

Structure Factor Check

3ABV

Title: CRYSTAL STRUCTURE OF PORCINE HEART MITOCHONDRIAL COMPLEX II
 N-BIPHENYL-3-YL-2-TRIFLUOROMETHYL-BENZAMIDE
 Date: 22-DEC-09
 PDB code: 3ABV

Crystal

Cell parameters:

a: 71.70 A b: 84.17 A c: 294.43 A
 α : 90.00 β : 90.00 γ : 90.00
 Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 37.6 – 3.23 A
 Reflections in file: 28950
 Unique reflections above 0: 28950
 above 1 σ : 28301
 above 3 σ : 22496

SFCHECK

Nominal resolution range: 37.6 – 3.24 A
\05max. from input data, min. from author\05
 Used reflections: 28919
 Reflections out of resolution: 31
 Completeness: 99.0 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.058
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.6497 0.6838 1.0000
 B_{overall} (by Patterson): 50.A²
 Optical resolution: 2.29 A
 Expected opt. resol. for complete data set: 2.29 A
 Estimated minimal error: 0.086 A

Model

8671 atoms
 Number of atoms with aniso_U: 8480
 Number of chains: 12
 Volume not occupied by model: 57.9 %
 $\langle B \rangle$ (for atomic model): 70.1 A²
 $\sigma(B)$: 15.47 A²
 Matthews coefficient: 3.66
 Corresponding solvent % : 66.12

Model vs. Structure Factors

R-factor for all reflections: 0.288
 Correlation factor: 0.811
 R-factor: 0.295
 for $F > 2.0\sigma$
 nom. resolution range: 37.63 – 3.24A
 reflections used: 28284

Rfree: 0.338
 Nfree: 1441
 R-factor without free-refl.: 0.292
 Non free-reflections: 26843
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.599 A
 Estimated maximal error: 0.237 A
 DPI: 0.449 A

Scaling

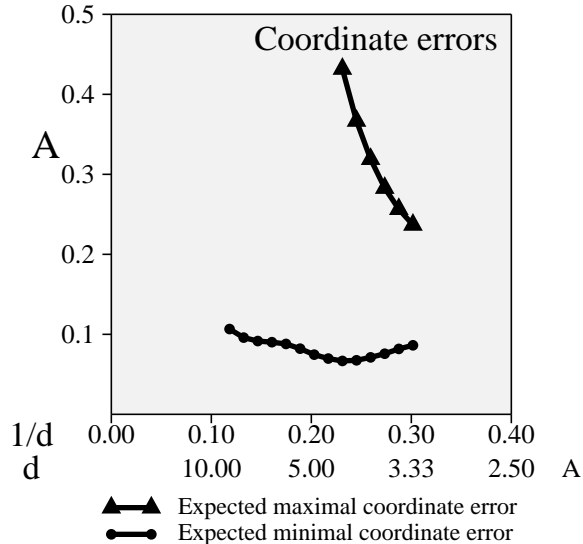
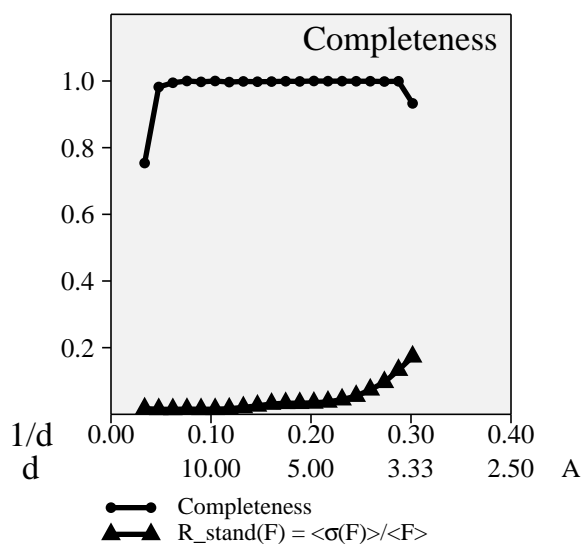
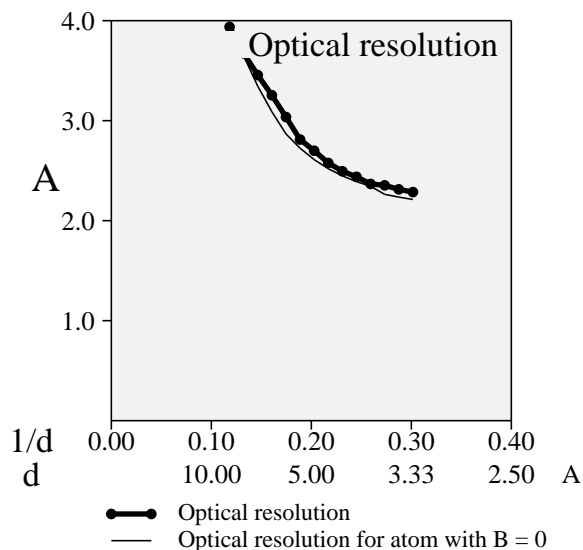
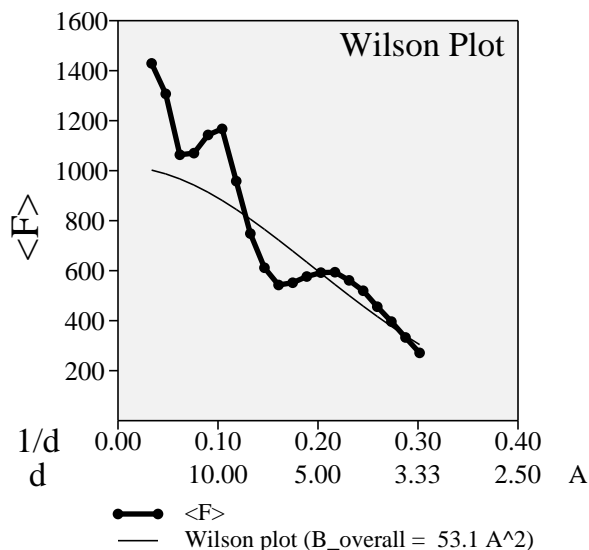
Scale: 0.893
 Bdiff: -8.53
 Anisothermal Scaling (Beta):
 -1.8915 -1.4536 3.6898 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.623 250.009

Refinement

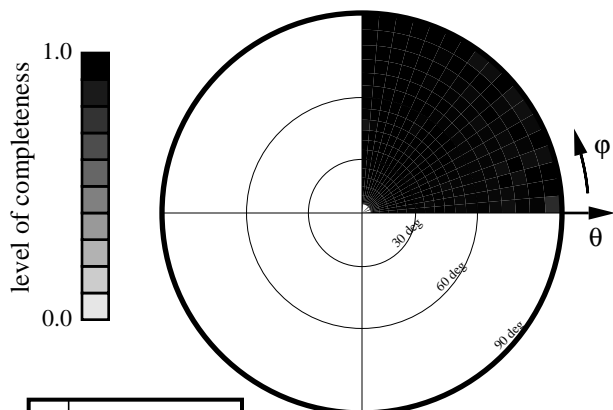
Program: REFMAC 5.5.0102
 Nominal resolution range: 37.6 – 3.24 A
 Reported R-factor: 0.203
 Number of reflections used: 28950
 Reported Rfree: 0.25
 Sigma cut-off: N.A.

