

Structure Factor Check

3CWB

Title: CHICKEN CYTOCHROME BC1 COMPLEX INHIBITED BY AN IODINATED ANA
THE POLYKETIDE CROCACIN-D
Date: 21-APR-08
PDB code: 3CWB

Crystal

Cell parameters:

a: 174.78 Å b: 182.66 Å c: 242.95 Å
α: 90.00 β: 90.00 γ: 90.00

Space group: P 21 21 21

Model

32696 atoms (16 water molecules)

Number of chains: 51

Volume not occupied by model: 62.8 %

 (for atomic model): 83.3 Å²

σ(B): 19.48 Å²

Matthews coefficient: 4.24

Corresponding solvent % : 70.74

Refinement

Program: CNS 1.1

Nominal resolution range: 22.0 – 3.51 Å

Reported R-factor: 0.285

Number of reflections used: 96135

Reported Rfree: 0.32

Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 44.9 – 3.51 Å

Reflections in file: 96516

Unique reflections above 0: 96516

above 1σ: 93637

above 3σ: 54723

SFCHECK

Nominal resolution range: 44.9 – 3.51 Å

\05max. from input data, min. from author\05

Used reflections: 96514

Reflections out of resolution: 2

Completeness: 98.9 %

R_stand(F) = <σ(F)>/<F> : 0.102

Anisotropic distribution of Structure Factors

ratio of eigen values: 1.0000 0.5074 0.7172

B_overall (by Patterson): 62.Å²

Optical resolution: 2.51 Å

Expected opt. resol. for complete data set: 2.51 Å

Estimated minimal error: 0.180 Å

Model vs. Structure Factors

R-factor for all reflections: 0.352

Correlation factor: 0.752

R-factor: 0.347

for F > 2.0 σ

nom. resolution range: 21.98 – 3.51 Å

reflections used: 93278

Rfree: 0.373

Nfree: 4749

R-factor without free-refl.: 0.345

Non free-reflections: 88529

<u> (error in coords by Luzzati plot): 0.796 Å

Estimated maximal error: 0.467 Å

DPI: 0.654 Å

Scaling

Scale: 0.877

Bdiff: -3.32

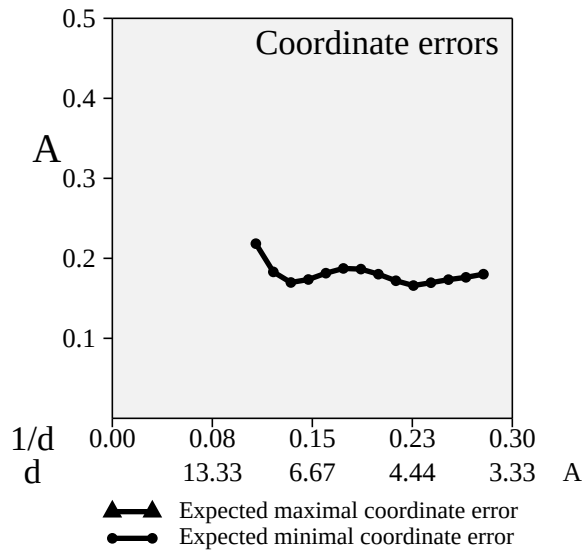
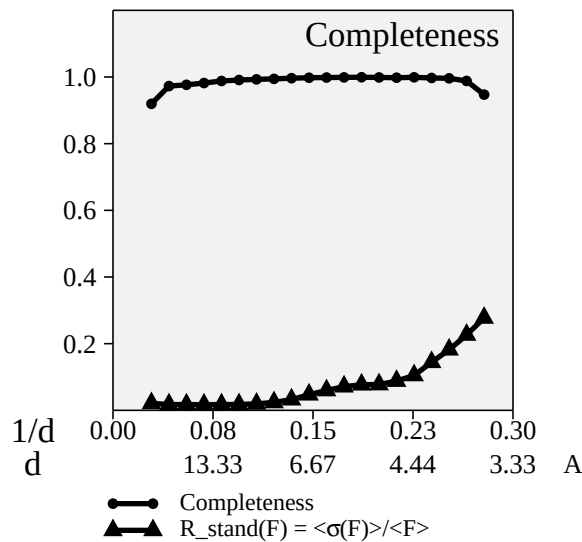
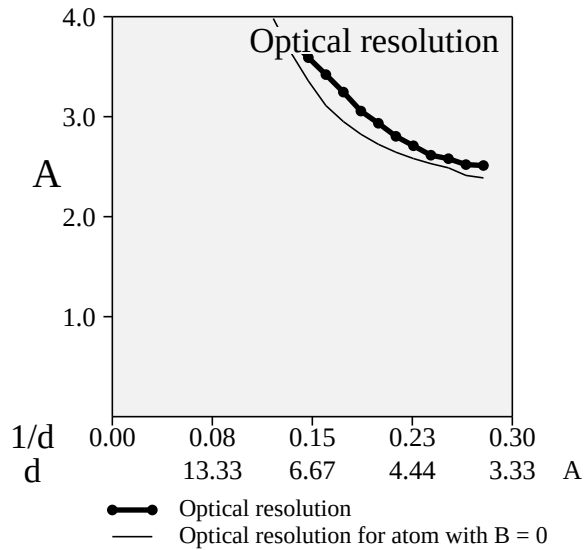
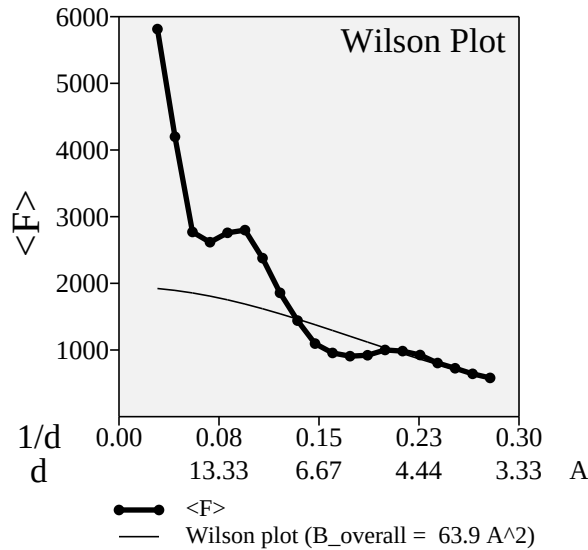
Anisothermal Scaling (Beta):

10.7163 -2.7174 4.6617 0.0000 0.0000 0.0000

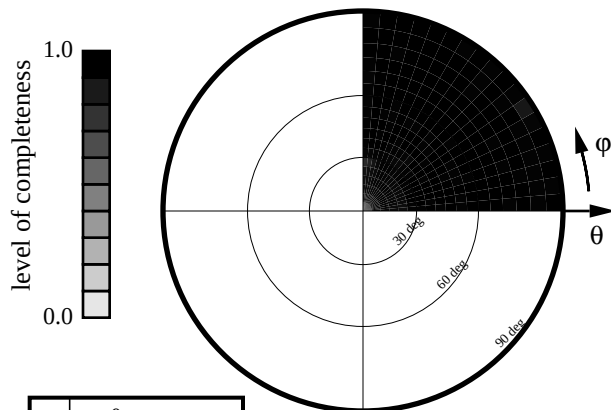
Solvent correction – Ks,Bs: 0.544 250.371

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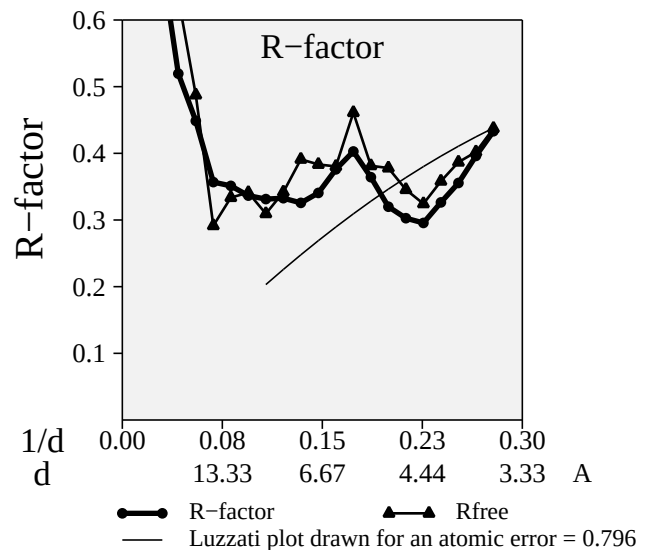


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

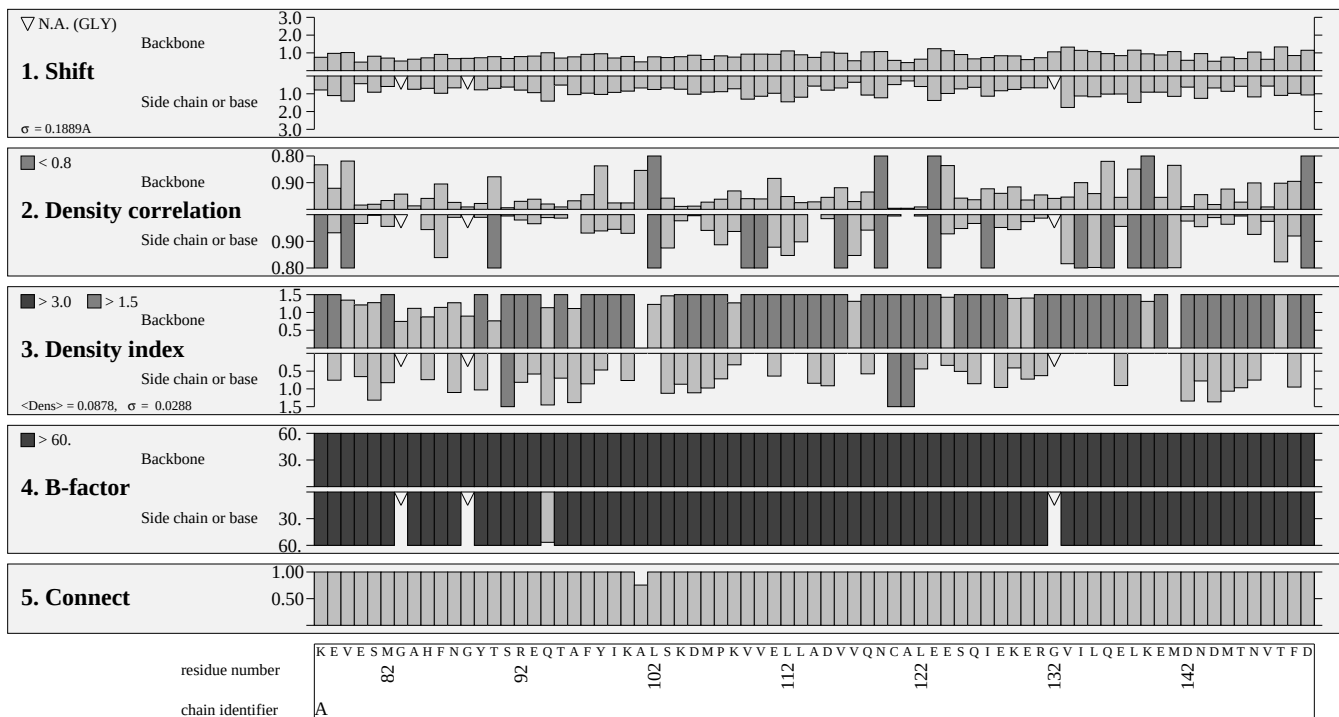
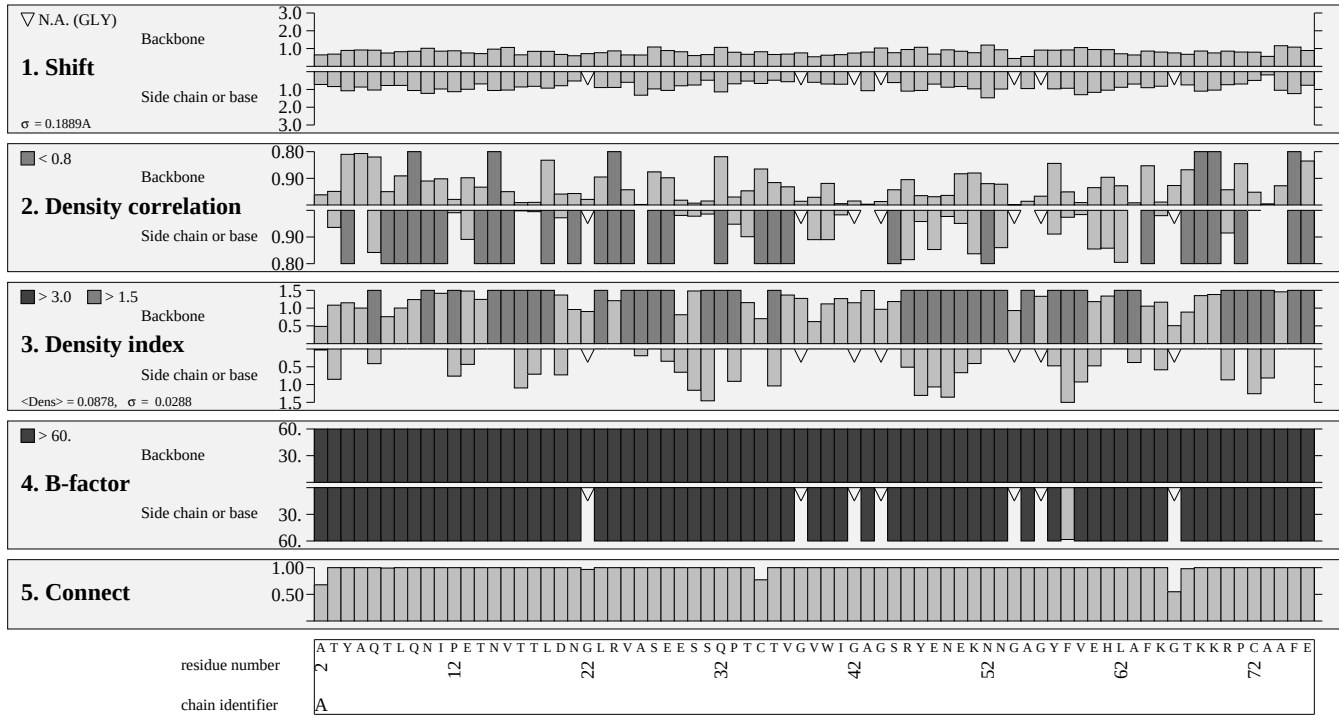
polar coordinates of the crystallographical axes



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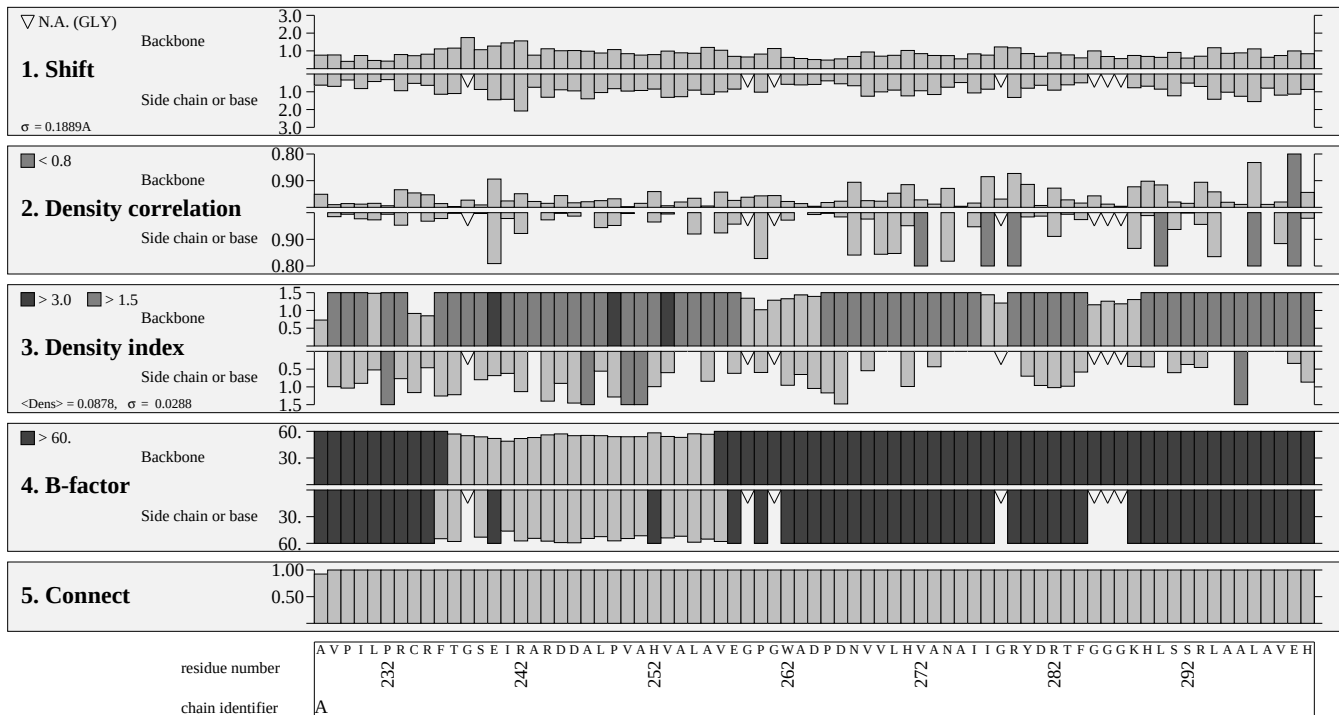
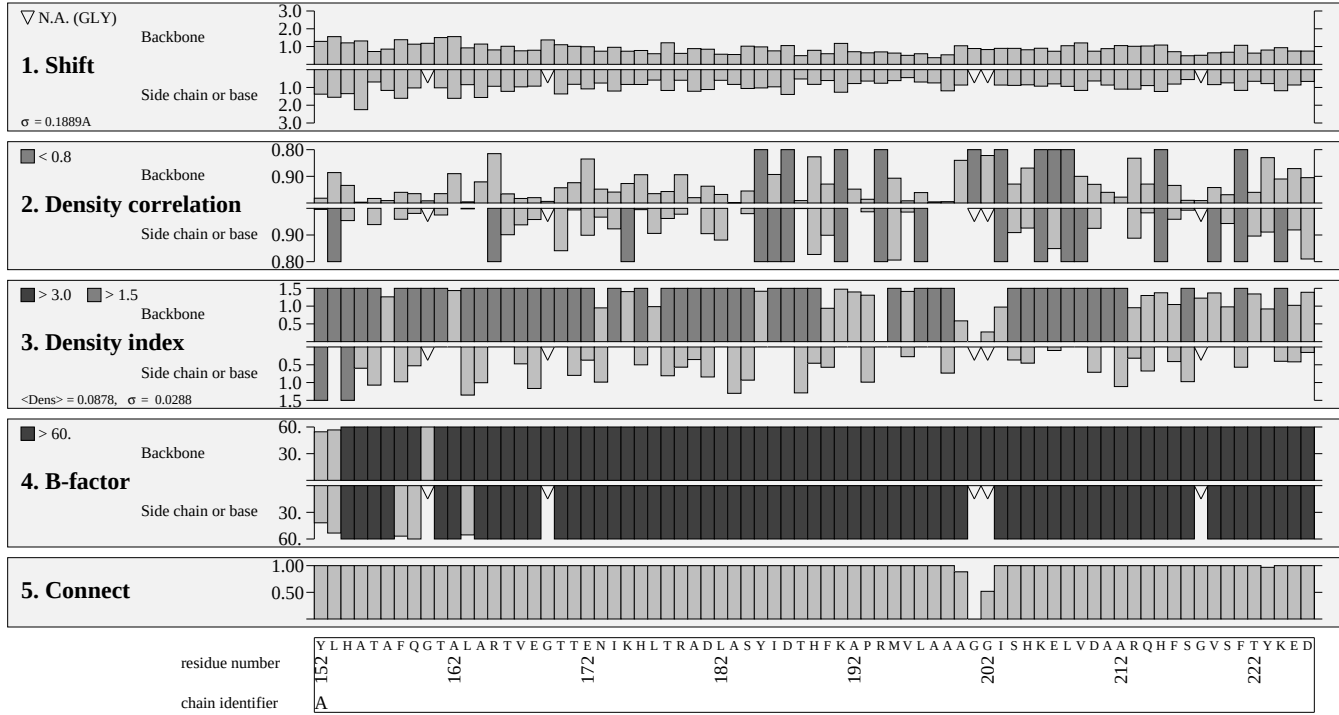
Local estimation



