

Structure Factor Check

1CFM

Title: CYTOCHROME F FROM CHLAMYDOMONAS REINHARDTII
 Date: 18-SEP-98
 PDB code: 1CFM

Crystal

Cell parameters:

a: 75.62 A b: 94.94 A c: 119.92 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Number of NCS-operators: 2
 NC-symmetry only for information

Structure Factors

Input

Nominal resolution range: 28.6 – 2.00 A
 Reflections in file: 47521
 Unique reflections above 0: 47521
 above 1 σ : 47054
 above 3 σ : 41783

SFCHECK

Nominal resolution range: 28.6 – 2.00 A
\05max. from input data, min. from author\05
 Used reflections: 47418
 Reflections out of resolution: 103
 Completeness: 80.4 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.021
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.7794 0.7589
 B_{overall} (by Patterson): 29. A²
 Optical resolution: 1.58 A
 Expected opt. resol. for complete data set: 1.58 A
 Estimated minimal error: 0.012 A

Model

6878 atoms (1001 water molecules)
 Number of chains: 9
 Volume not occupied by model: 26.7 %
 $\langle B \rangle$ (for atomic model): 26.9 A²
 $\sigma(B)$: 12.40 A²
 Matthews coefficient: 2.24
 Corresponding solvent % : 44.55

Model vs. Structure Factors

R-factor for all reflections: 0.230
 Correlation factor: 0.918
 R-factor: 0.231
 for $F > 2.0\sigma$
 nom. resolution range: 25.00 – 2.00A
 reflections used: 46961
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.263 A
 Estimated maximal error: 0.108 A
 DPI: 0.221 A

Scaling

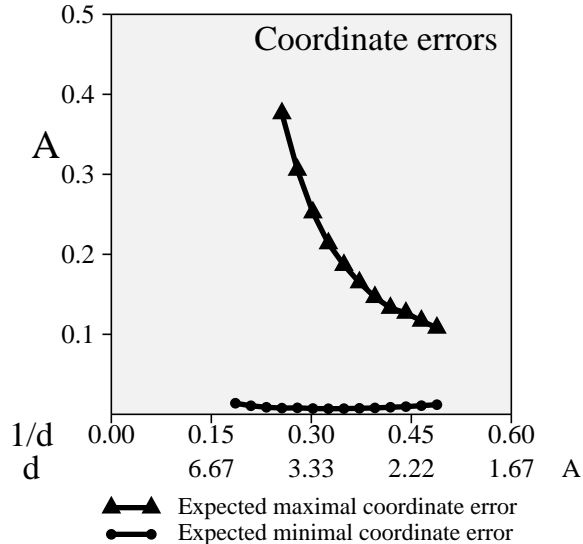
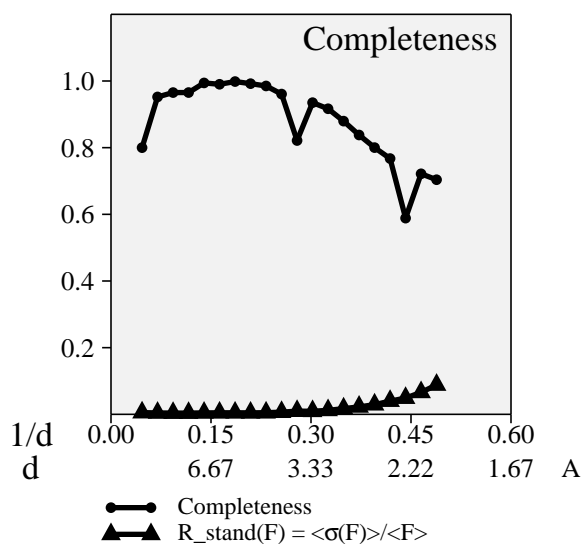
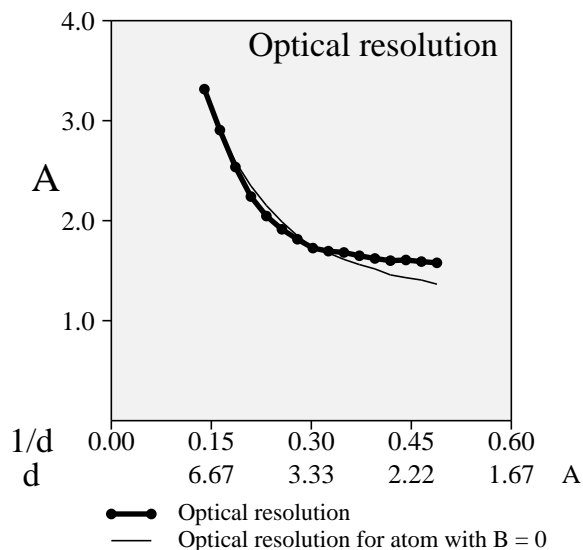
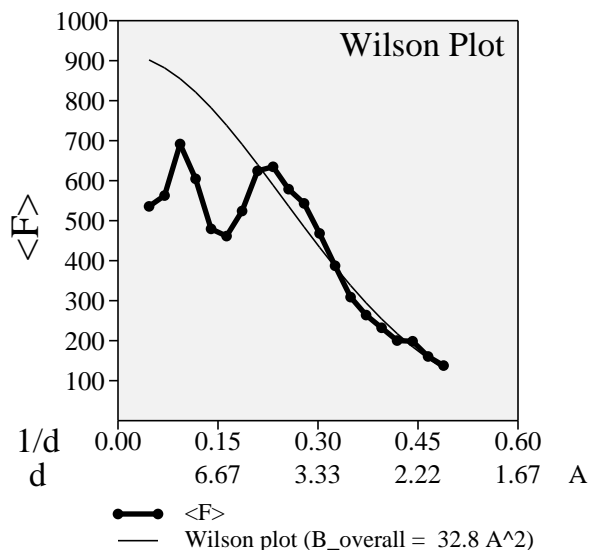
Scale: 0.828
 Bdiff: 0.13
 Anisothermal Scaling (Beta):
 1.3460 0.1195 -0.9334 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.837 250.002

Refinement

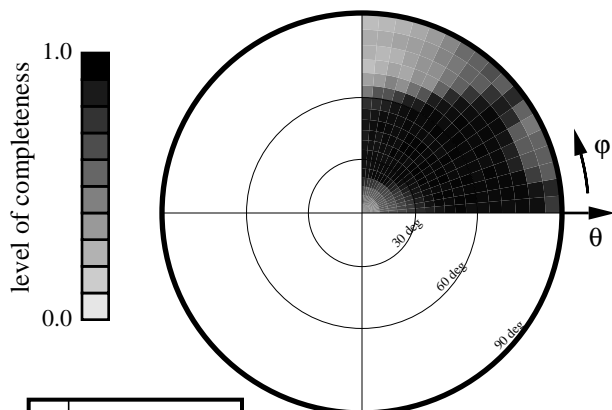
Program: CNS 0.1
 Nominal resolution range: 25.0 – 2.00 A
 Reported R-factor: 0.214
 Number of reflections used: 46907
 Reported Rfree: 0.27
 Sigma cut-off (F): 2.00

