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

Structure Factor Check

4E9M

Title:	NOD1 CARD DOMAIN WITH THREE DISULFIDE−CLINCHED, DOMAIN−SWAPP IN THE ASYMMETRIC UNIT
Date:	21−MAR−12
PDB code:	4E9M

Crystal

Cell parameters:

a: 82.85 A b: 85.33 A c: 113.68 A

α: 90.00 β: 90.00 γ: 90.00

Space group: P 21 21 21

Model

4641 atoms (88 water molecules)

Number of chains:	13
Volume not occupied by model:	49.9 %
<B> (for atomic model):	49.6 A^2
σ(B):	23.79 A^2
Matthews coefficient:	3.09
Corresponding solvent % :	59.91

Refinement

Program:	CNS 1.1
Nominal resolution range:	24.8 − 2.15 A
Reported R−factor:	0.245
Number of reflections used:	34213
Reported Rfree:	0.28
Sigma cut−off:	N.A.

Structure Factors

Input

Nominal resolution range:		24.8 − 2.15 A
Reflections in file:		34213
Unique reflections	above 0:	34213
	above 1σ:	33263
	above 3σ:	22746

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Nominal resolution range: 24.8 − 2.15 A

\05max. from input data, min. from author\05

Used reflections:	34213
Completeness:	76.9 %
R_stand(F) = <σ(F)>/<F> :	0.074
Anisotropic distribution of Structure Factors	
ratio of eigen values:	1.0000 0.9542 0.9992
B_overall (by Patterson):	37.A^2
Optical resolution:	1.75 A
Expected opt. resol. for complete data set:	1.75 A
Estimated minimal error:	0.051 A

Model vs. Structure Factors

R−factor for all reflections:	0.273
Correlation factor:	0.883
R−factor:	0.275
for F > 2.0 σ	
nom. resolution range:	24.84 − 2.15A
reflections used:	33266
Rfree:	0.304
Nfree:	1662
R−factor without free−refl.:	0.273
Non free−reflections:	31604
<u> (error in coords by Luzzati plot):	0.343 A
Estimated maximal error:	0.184 A
DPI:	0.238 A

Scaling

Scale:	1.013
Bdiff:	−2.78

Anisothermal Scaling (Beta):

