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

Structure Factor Check

2BCC

Title: STIGMATELLIN−BOUND CYTOCHROME BC1 COMPLEX FROM CHICKEN
Date: 18−SEP−98
PDB code: 2BCC

Crystal

Cell parameters:

a: 173.46 A b: 182.45 A c: 241.33 A
α: 90.00 β: 90.00 γ: 90.00

Space group: P 21 21 21

Number of NCS−operators: 1
NC−symmetry only for information

Model

15754 atoms

Number of chains:	19
Volume not occupied by model:	64.3 %
<B> (for atomic model):	55.9 A^2
σ(B):	24.16 A^2
Matthews coefficient:	8.66
Corresponding solvent % :	85.68

Refinement

Program:	CNS 0.1
Nominal resolution range:	12.0 − 3.50 A
Reported R−factor:	0.284
Number of reflections used:	80760
Reported Rfree:	0.32
Sigma cut−off:	N.A.

Structure Factors

Input

Nominal resolution range:		49.5 − 3.02 A
Reflections in file:		118814
Unique reflections	above 0:	106582
	above 1σ:	96009
	above 3σ:	75336
Reflections > 0:		12232

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Nominal resolution range: 49.5 − 3.50 A
\05max. from input data, min. from author\05

Used reflections:	79550
Reflections out of resolution:	27032
Completeness:	82.1 %
R_stand(F) = <σ(F)>/<F> :	0.099

Anisotropic distribution of Structure Factors
ratio of eigen values: 1.0000 0.6958 0.7364

B_overall (by Patterson):	58.A^2
Optical resolution:	2.46 A
Expected opt. resol. for complete data set:	2.46 A
Estimated minimal error:	1.026 A

Model vs. Structure Factors

R−factor for all reflections:	0.299
Correlation factor:	0.736
R−factor:	0.294

for F > 2.0 σ
nom. resolution range: 12.00 − 3.50A
reflections used: 73382

<u> (error in coords by Luzzati plot):	0.653 A
Estimated maximal error:	0.407 A
DPI:	0.393 A

Scaling

Scale:	0.034
Bdiff:	−1.48

Anisothermal Scaling (Beta):
6.1351 1.5718 2.3300 0.0000 0.0000 0.0000

Solvent correction − Ks,Bs: 0.730 250.261

Structure Factor Check

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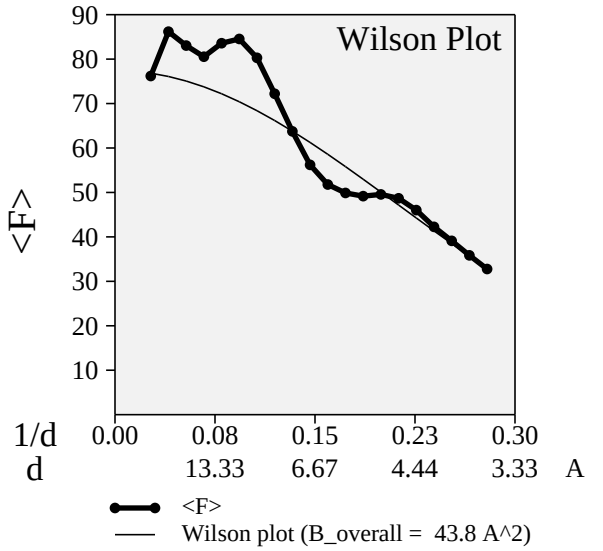
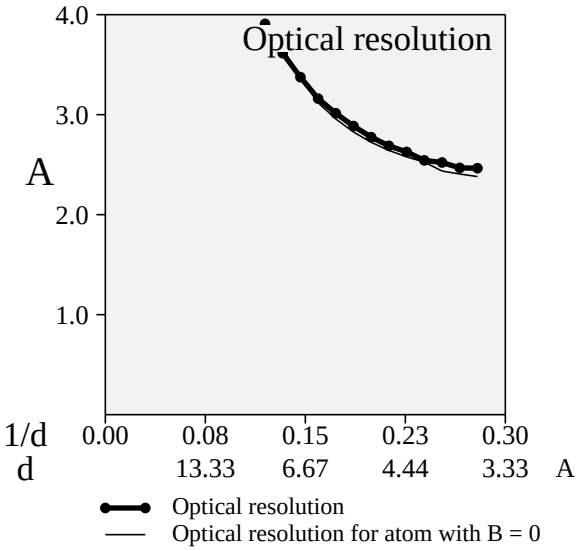
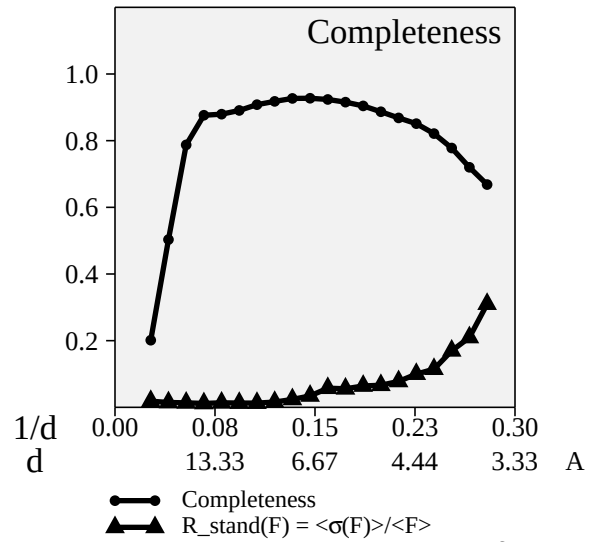
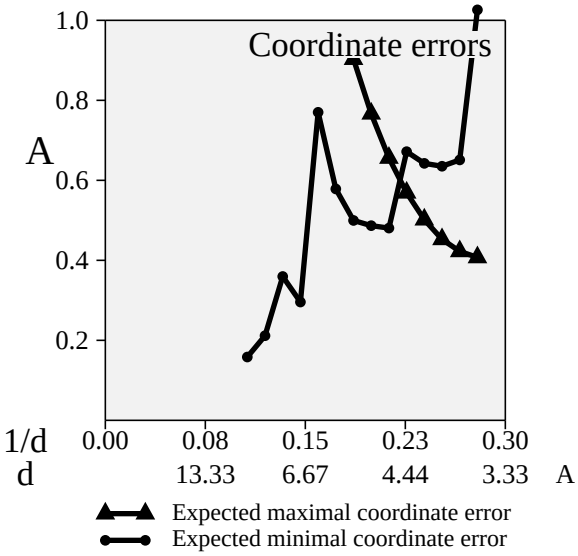
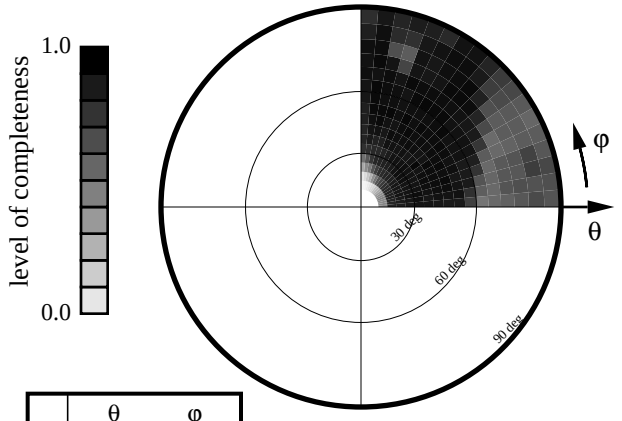