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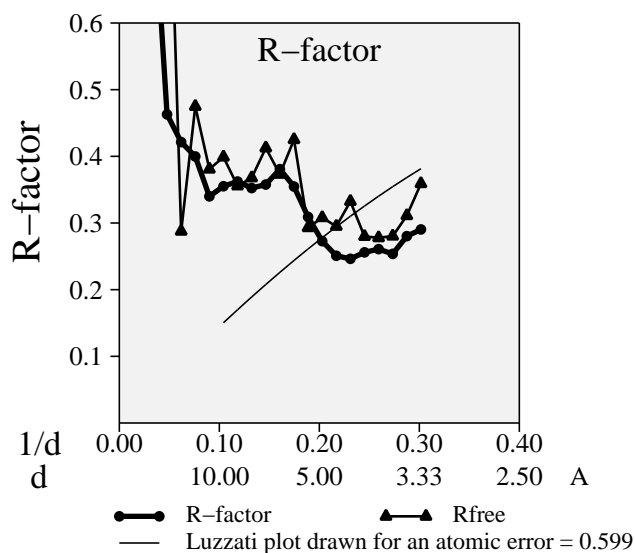


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

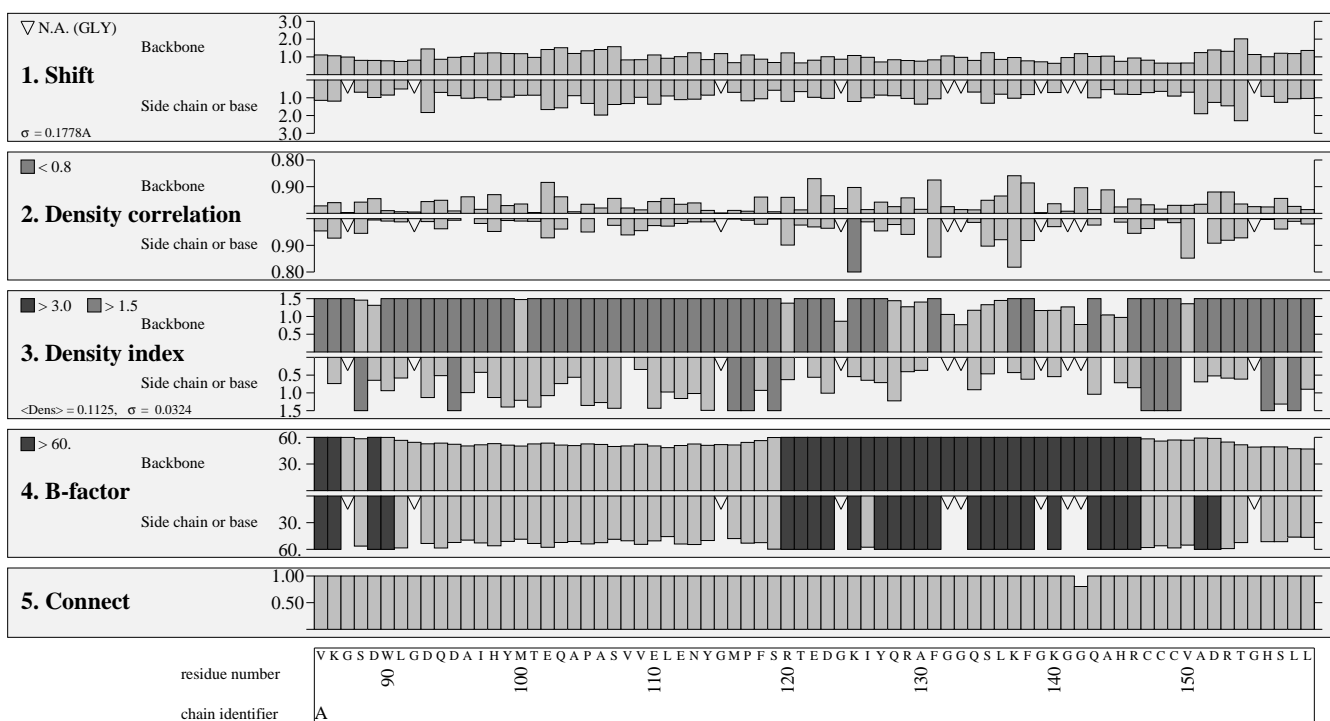
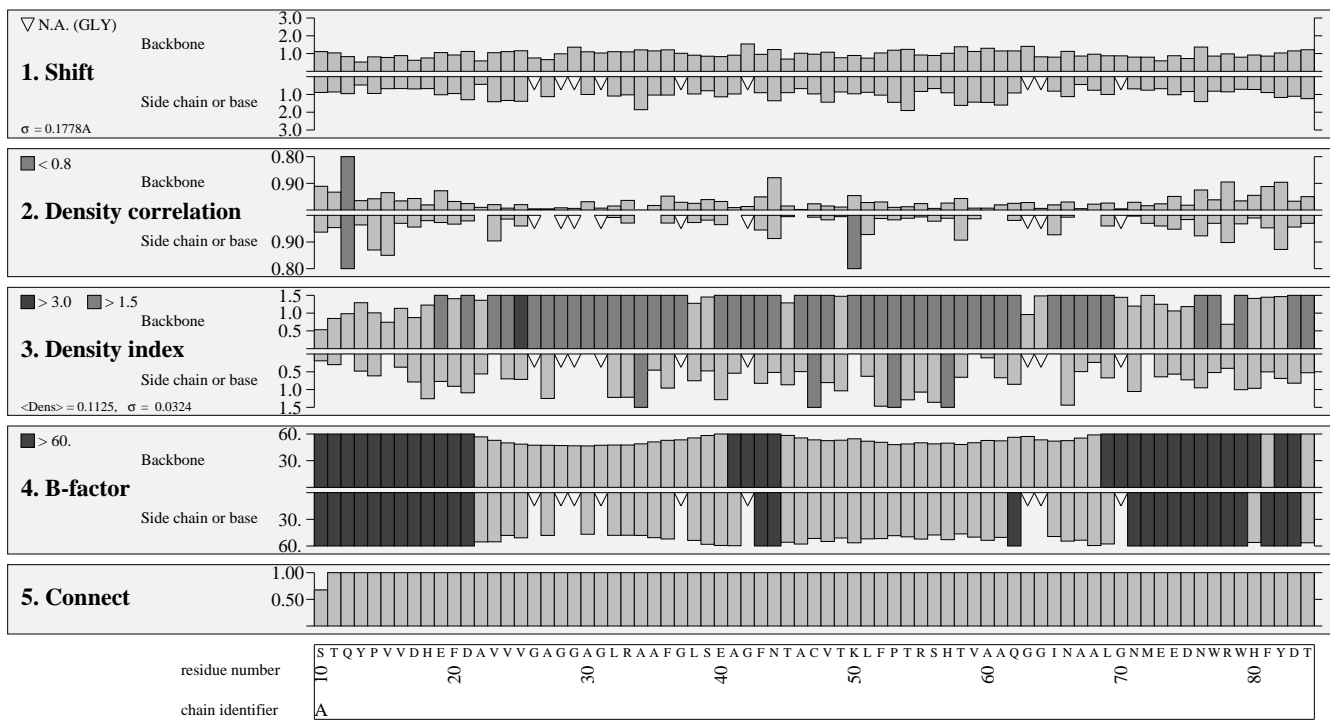
polar coordinates of the crystallographical axes



