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

Structure Factor Check

2FBW

Title: AVIAN RESPIRATORY COMPLEX II WITH CARBOXIN BOUND
Date: 10−DEC−05
PDB code: 2FBW

Crystal

Cell parameters:

a: 118.70 A b: 200.75 A c: 67.63 A
α: 90.00 β: 90.06 γ: 90.00

Space group: P 1 21 1

Model

19494 atoms (2000 water molecules)

Number of chains:	51
Volume not occupied by model:	46.8 %
<B> (for atomic model):	30.4 A^2
σ(B):	14.95 A^2
Matthews coefficient:	2.95
Corresponding solvent % :	58.01

Refinement

Program:	CNS 1.1
Nominal resolution range:	64.1 − 2.10 A
Reported R−factor:	0.187
Number of reflections used:	162208
Reported Rfree:	0.23
Sigma cut−off:	N.A.

Structure Factors

Input

Nominal resolution range:		64.1 − 2.05 A
Reflections in file:		166892
Unique reflections	above 0:	166892
	above 1σ:	166666
	above 3σ:	153945

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Nominal resolution range: 64.1 − 2.10 A
\05max. from input data, min. from author\05

Used reflections:	162211
Reflections out of resolution:	4681
Completeness:	88.3 %
R_stand(F) = <σ(F)>/<F> :	0.035

Anisotropic distribution of Structure Factors
ratio of eigen values: 0.7481 1.0000 0.6648

B_overall (by Patterson):	30.A^2
Optical resolution:	1.63 A
Expected opt. resol. for complete data set:	1.63 A
Estimated minimal error:	0.019 A

Model vs. Structure Factors

R−factor for all reflections:	0.193
Correlation factor:	0.935
R−factor:	0.198

for F > 2.0 σ
nom. resolution range: 64.09 − 2.10A
reflections used: 162012

Rfree:	0.235
Nfree:	8000
R−factor without free−refl.:	0.197
Non free−reflections:	154012
<u> (error in coords by Luzzati plot):	0.232 A
Estimated maximal error:	0.111 A
DPI:	0.166 A

Scaling

Scale:	1.056
Bdiff:	−0.67

Anisothermal Scaling (Beta):
−0.3776 2.1252 −0.5333 0.0000 −0.2013 0.0000

Solvent correction − Ks,Bs: 0.900 492.305

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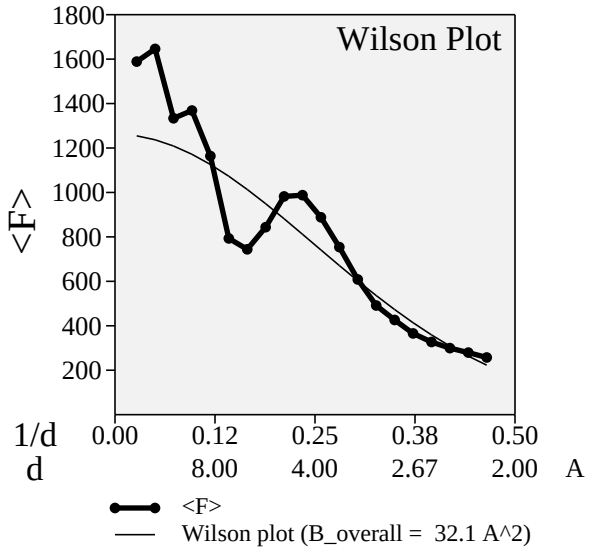
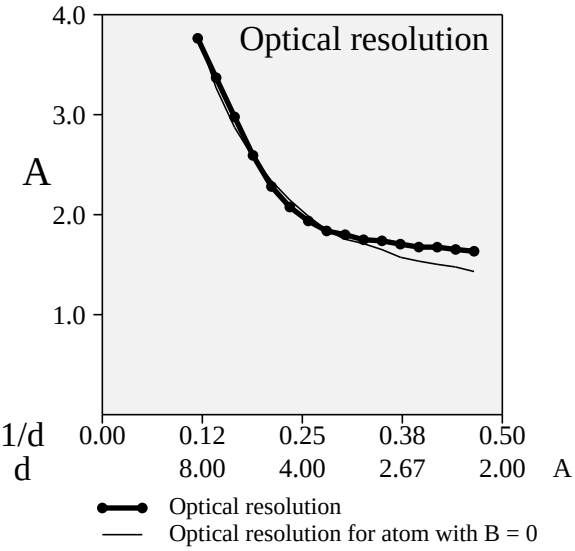
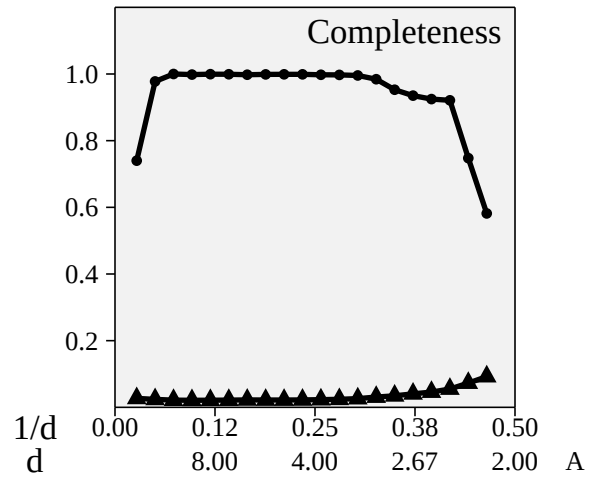


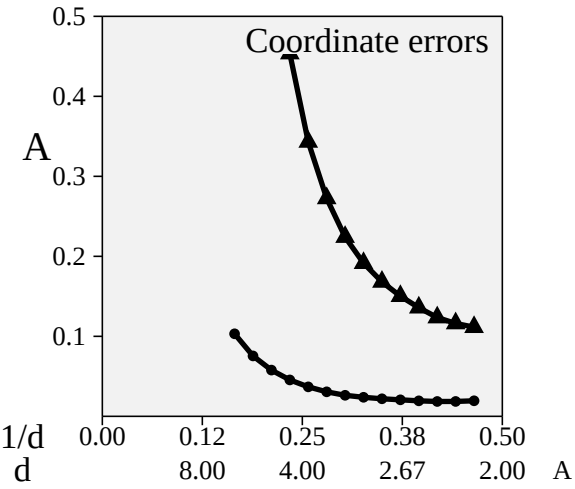
<F>
Wilson plot (B_overall = 32.1 A^2)



Optical resolution
Optical resolution for atom with B = 0

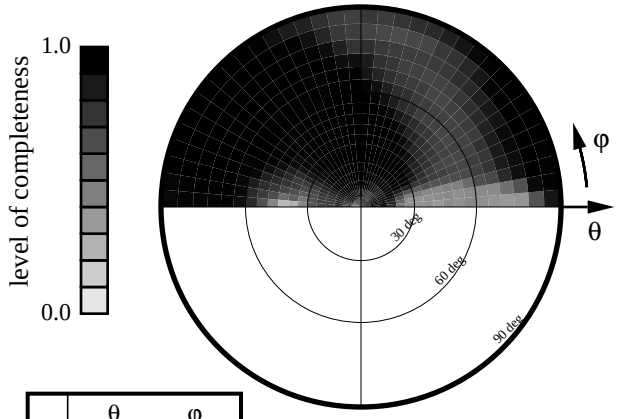


Completeness
R_stand(F) = <σ(F)>/<F>



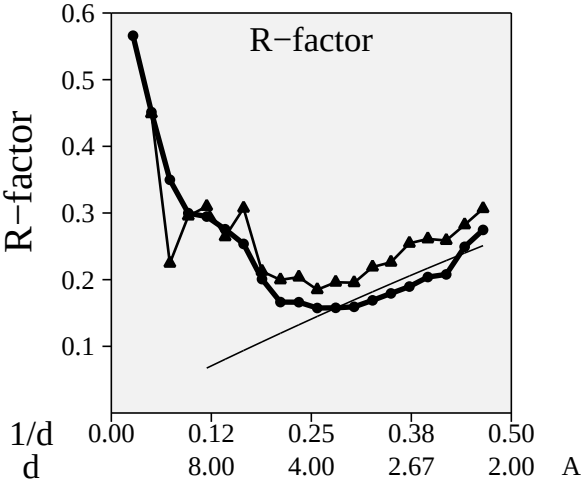
Expected maximal coordinate error
Expected minimal coordinate error

Stereographic projection of
the averaged radial completeness



	θ	φ
h	89.94	0.00
k	90.00	90.00
l	0.00	0.00

polar coordinates of the
crystallographical axes



R−factor
Rfree
Luzzati plot drawn for an atomic error = 0.232

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Structure Factor Check

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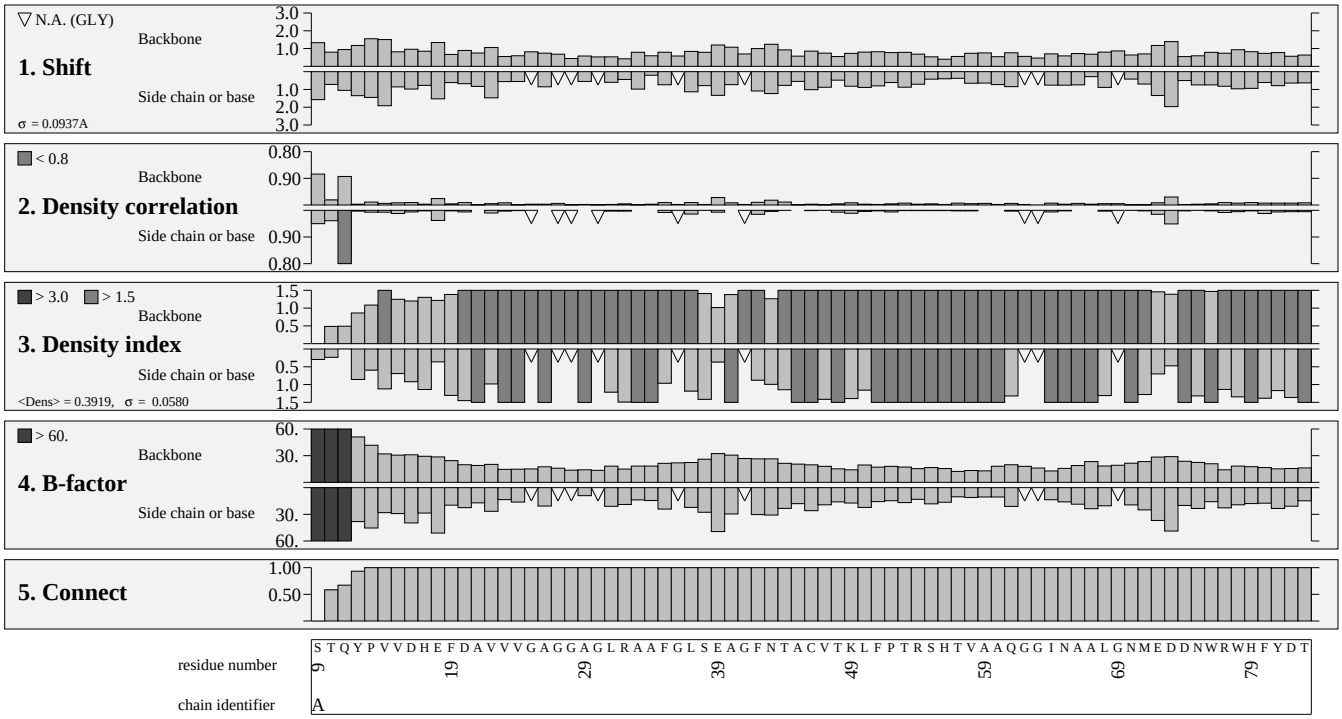
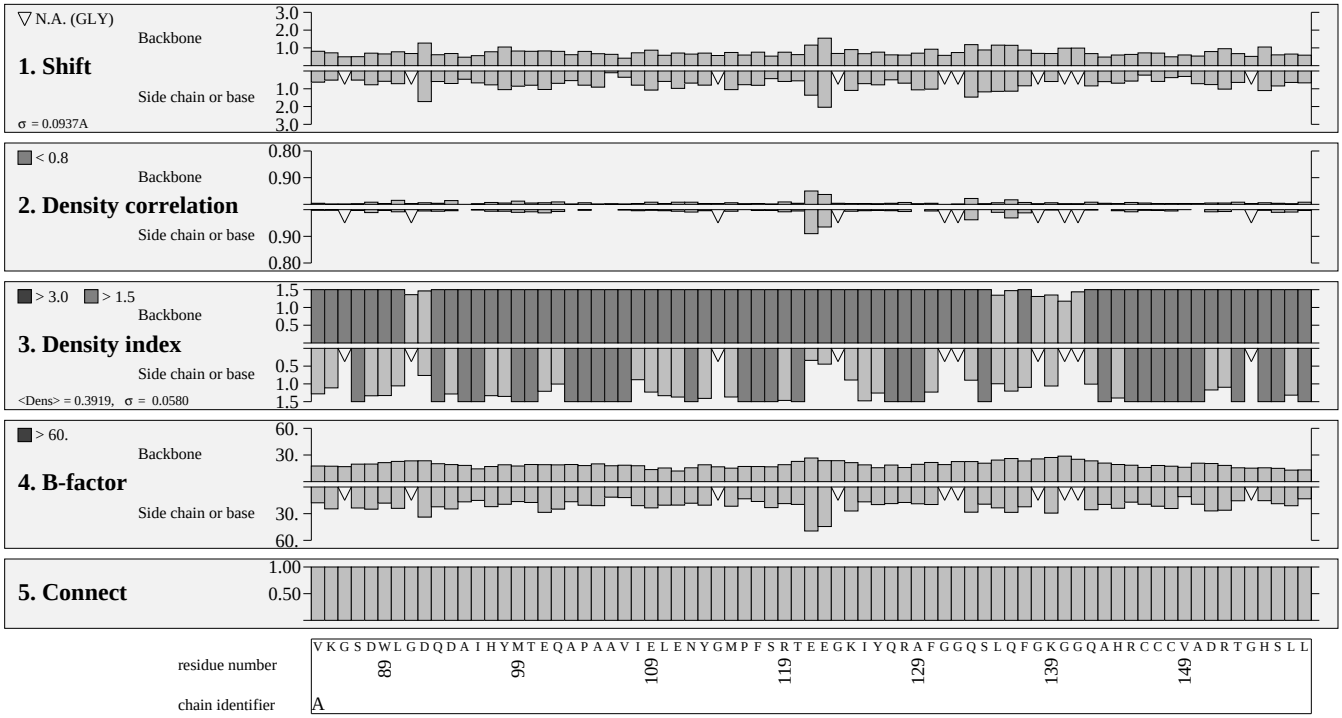
Local estimation