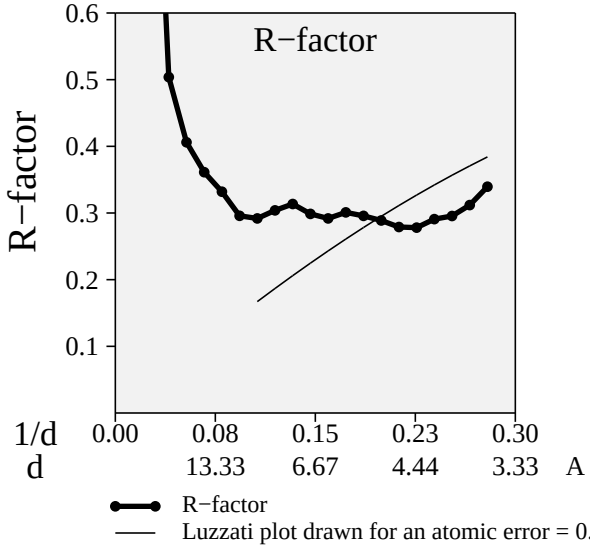


Stereographic projection of
the averaged radial completeness



	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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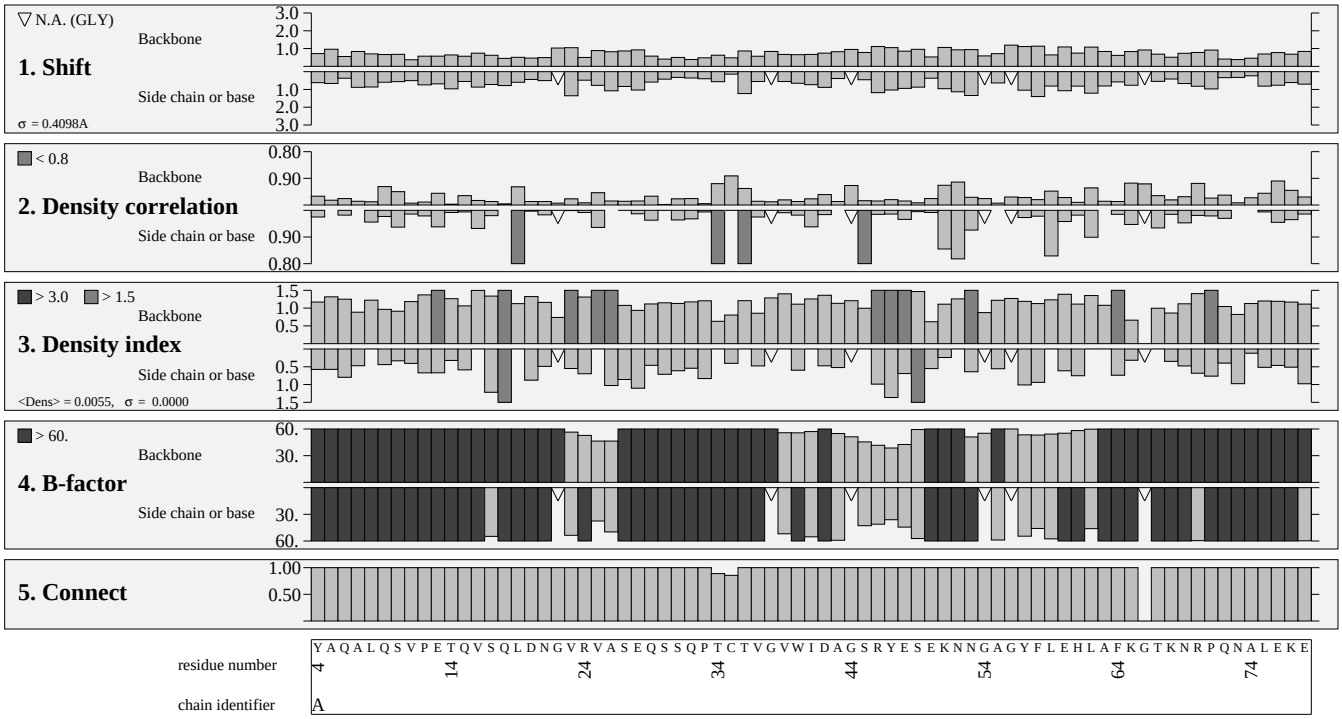
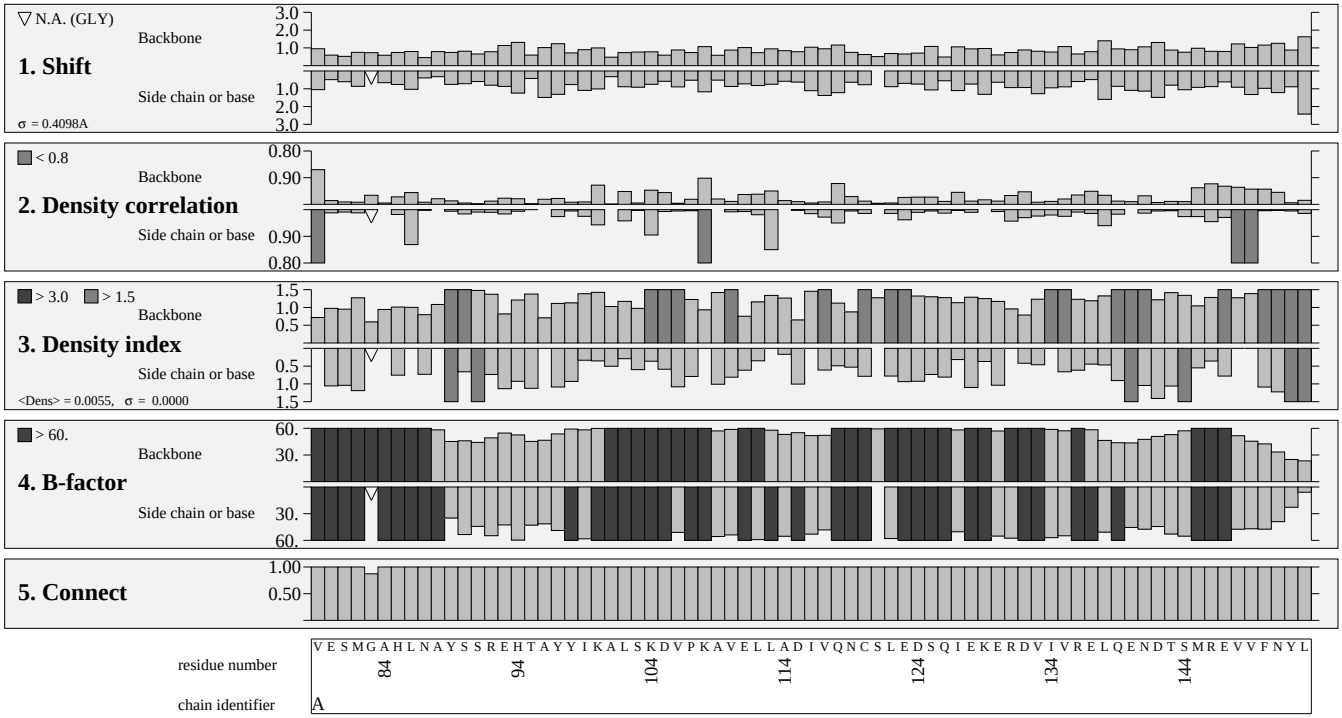
Structure Factor Check

2BCC

Local estimation





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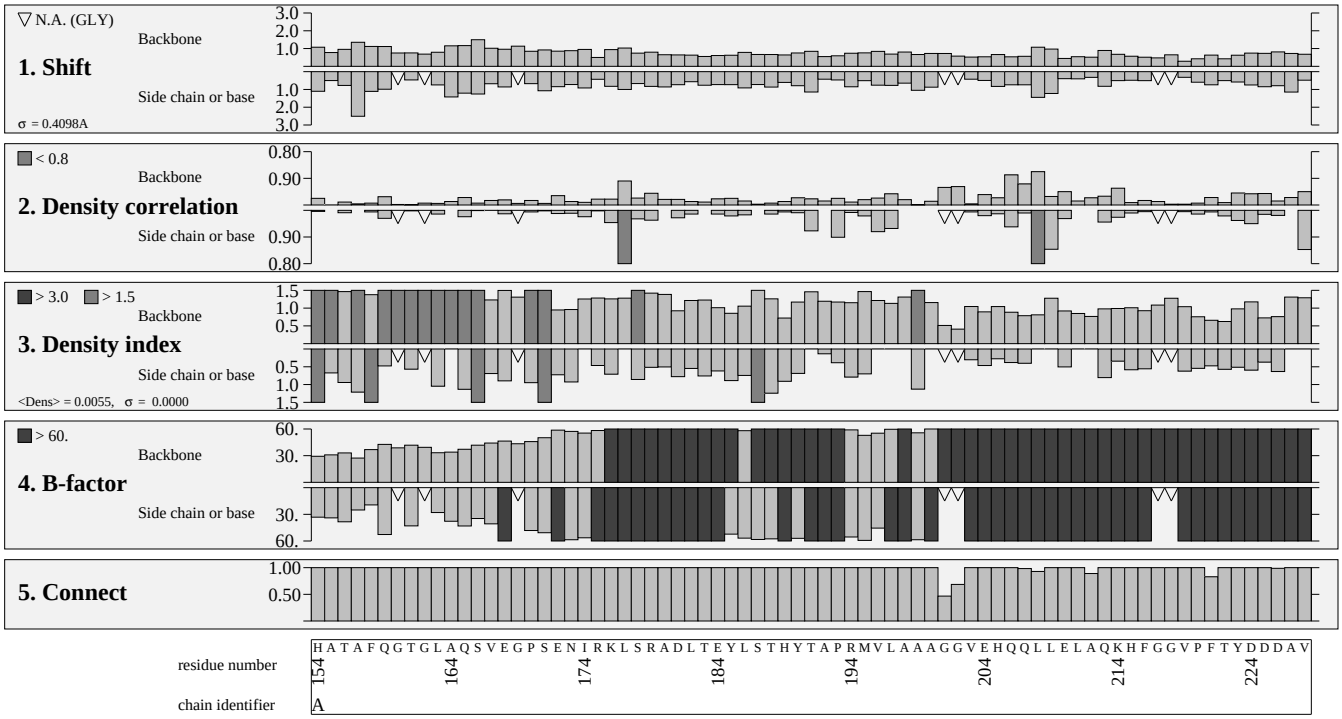
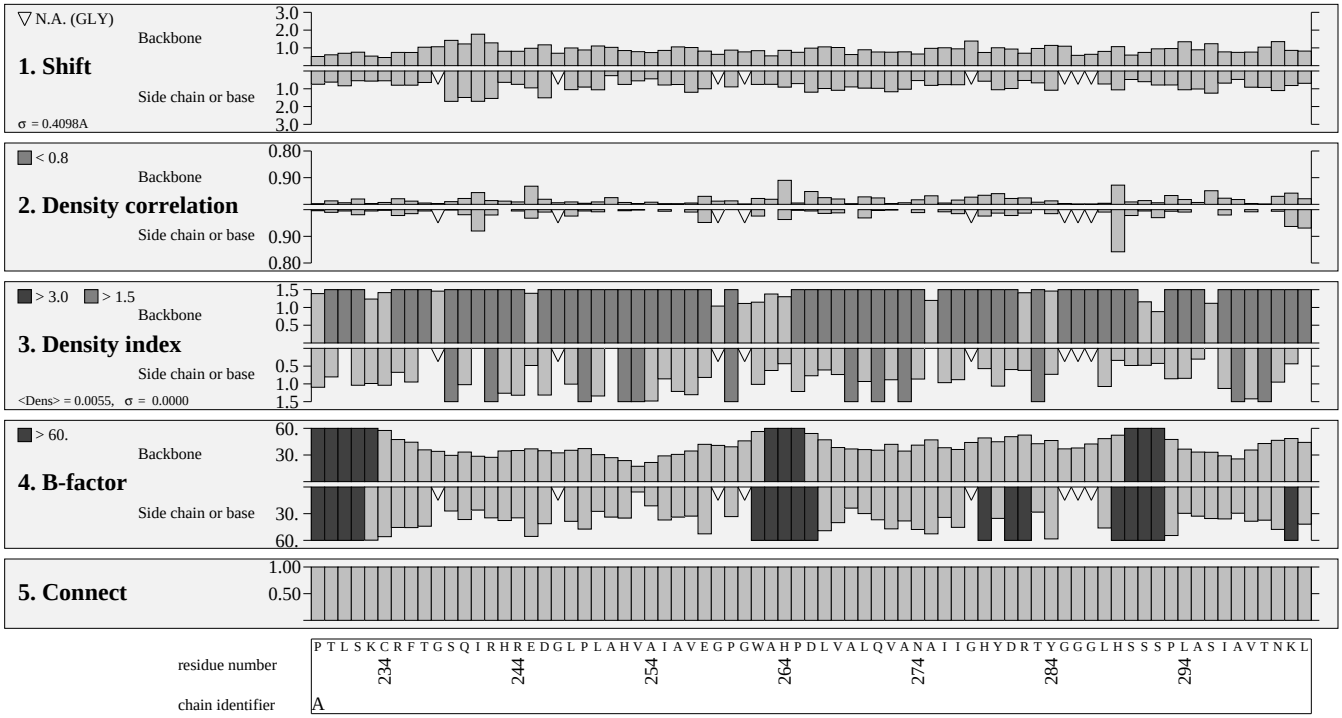
Structure Factor Check

2BCC

Local estimation (2)





