

Structure Factor Check

6MYO

Title: AVIAN MITOCHONDRIAL COMPLEX II WITH FLUTOLANYL BOUND
 Date: 02-NOV-18
 PDB code: 6MYO

Crystal

Cell parameters:

a: 69.64 A b: 83.78 A c: 289.58 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 47.6 – 2.20 A
 Reflections in file: 87121
 Unique reflections above 0: 75089
 above 1 σ : 71145
 above 3 σ : 61446
 Reflections > 0: 12032

SF CHECK

Nominal resolution range: 47.6 – 2.20 A
\05max. from input data, min. from author\05
 Used reflections: 75089
 Completeness: 86.3 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.052
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.9575 1.0000 0.6915
 B_{overall} (by Patterson): 65. A²
 Optical resolution: 2.13 A
 Expected opt. resol. for complete data set: 2.13 A
 Estimated minimal error: 0.031 A

Model

9321 atoms (426 water molecules)
 Number of atoms with aniso_U: 9321
 Number of chains: 51
 Volume not occupied by model: 53.6 %
 $\langle B \rangle$ (for atomic model): 57.0 A²
 $\sigma(B)$: 13.85 A²
 Matthews coefficient: 3.24
 Corresponding solvent % : 61.70

Model vs. Structure Factors

R-factor for all reflections: 0.267
 Correlation factor: 0.895
 R-factor: 0.266
 for $F > 2.0\sigma$
 nom. resolution range: 47.64 – 2.20A
 reflections used: 71154

Rfree: 0.295
 Nfree: 2130
 R-factor without free-refl.: 0.265
 Non free-reflections: 69024
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.358 A
 Estimated maximal error: 0.125 A
 DPI: 0.185 A

Scaling

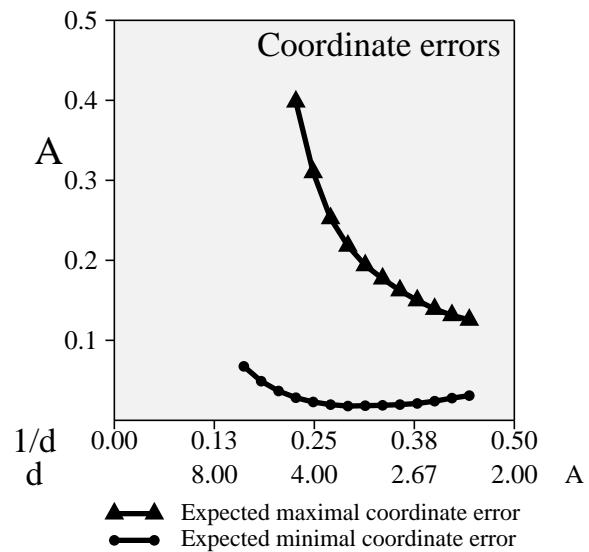
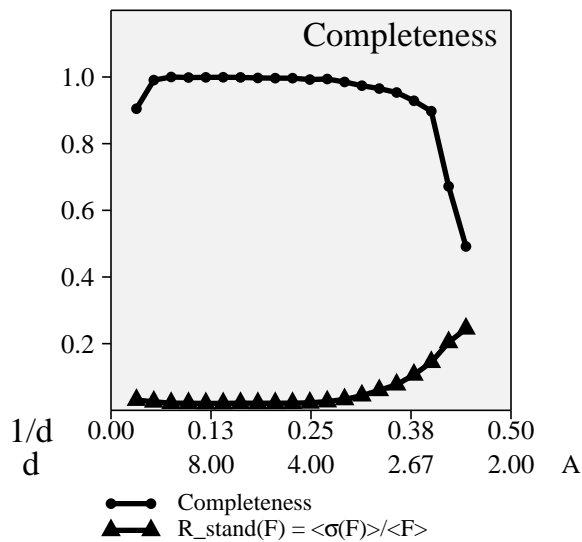
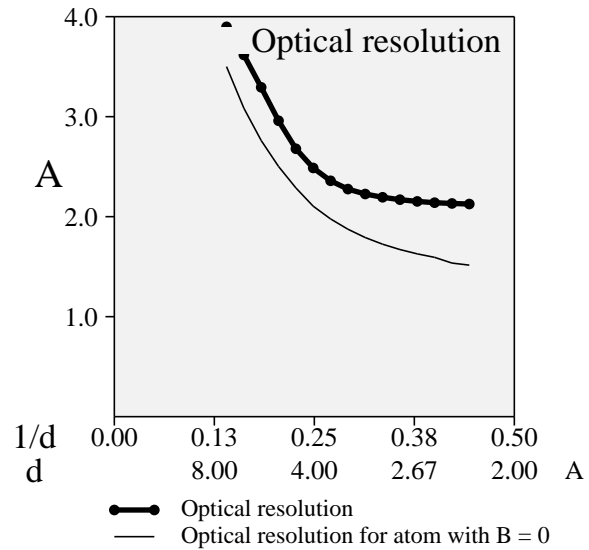
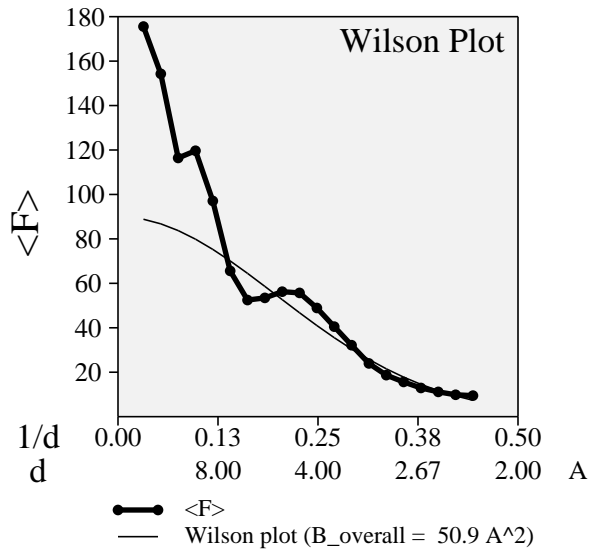
Scale: 0.067
 Bdiff: -18.15
 Anisothermal Scaling (Beta):
 5.1204 5.4667 1.0207 -0.0000 0.0000 -0.0000
 Solvent correction – Ks, Bs: 0.440 250.096

Refinement

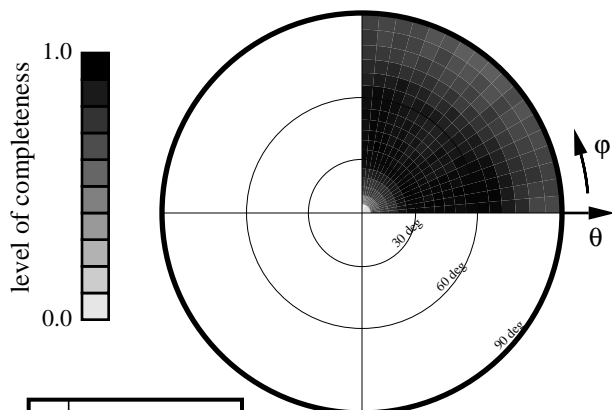
Program: PHENIX DEV_3150
 Nominal resolution range: 47.6 – 2.20 A
 Reported R-factor: 0.189
 Number of reflections used: 79336
 Reported Rfree: 0.23
 Sigma cut-off: N.A.

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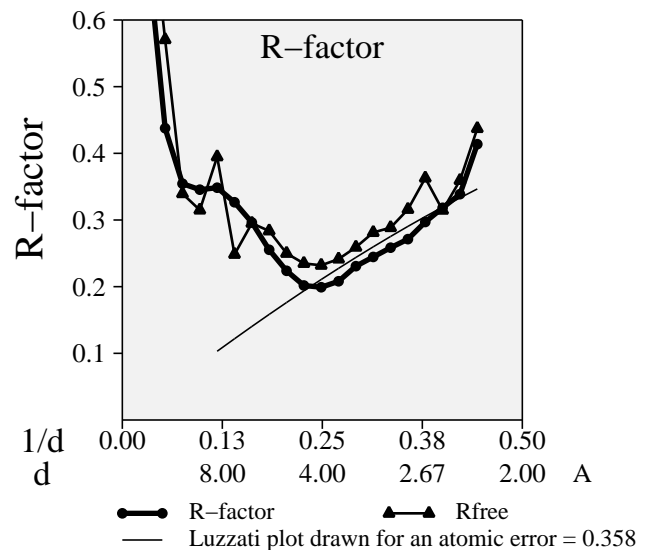