Structure Factor Check

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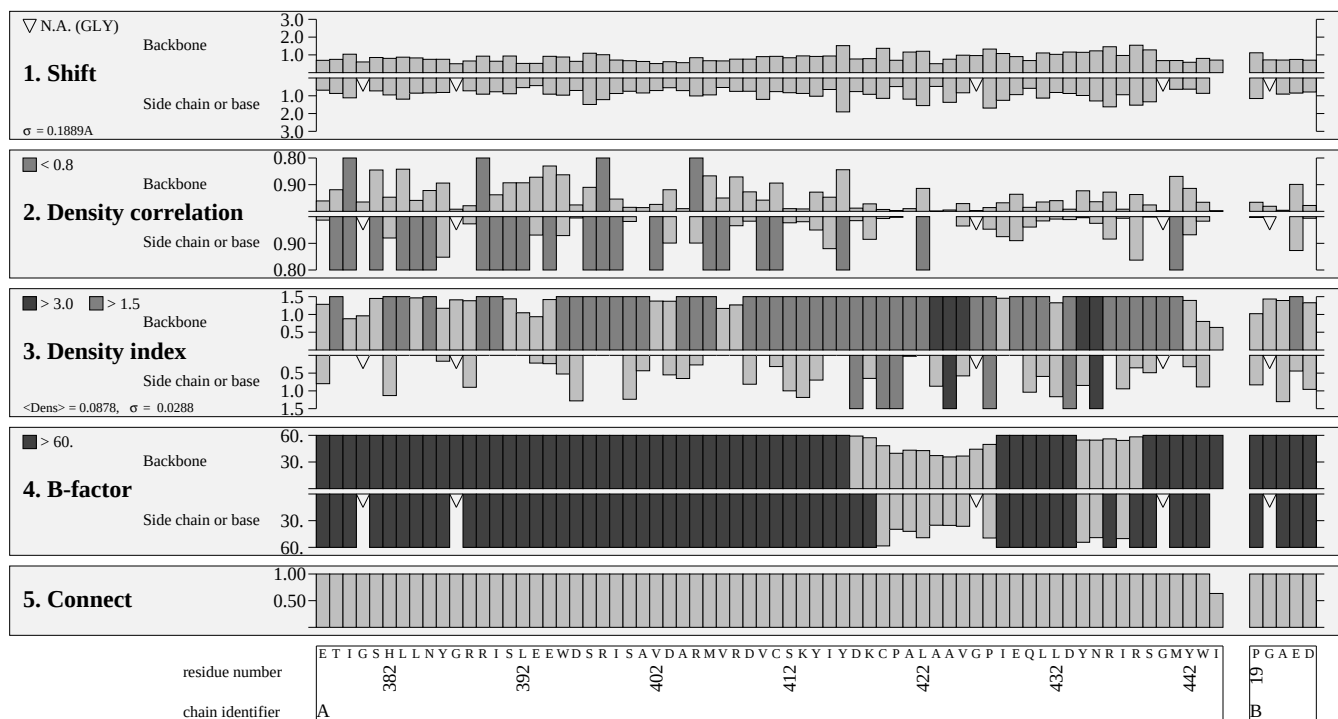
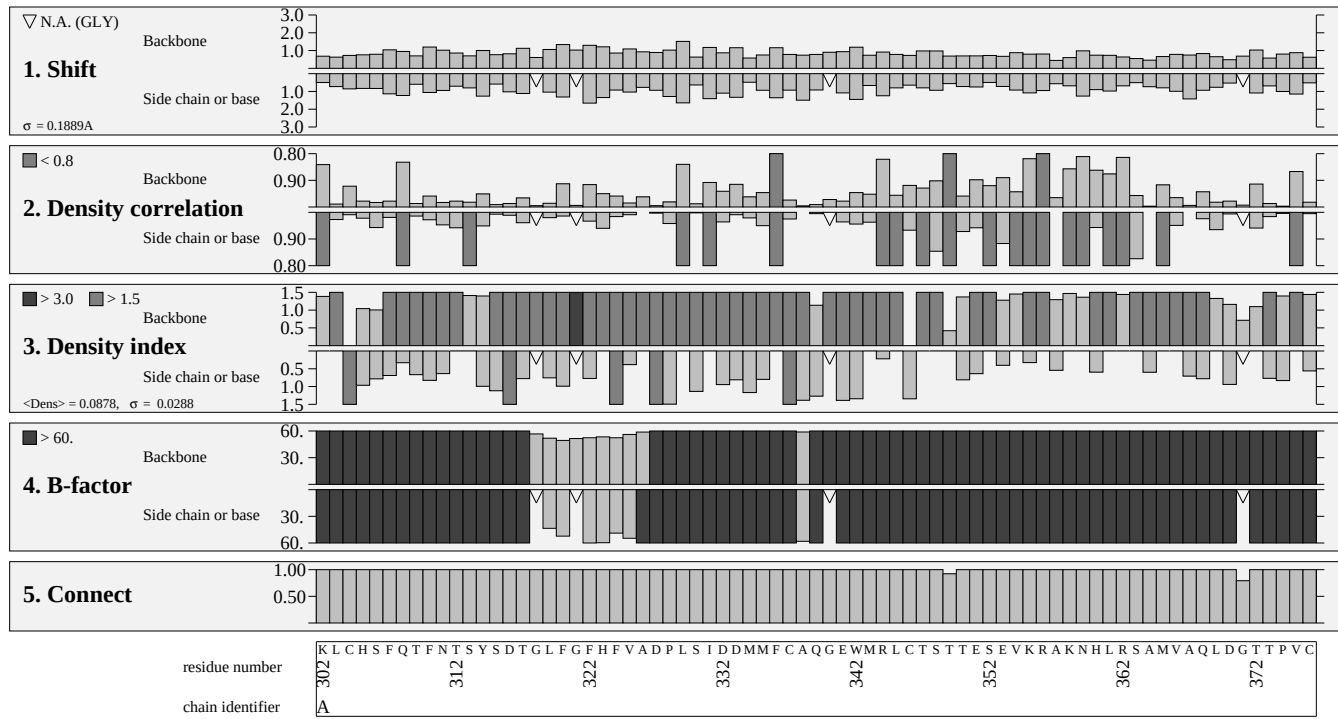
Local estimation (2)



Structure Factor Check

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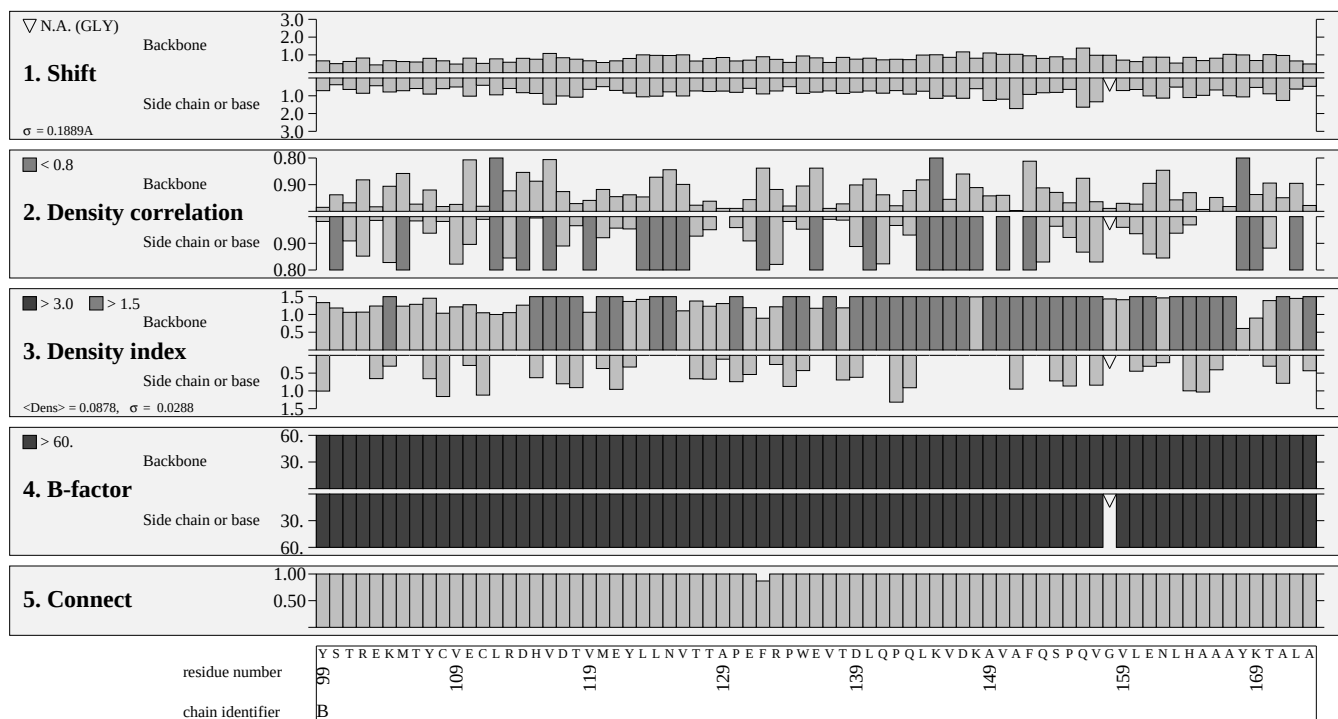
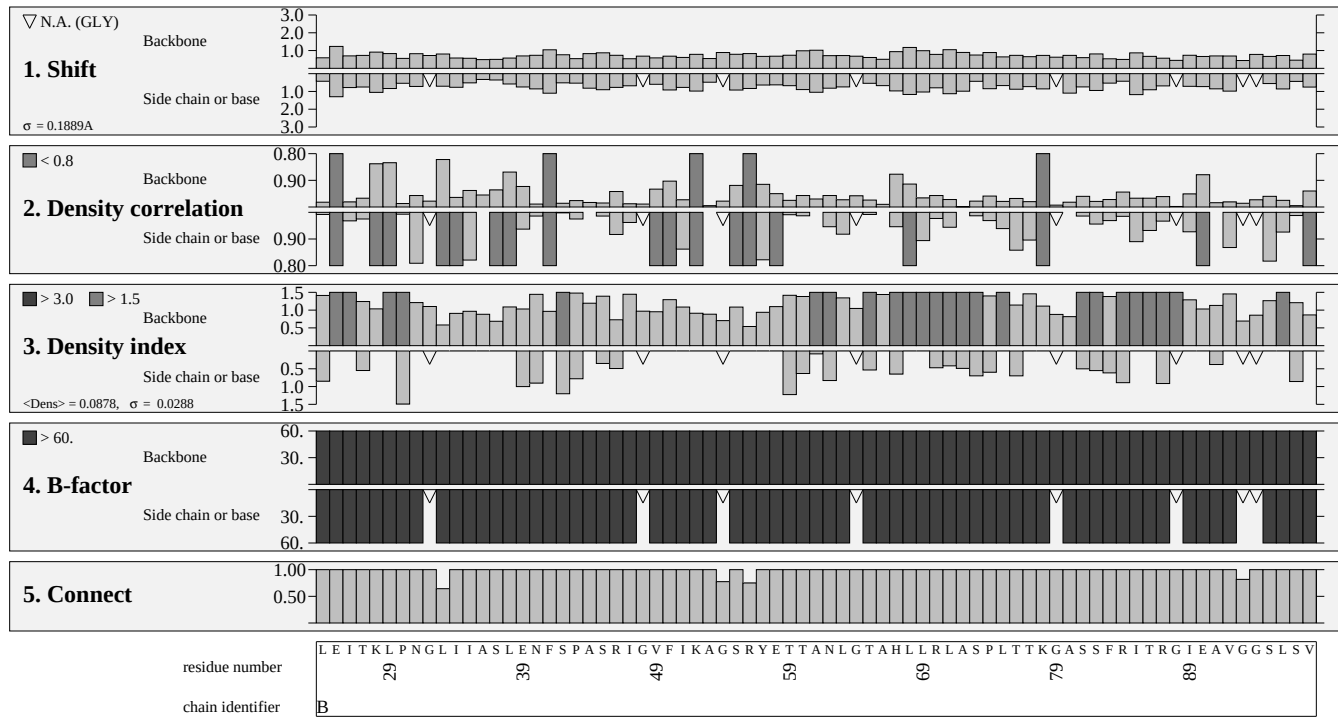
Local estimation (3)



Structure Factor Check

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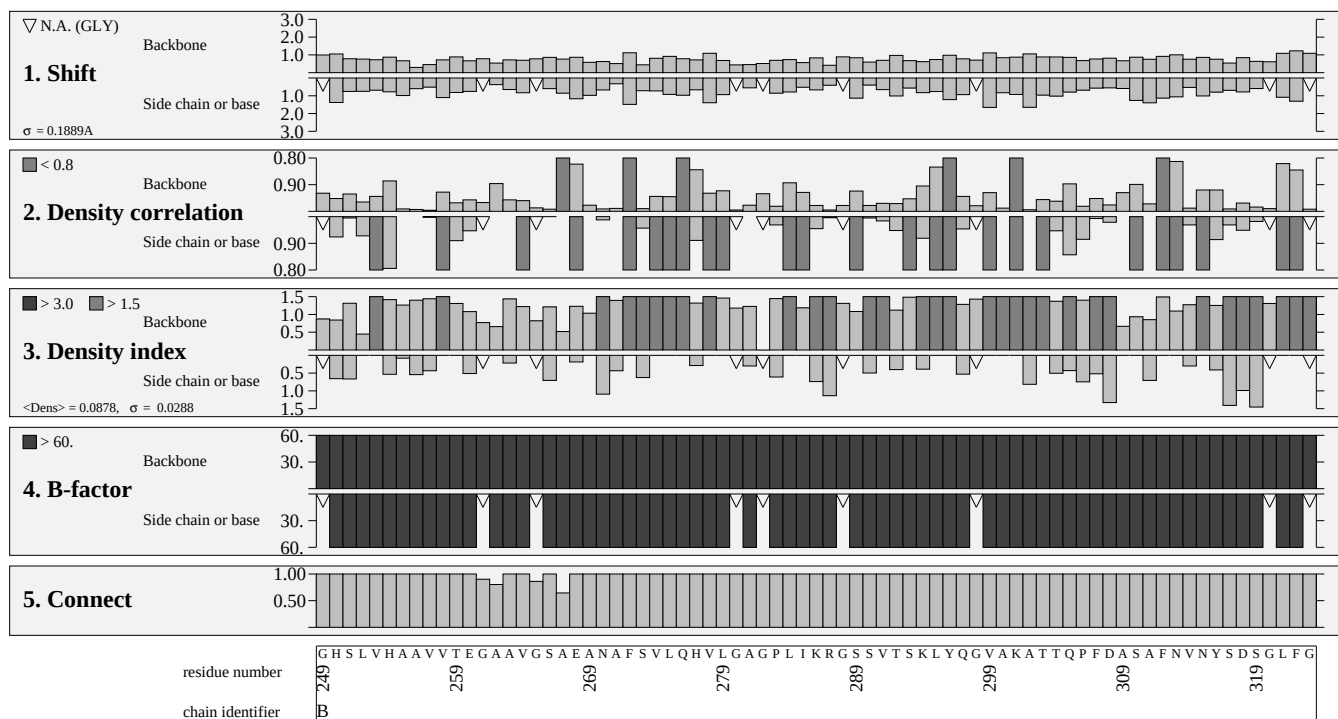
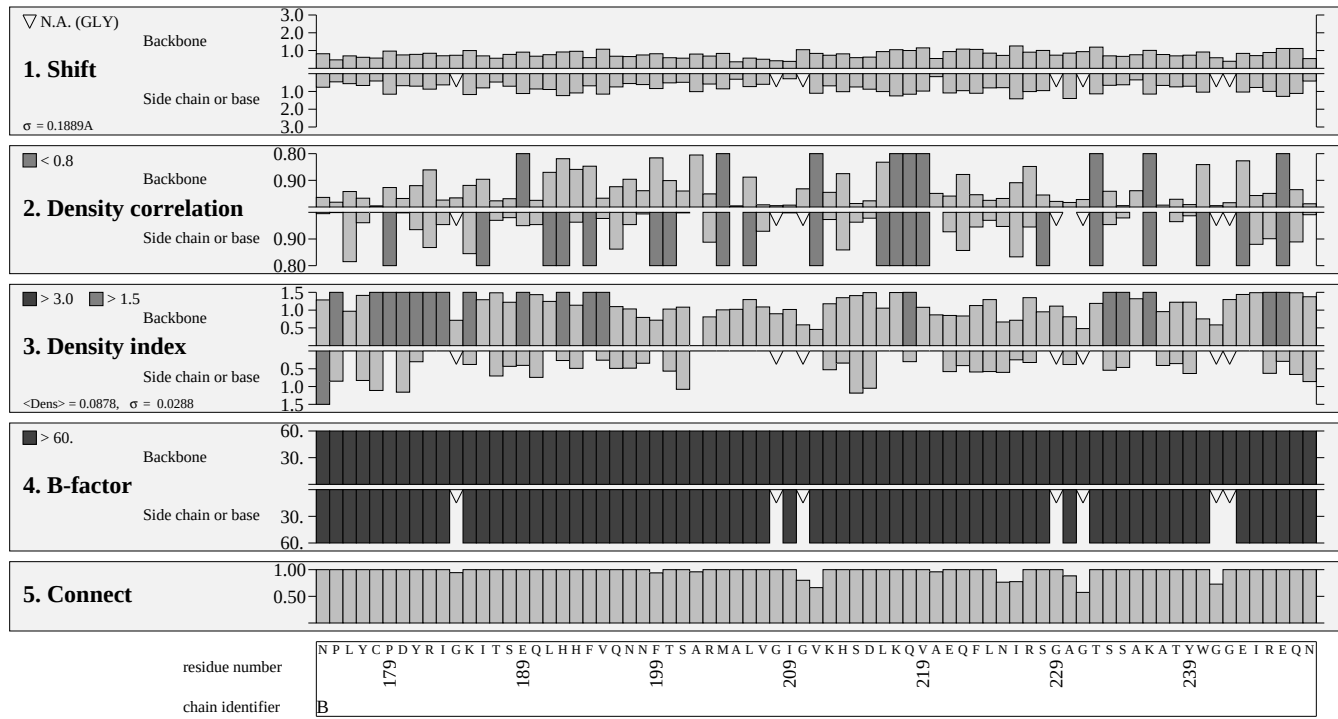
Local estimation (4)



Structure Factor Check

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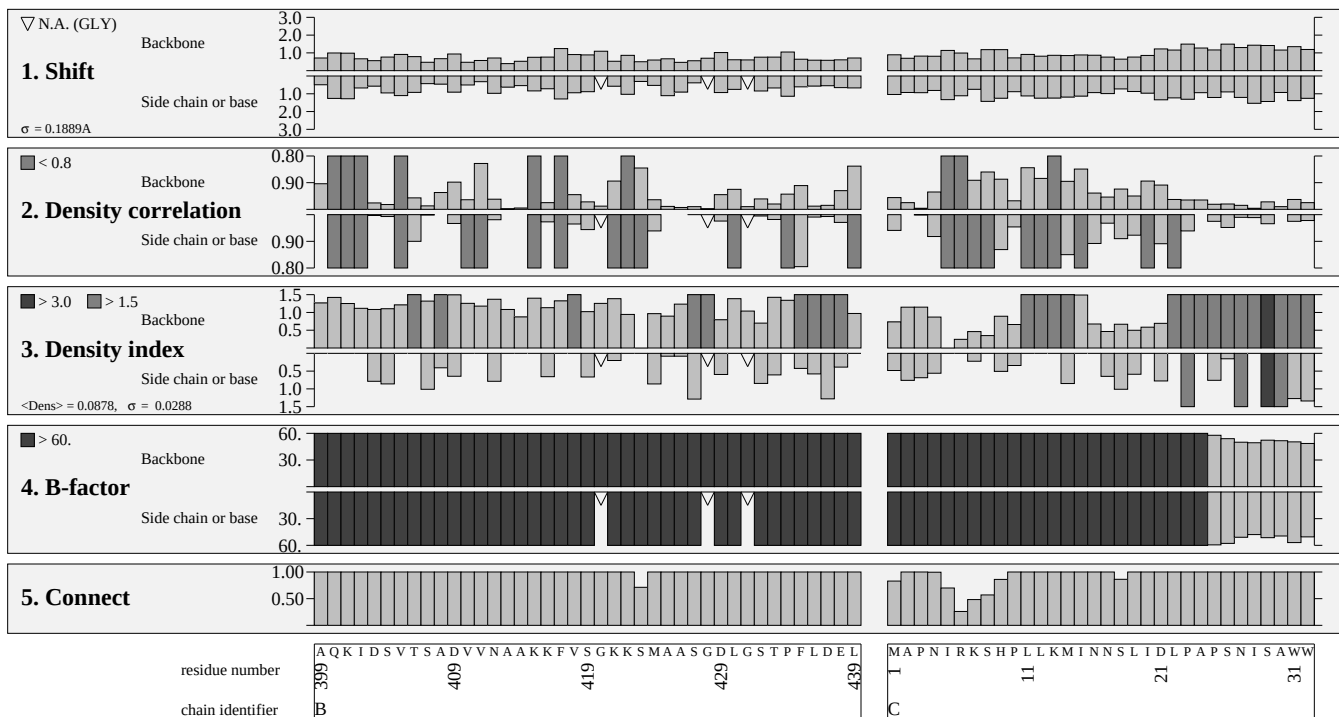
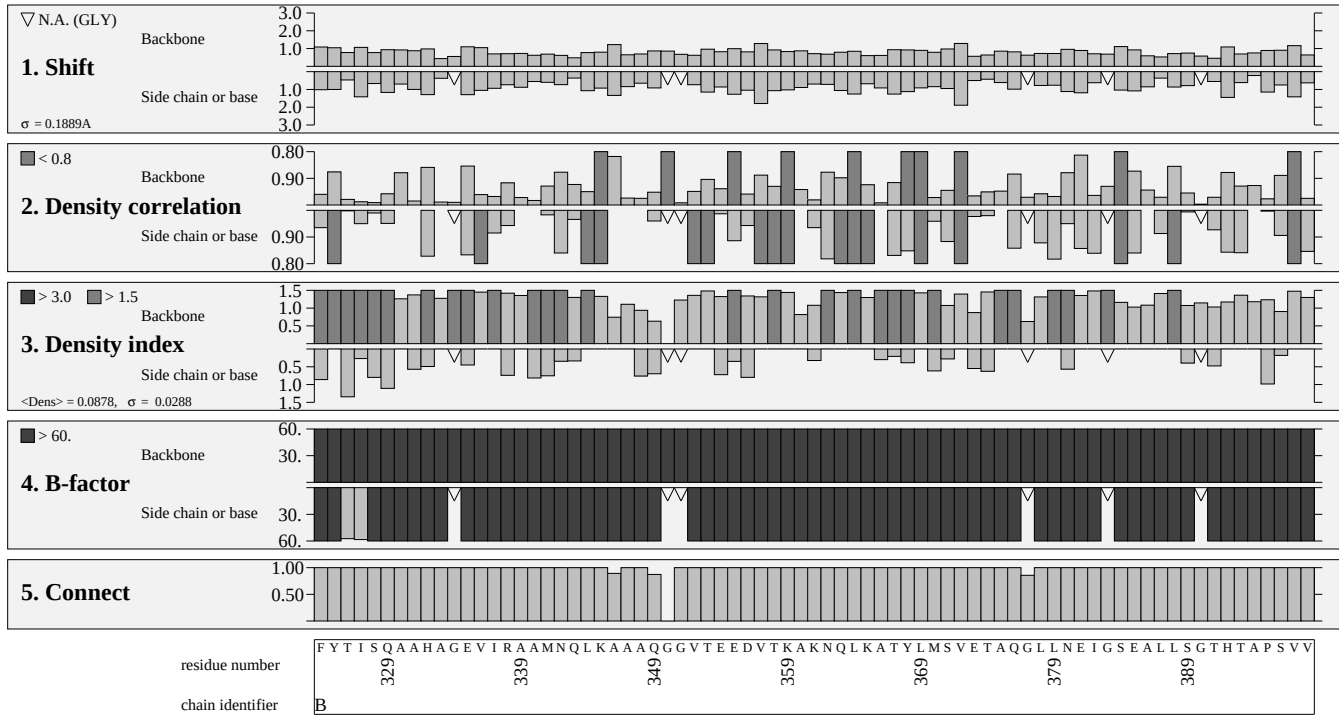
Local estimation (5)



