"Judge not, that you be not judged" Bible, Matthew, ch.7

Structure Factor Check

1JGC

Title:	THE 2.6 A STRUCTURE RESOLUTION OF RHODOBACTER CAPSULATUS BACTERIOFERRITIN WITH METAL−FREE DINUCLEAR SITE AND HEME IR CRYSTALLOGRAPHIC SPECIAL POSITION
Date:	24−JUN−01
PDB code:	1JGC

Crystal

Cell parameters:

a: 142.37 A b: 142.37 A c: 140.88 A

α: 90.00 β: 90.00 γ: 90.00

Space group: I 4 2 2

Model

3981 atoms (21 water molecules)

Number of chains:	9
Volume not occupied by model:	53.6 %
<B> (for atomic model):	26.2 A^2
σ(B):	5.83 A^2
Matthews coefficient:	3.20
Corresponding solvent % :	61.29

Refinement

Program:	CNS
Nominal resolution range:	21.4 − 2.60 A
Reported R−factor:	0.225
Number of reflections used:	22526
Reported Rfree:	0.24
Sigma cut−off:	N.A.

Structure Factors

Input

Nominal resolution range:		21.4 − 2.59 A
Reflections in file:		22679
Unique reflections	above 0:	22679
	above 1σ:	22315
	above 3σ:	19828

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Nominal resolution range:	21.4 − 2.60 A
\05max. from input data, min. from author\05	
Used reflections:	22525
Reflections out of resolution:	154
Completeness:	100.0 %
R_stand(F) = <σ(F)>/<F> :	0.027
Anisotropic distribution of Structure Factors	
ratio of eigen values:	1.0000 1.0000 0.7325
B_overall (by Patterson):	36.A^2
Optical resolution:	1.89 A
Estimated minimal error:	0.028 A

Model vs. Structure Factors

R−factor for all reflections:	0.267
Correlation factor:	0.865
R−factor:	0.269
for F > 2.0 σ	
nom. resolution range:	21.44 − 2.60A
reflections used:	22162
Rfree:	0.286
Nfree:	1078
R−factor without free−refl.:	0.268
Non free−reflections:	21084
<u> (error in coords by Luzzati plot):	0.371 A
Estimated maximal error:	0.219 A
DPI:	0.263 A

Scaling

Scale:	0.422
Bdiff:	−3.54

Anisothermal Scaling (Beta):