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

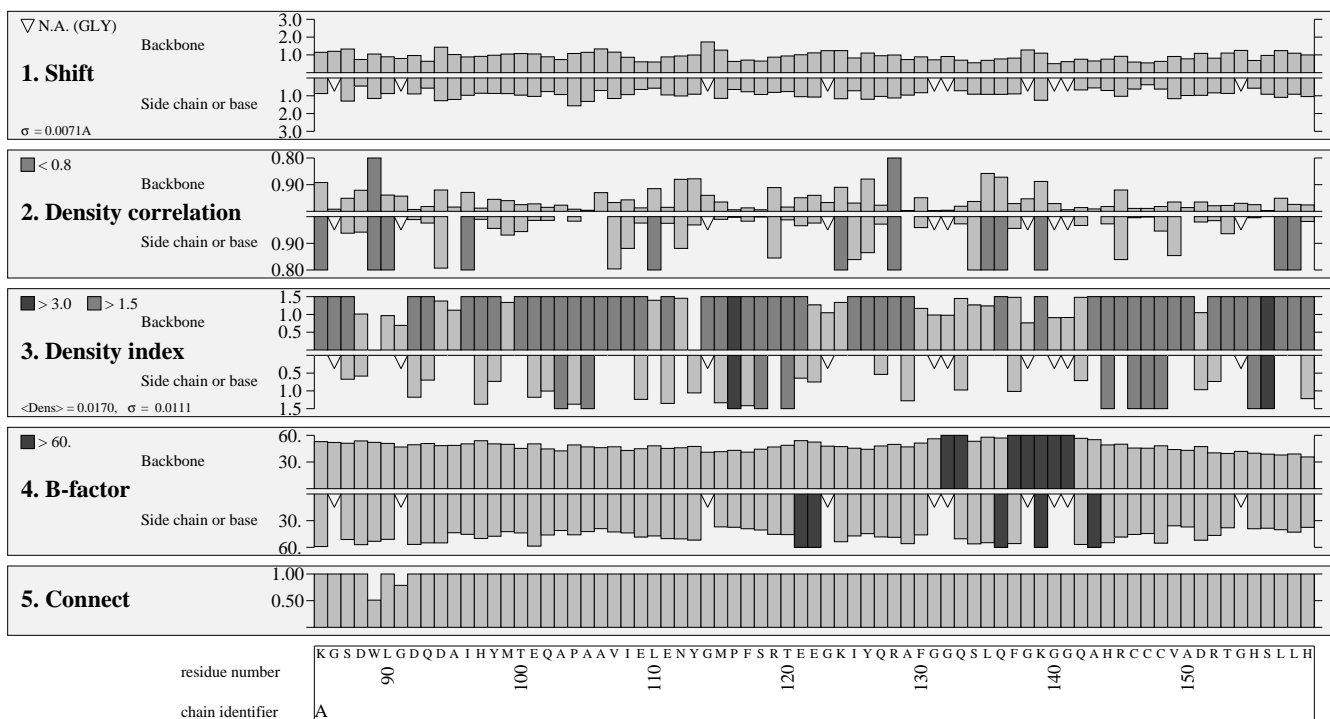
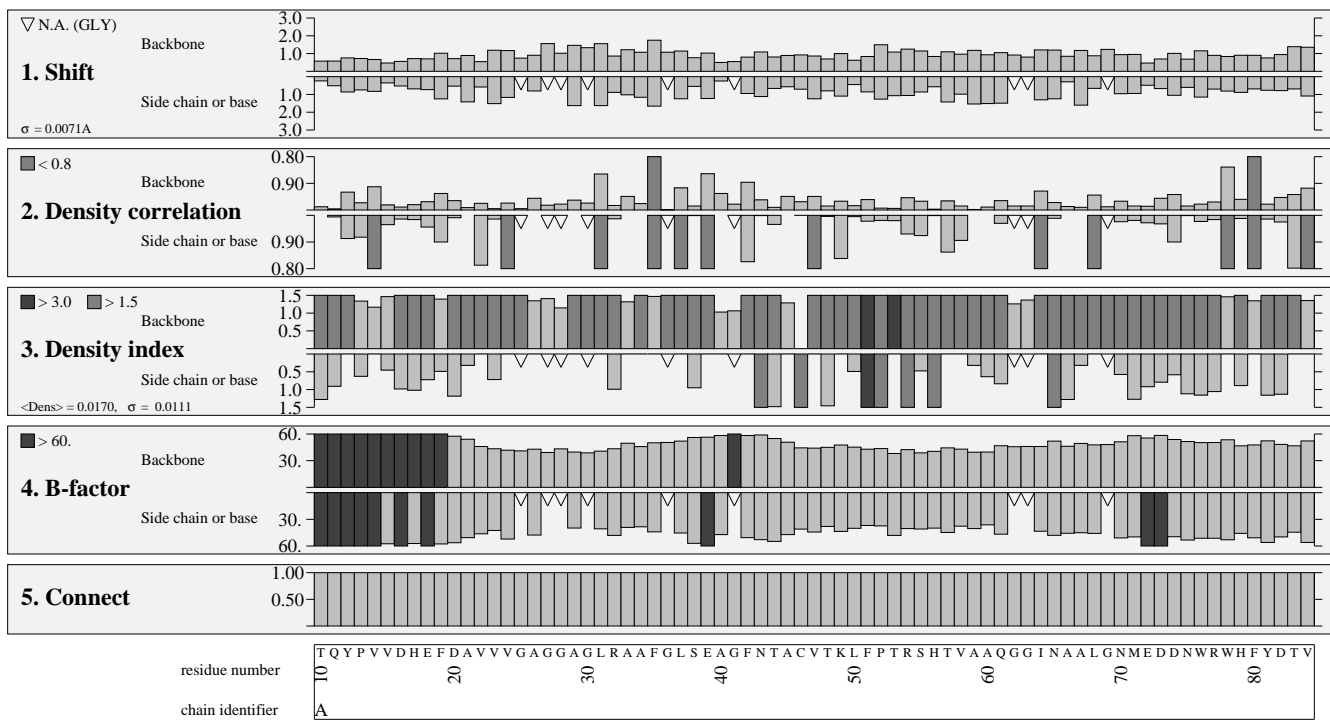
polar coordinates of the crystallographical axes



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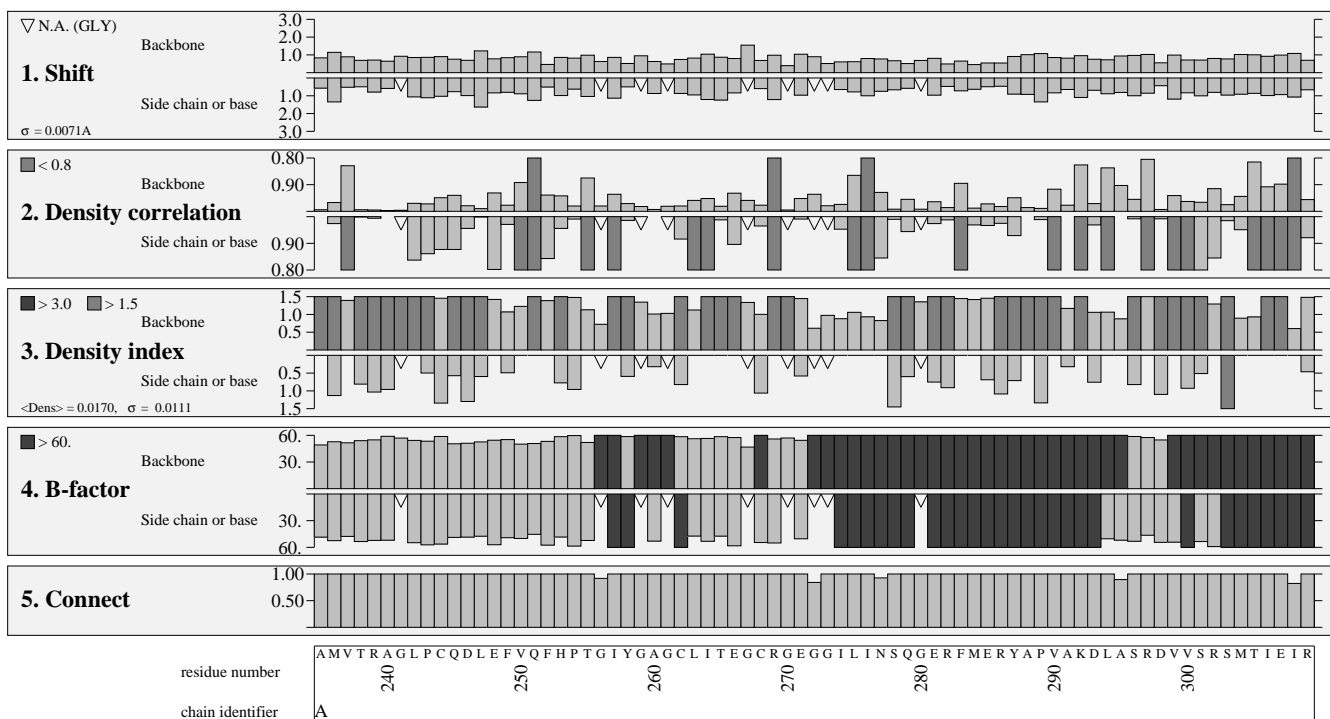
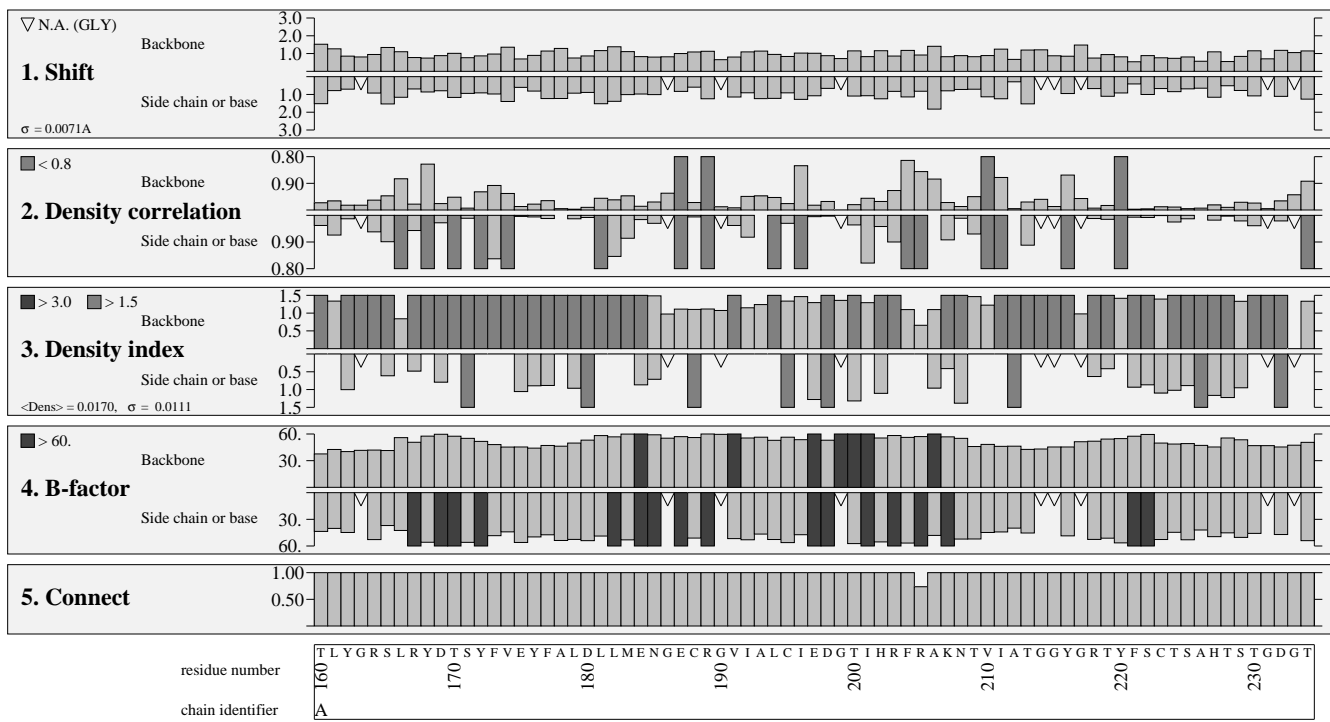
Local estimation