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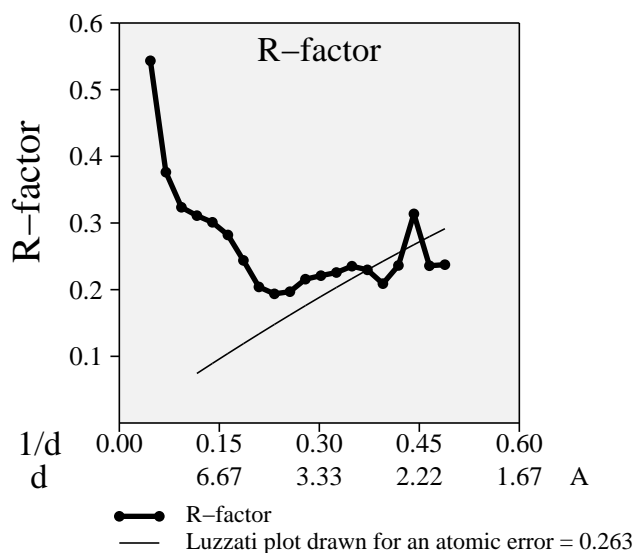


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

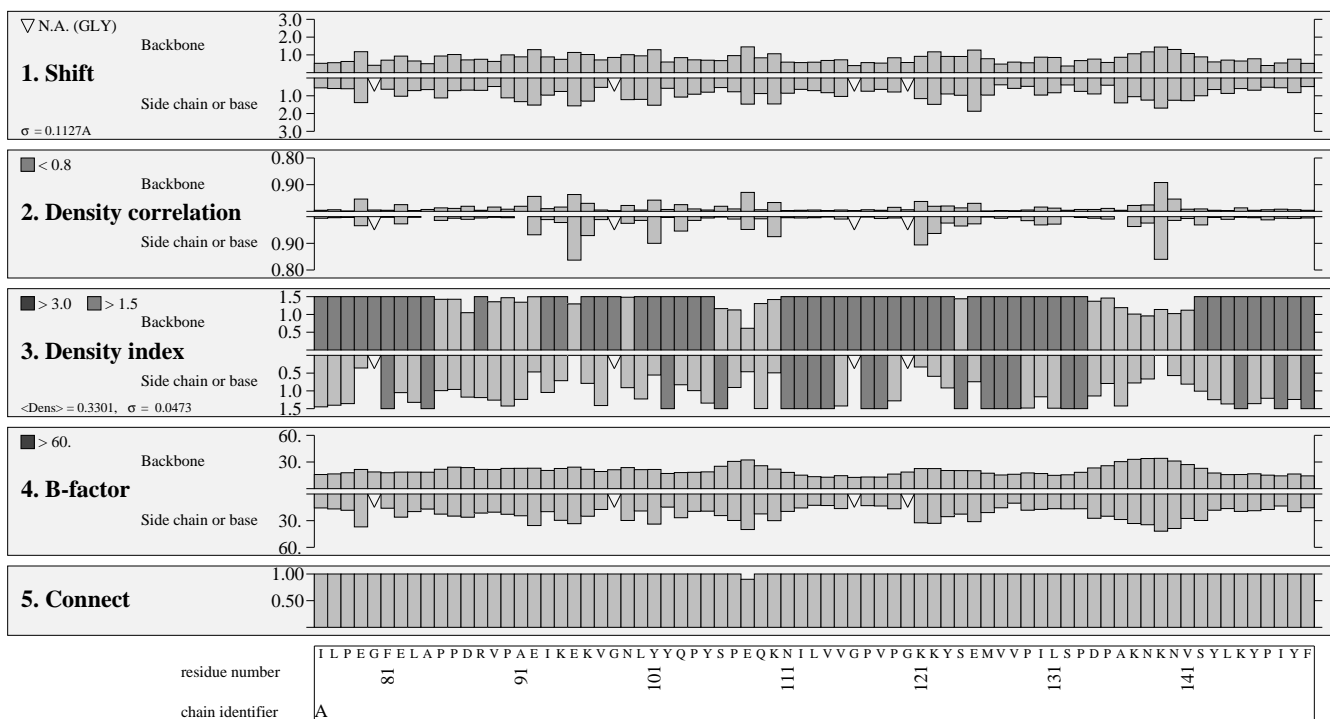
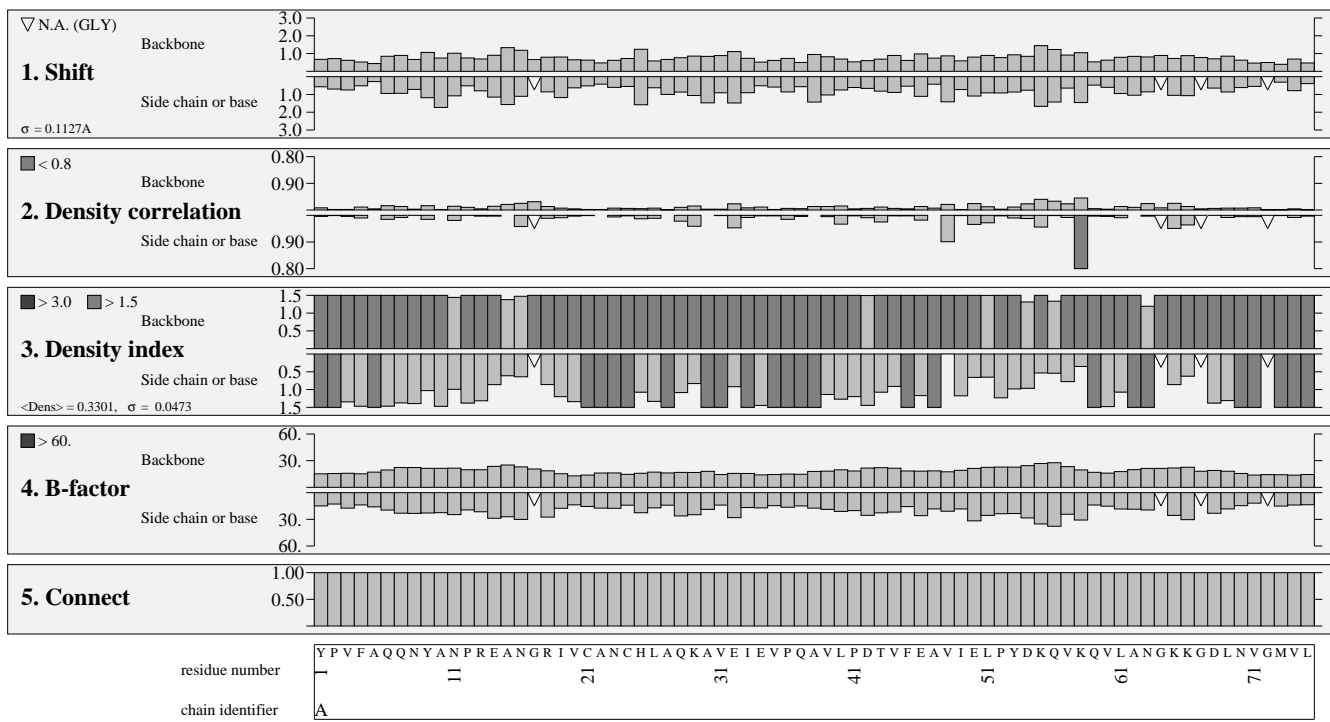
polar coordinates of the crystallographical axes