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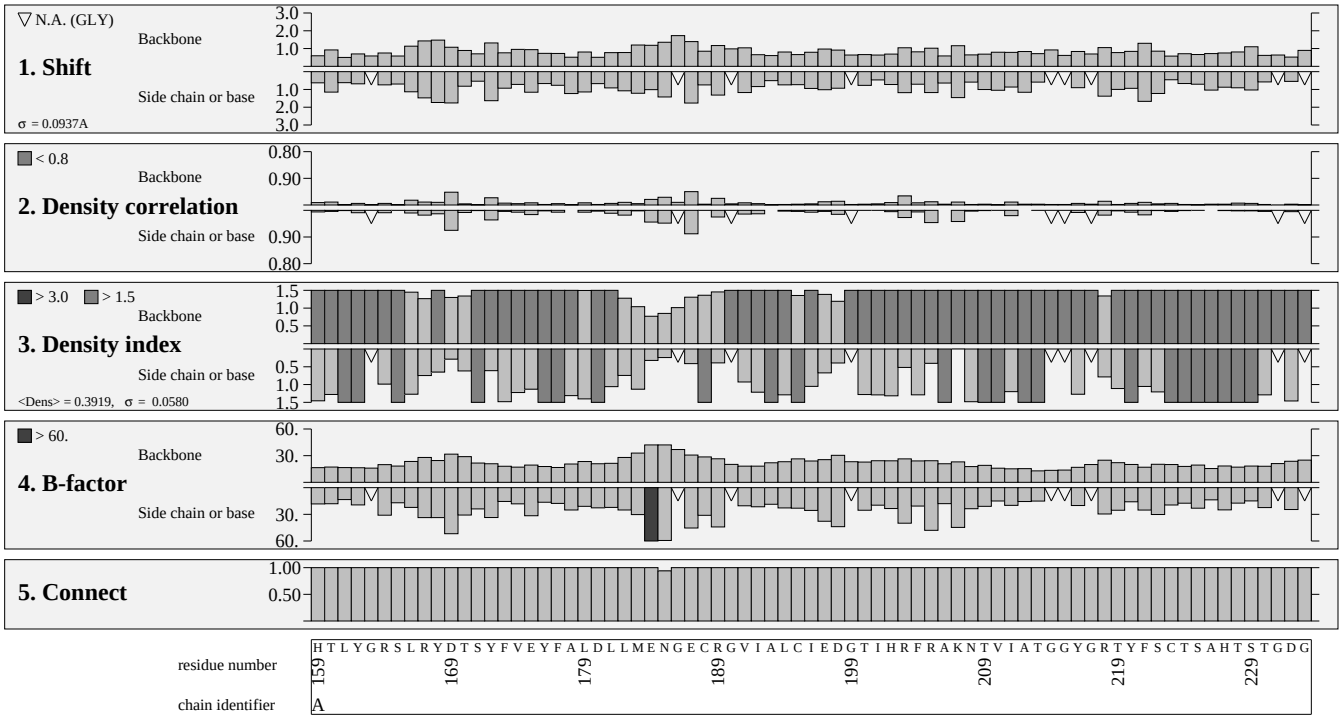
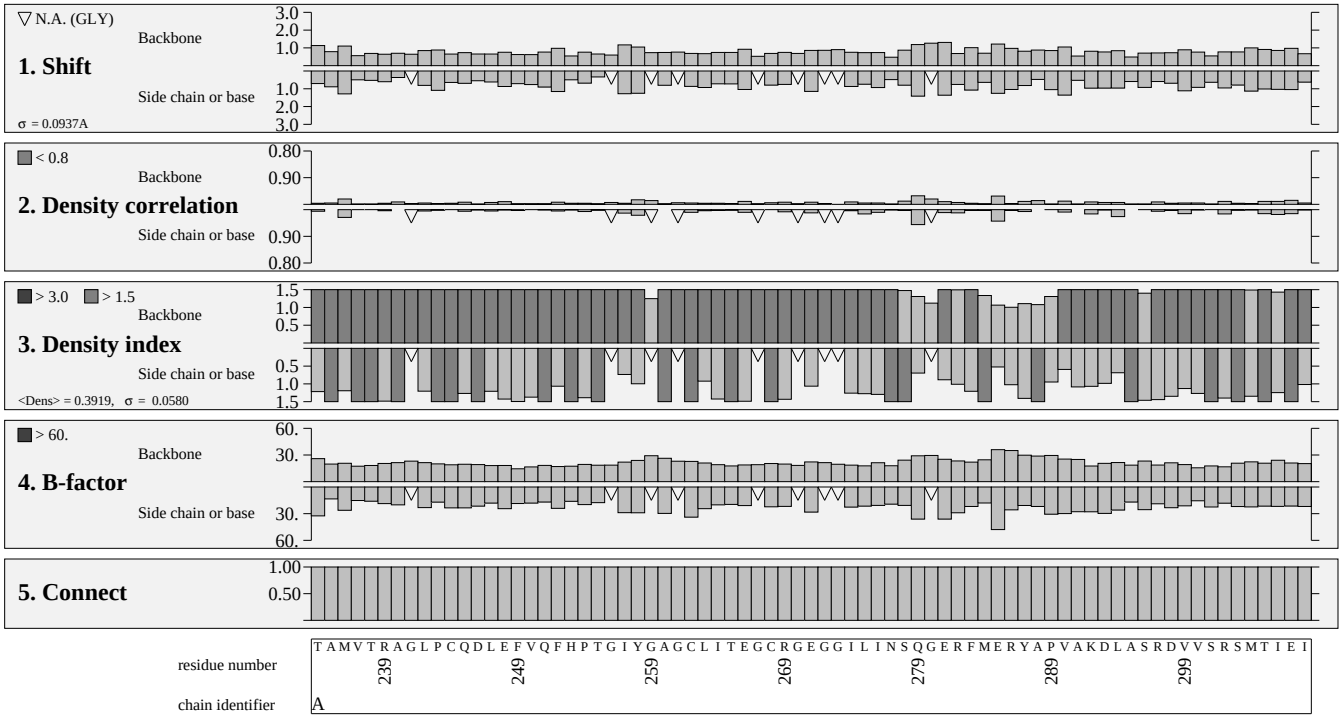
Structure Factor Check

2FBW

Local estimation (2)





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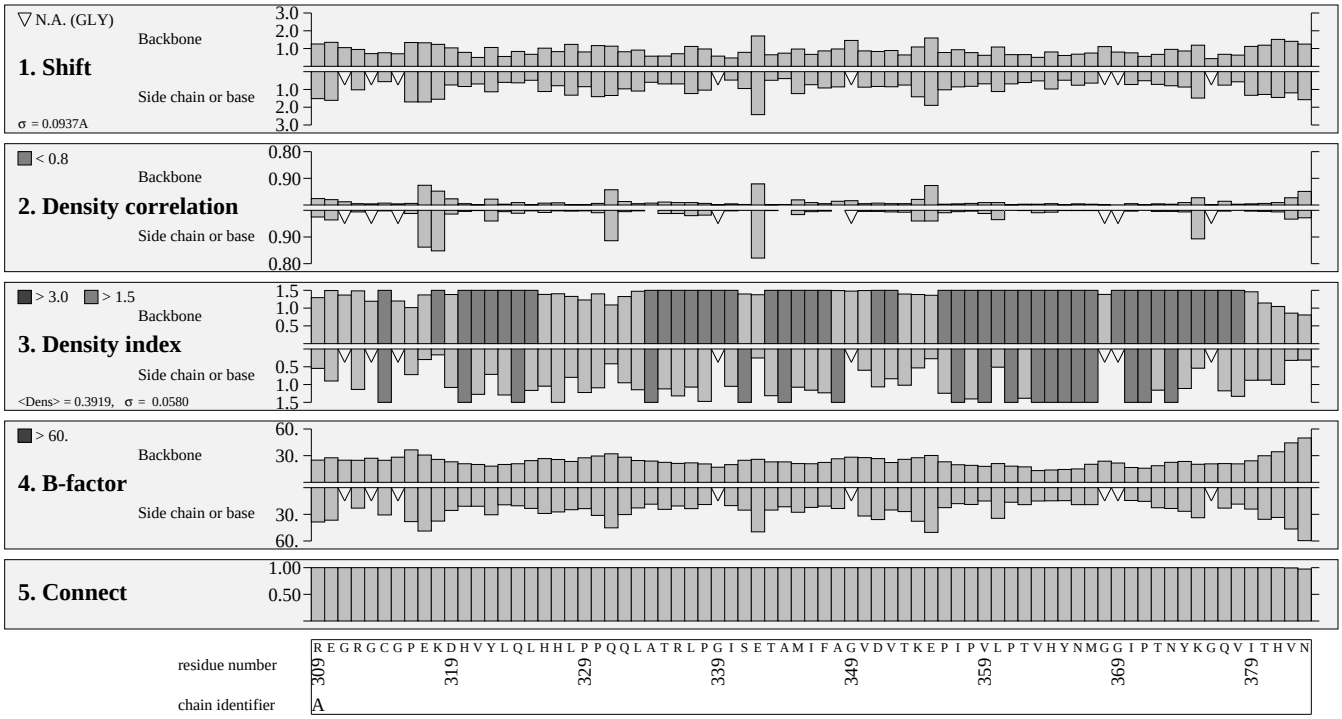
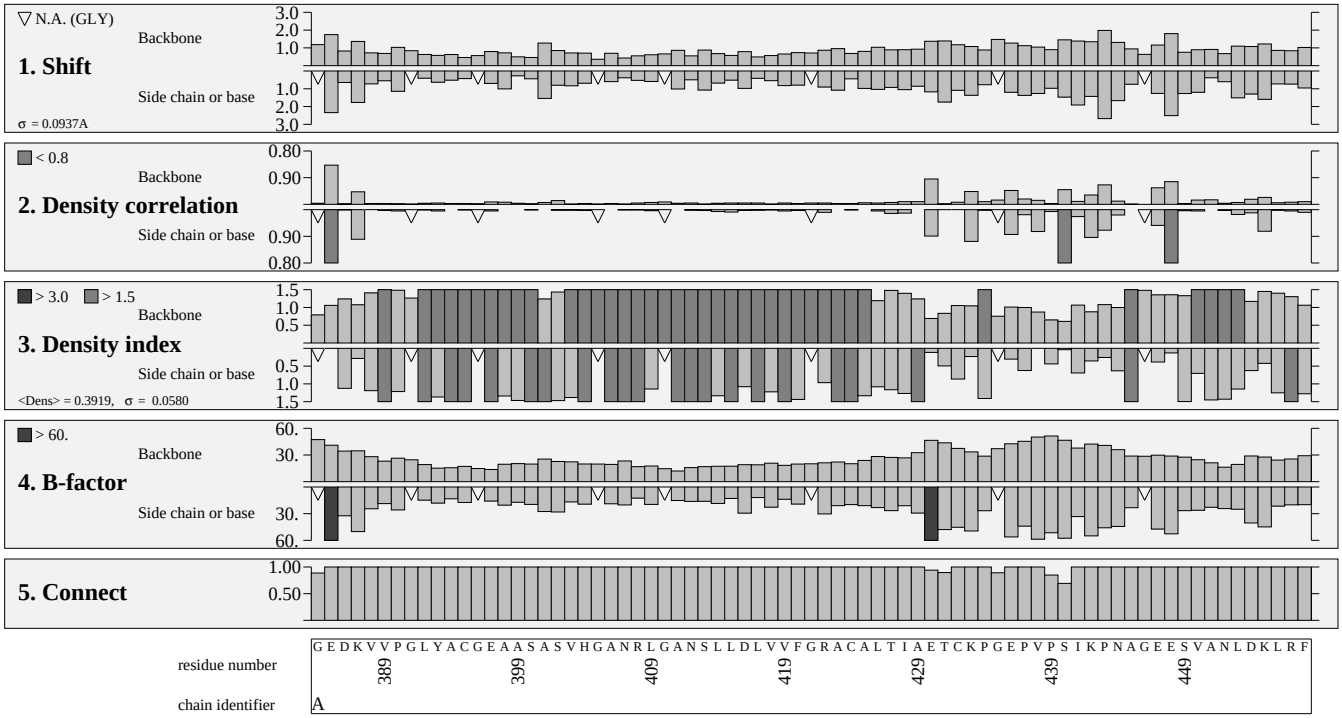
Structure Factor Check