0.9292 −0.2039 0.7260 0.0000 0.0000 0.0000

Solvent correction − Ks,Bs: 0.762 250.011

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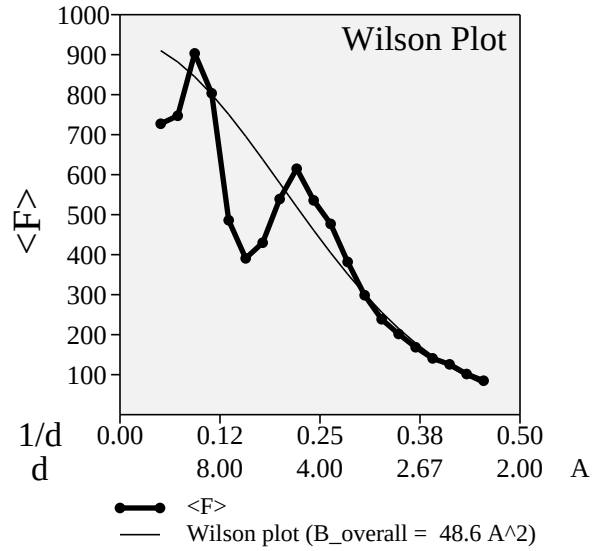
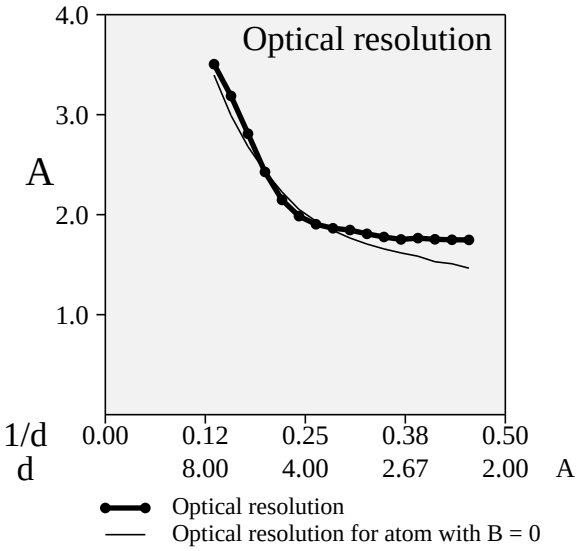
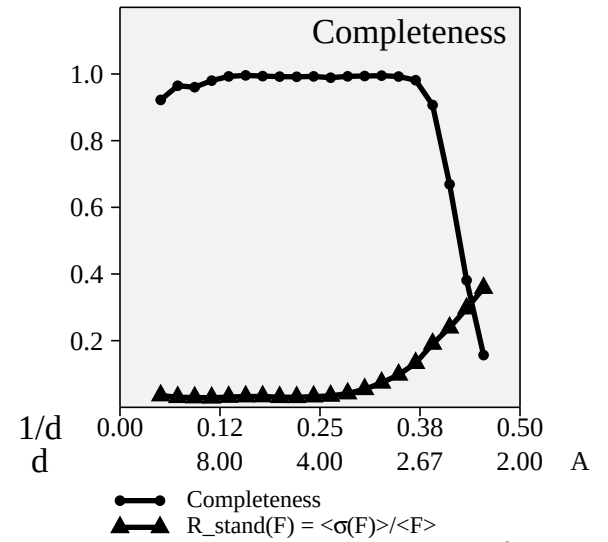
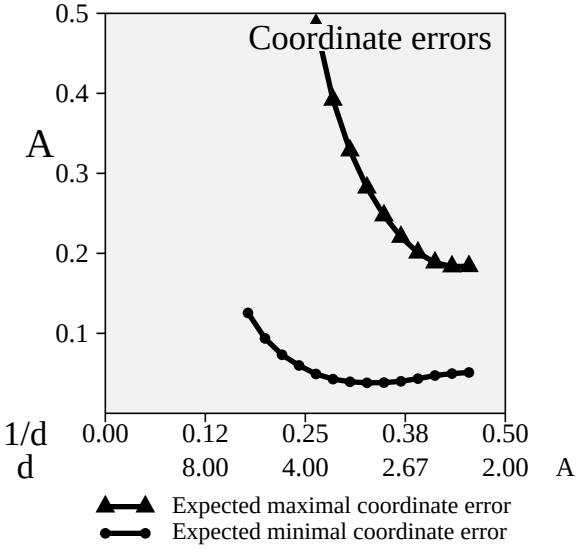
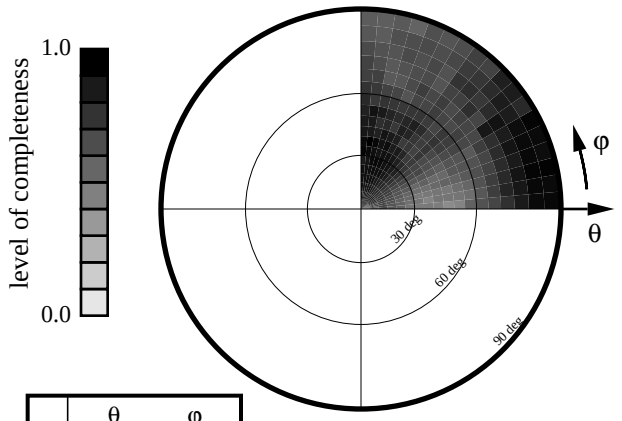