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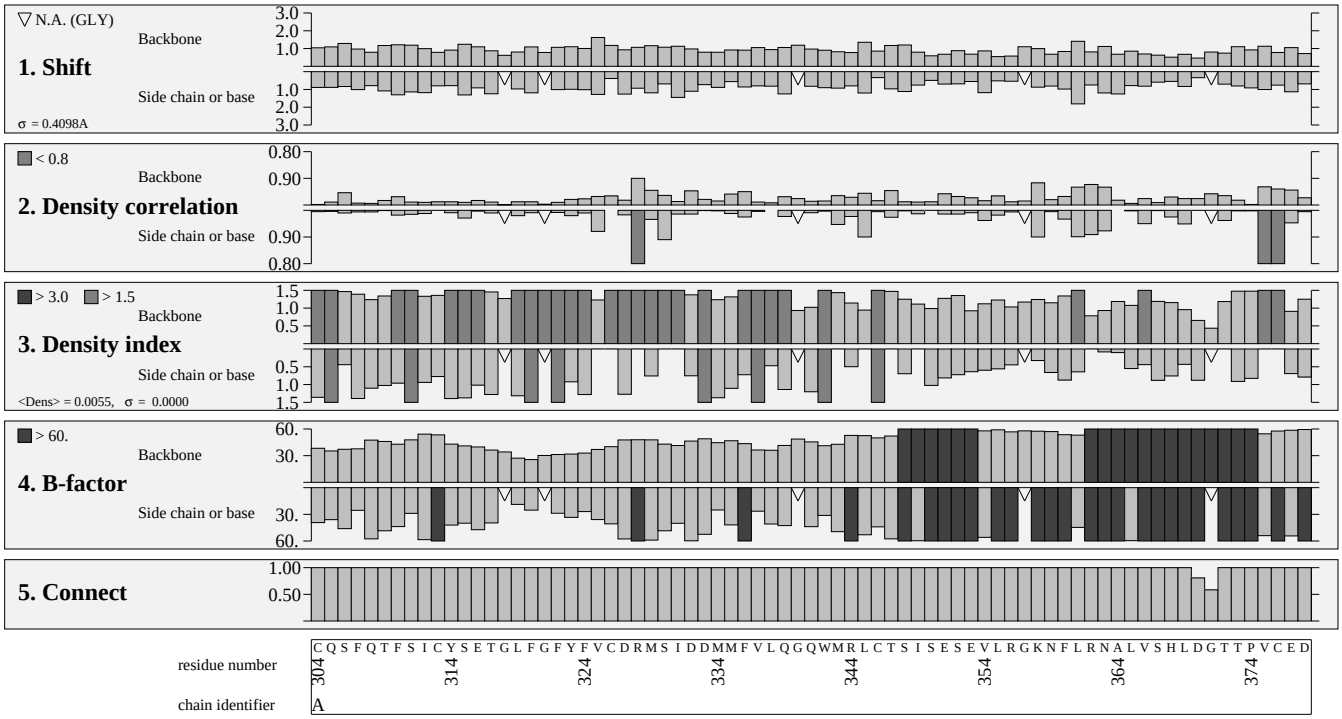
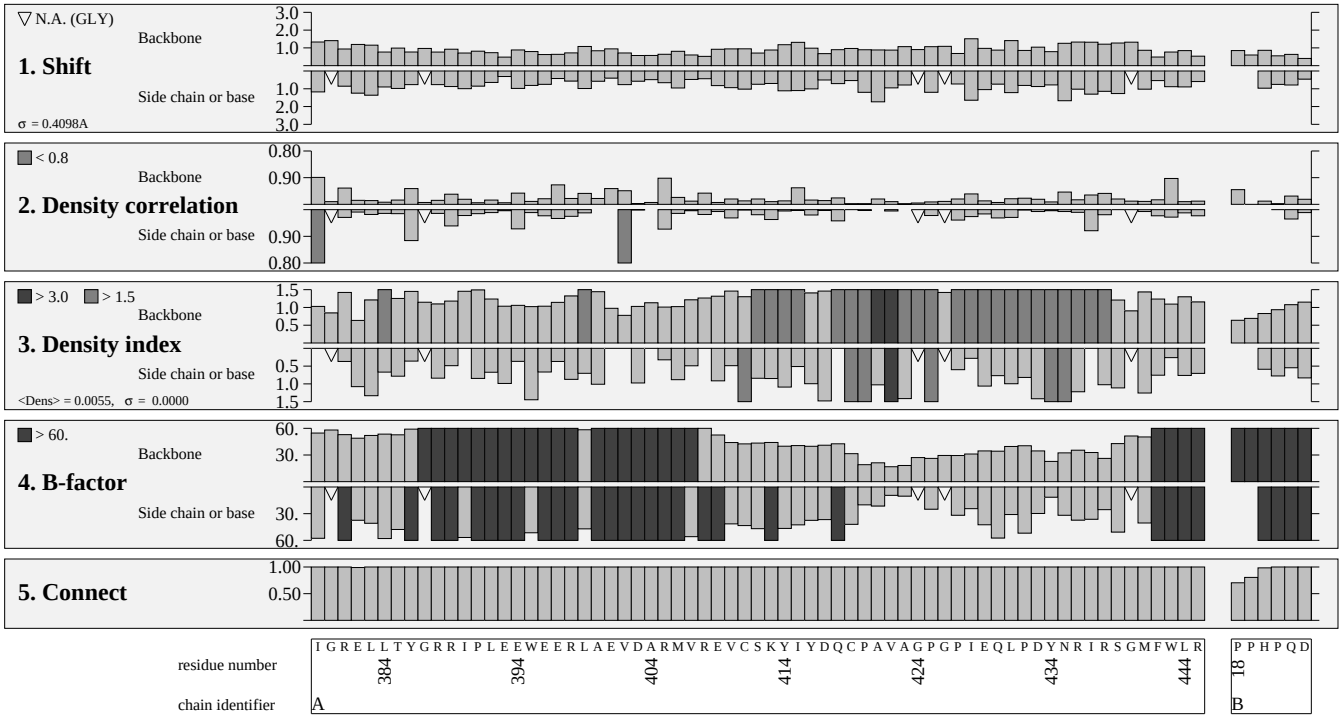
2BCC

Local estimation (3)





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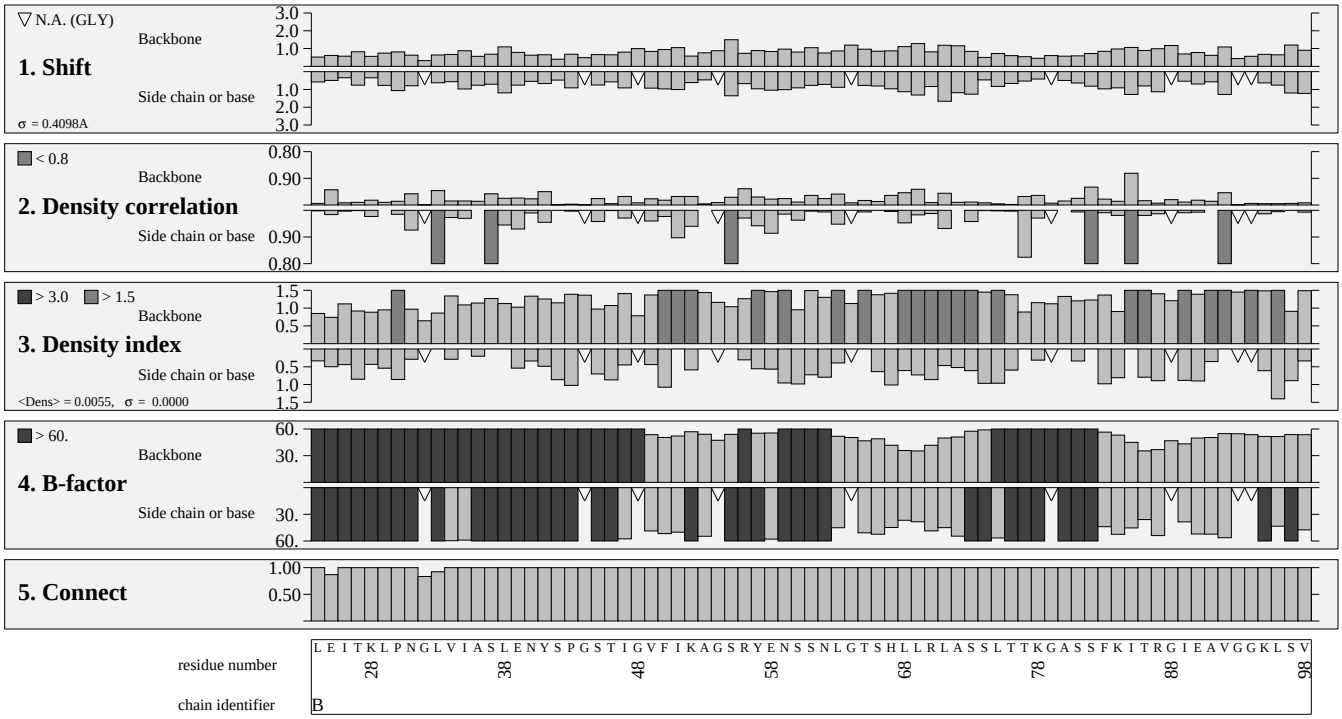
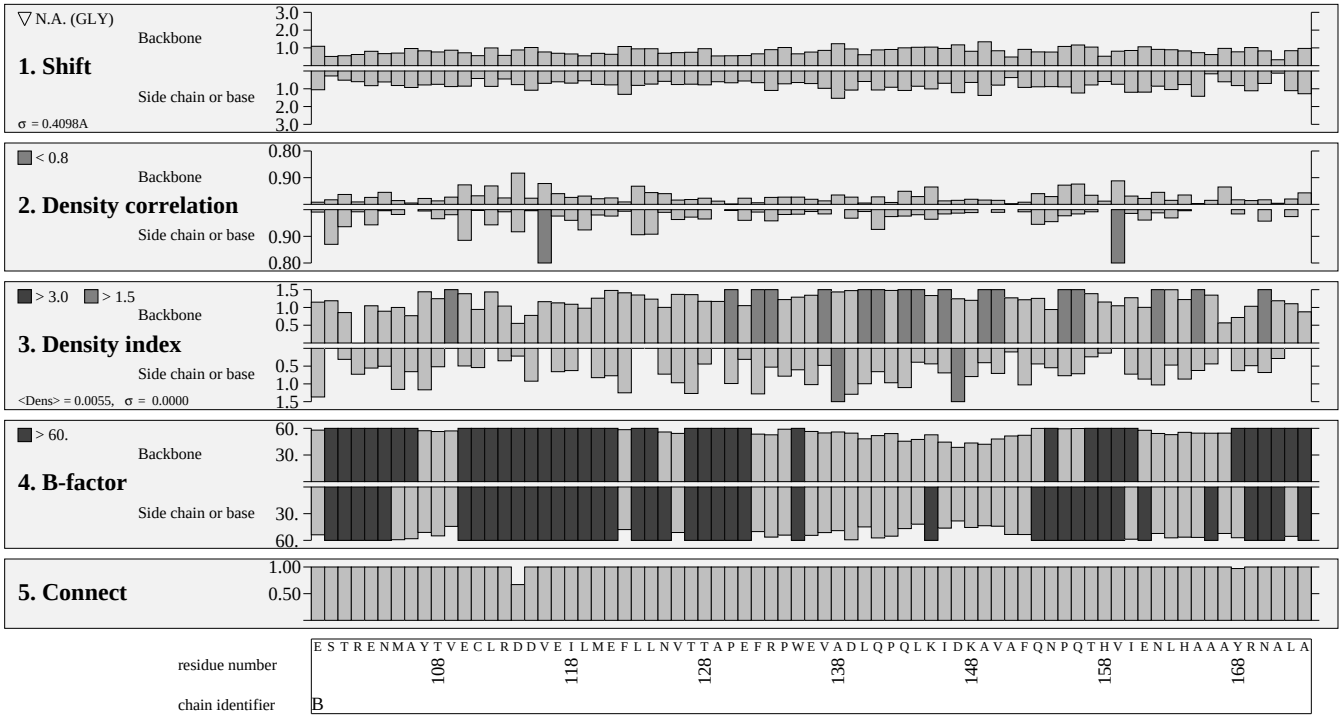
Local estimation (4)





