

Structure Factor Check

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Title: BOVINE CYTOCHROME BC1 COMPLEX WITH STIGMATELLIN BOUND
Date: XX-XXX-XX
PDB code: XXXX

Crystal

Cell parameters:

a: 128.25 Å b: 168.80 Å c: 230.82 Å
 α : 90.00° β : 90.00° γ : 90.00°

Space group: P 21 21 21

Number of NCS-operators: 1
NC-symmetry only for information

Structure Factors

Input

Nominal resolution range: 37.9 – 2.00 Å
Reflections in file: 308086
Unique reflections above 0: 308086
 above 1 σ : 300977
 above 3 σ : 180169

SFCHECK

Nominal resolution range: 37.9 – 2.10 Å
(max. from input data, min. from author)
Used reflections: 276806
Reflections out of resolution: 31280
Completeness: 95.3 %
R_{stand}(F) = $\langle \sigma(F) \rangle / \langle F \rangle$: 0.057
Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.9620 1.0000 0.8986
B_{overall} (by Patterson): 36.6 Å²
Optical resolution: 1.73 Å
Expected opt. resol. for complete data set: 1.73 Å
Estimated minimal error: 0.033 Å

Model

33890 atoms (1612 water molecules)
Number of chains: 51
Volume not occupied by model: 44.9 %
 (for atomic model): 48.1 Å²
 σ (B): 16.67 Å²
Matthews coefficient: 2.76
Corresponding solvent % : 55.16

Model vs. Structure Factors

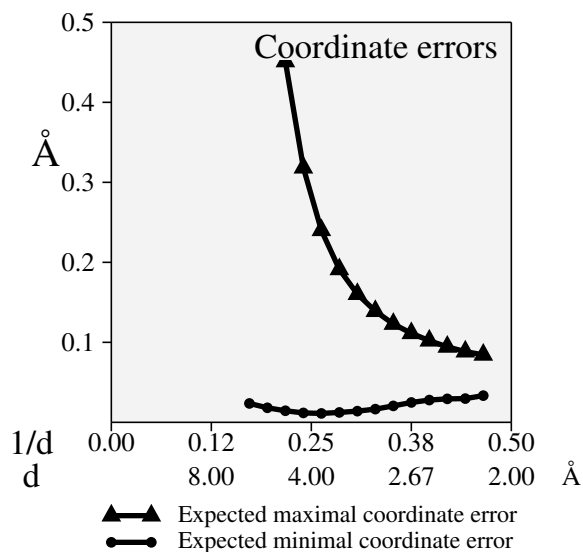
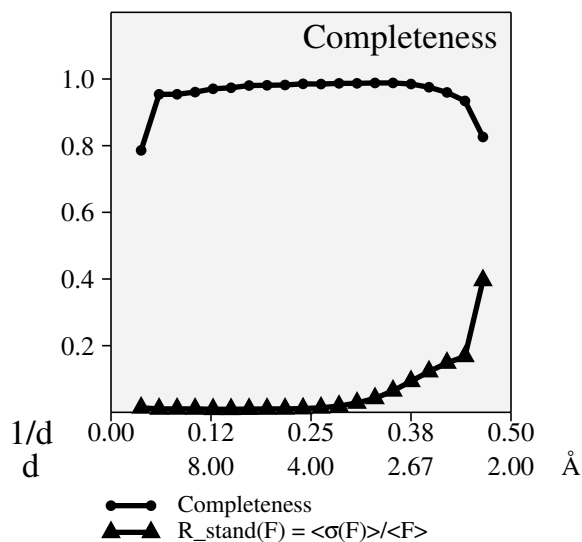
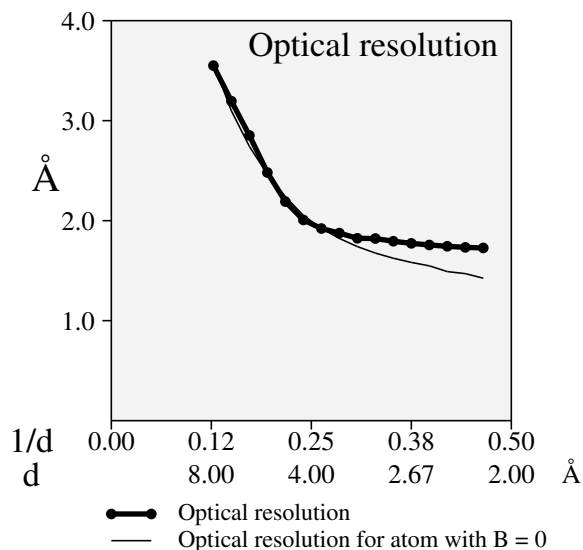
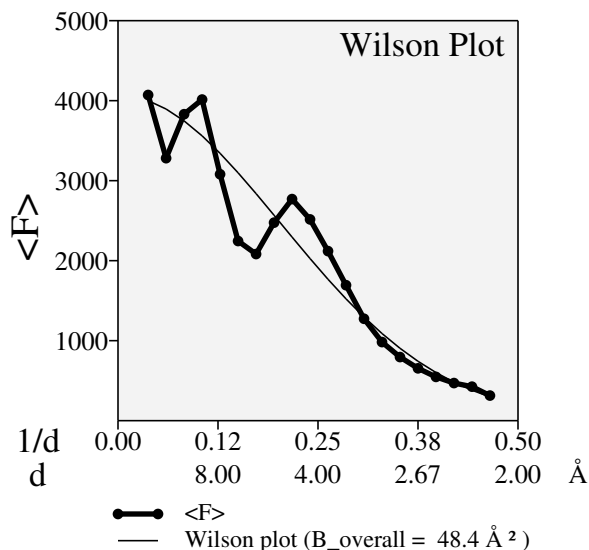
R-factor for all reflections: 0.238
Correlation factor: 0.933
R-factor: 0.243
 for F > 2.0 σ
 nom. resolution range: 37.87 – 2.10 Å
 reflections used: 271206
Rfree: 0.282
Nfree: 13477
R-factor without free-refl.: 0.241
Non free-reflections: 257729
<u> (error in coords by Luzzati plot): 0.300 Å
Estimated maximal error: 0.084 Å
DPI: 0.174 Å
Scaling
Scale: 1.718
Bdiff: -4.66
Anisothermal Scaling (Beta):
 1.9763 2.2038 0.7639 0.0000 0.0000 0.0000
Solvent correction – Ks,Bs: 0.832 250.036

Refinement

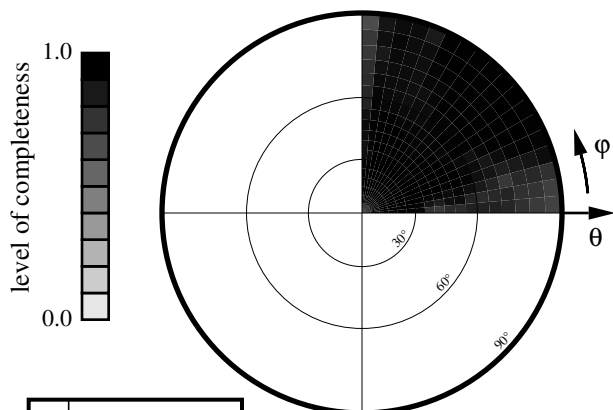
Program: CNS 1.1
Nominal resolution range: 37.9 – 2.10 Å
Reported R-factor: 0.222
Number of reflections used: 276810
Reported Rfree: 0.26
Sigma cut-off: N.A.

Structure Factor Check

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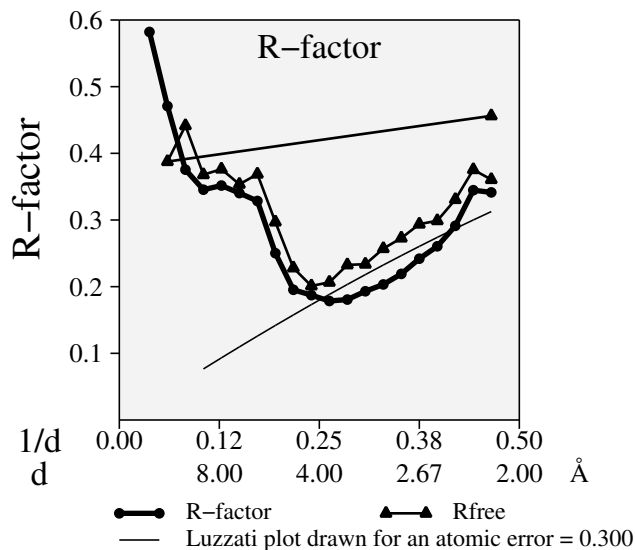


Stereographic projection of the averaged radial completeness



	θ	φ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

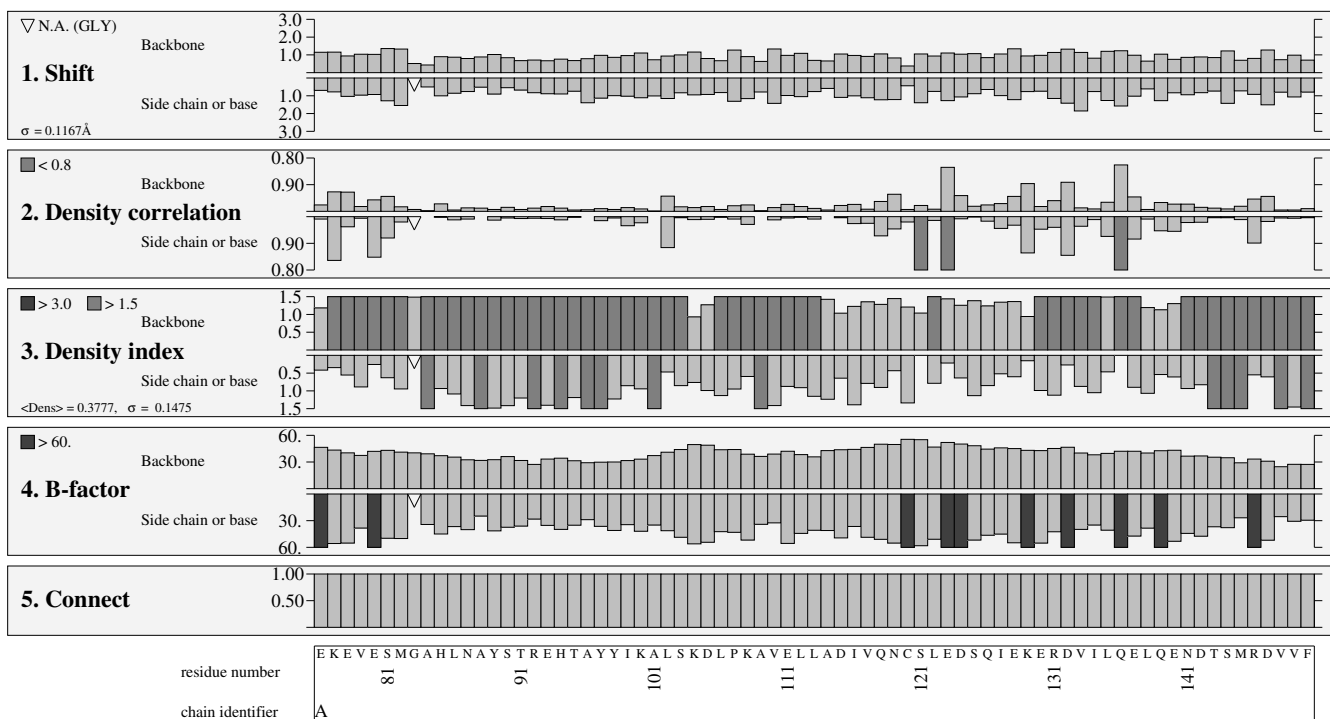
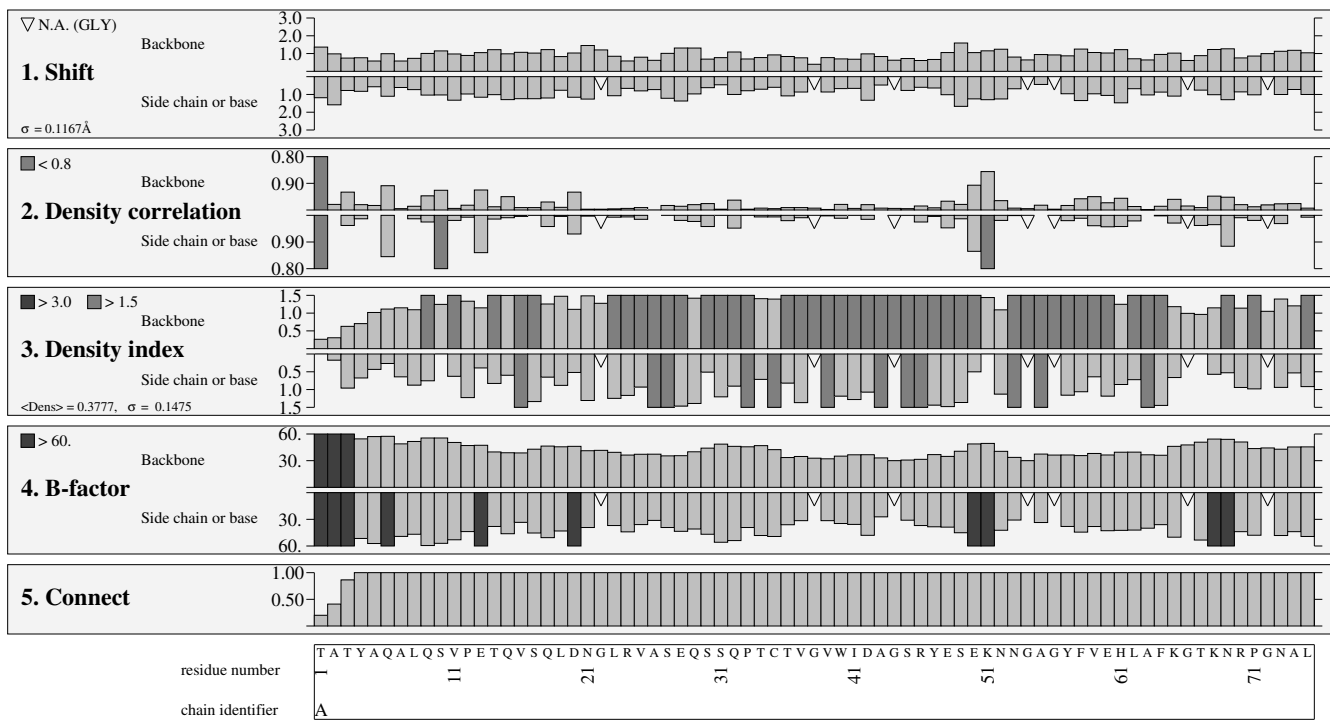
polar coordinates of the crystallographical axes



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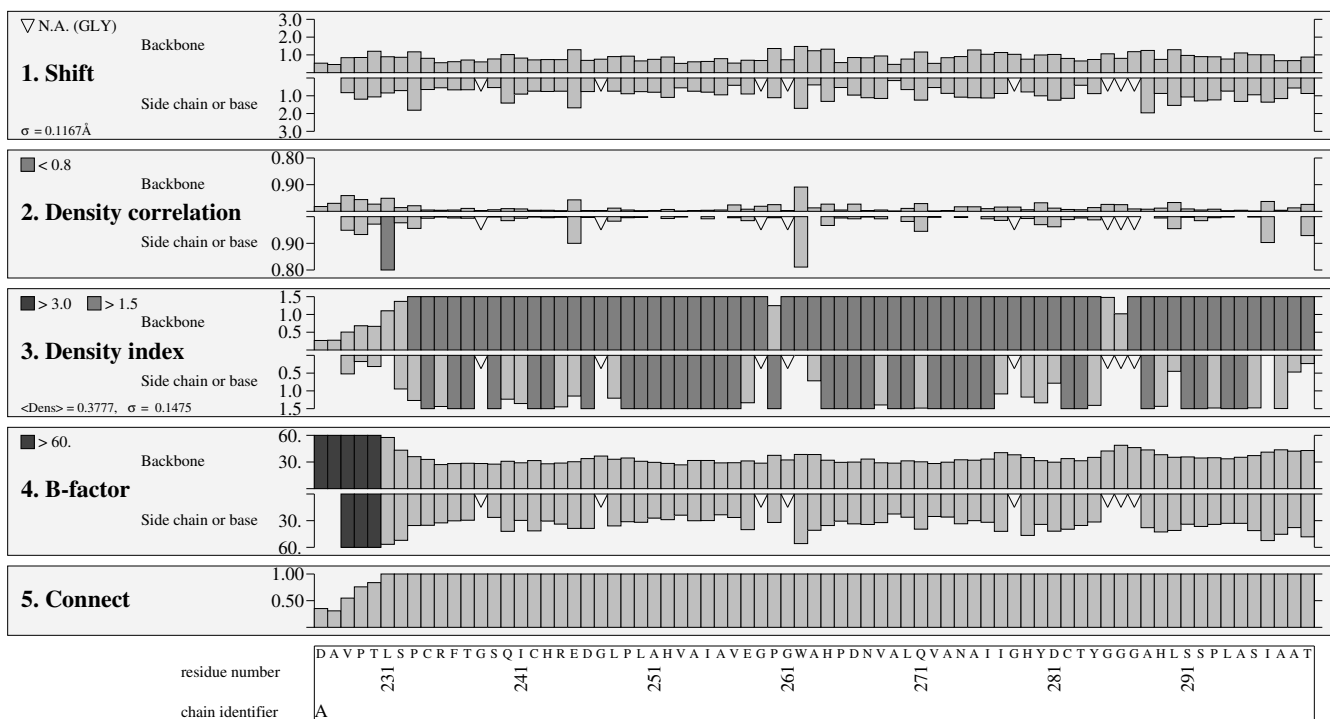
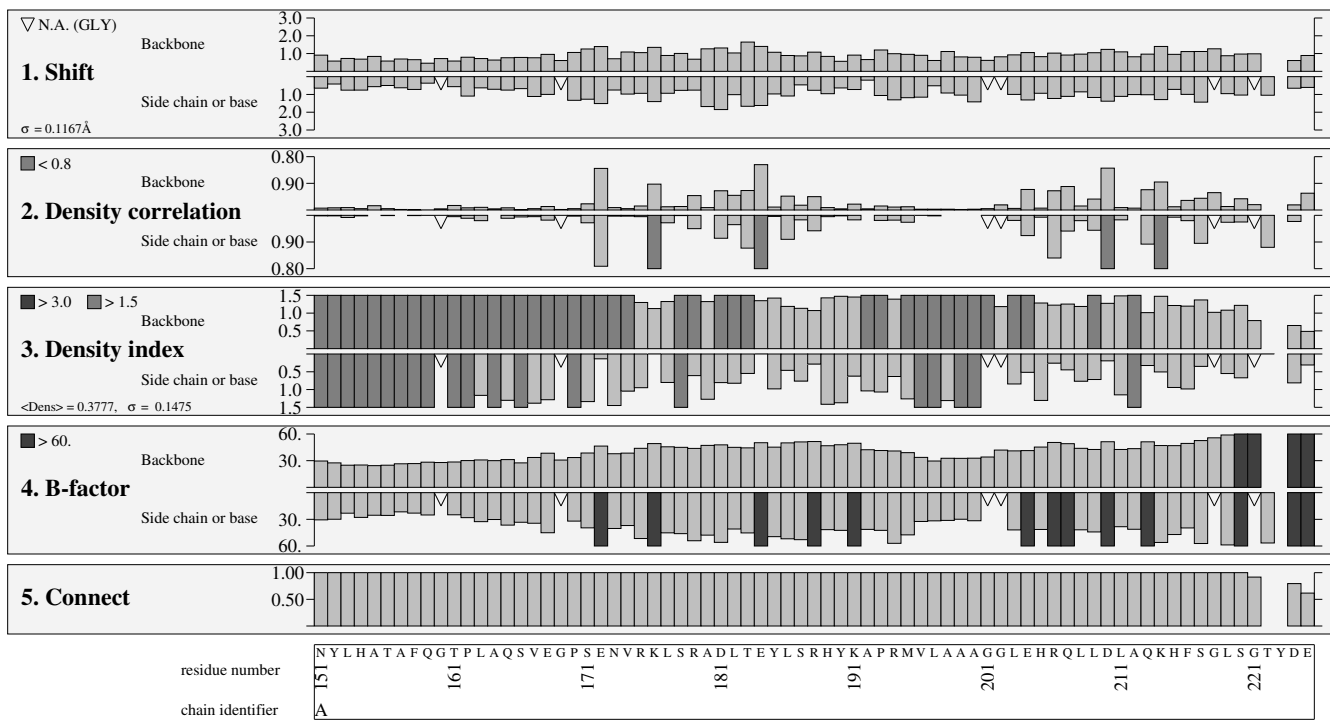
Local estimation



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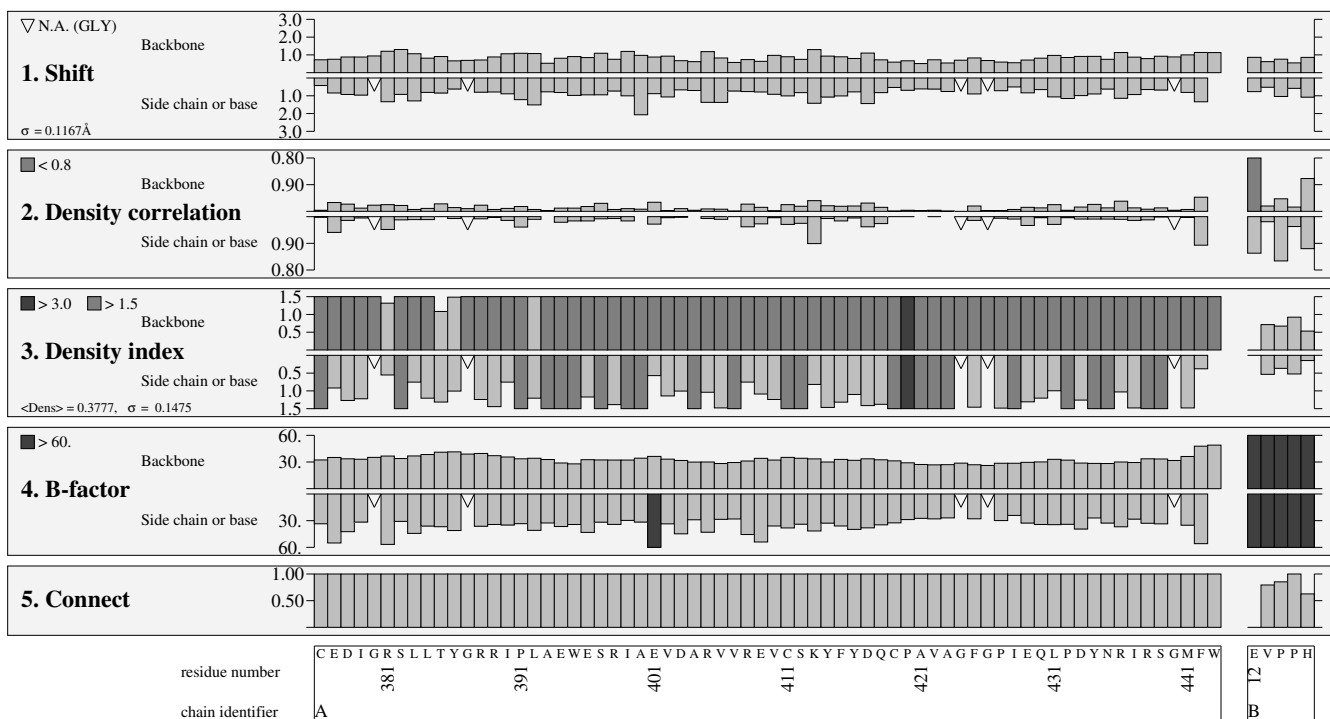
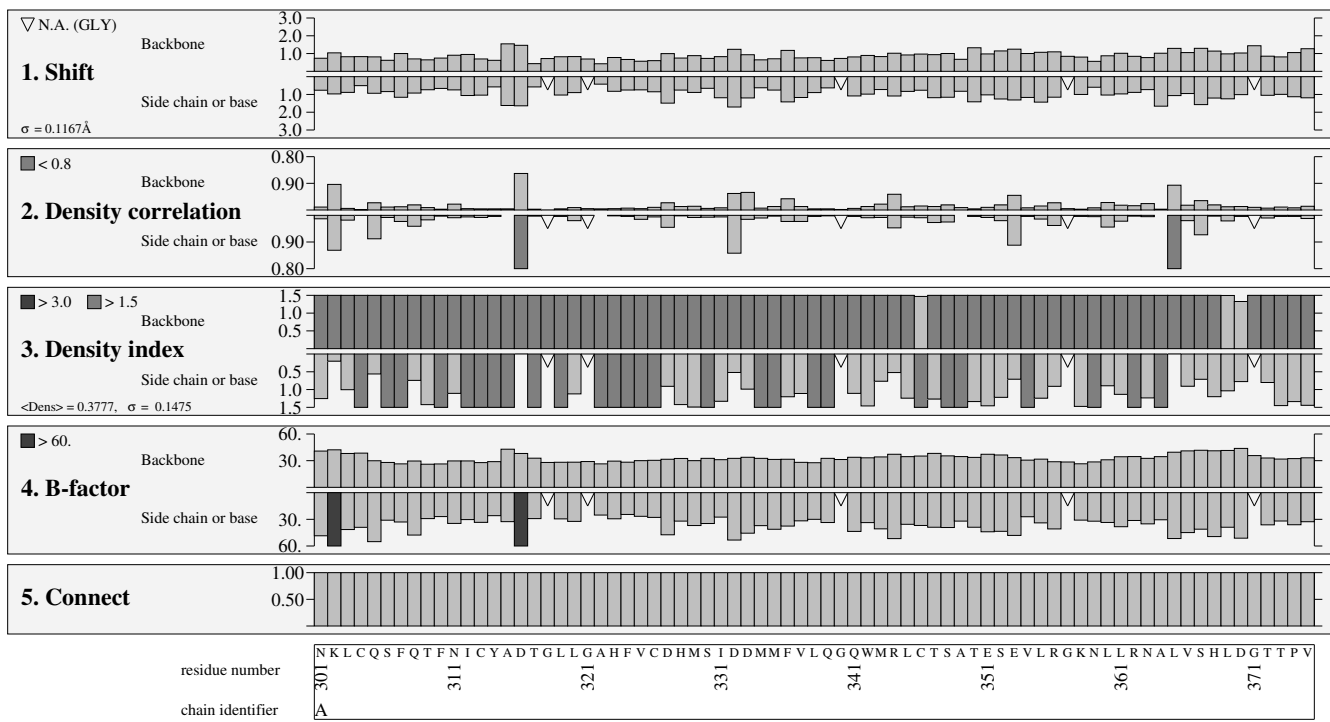
Local estimation (2)