1.0648 1.0648 −1.4513 0.0000 0.0000 0.0000

Solvent correction − Ks,Bs: 0.649 250.006

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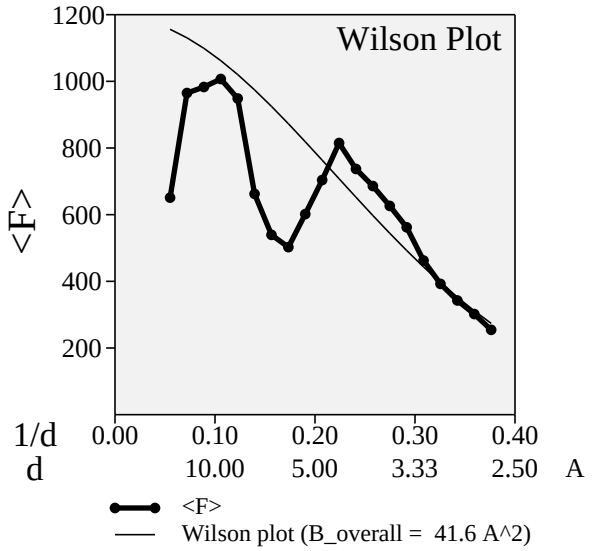
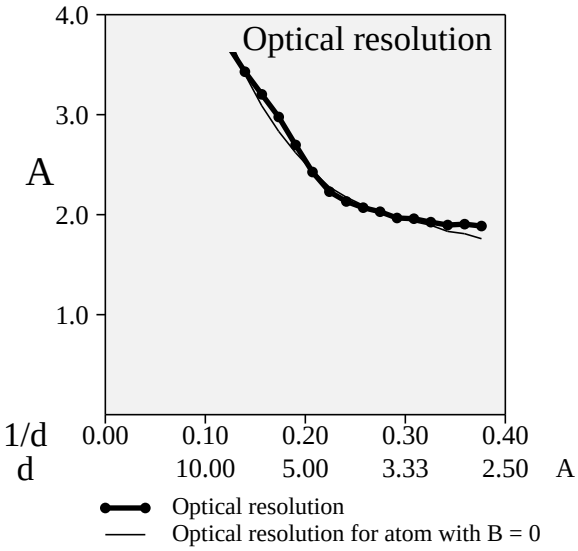
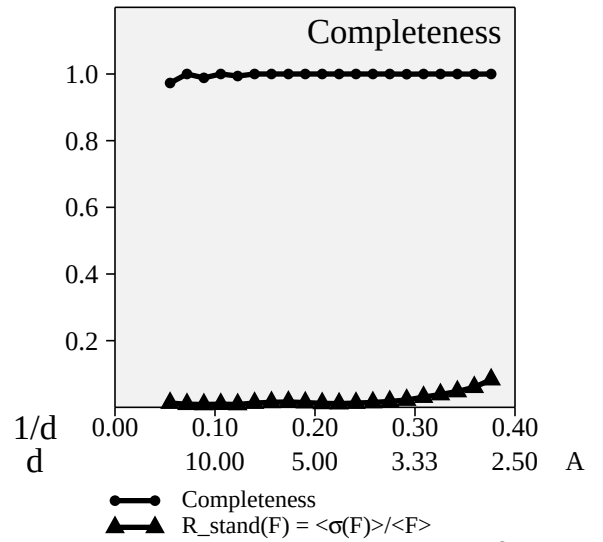
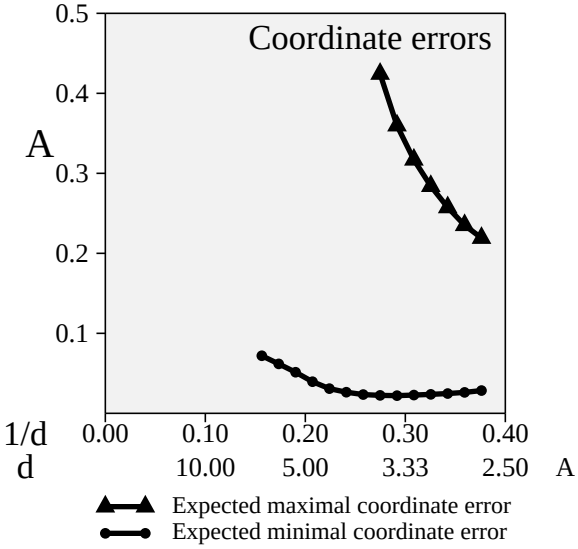
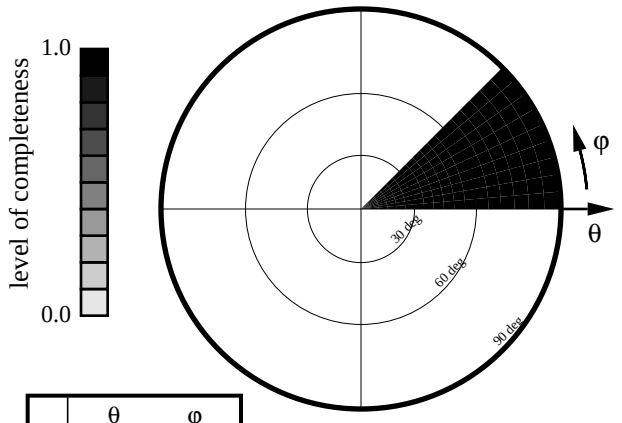