Structure Factor Check

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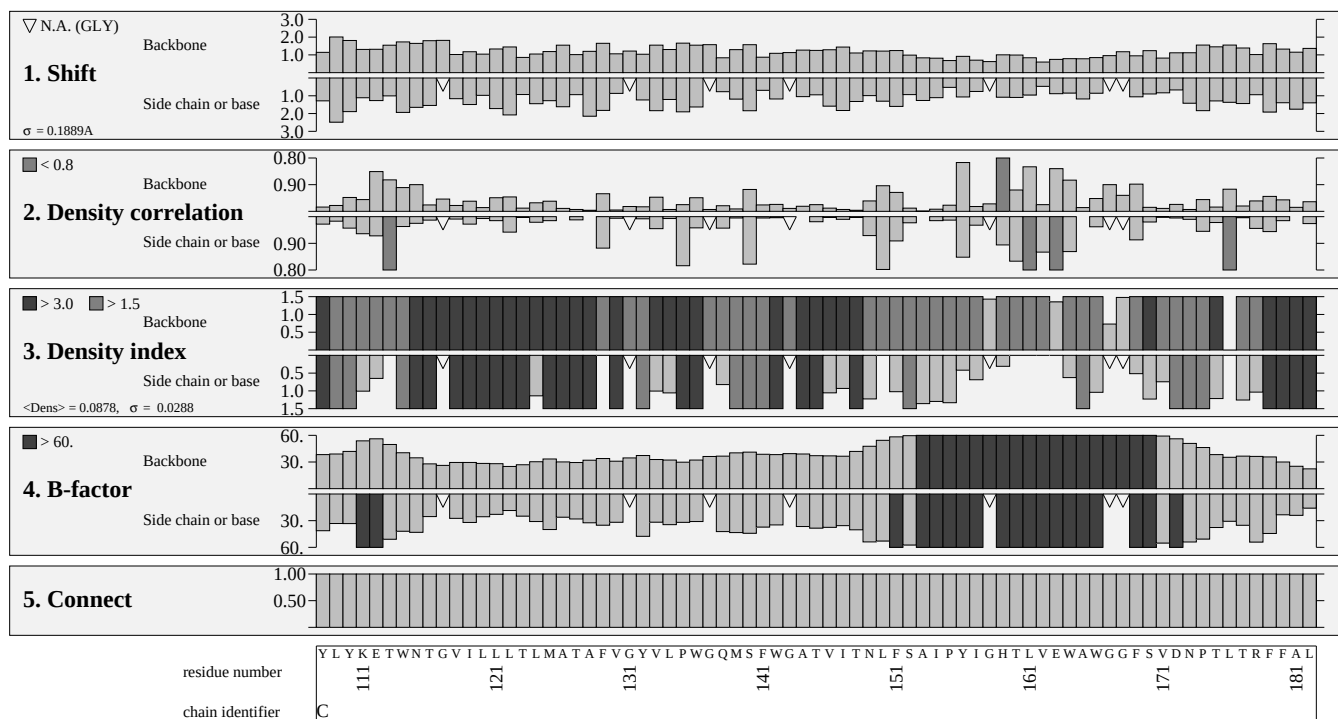
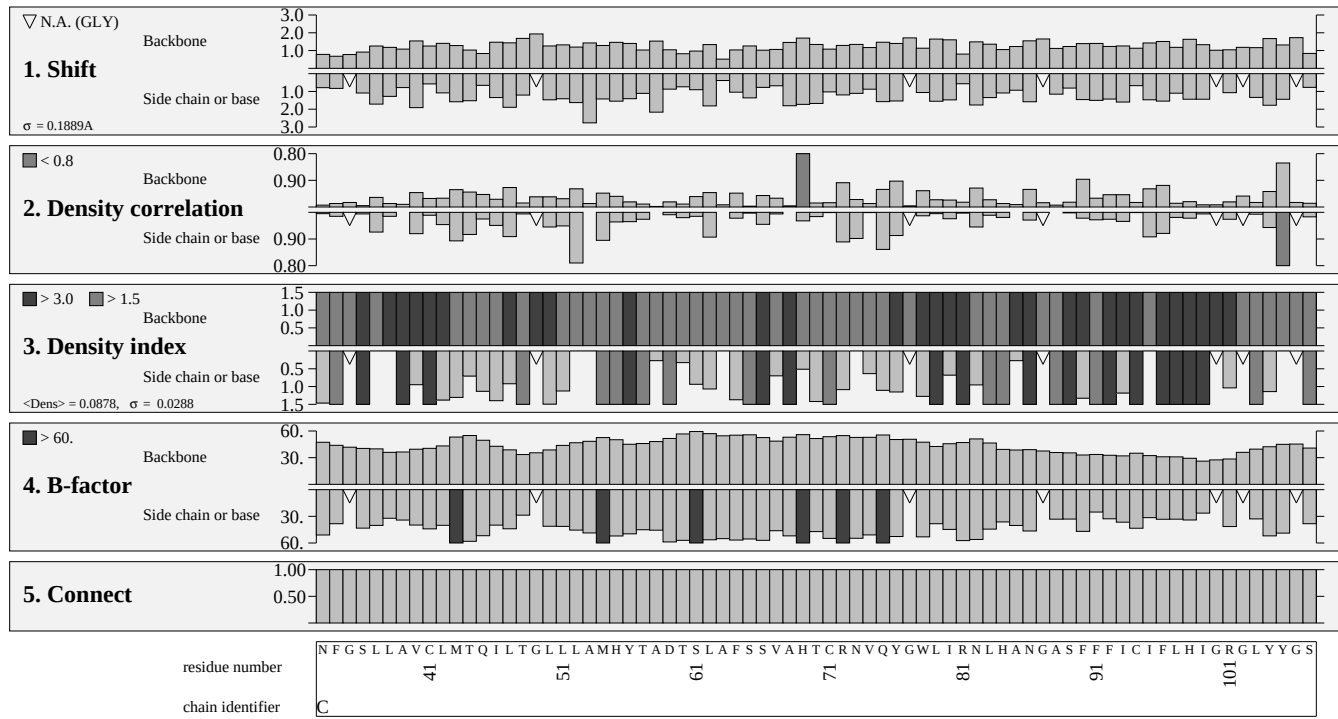
Local estimation (6)



Structure Factor Check

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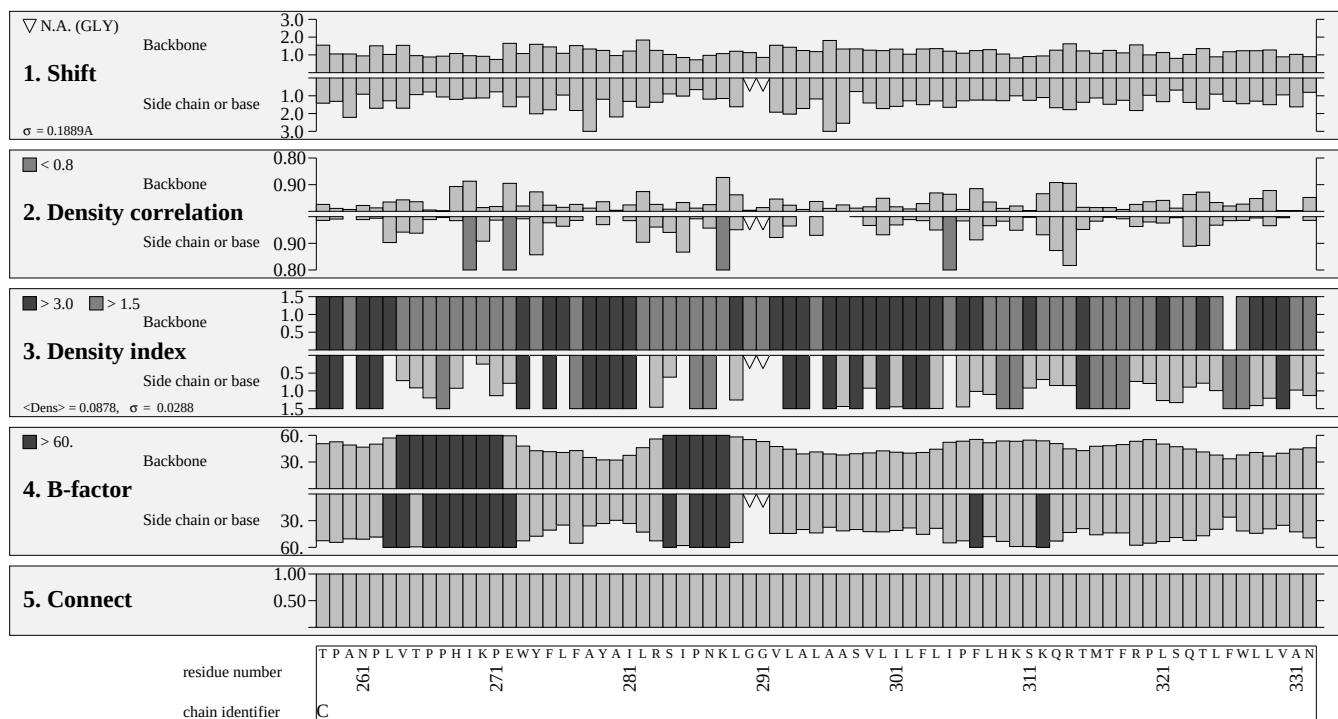
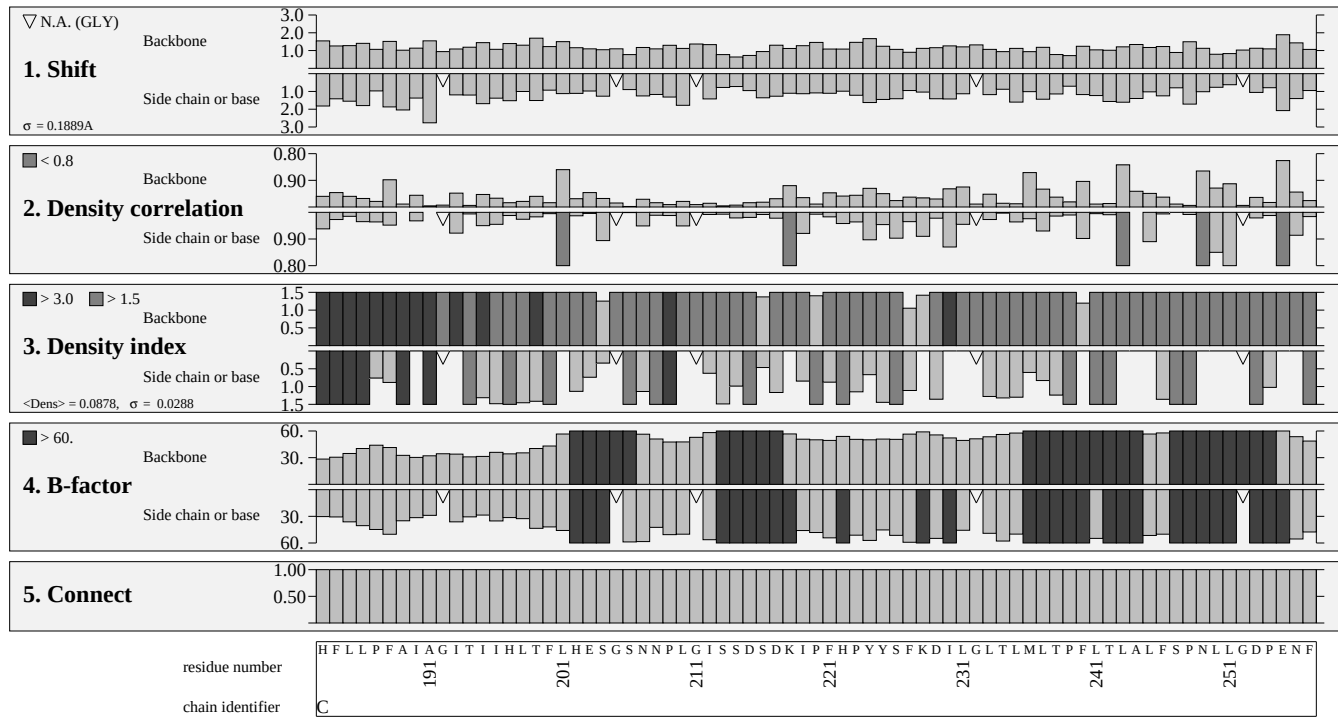
Local estimation (7)



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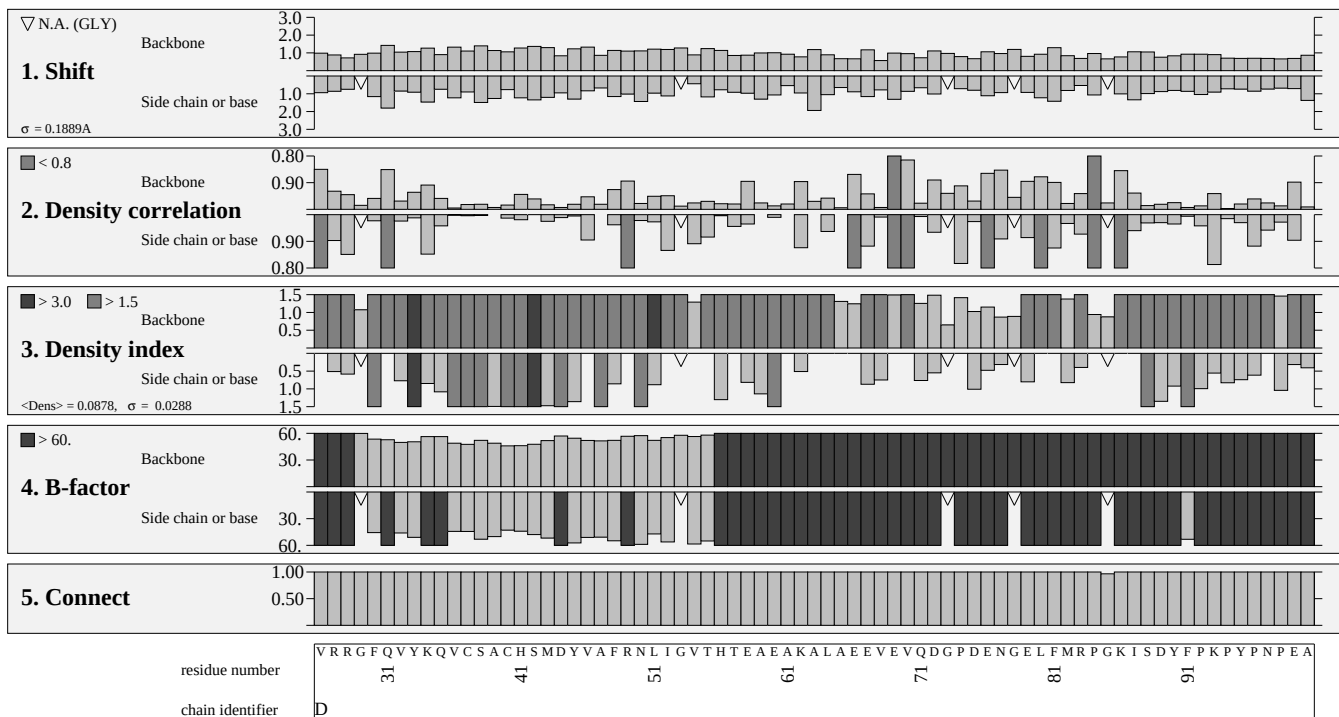
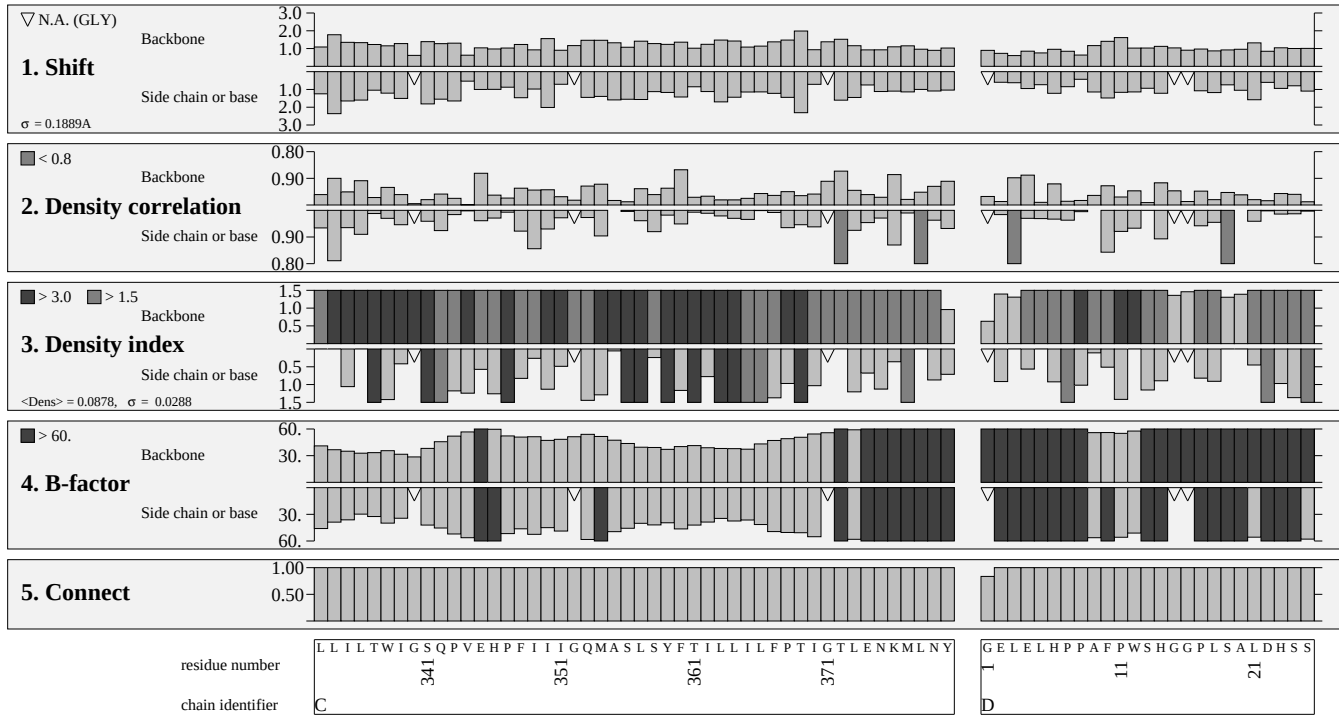
Local estimation (8)



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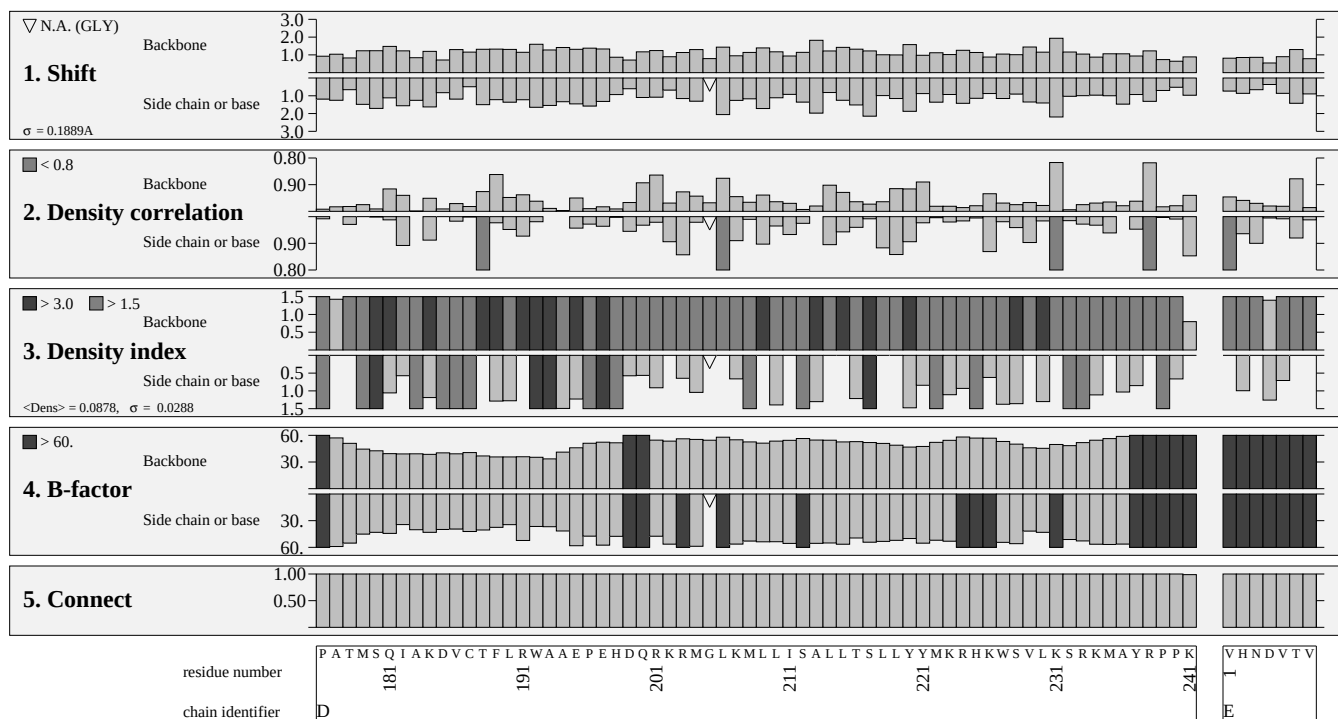
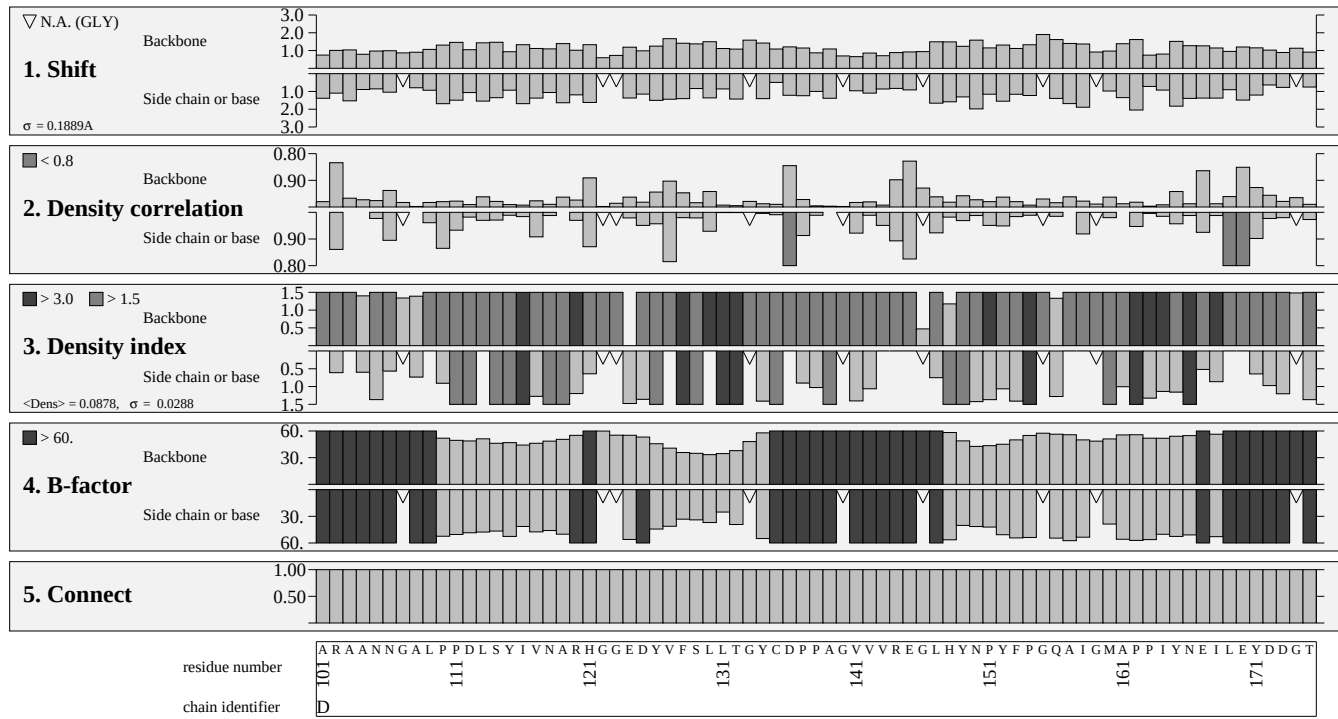
Local estimation (9)