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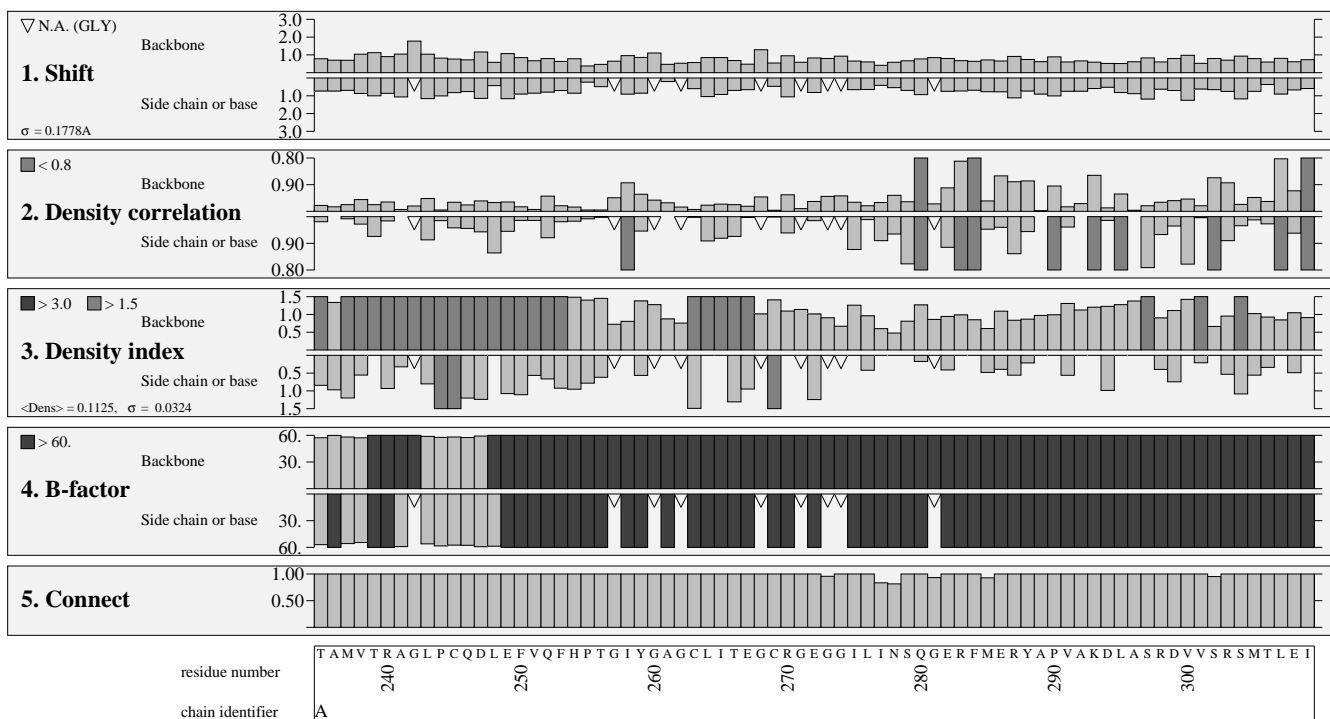
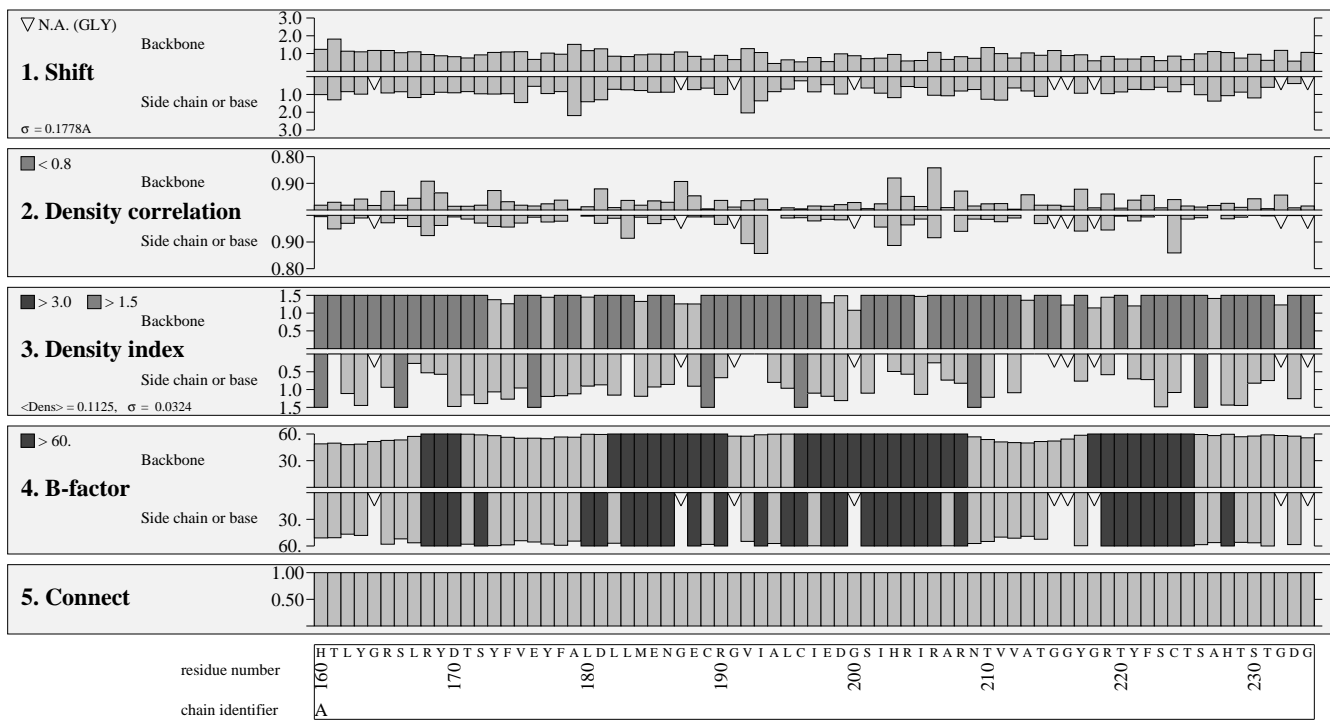
Local estimation