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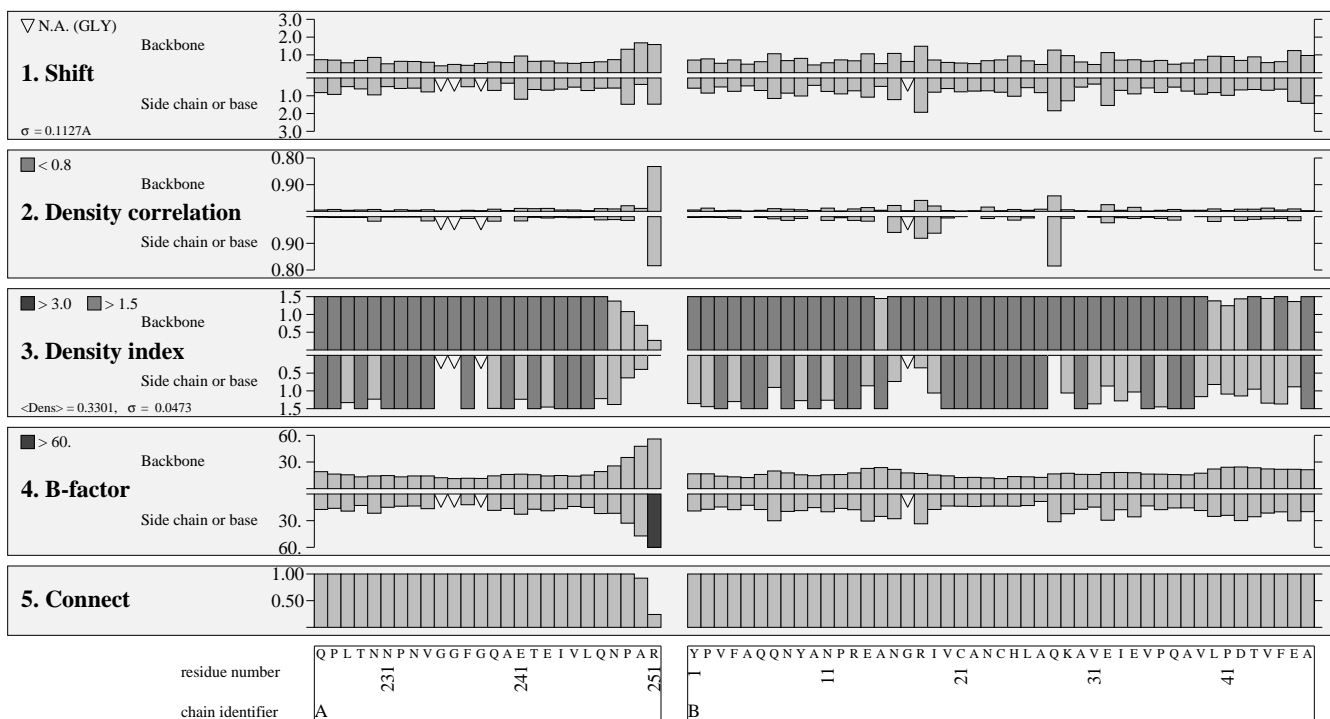
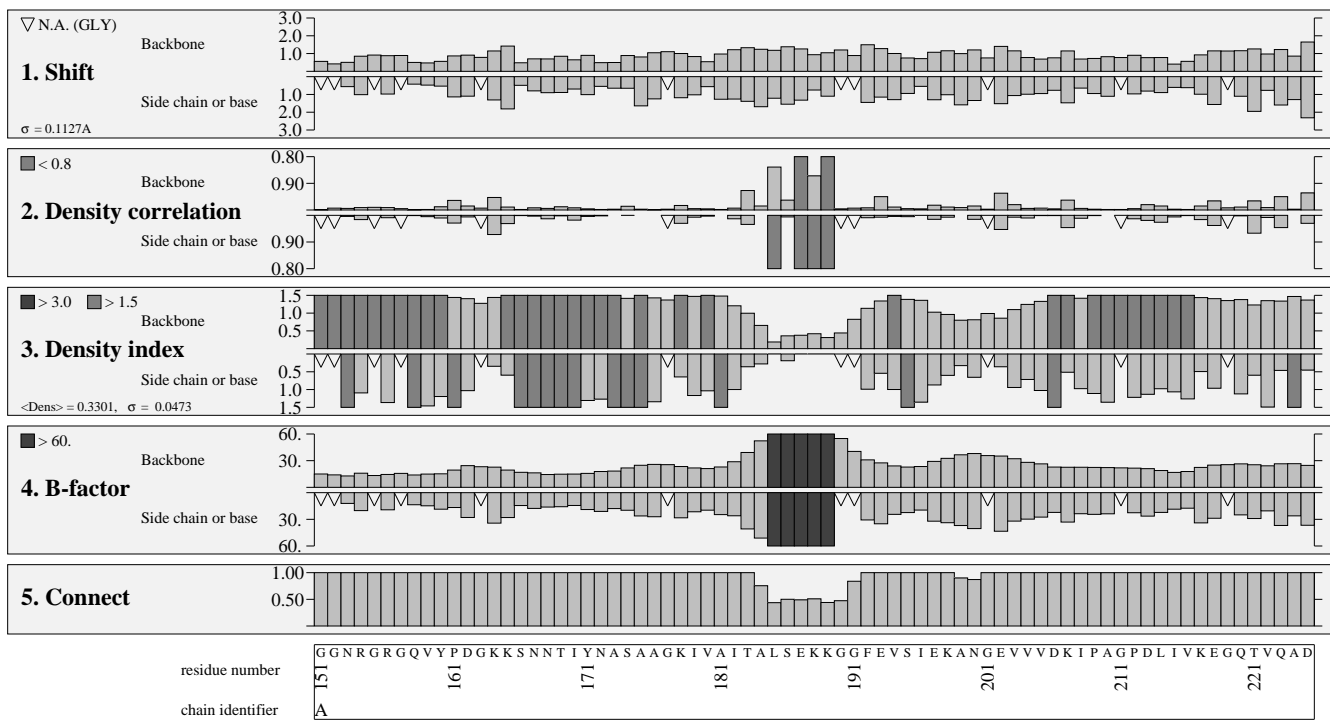
Local estimation