Structure Factor Check

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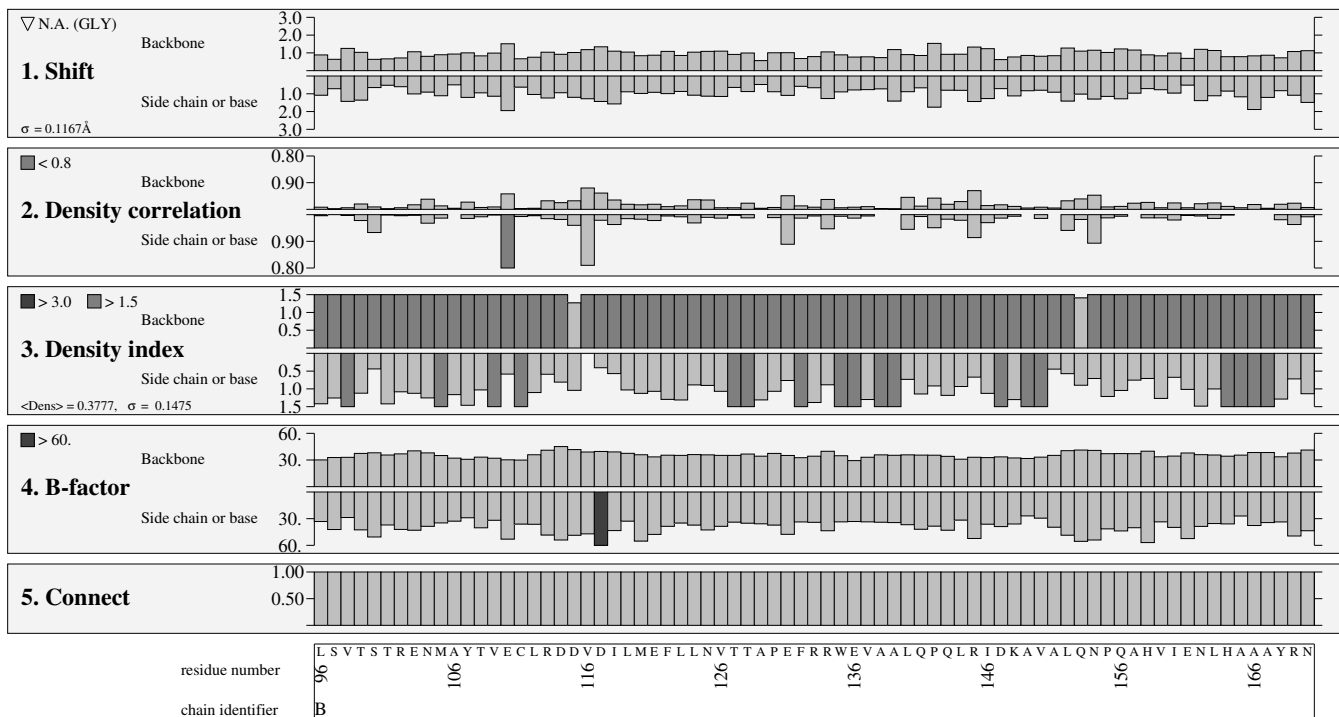
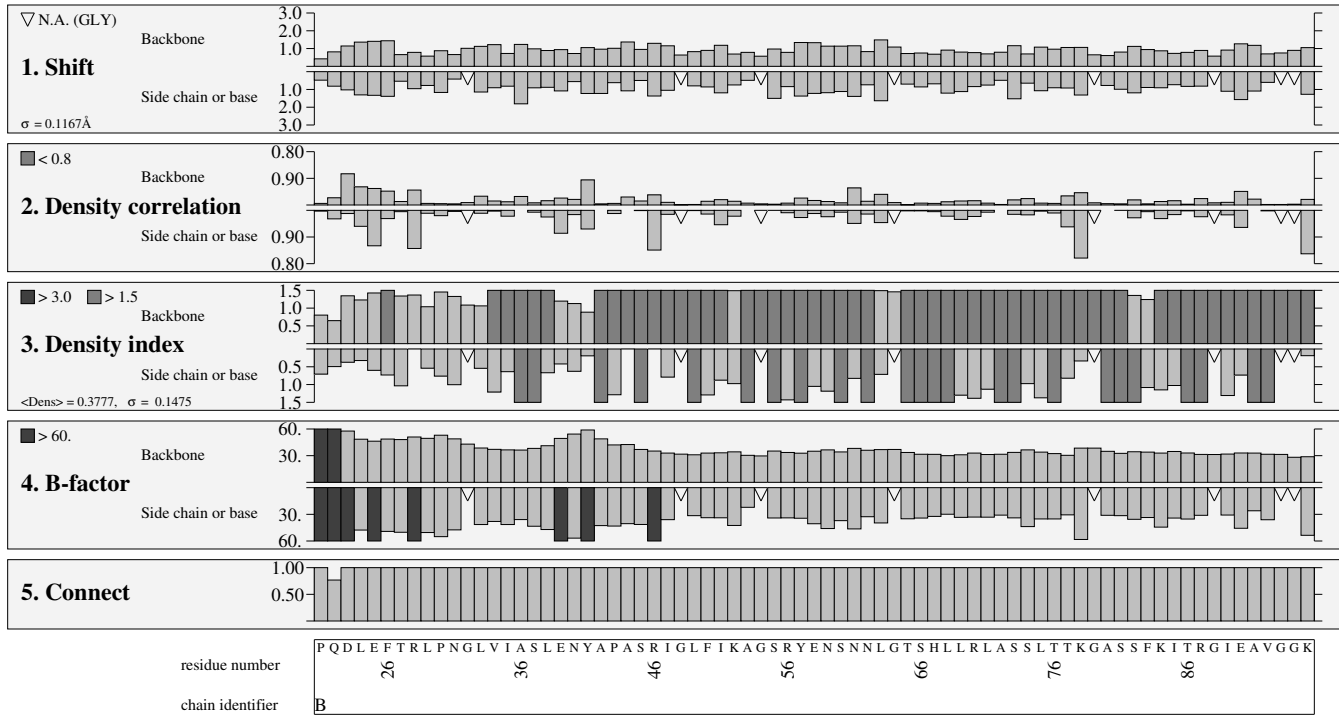
Local estimation (3)



Structure Factor Check

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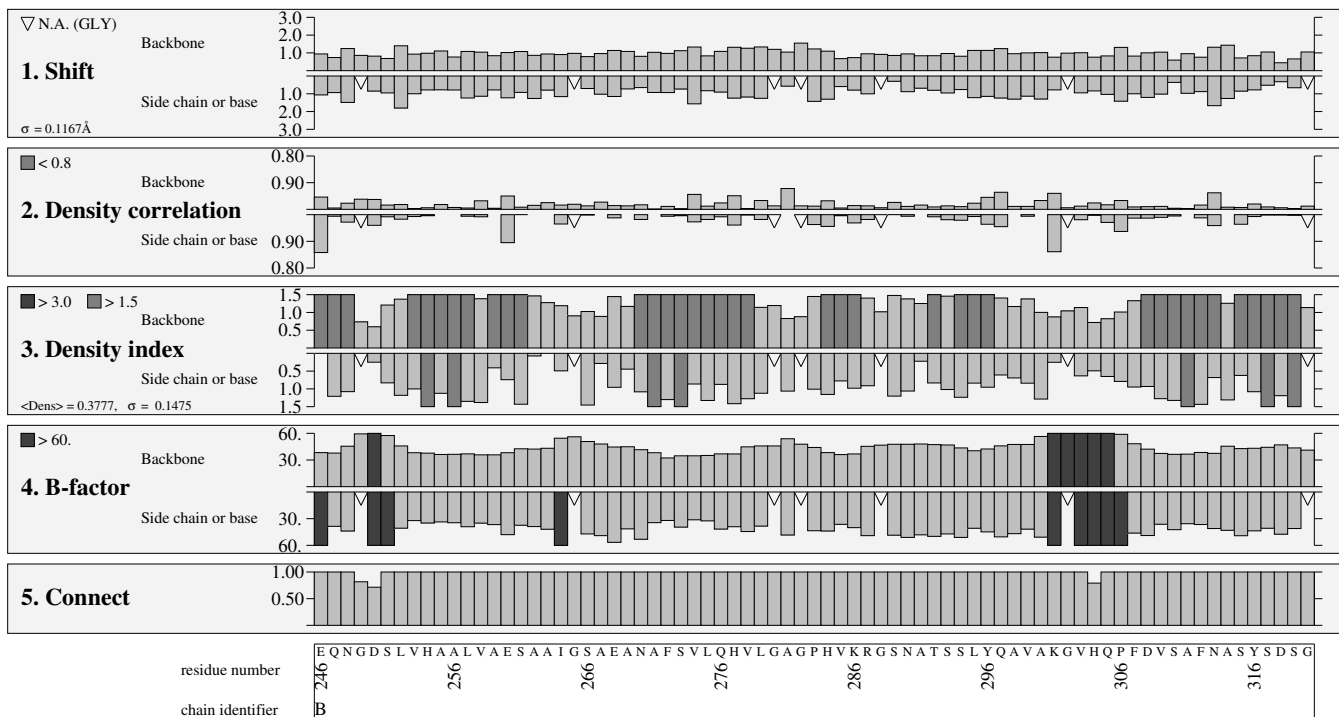
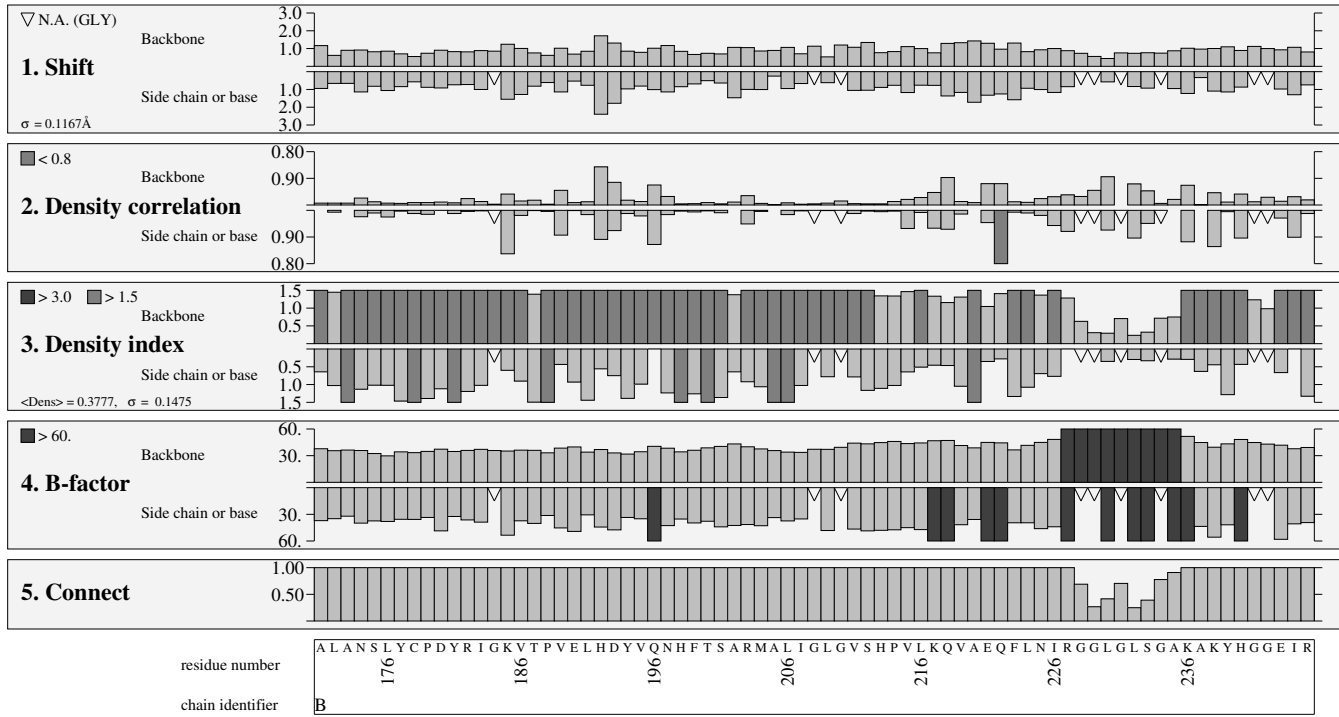
Local estimation (4)



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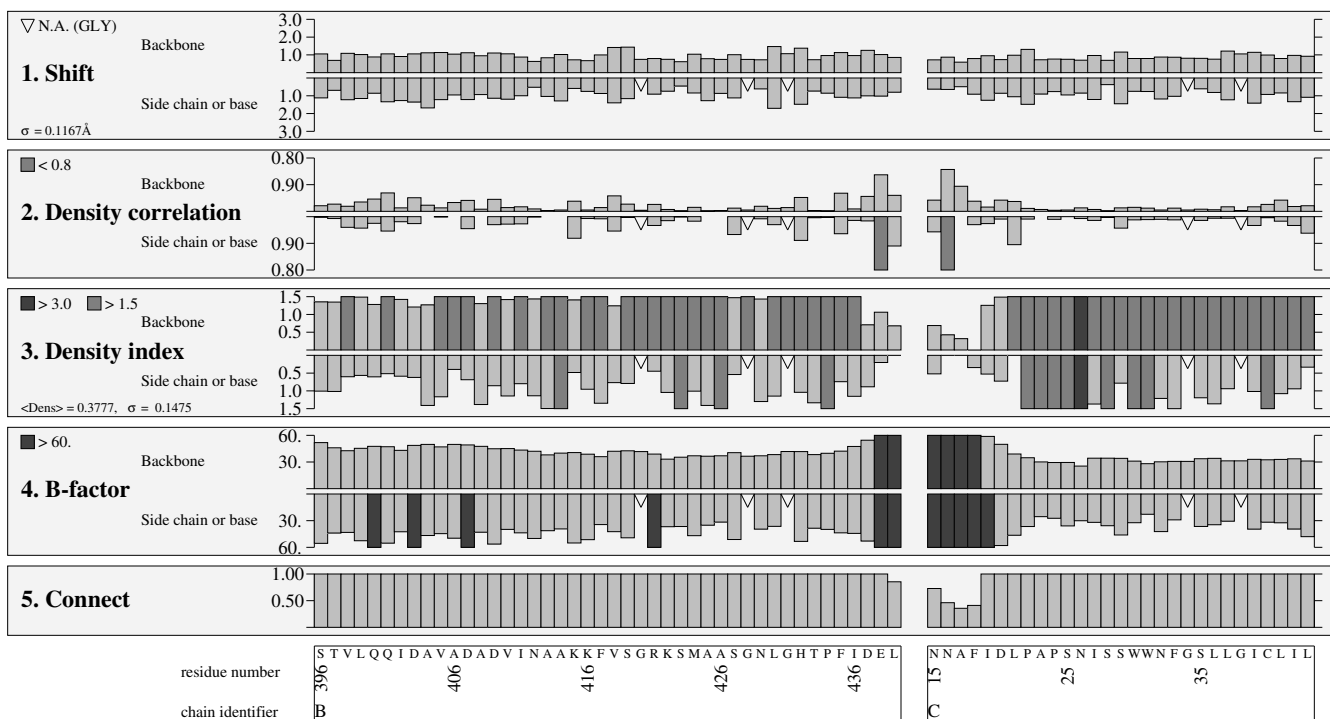
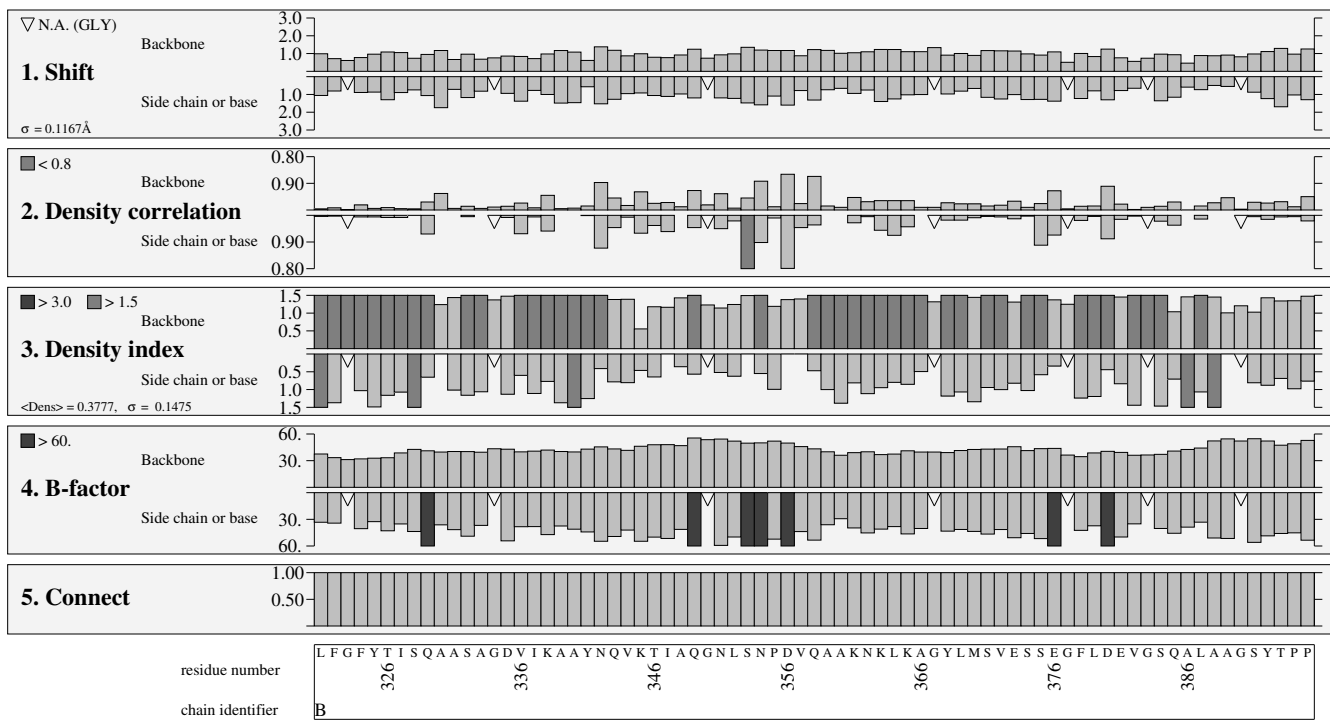
Local estimation (5)



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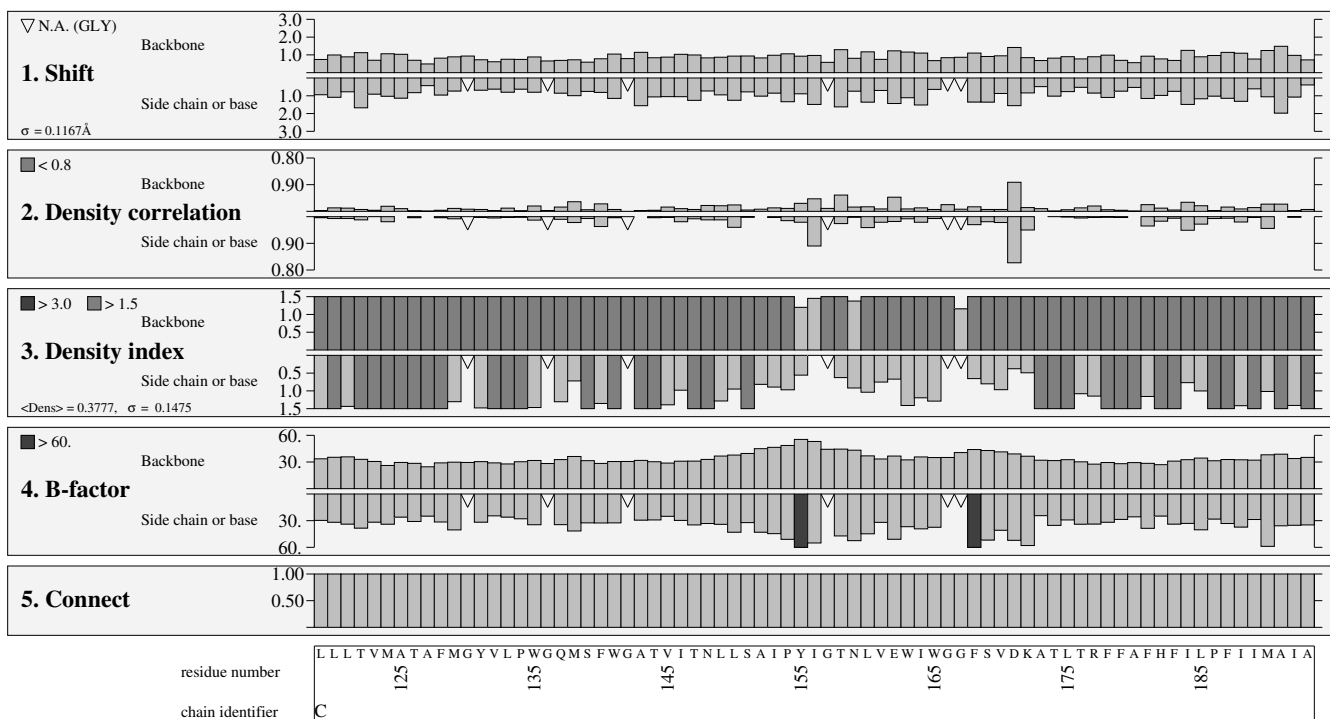
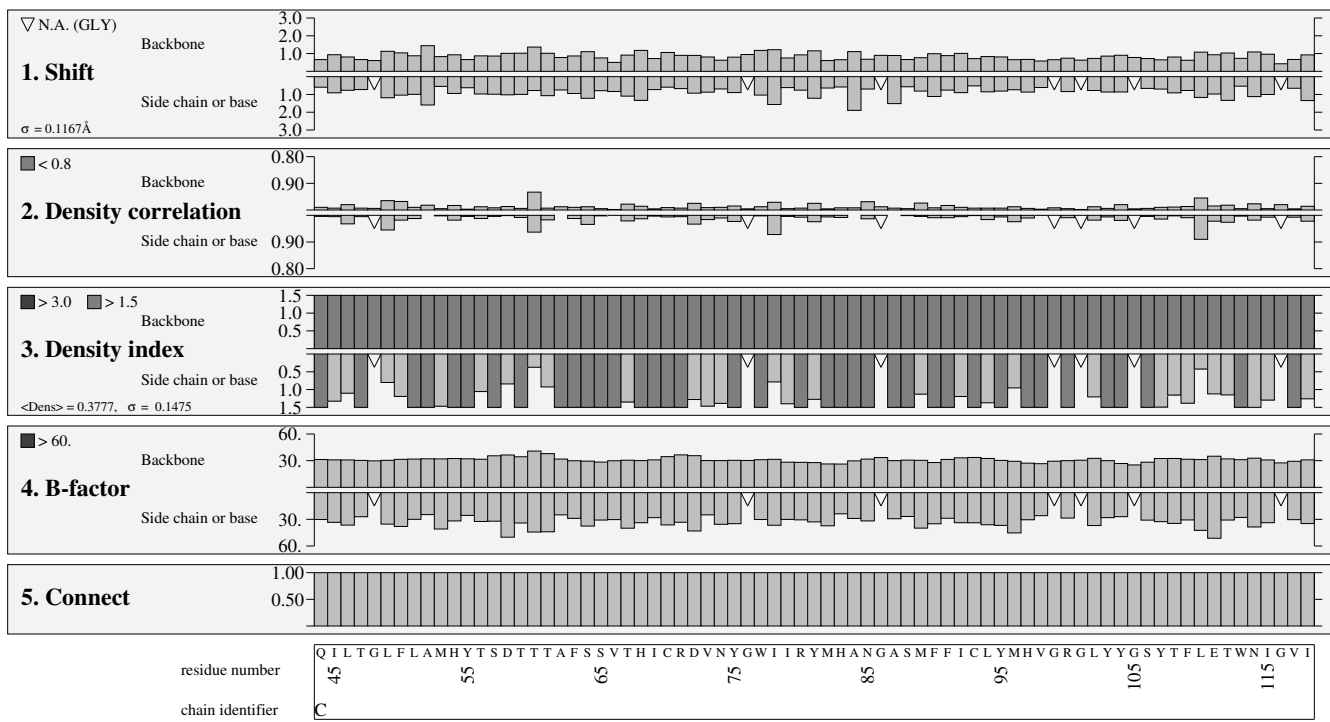
Local estimation (6)