Structure Factor Check

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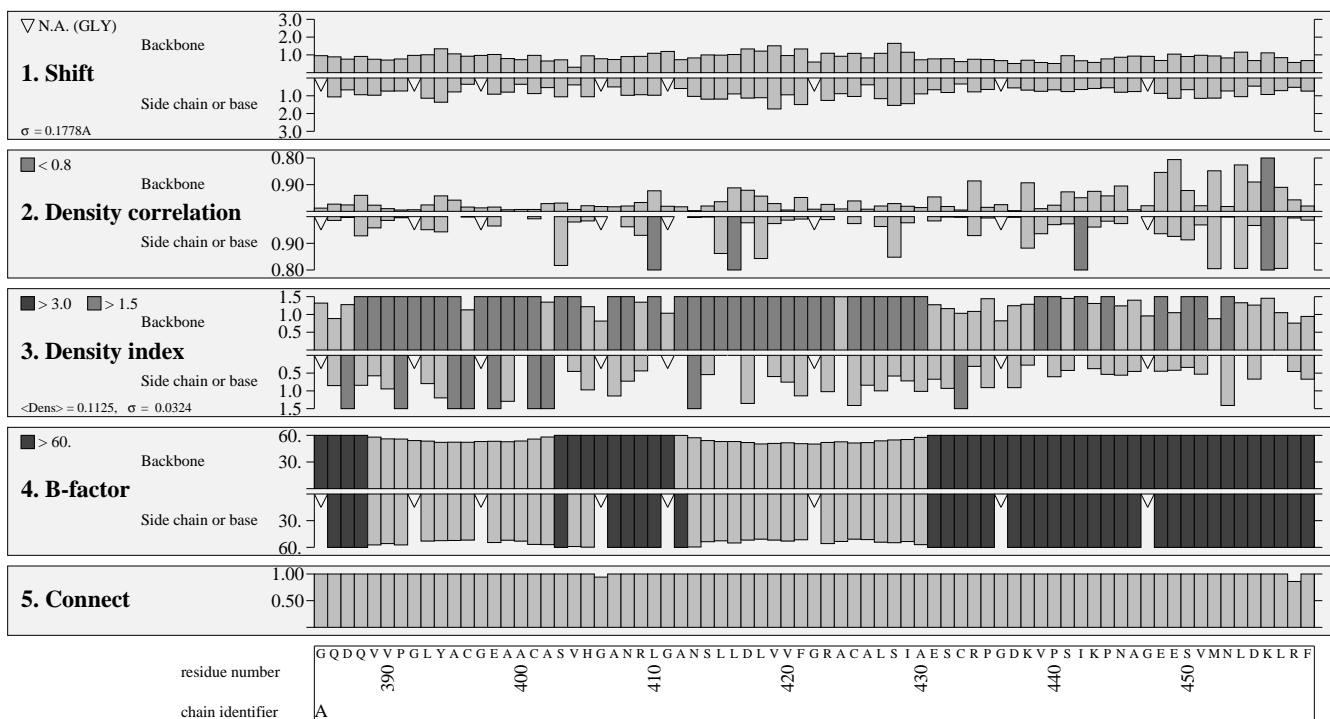
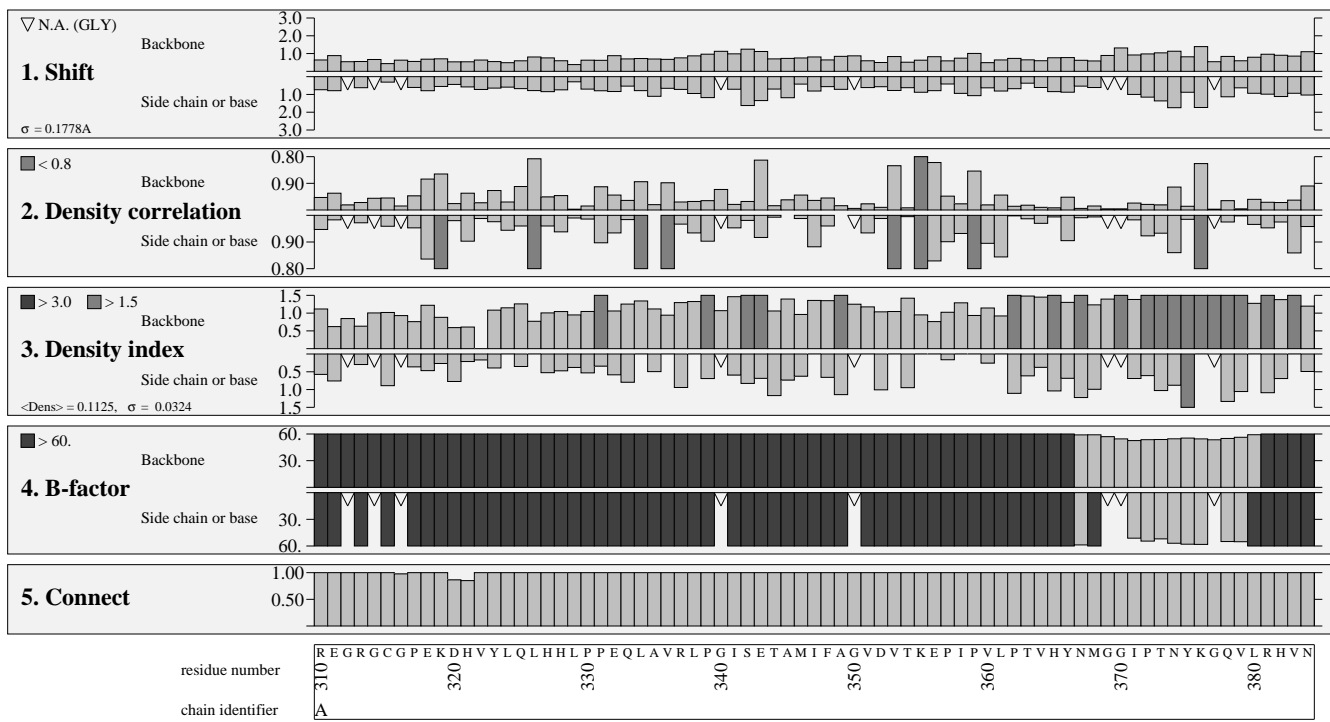
Local estimation (2)



