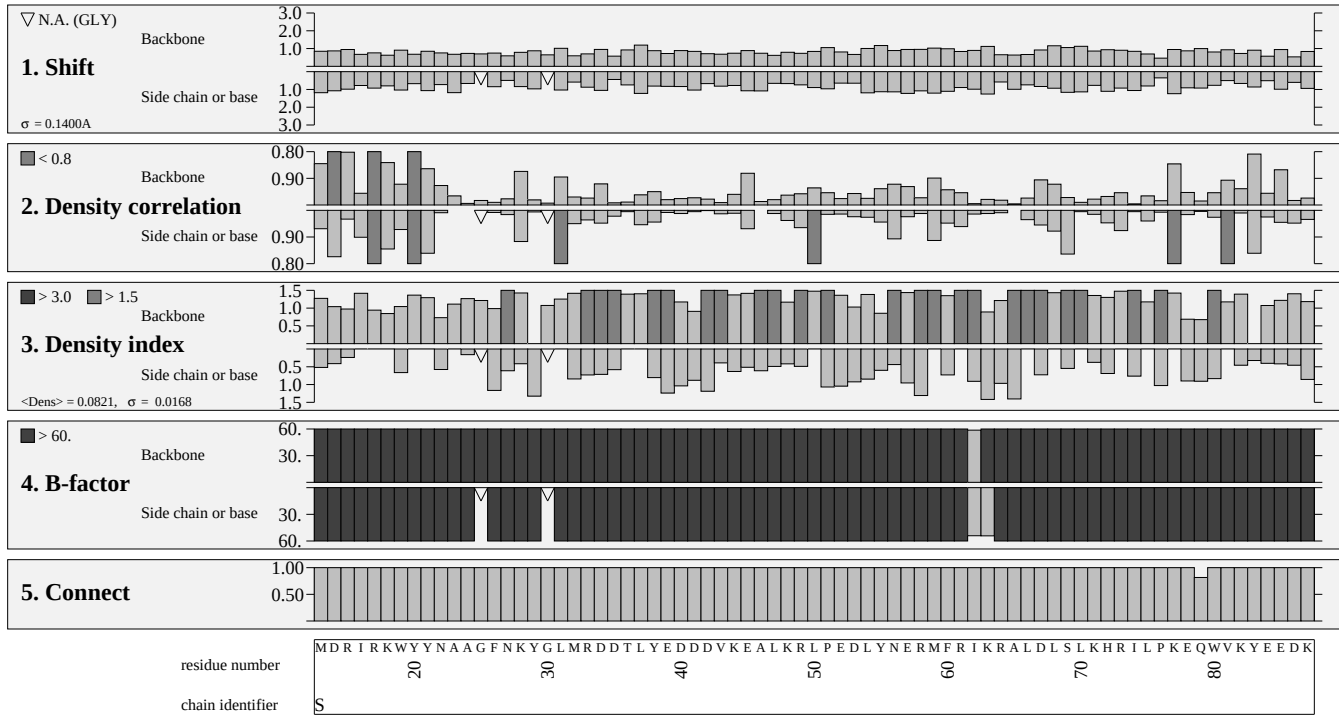
Local estimation (25)