2FBW

Local estimation (3)





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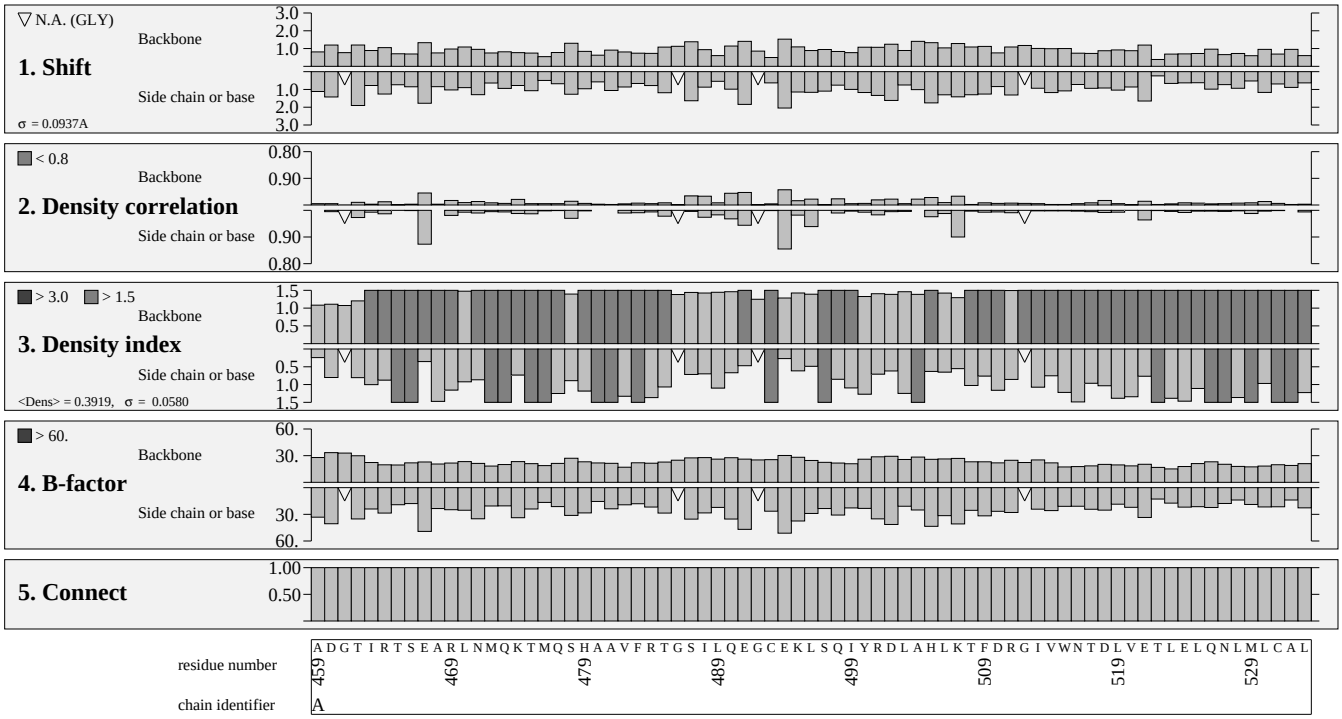
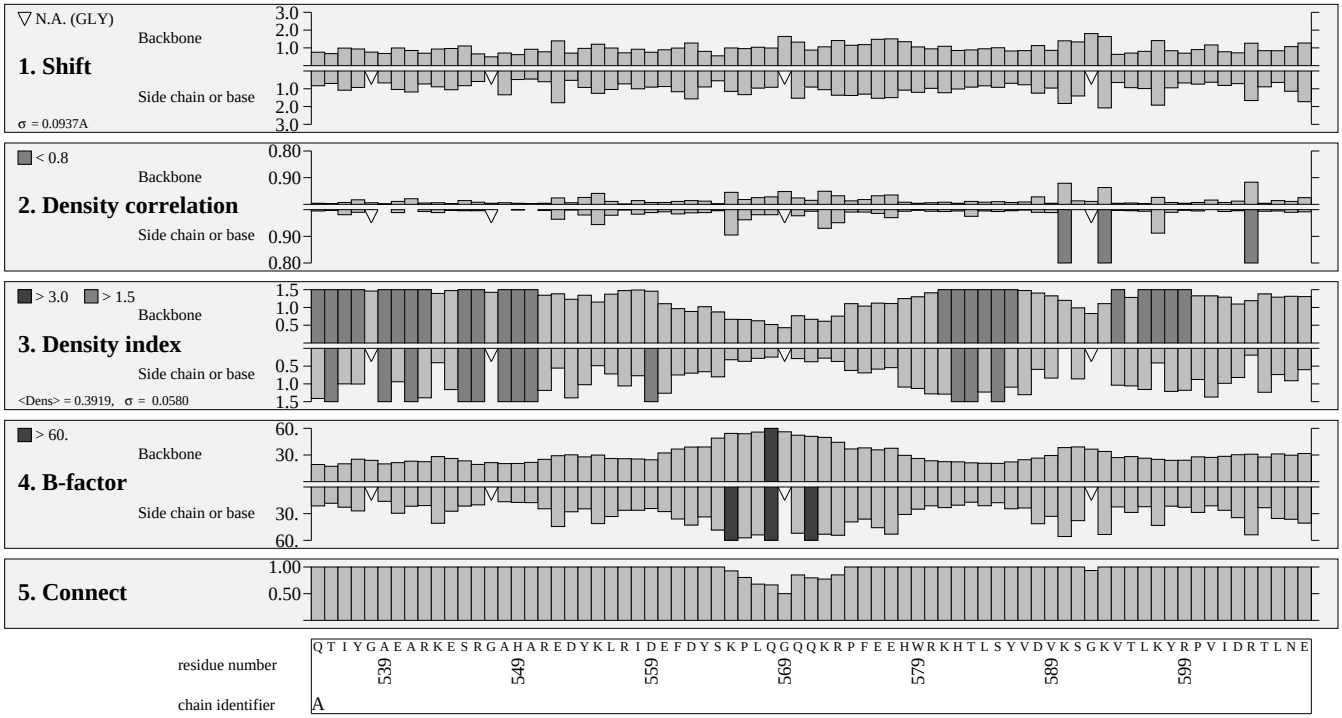
Structure Factor Check

2FBW

Local estimation (4)





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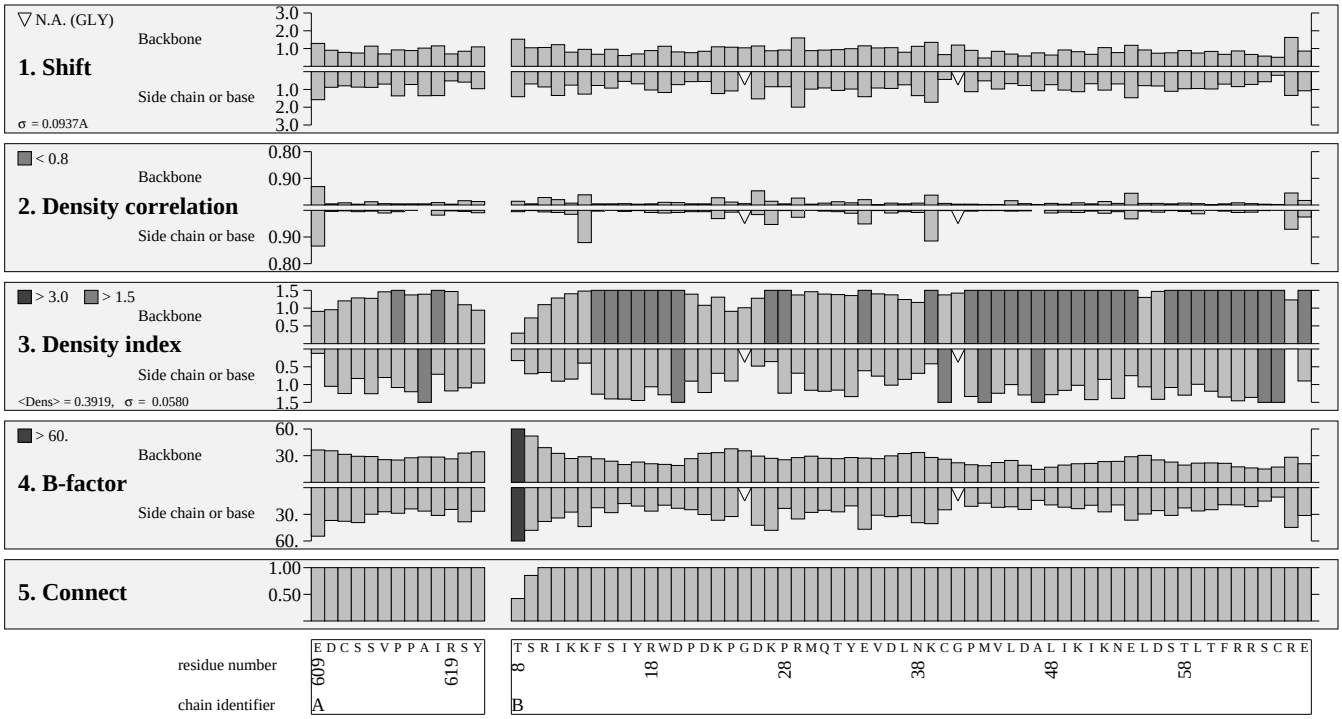
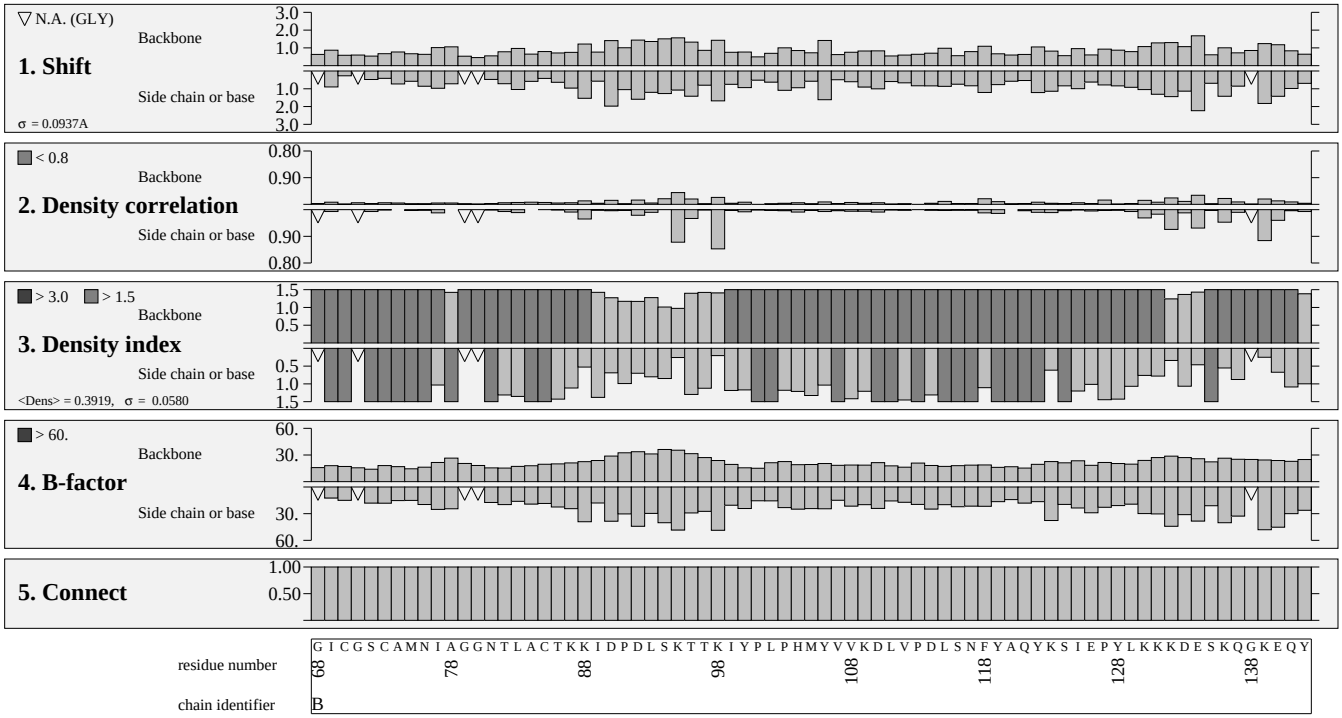
Structure Factor Check