Structure Factor Check

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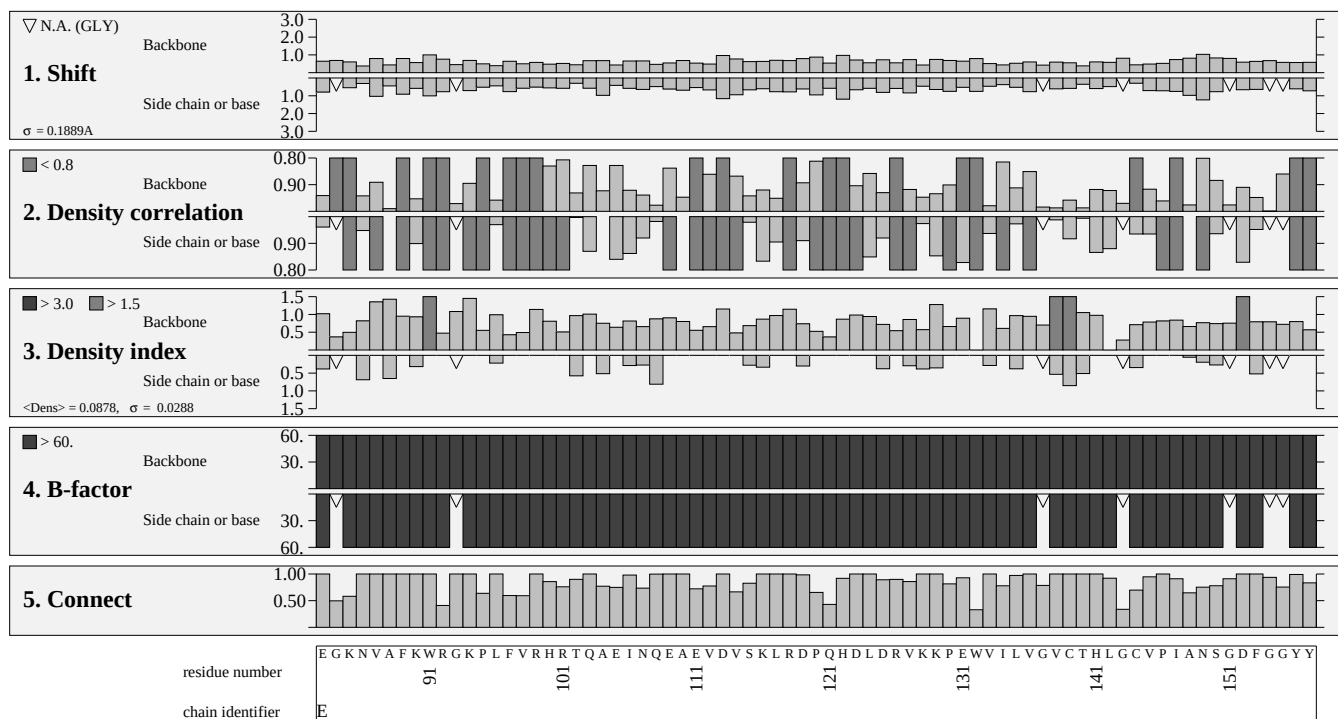
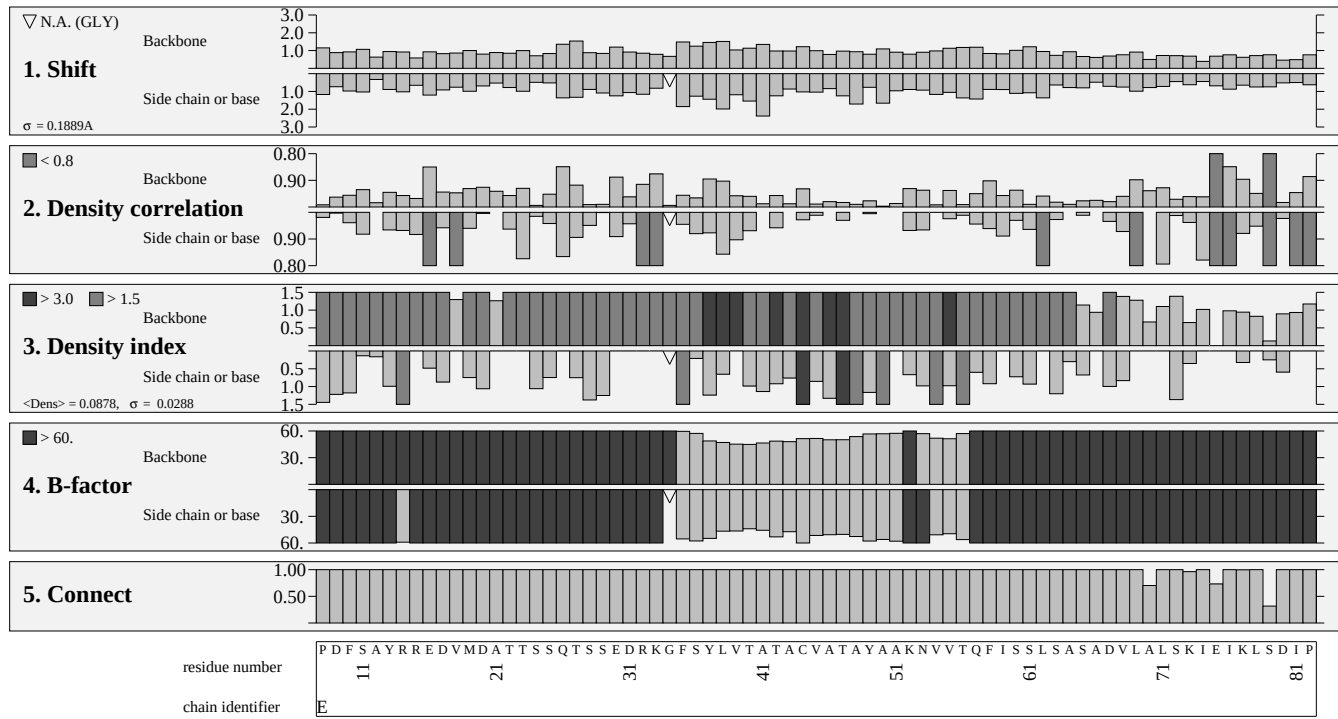
Local estimation (10)



Structure Factor Check

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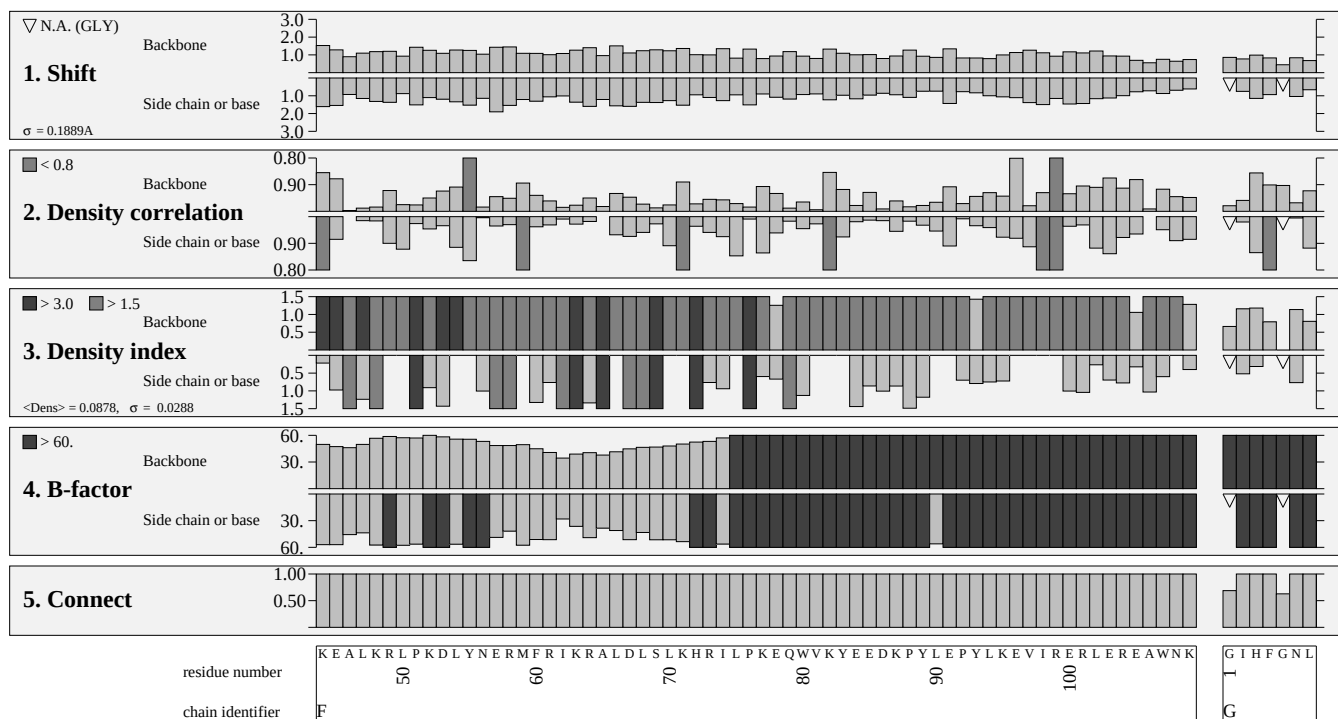
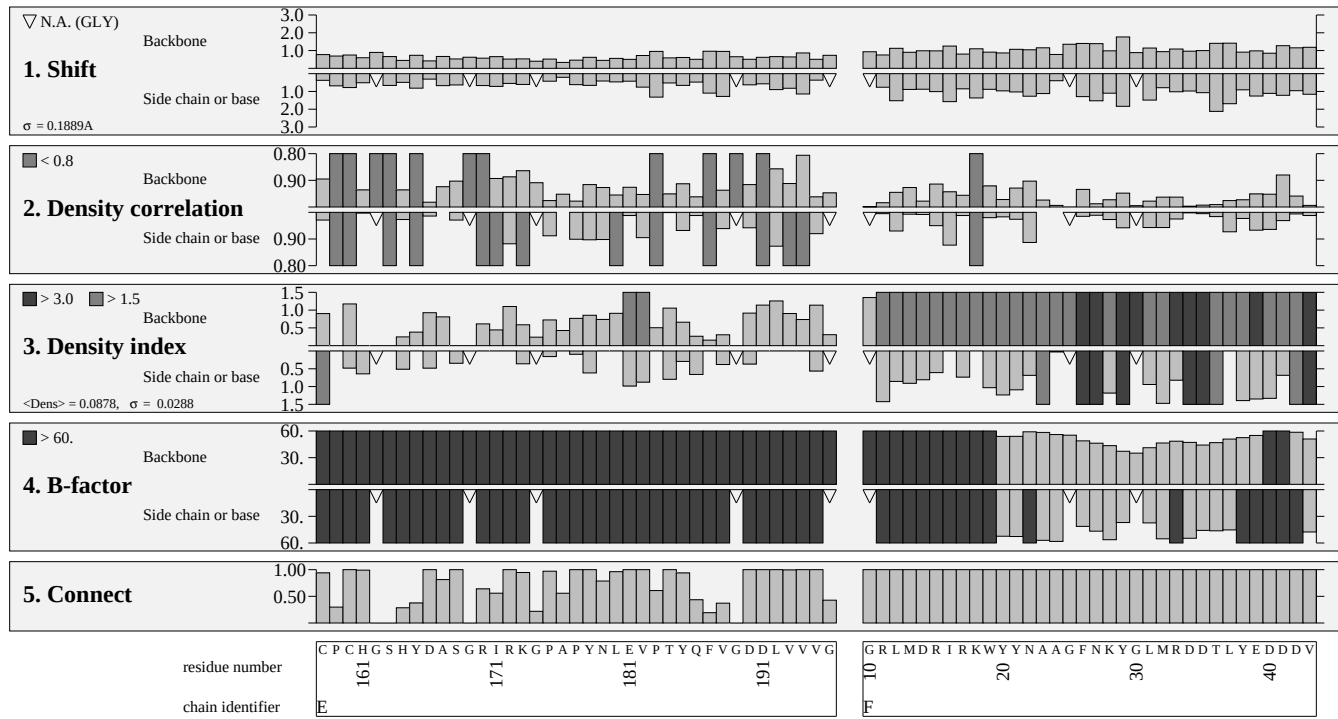
Local estimation (11)



Structure Factor Check

3CWB

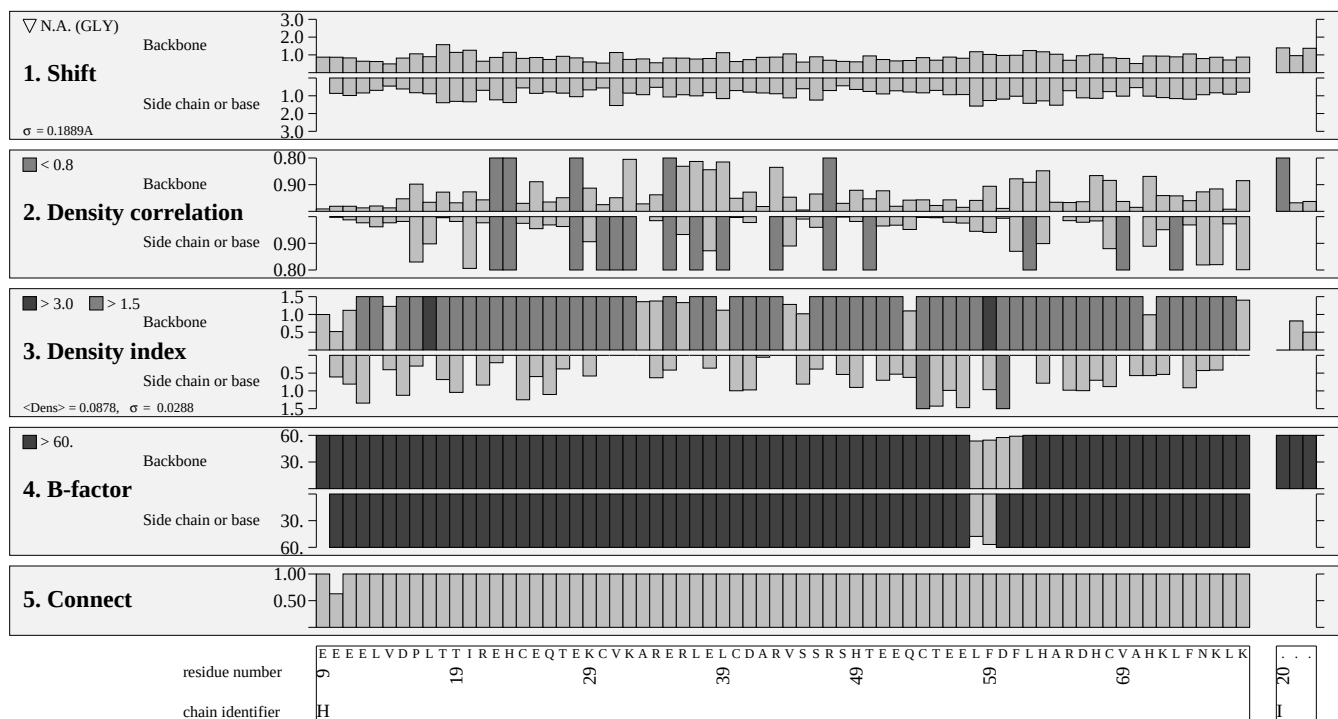
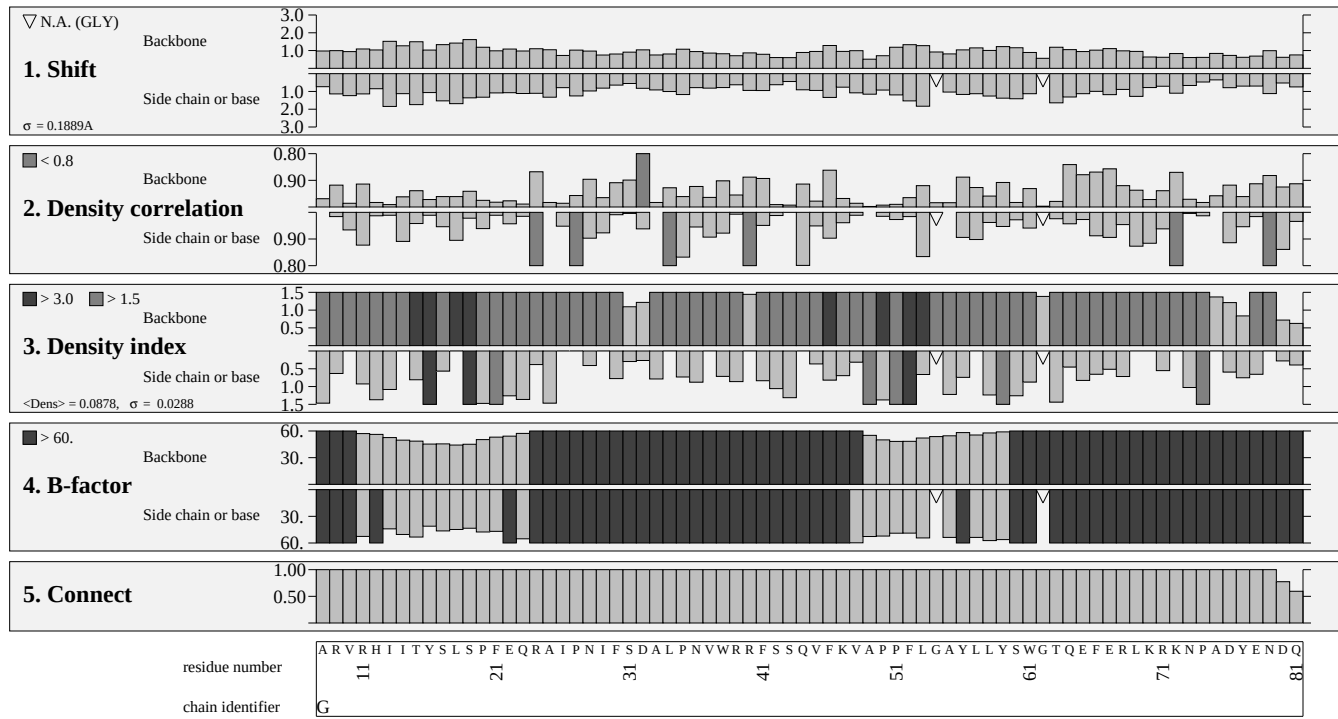
Local estimation (12)



Structure Factor Check

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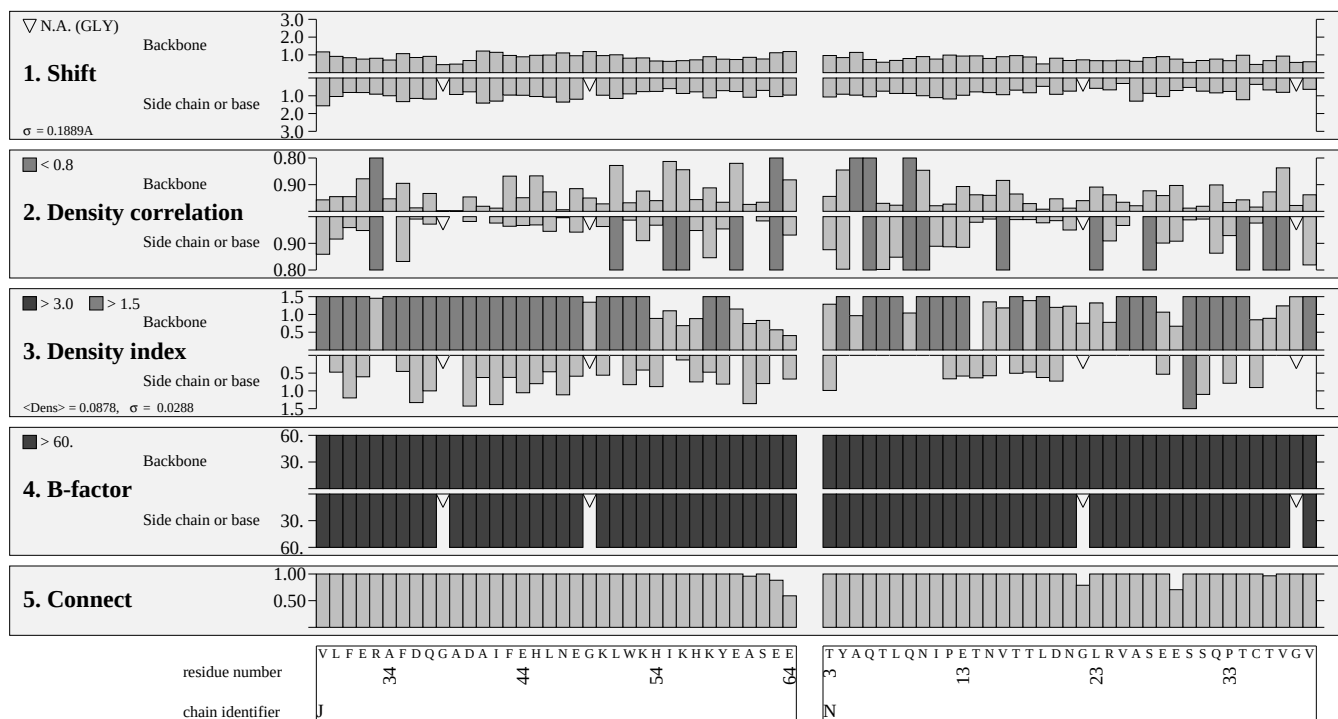
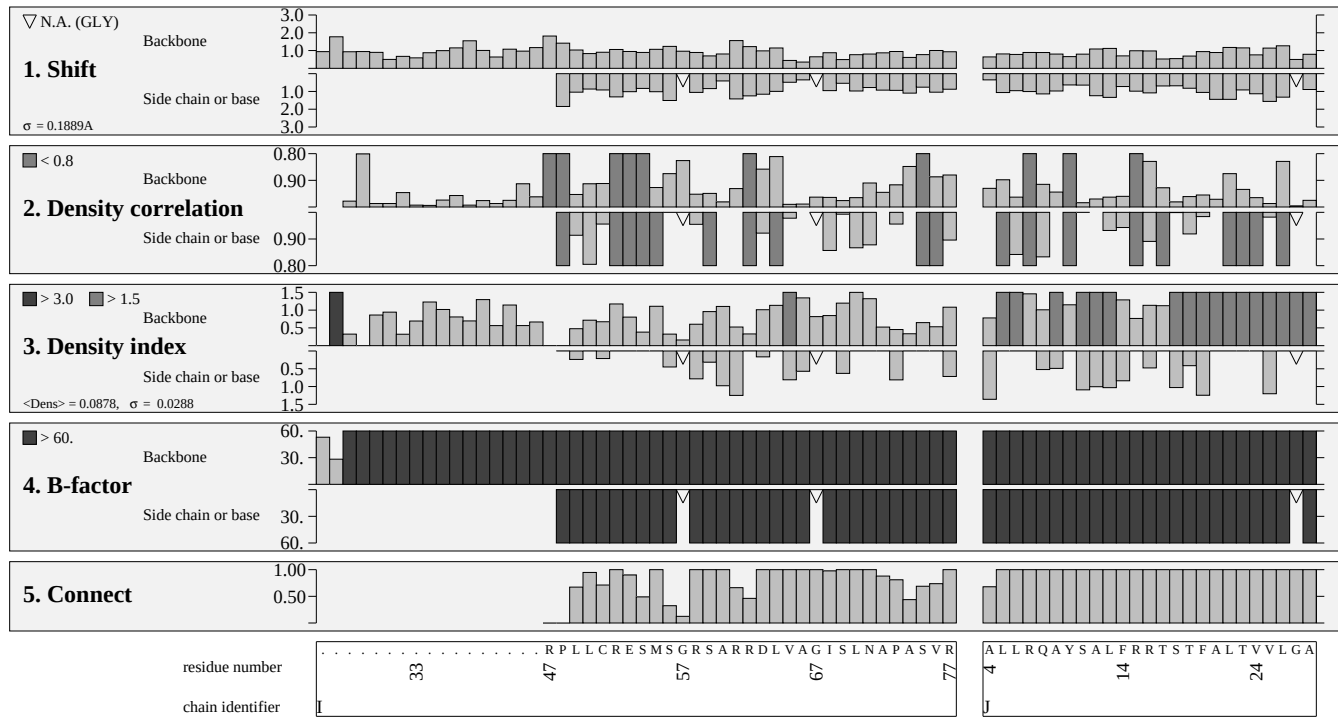
Local estimation (13)