Structure Factor Check

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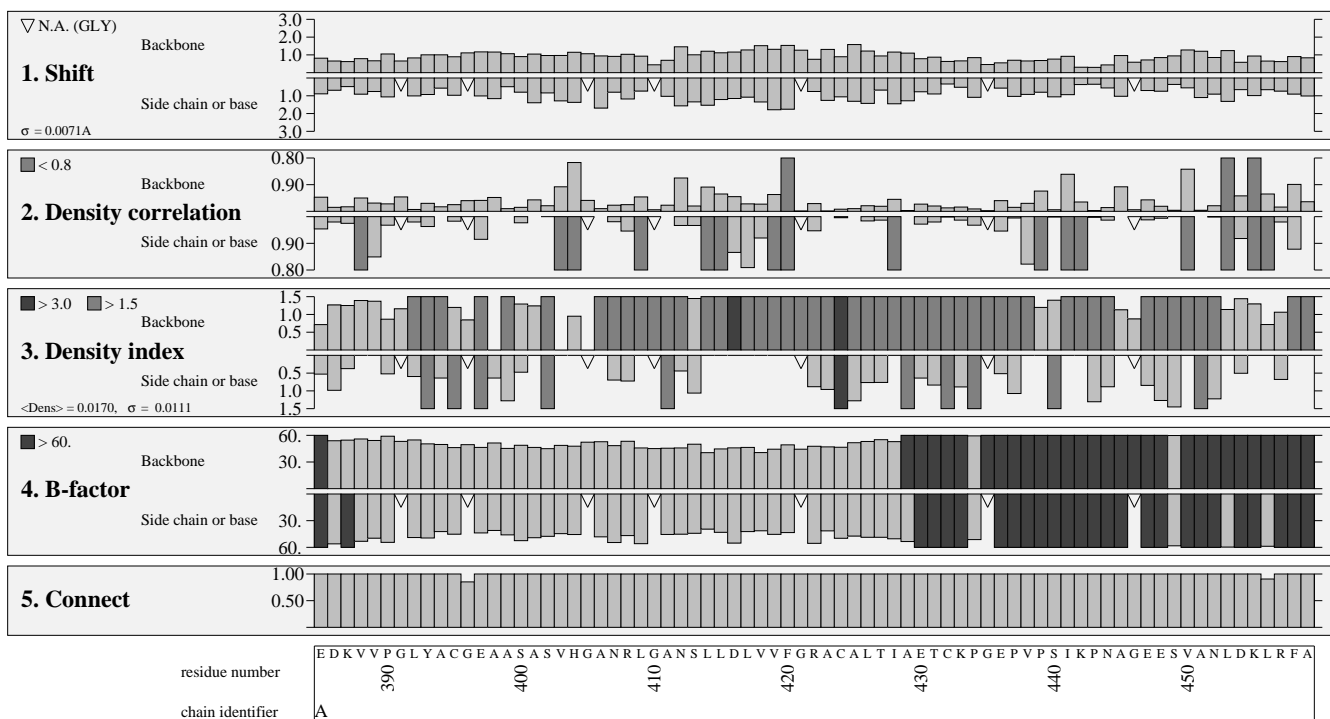
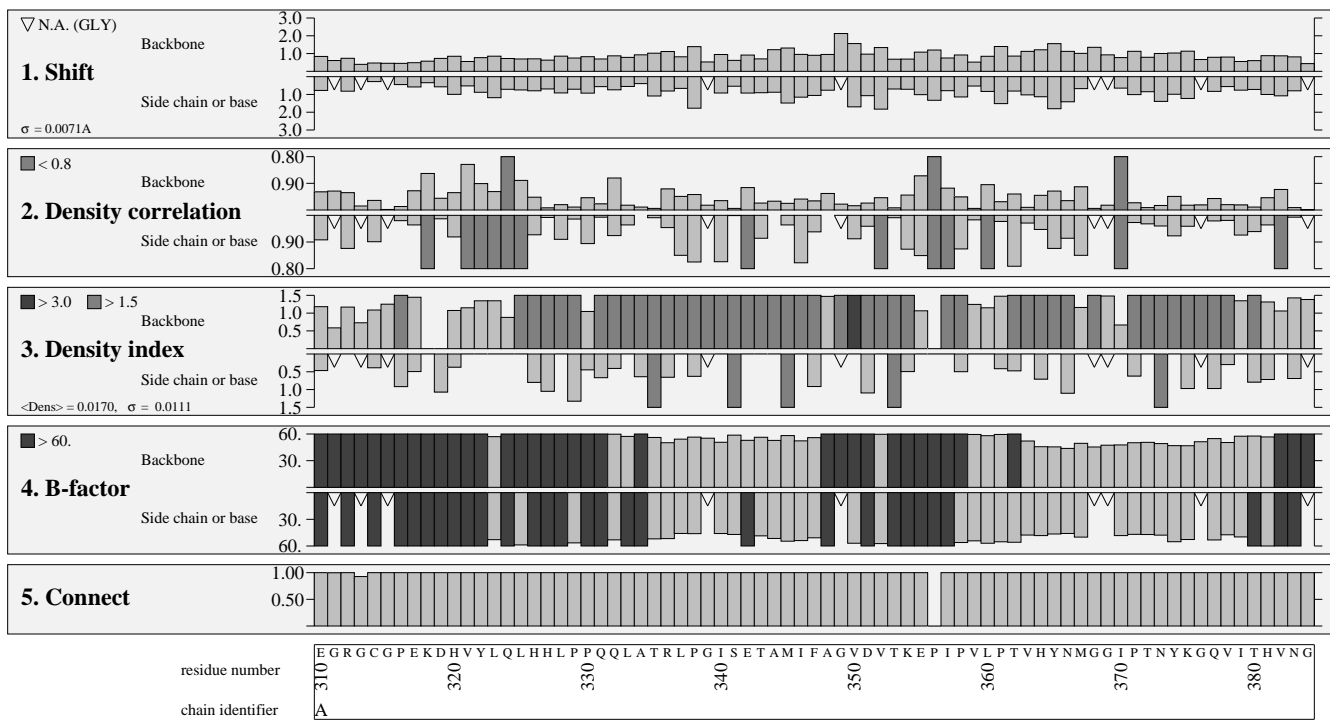
Local estimation (2)