2FBW

Local estimation (5)





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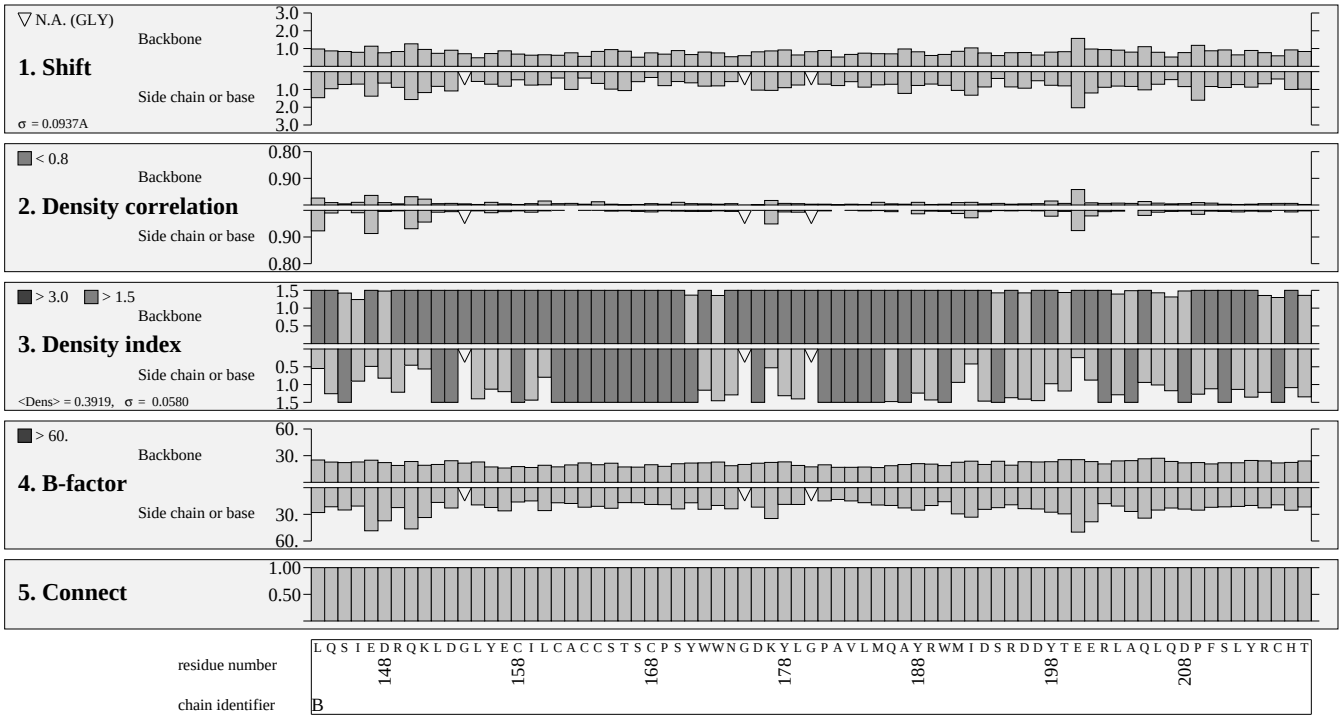
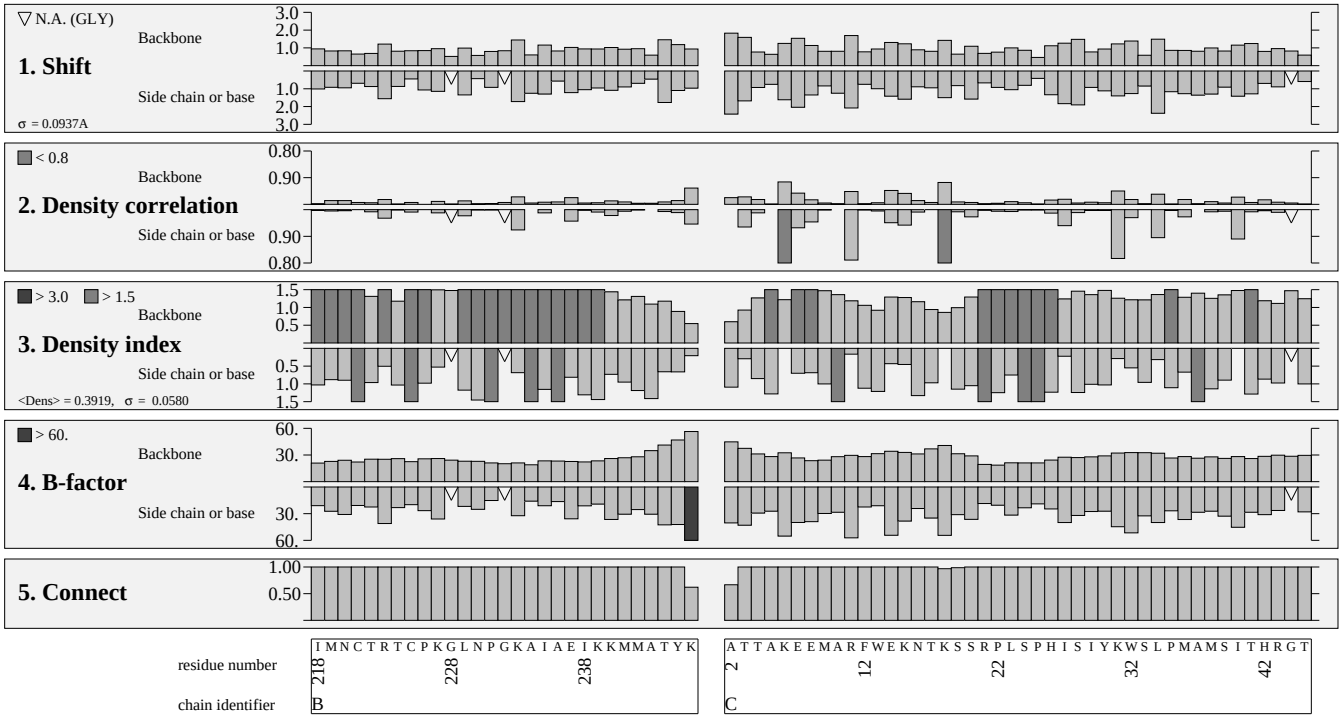
Structure Factor Check

2FBW

Local estimation (6)





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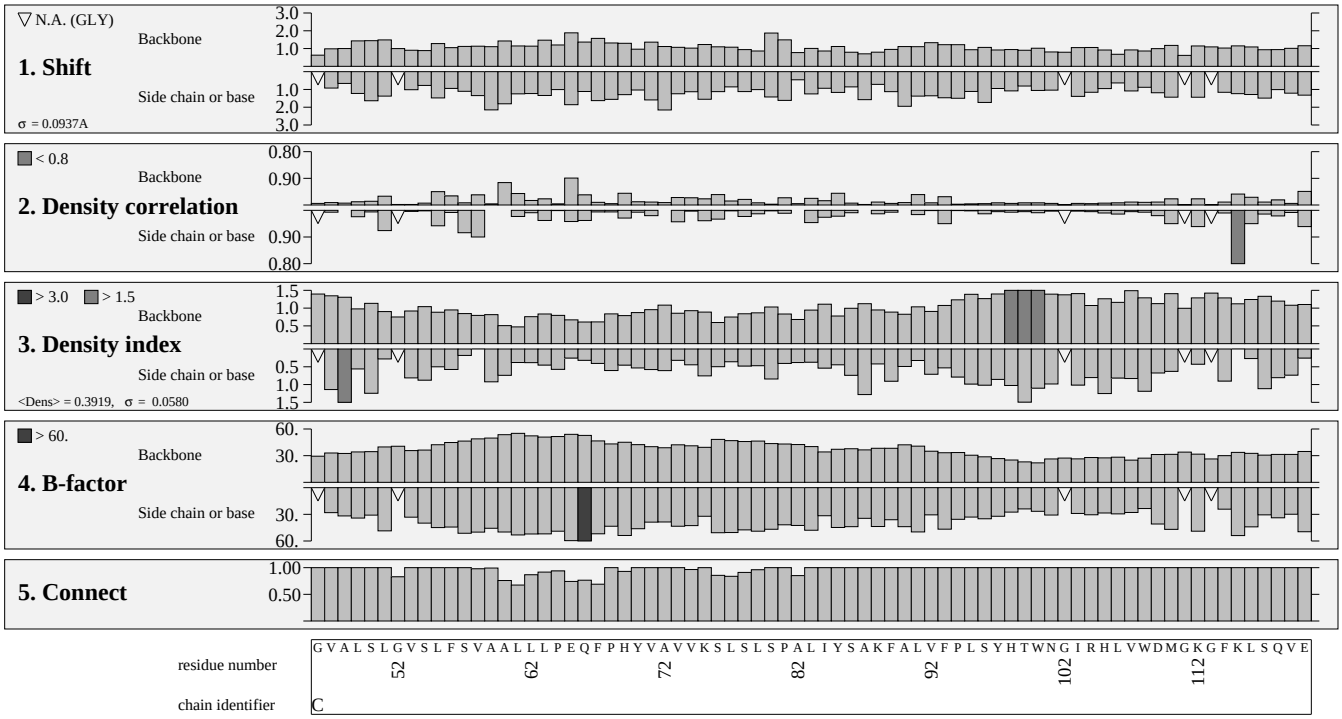
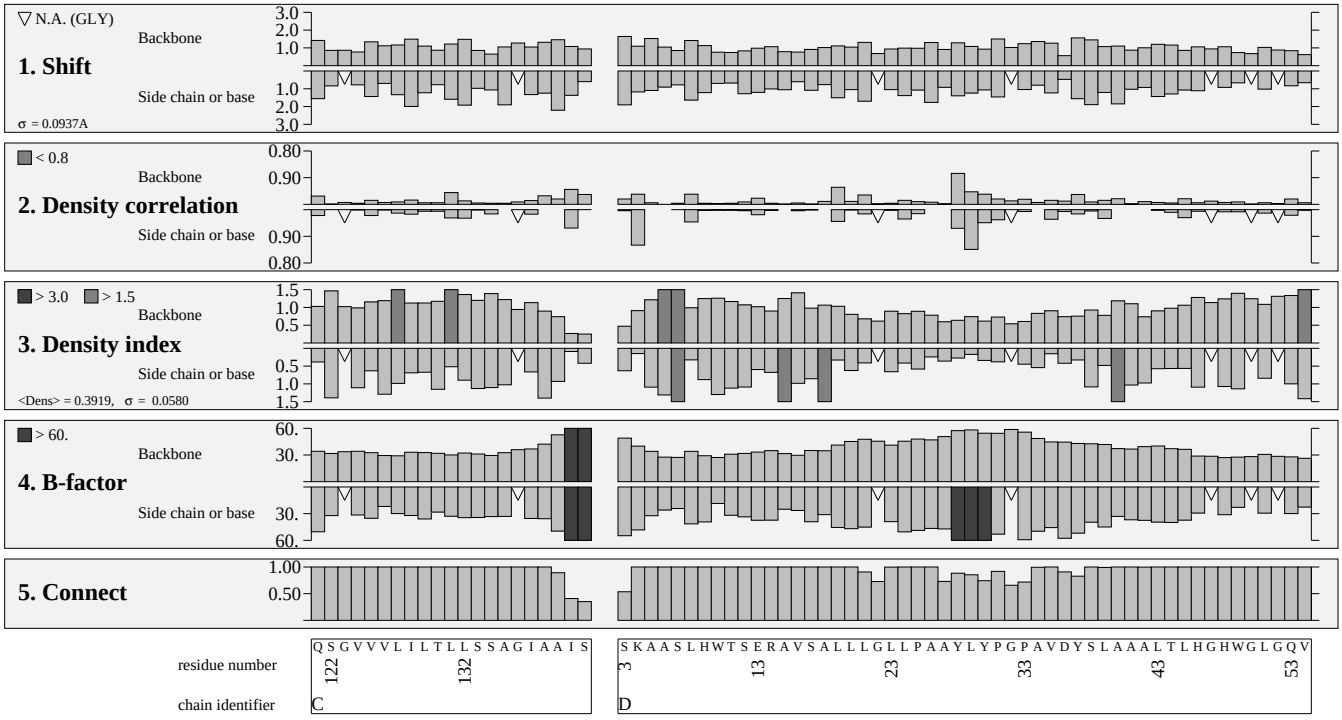
Structure Factor Check