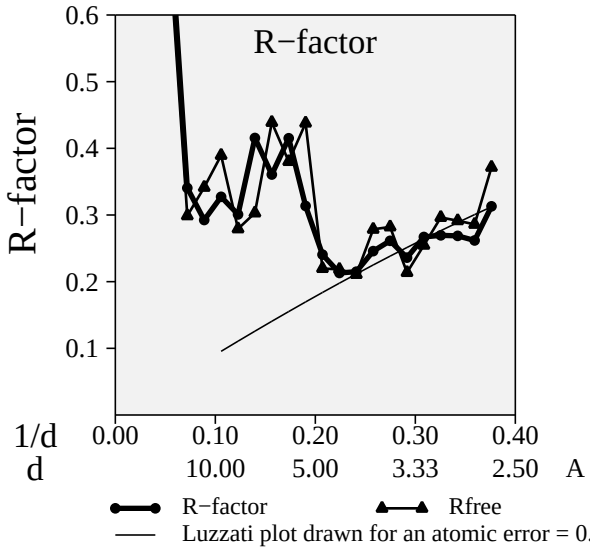


Stereographic projection of
the averaged radial completeness



	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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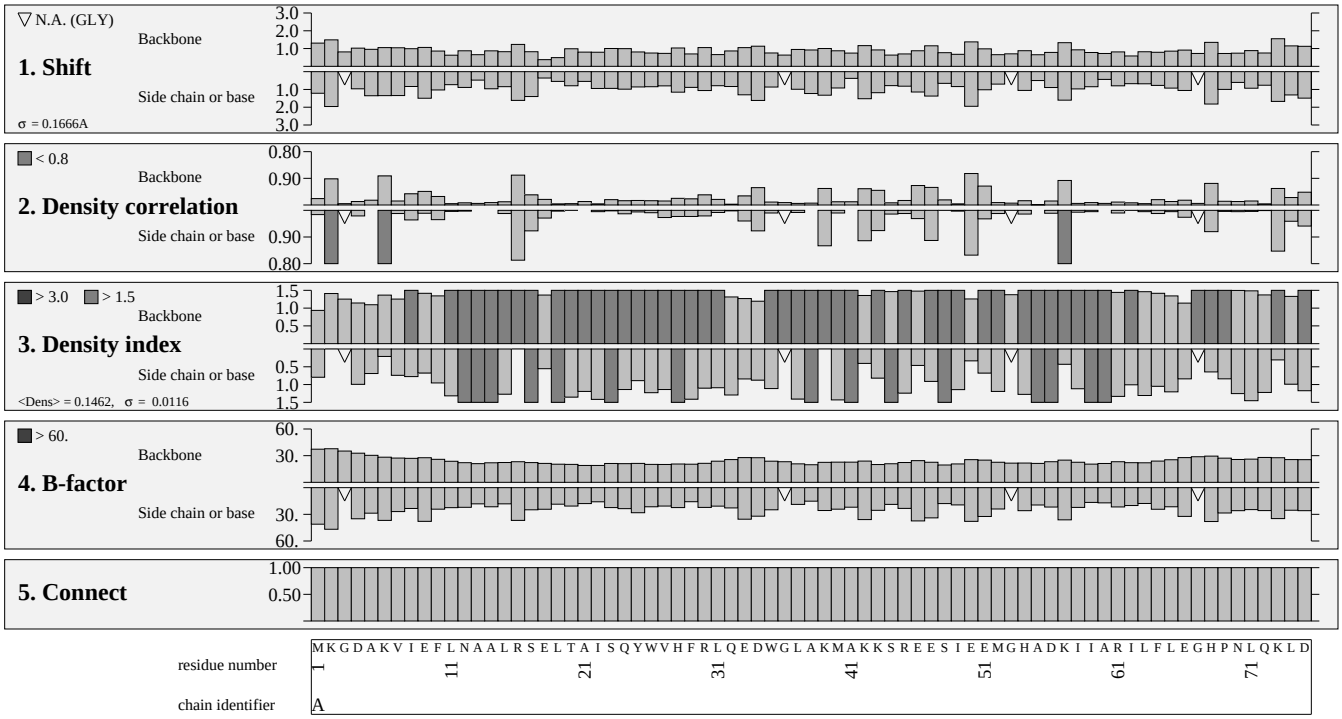
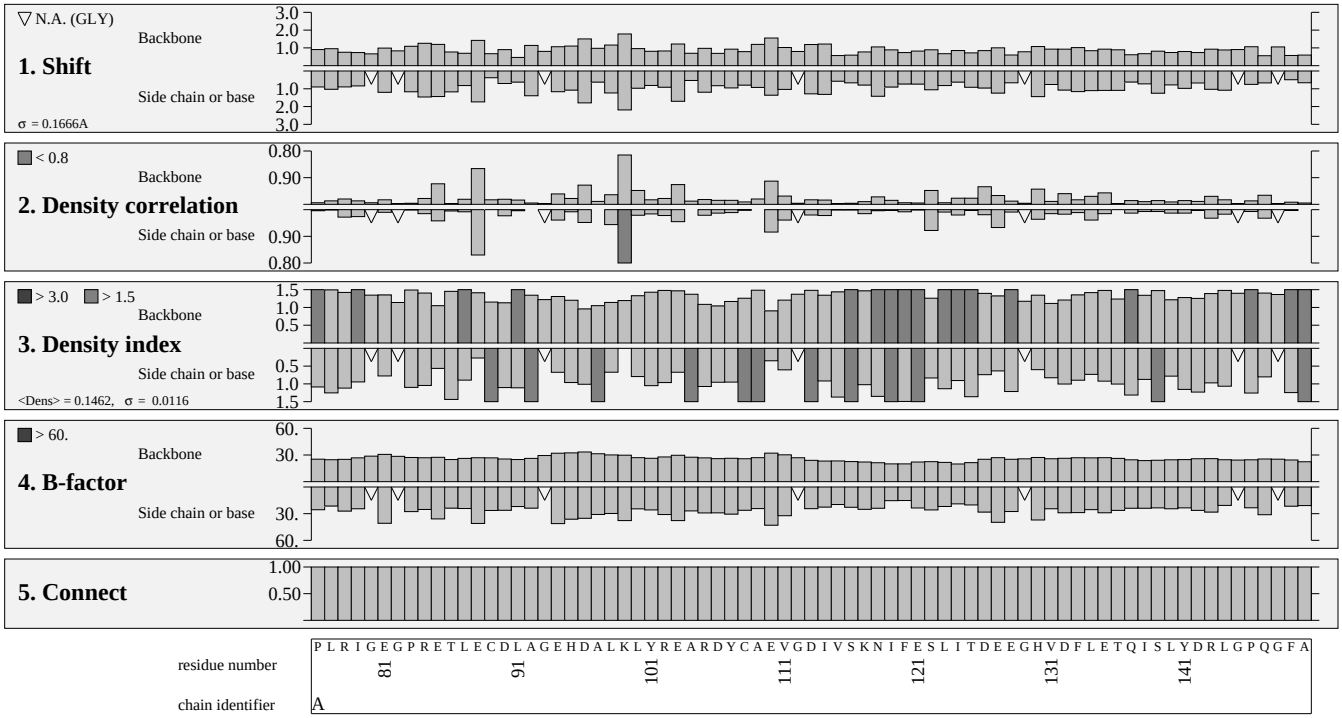
Local estimation