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Structure Factor Check

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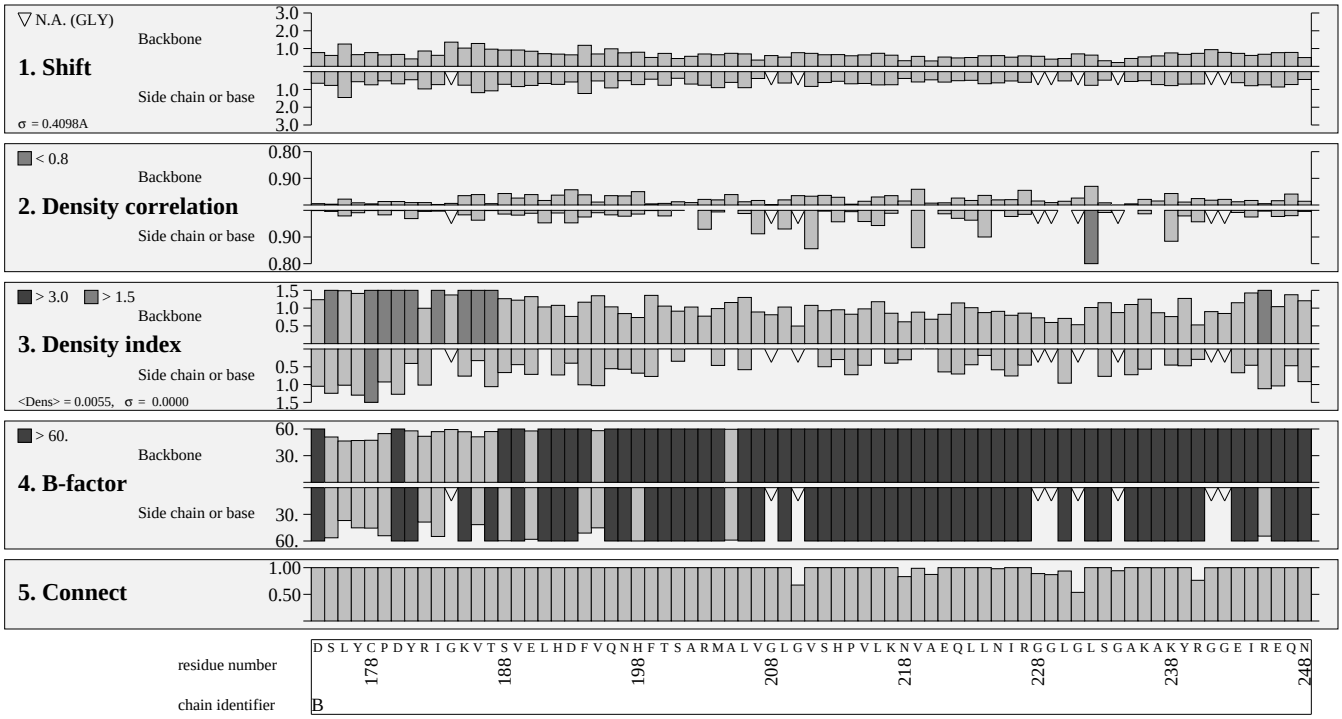
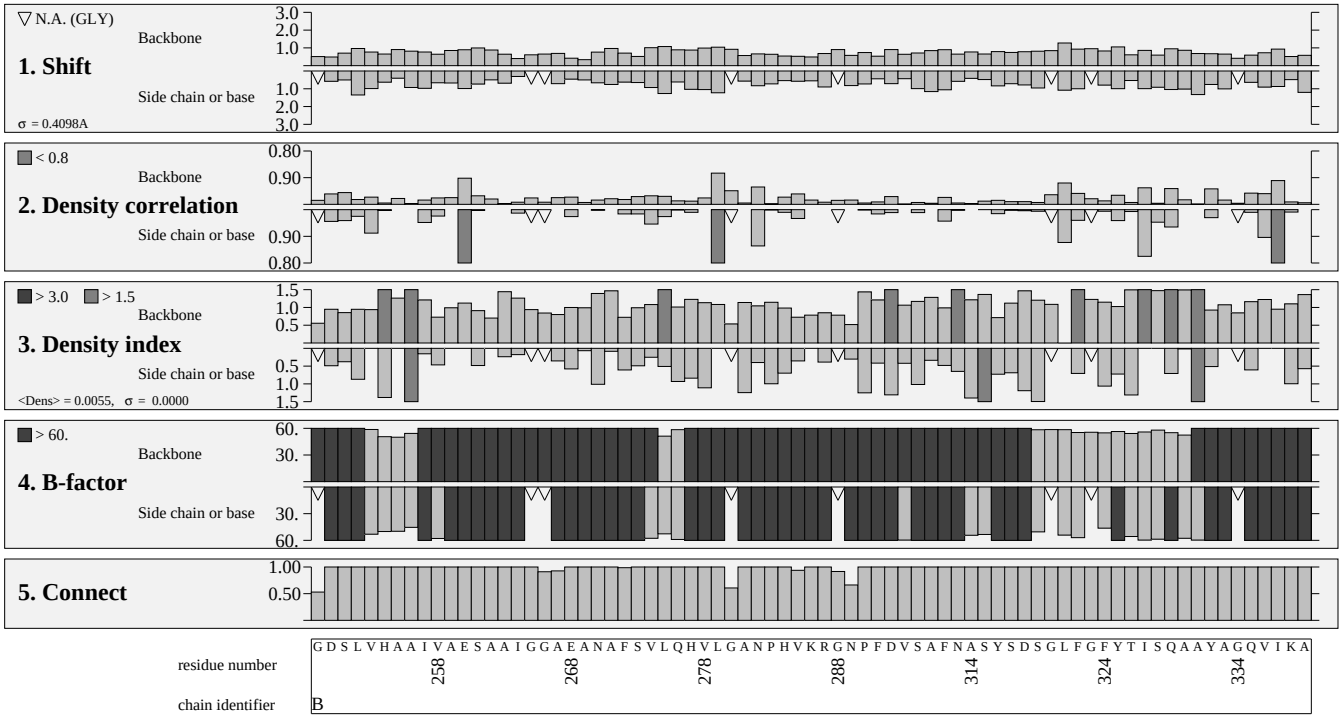
Local estimation (5)





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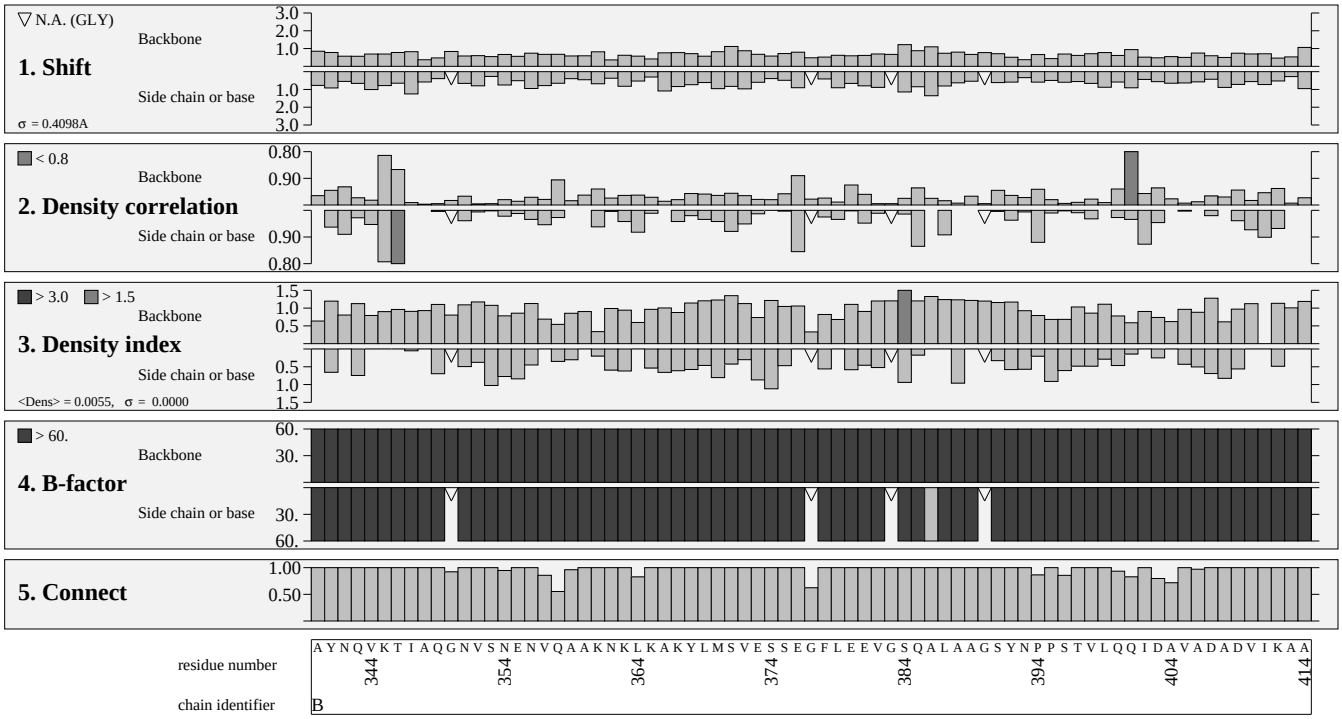
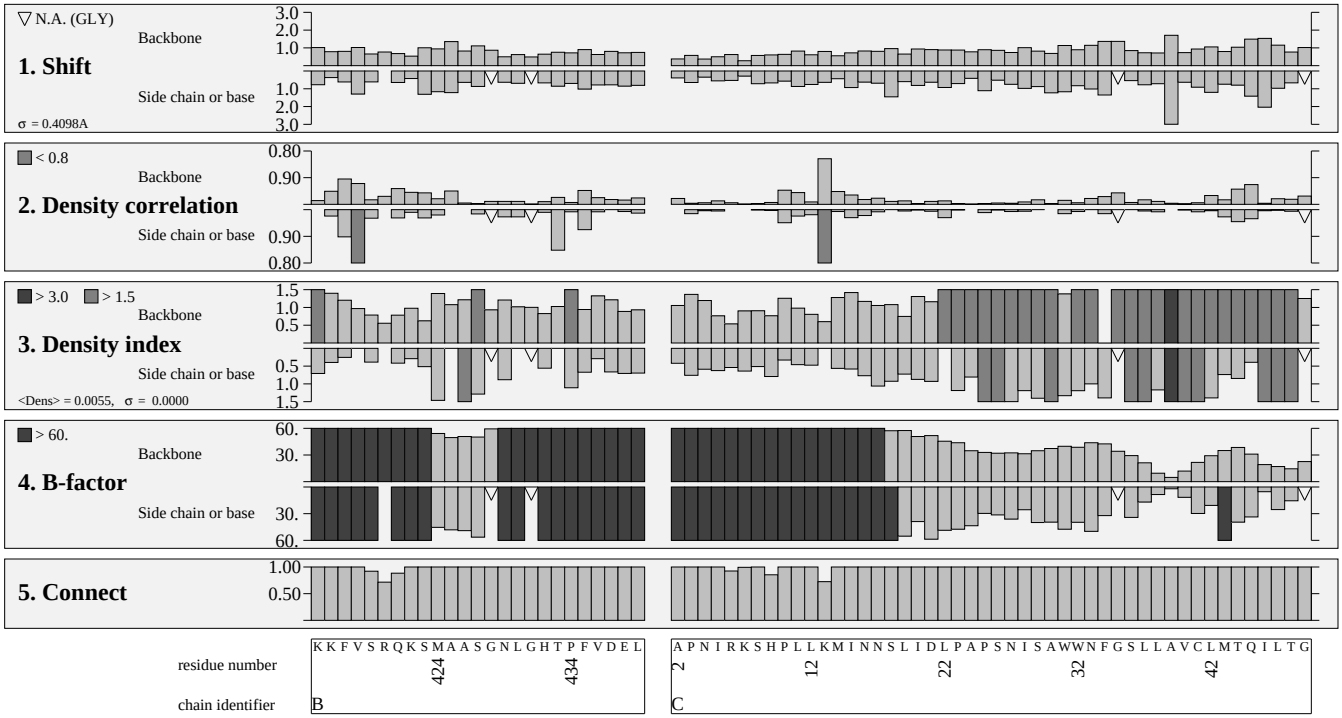
Structure Factor Check