2FBW

Local estimation (7)





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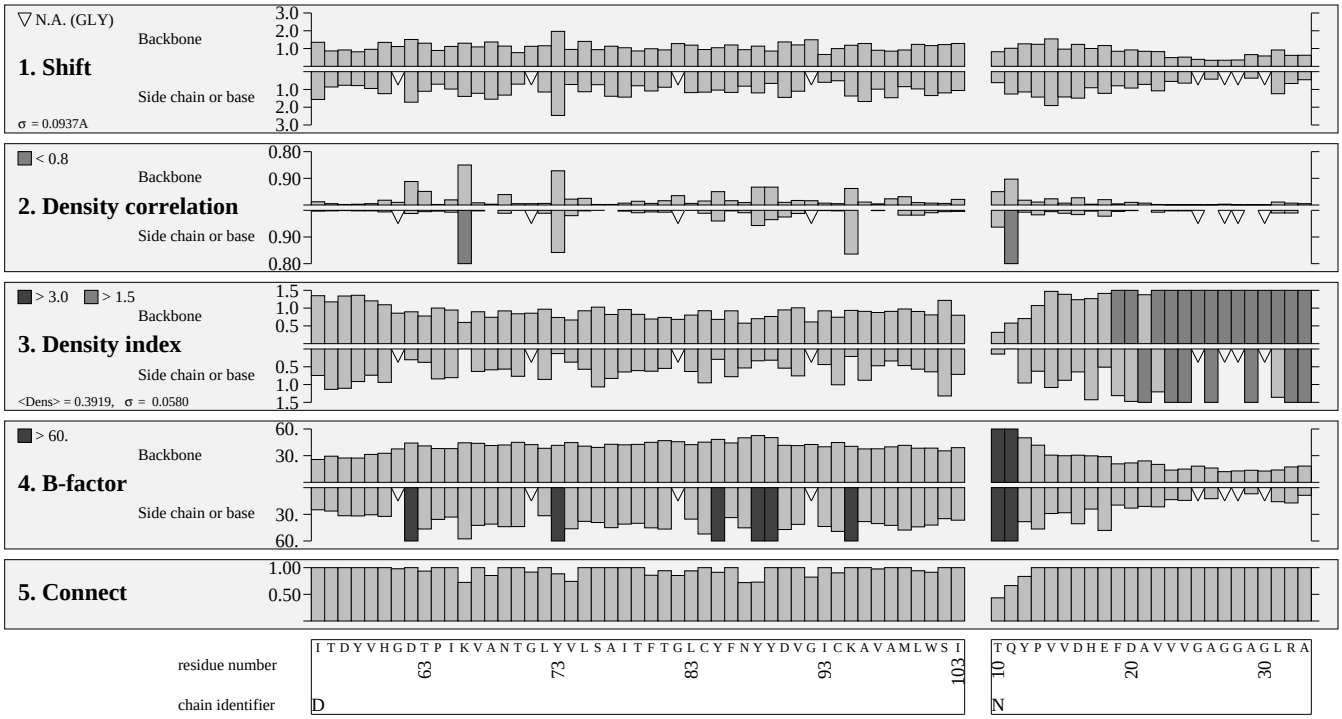
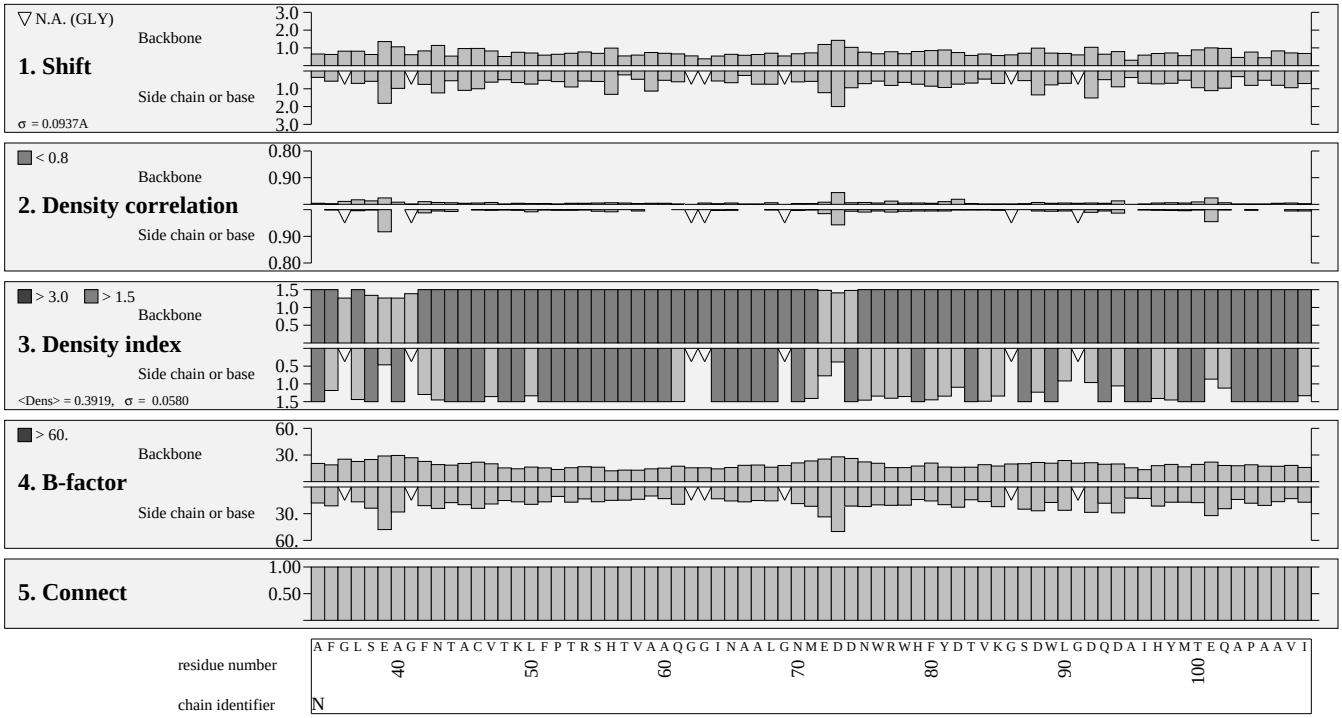
Structure Factor Check

2FBW

Local estimation (8)





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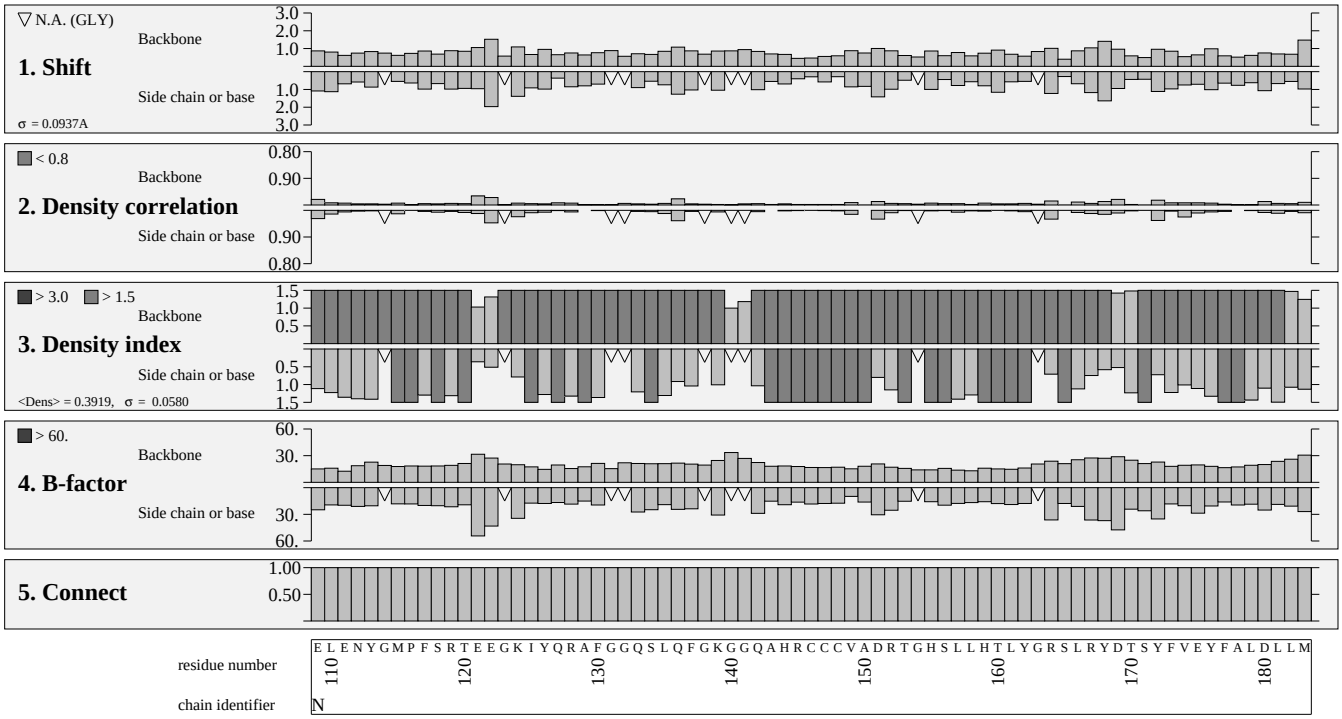
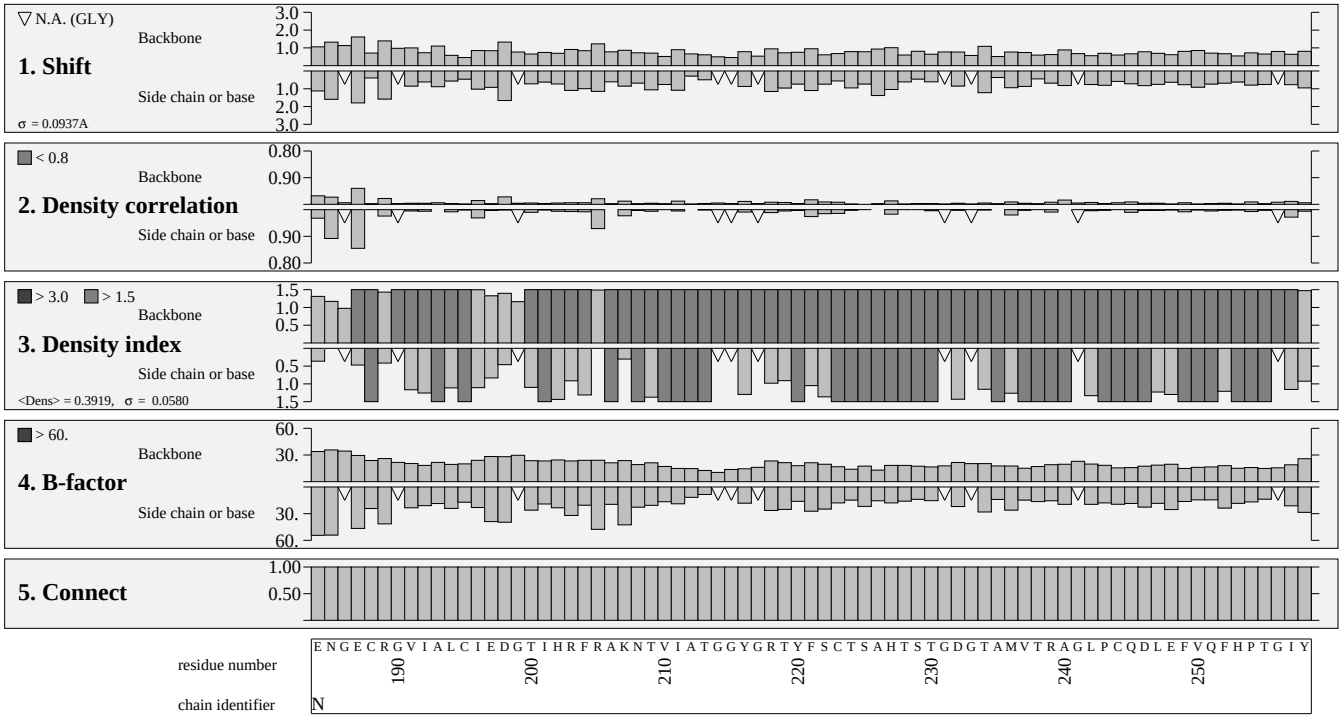
Structure Factor Check