Structure Factor Check

3CWB

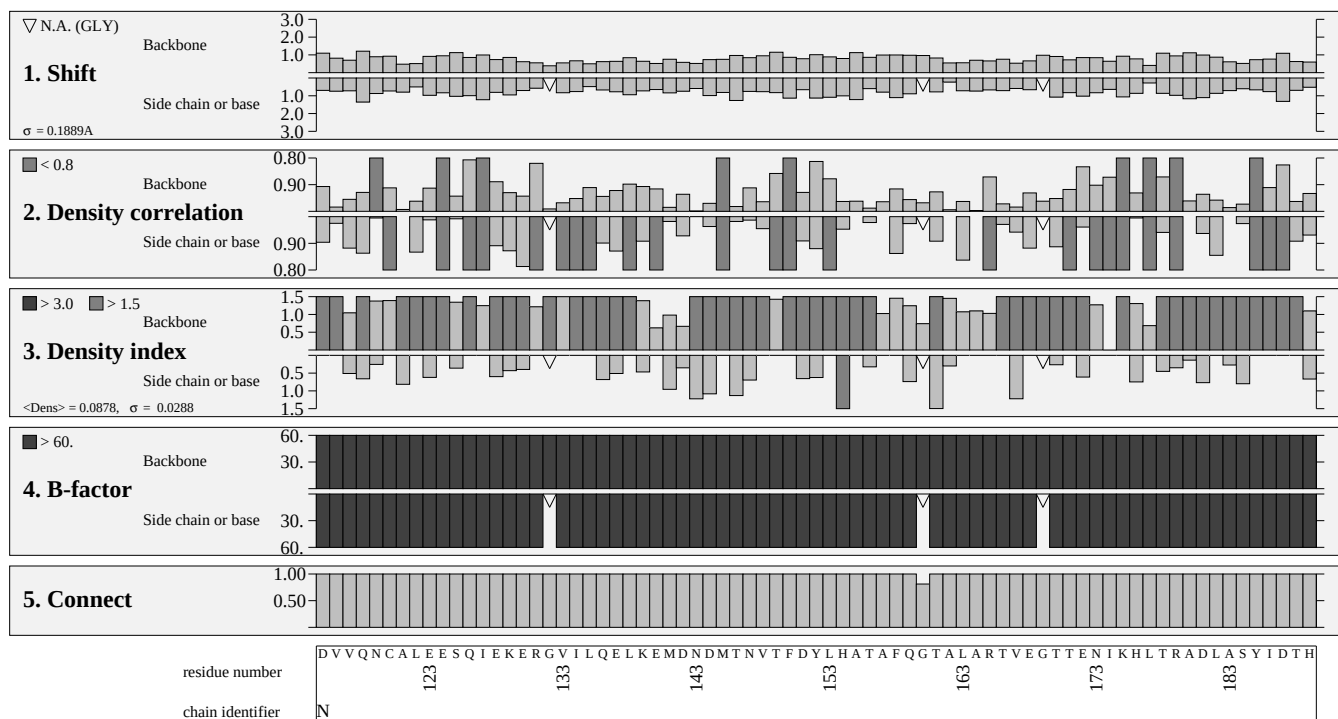
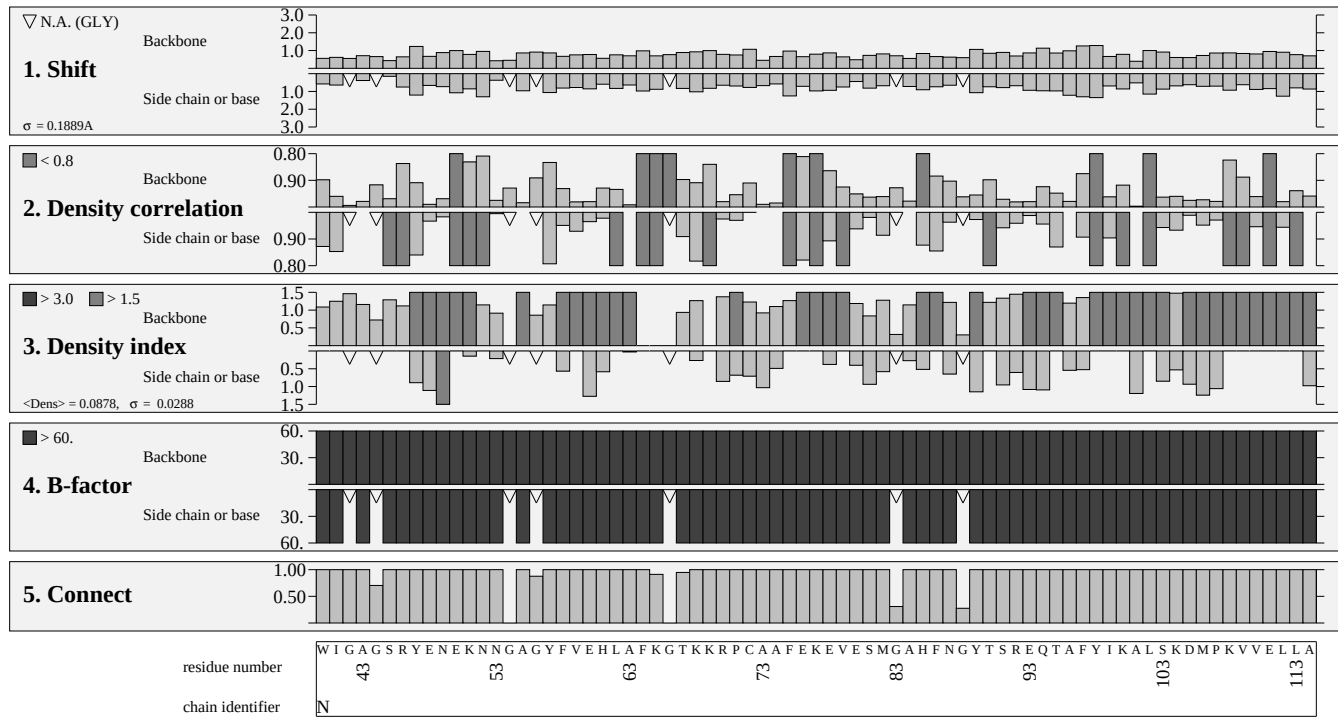
Local estimation (14)



Structure Factor Check

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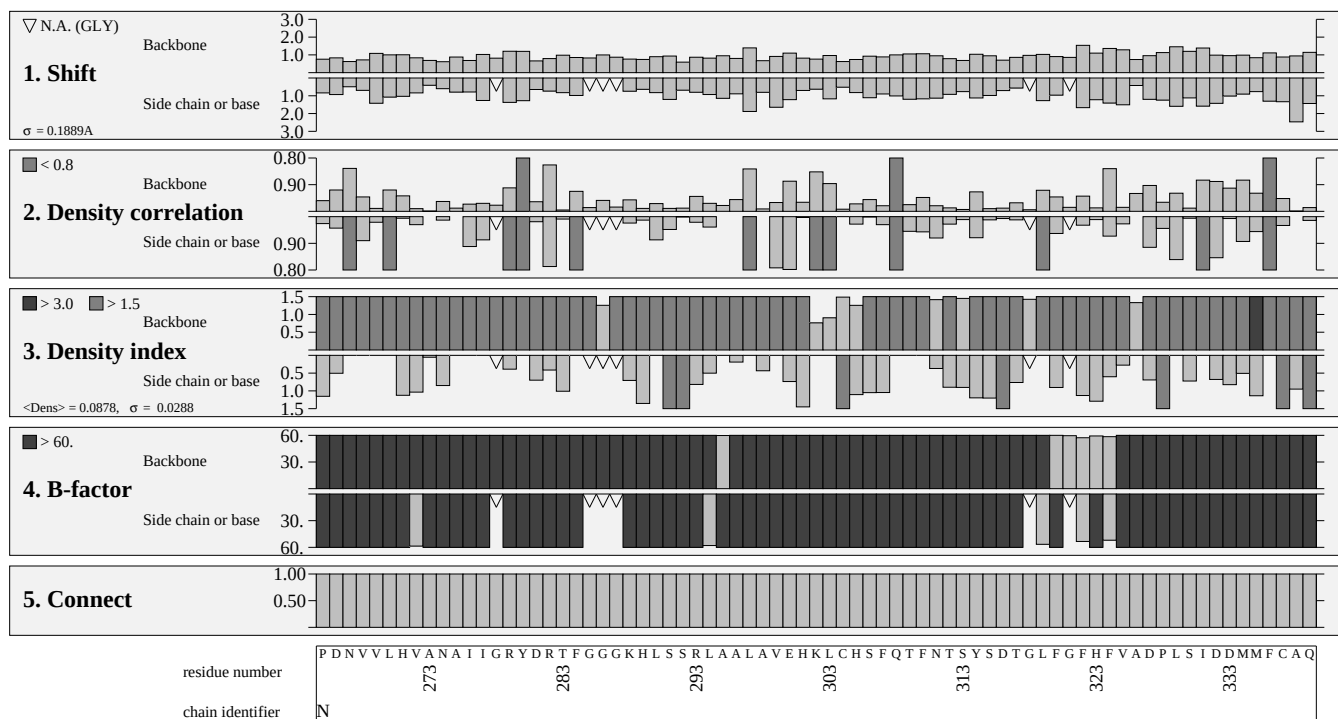
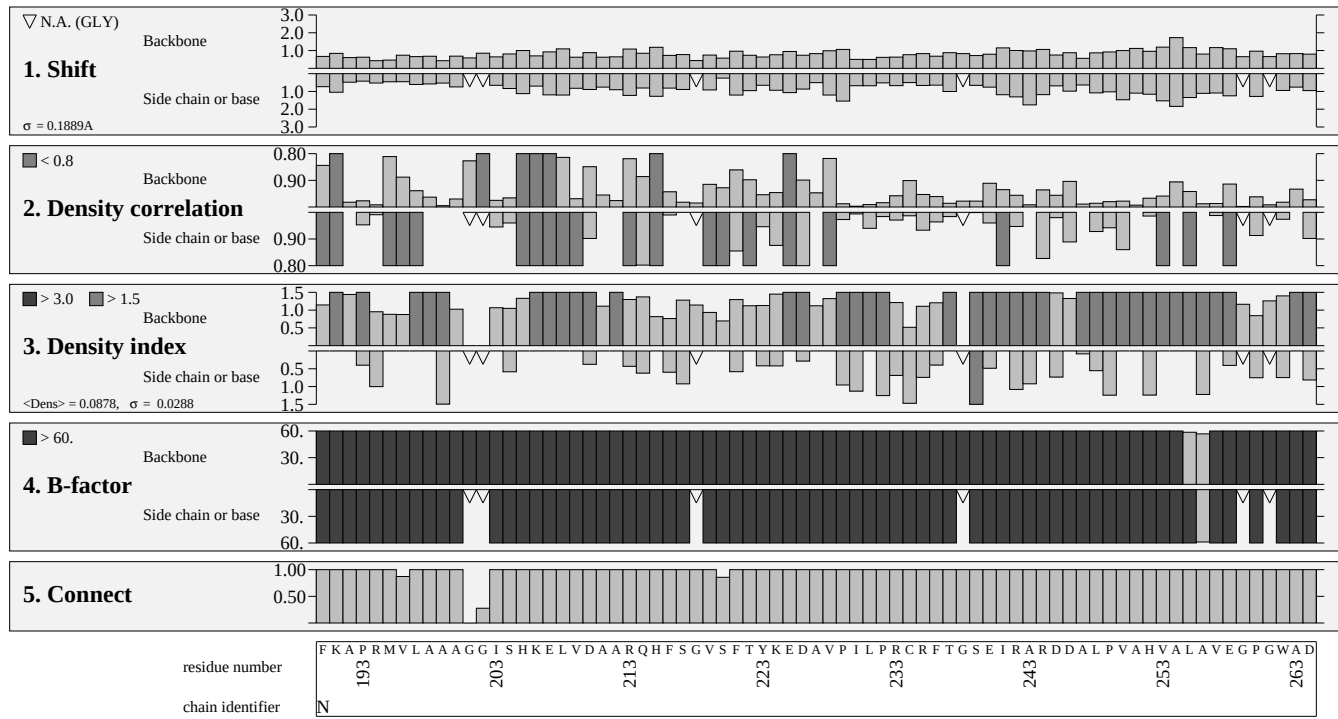
Local estimation (15)



Structure Factor Check

3CWB

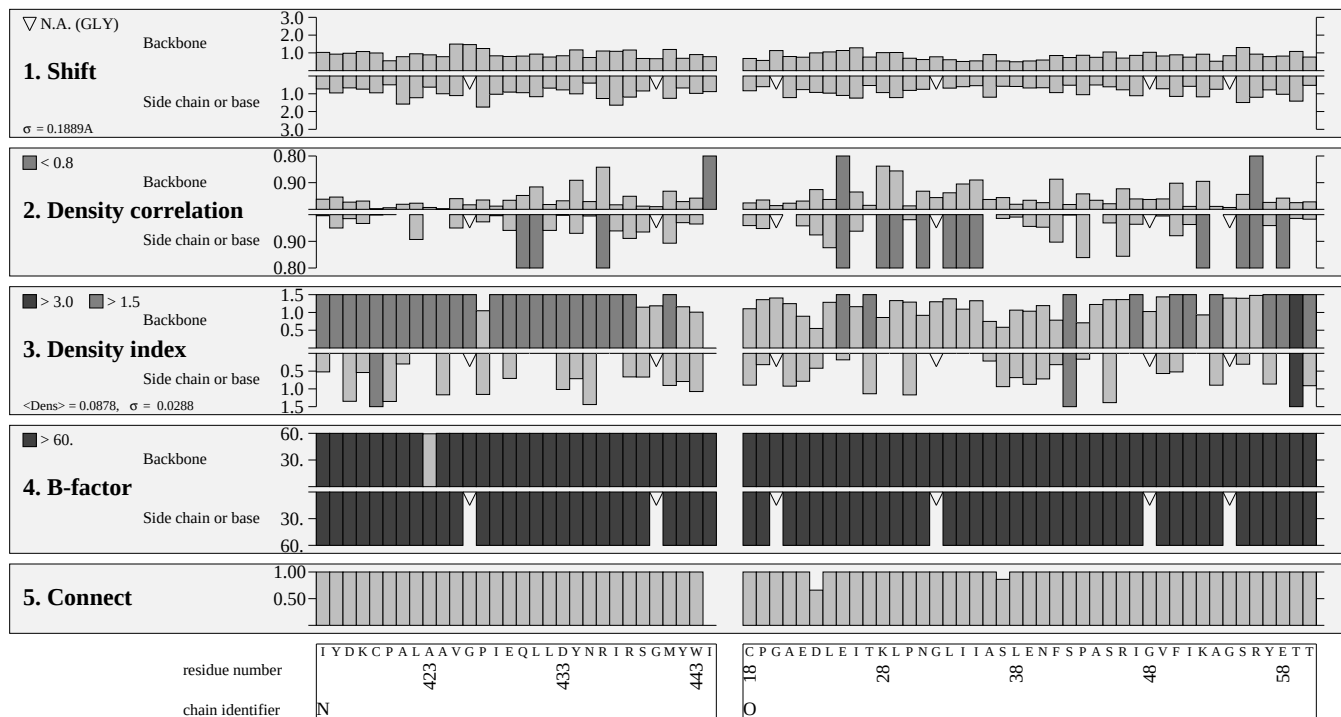
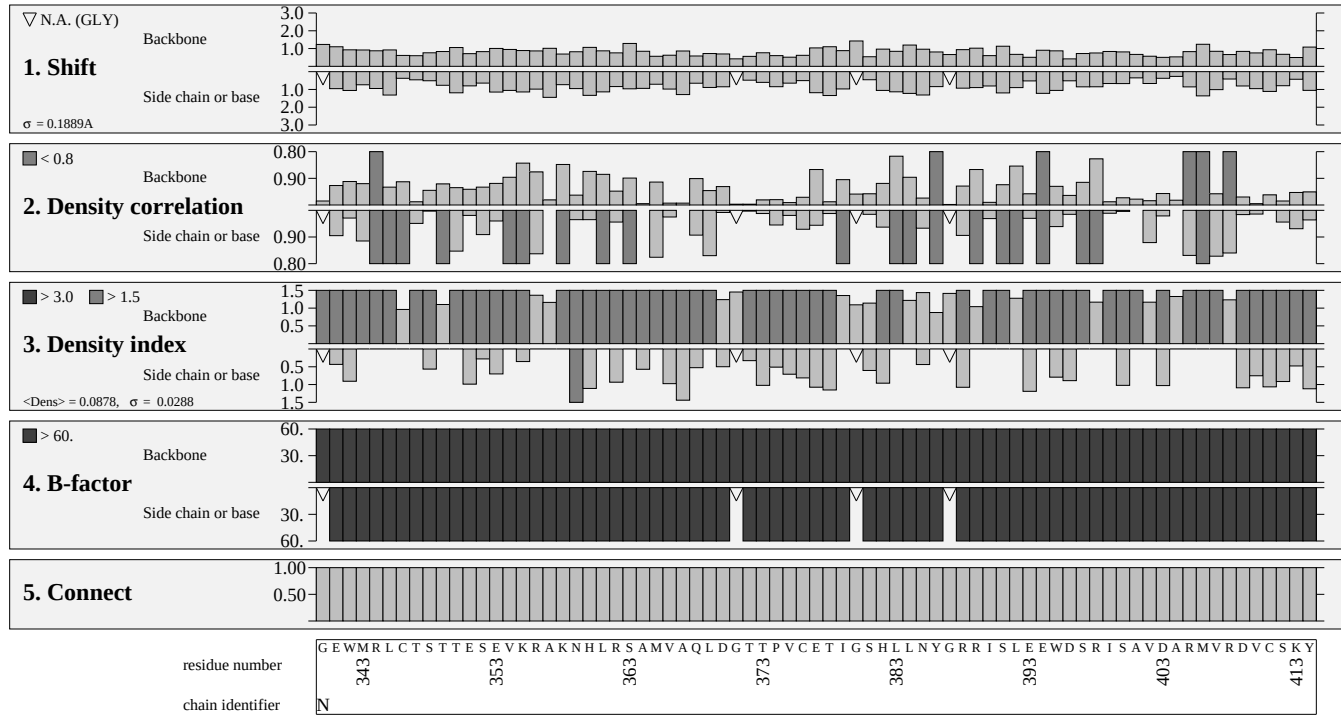
Local estimation (16)