Structure Factor Check

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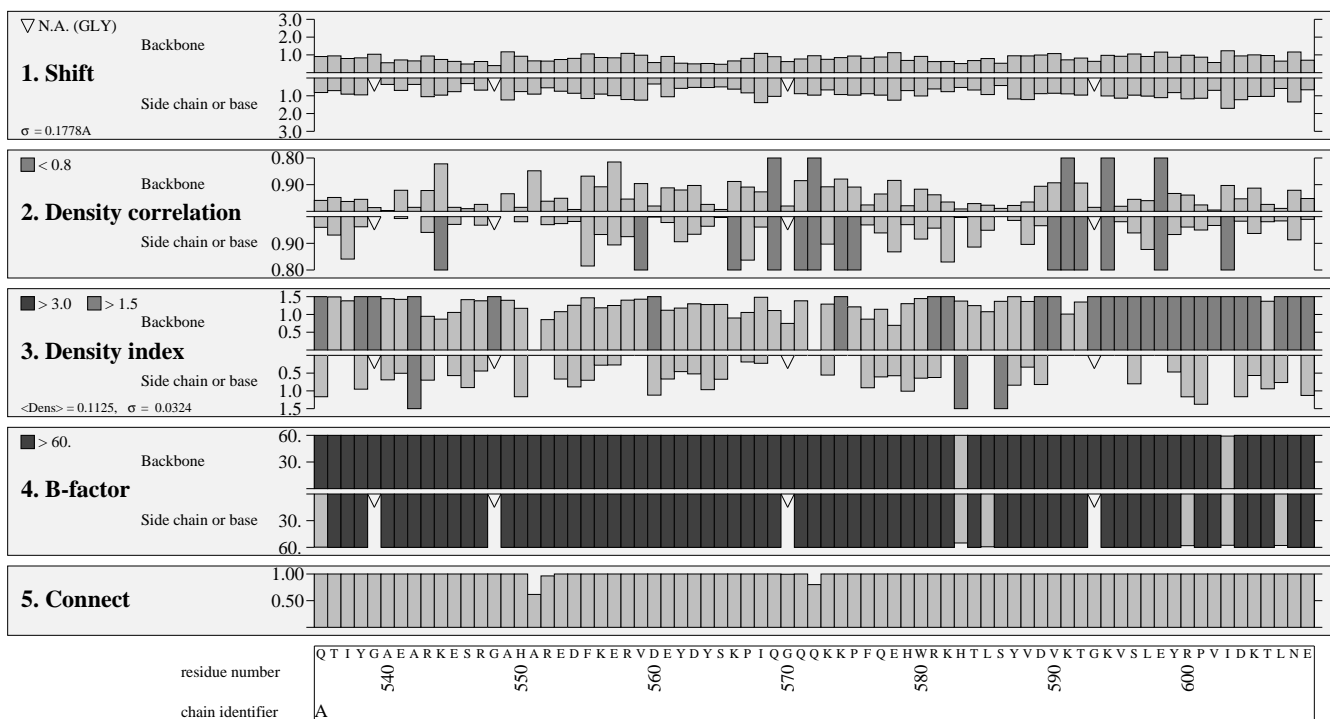
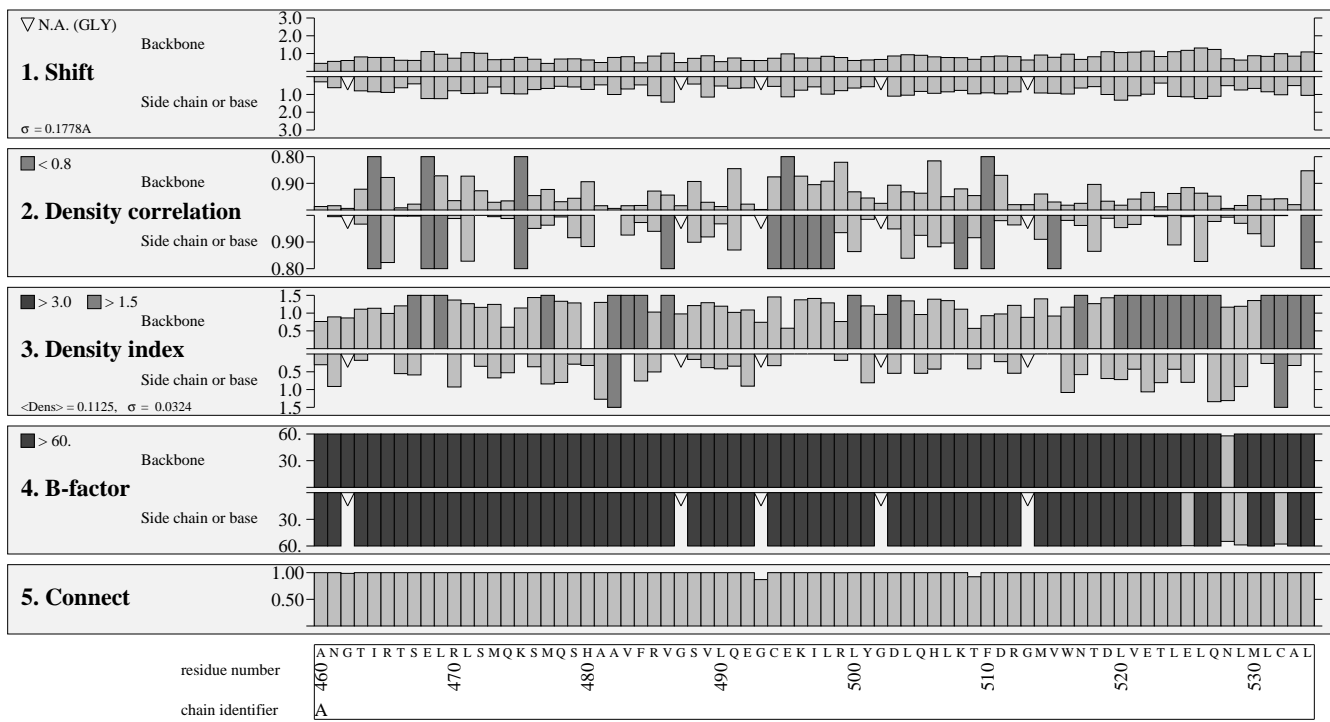
Local estimation (3)