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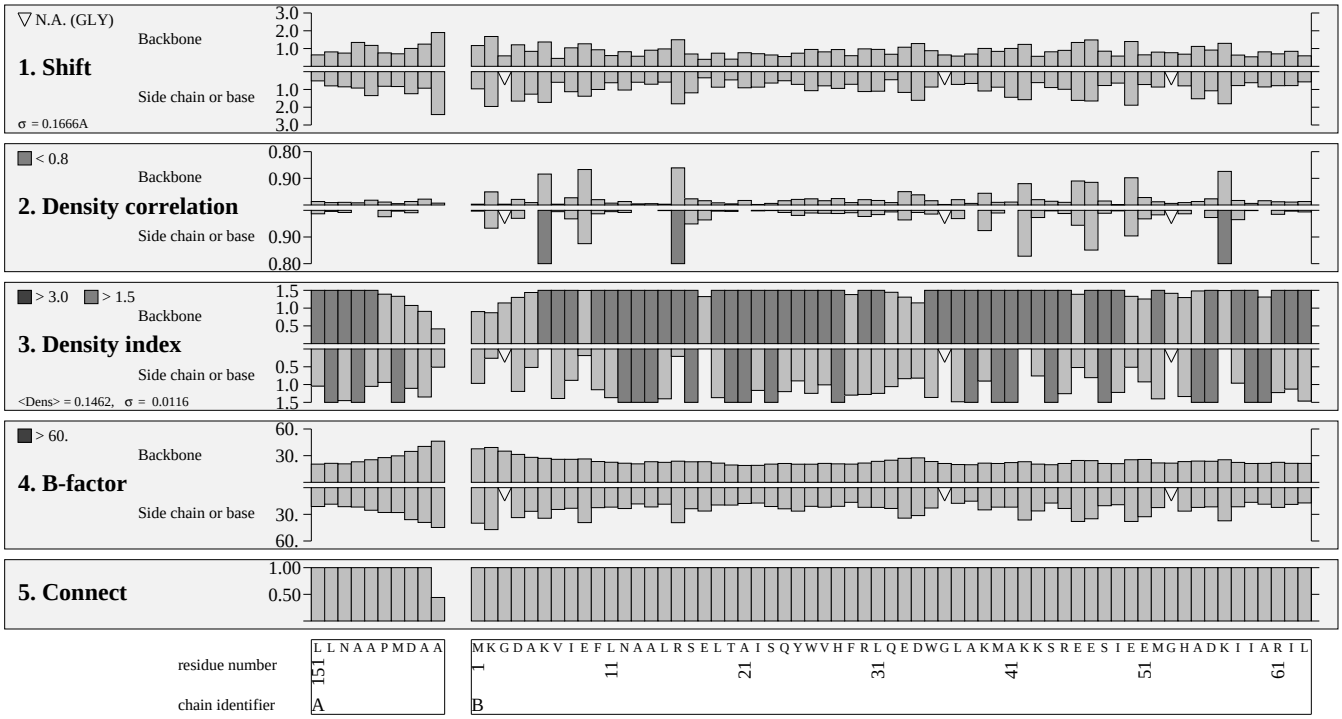
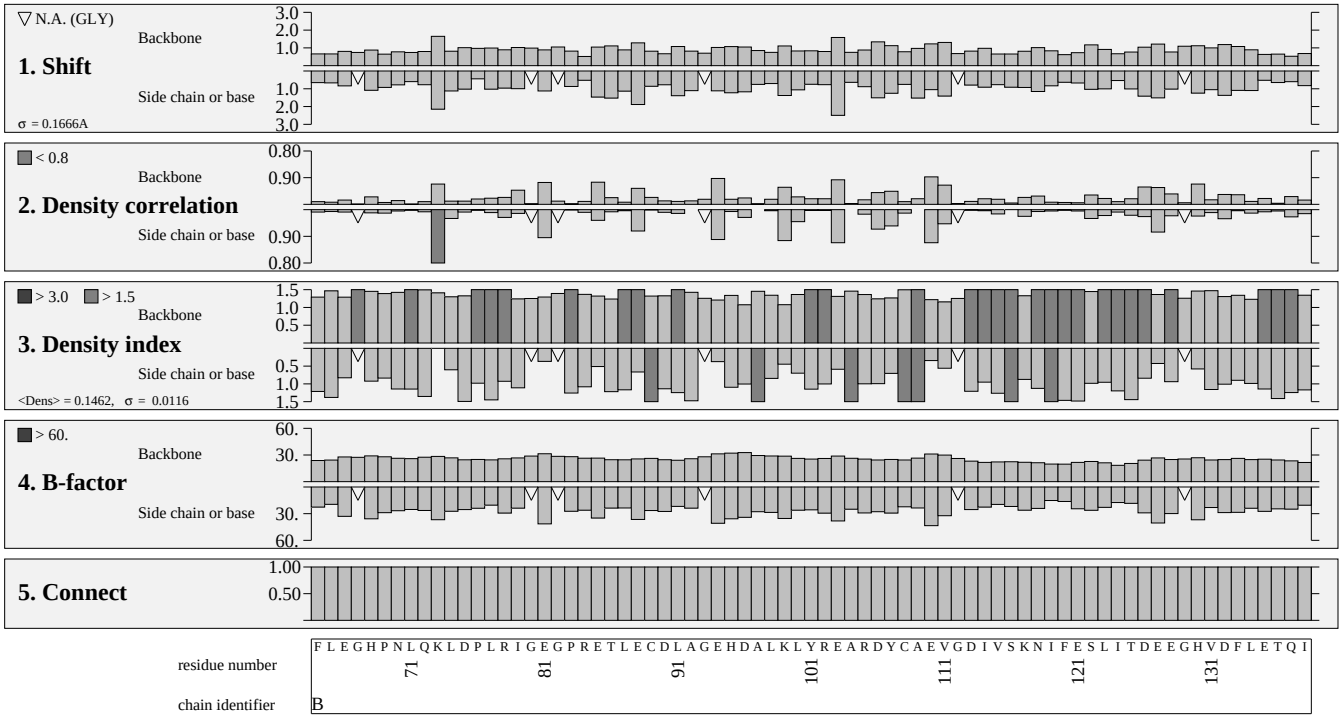
Local estimation (2)