Structure Factor Check

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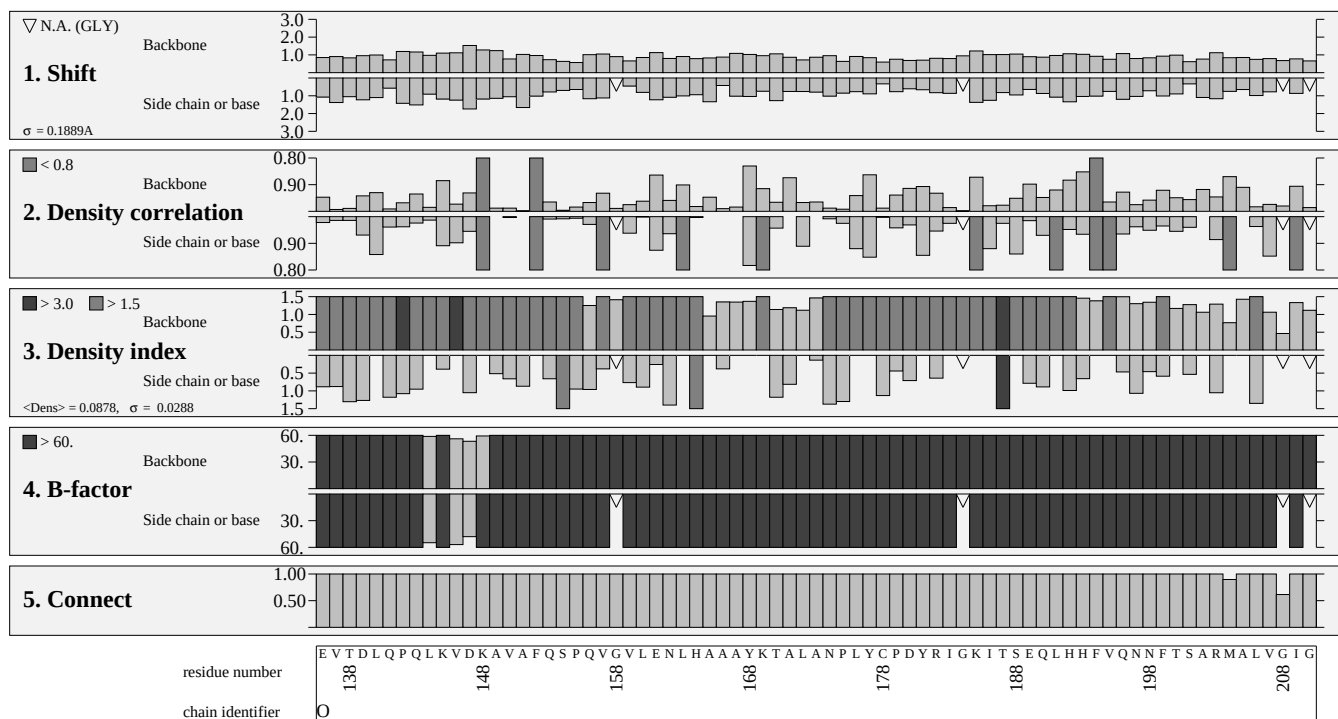
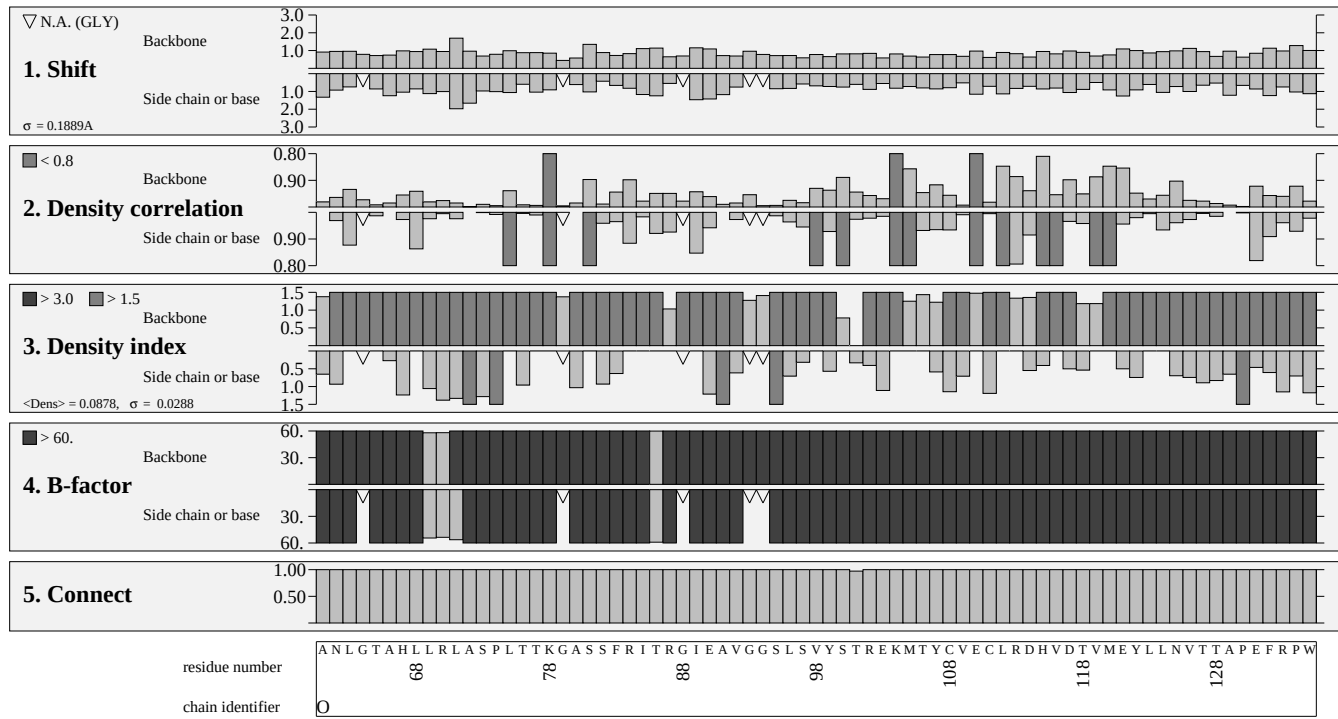
Local estimation (17)



Structure Factor Check

3CWB

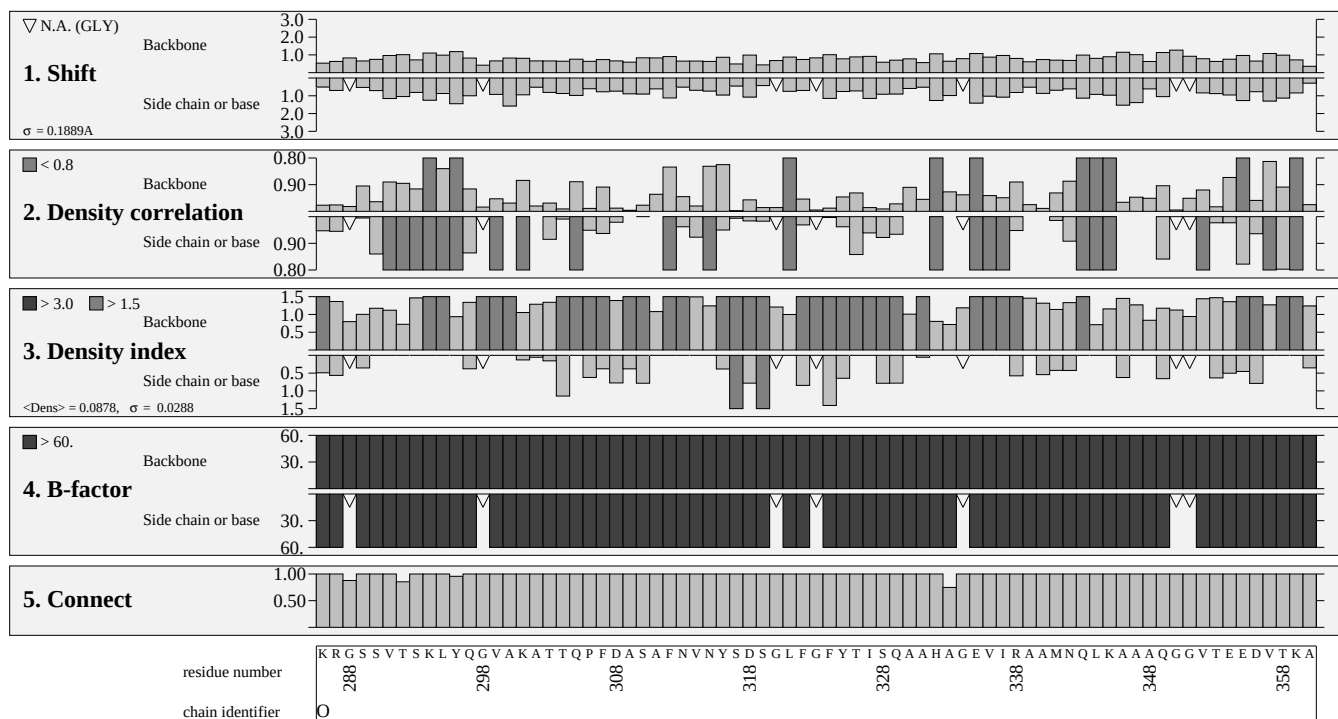
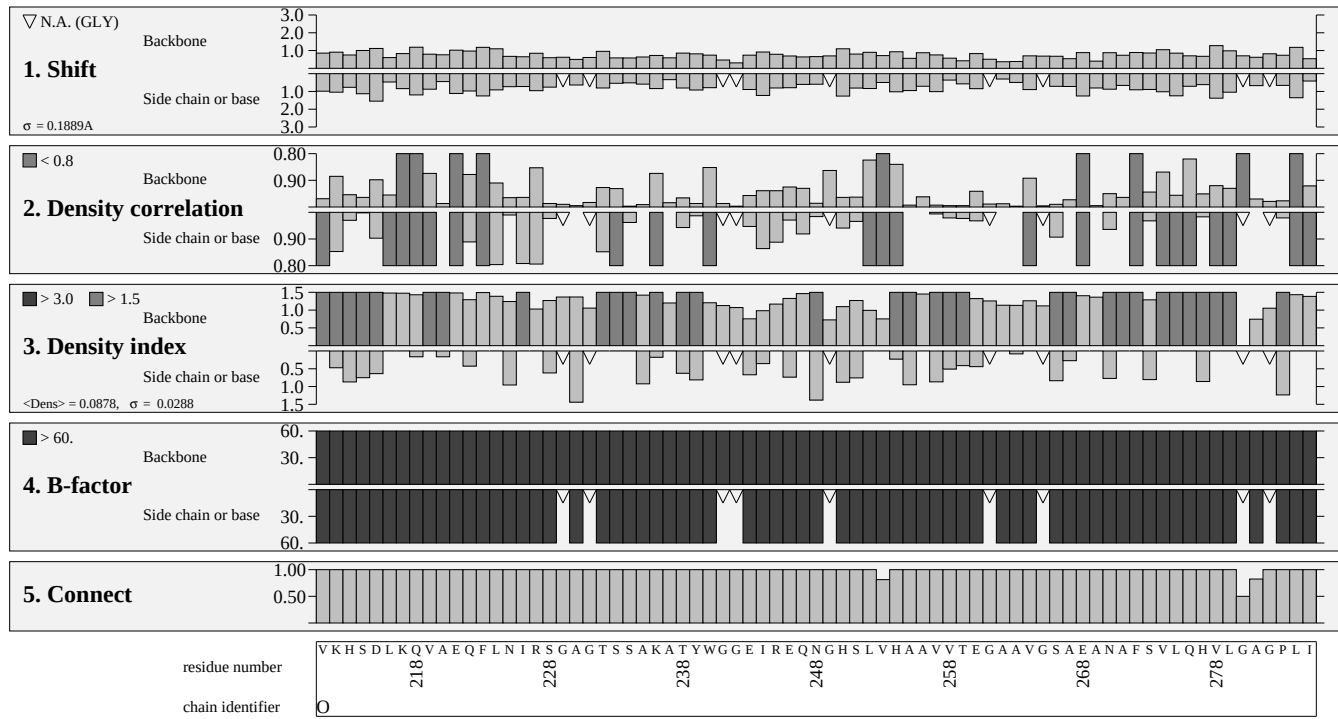
Local estimation (18)



Structure Factor Check

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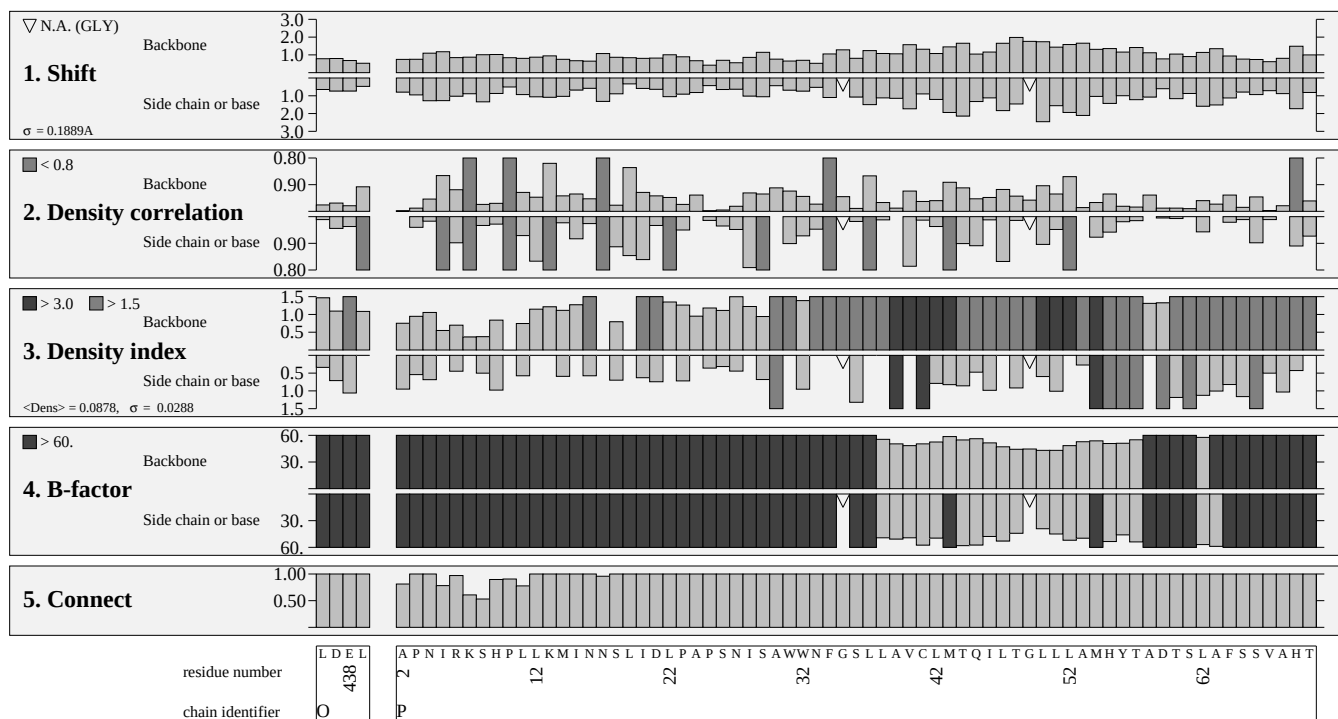
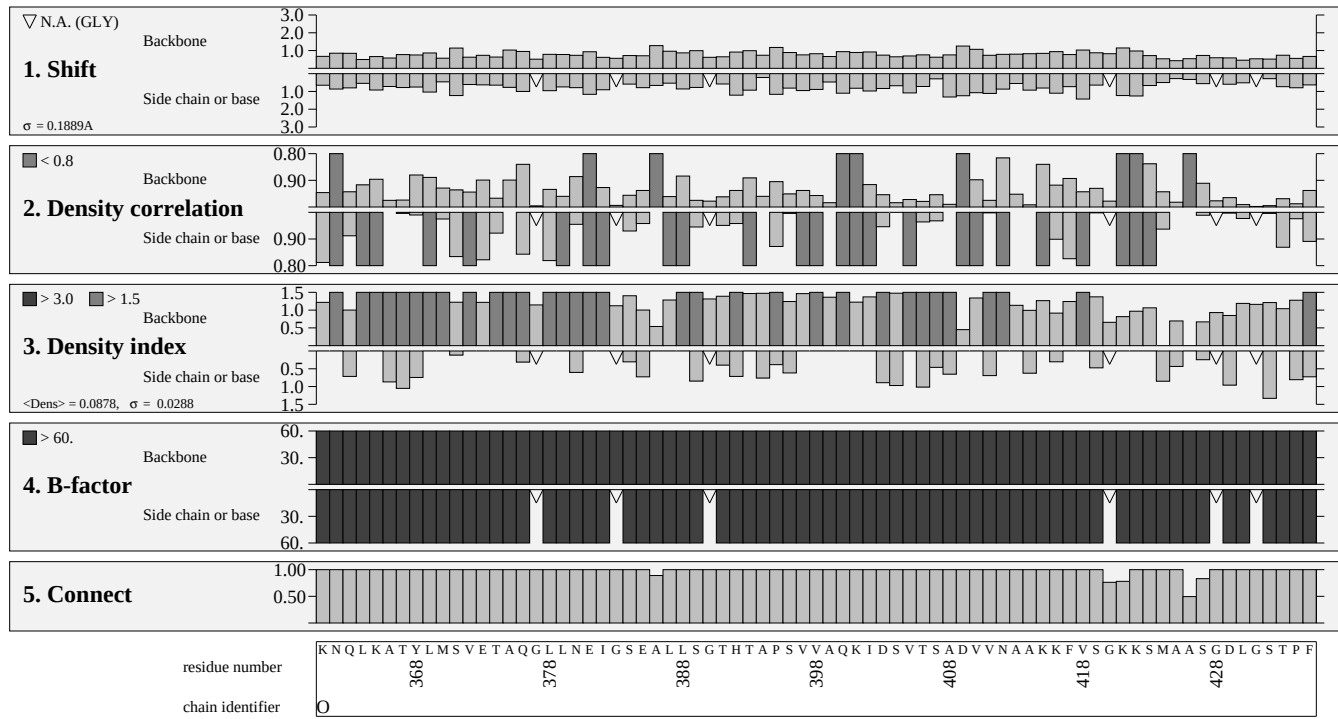
Local estimation (19)



Structure Factor Check

3CWB

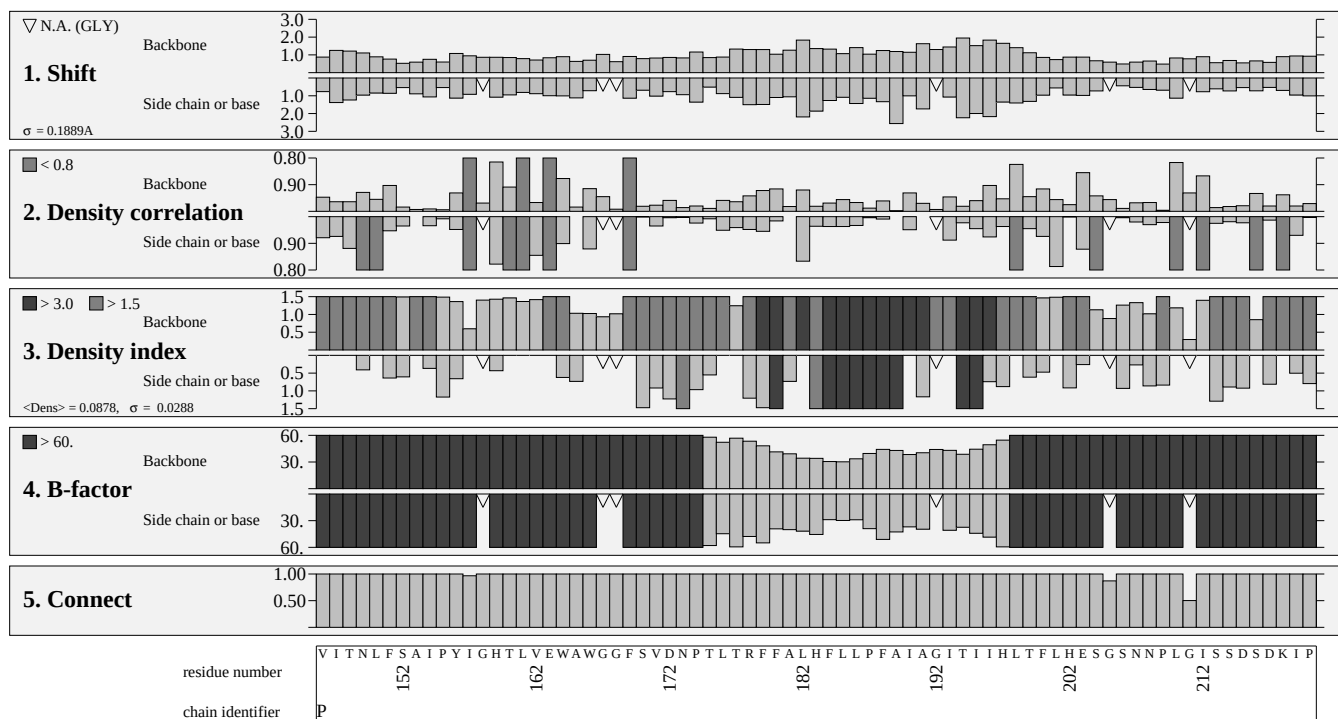
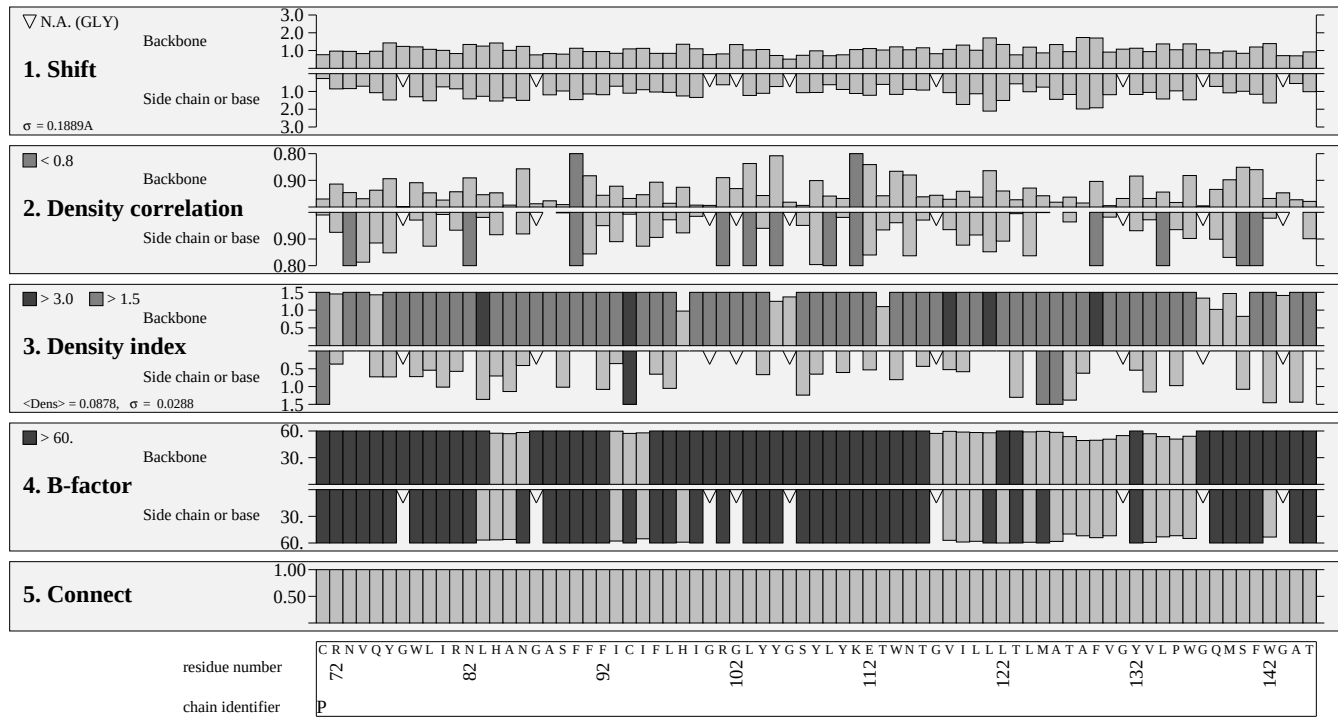
Local estimation (20)