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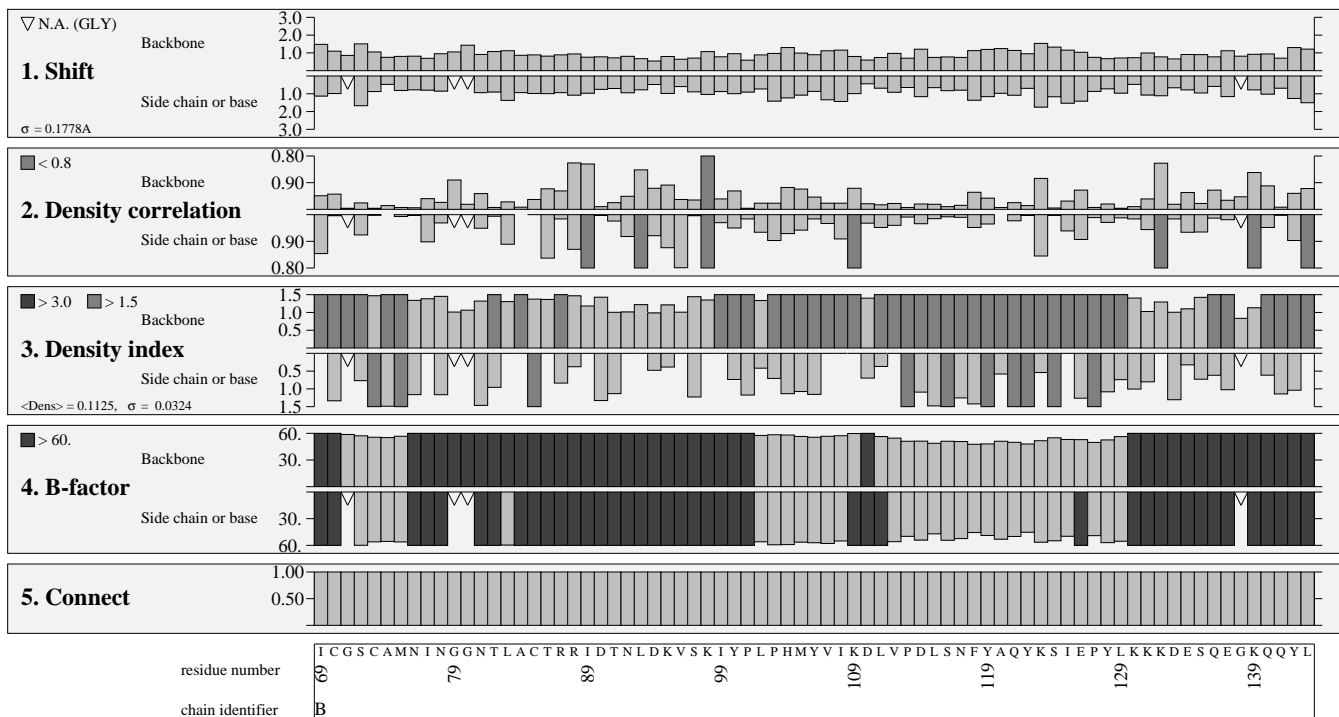
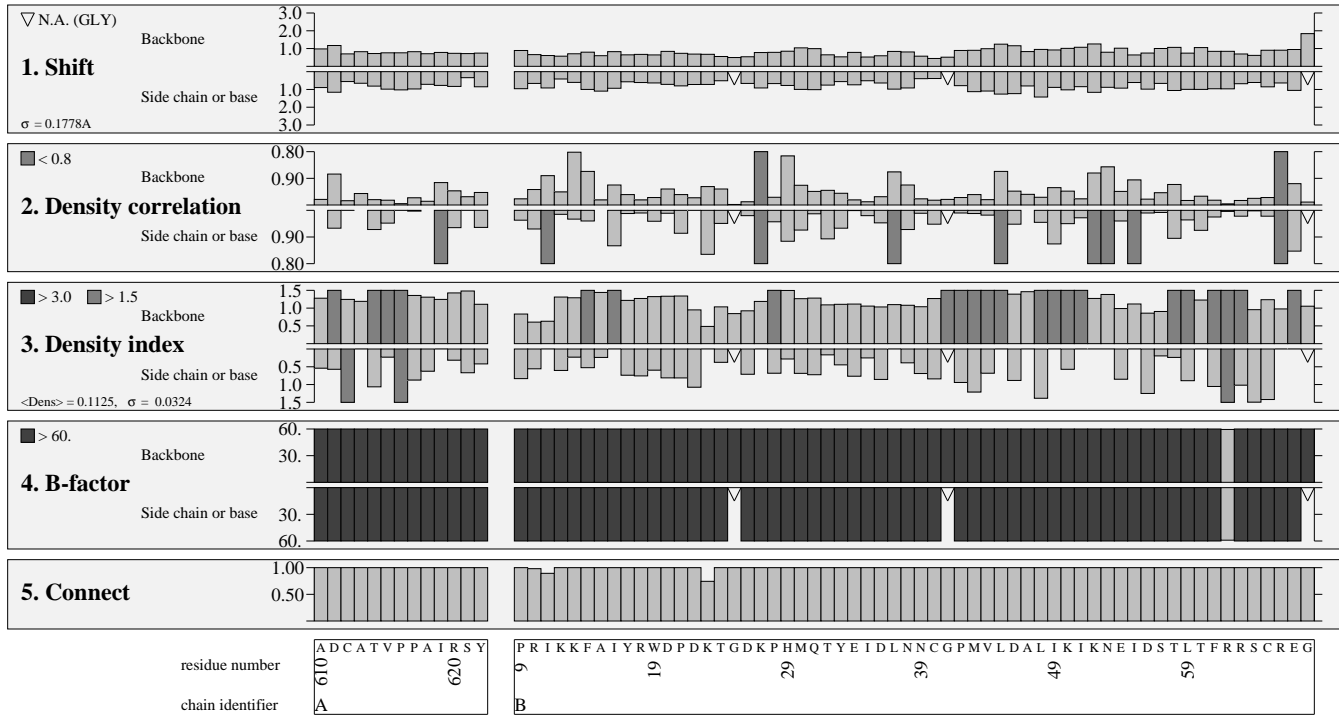
Local estimation (4)