Structure Factor Check

3H1H

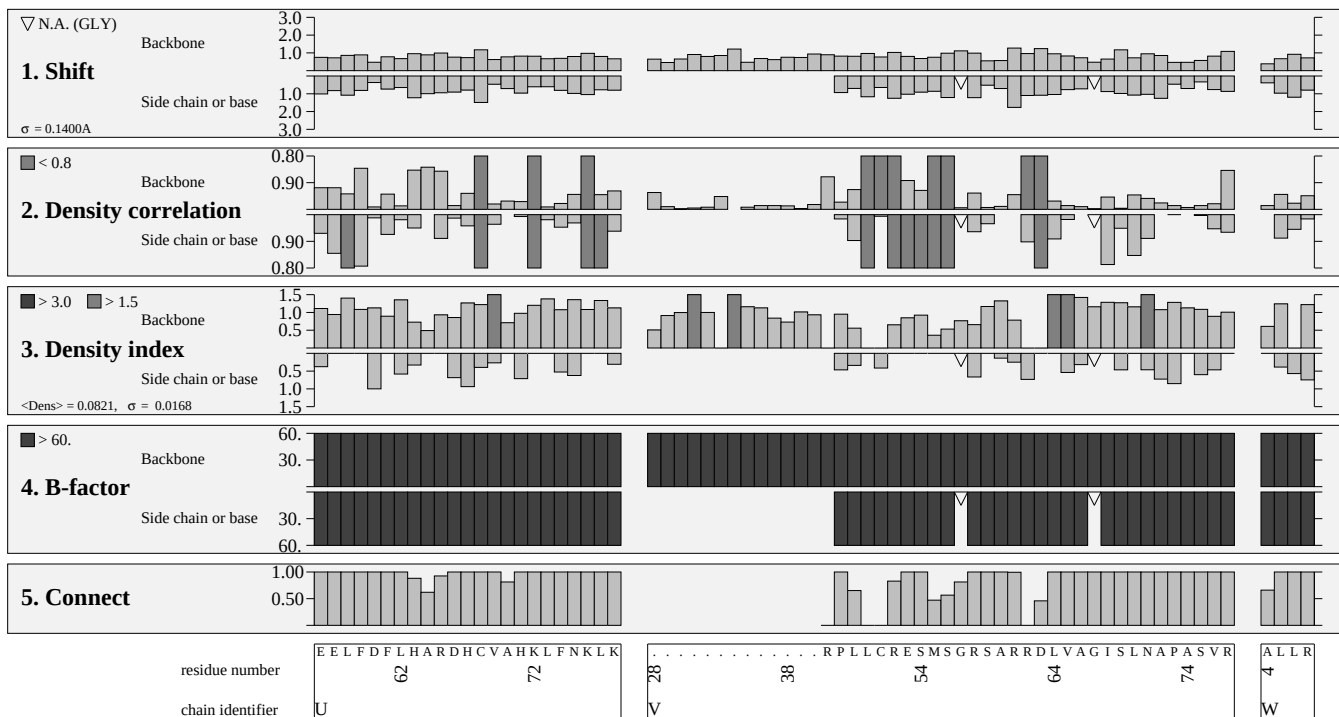
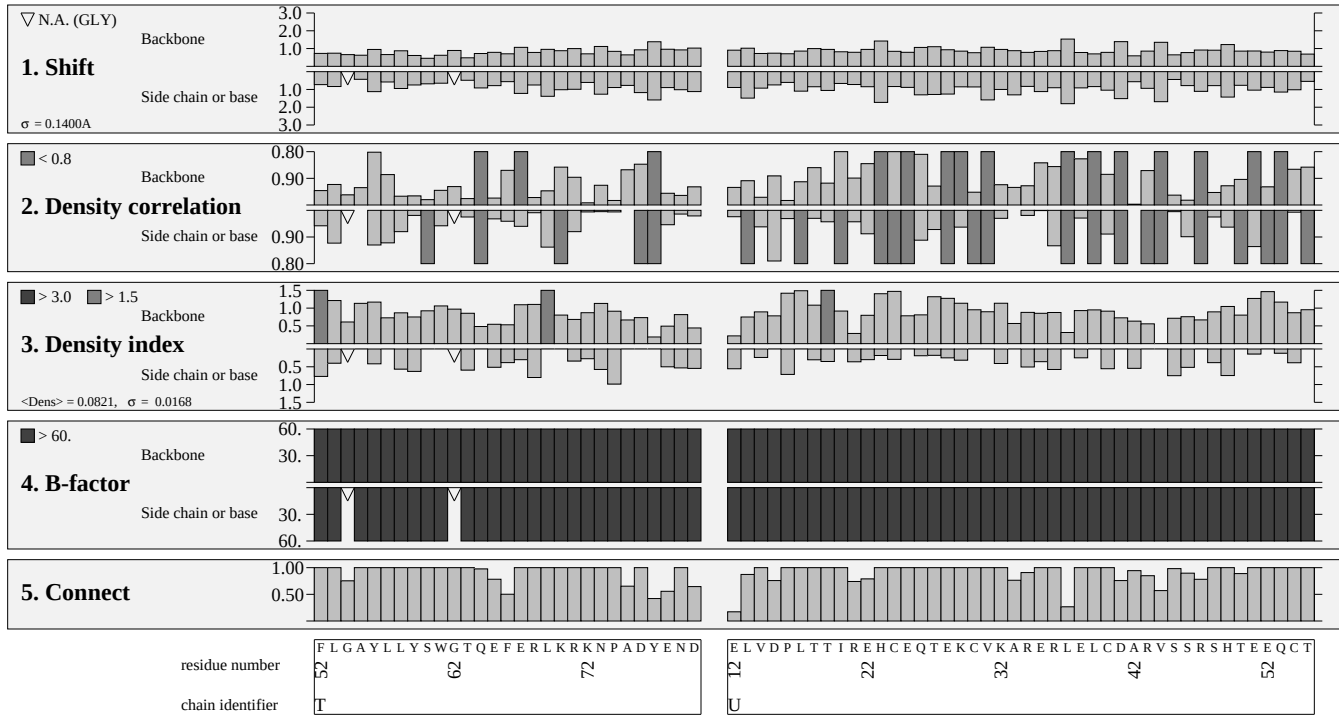
Local estimation (26)