Structure Factor Check

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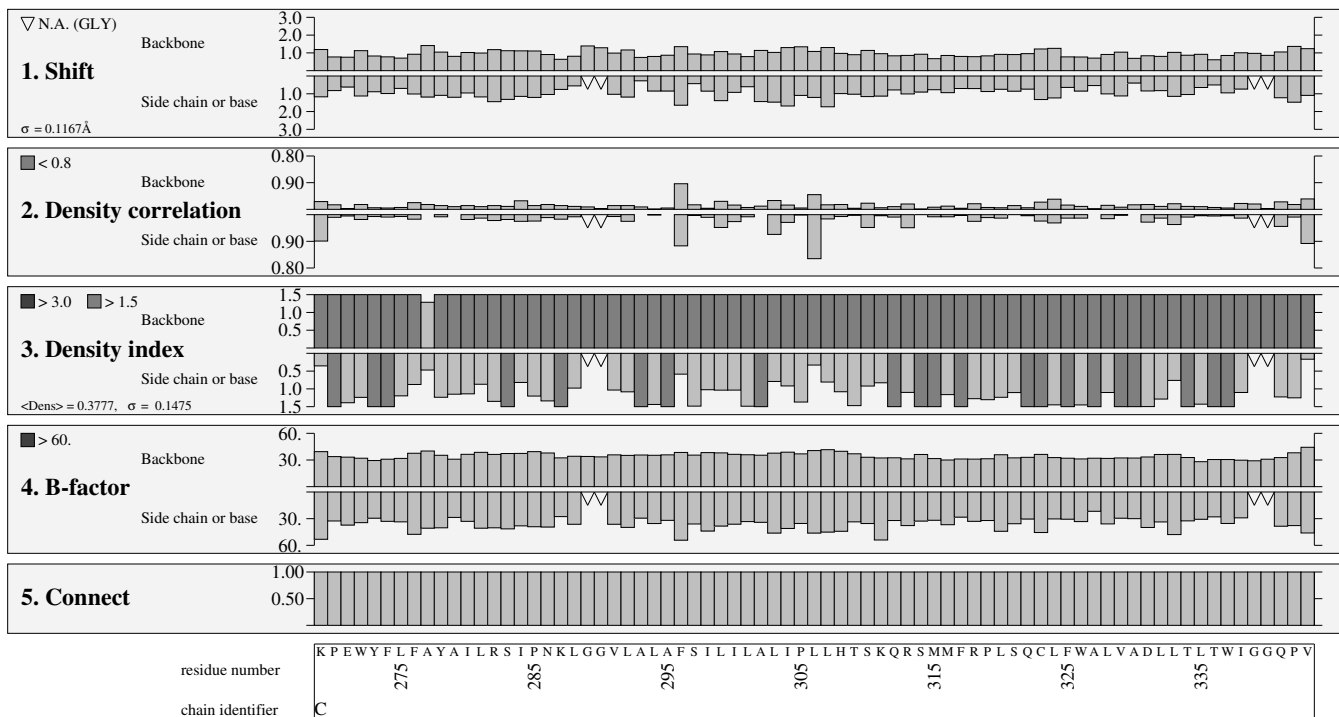
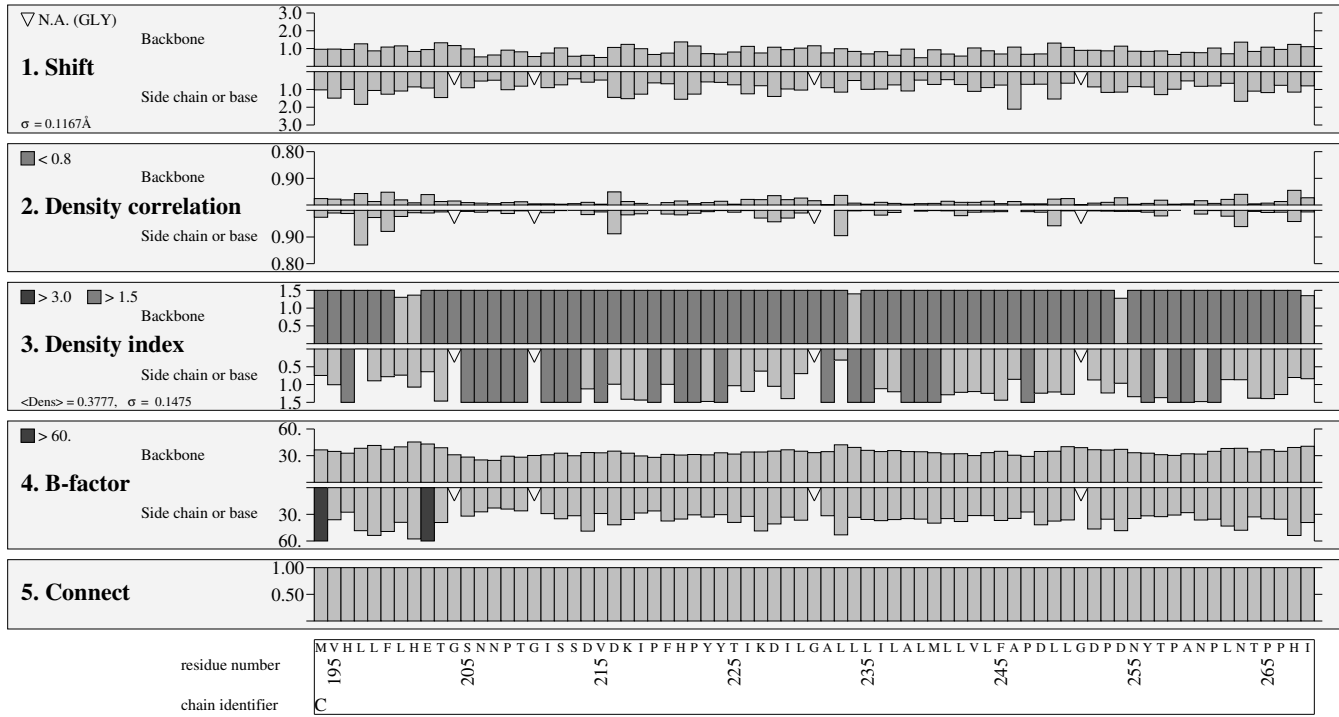
Local estimation (7)



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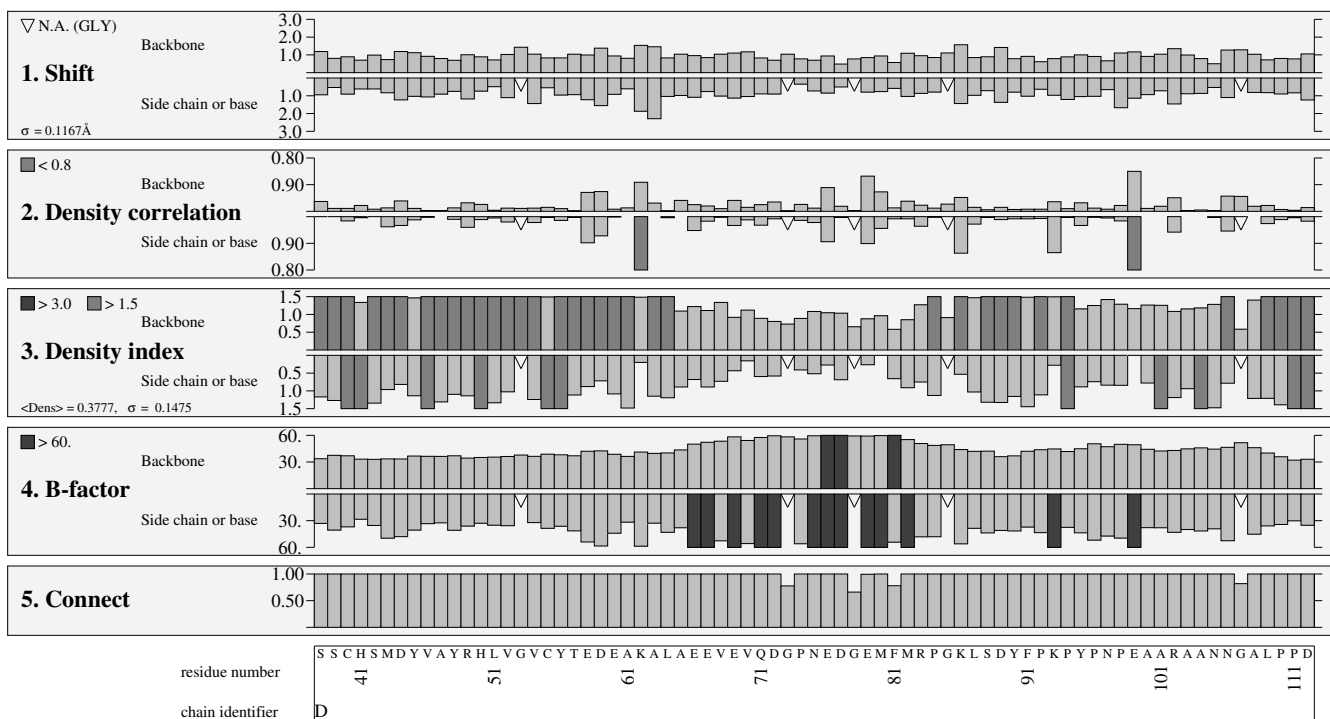
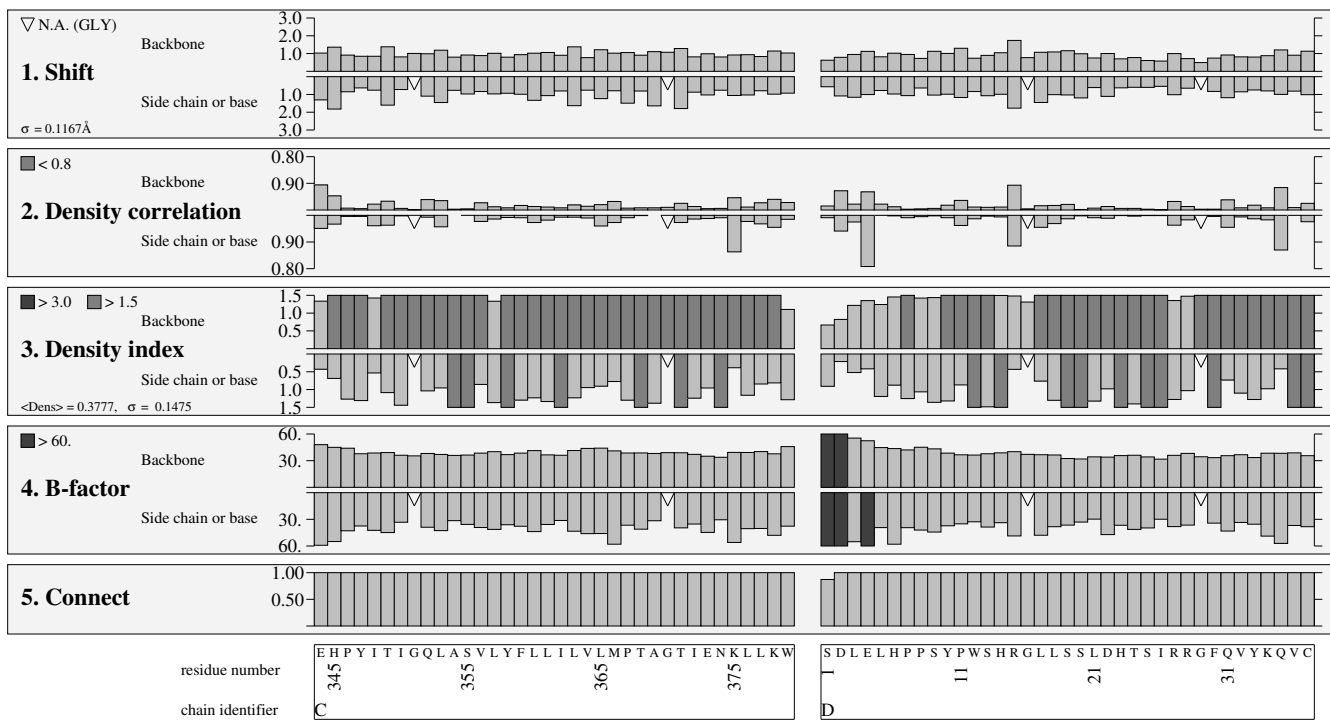
Local estimation (8)



Structure Factor Check

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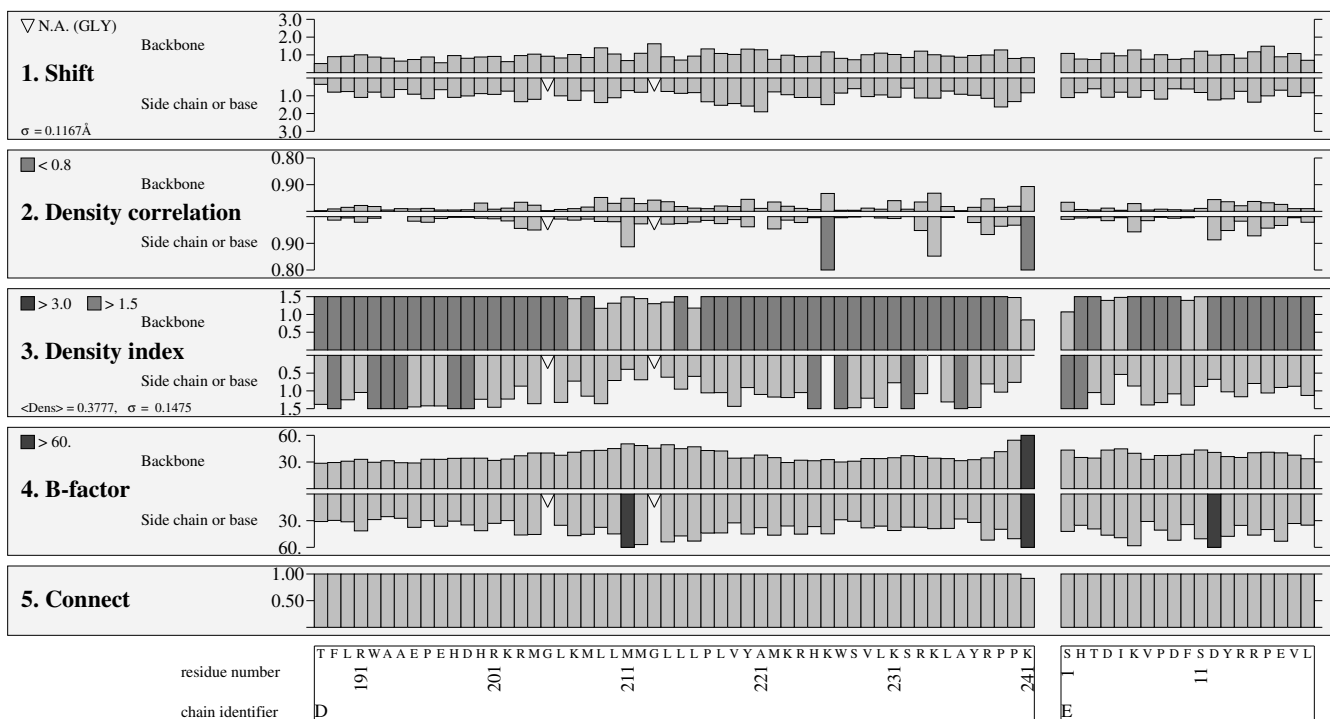
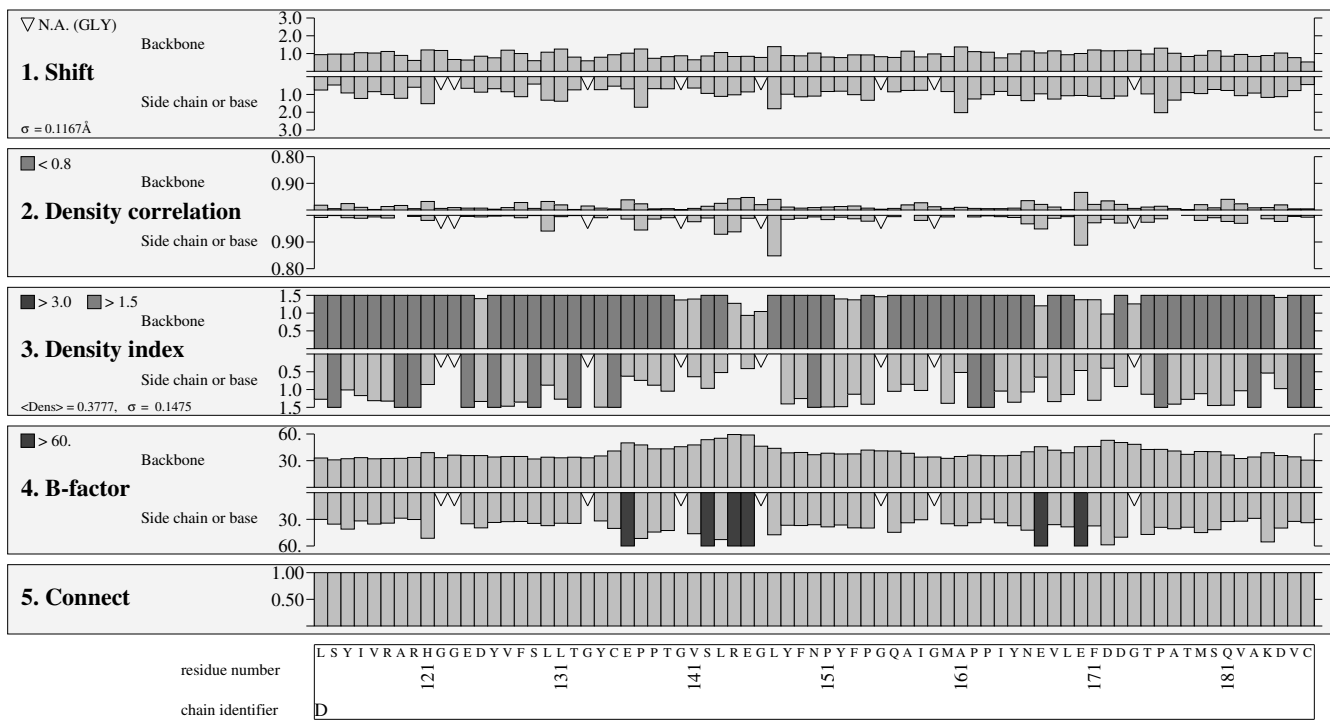
Local estimation (9)



Structure Factor Check

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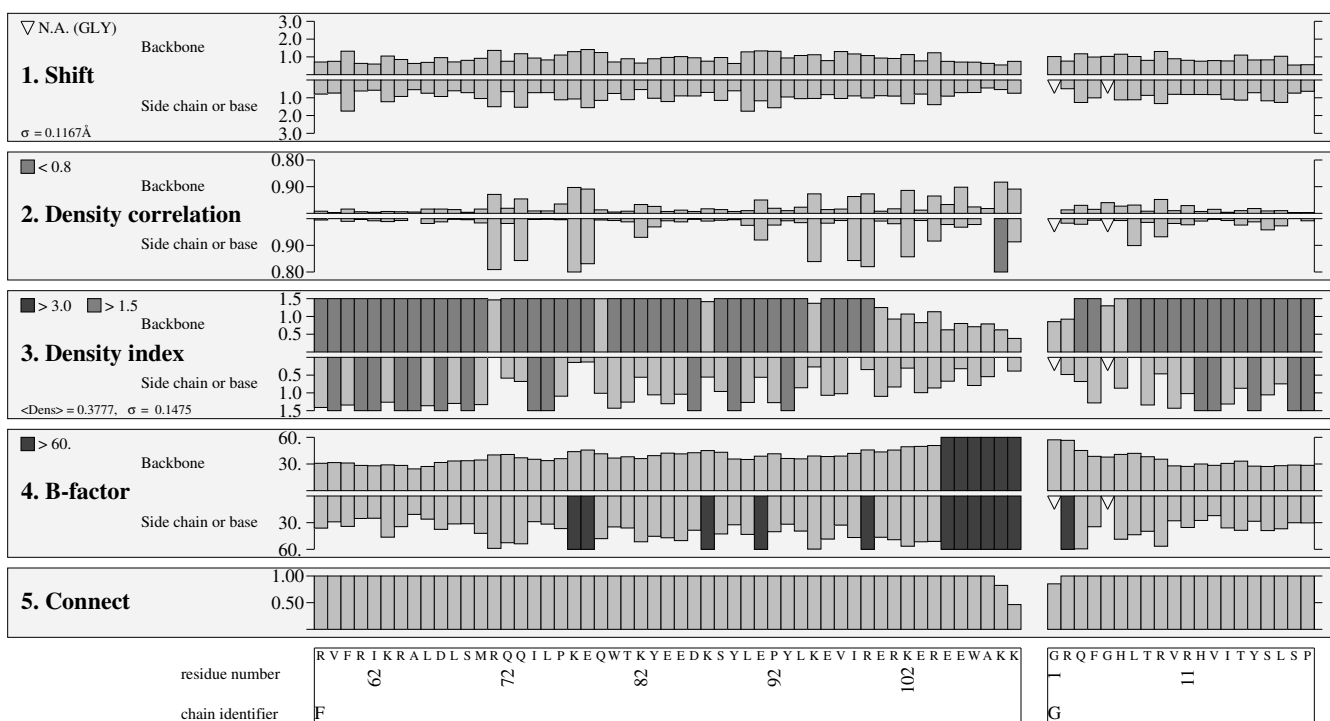
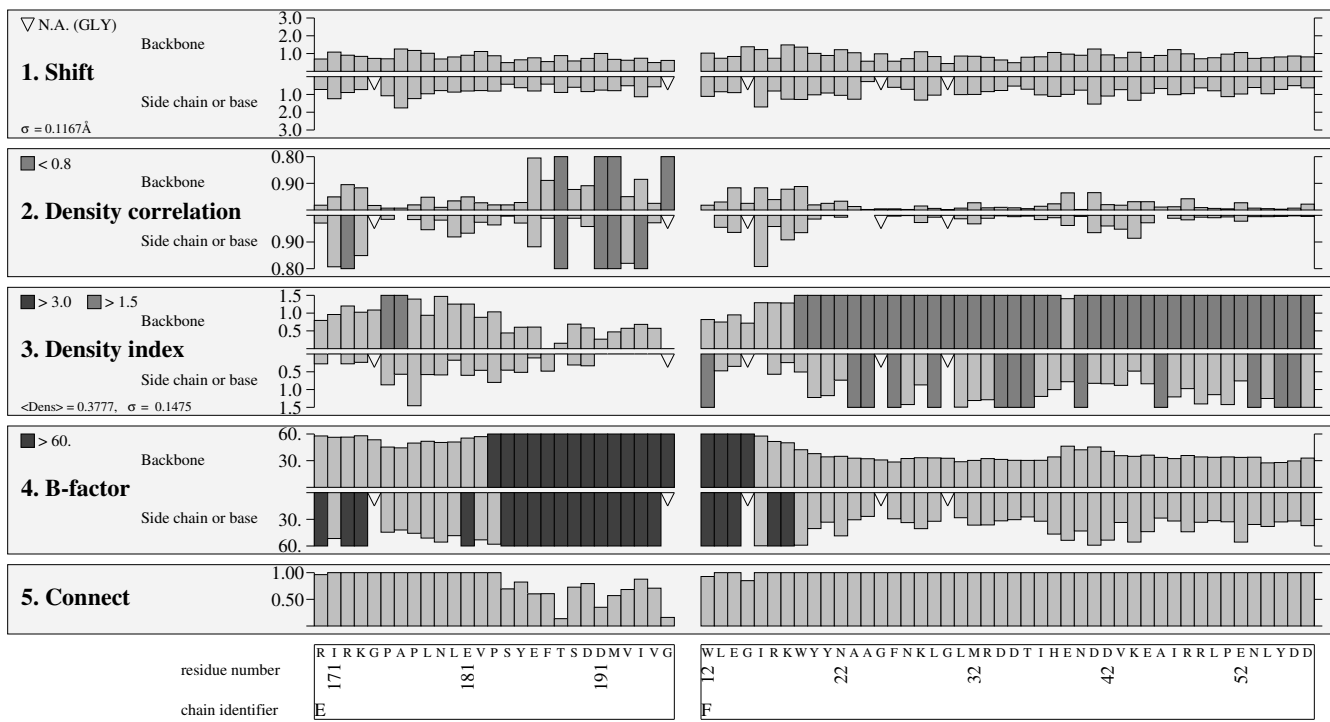
Local estimation (10)



Structure Factor Check

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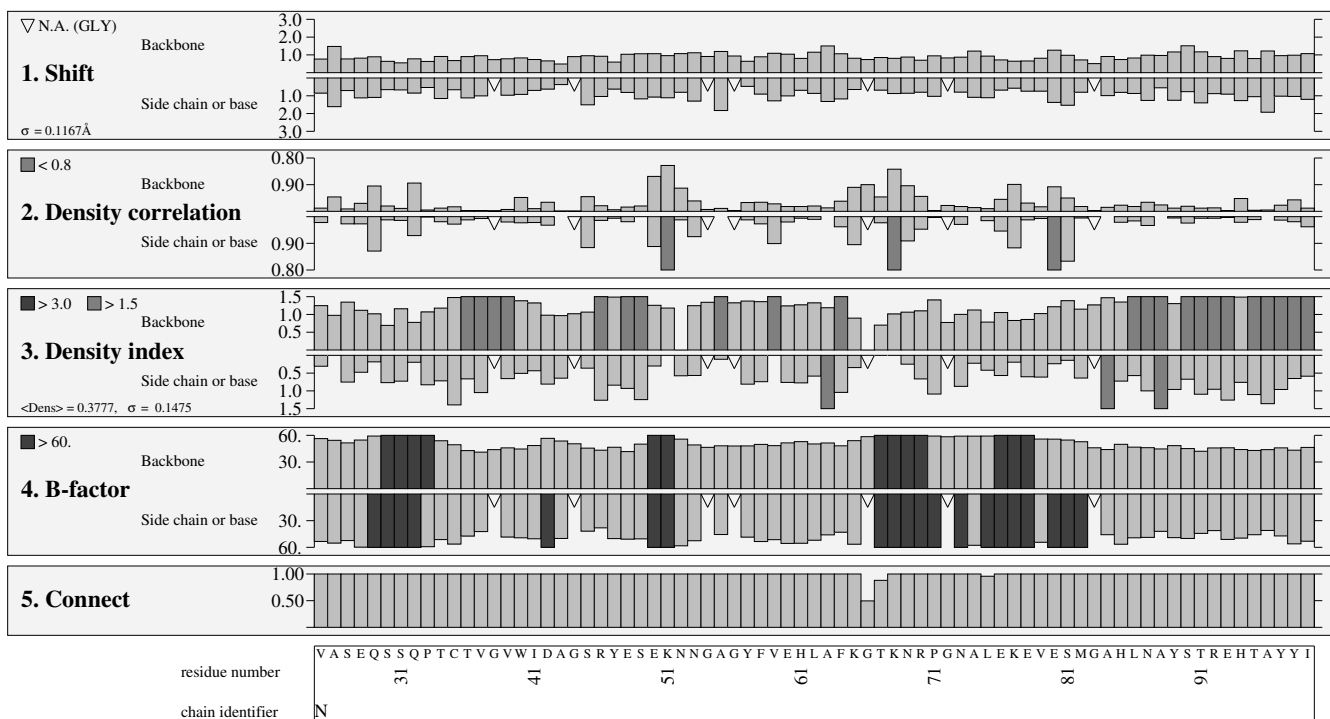
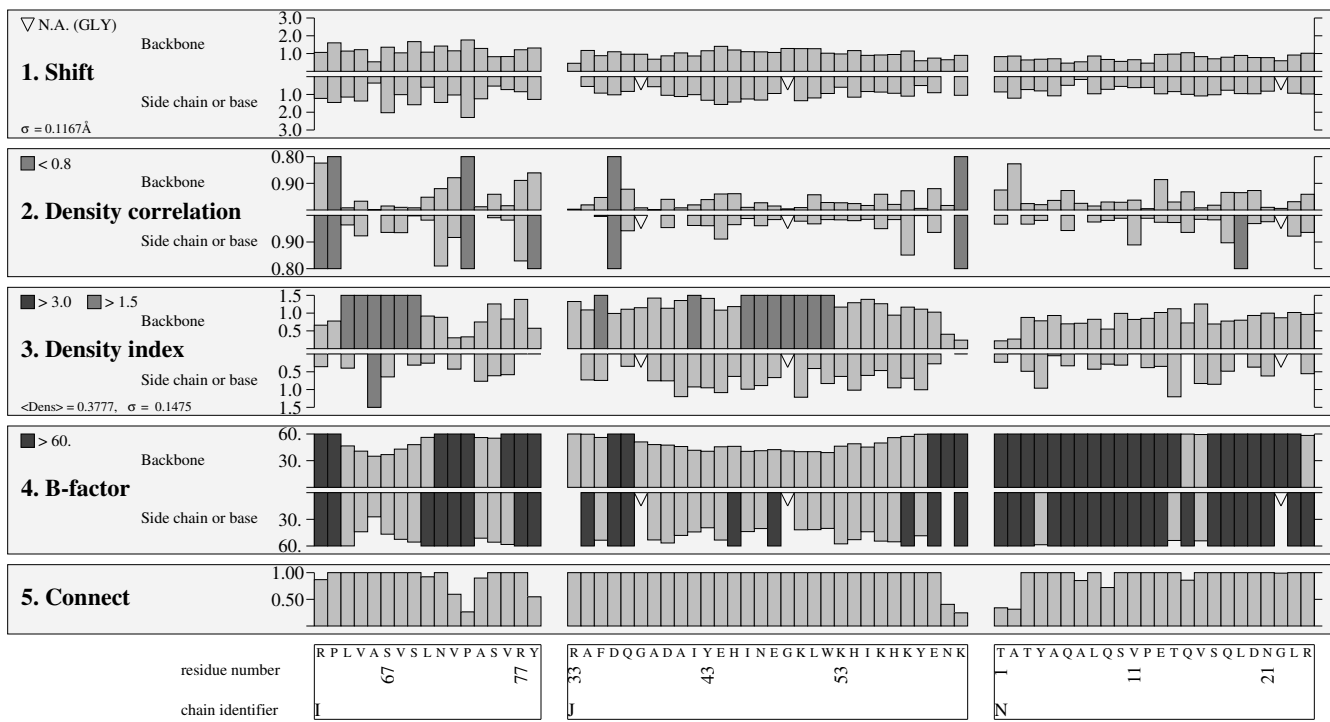
Local estimation (12)