Structure Factor Check

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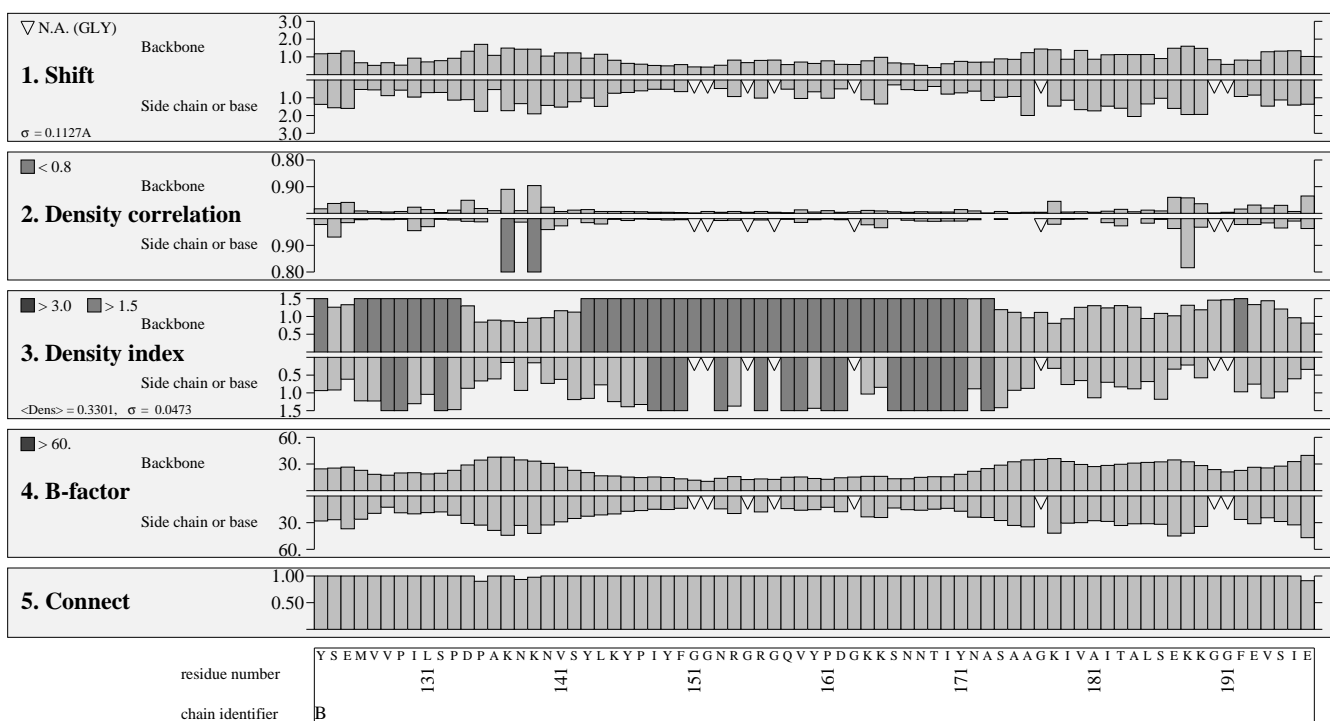
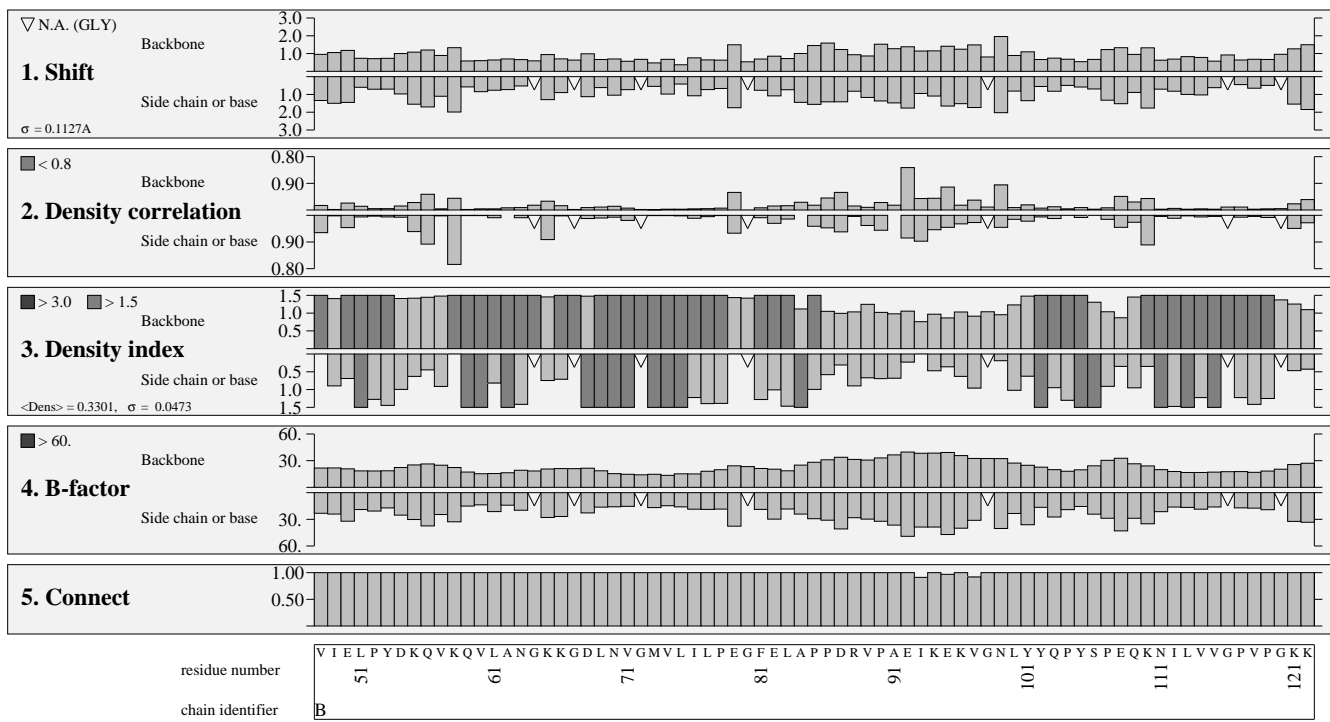
Local estimation (2)