2FBW

Local estimation (9)





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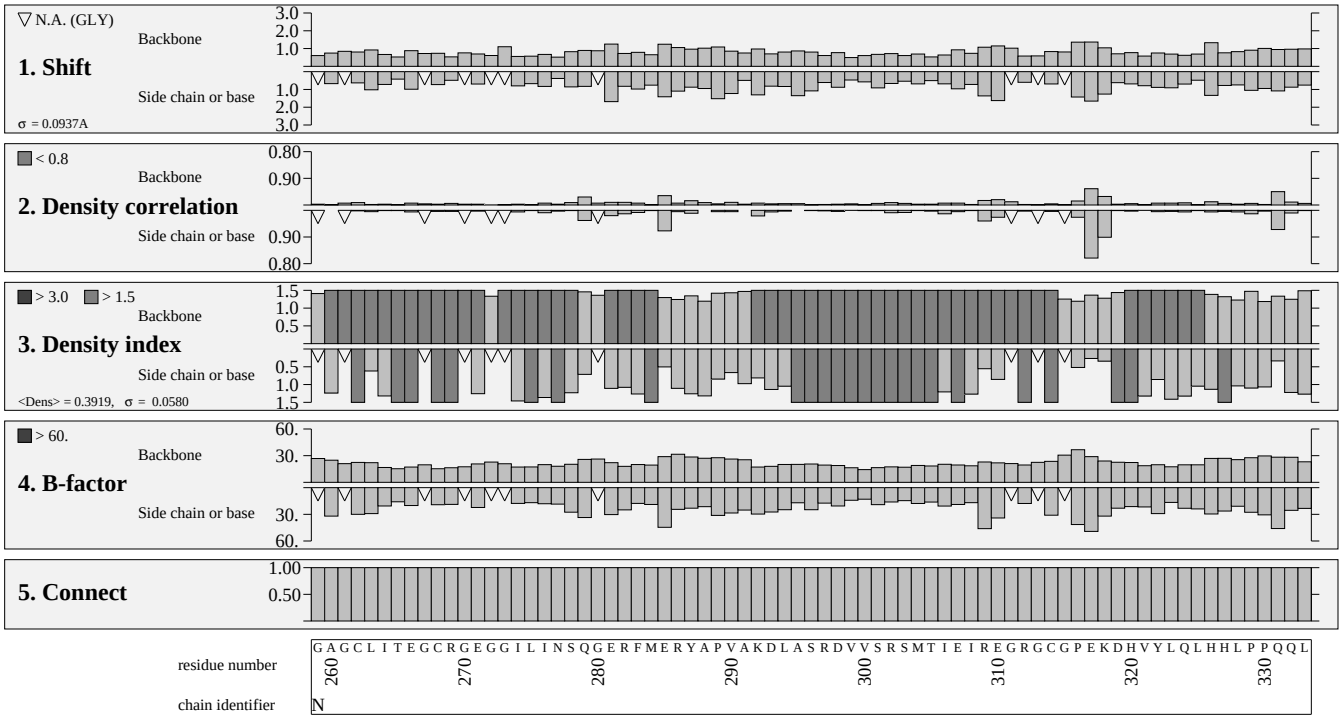
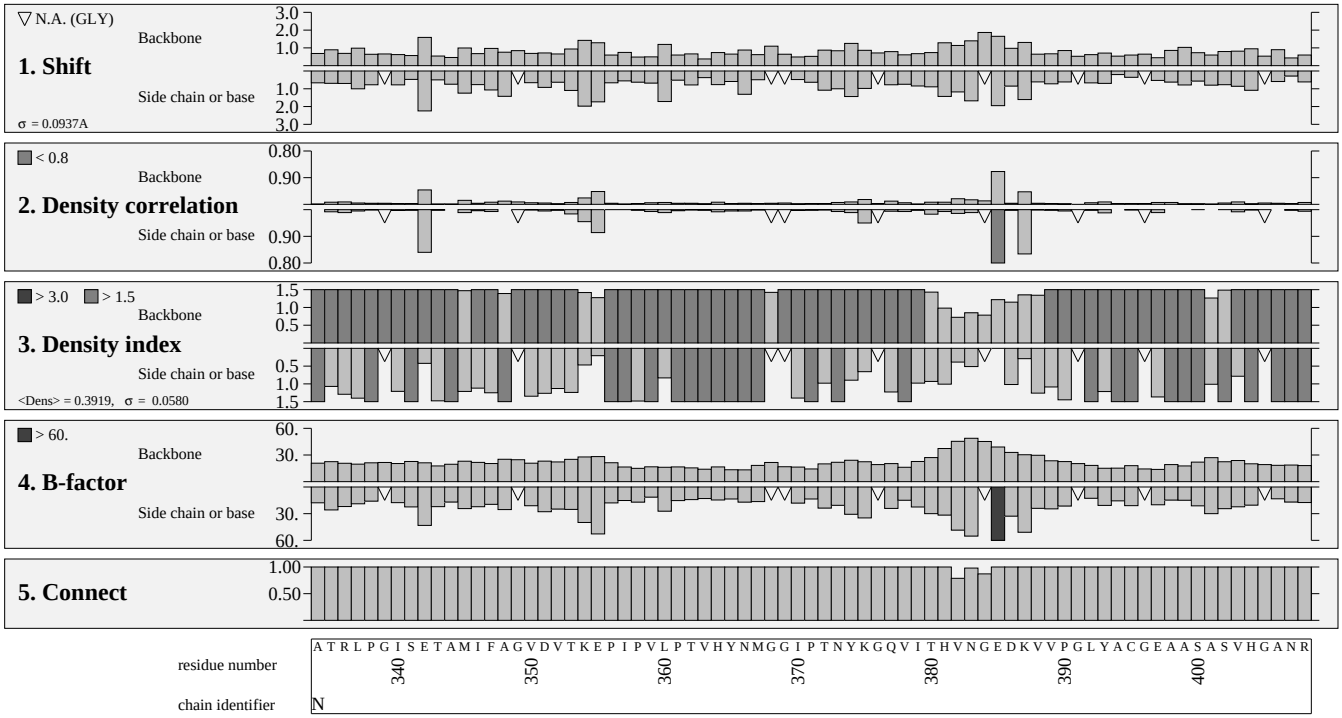
Structure Factor Check

2FBW

Local estimation (10)





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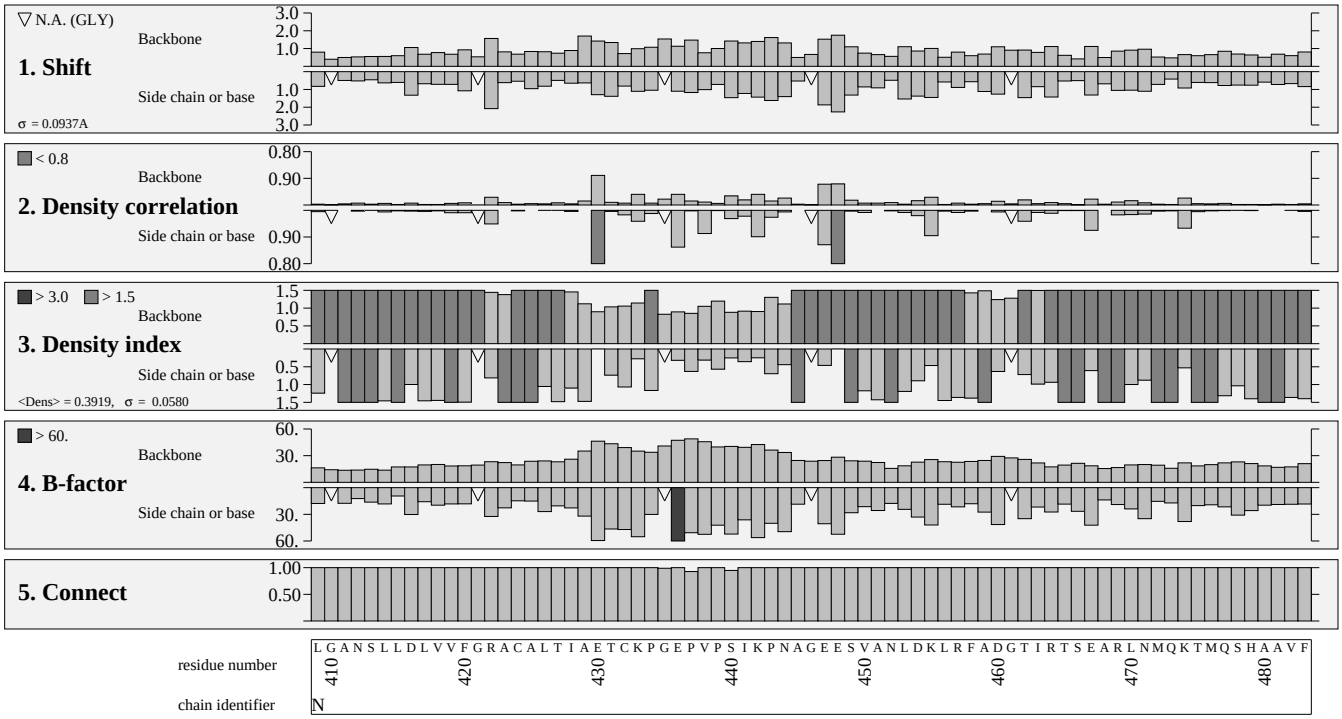
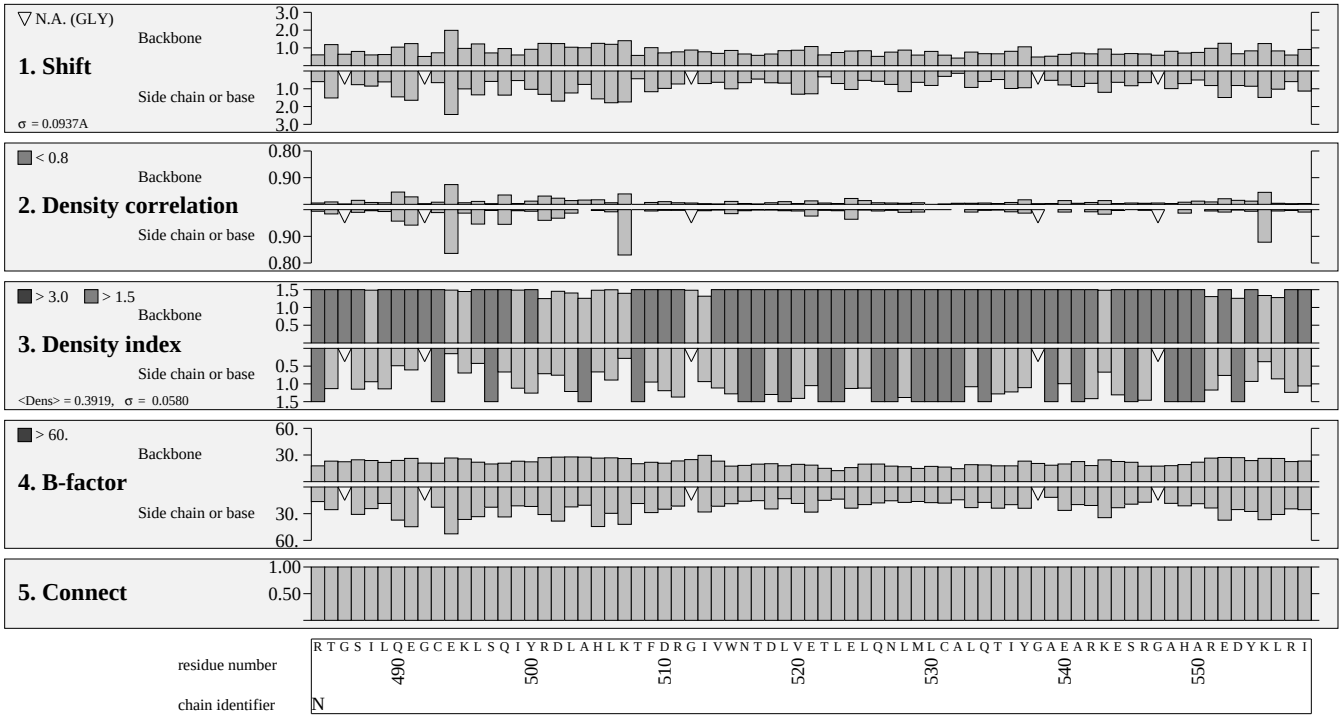
Structure Factor Check