Structure Factor Check

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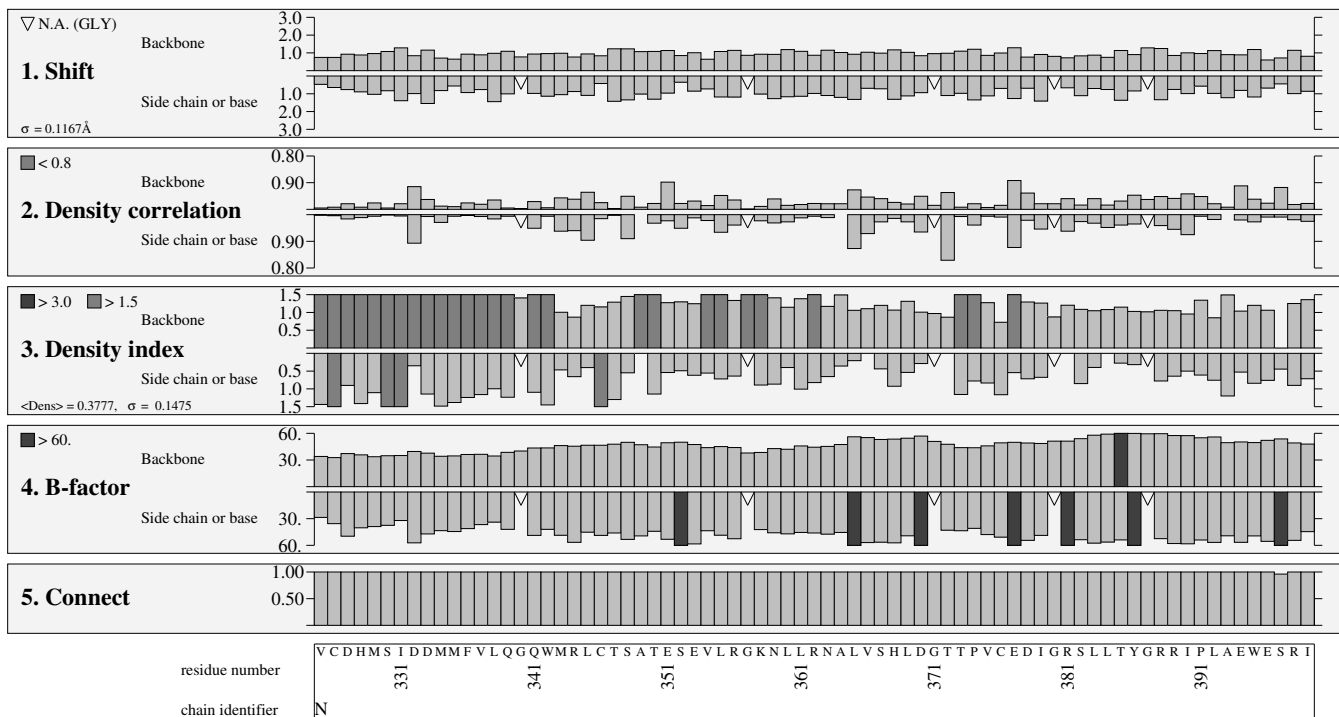
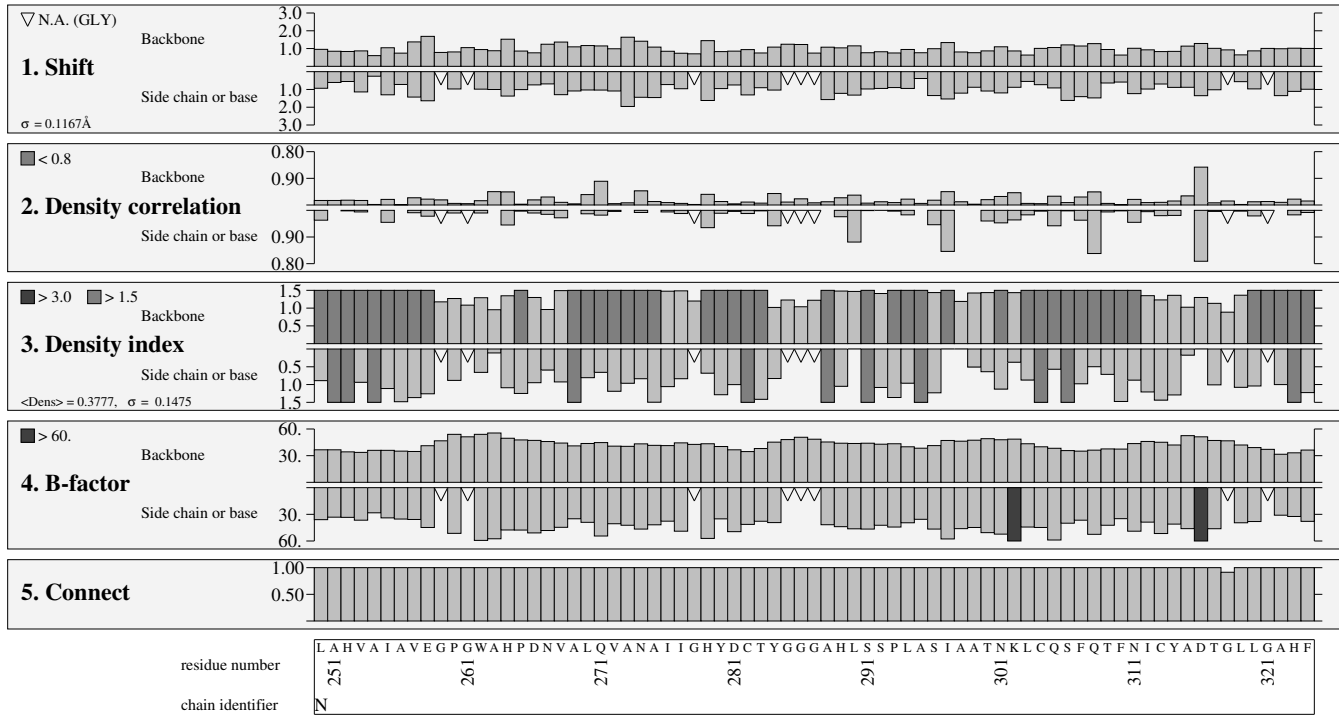
Local estimation (14)



Structure Factor Check

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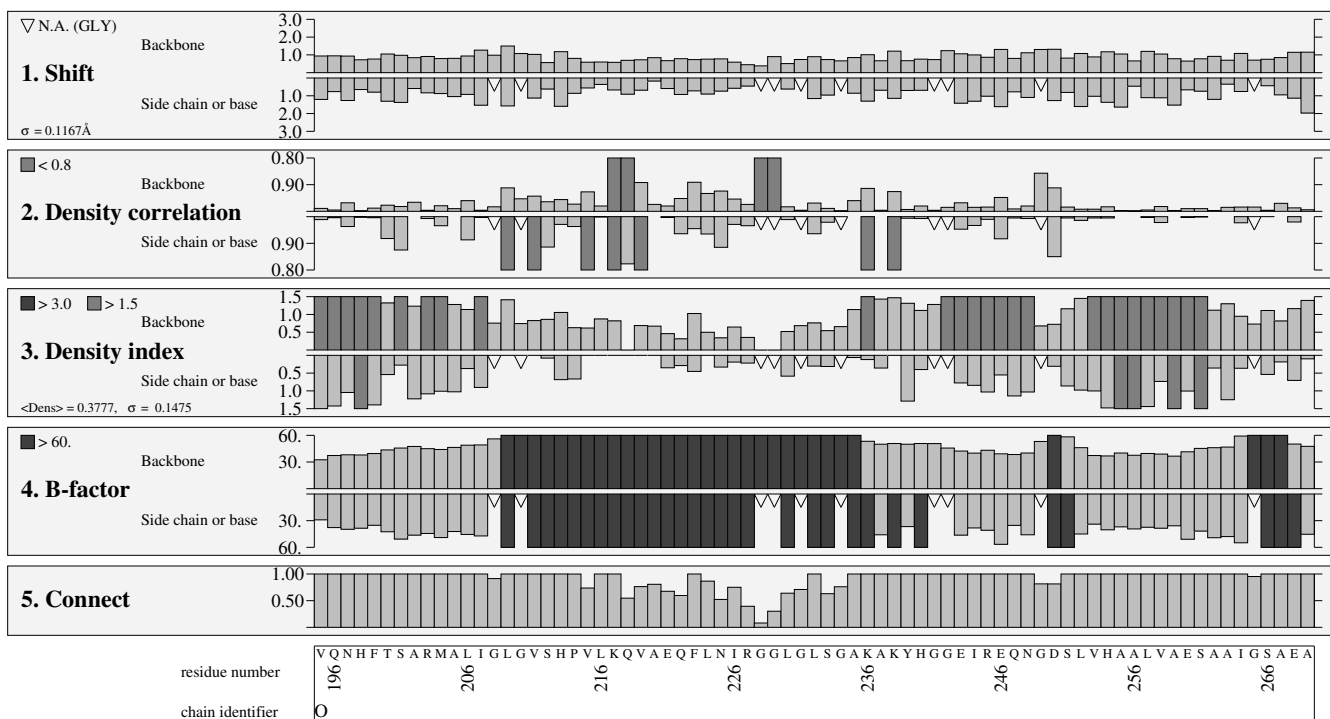
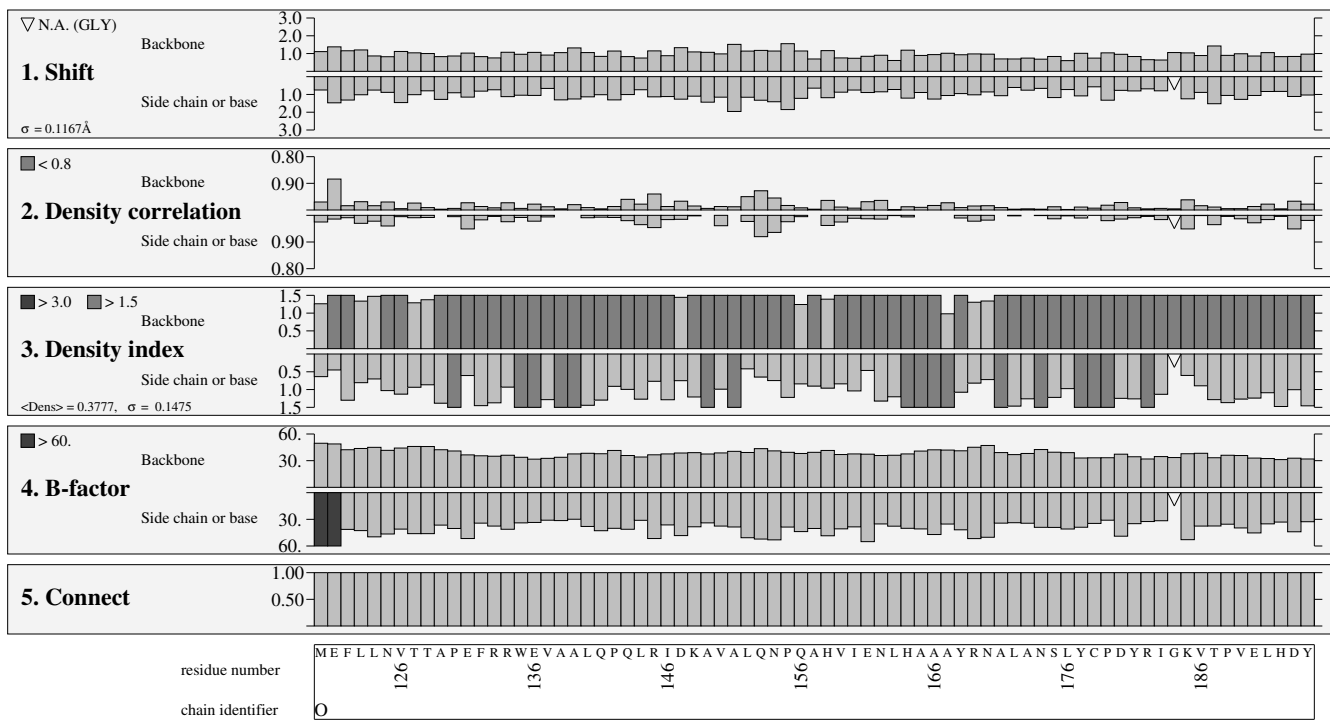
Local estimation (16)



Structure Factor Check

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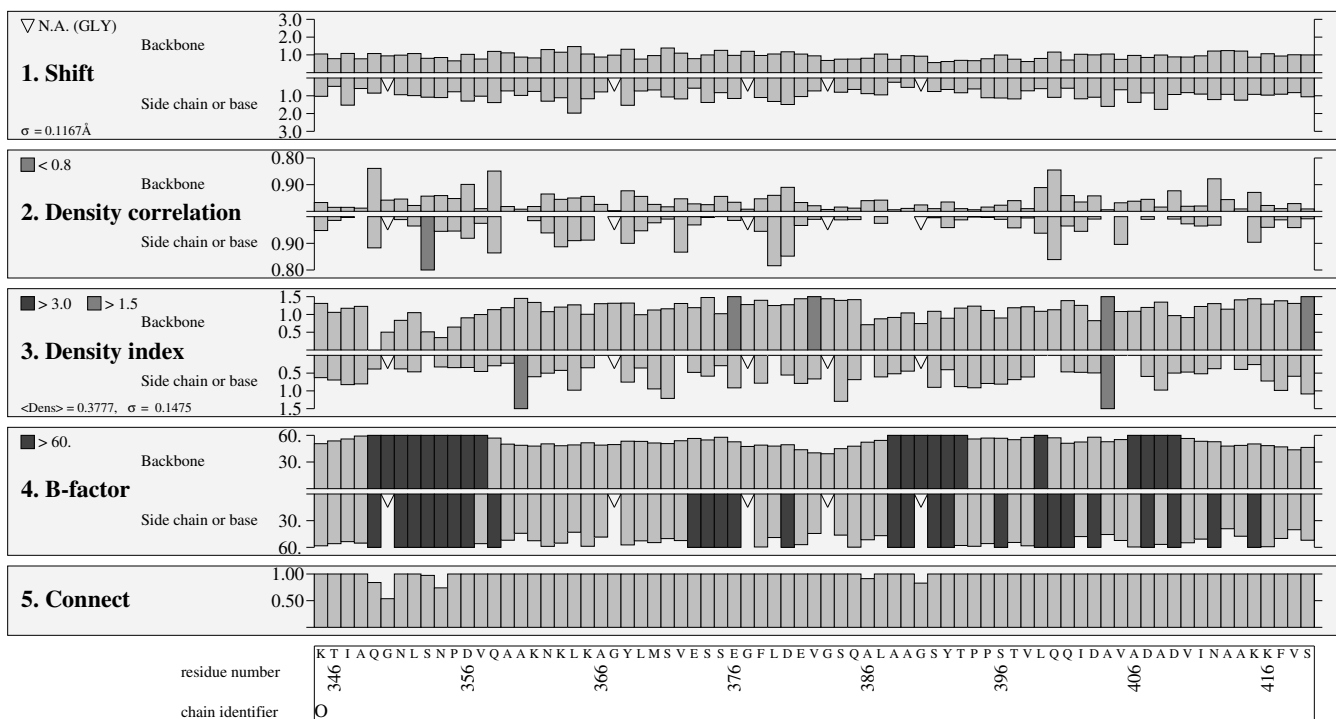
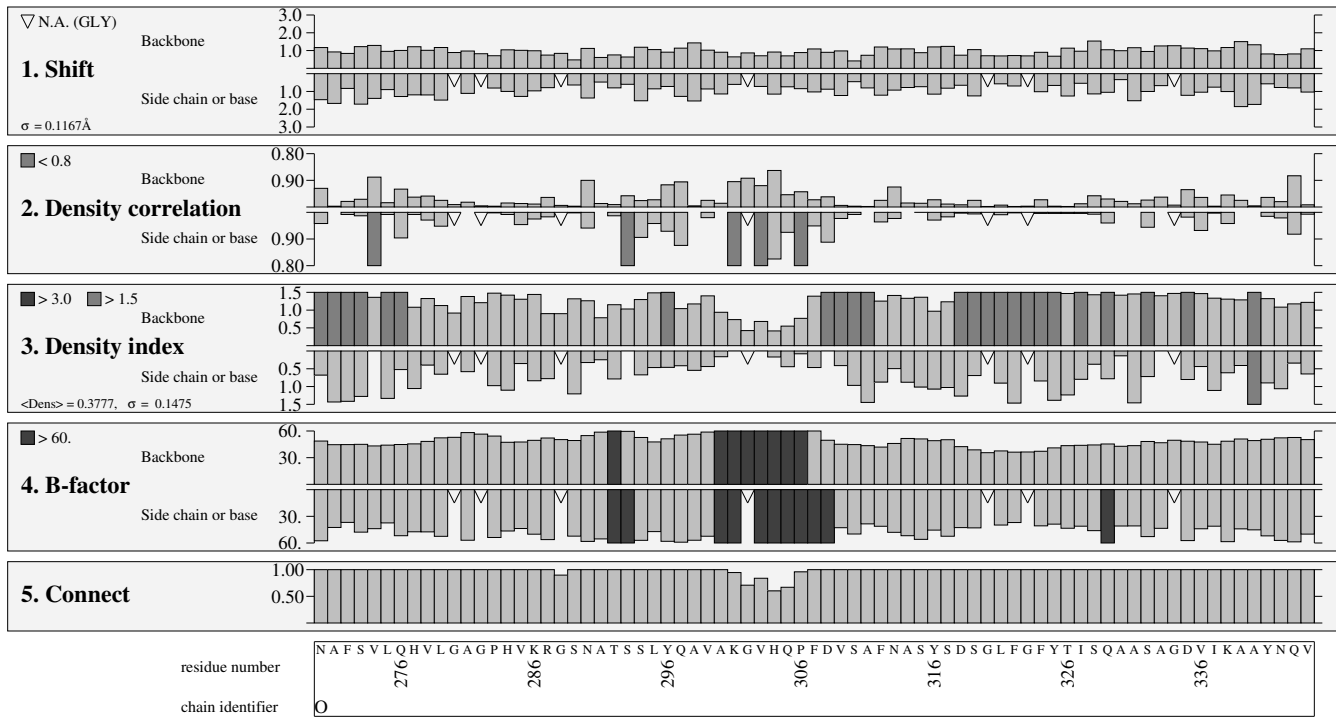
Local estimation (18)



Structure Factor Check

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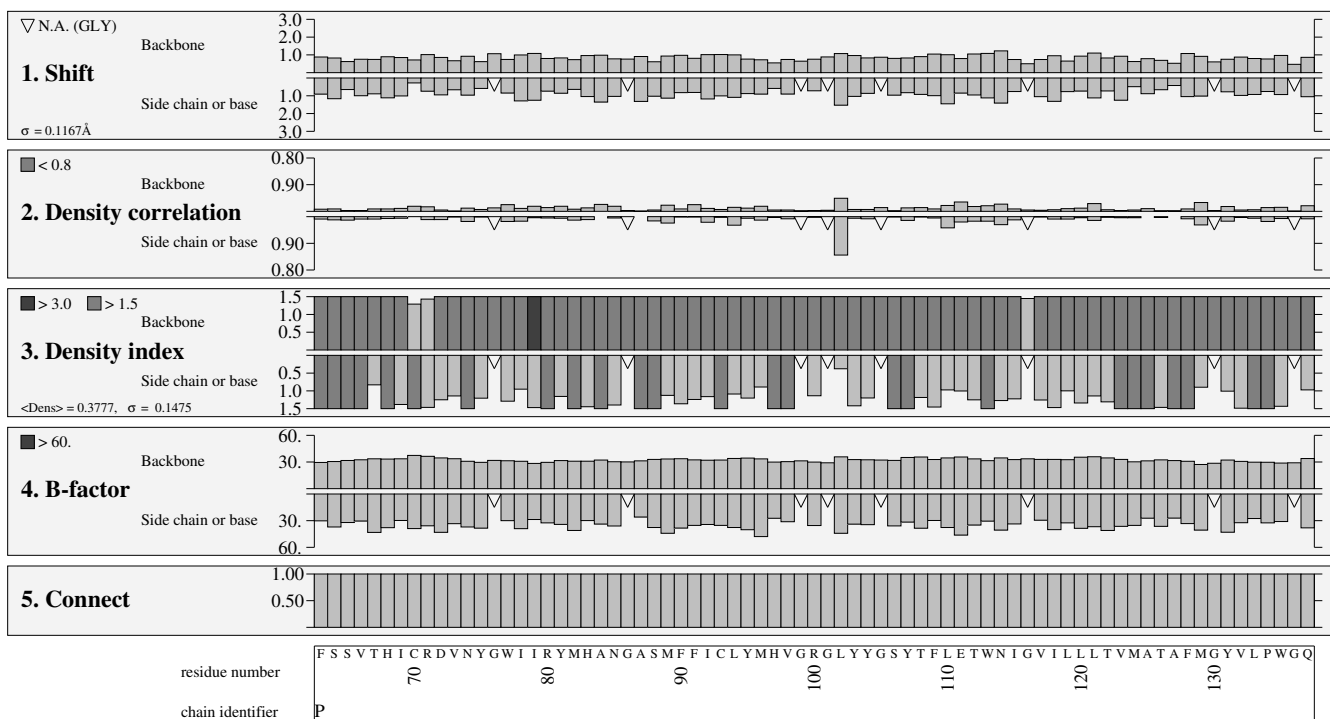
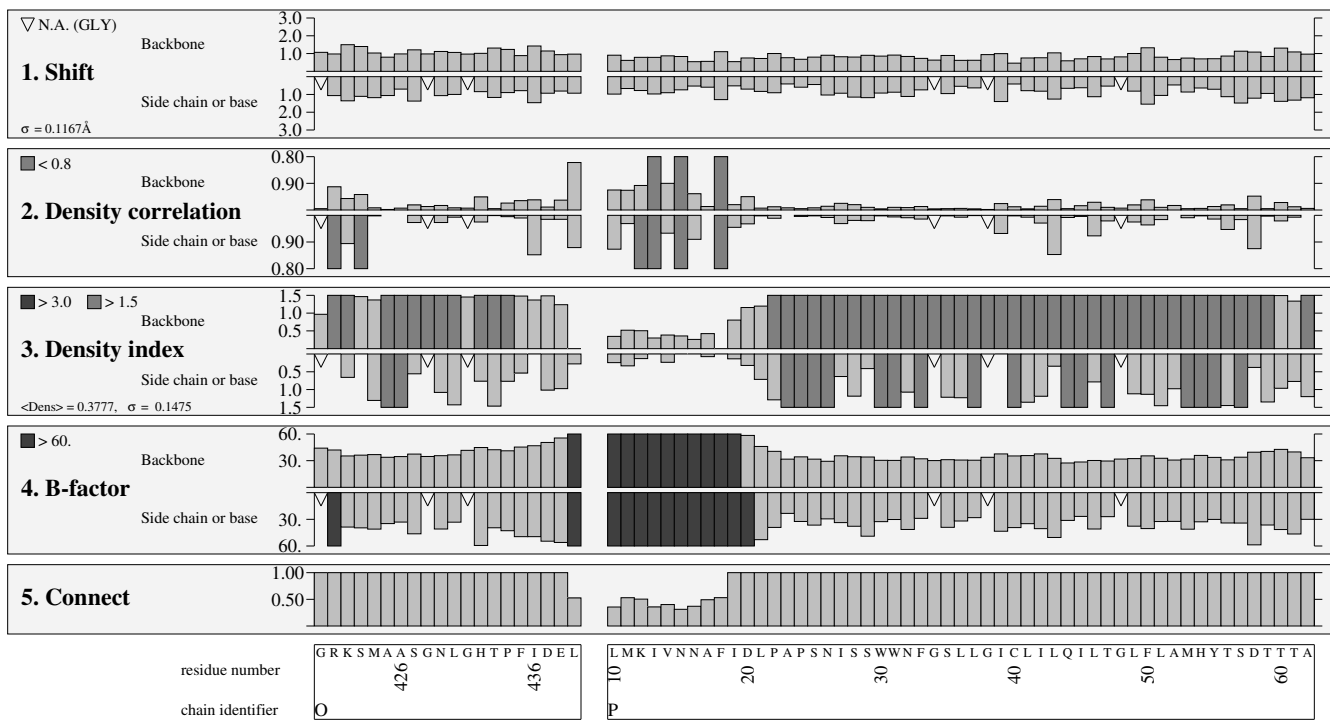
Local estimation (19)