Structure Factor Check

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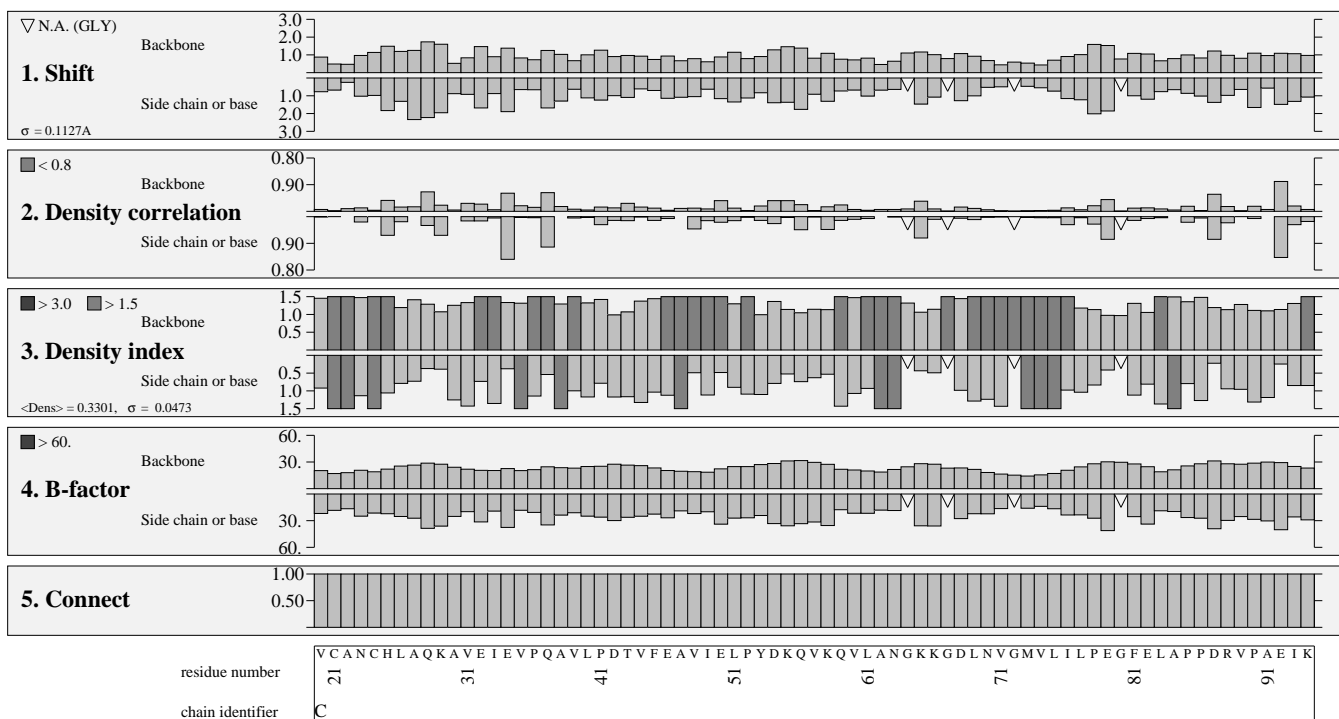
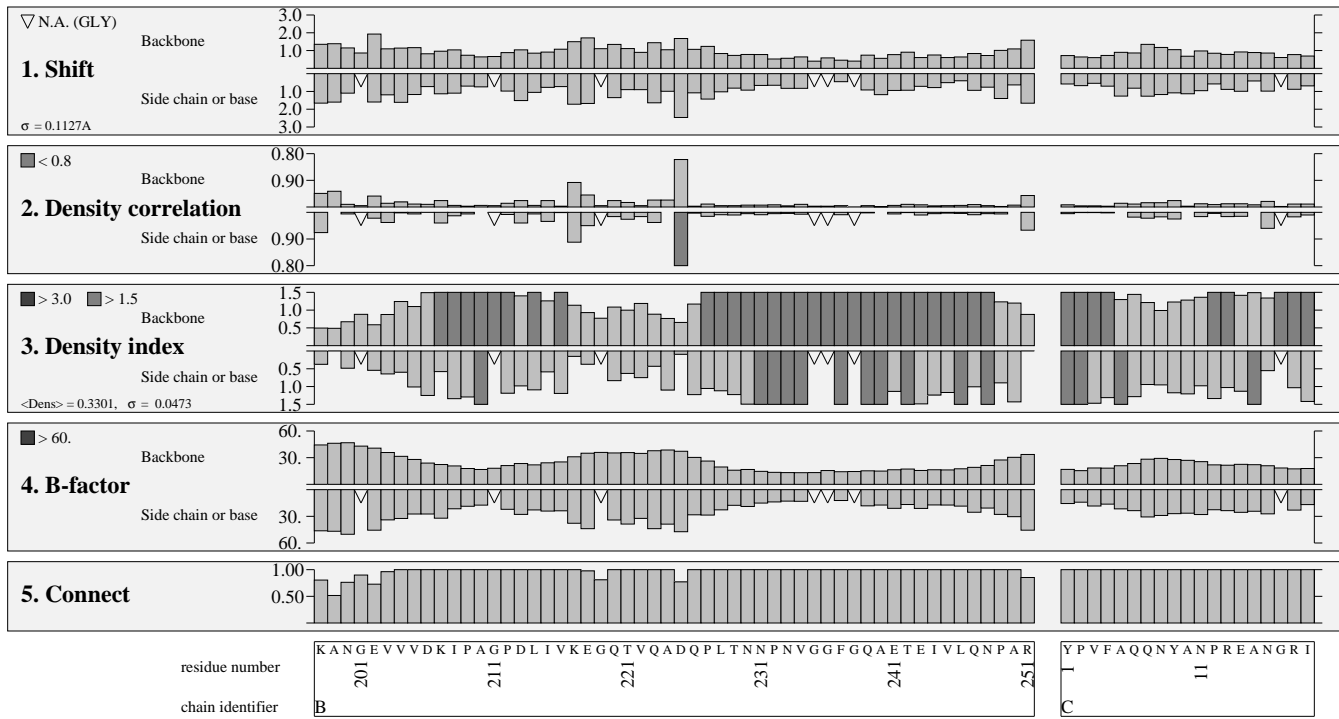
Local estimation (3)



Structure Factor Check

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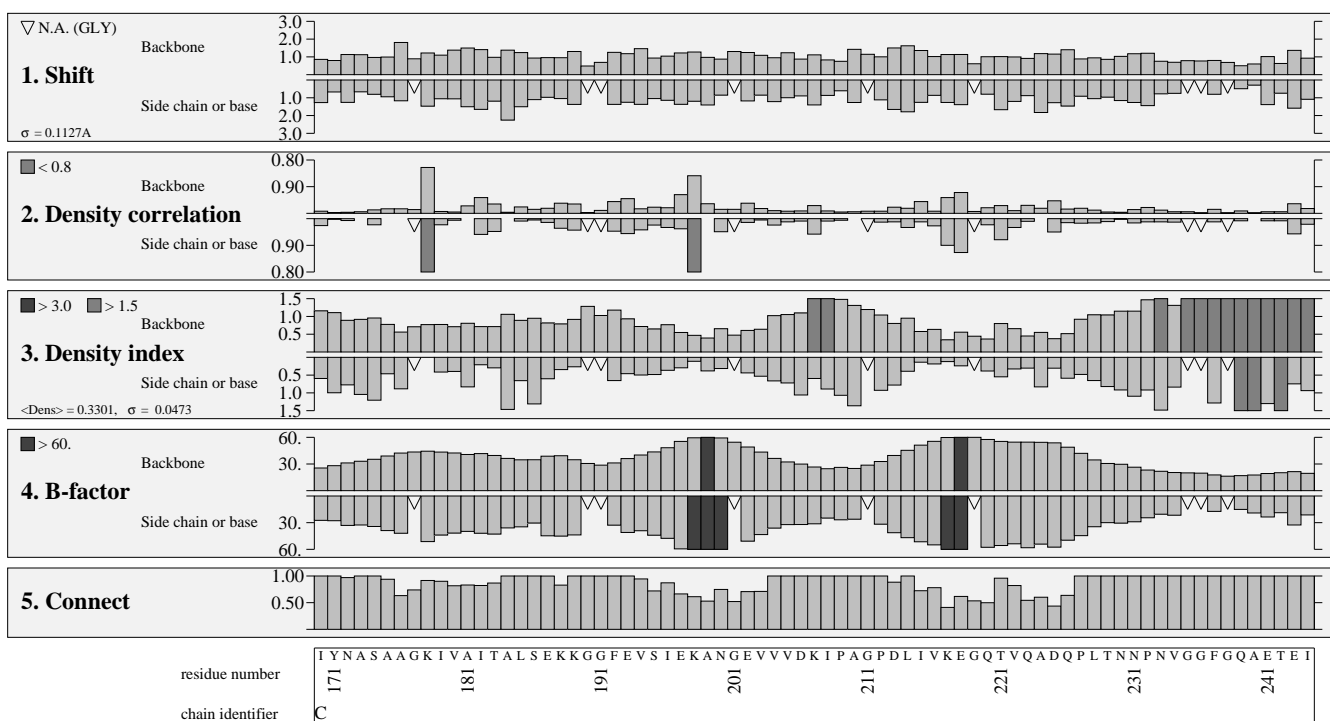
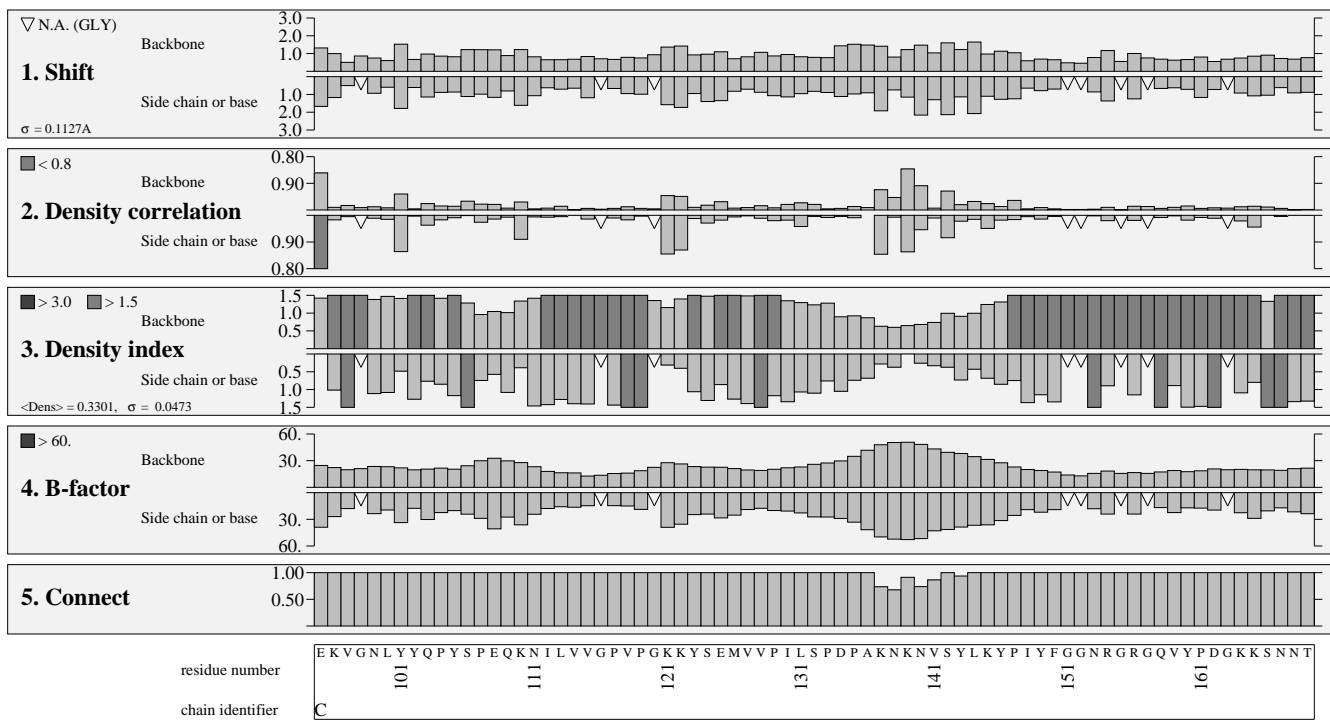
Local estimation (4)