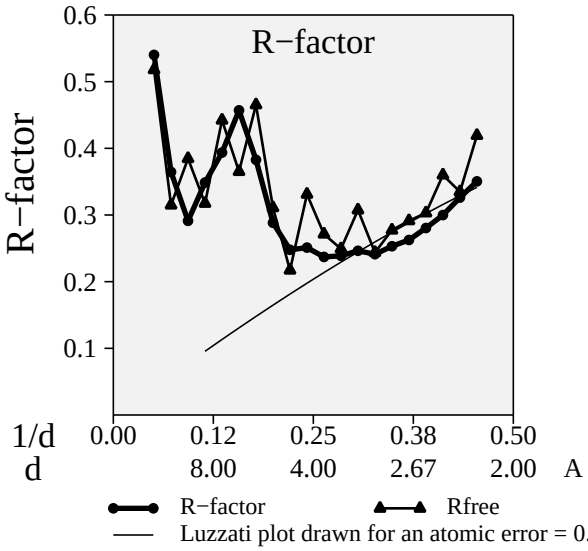


Stereographic projection of
the averaged radial completeness



	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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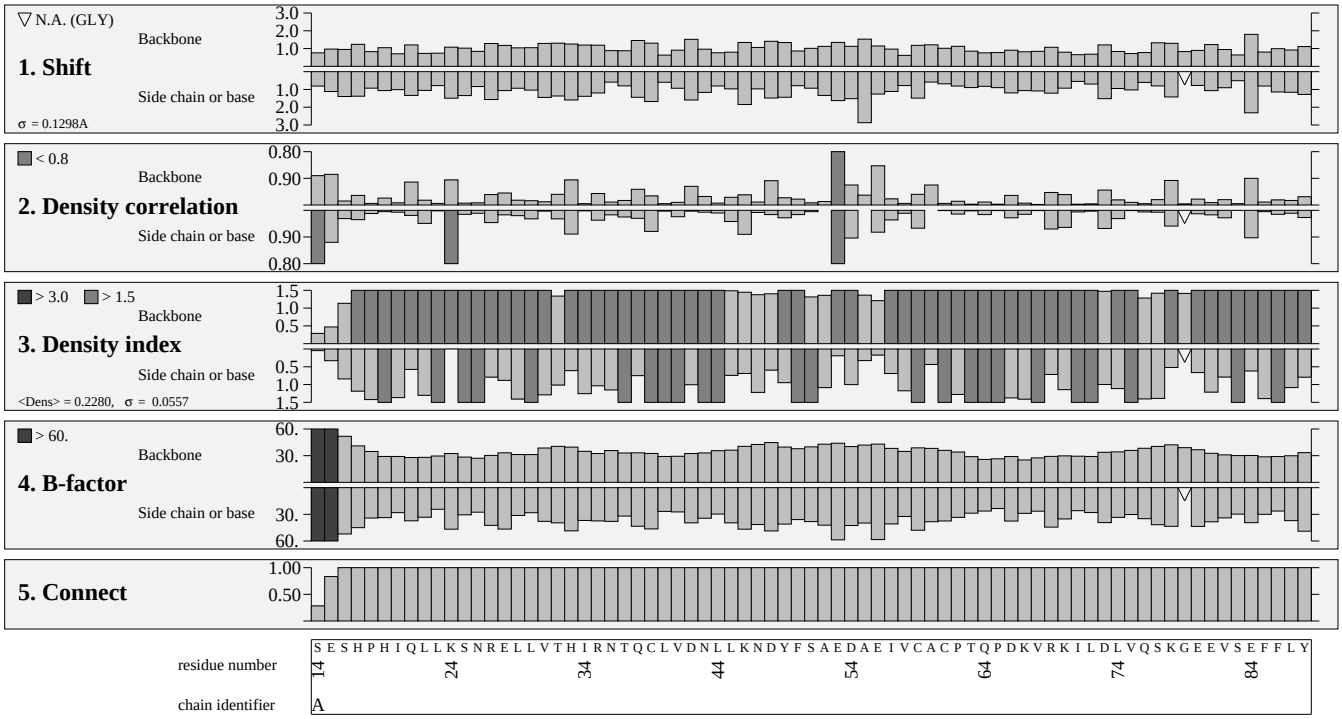
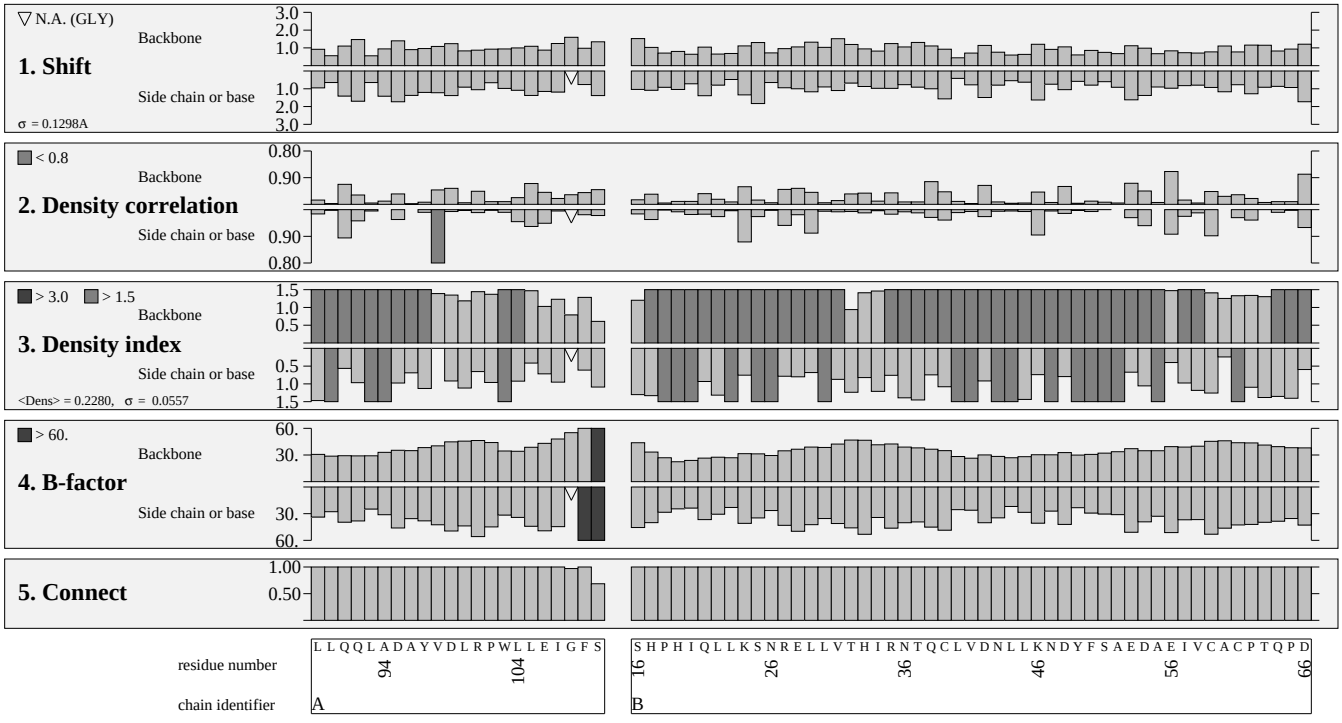
Local estimation