Structure Factor Check

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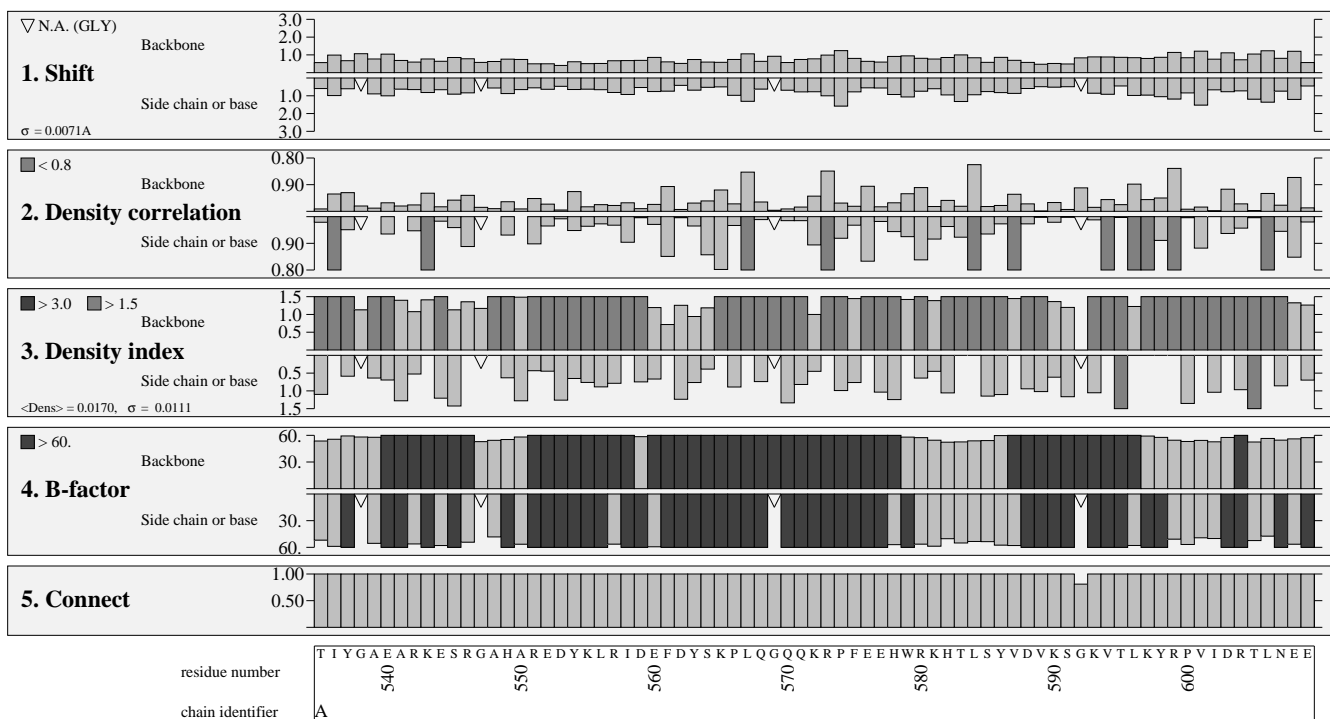
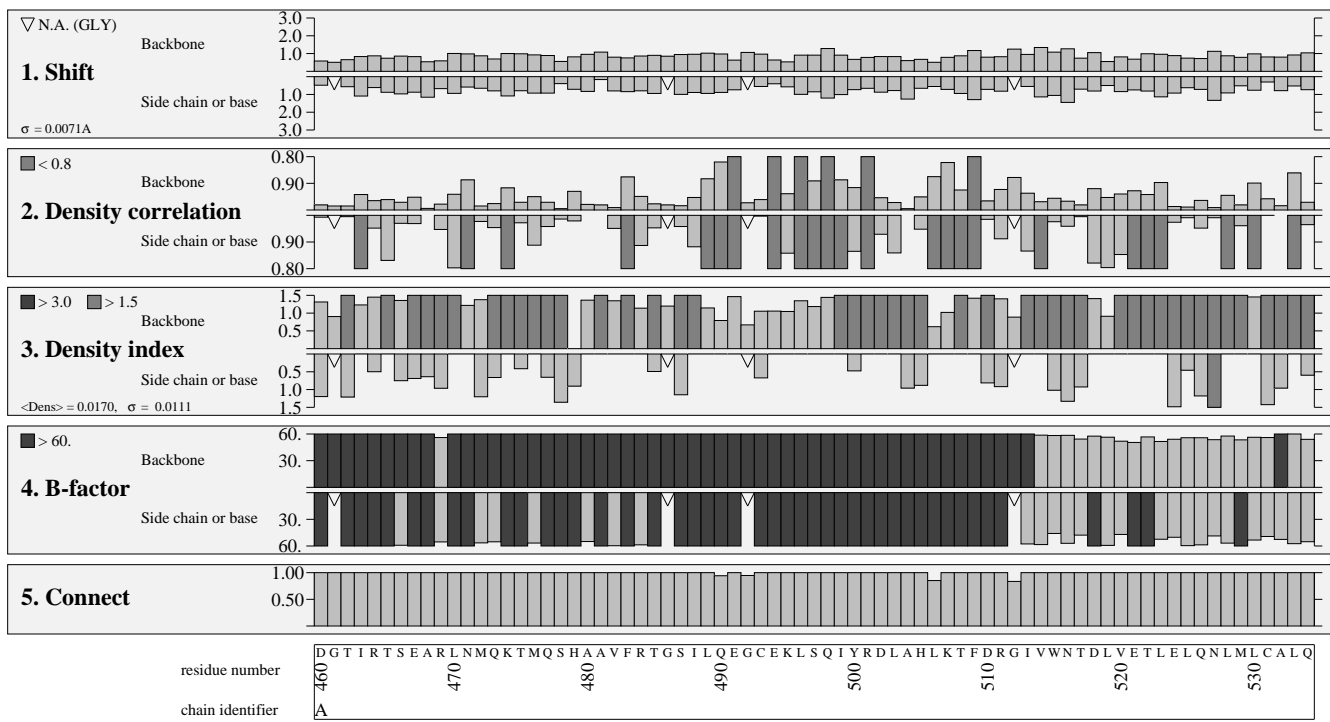
Local estimation (3)