2FBW

Local estimation (11)





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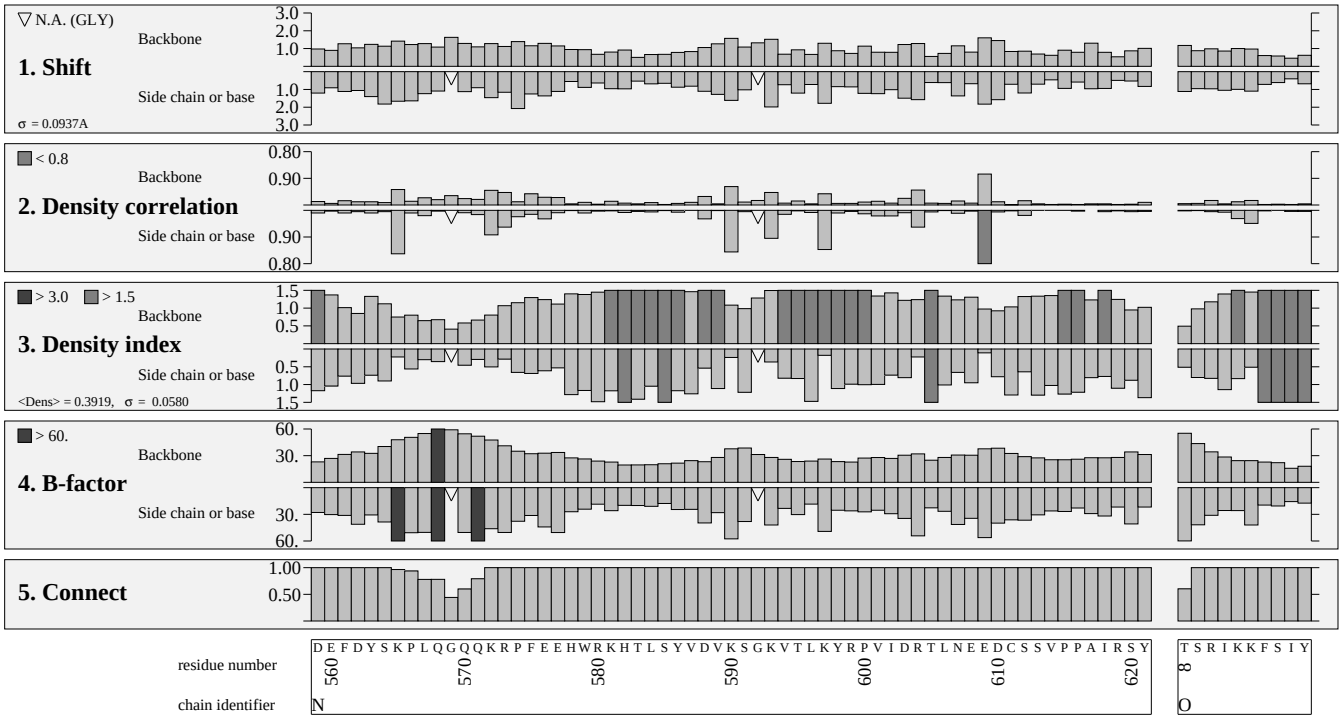
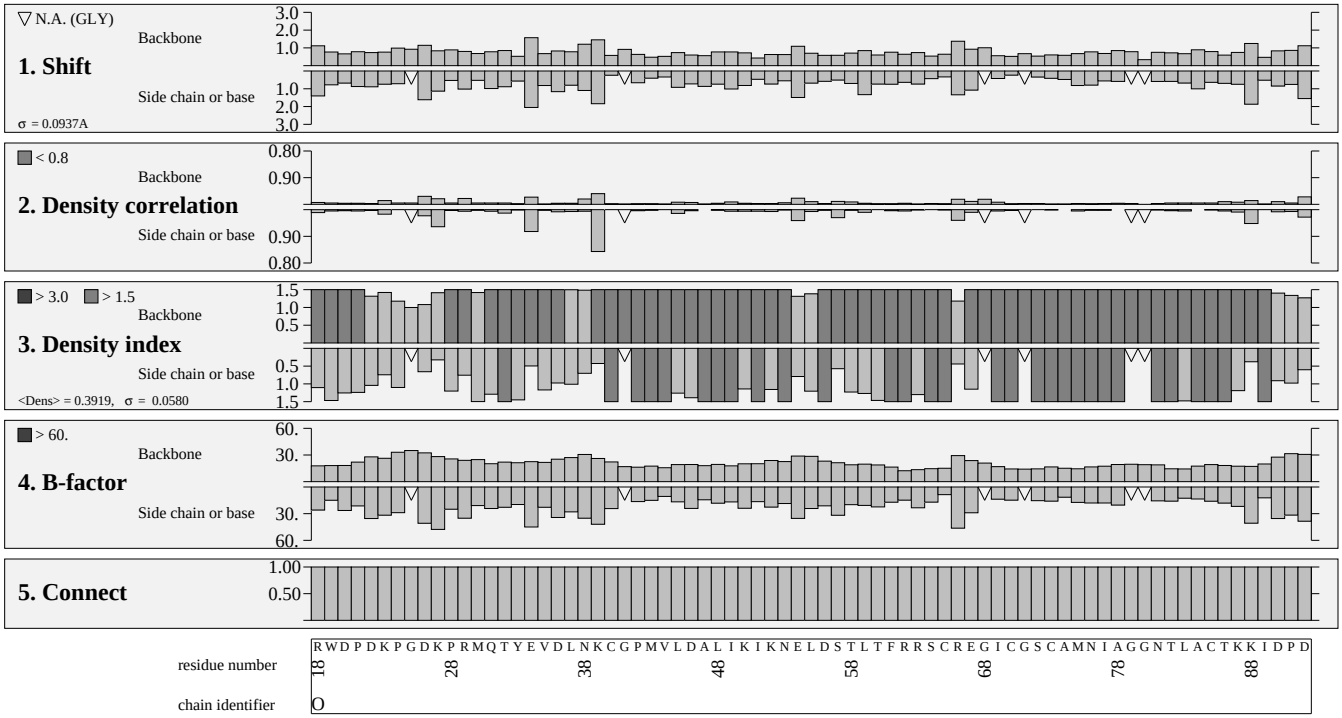
Structure Factor Check

2FBW

Local estimation (12)



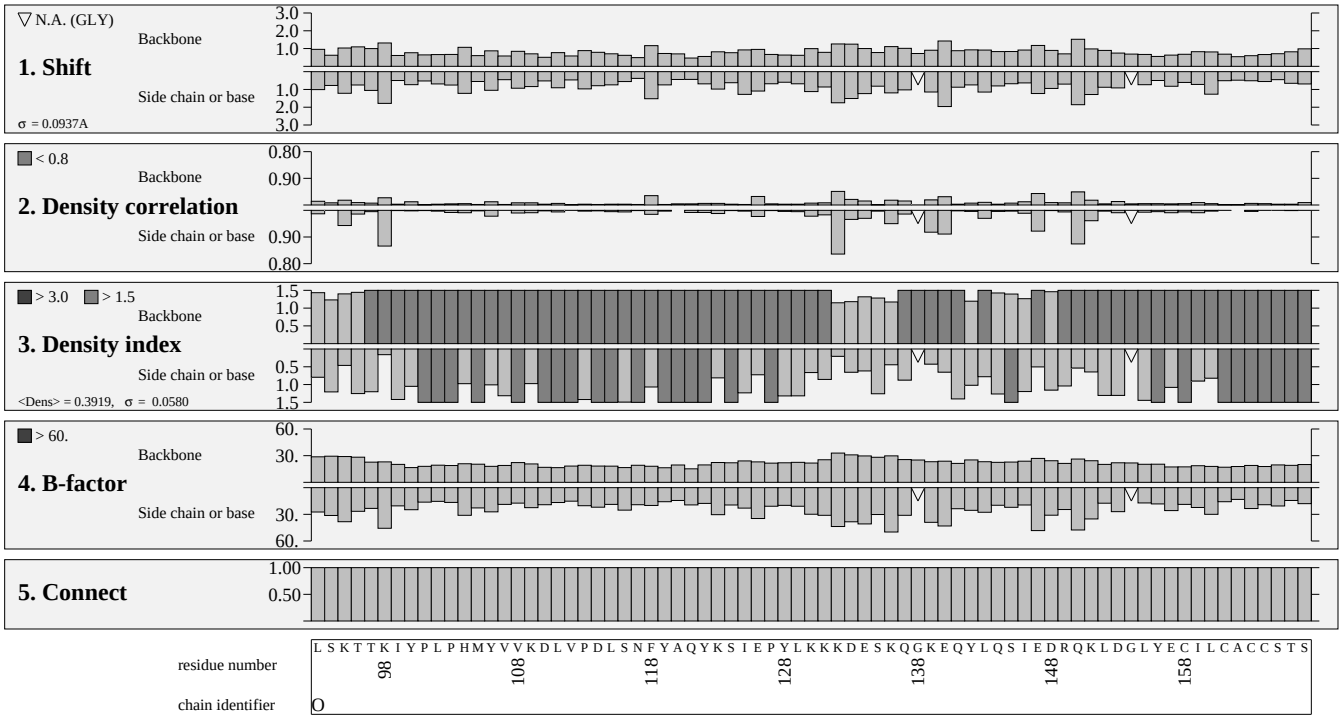


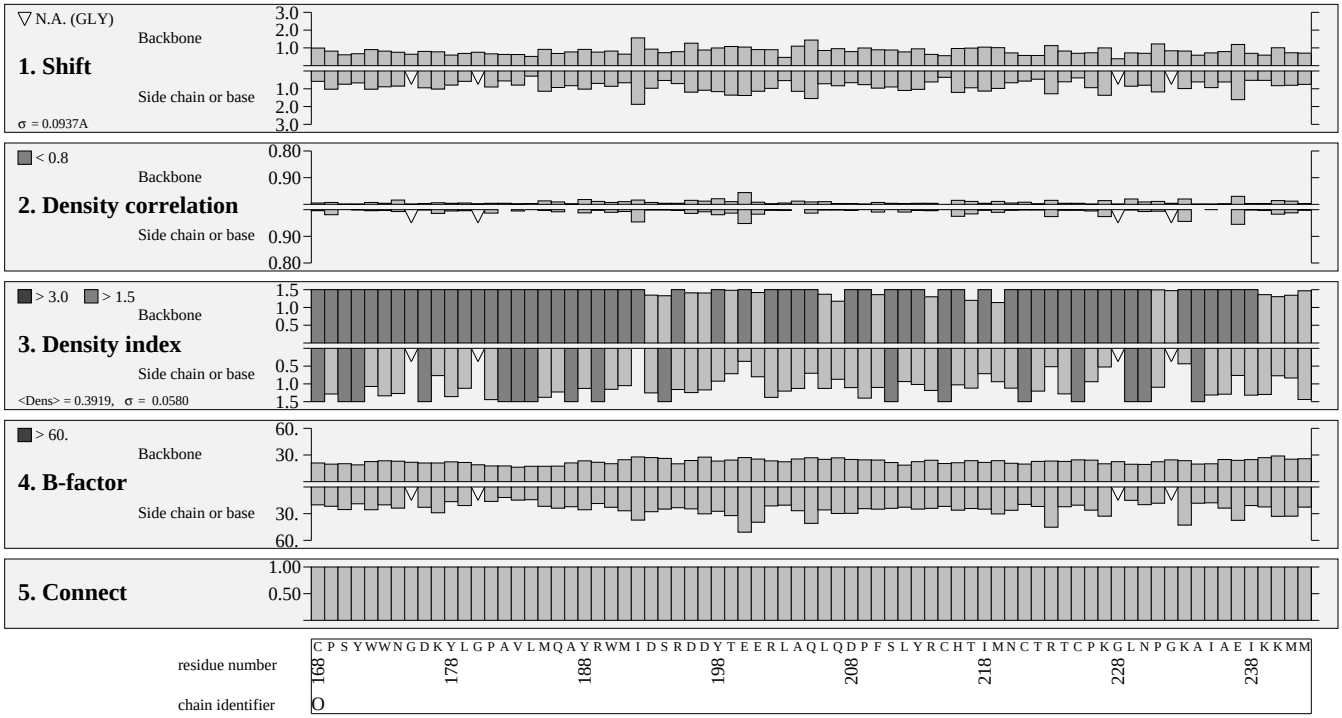
SFCHECK 7.03.16

Structure Factor Check

2FBW

Local estimation (13)