Structure Factor Check

3CWB

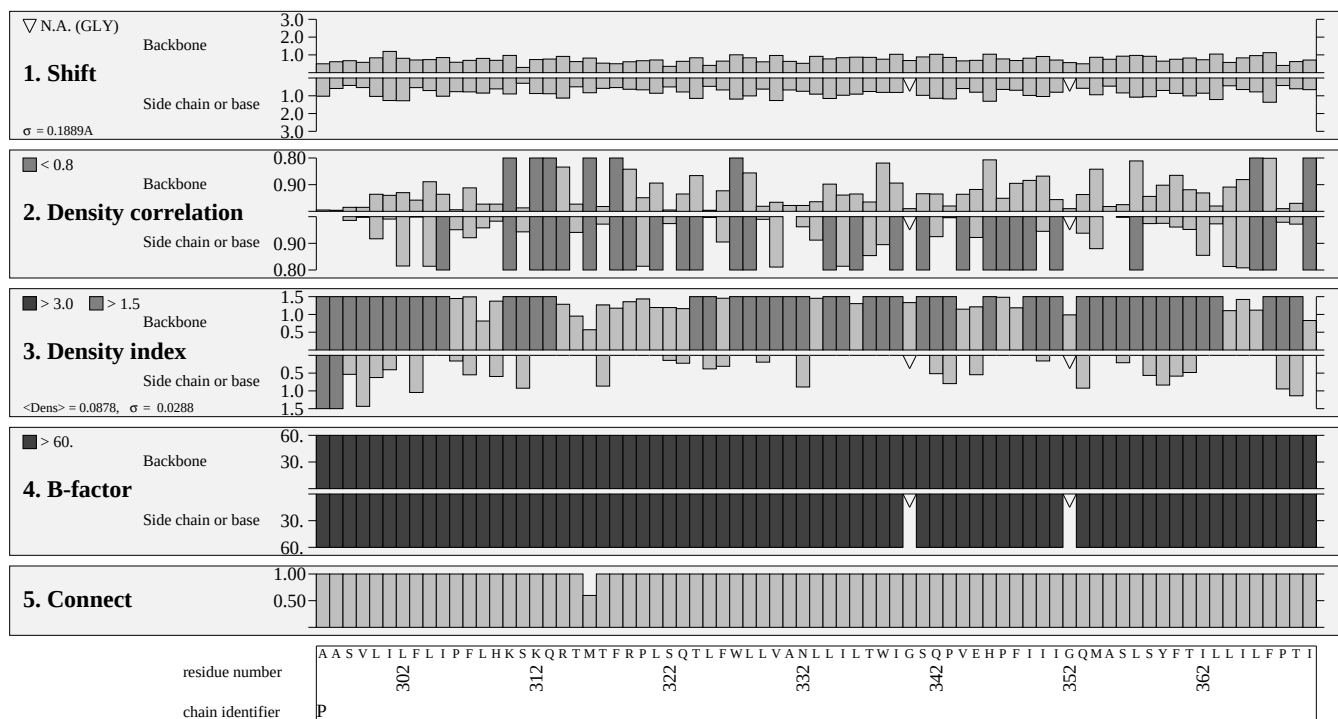
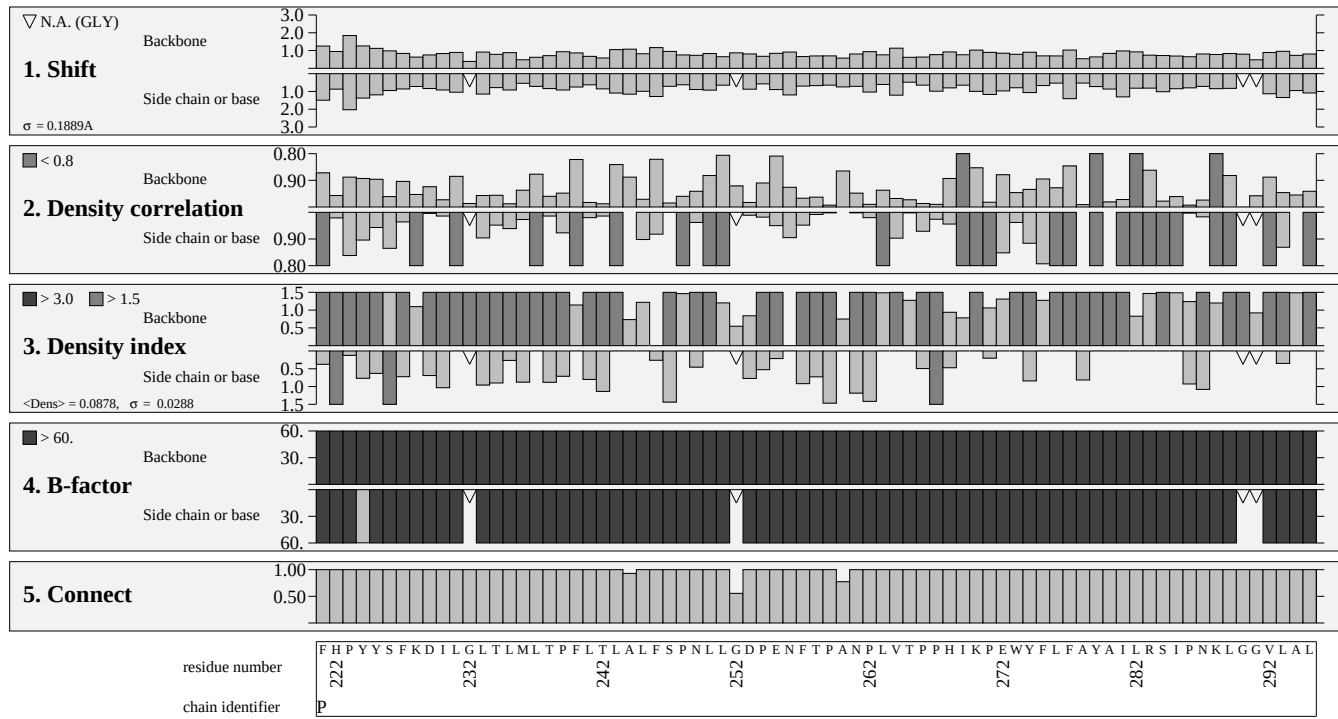
Local estimation (21)



Structure Factor Check

3CWB

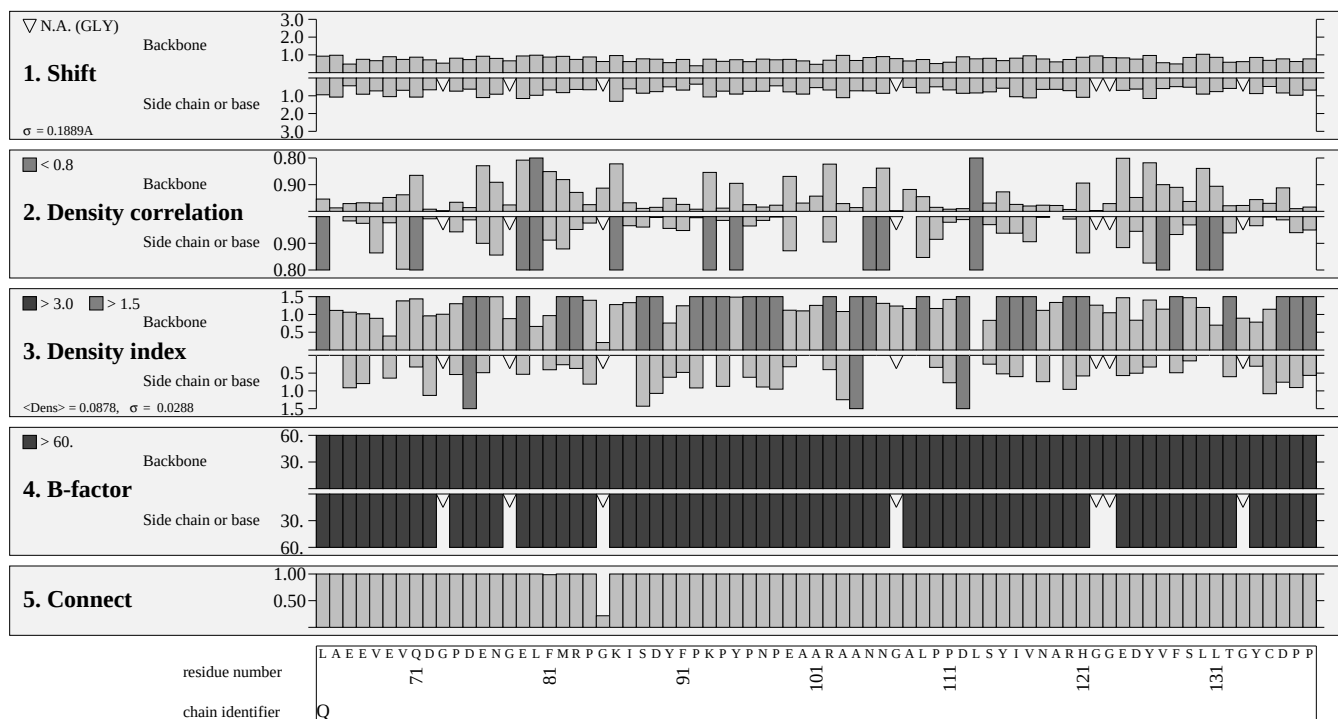
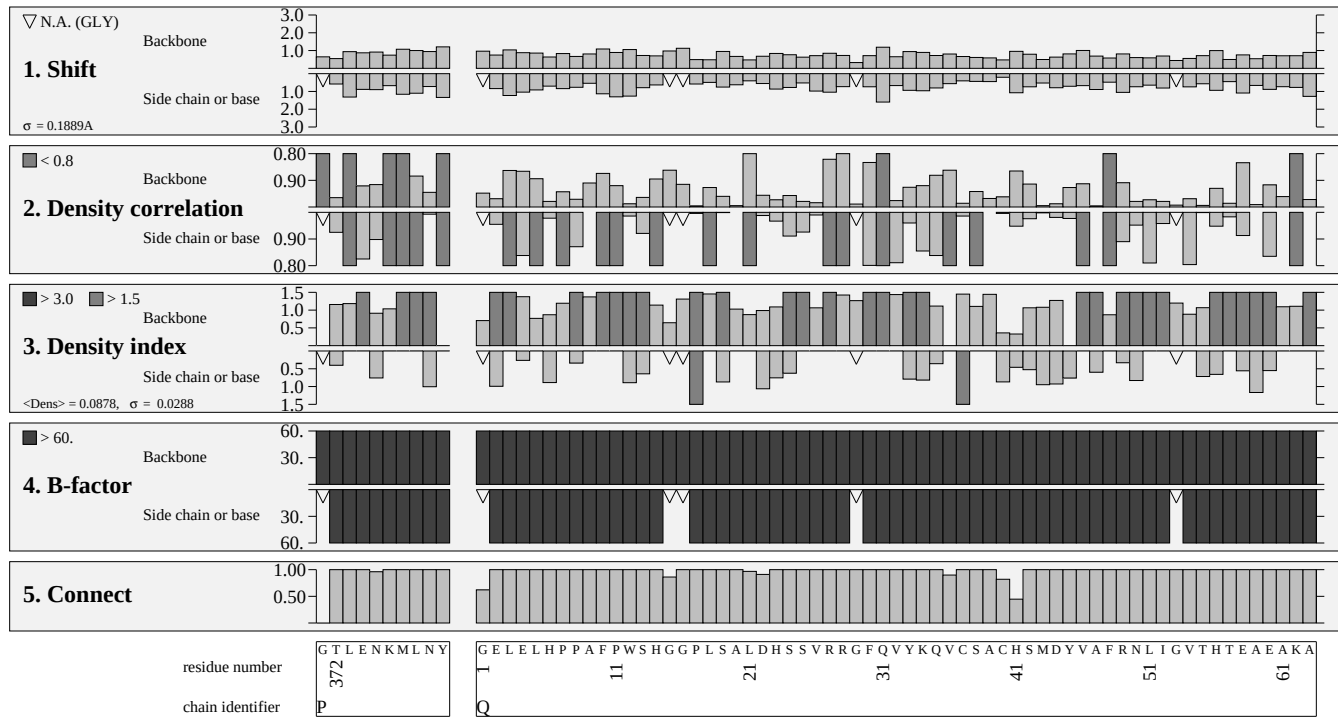
Local estimation (22)



Structure Factor Check

3CWB

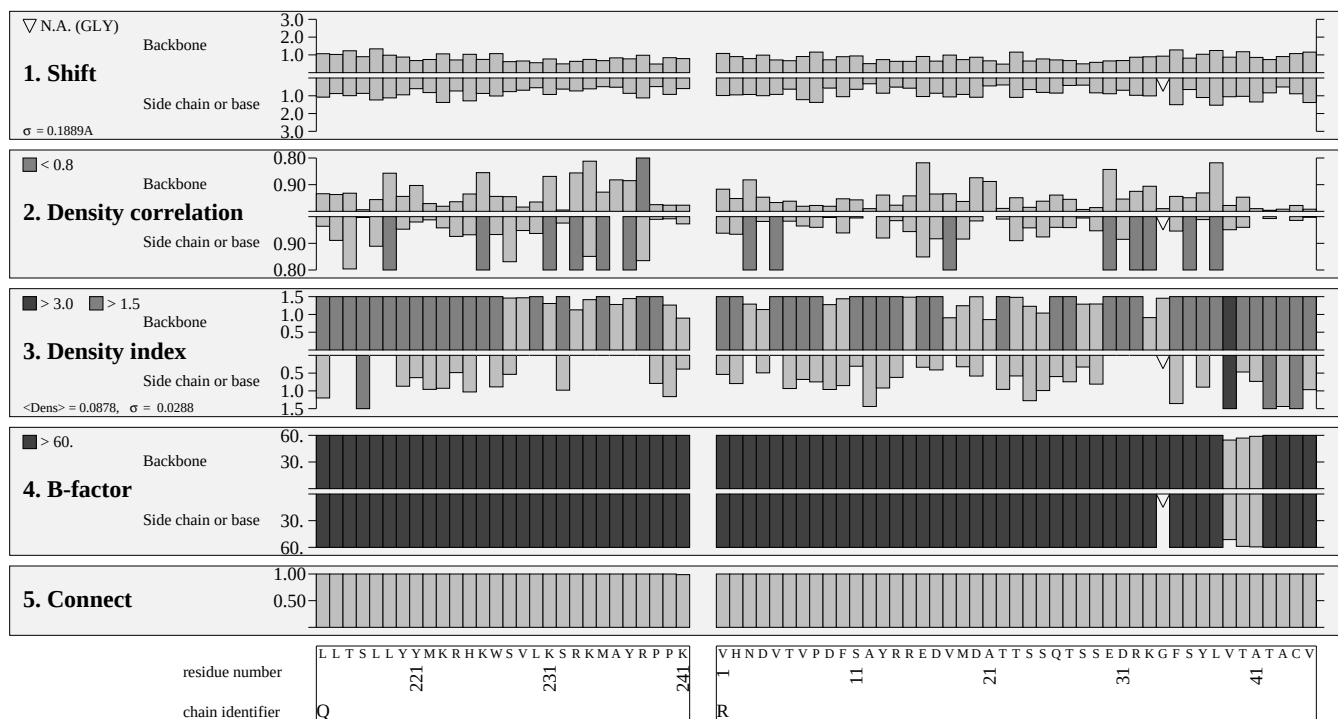
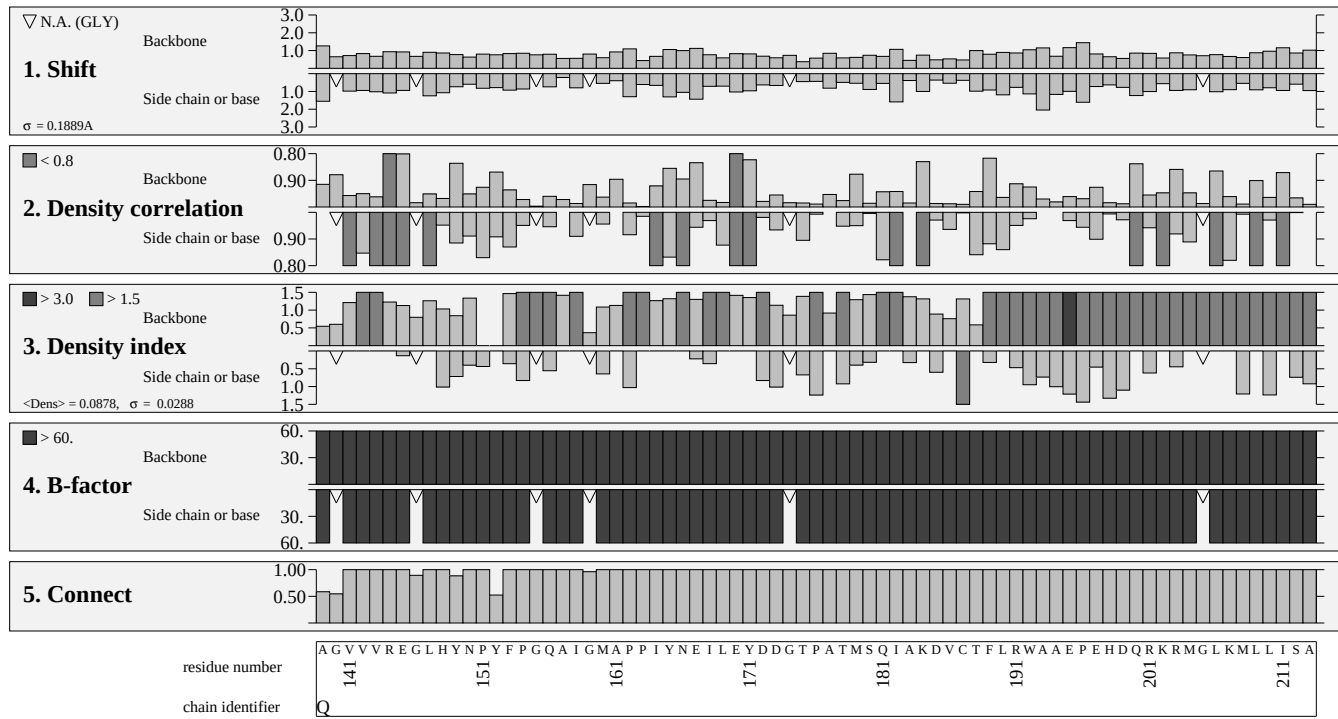
Local estimation (23)



Structure Factor Check

3CWB

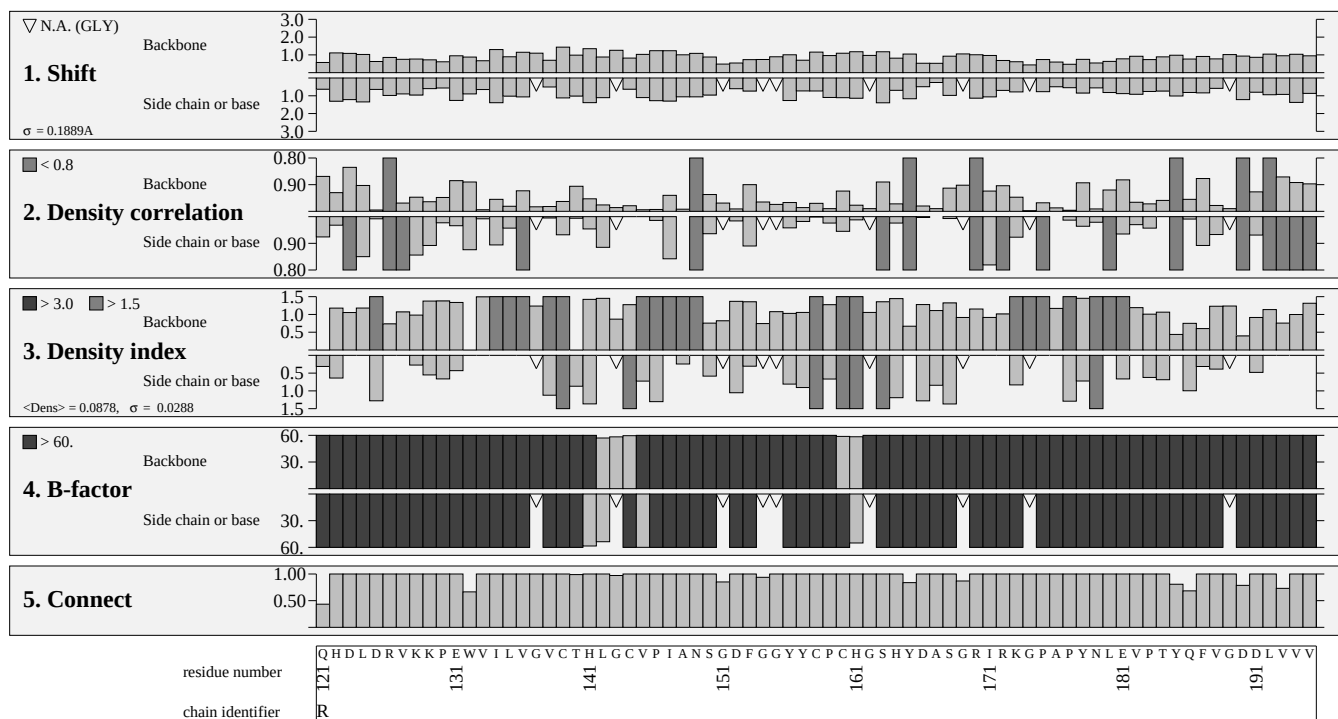
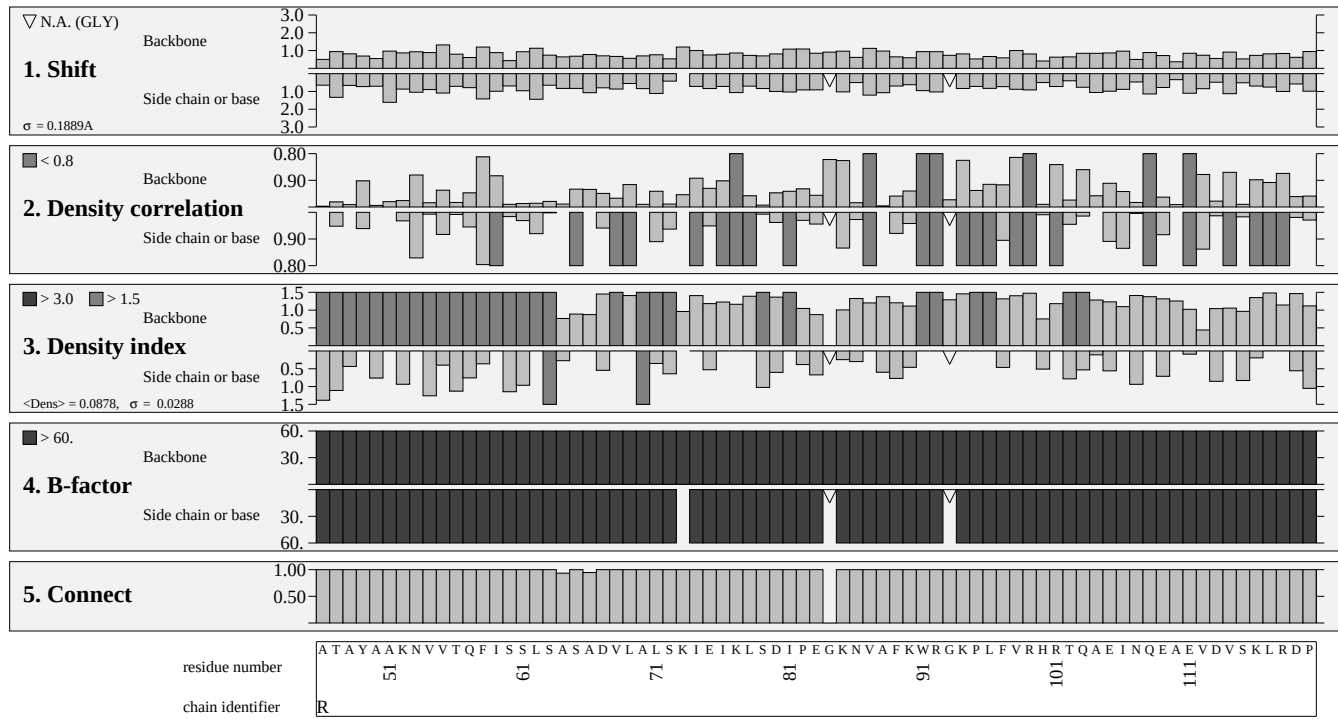
Local estimation (24)