Structure Factor Check

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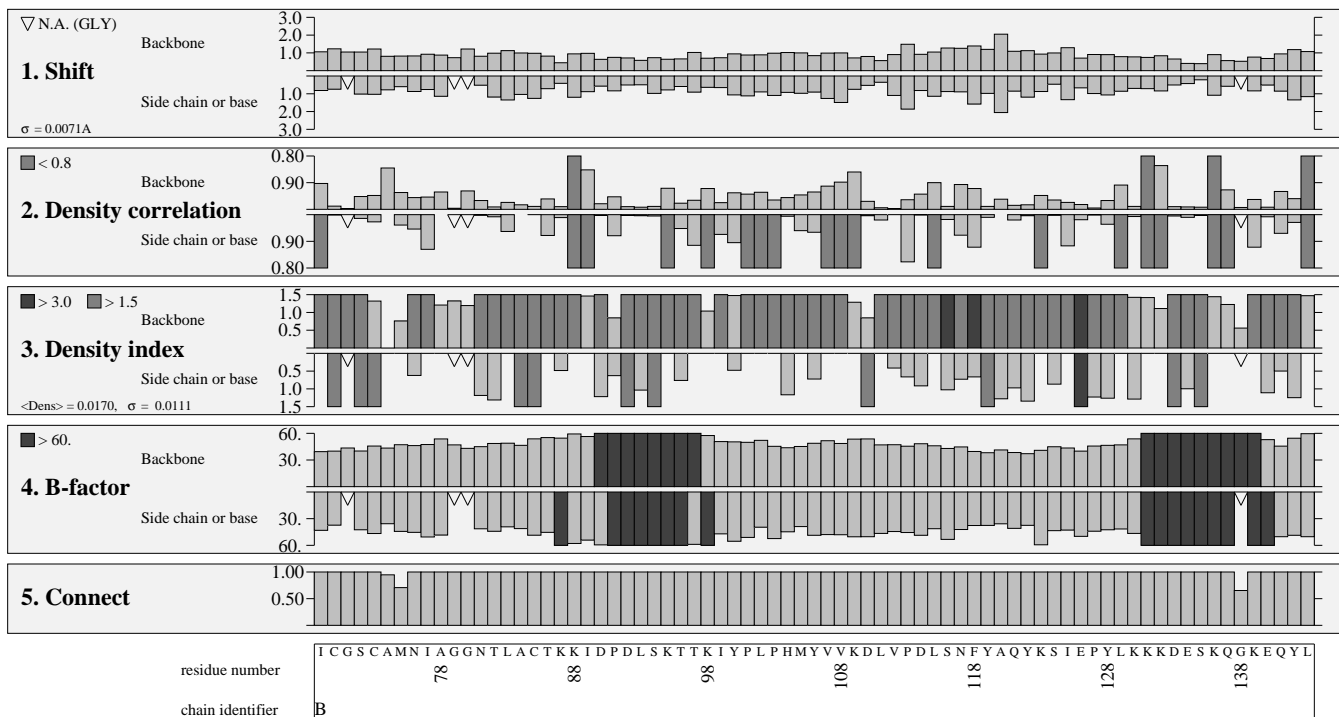
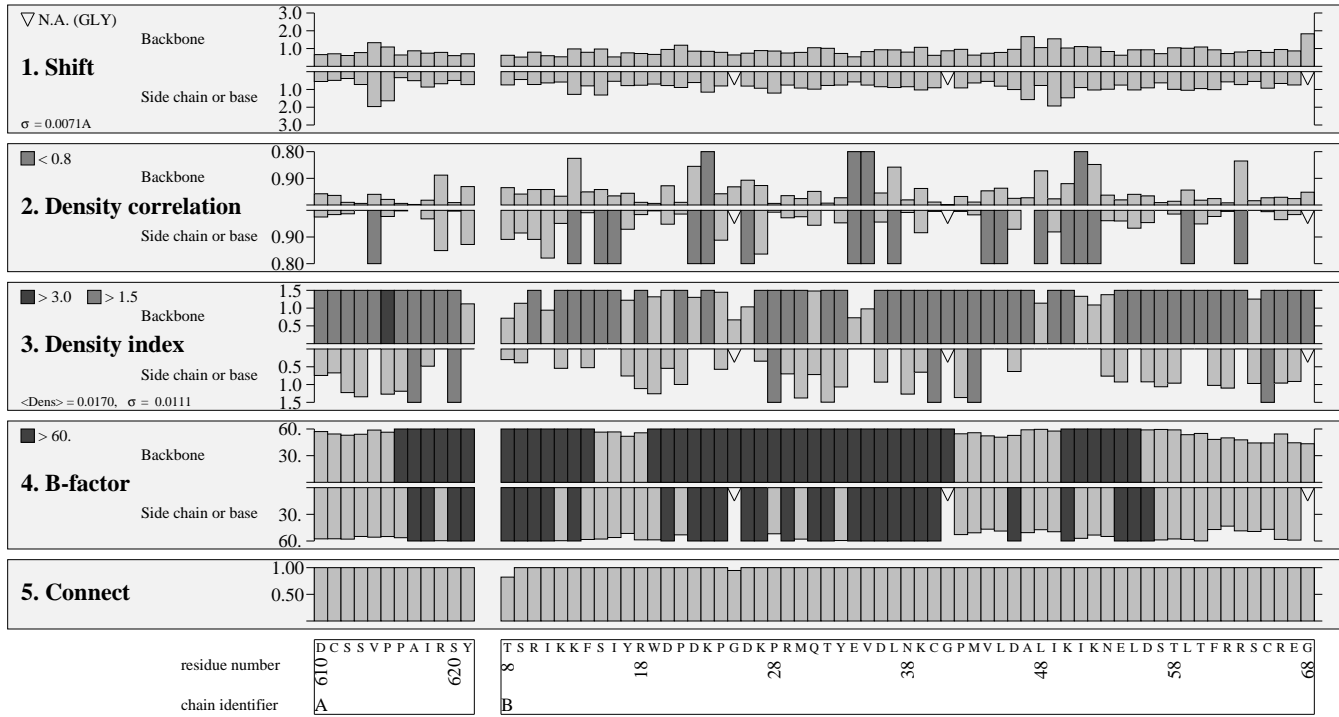
Local estimation (4)



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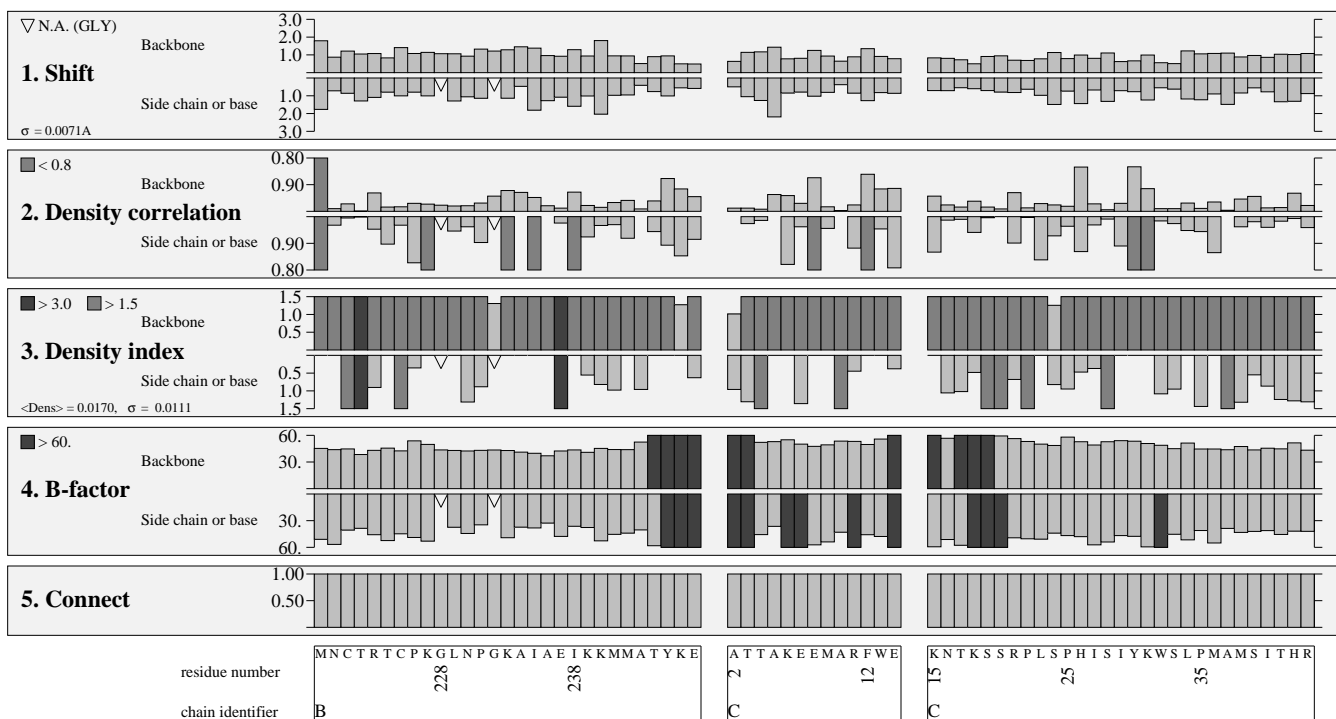
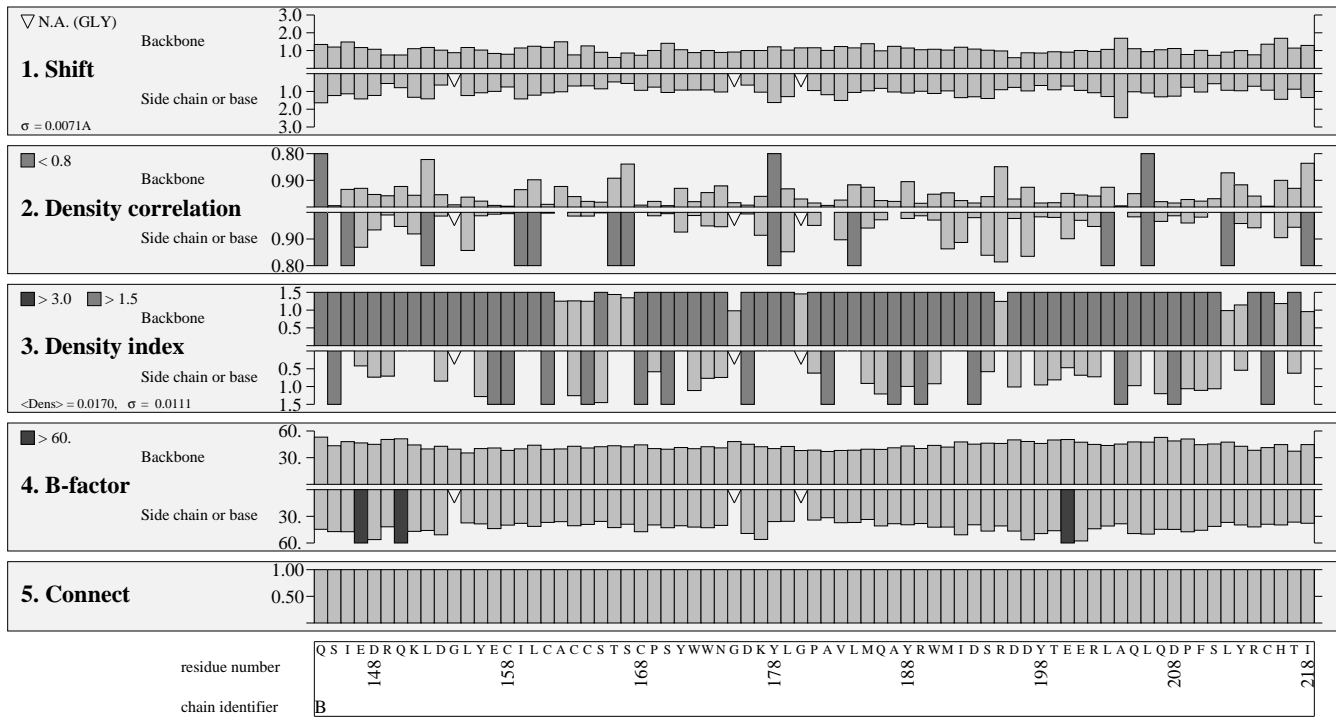
Local estimation (5)