2BCC

Local estimation (6)





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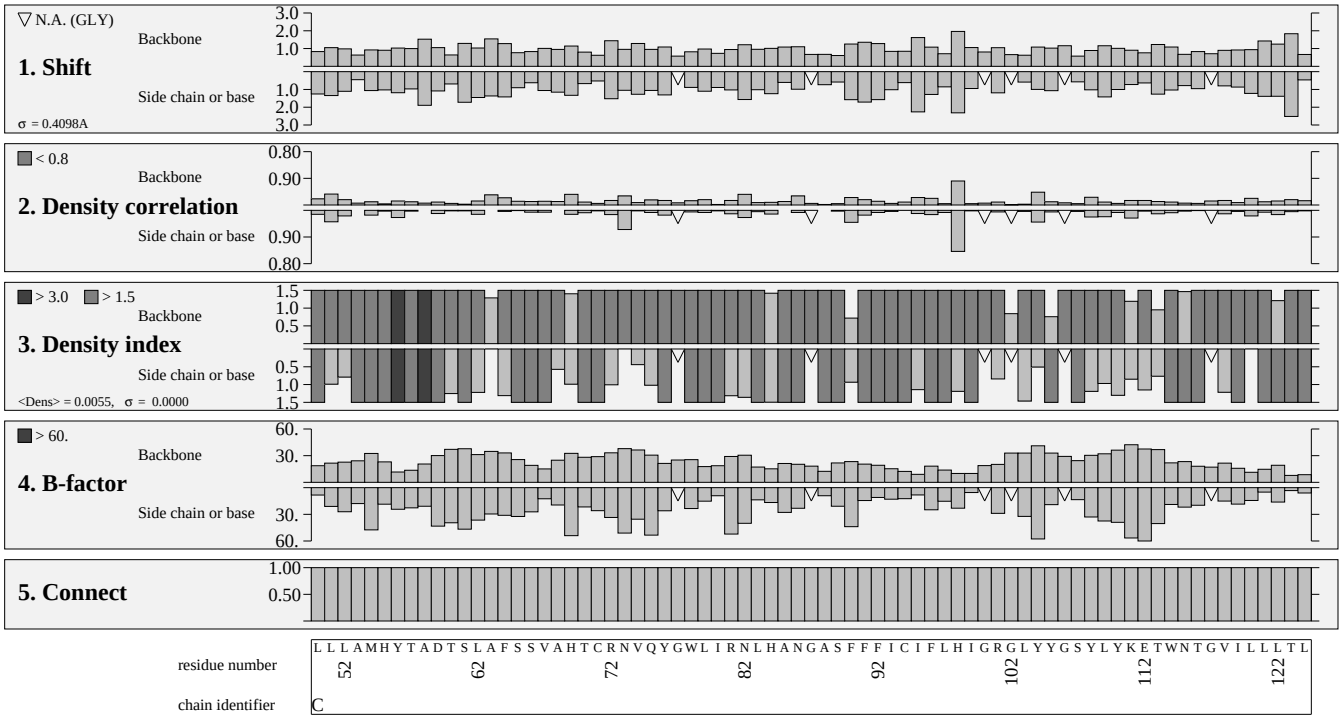
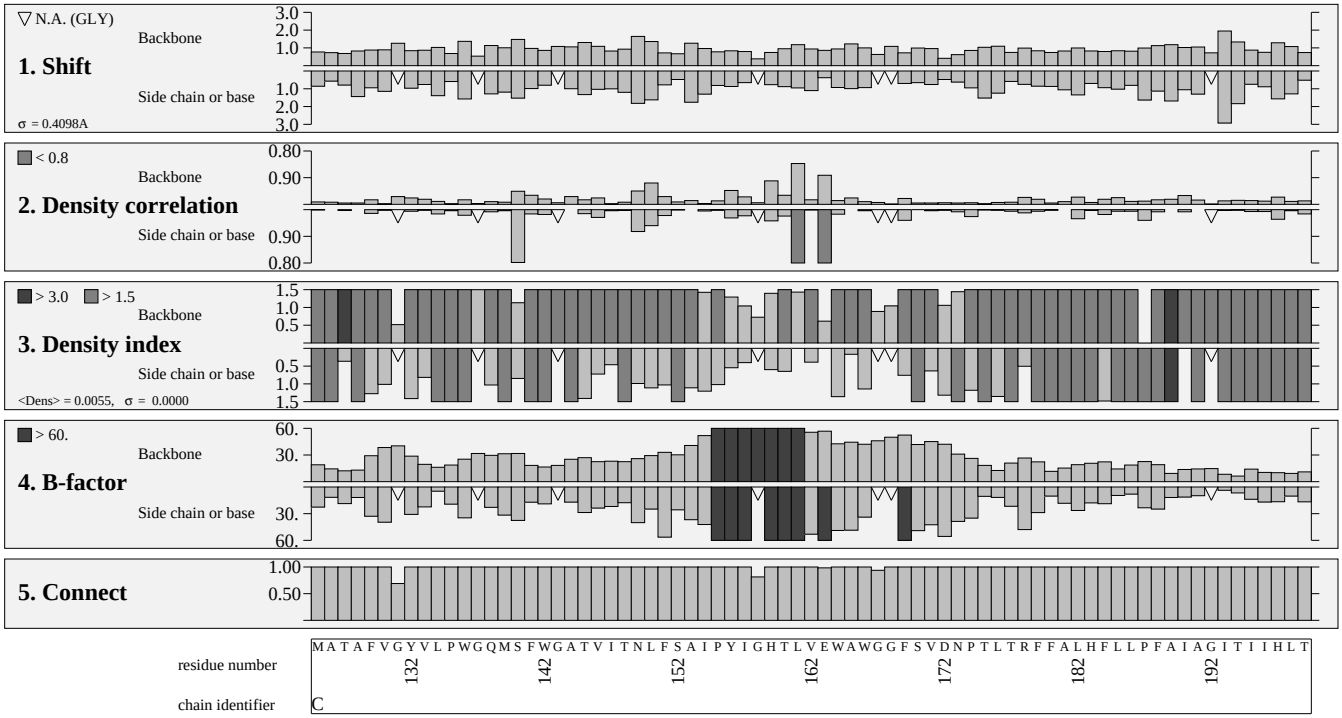
Structure Factor Check

2BCC

Local estimation (7)





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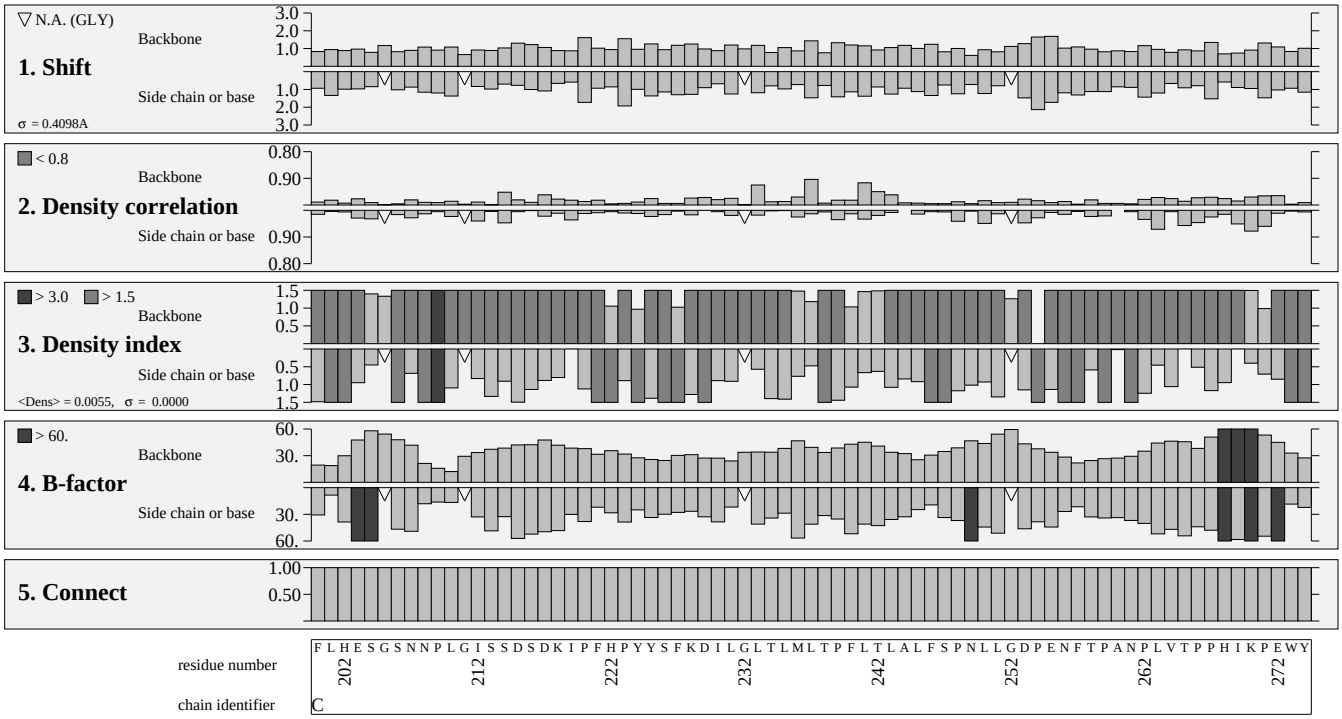
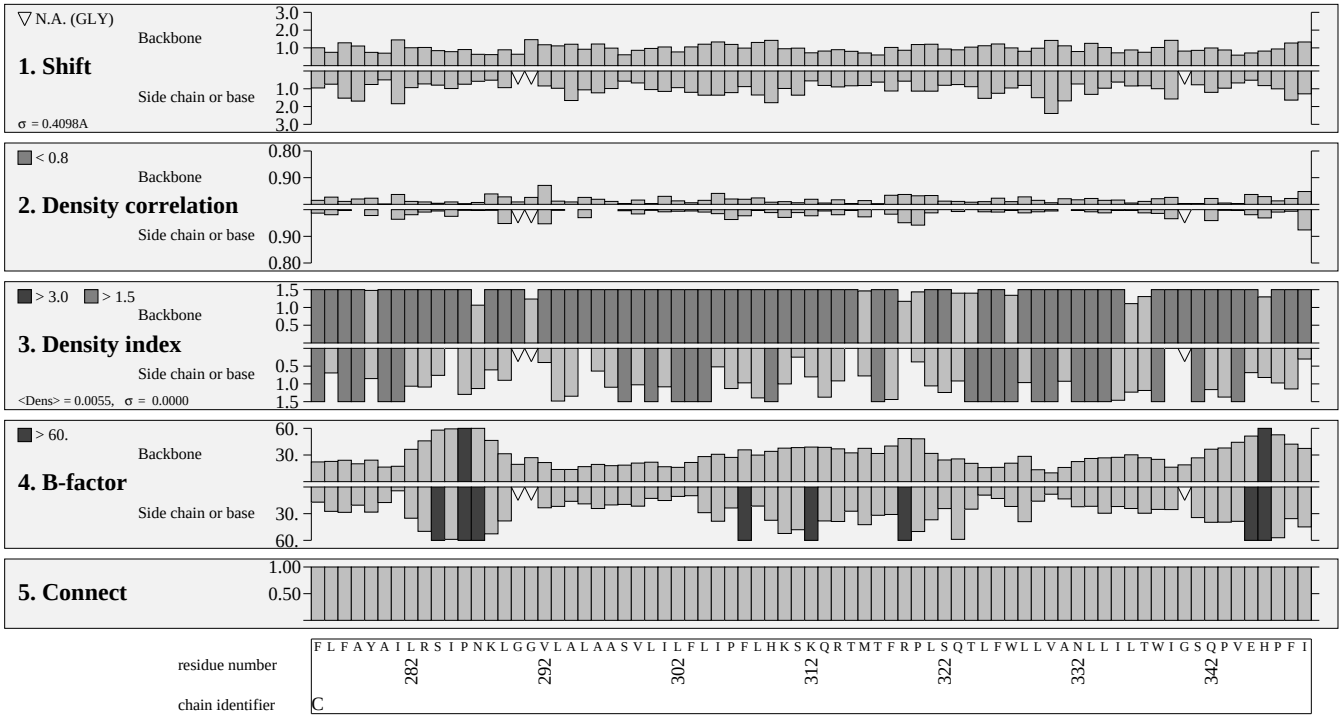
Structure Factor Check