Structure Factor Check

3CWB

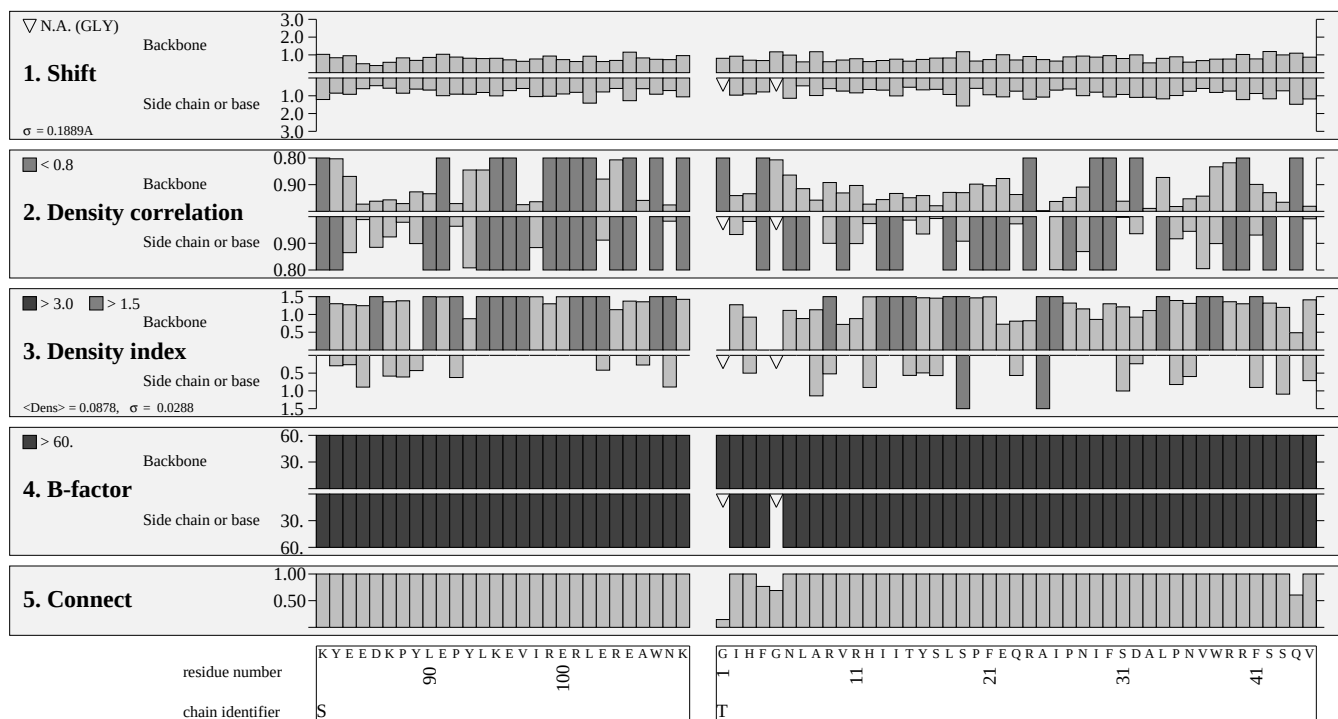
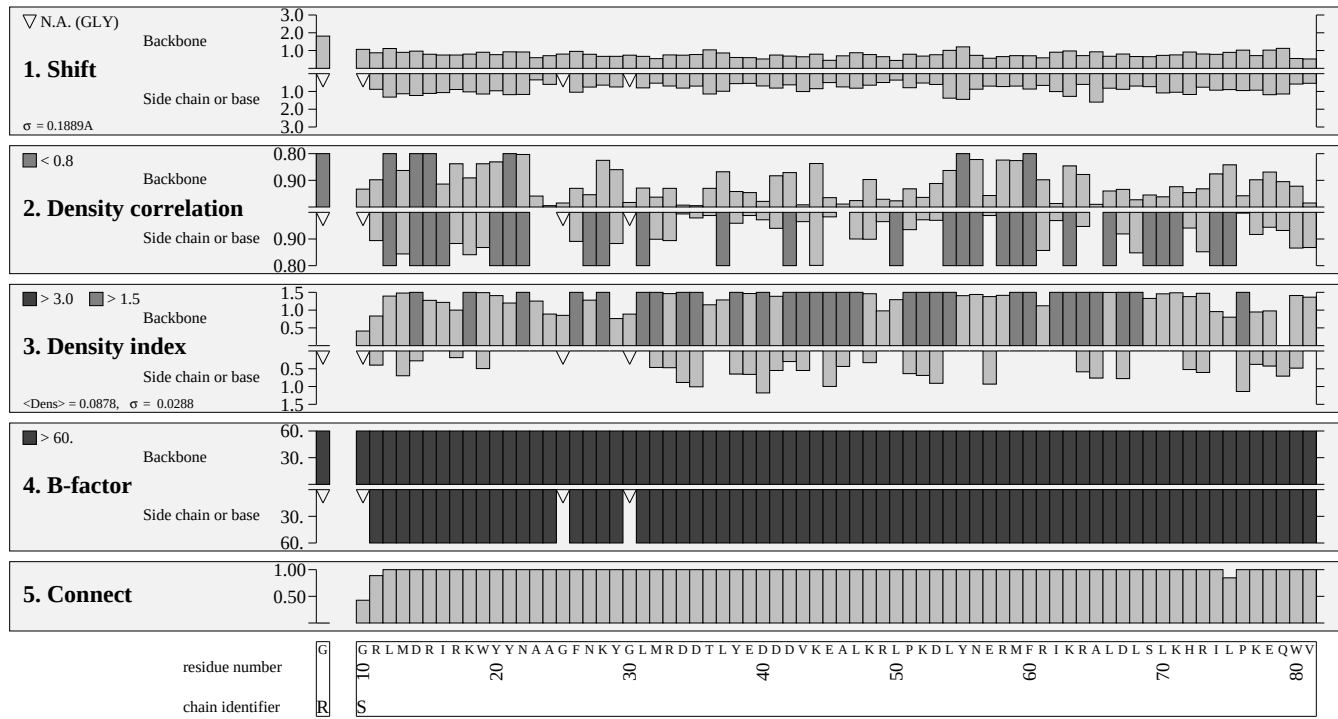
Local estimation (25)



Structure Factor Check

3CWB

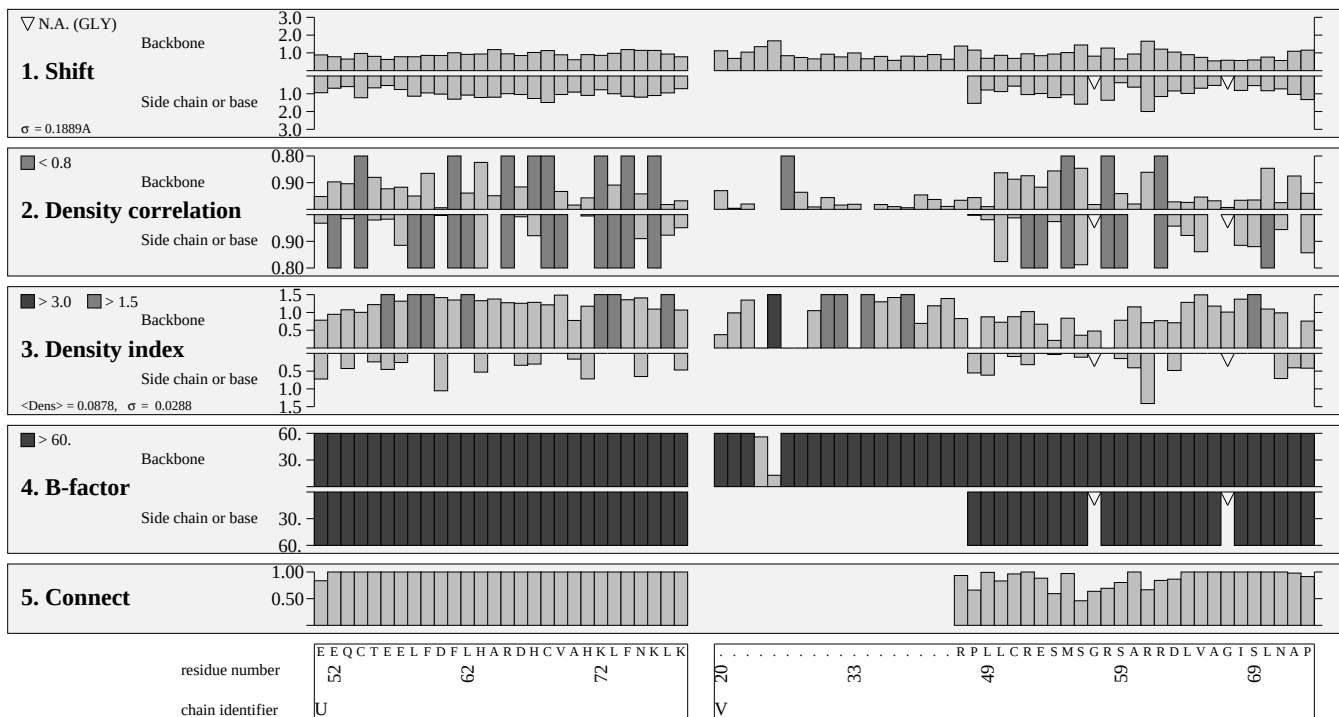
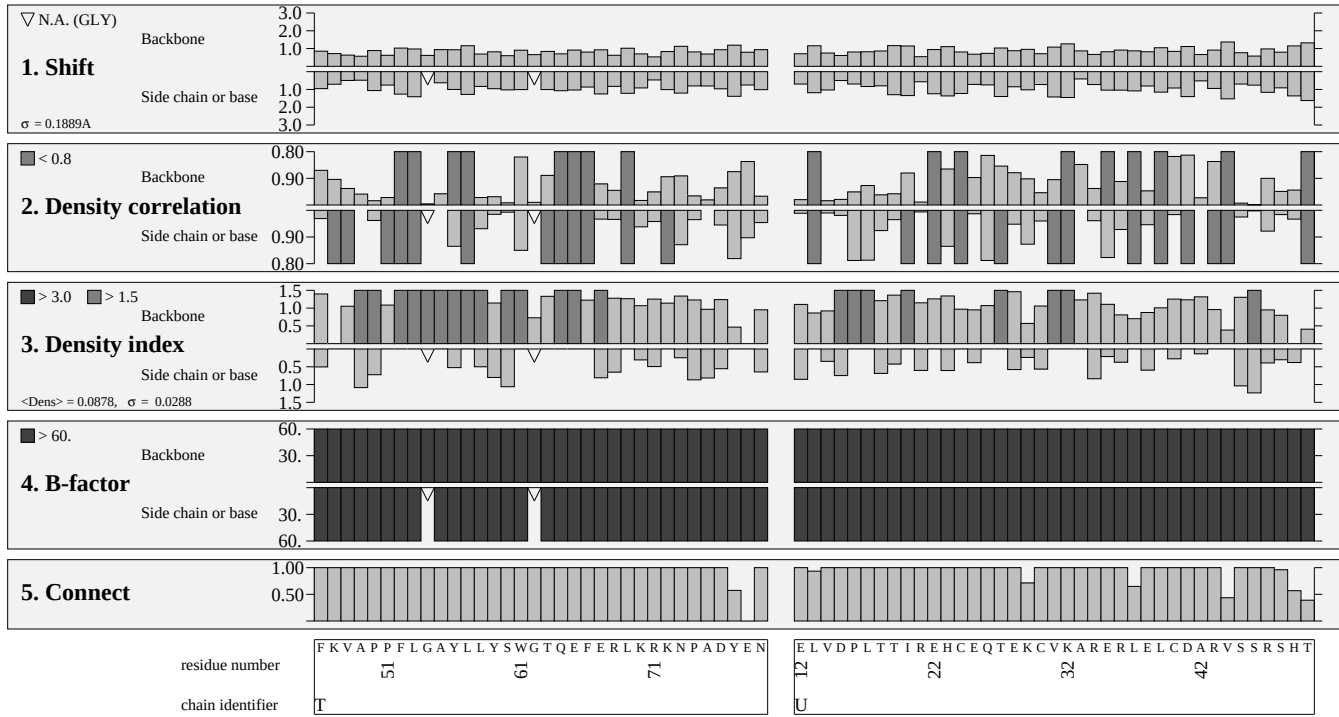
Local estimation (26)



Structure Factor Check

3CWB

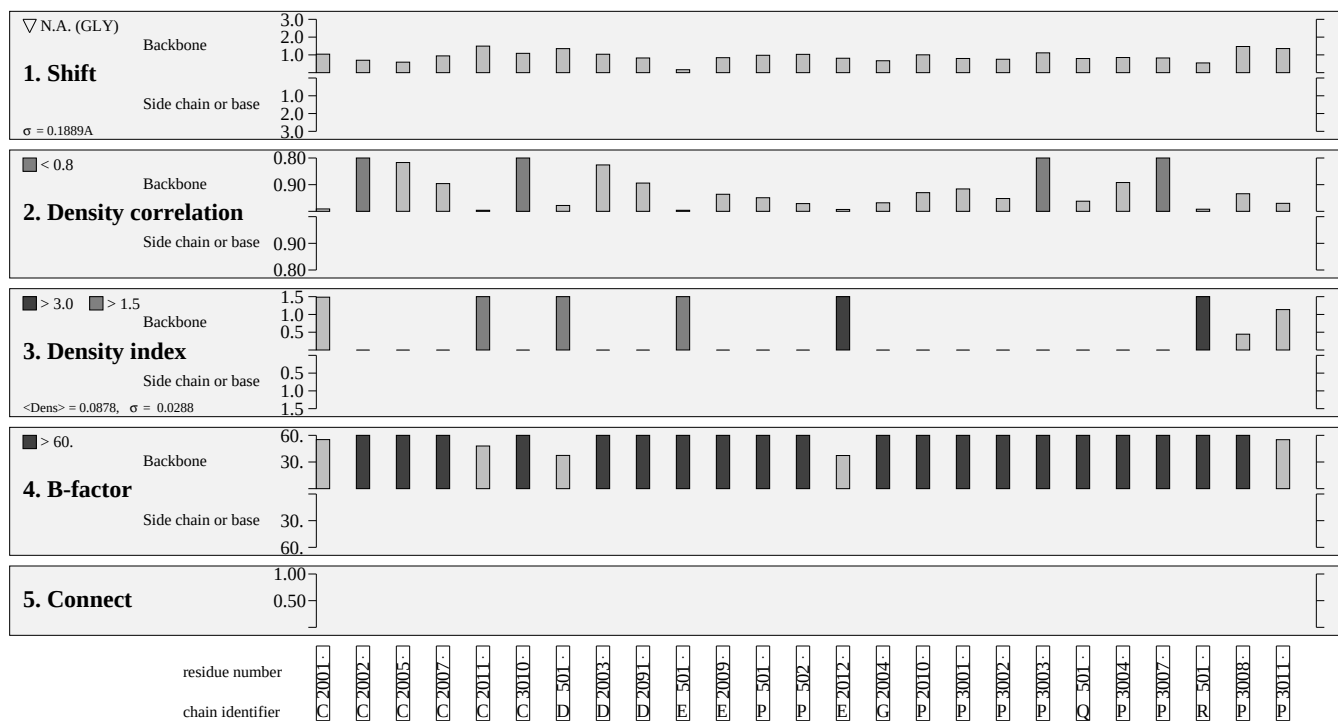
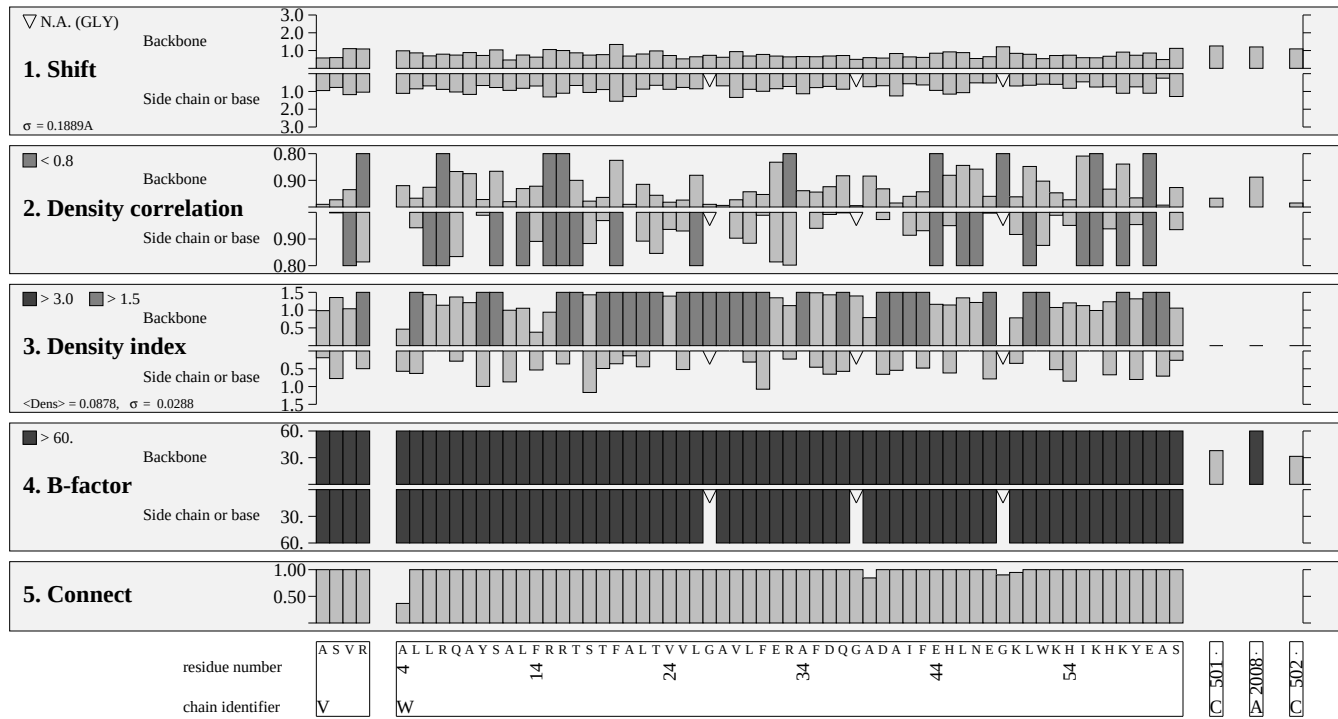
Local estimation (27)



Structure Factor Check

3CWB

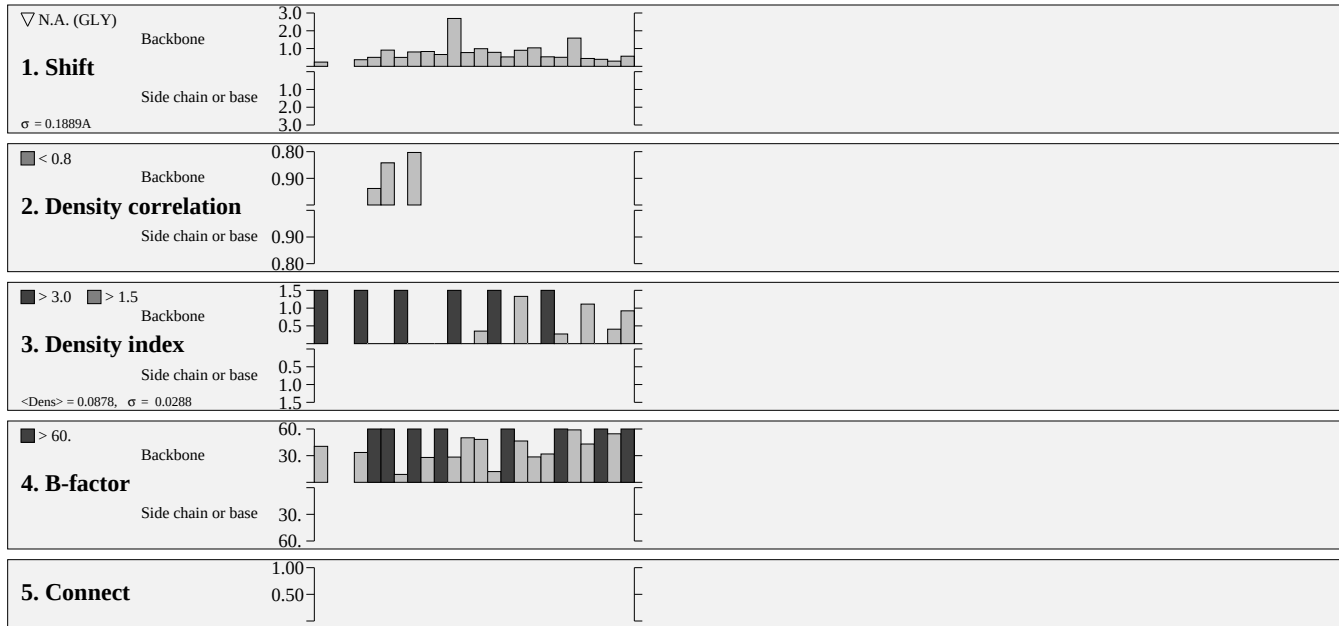
Local estimation (28)



Structure Factor Check

3CWB

Local estimation (29)



residue number	3013	3014	3015	3016	3017	3018	3019	3020	3021	3022	3023	3024	3025	3026	3027	3028	3029	3030	3031	3032	3033
chain identifier	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q	Q