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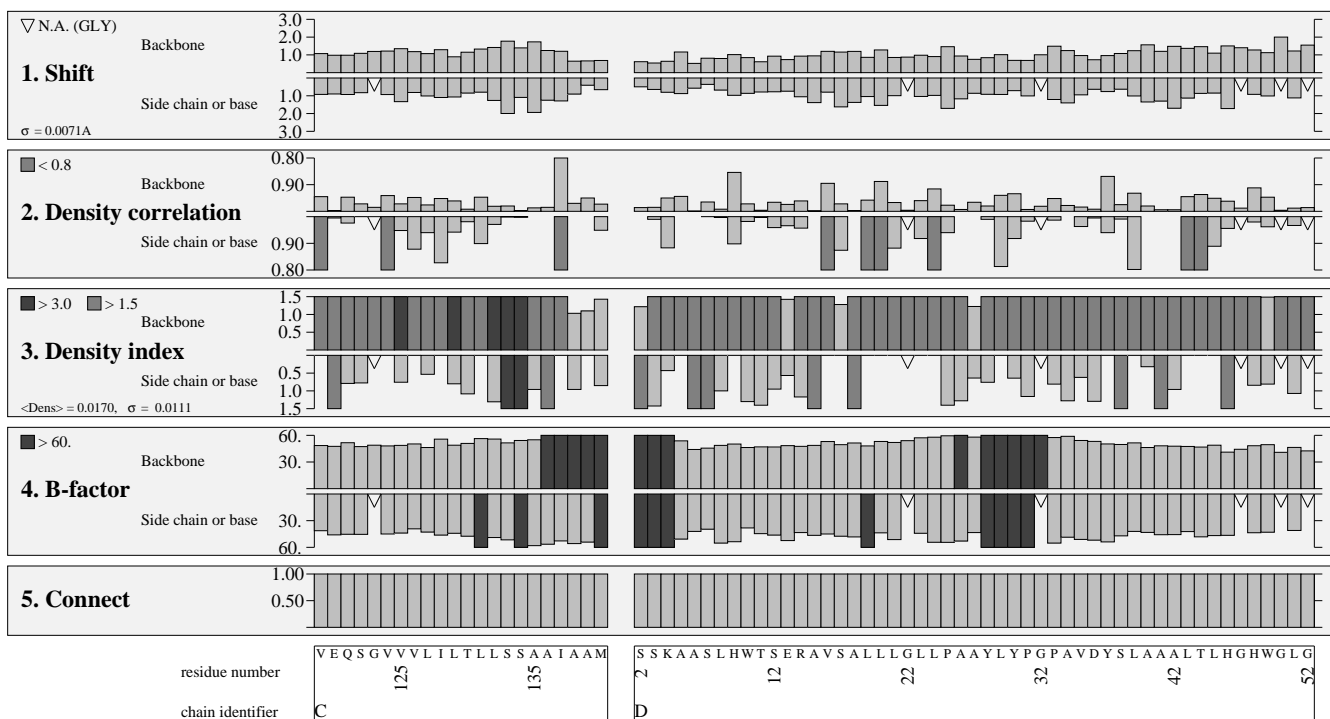
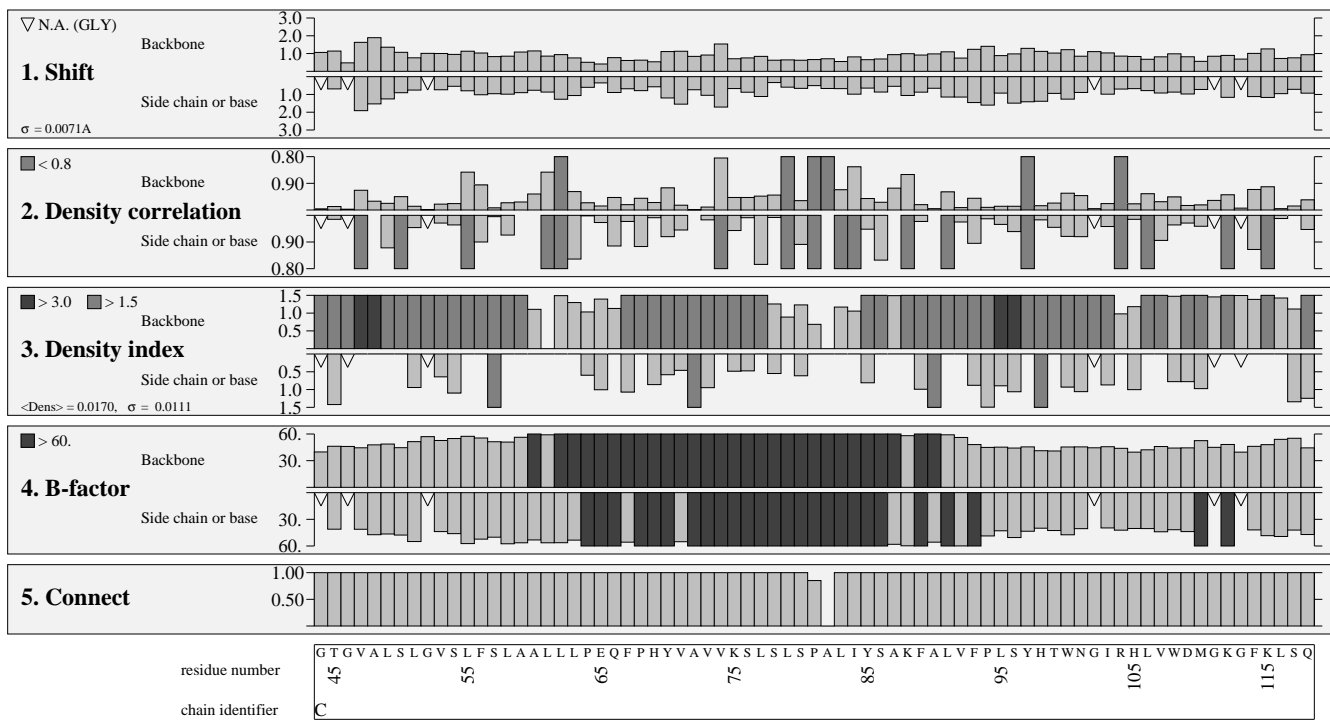
Local estimation (6)