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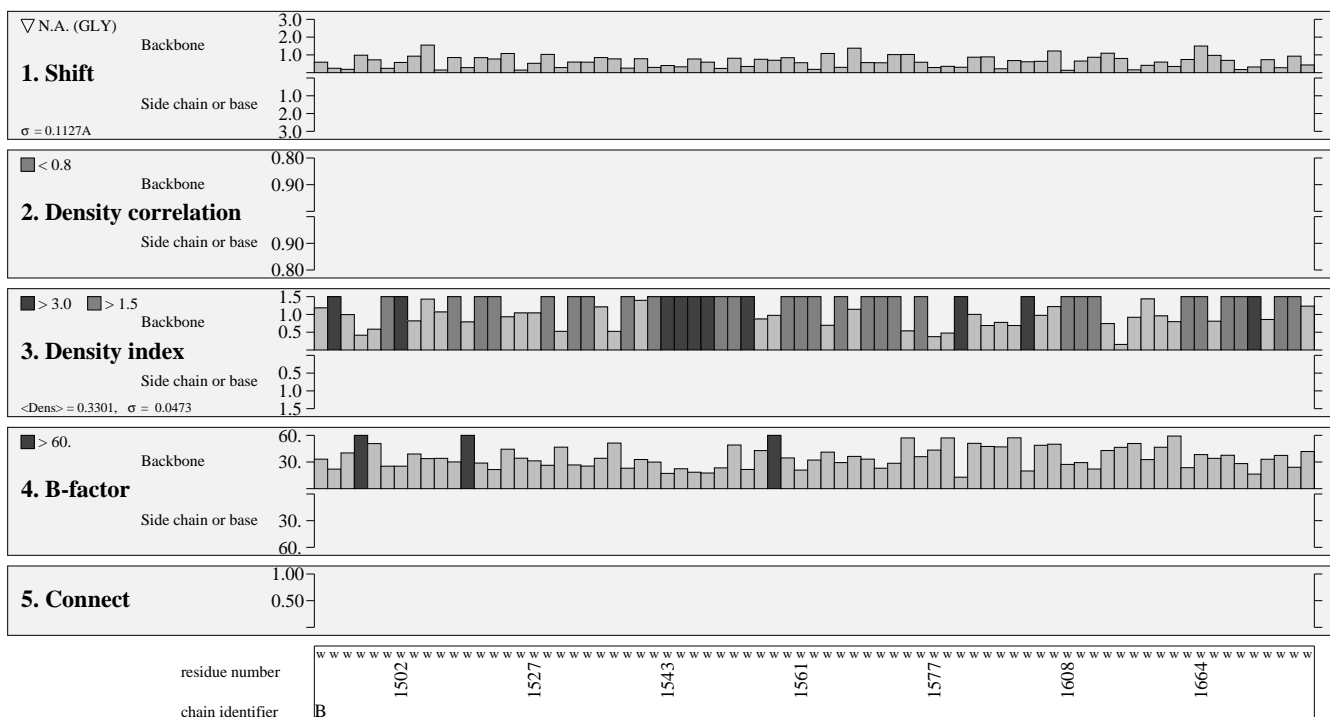
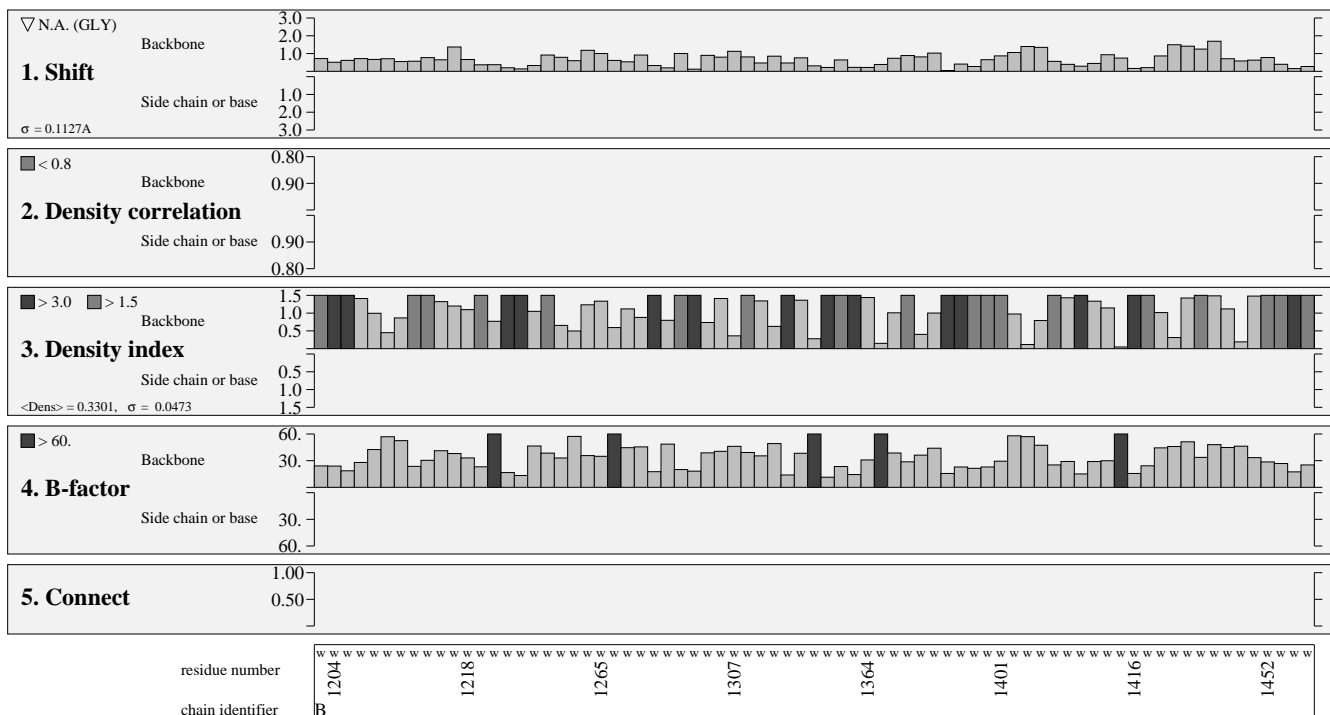
Local estimation (5)