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Structure Factor Check

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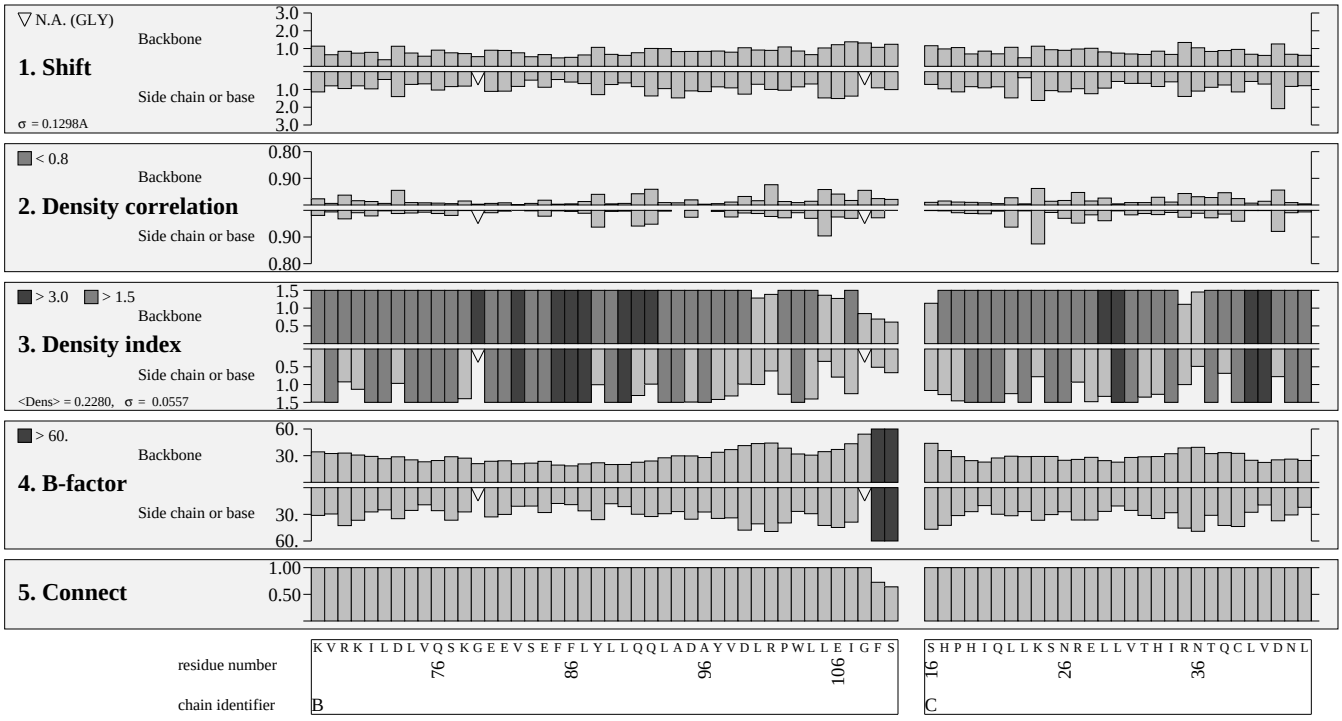
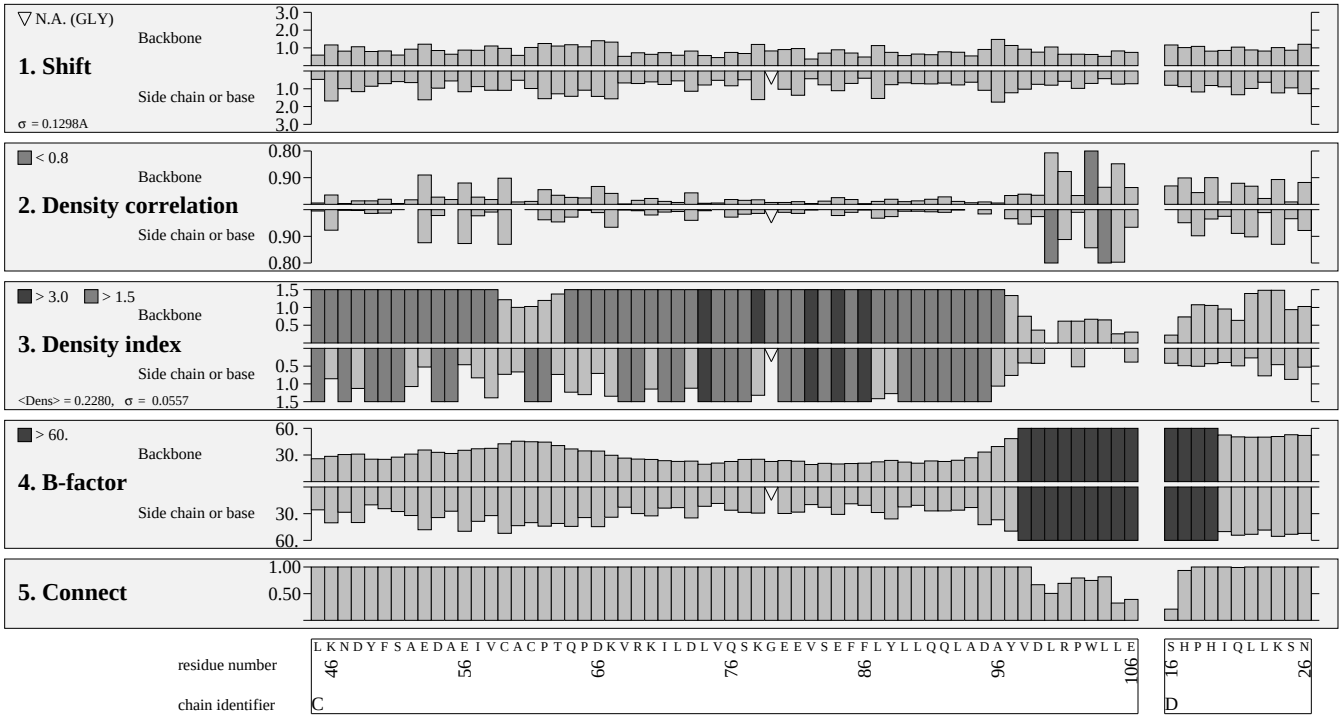
Local estimation (2)