Structure Factor Check

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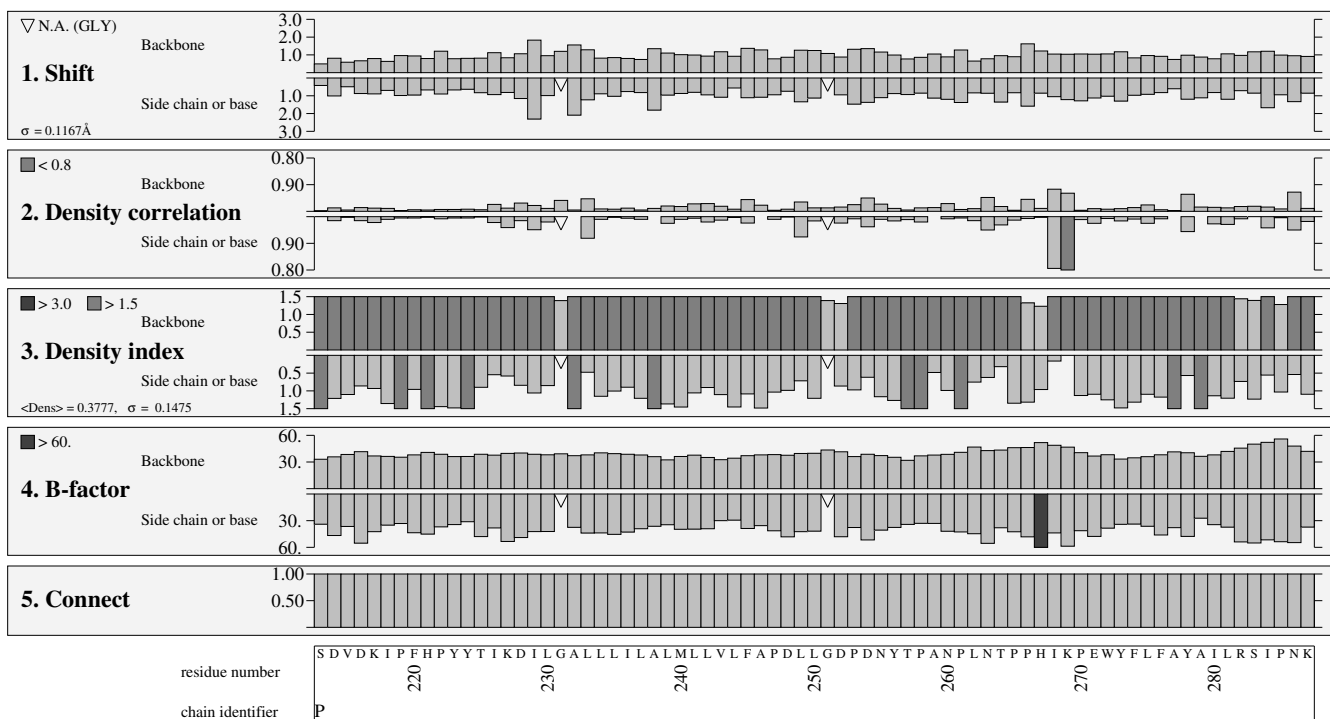
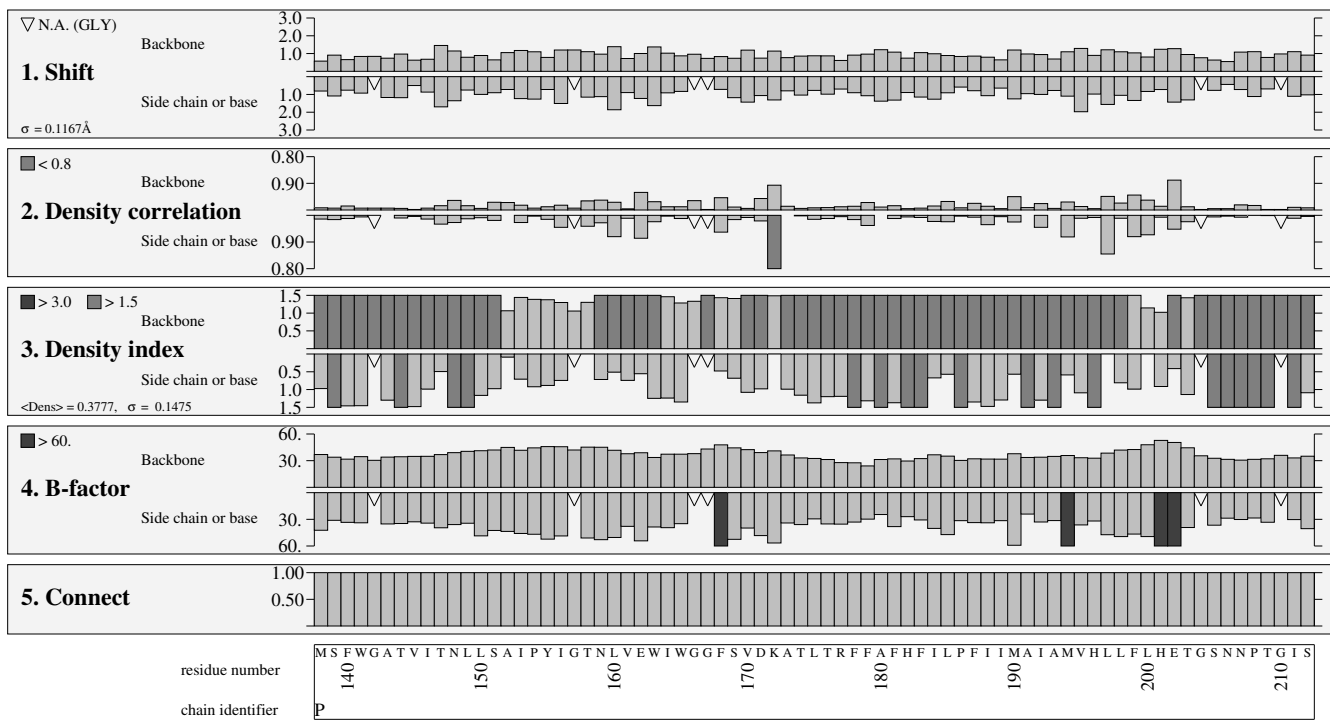
Local estimation (20)



Structure Factor Check

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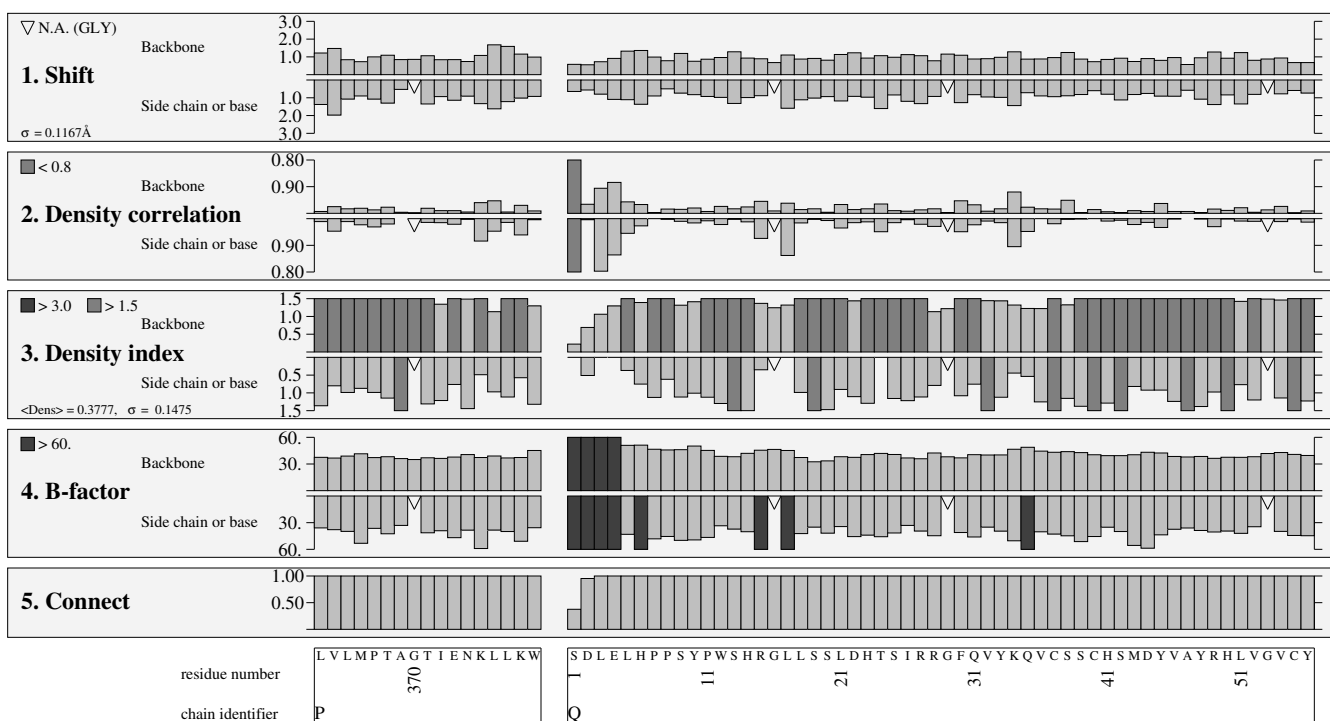
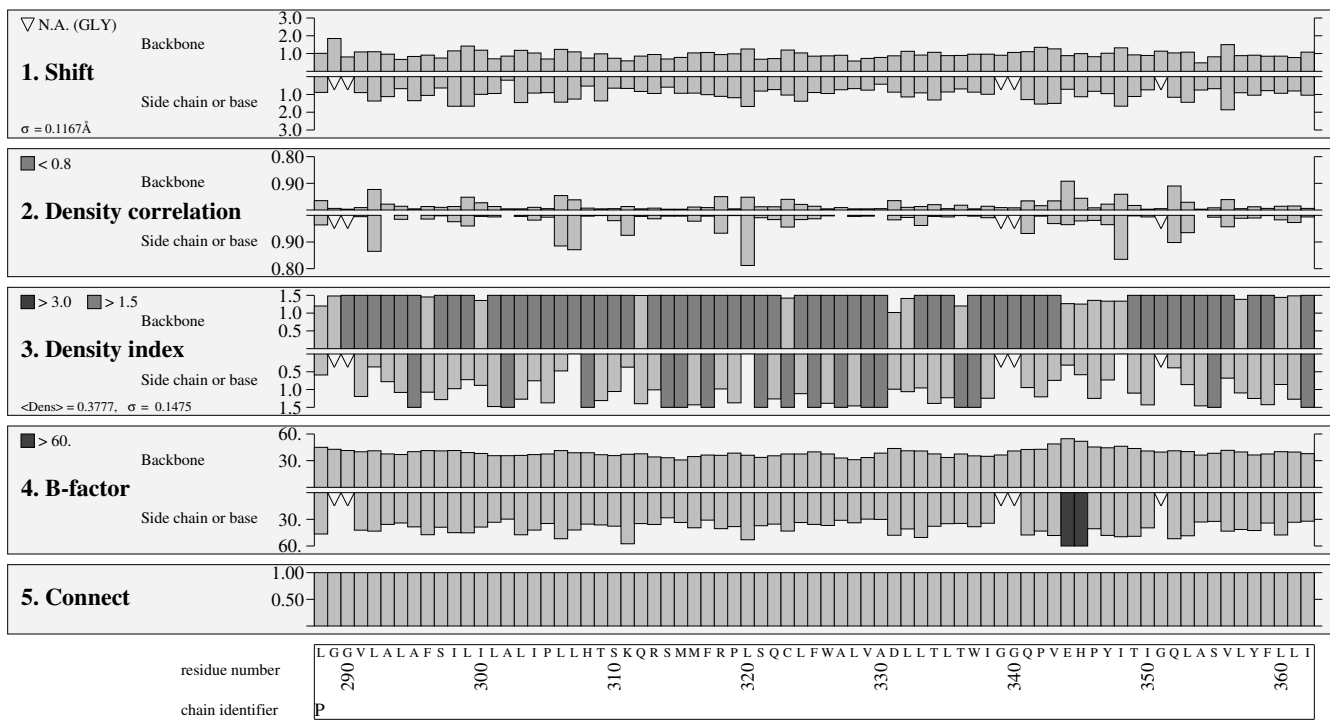
Local estimation (21)



Structure Factor Check

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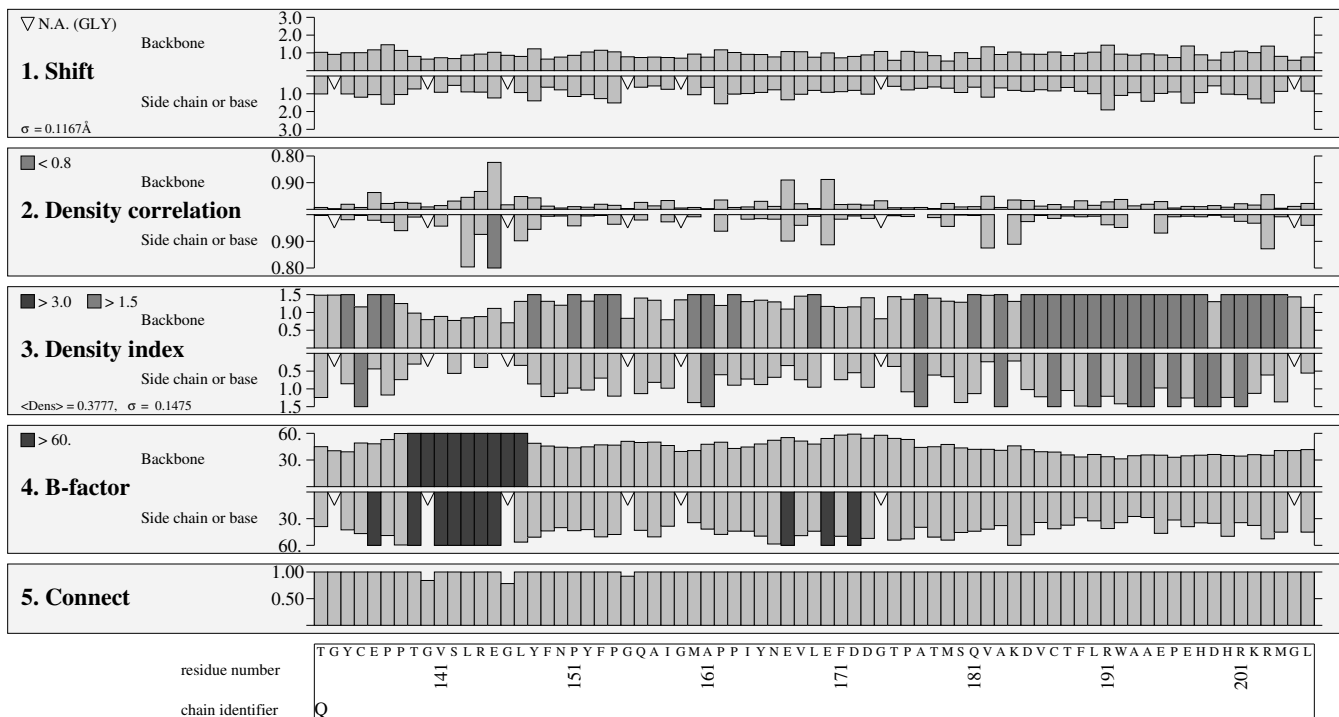
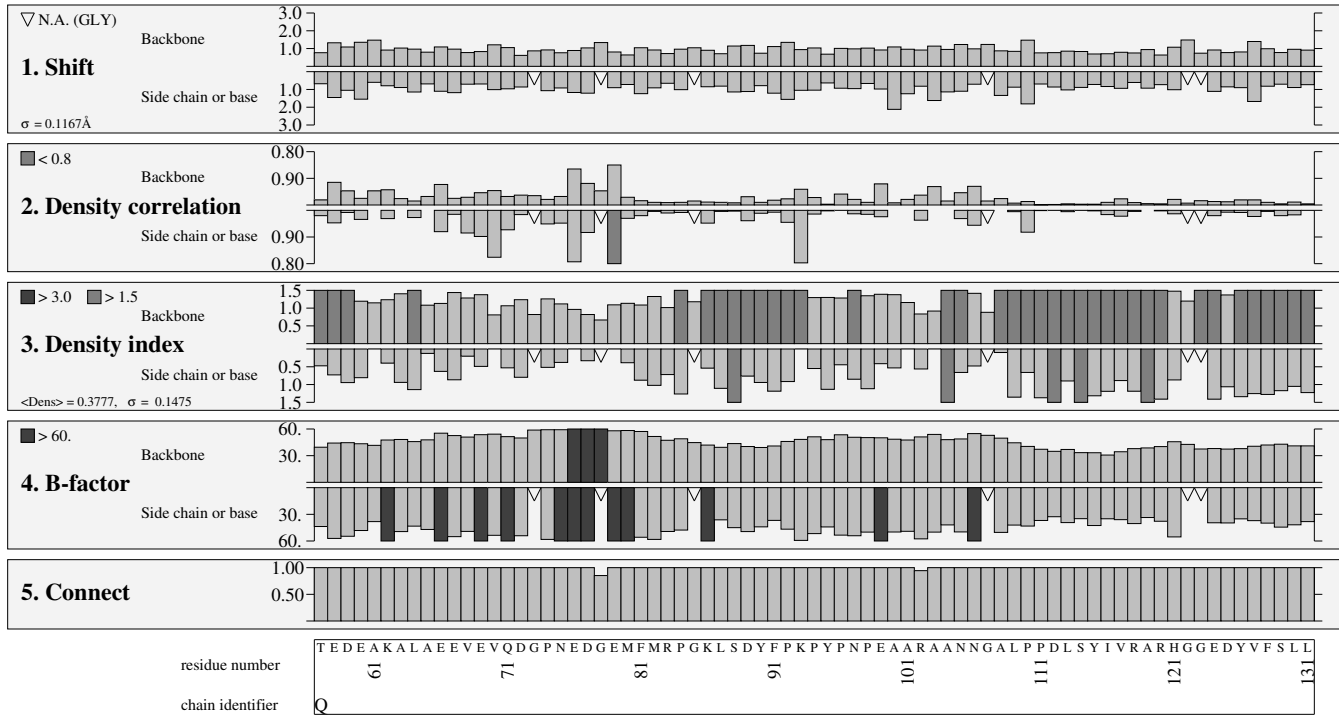
Local estimation (22)



Structure Factor Check

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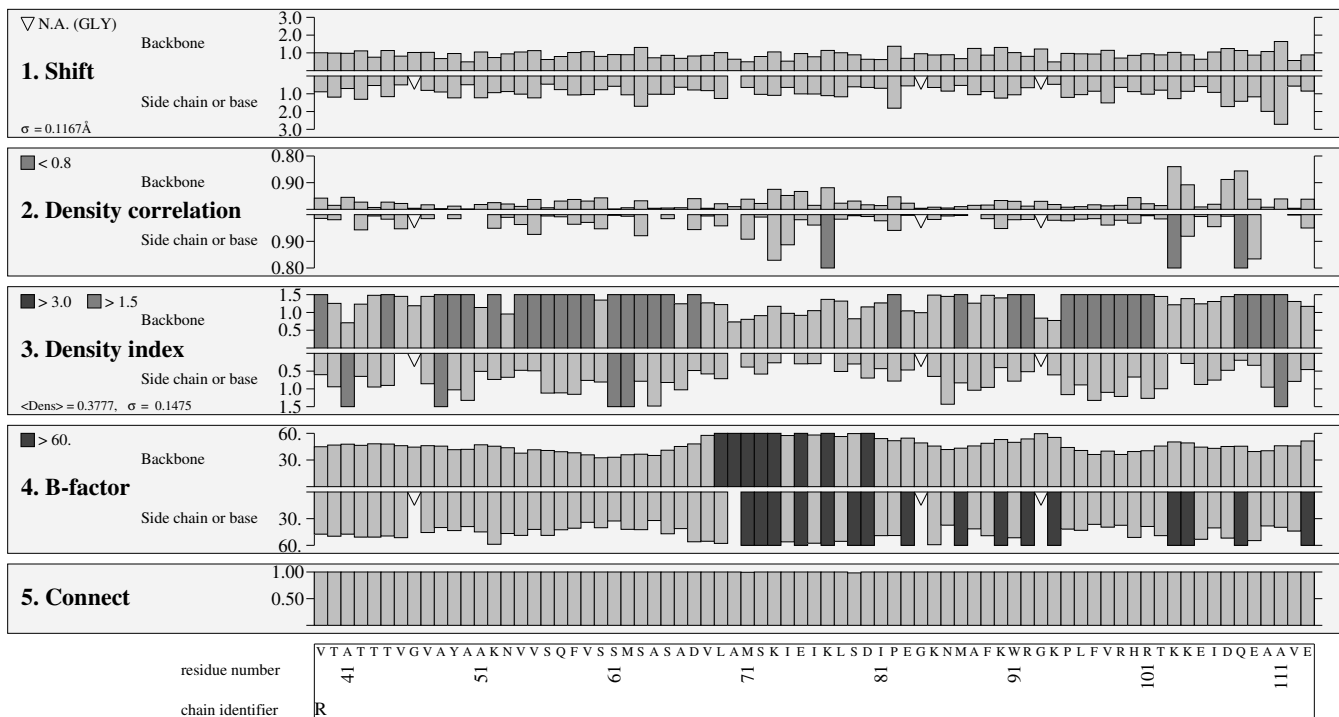
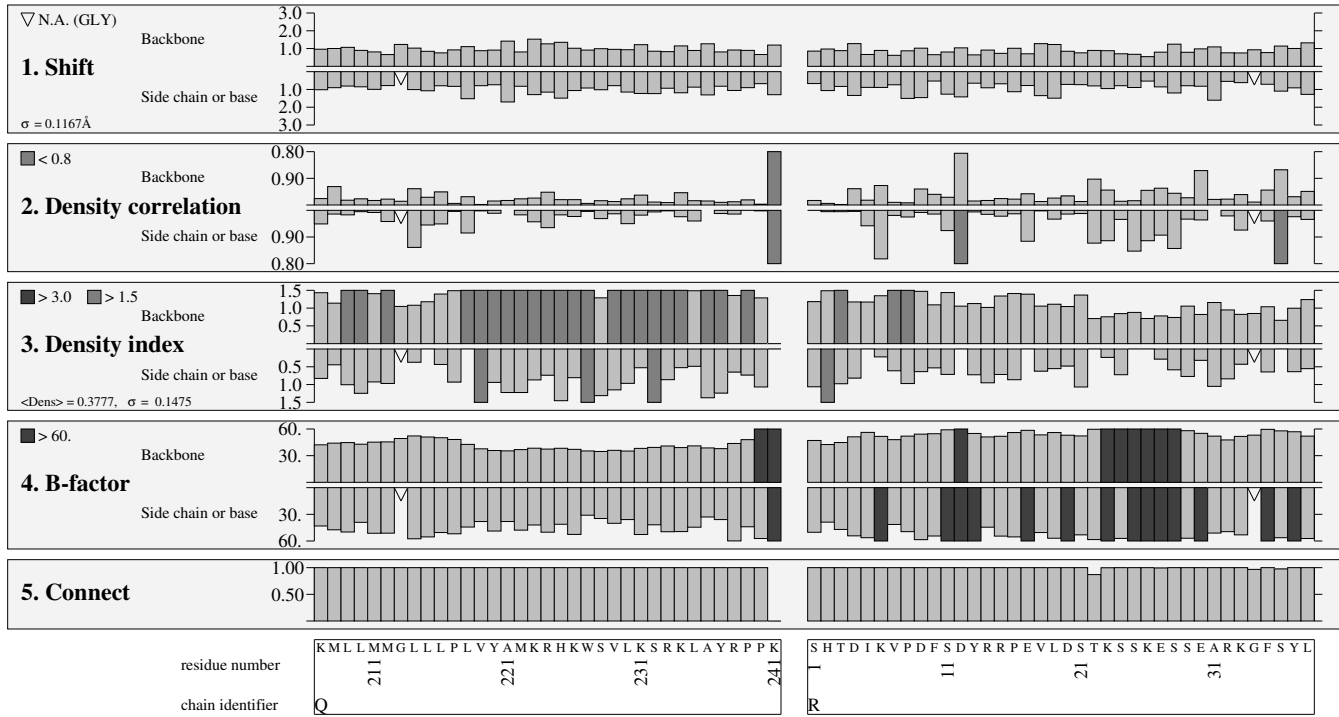
Local estimation (23)



Structure Factor Check

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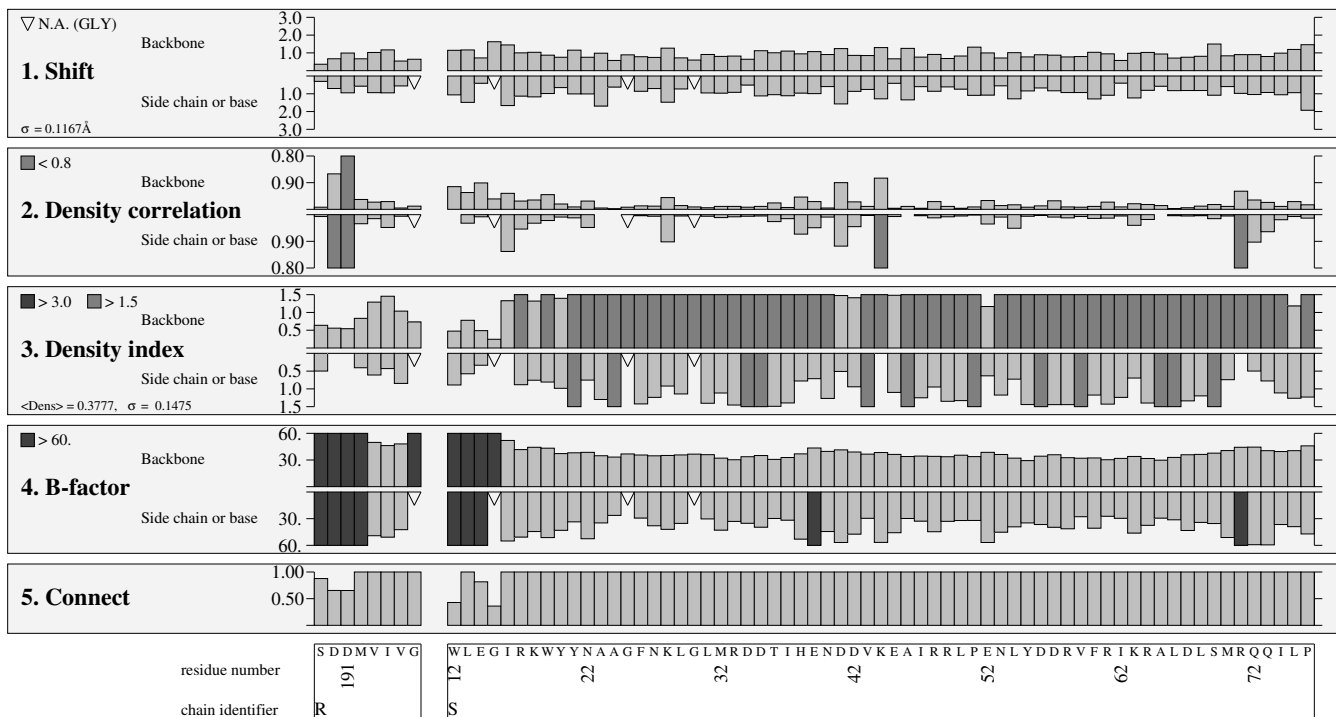
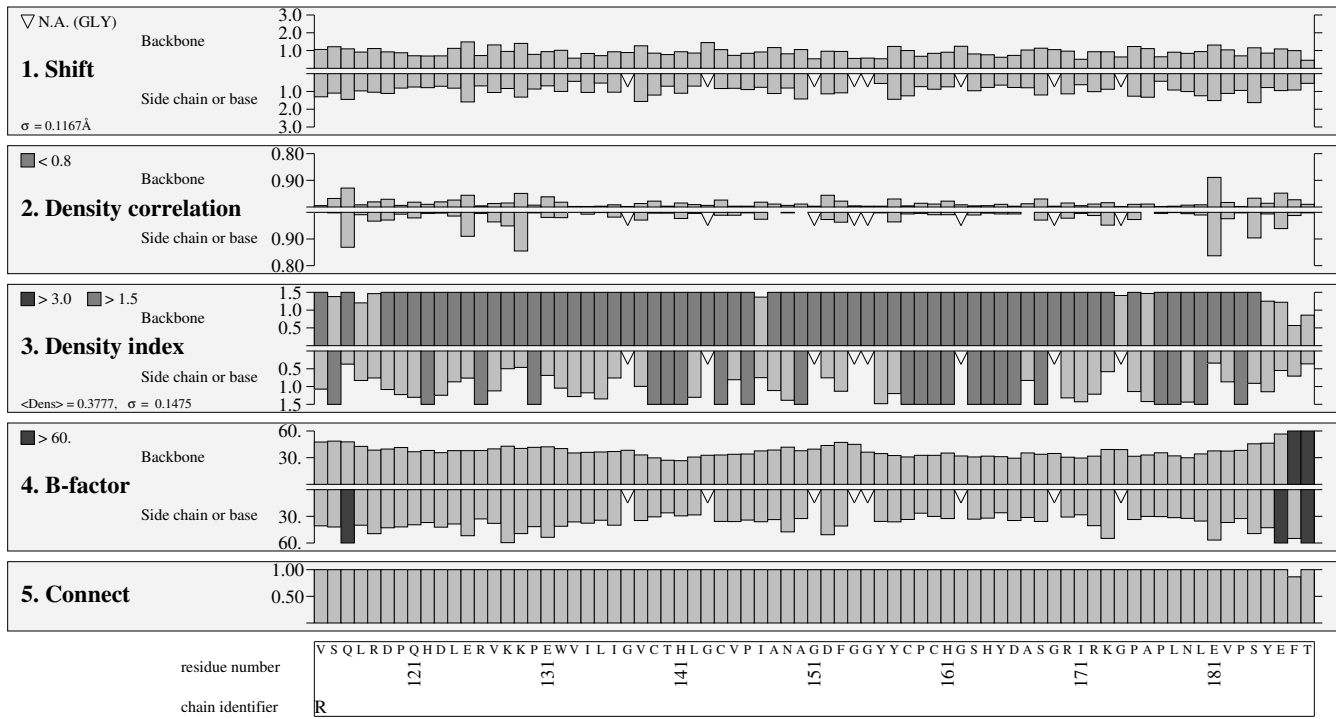
Local estimation (24)