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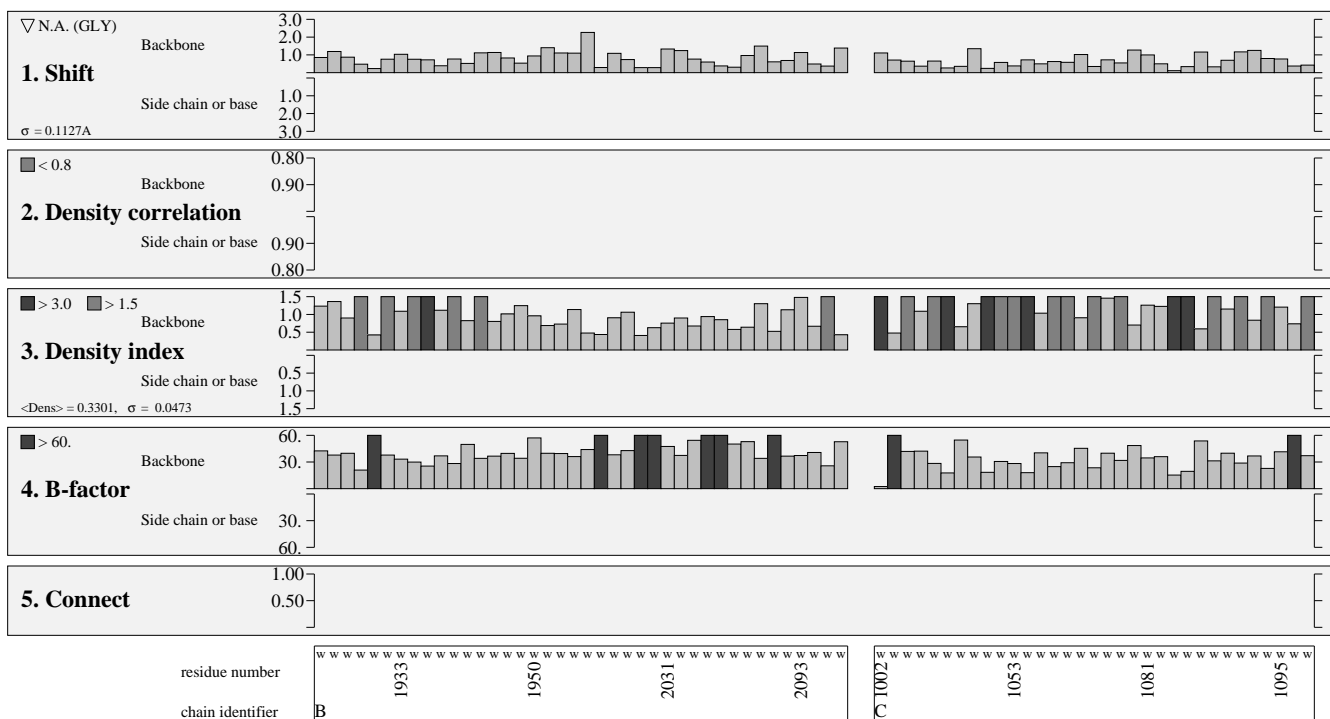
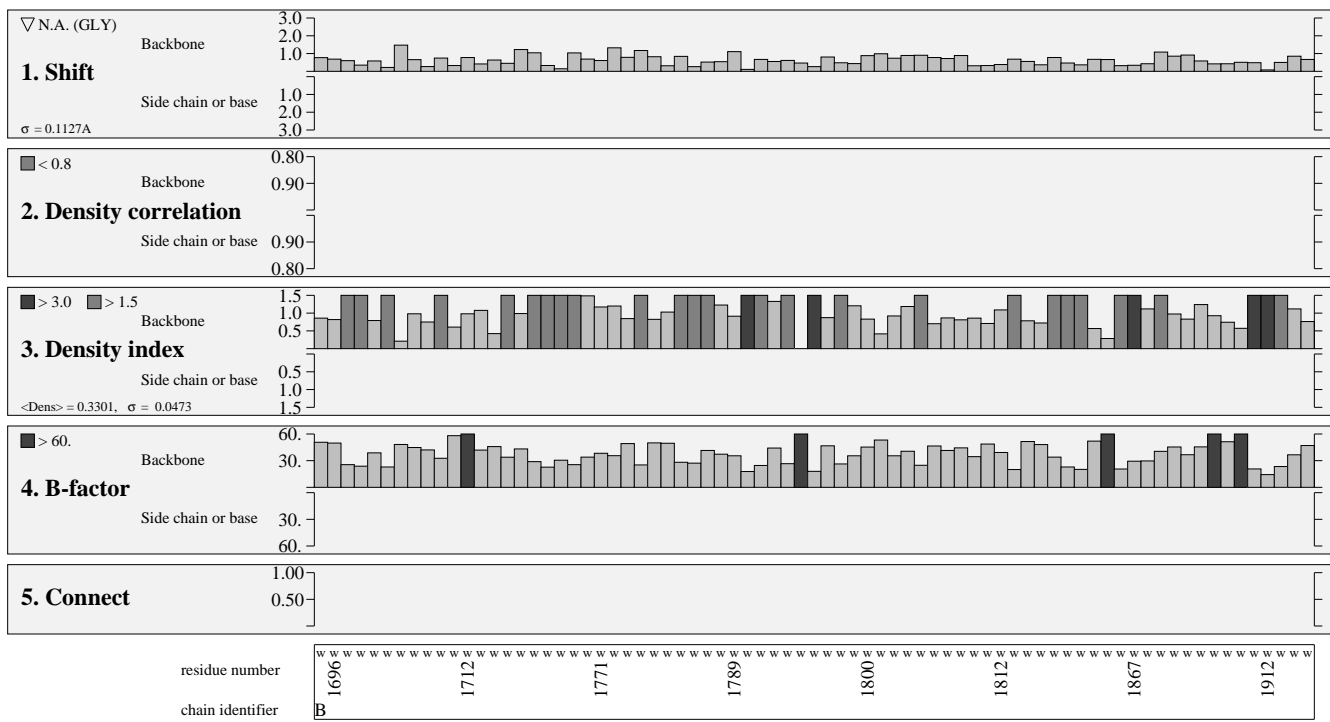
Local estimation (9)