2BCC

Local estimation (8)





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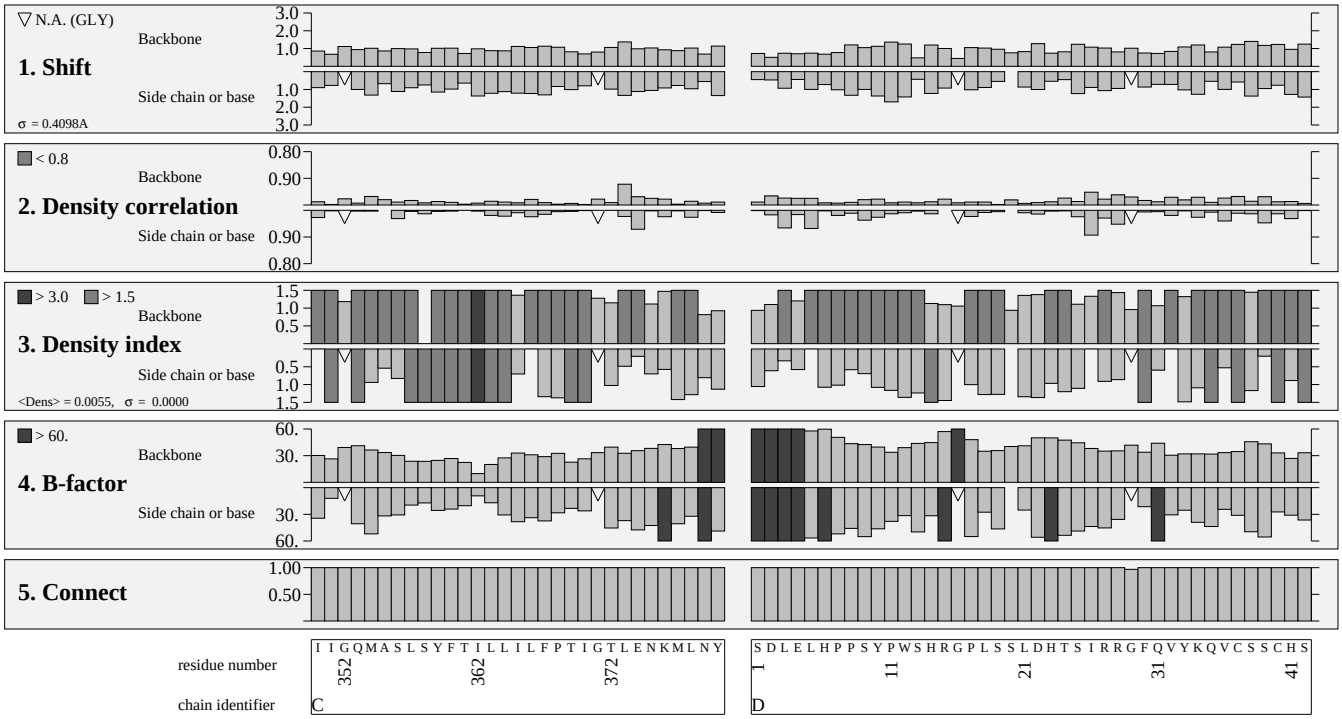
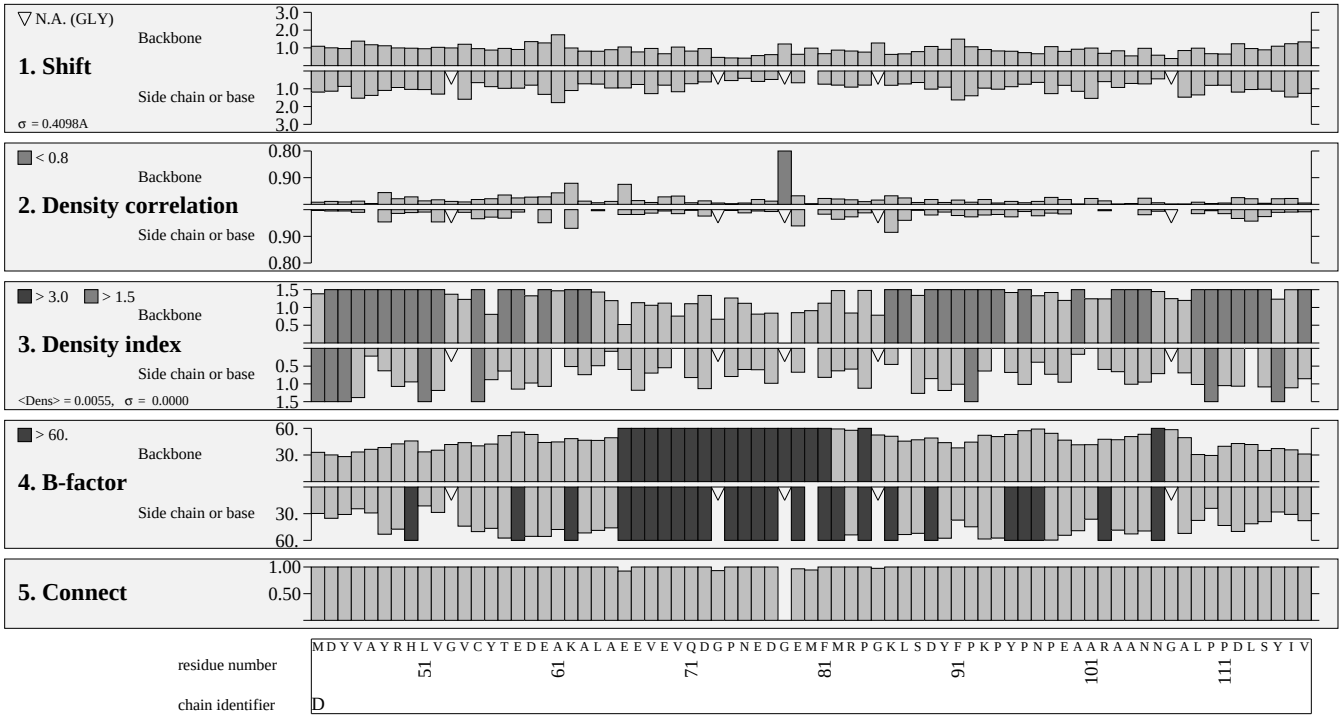
Structure Factor Check

2BCC

Local estimation (9)