Structure Factor Check

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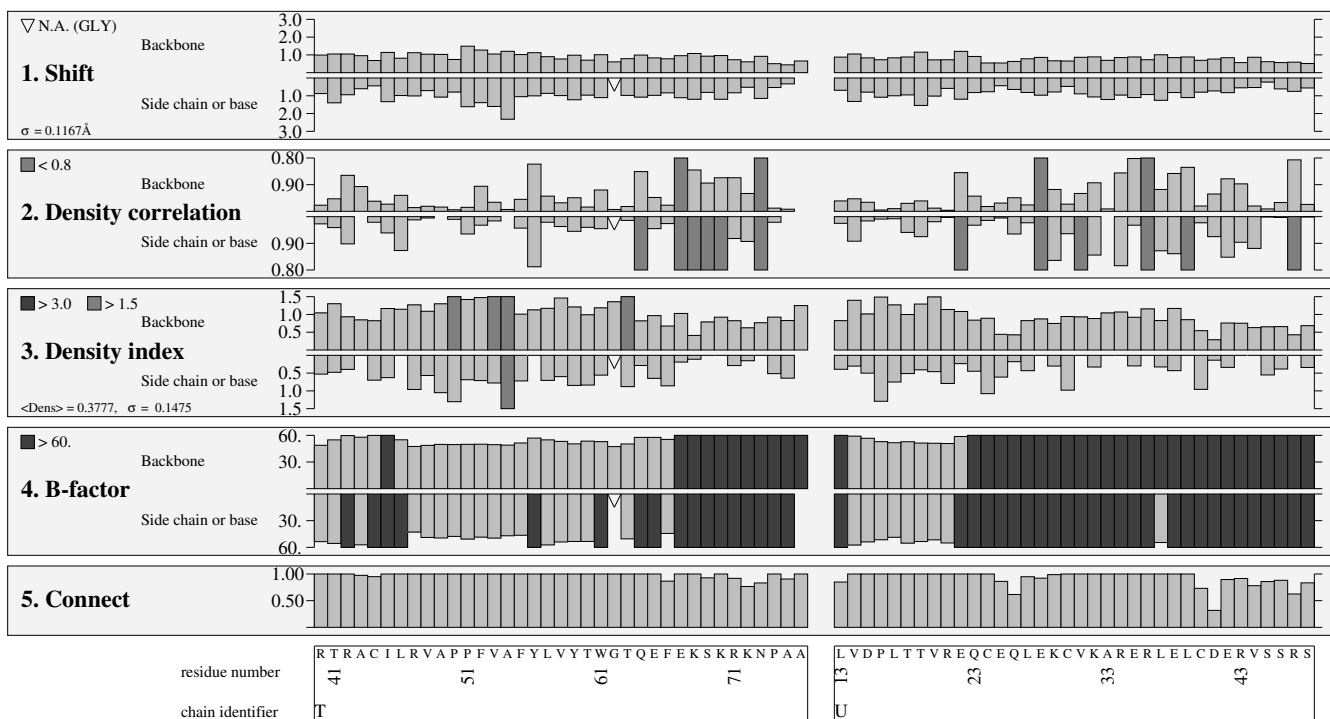
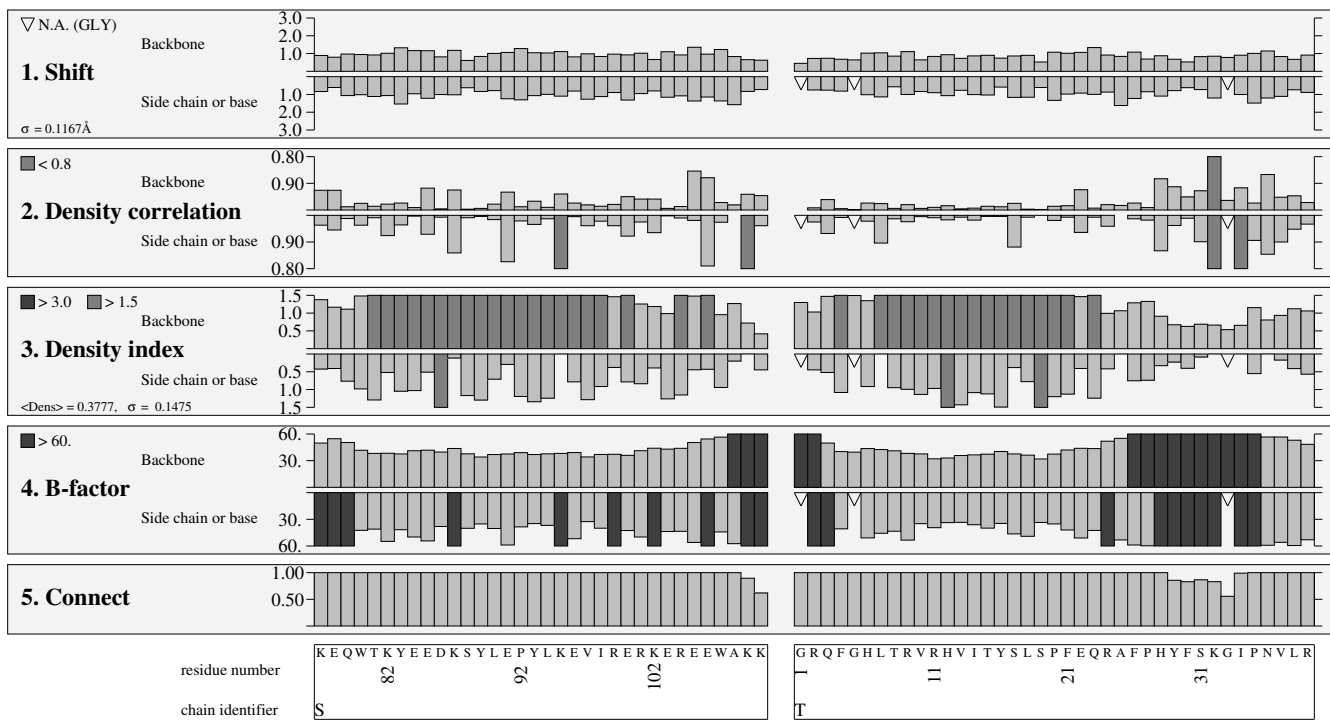
Local estimation (25)



Structure Factor Check

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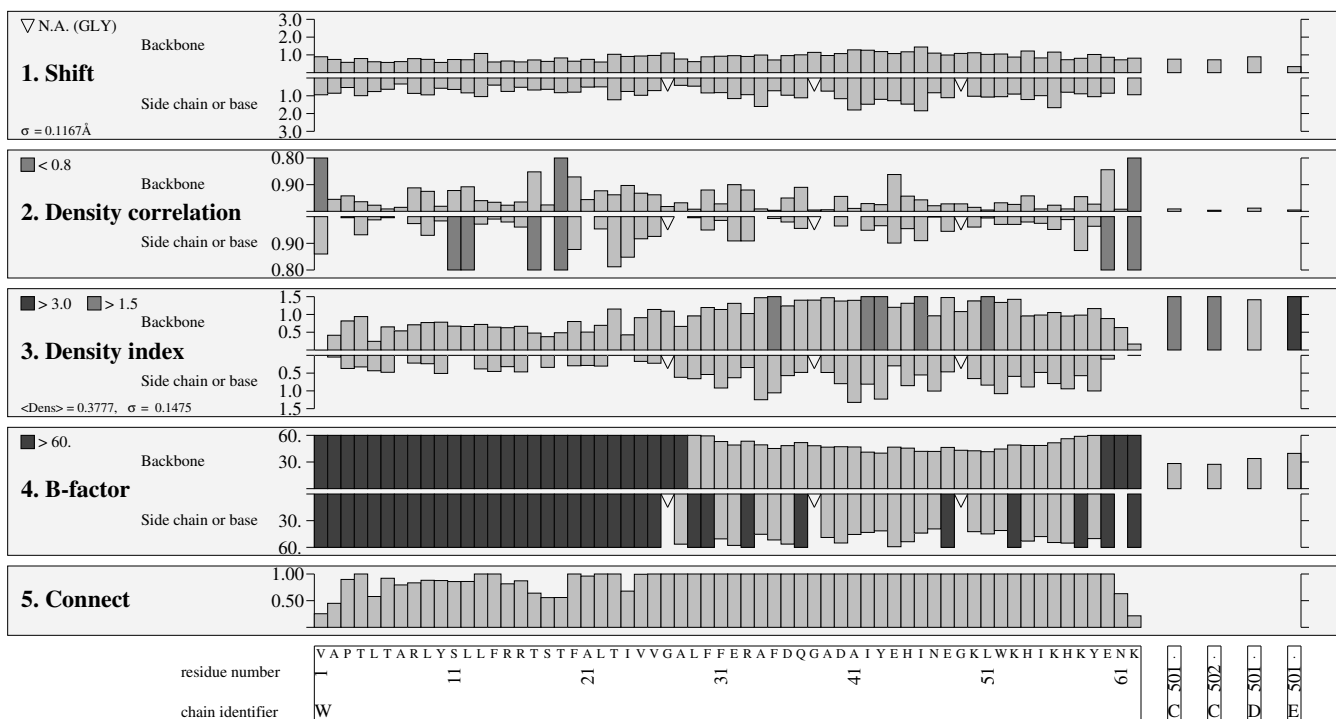
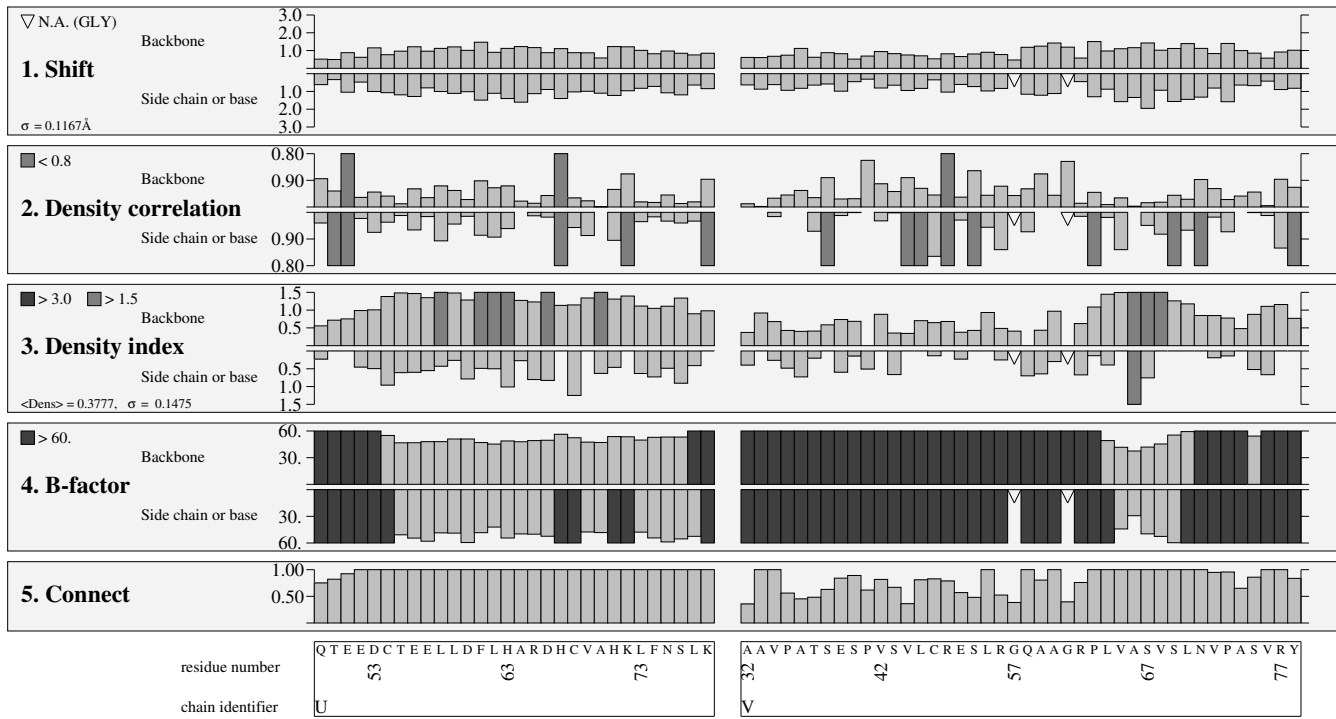
Local estimation (26)



Structure Factor Check

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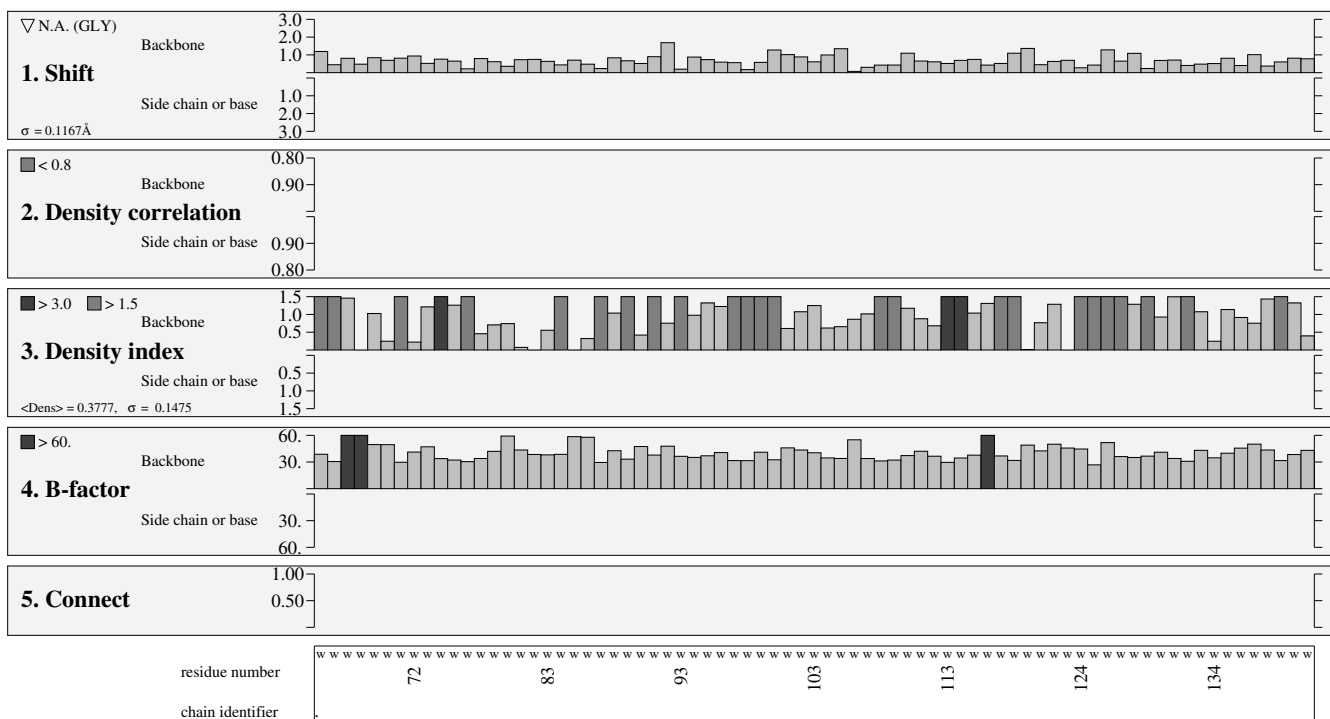
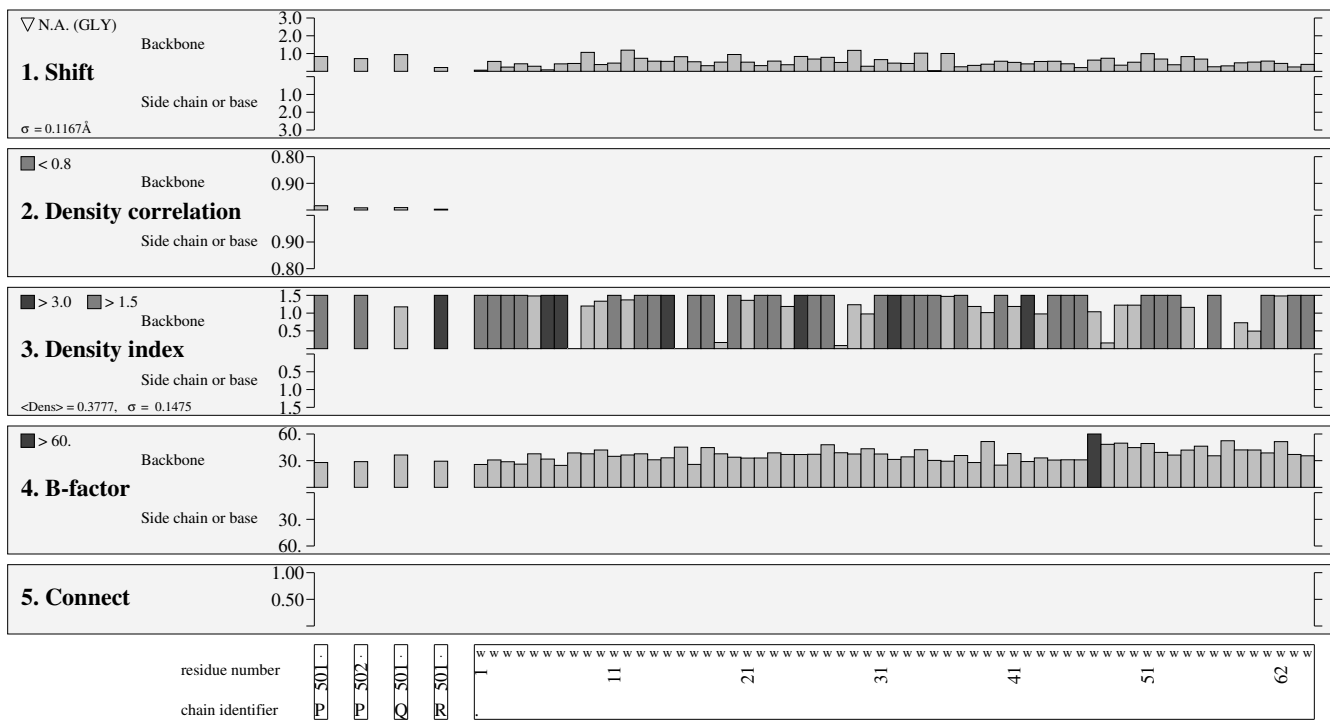
Local estimation (27)



Structure Factor Check

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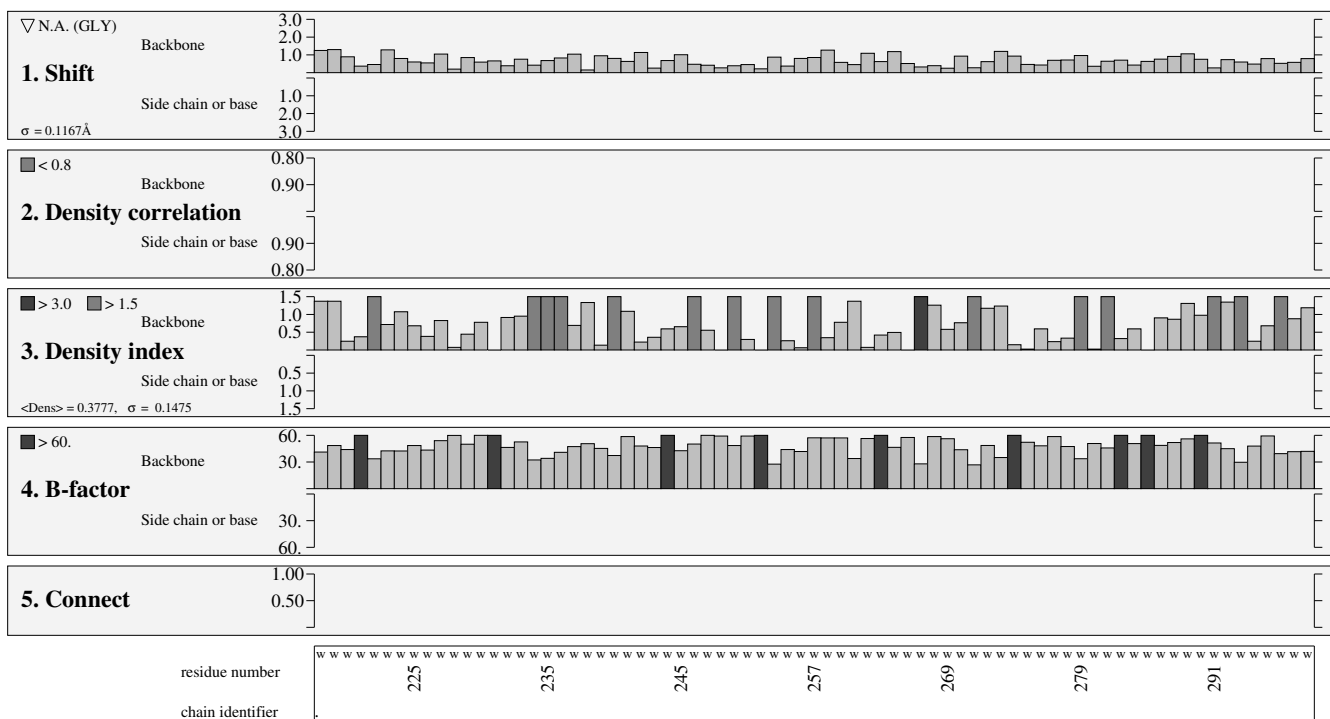
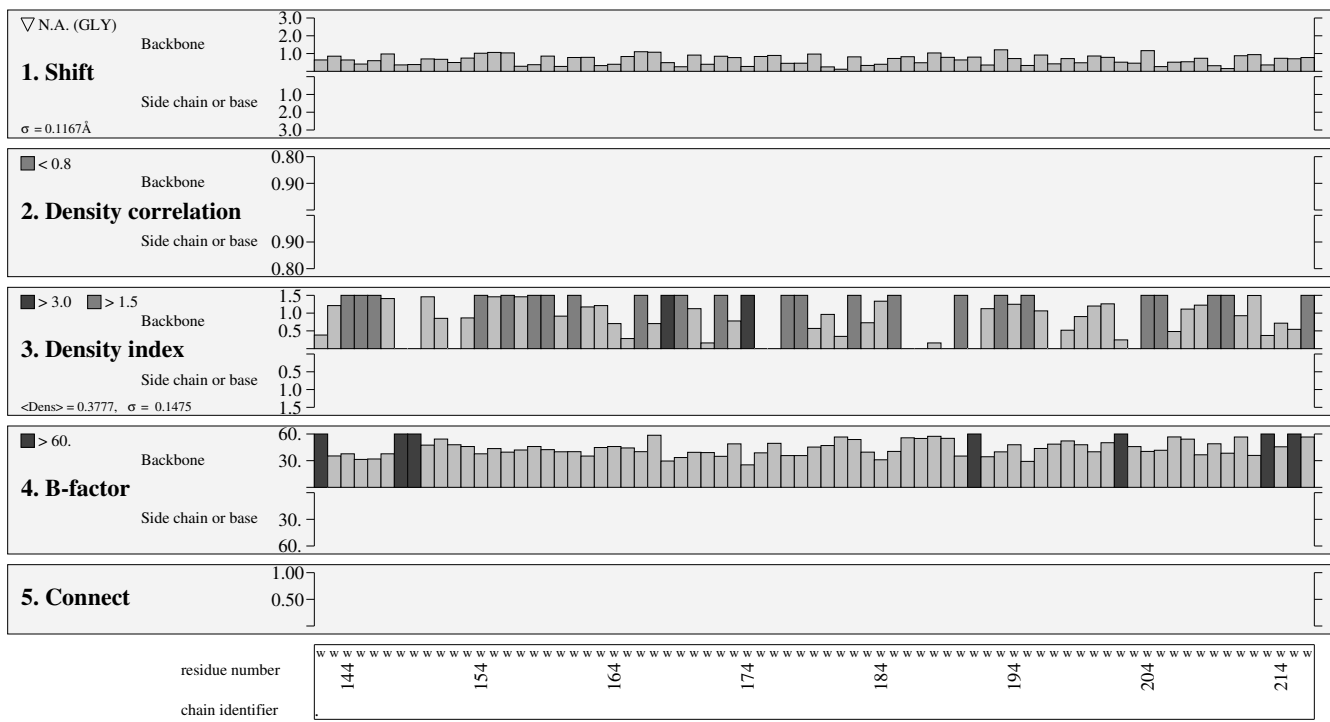
Local estimation (28)