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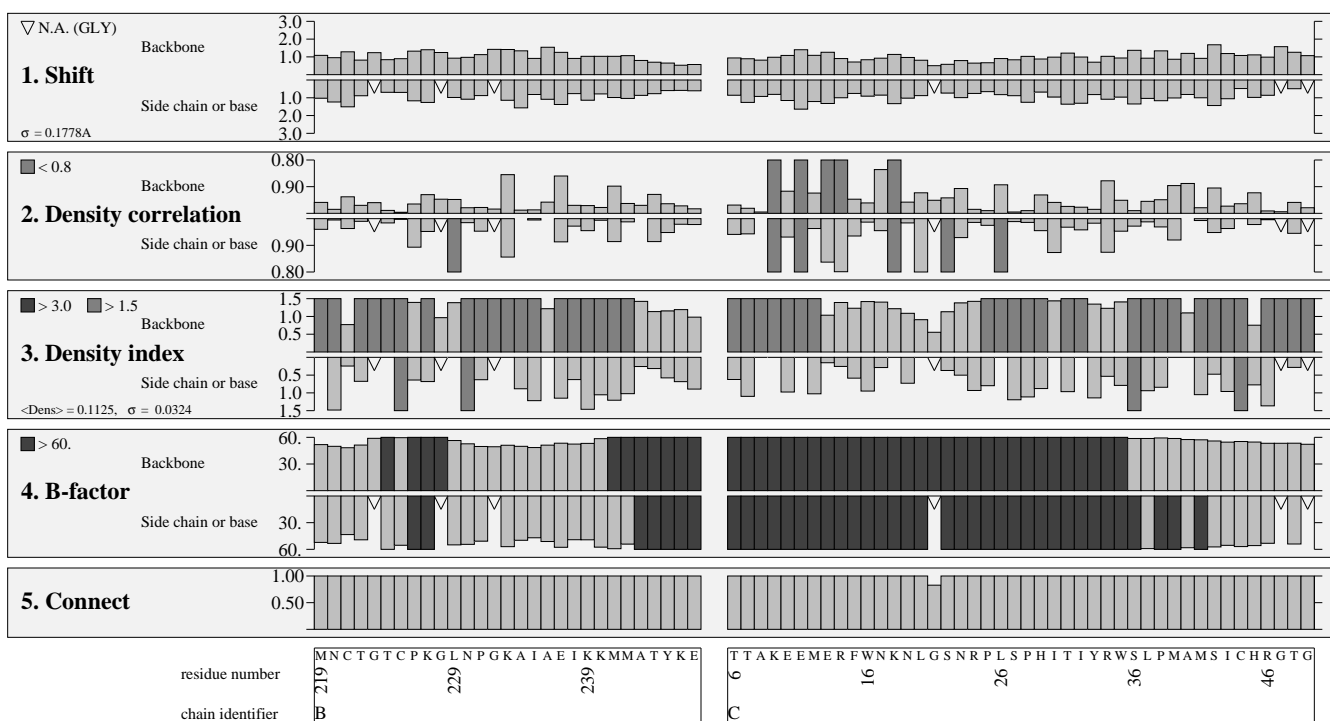
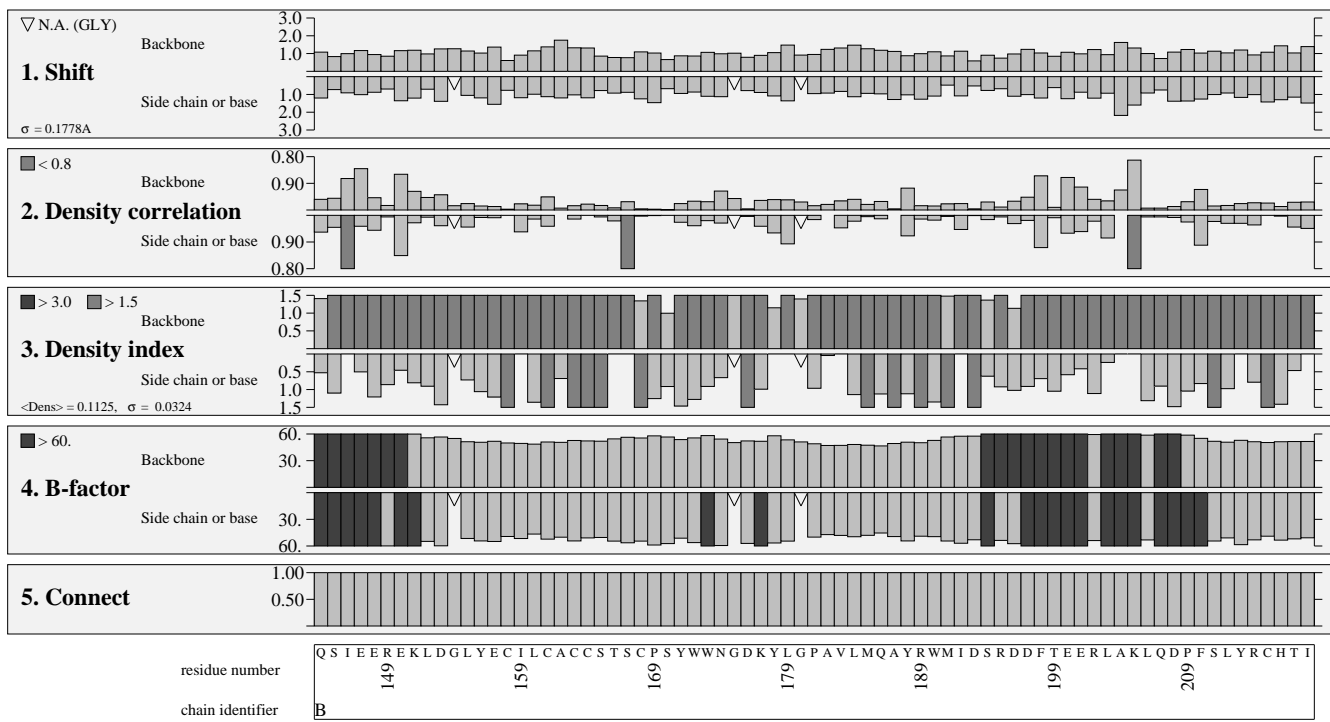
Local estimation (5)