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Structure Factor Check

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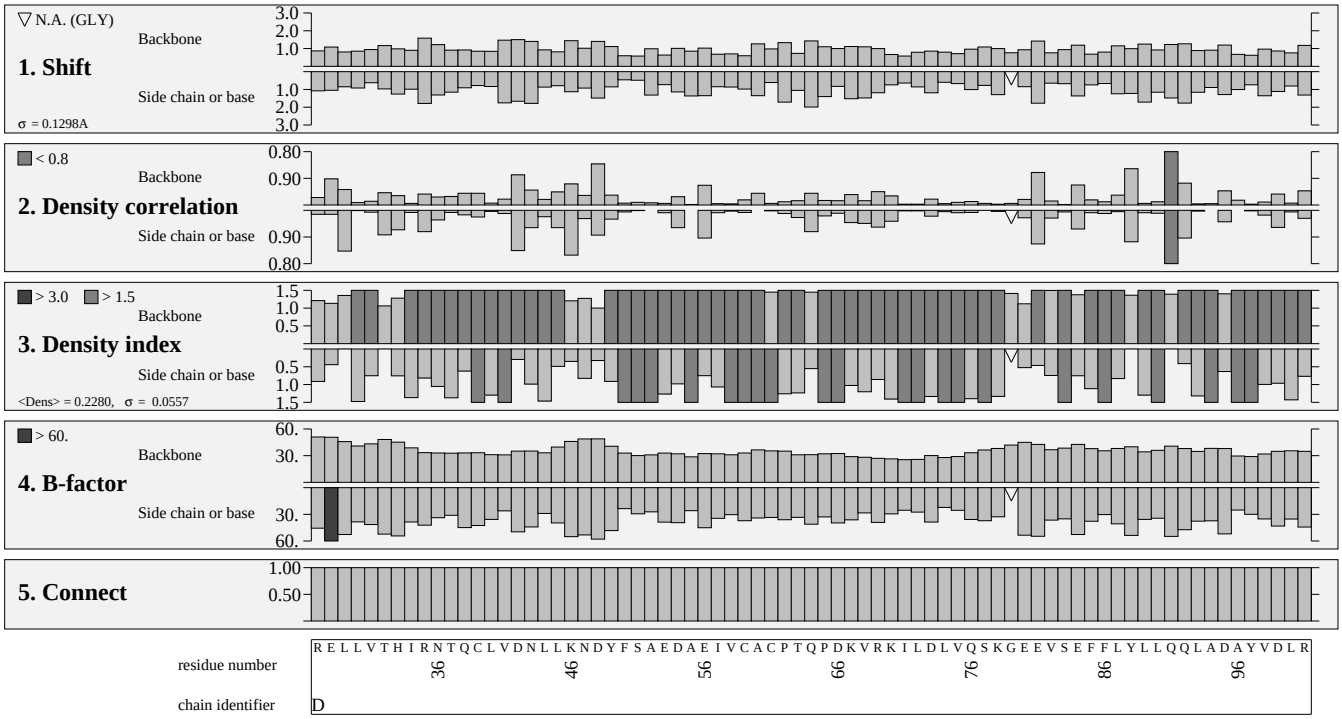
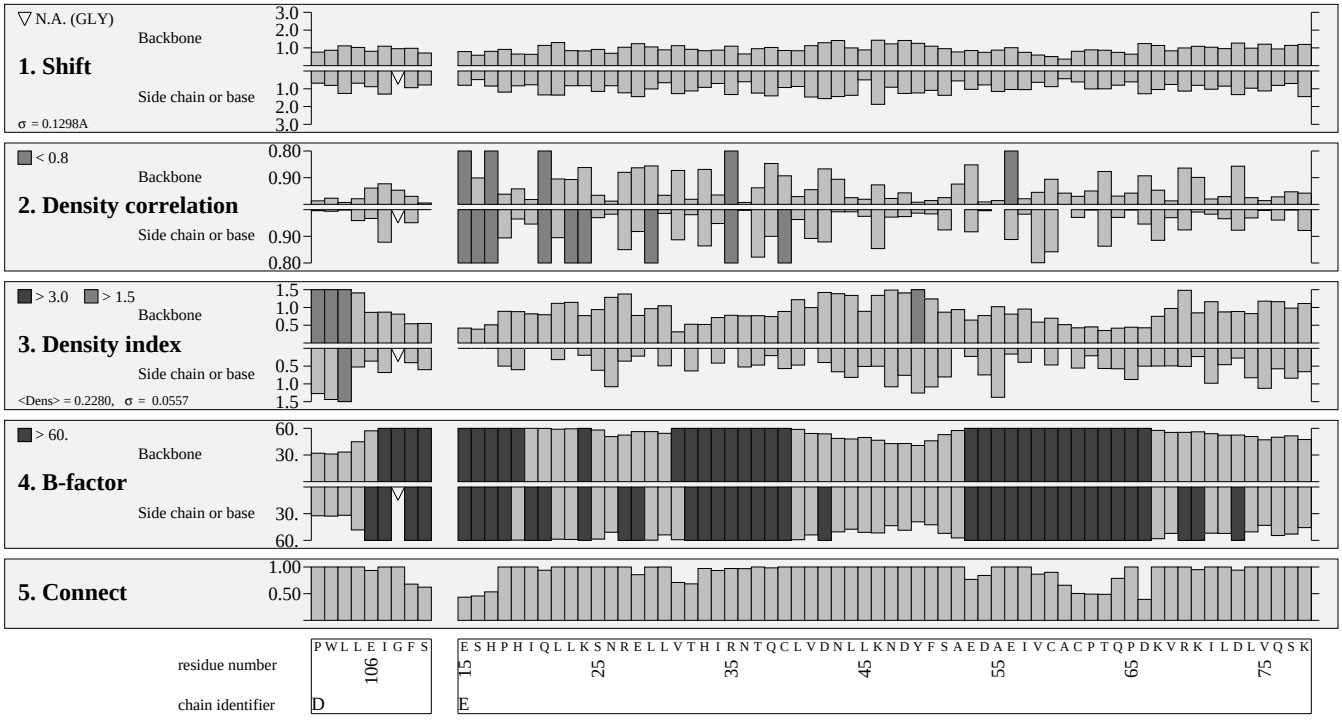
Local estimation (3)