Structure Factor Check

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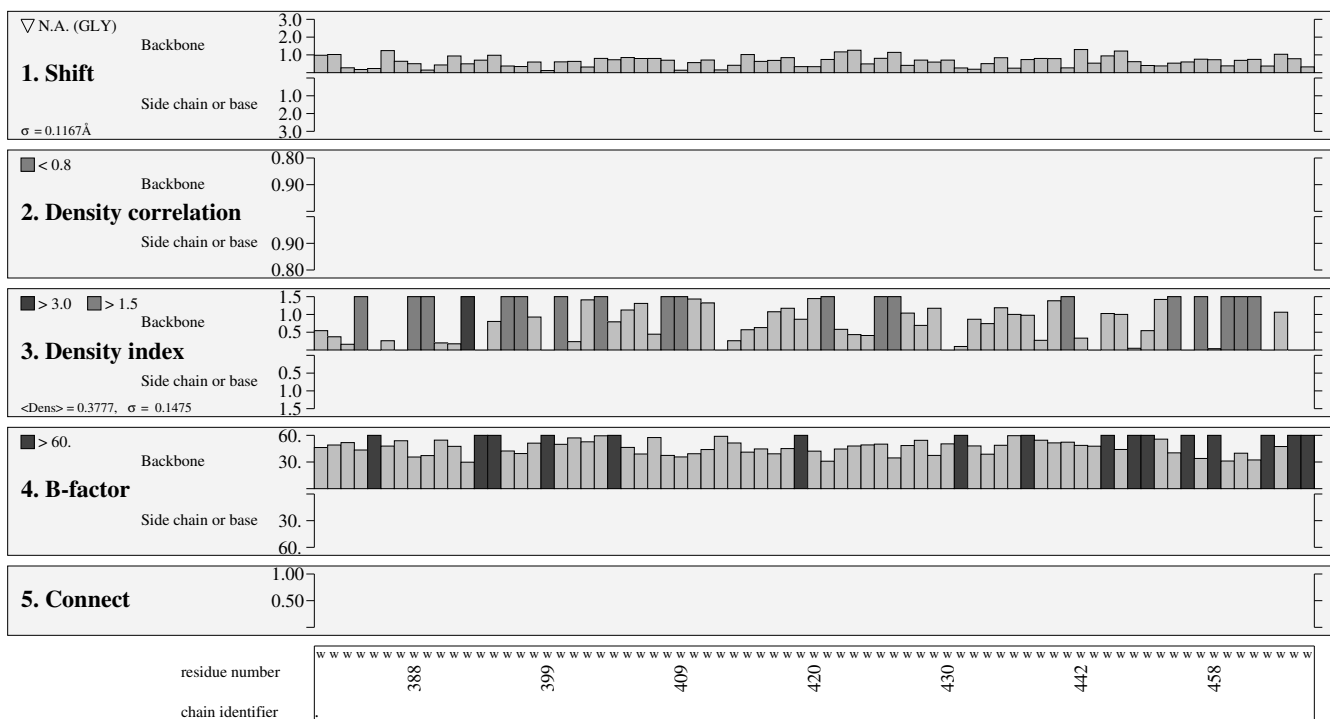
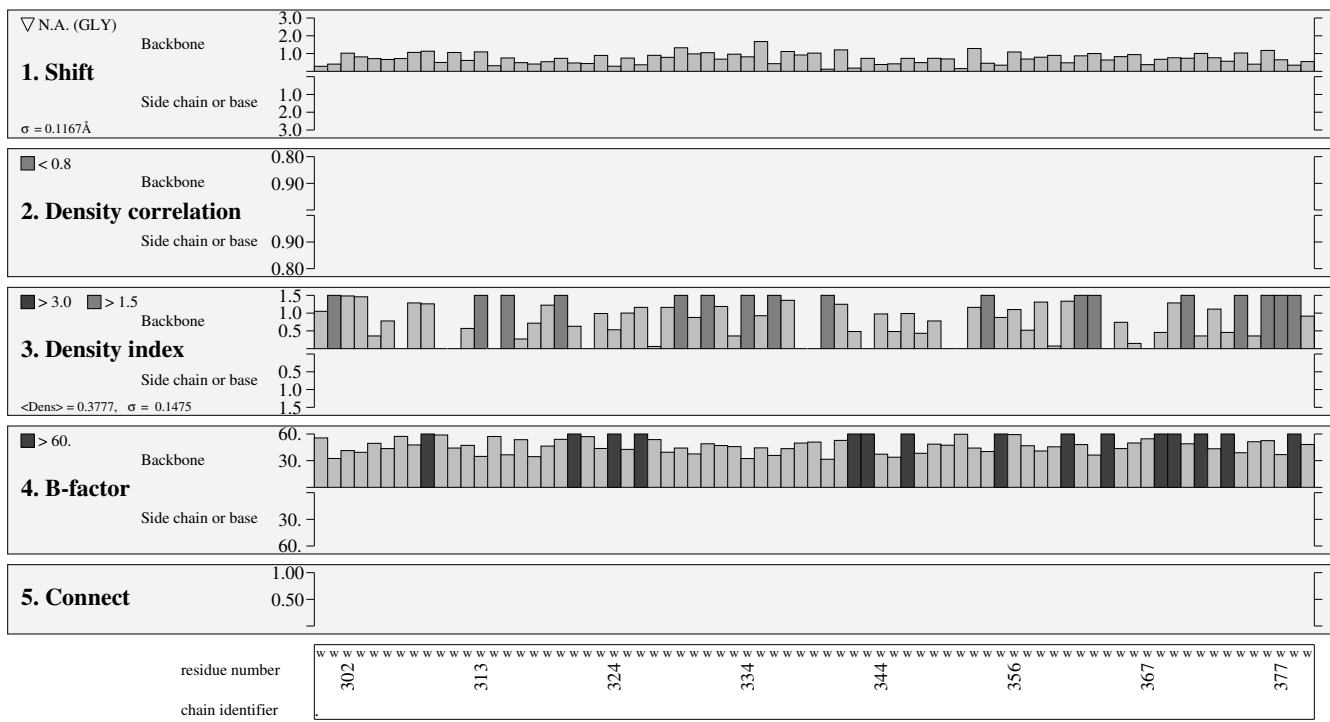
Local estimation (29)



Structure Factor Check

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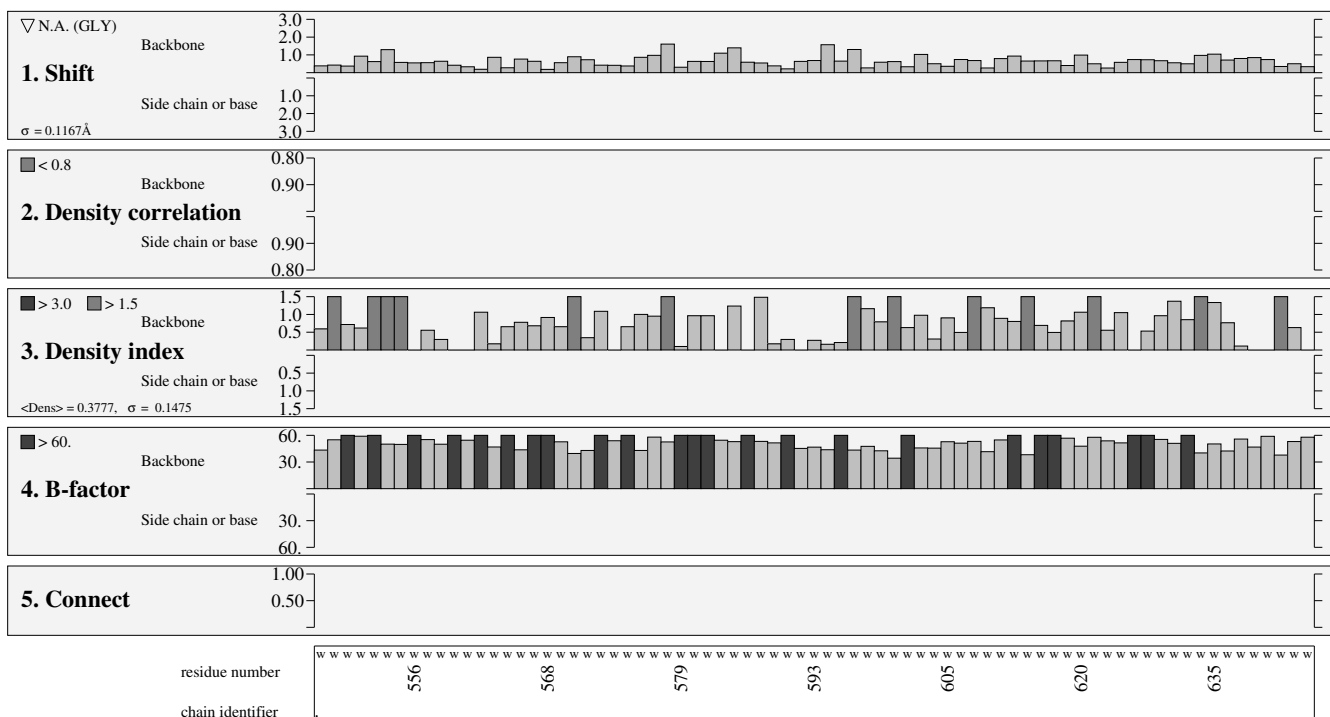
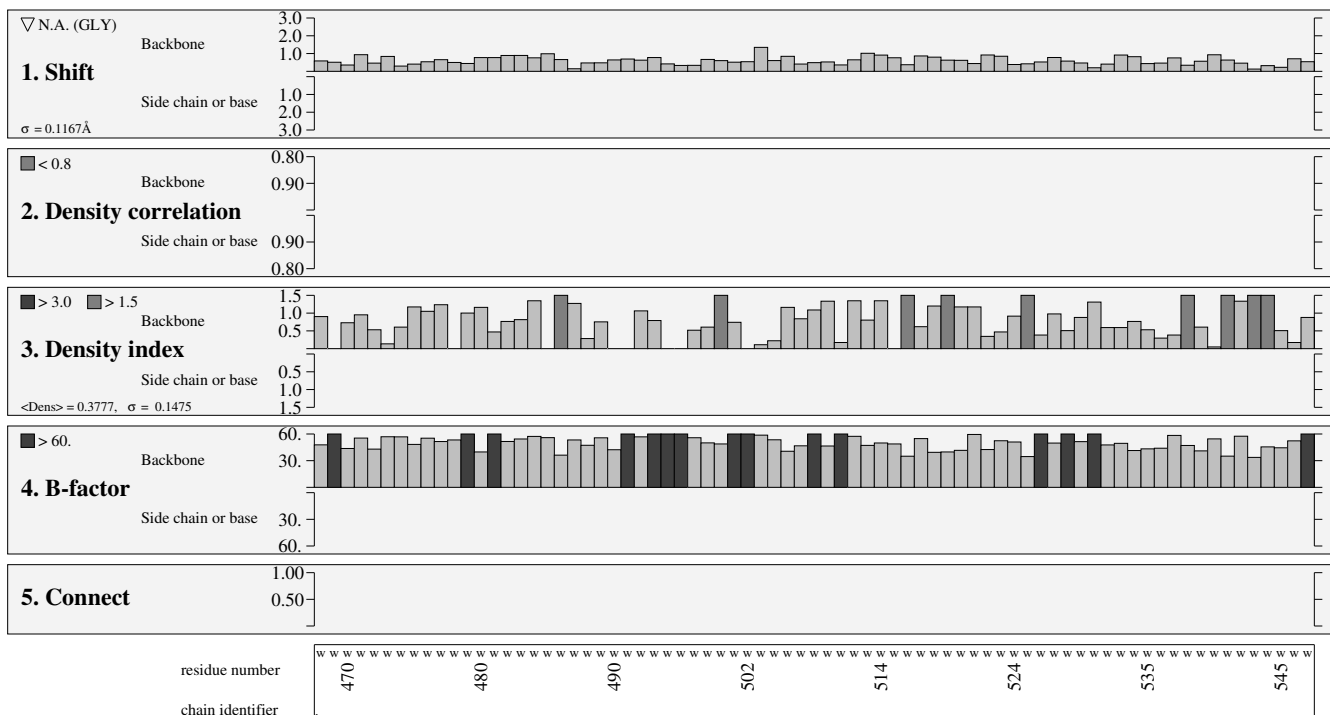
Local estimation (30)



Structure Factor Check

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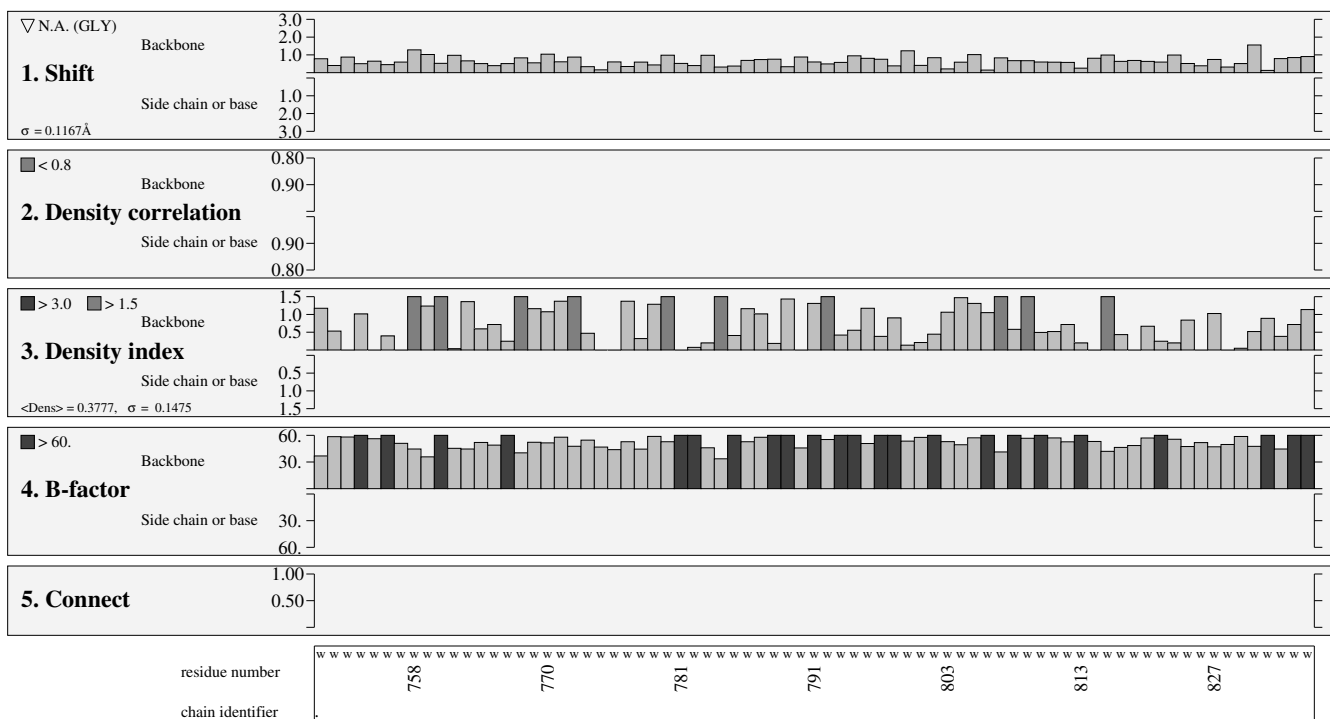
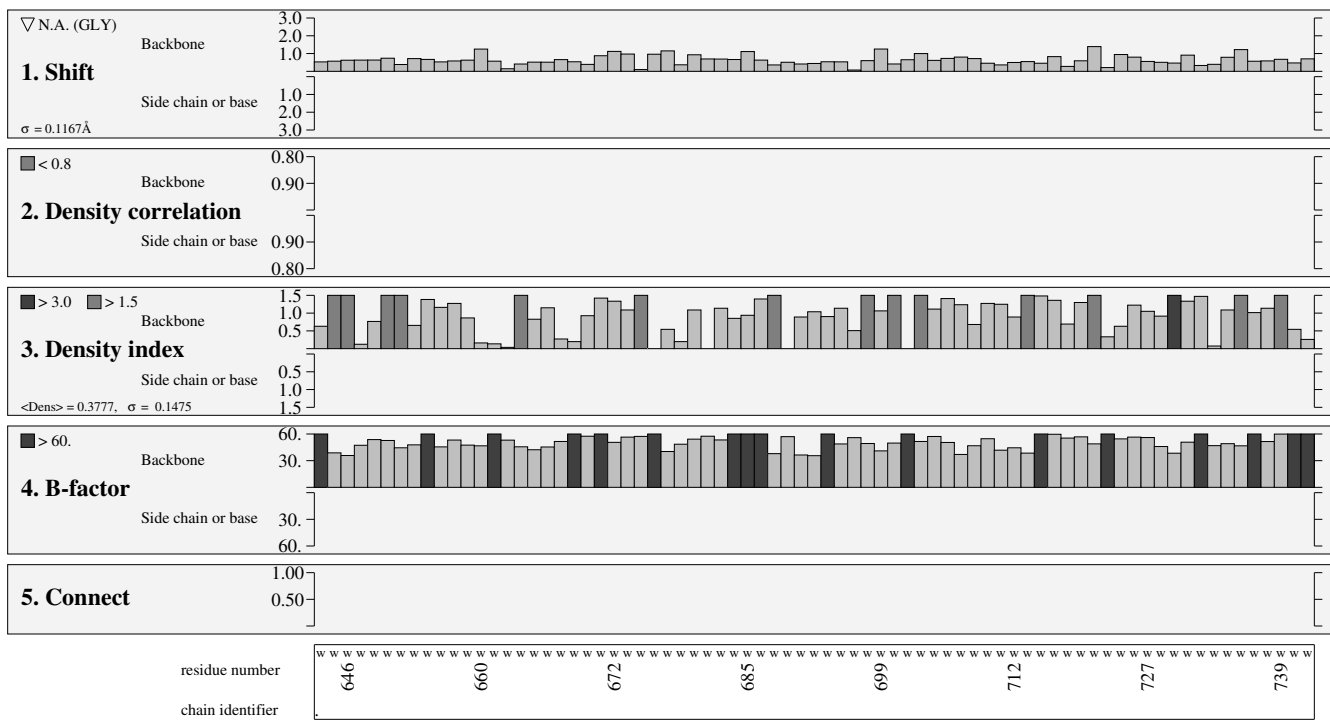
Local estimation (31)



Structure Factor Check

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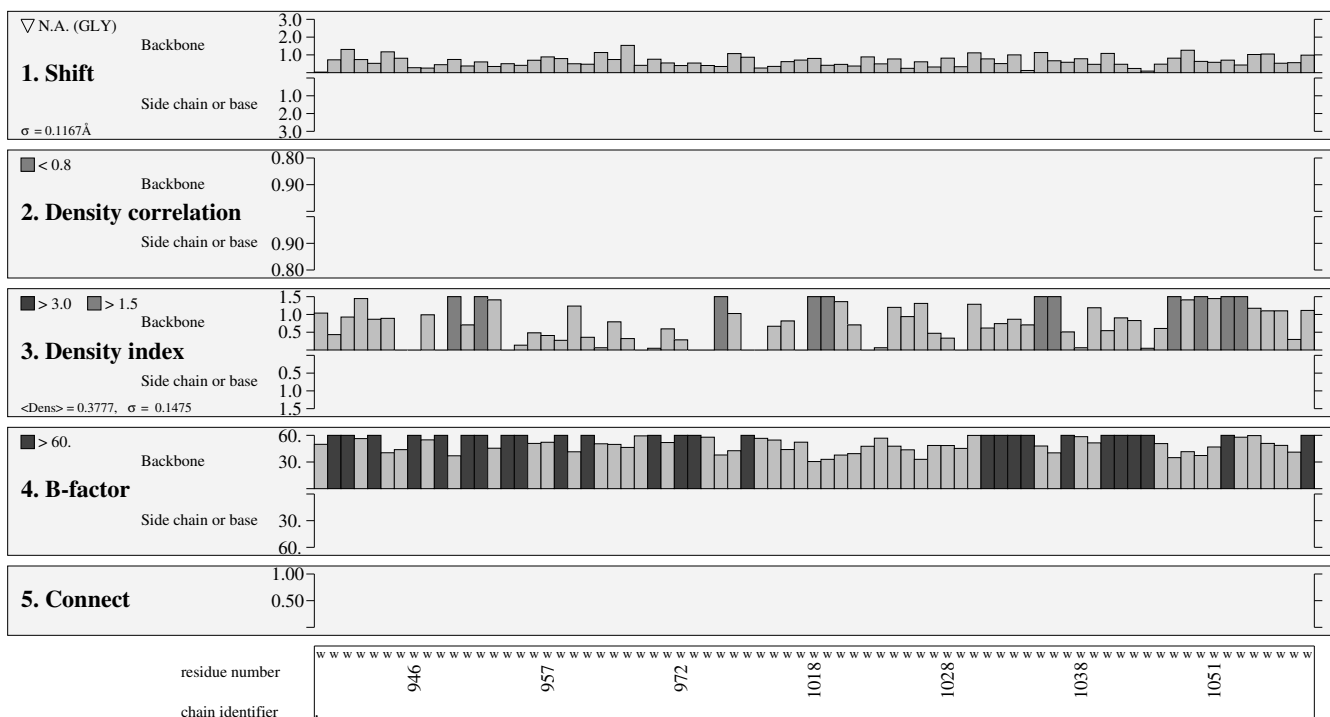
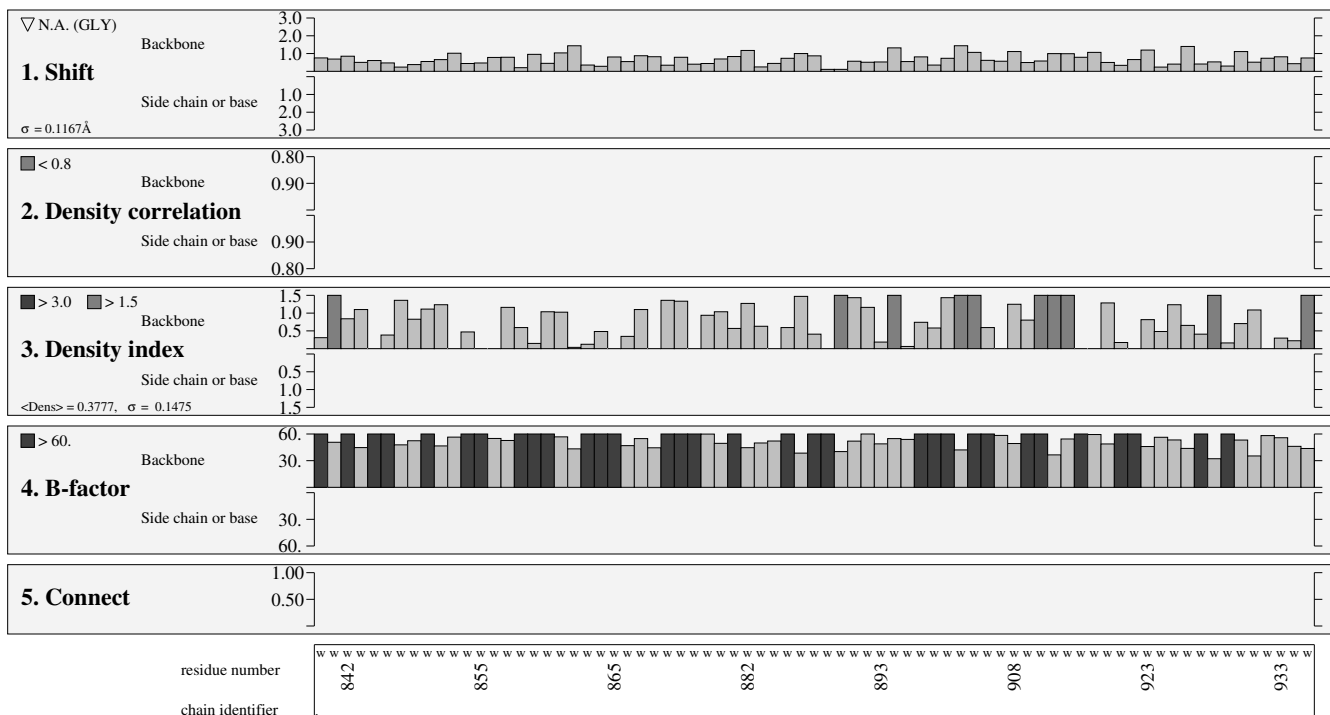
Local estimation (32)



Structure Factor Check

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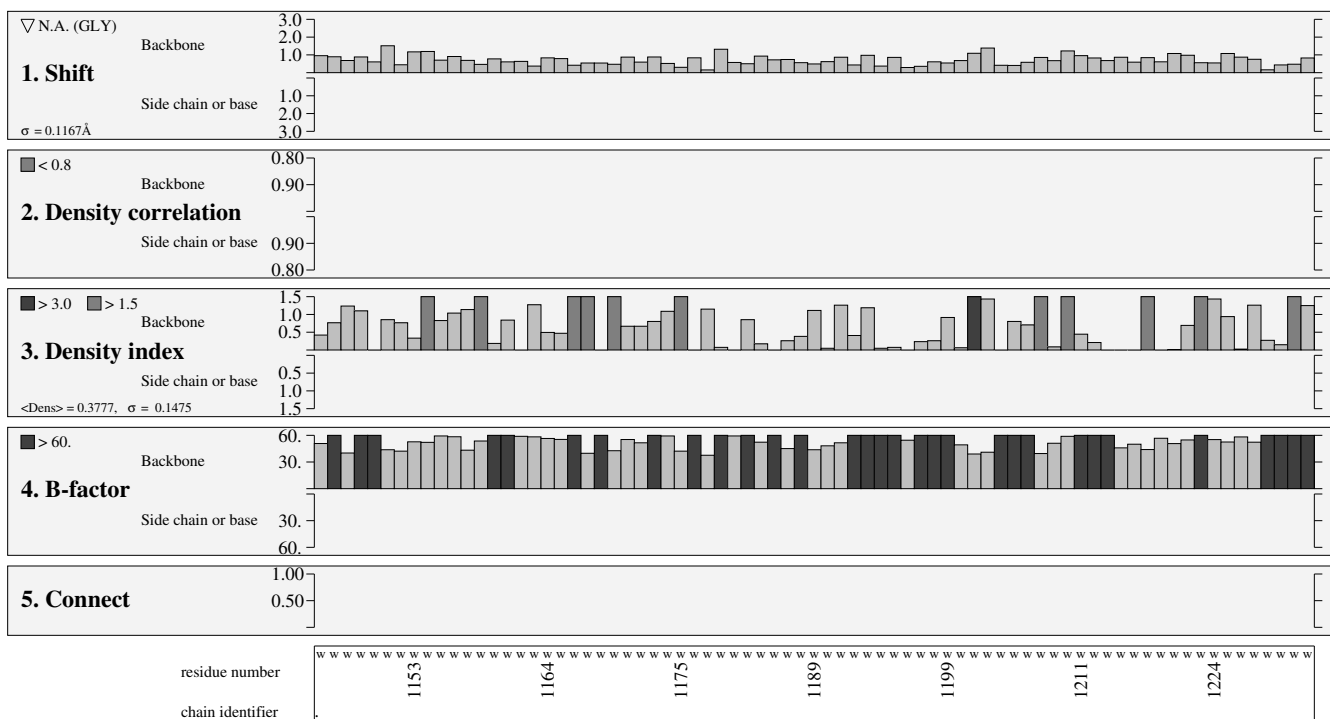
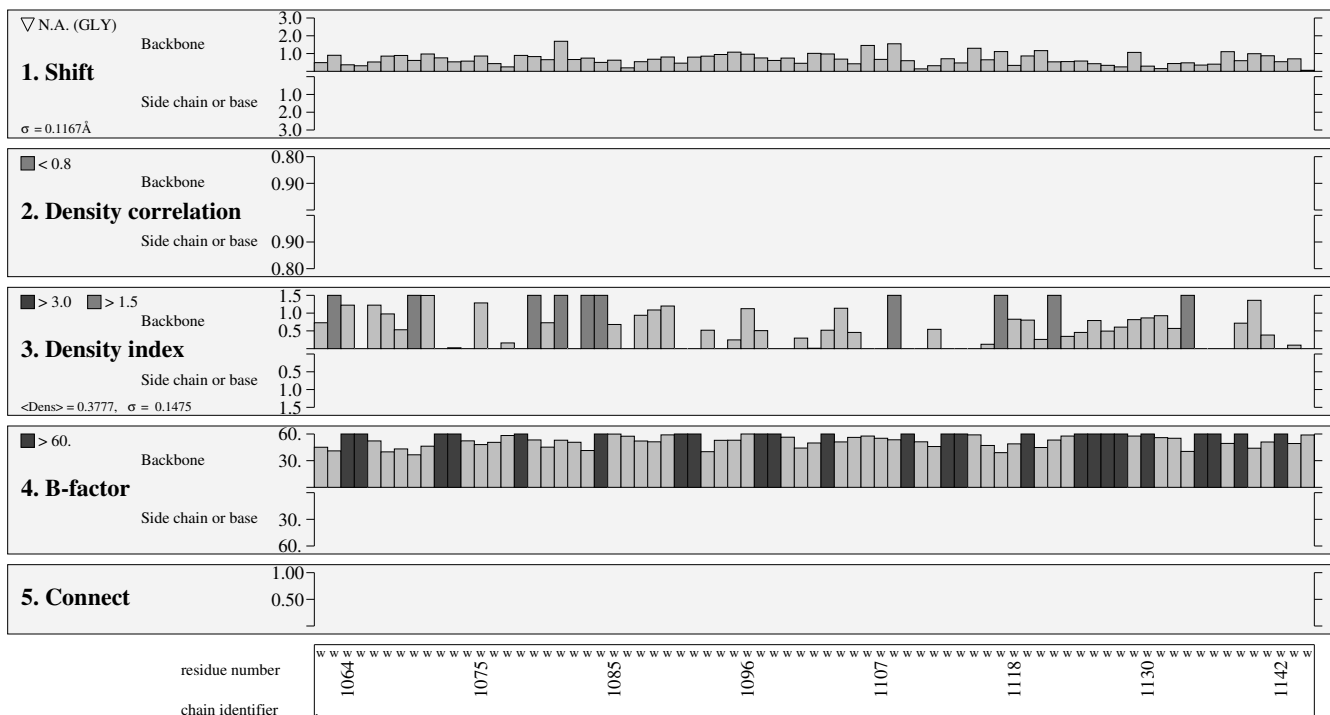
Local estimation (33)