Structure Factor Check

3H1H

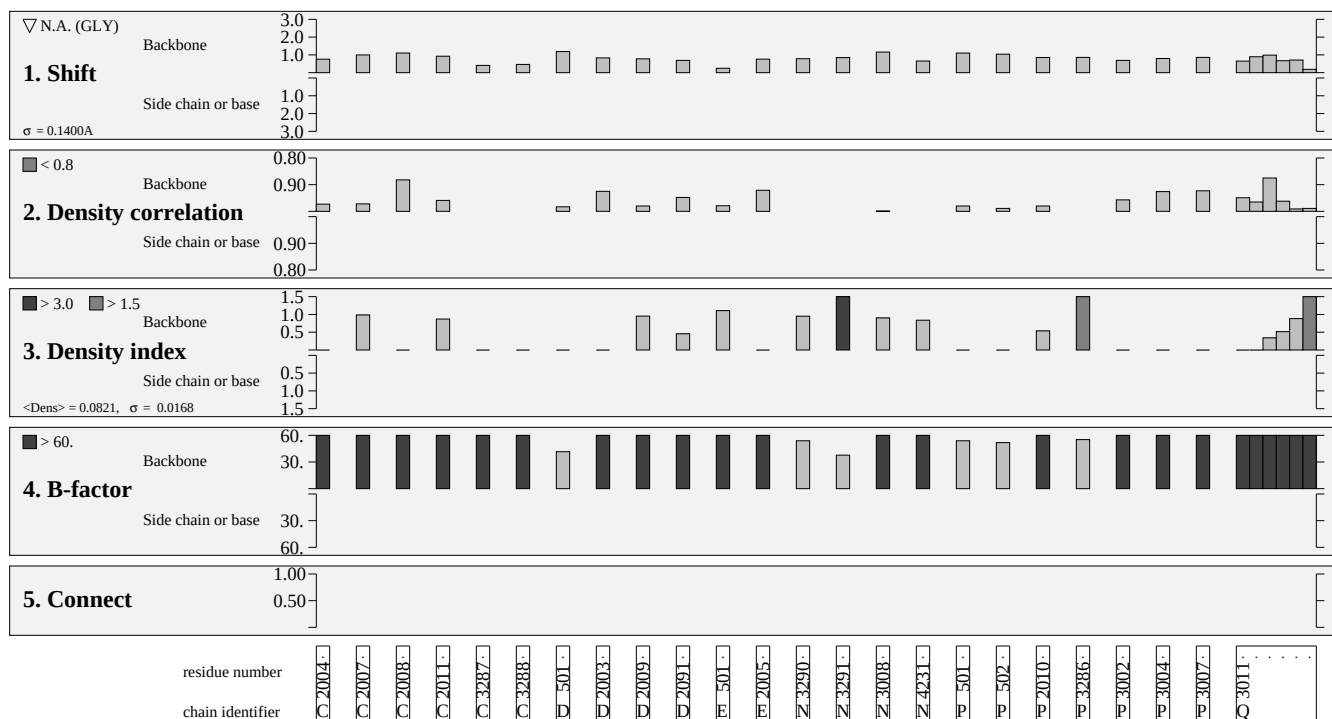
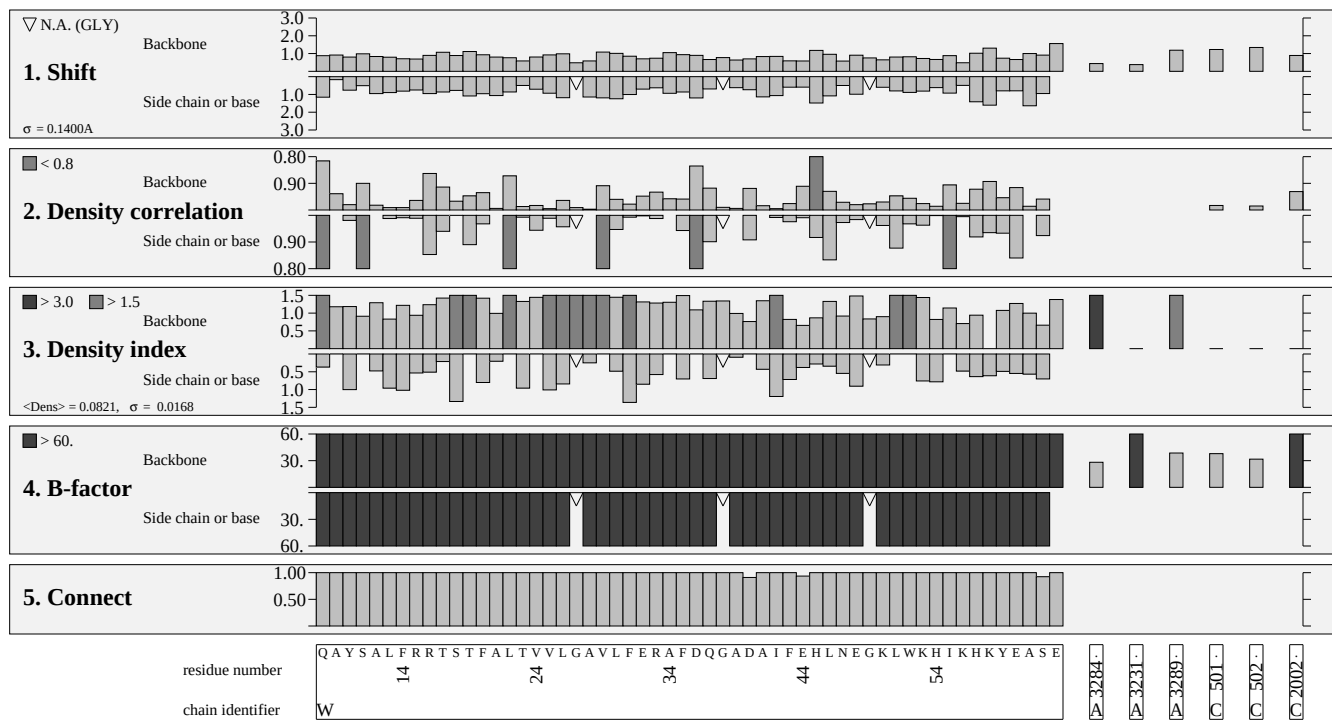
Local estimation (27)



Structure Factor Check

3H1H

Local estimation (28)



Local estimation (29)



chain identifier

384 385