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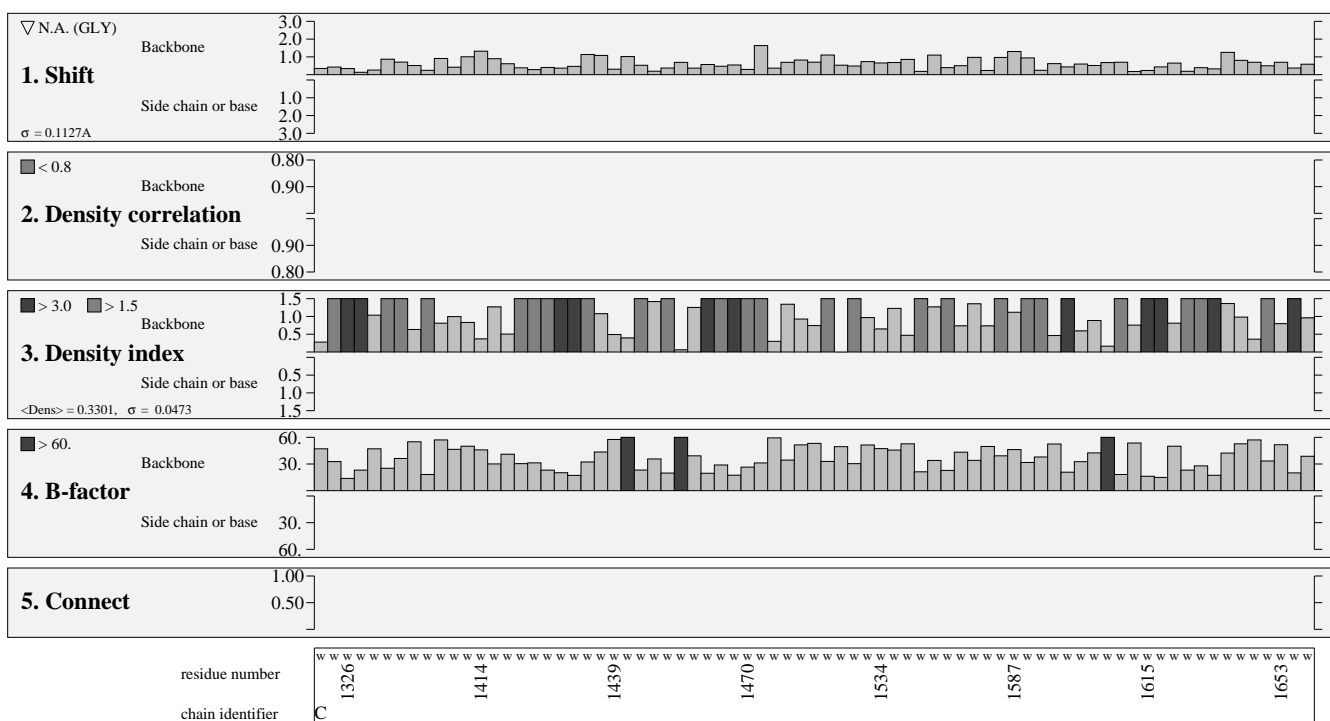
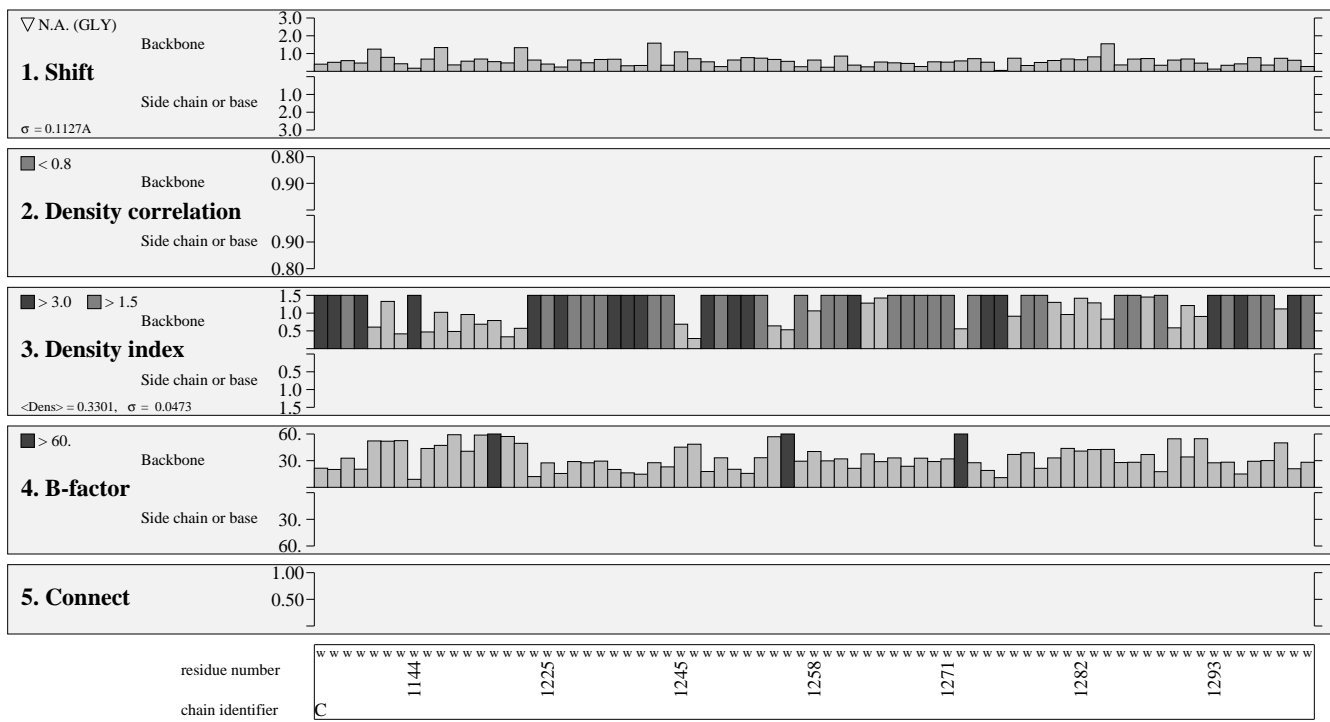
Local estimation (10)



Structure Factor Check

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Local estimation (11)



Structure Factor Check

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Local estimation (12)