Structure Factor Check

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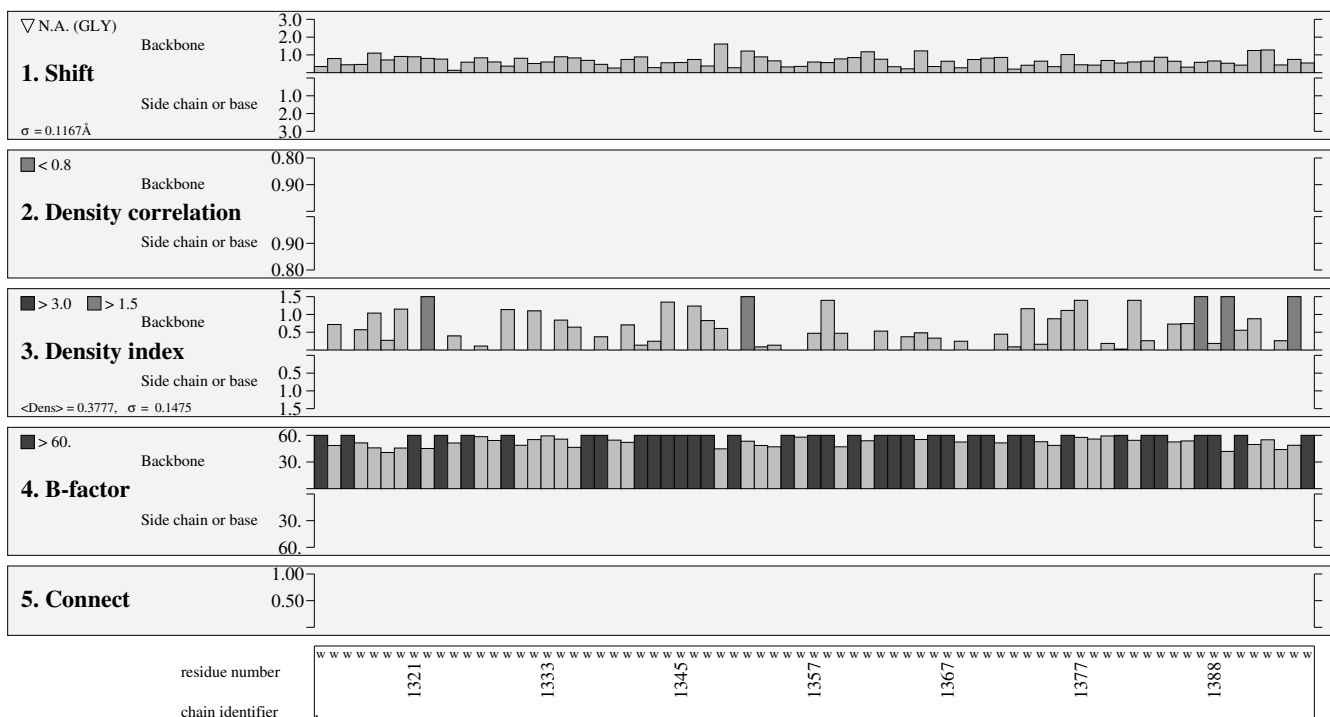
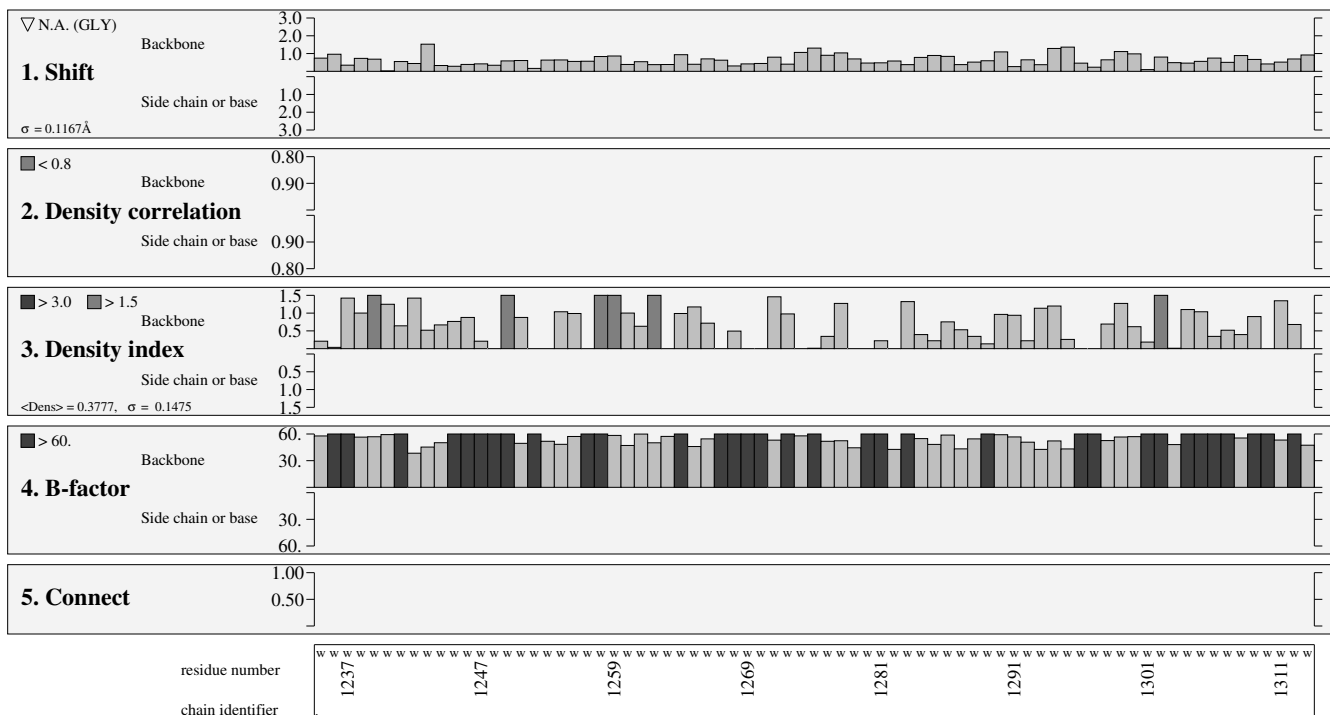
Local estimation (34)



Structure Factor Check

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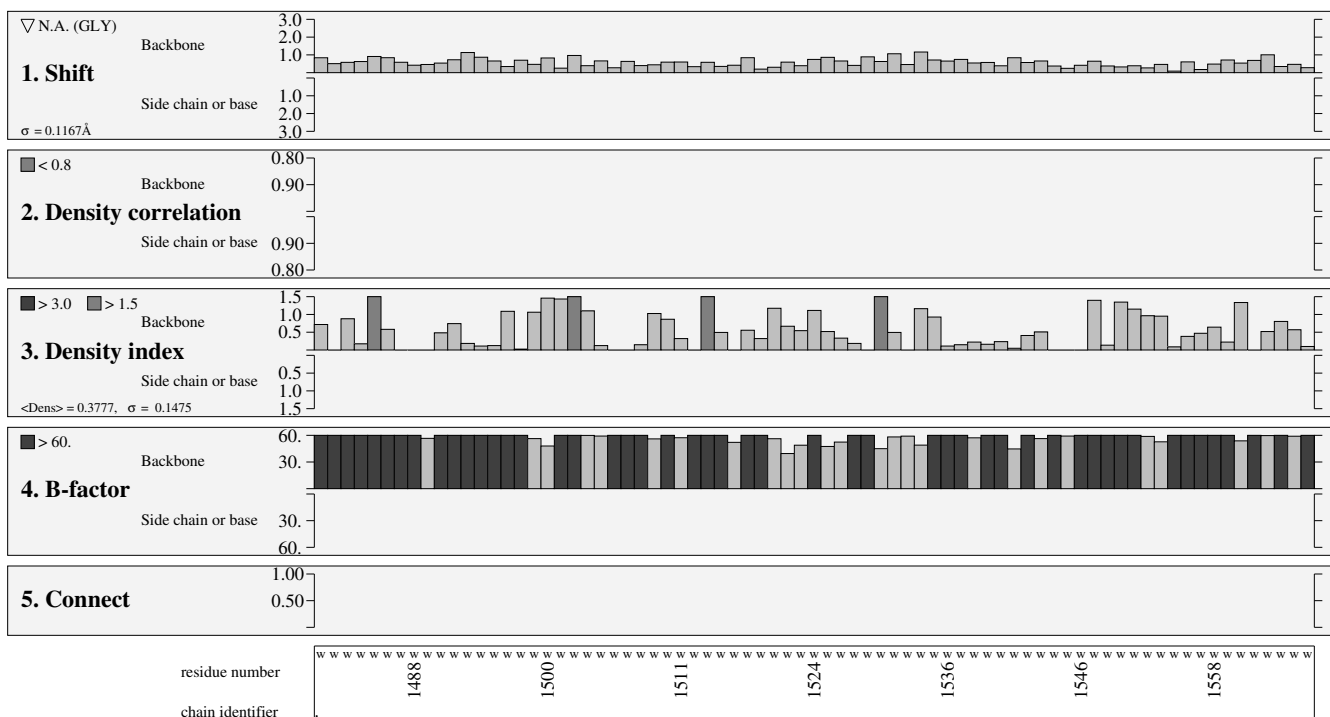
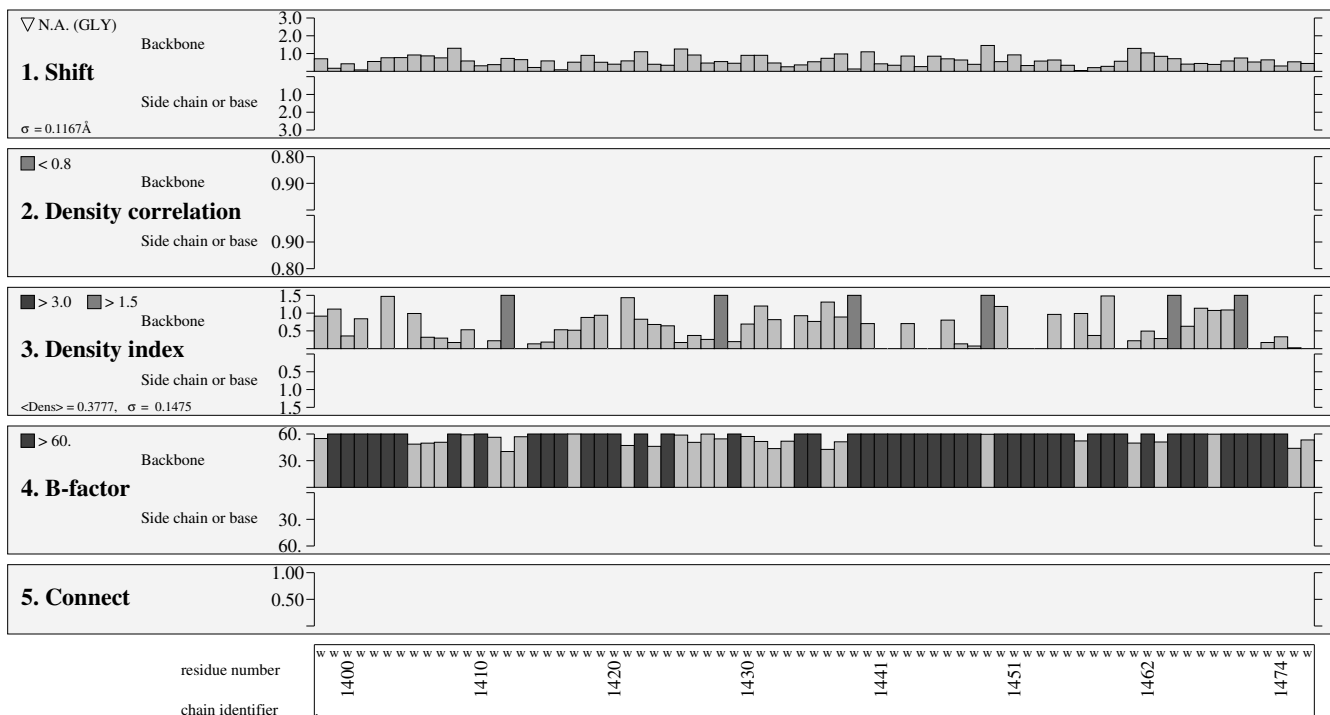
Local estimation (35)



Structure Factor Check

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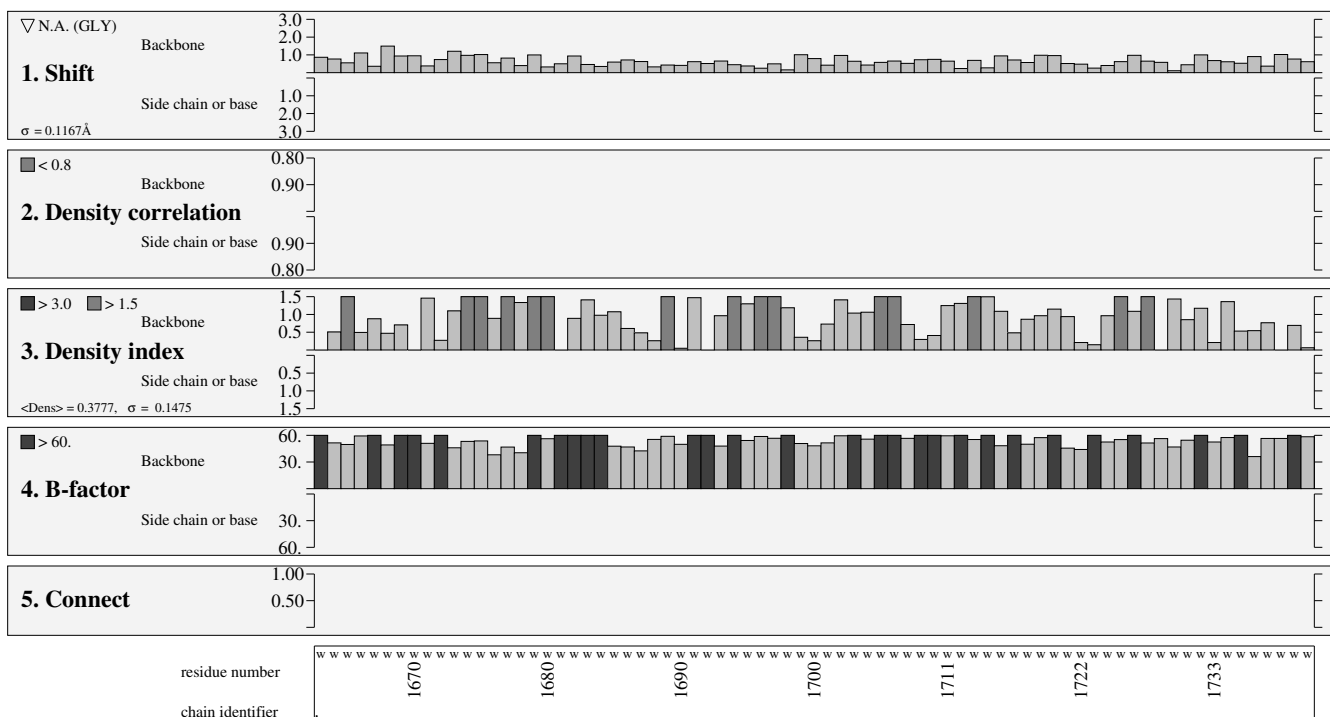
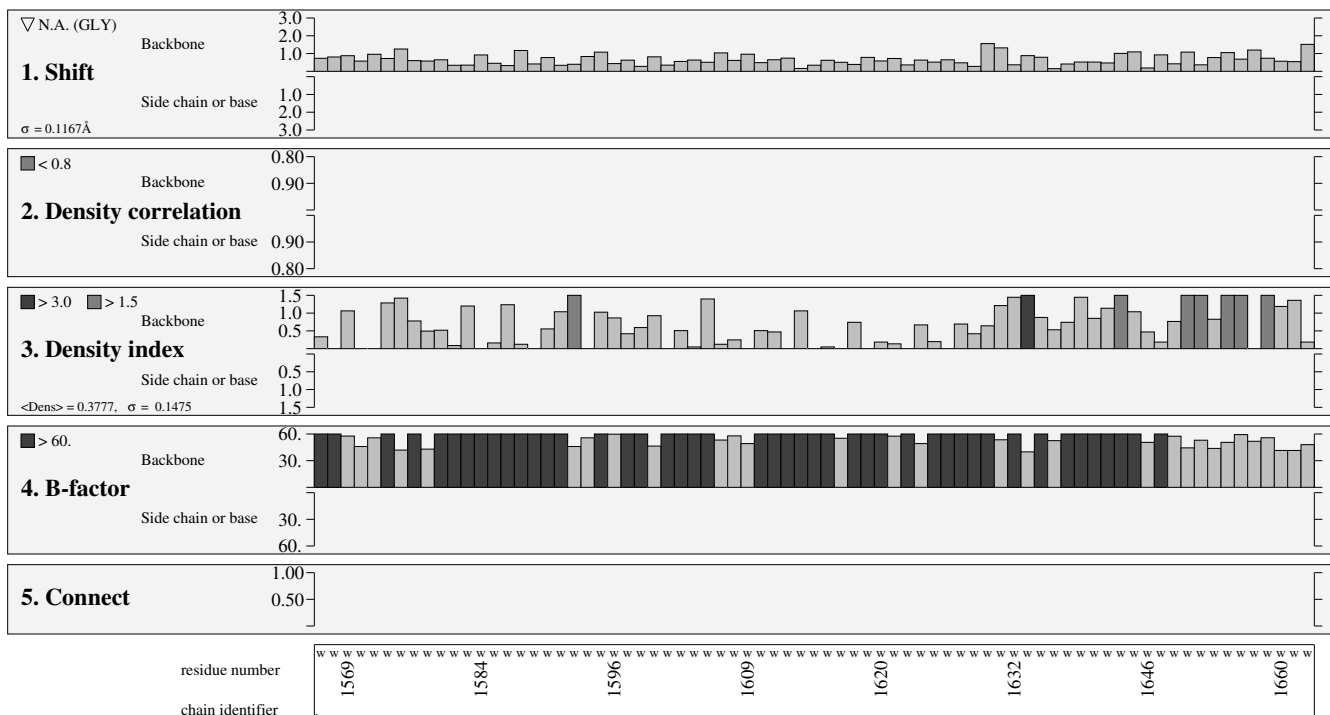
Local estimation (36)



Structure Factor Check

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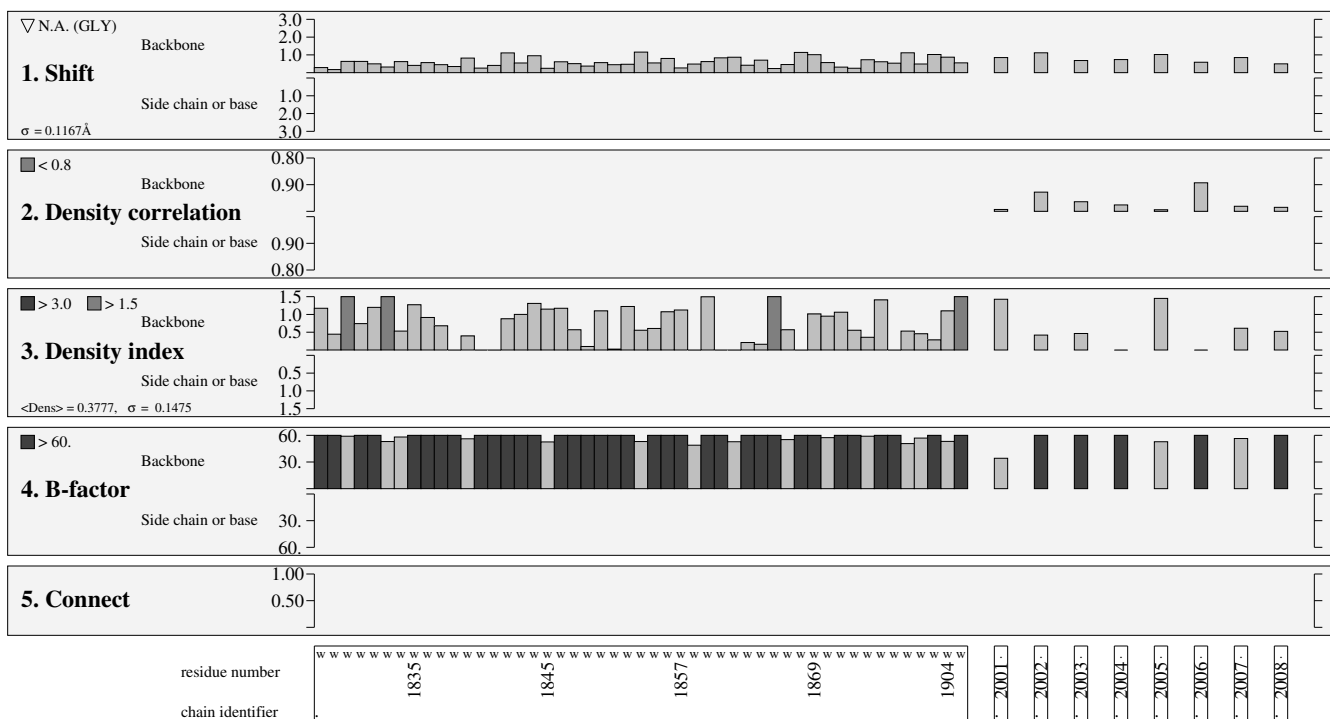
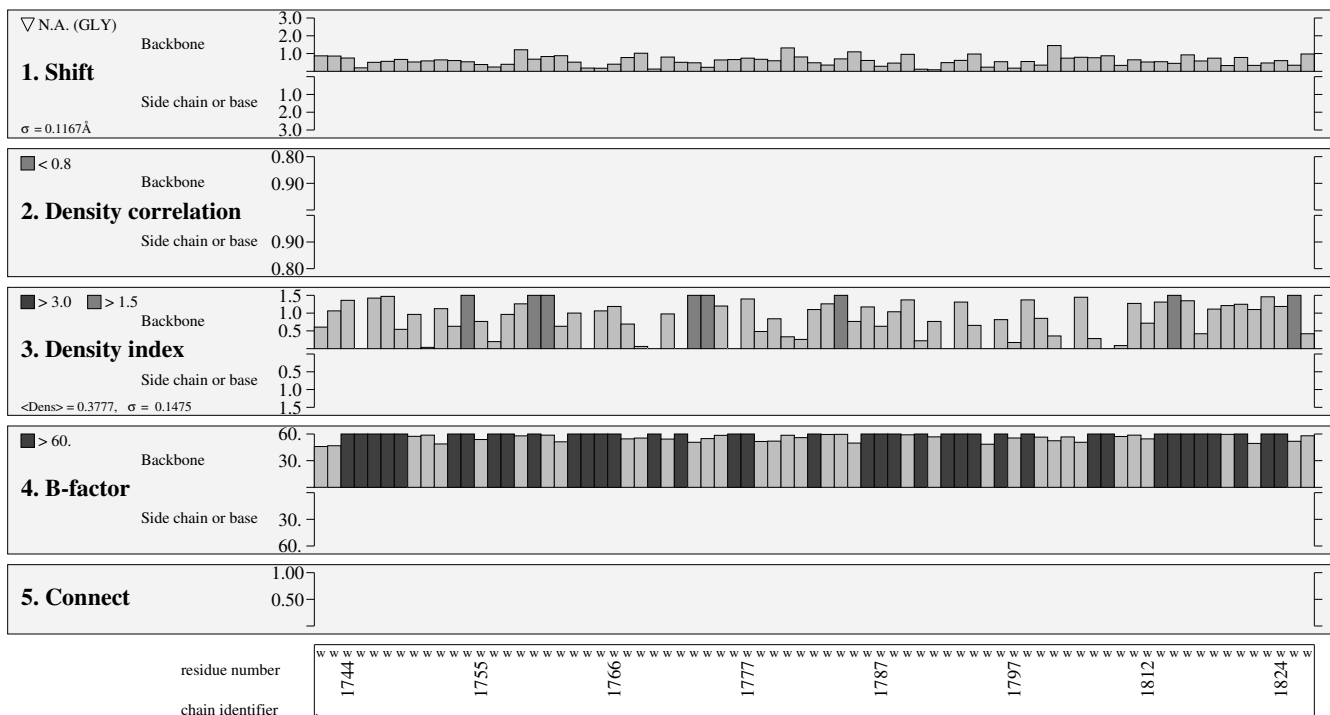
Local estimation (37)



Structure Factor Check

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Local estimation (38)



Structure Factor Check

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Local estimation (39)