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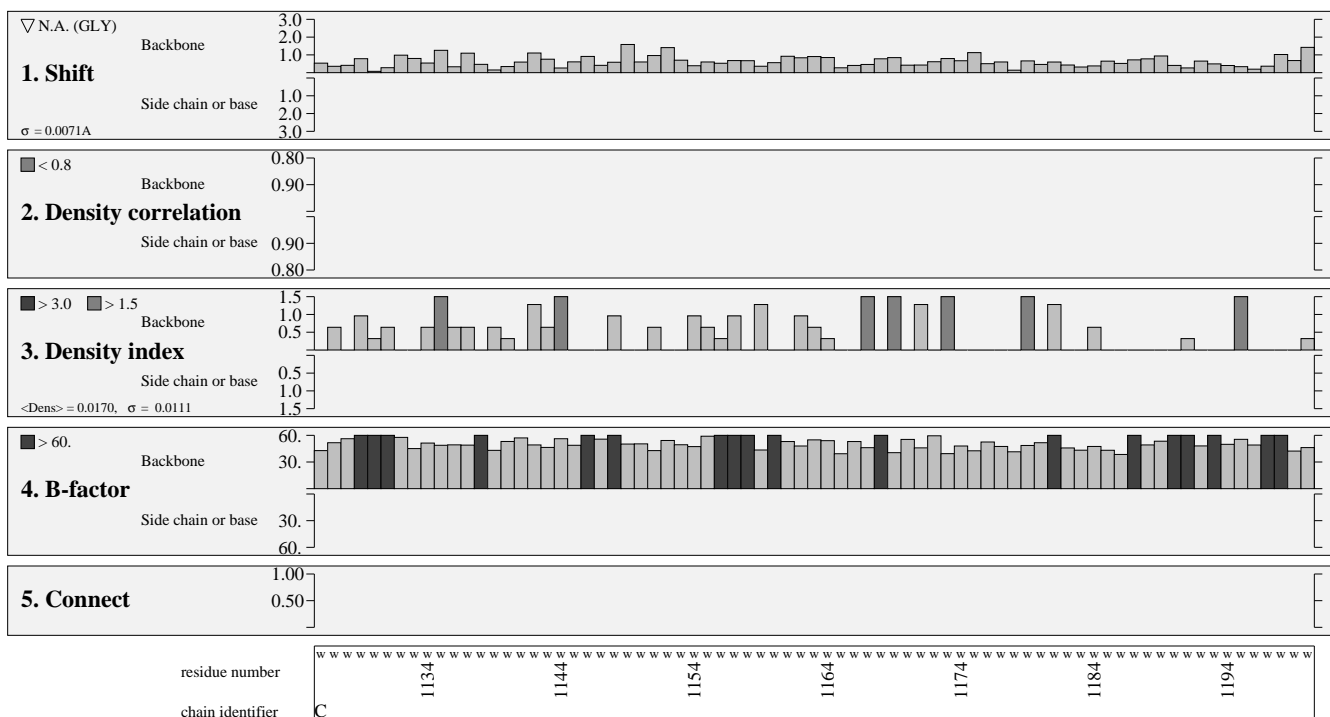
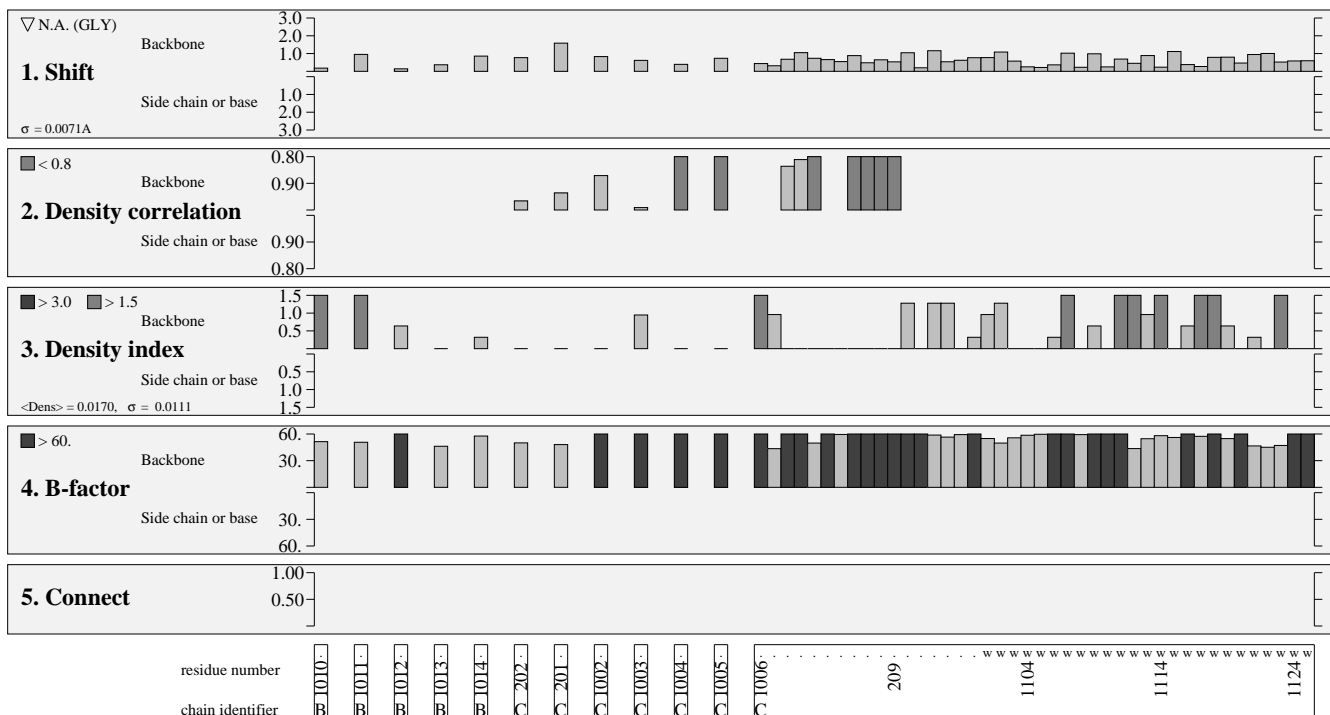
Local estimation (7)



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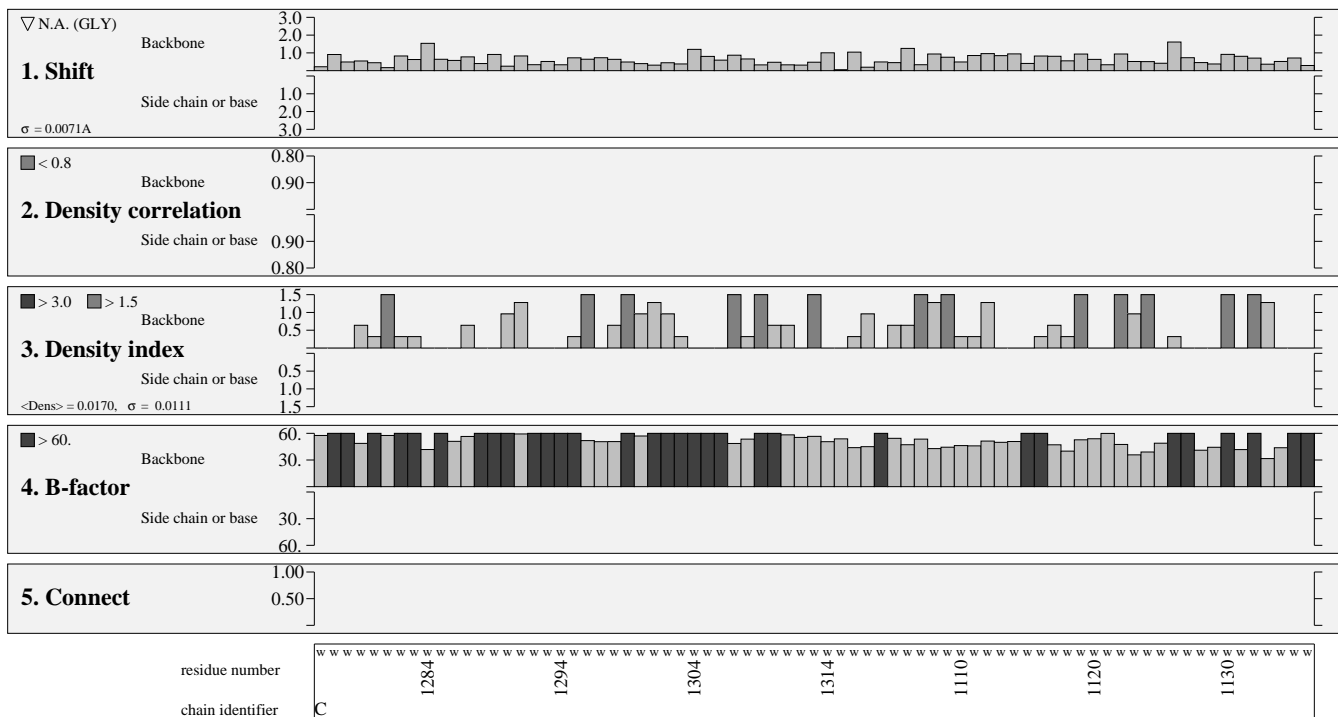
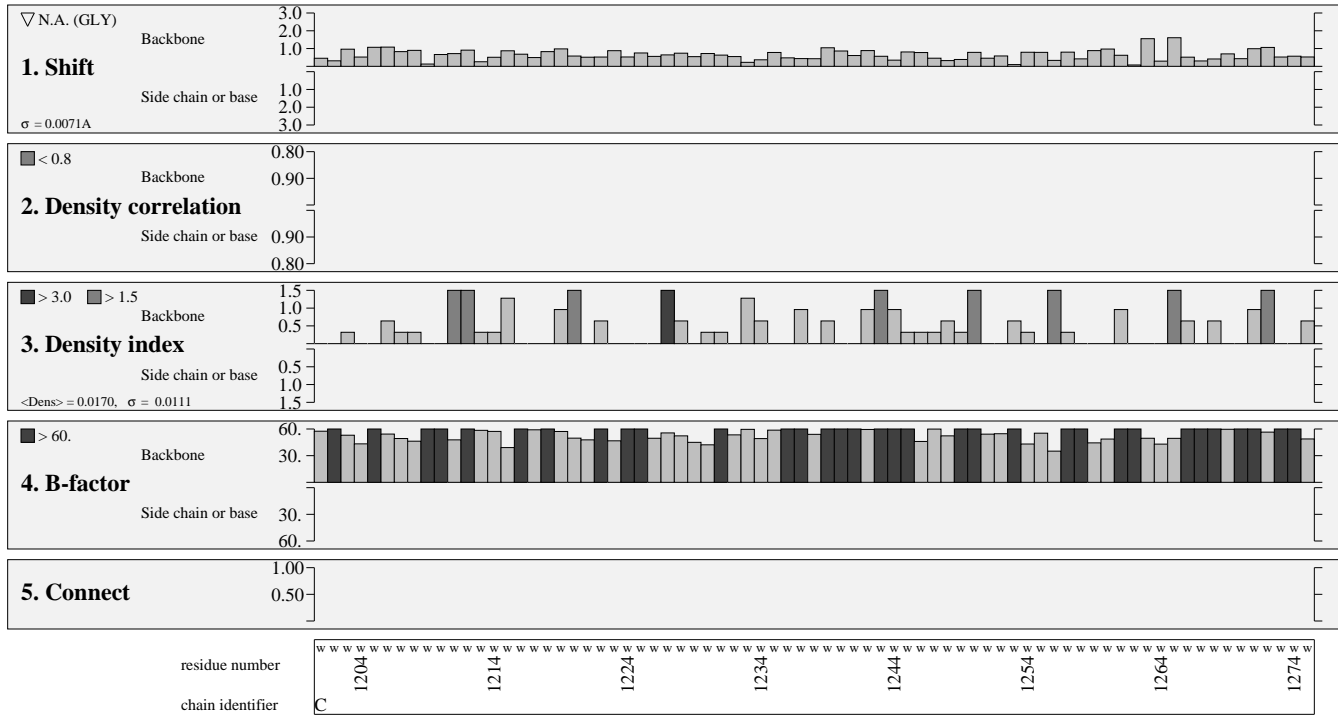
Local estimation (9)