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Structure Factor Check

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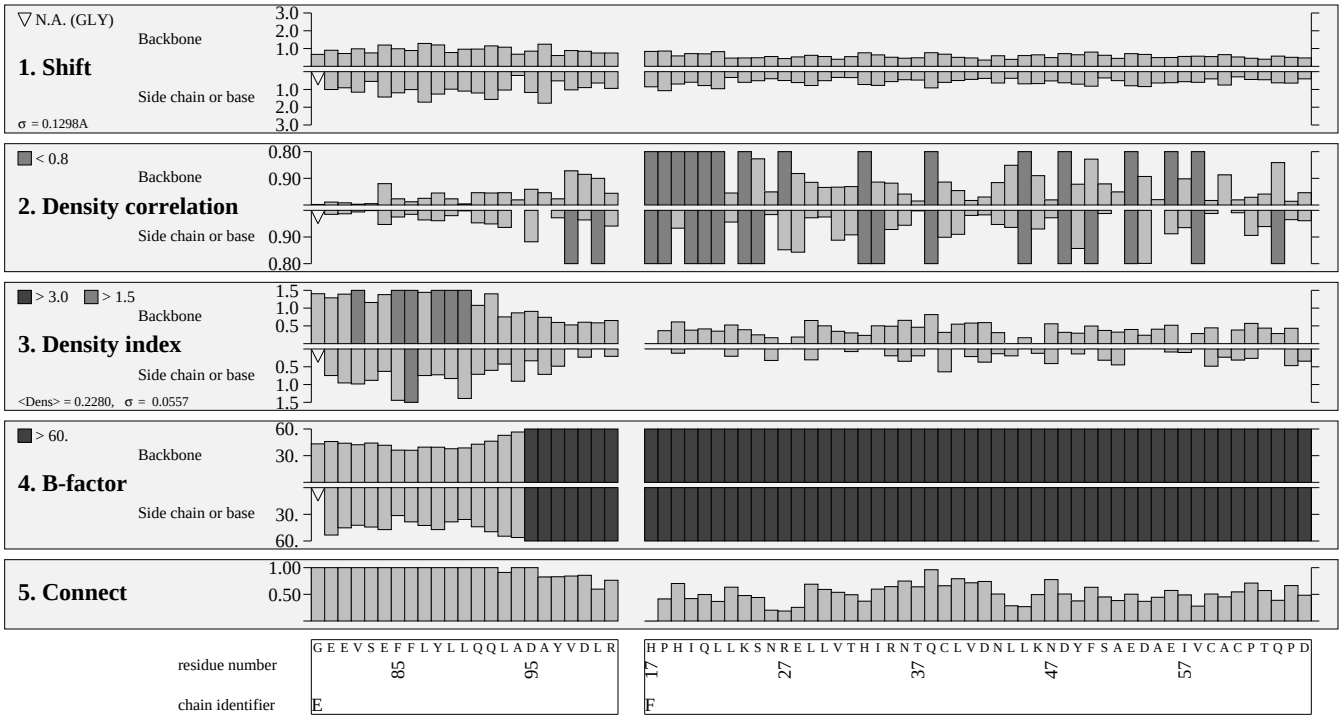