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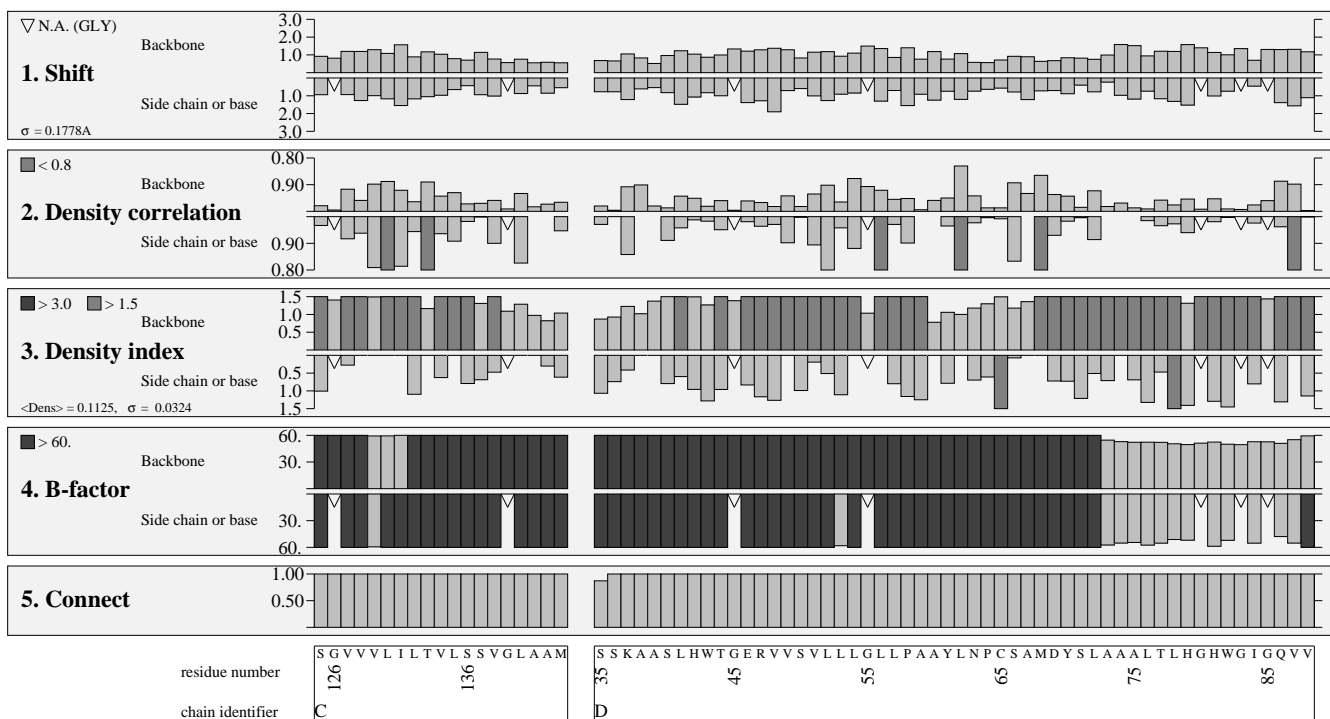
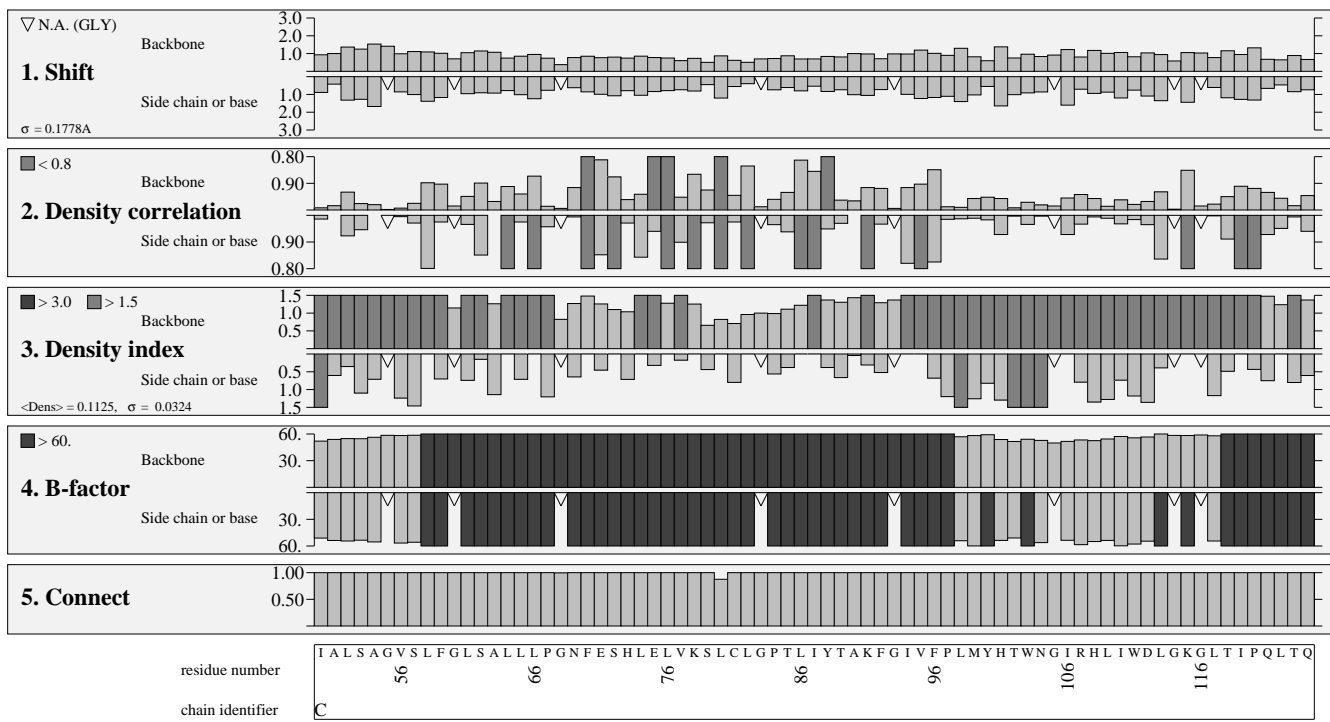
Local estimation (6)



Structure Factor Check

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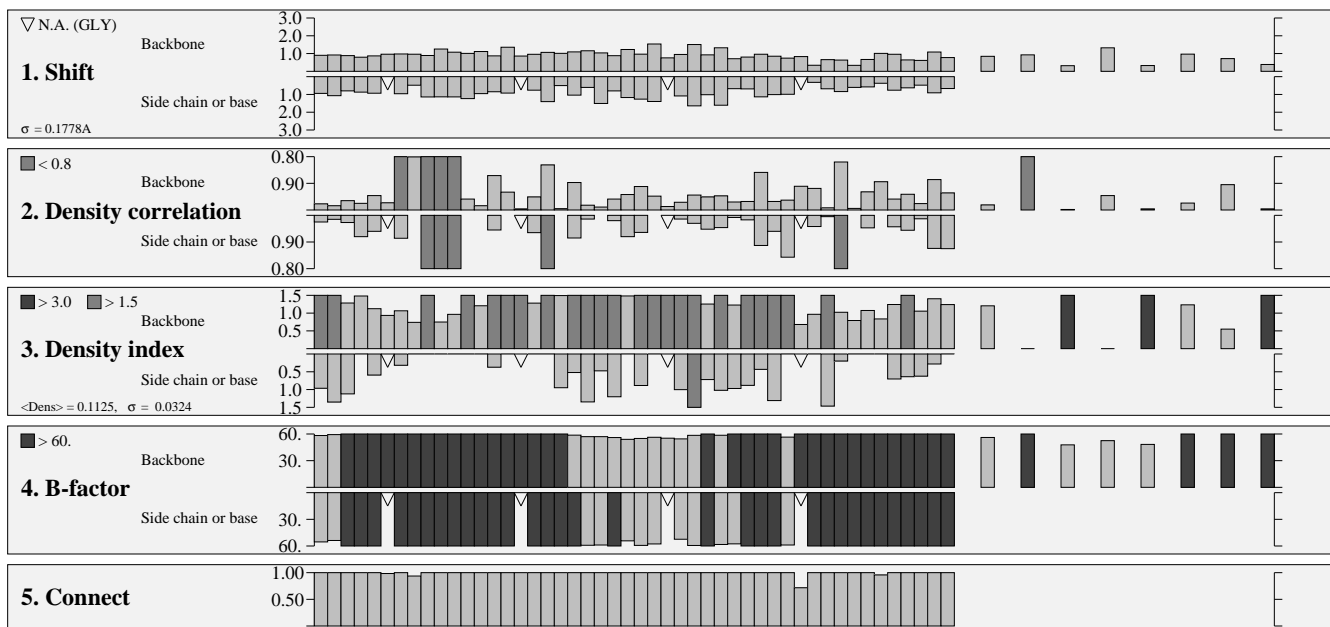
Local estimation (7)



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Local estimation (8)



residue number

chain identifier

T D Y V R G D A L Q K A A K A G L L A L S A F T F A G L C Y F N Y H D V G I C K A V A M L W K L
95 105 115 125 135

A 700

A 701

B 302

C 1305

B 303

B 1201

B 1306

B 304