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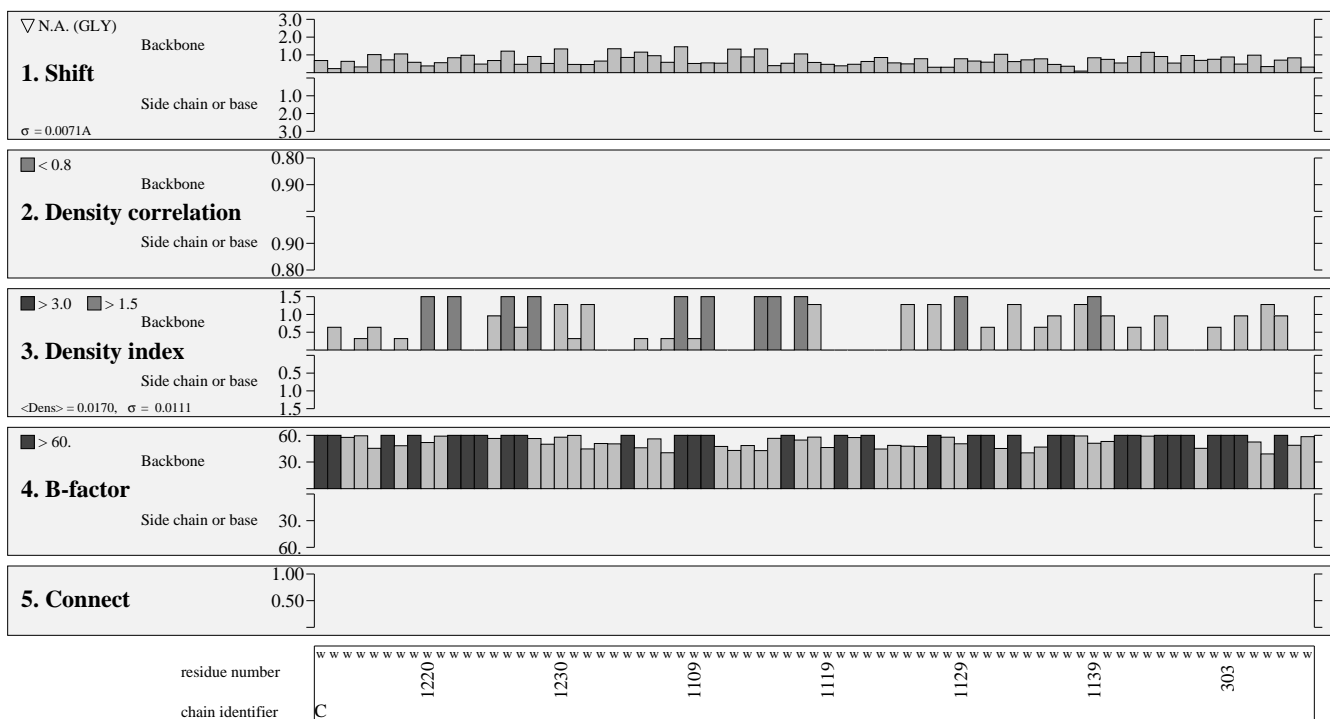
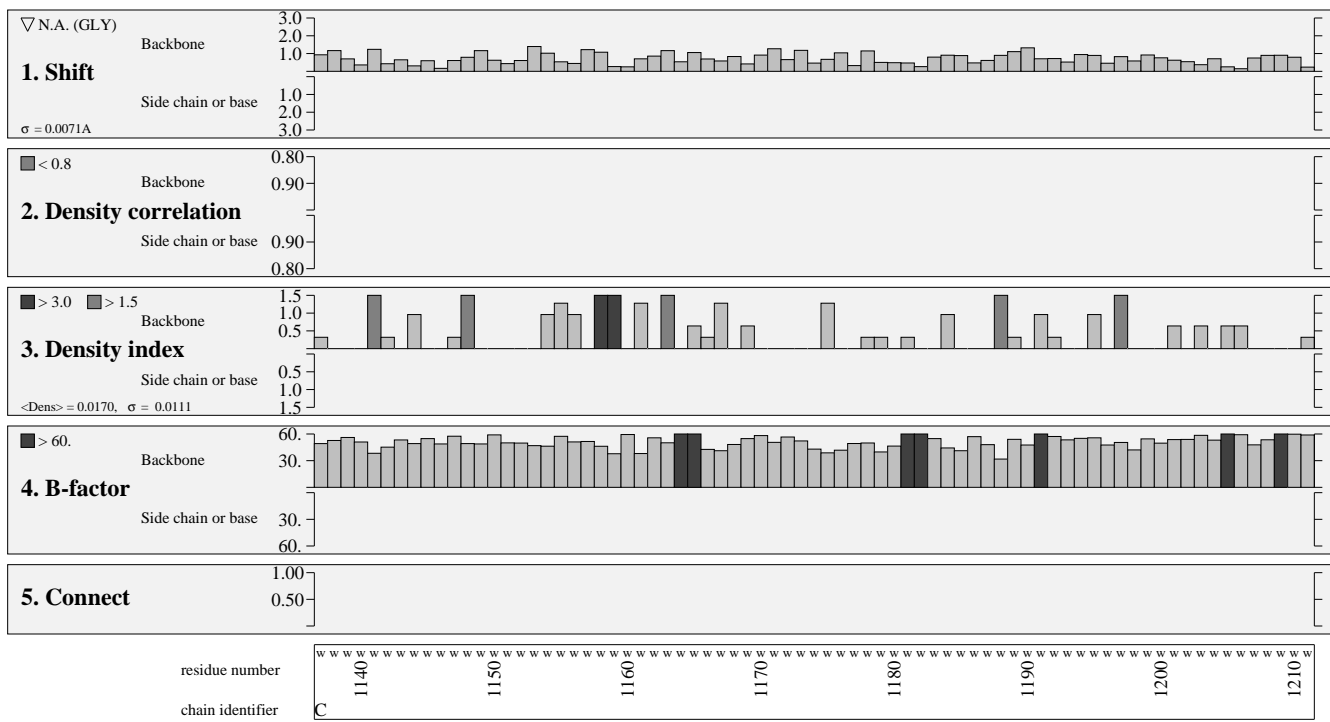
Local estimation (10)



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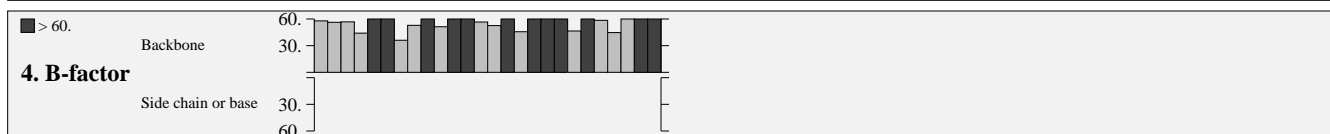
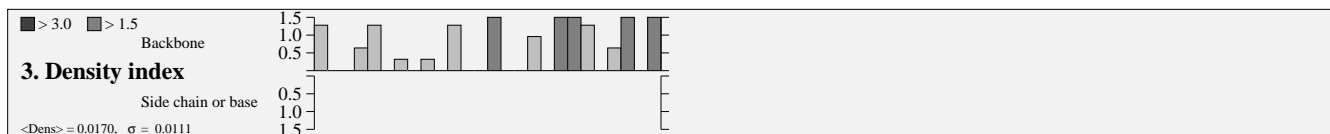
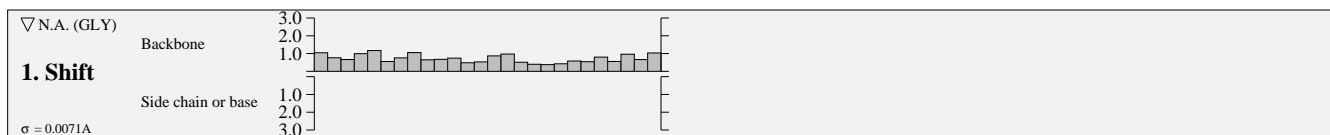
Local estimation (11)



Structure Factor Check

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Local estimation (12)



residue number	w w
chain identifier	C 313 323 333