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Structure Factor Check

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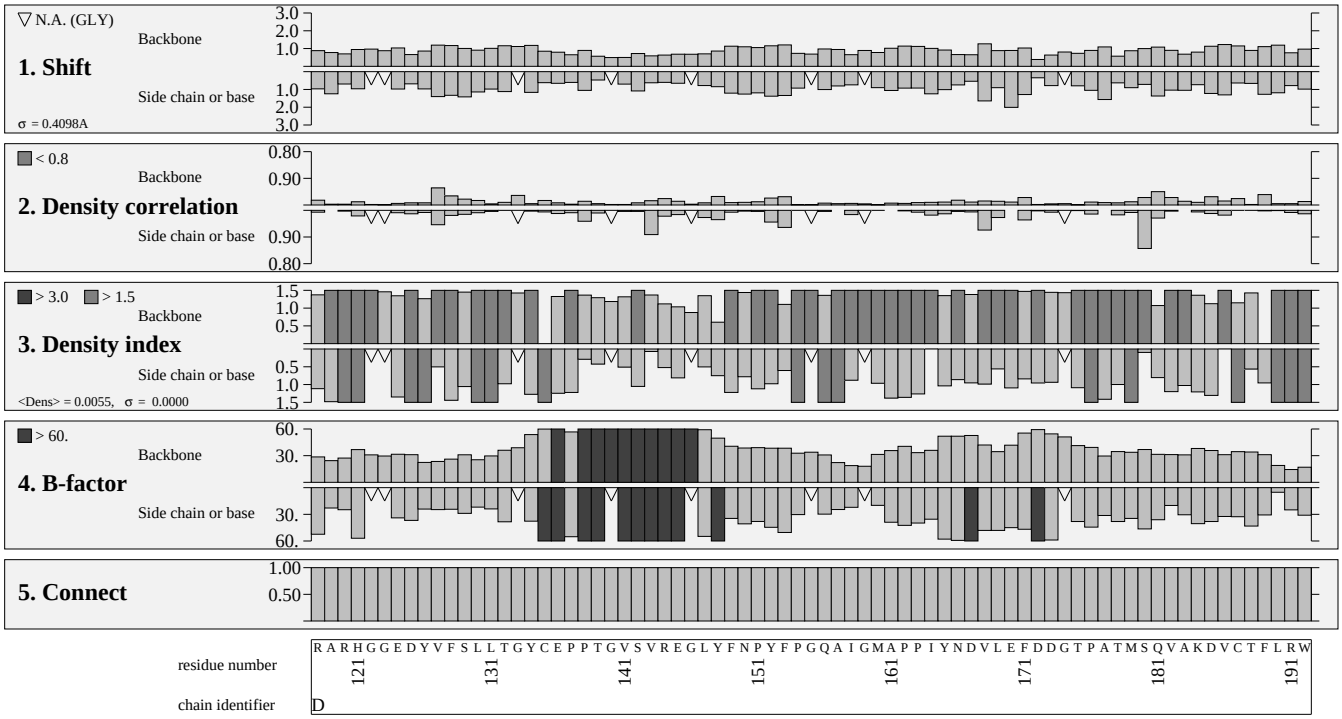
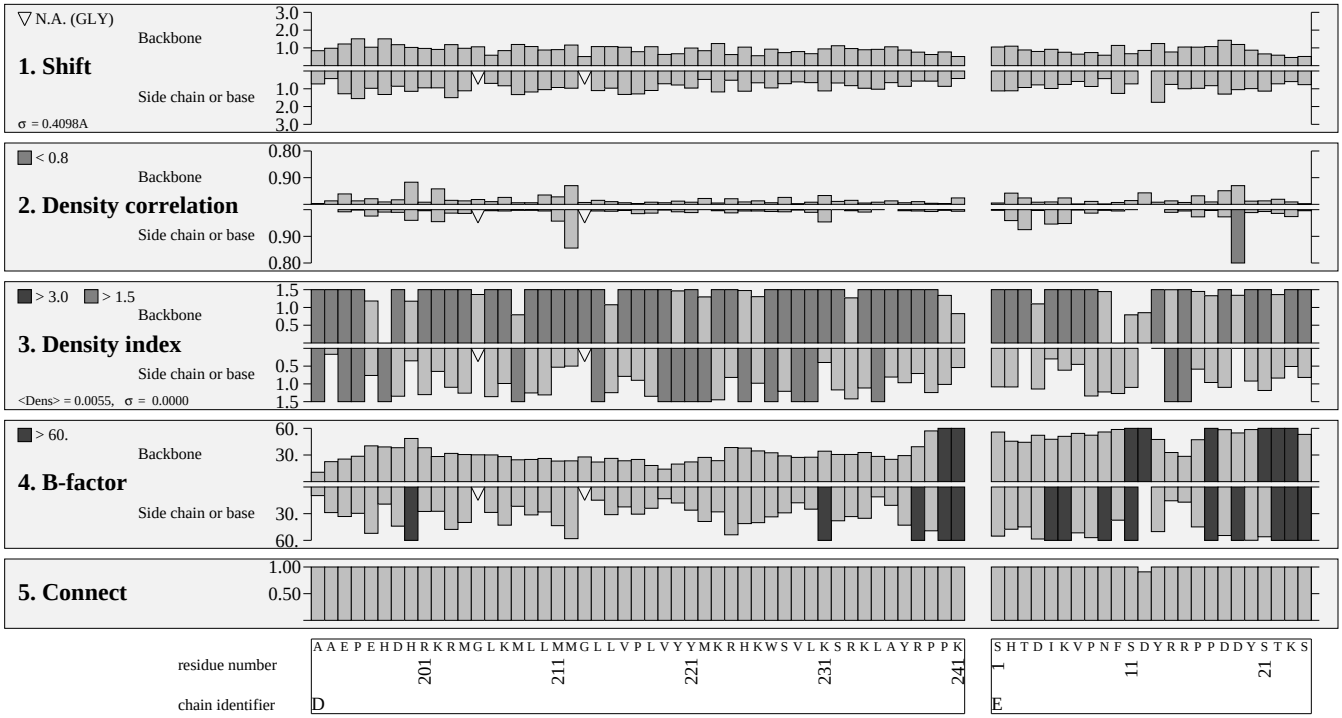
Local estimation (10)





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Structure Factor Check

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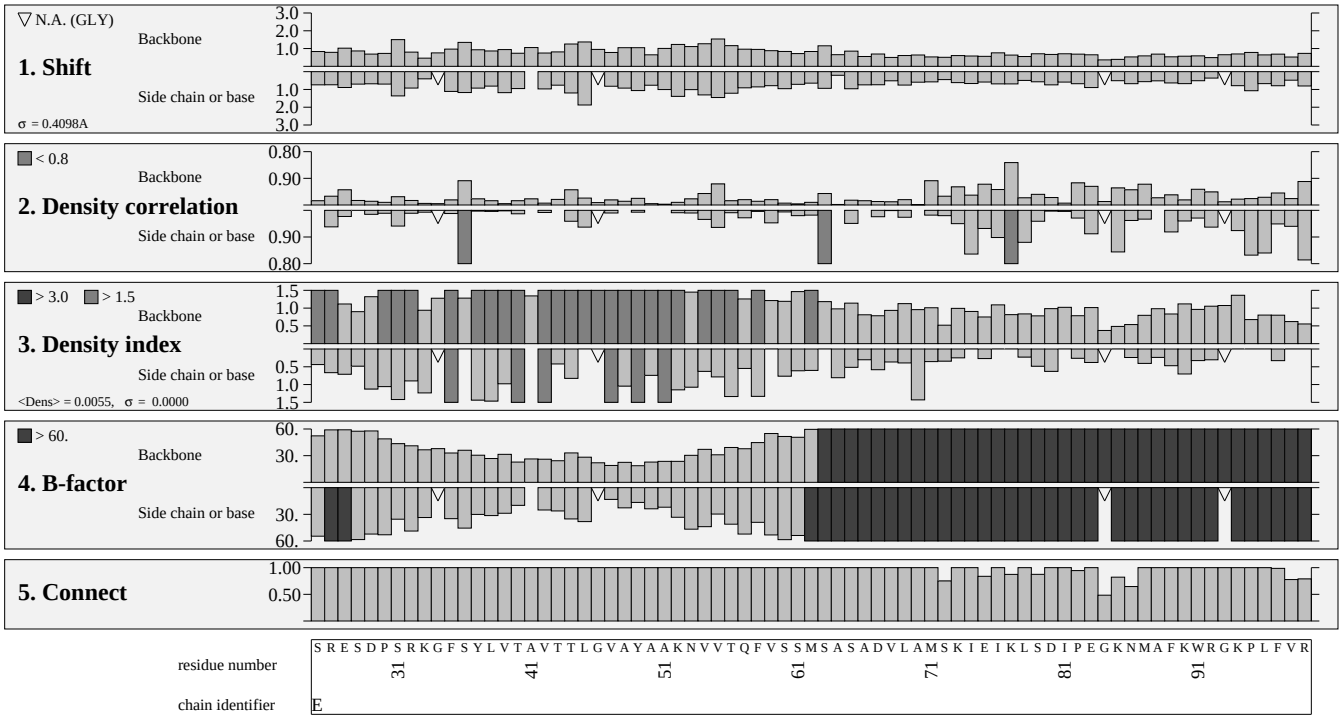
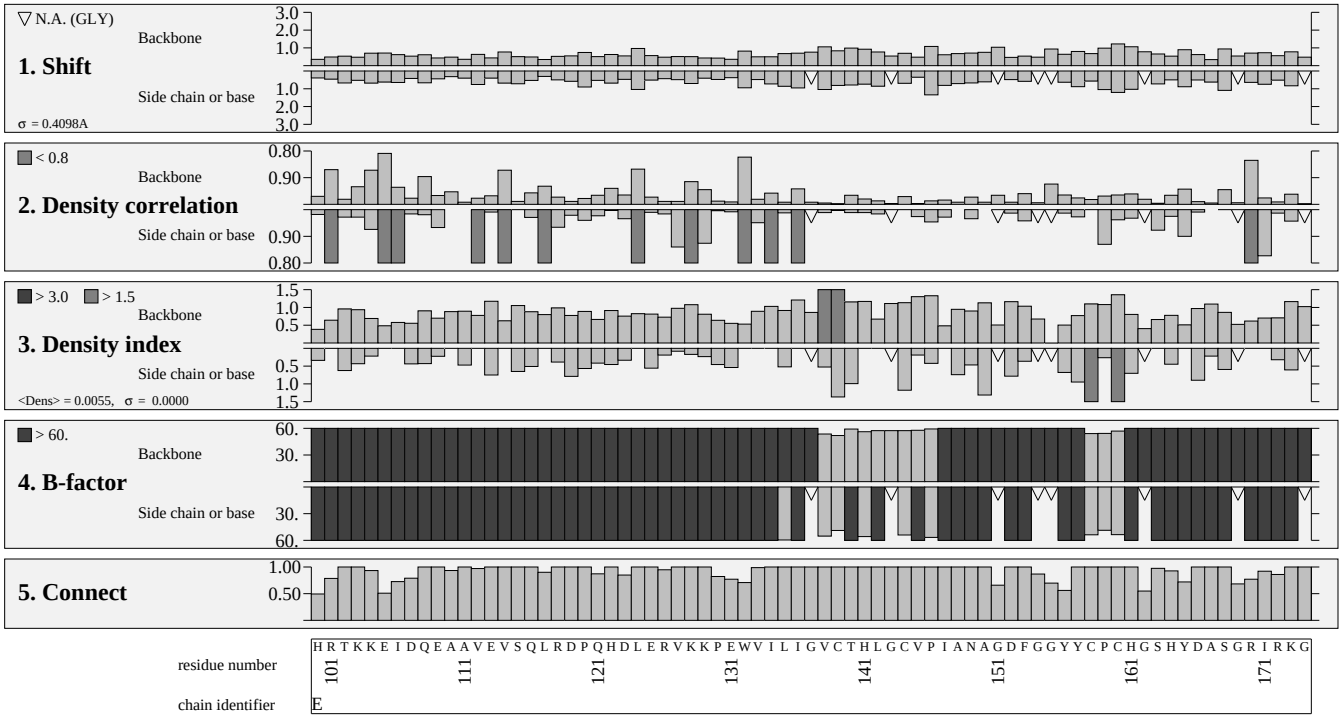
Local estimation (11)