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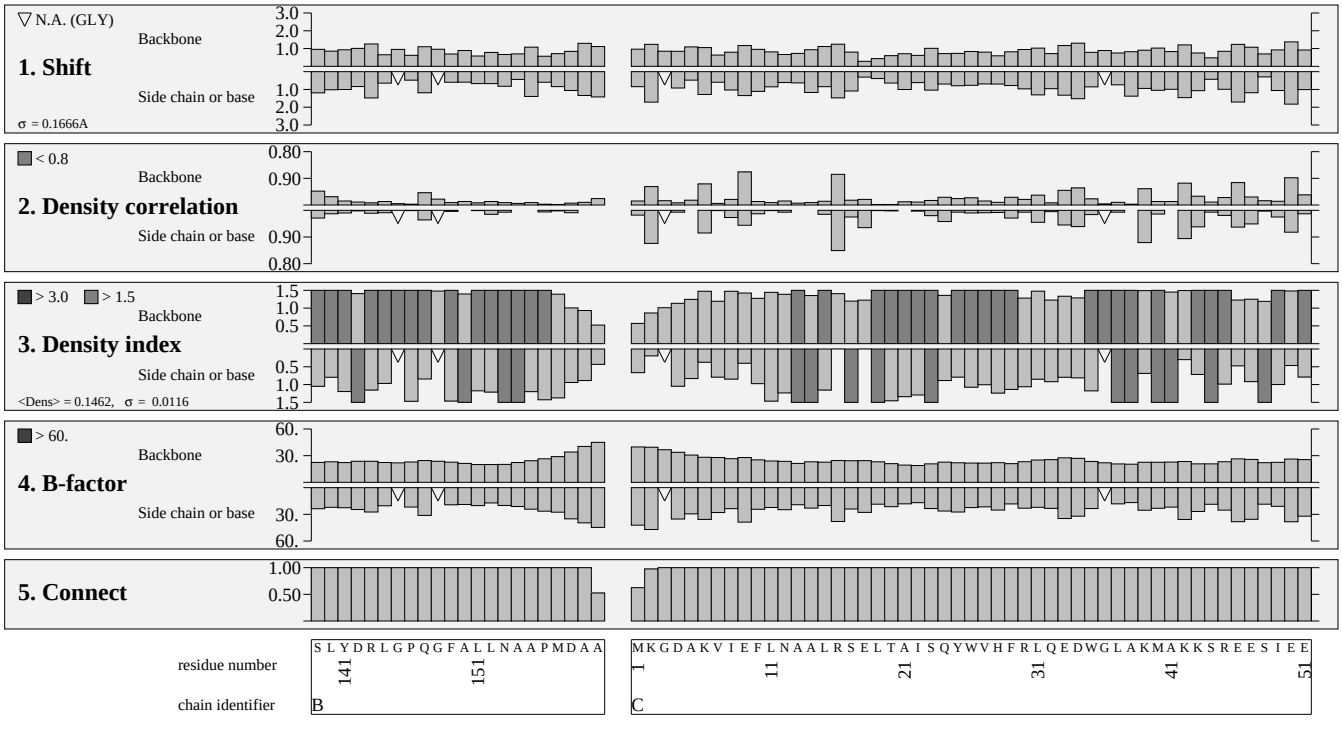
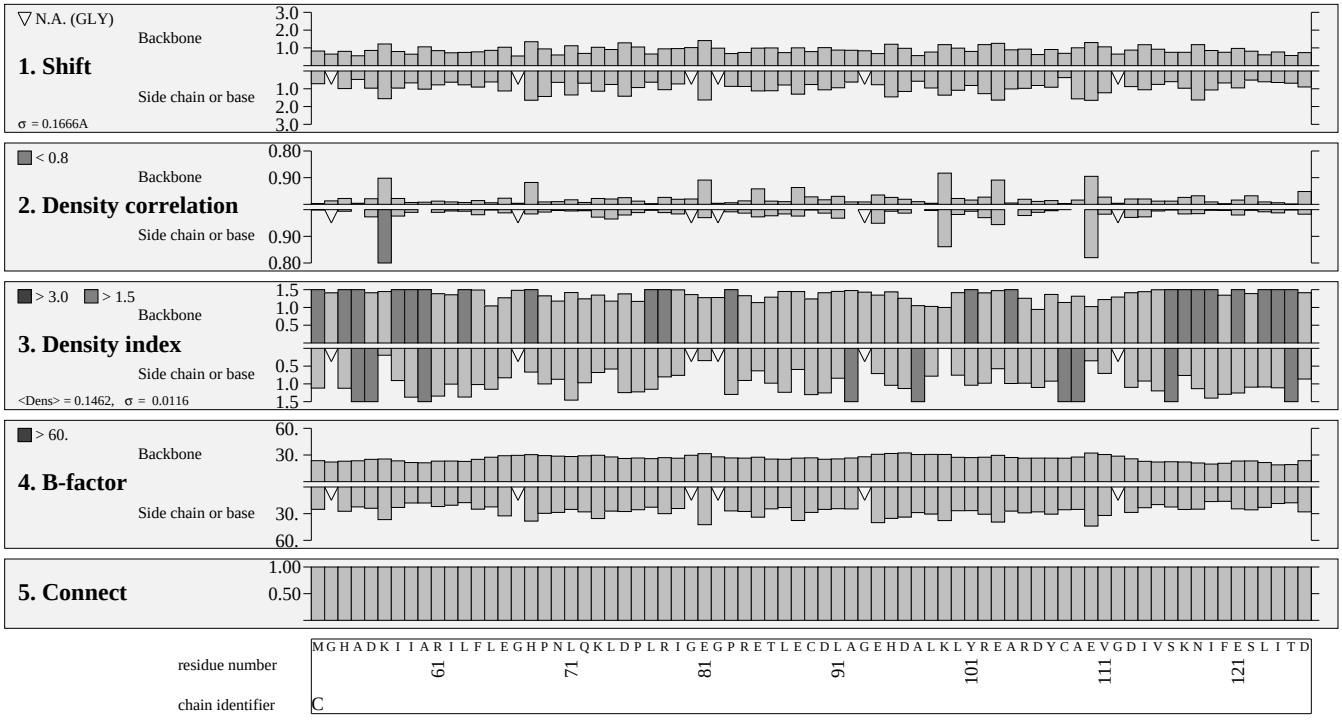
Local estimation (3)





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Local estimation (4)