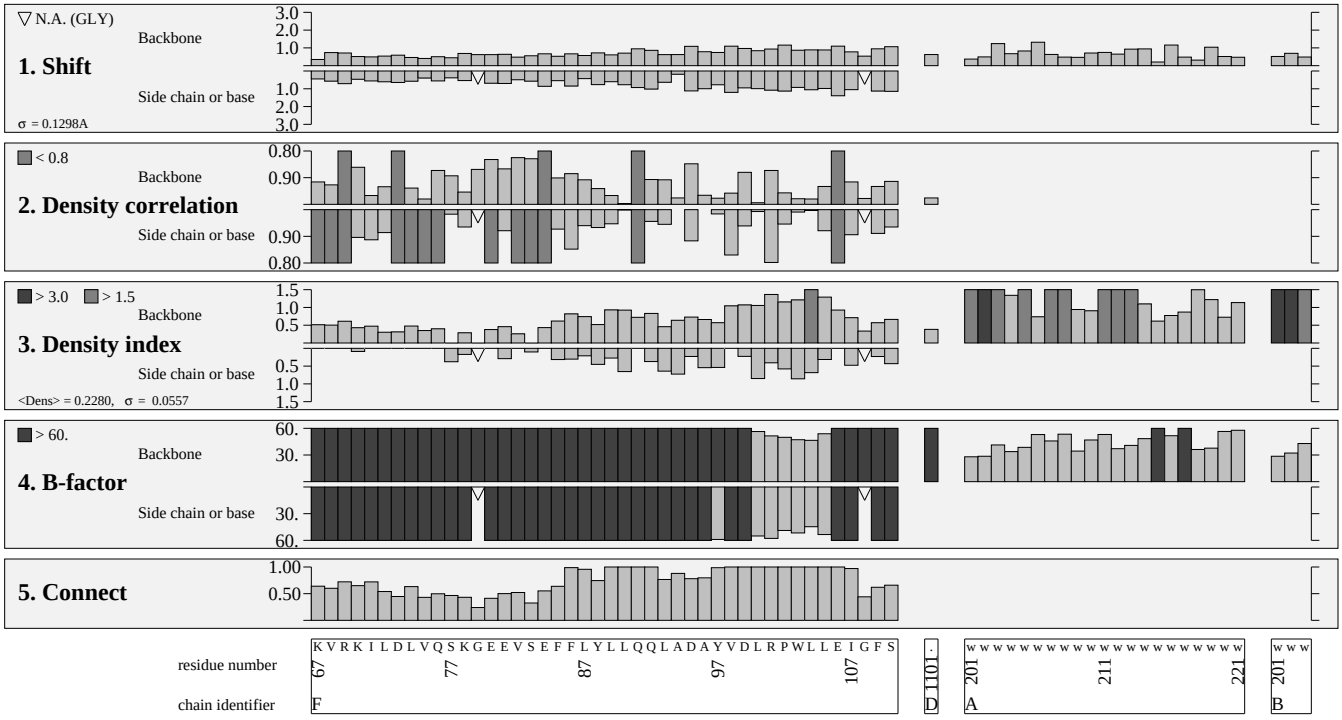
Local estimation (4)





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Local estimation (5)