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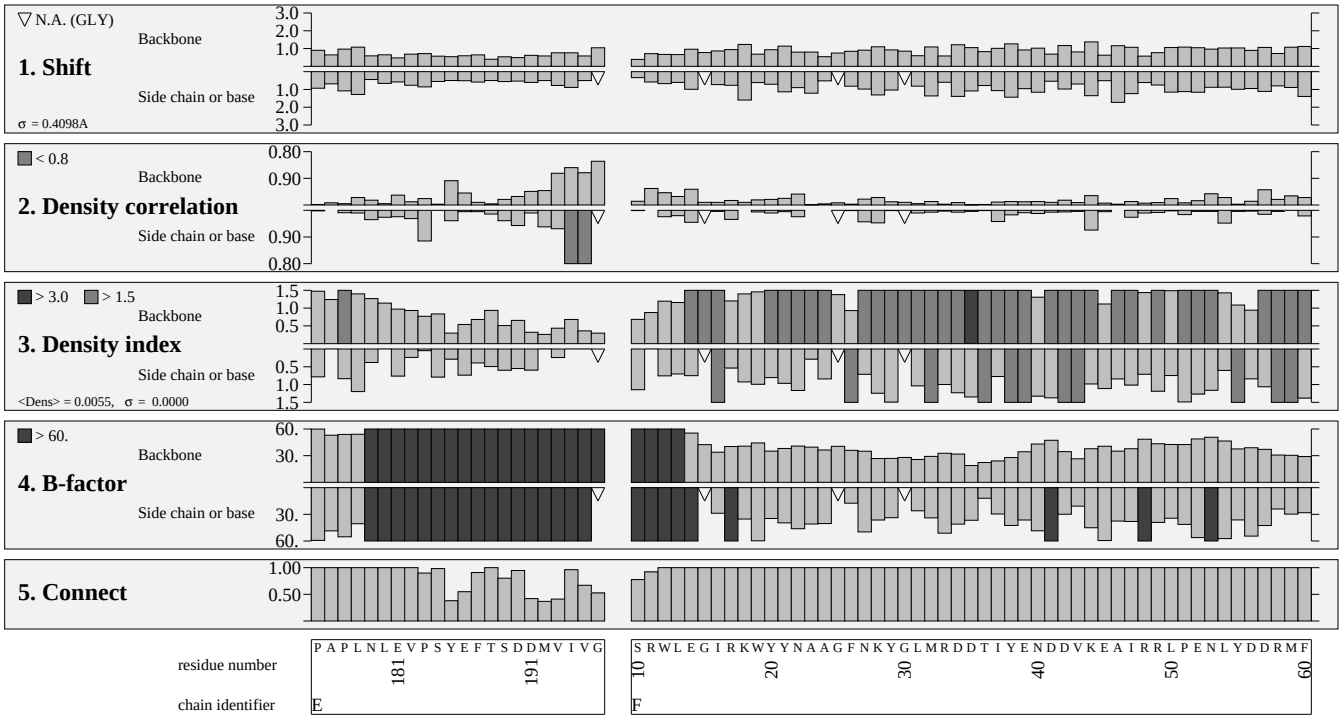
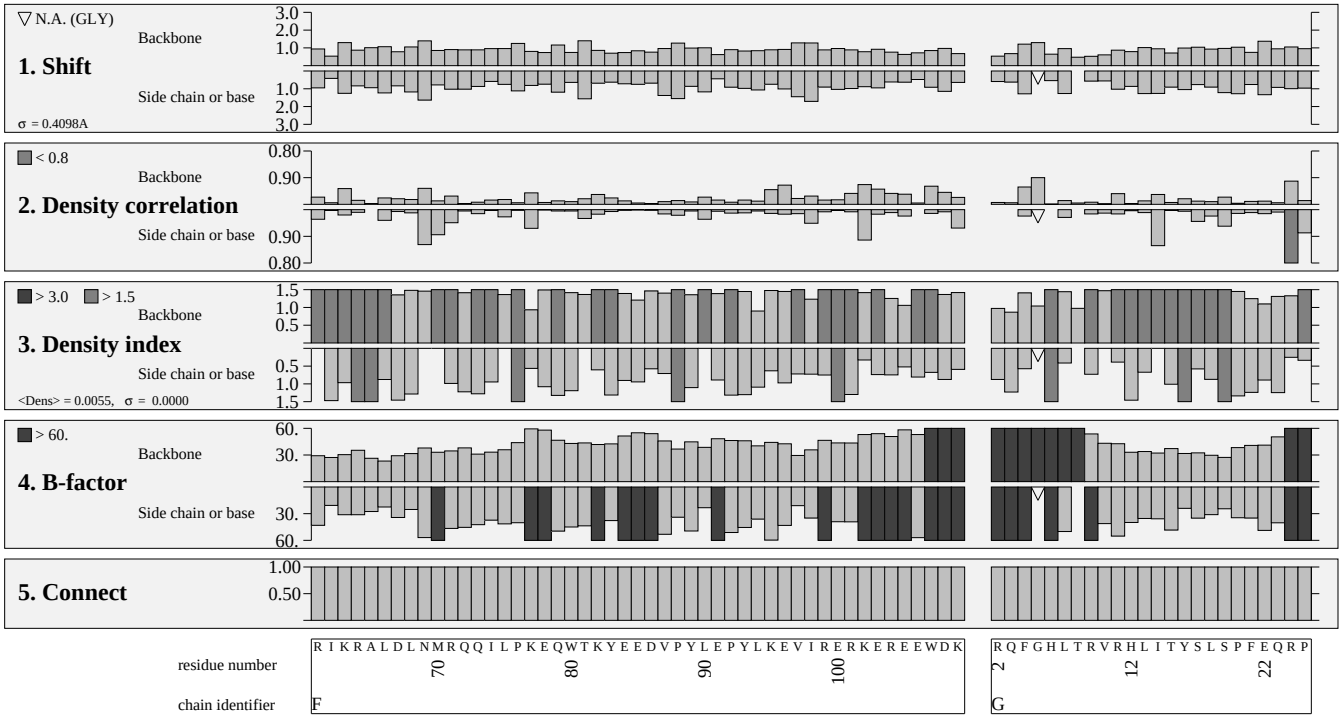
Structure Factor Check

2BCC

Local estimation (12)





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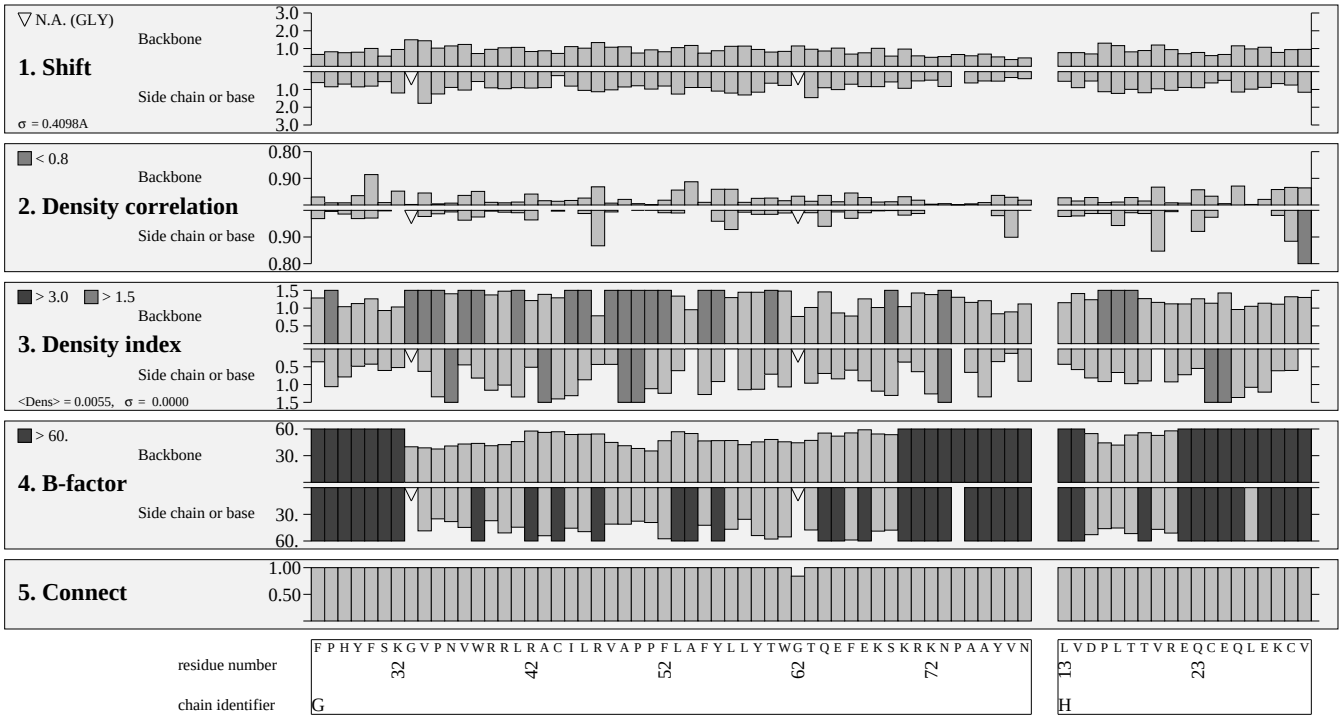
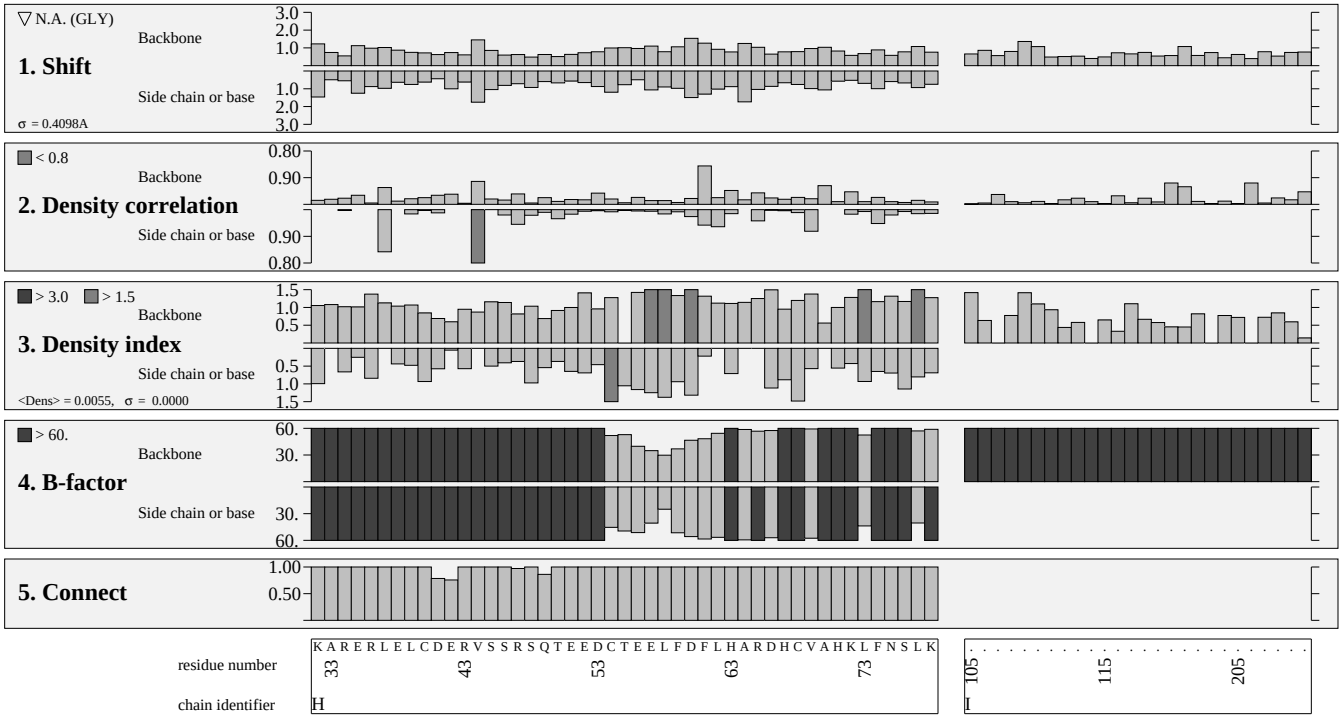
Structure Factor Check

2BCC

Local estimation (13)





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Structure Factor Check

2BCC

Local estimation (14)