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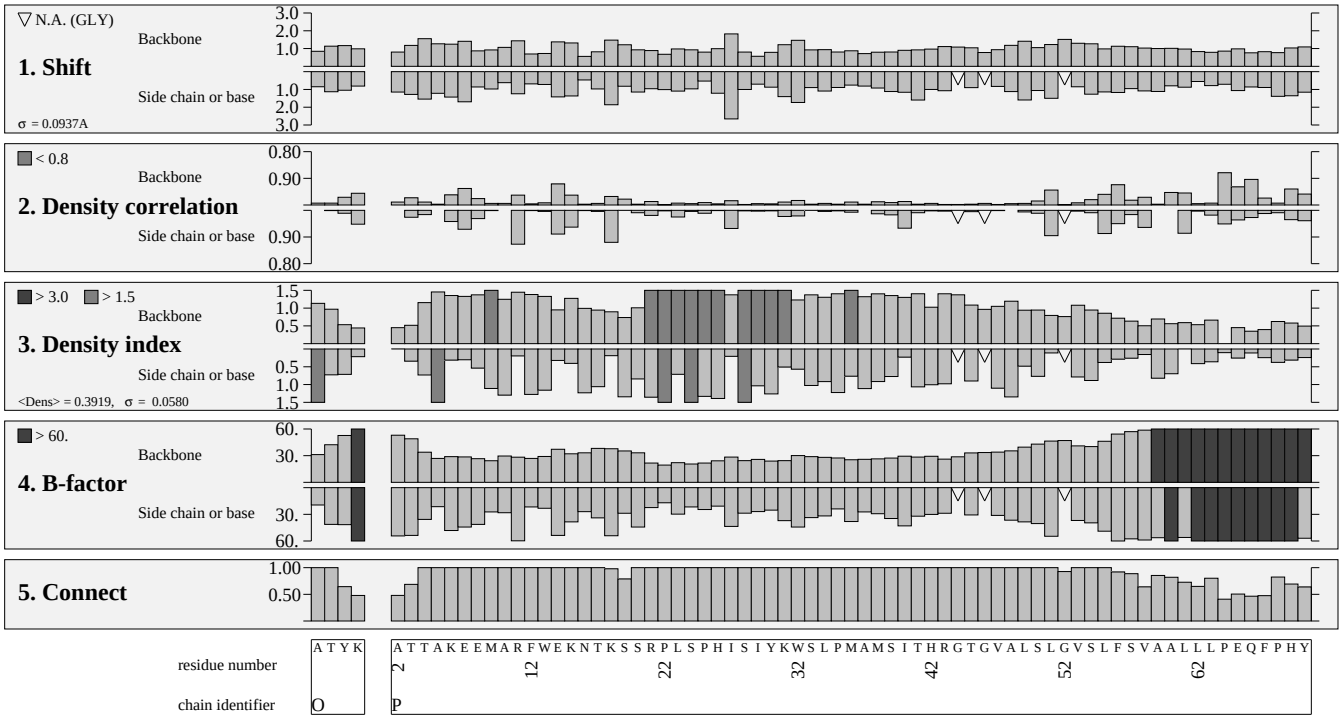
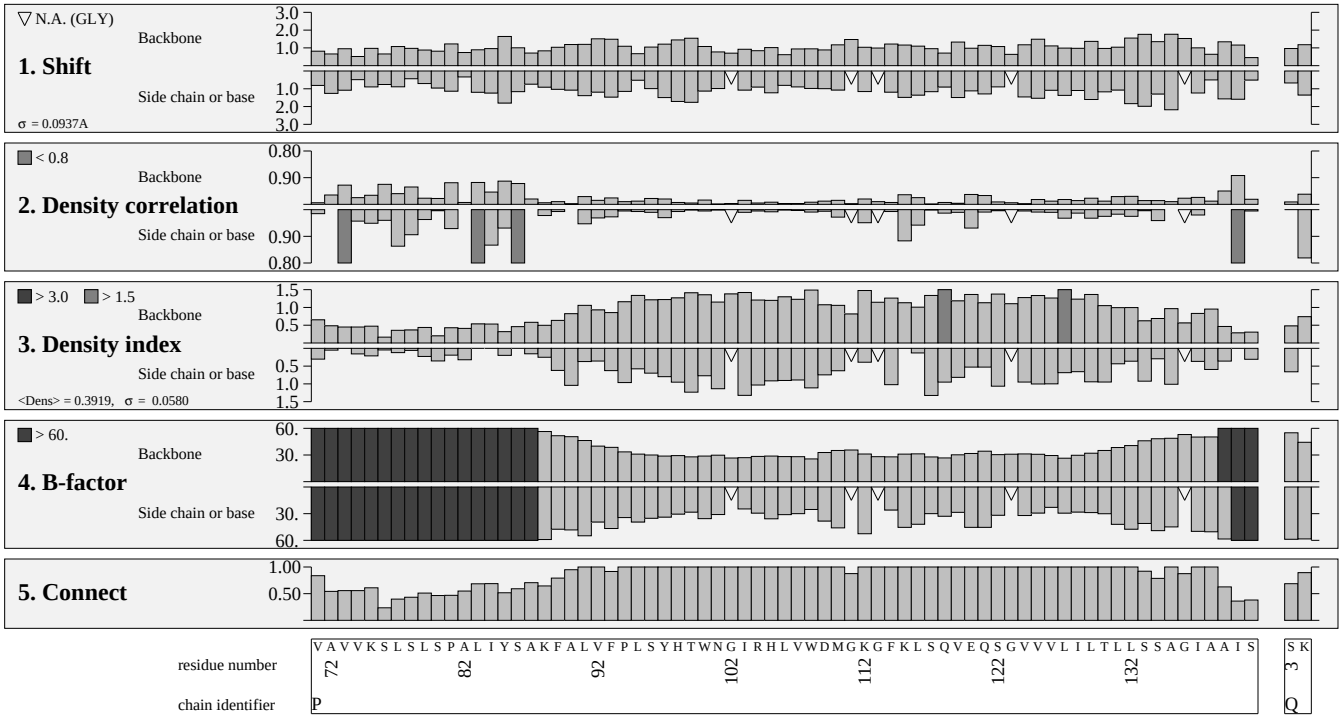
Structure Factor Check

2FBW

Local estimation (14)





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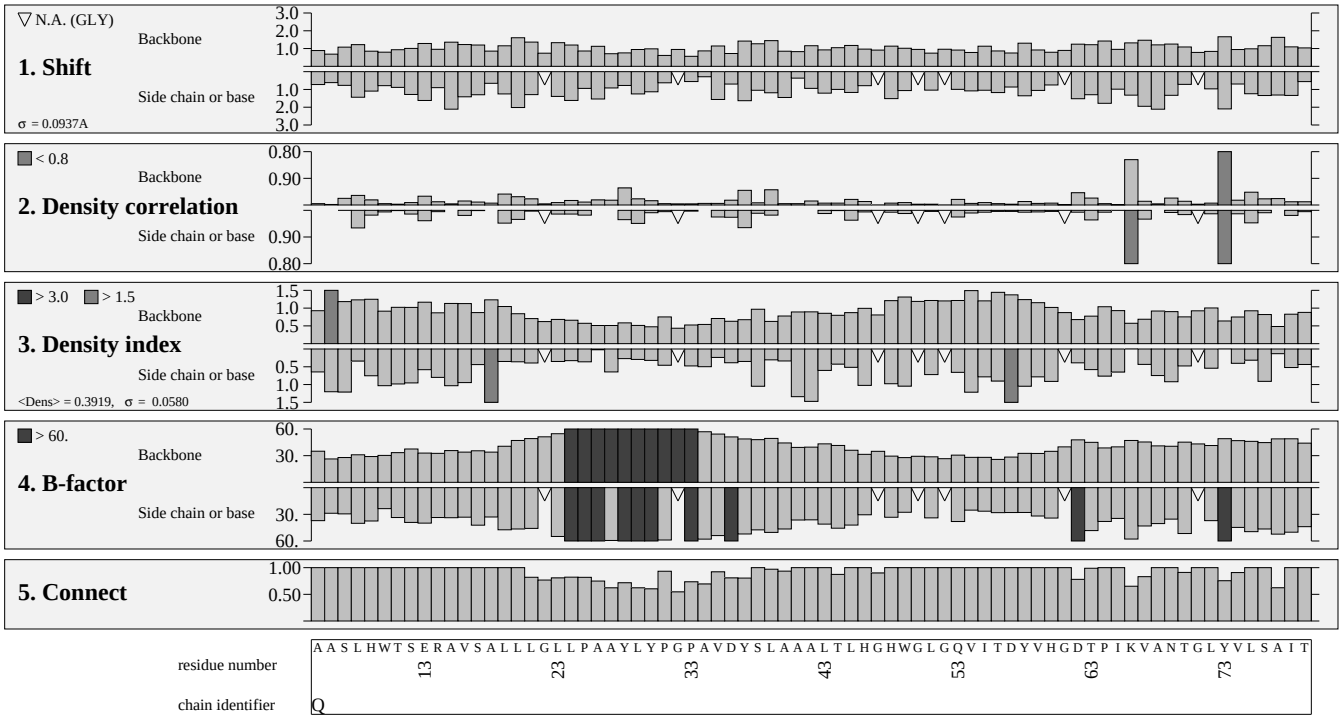
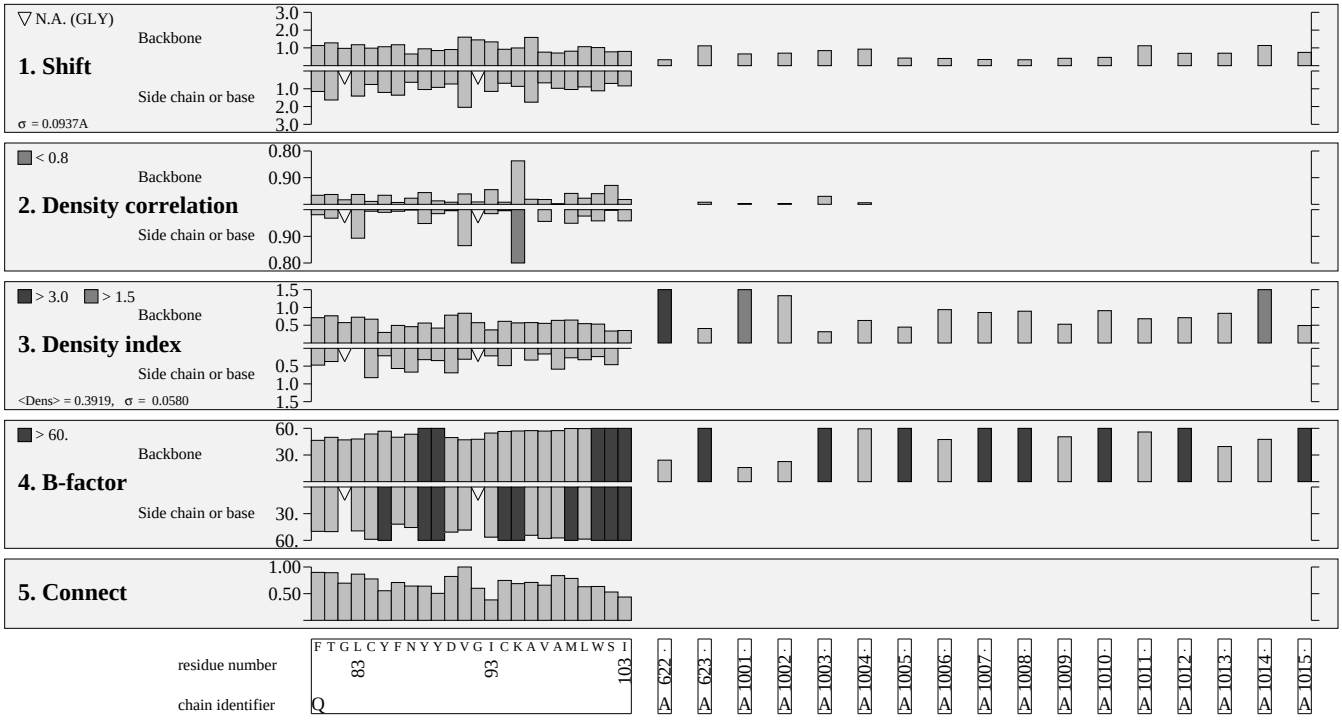
Structure Factor Check

2FBW

Local estimation (15)



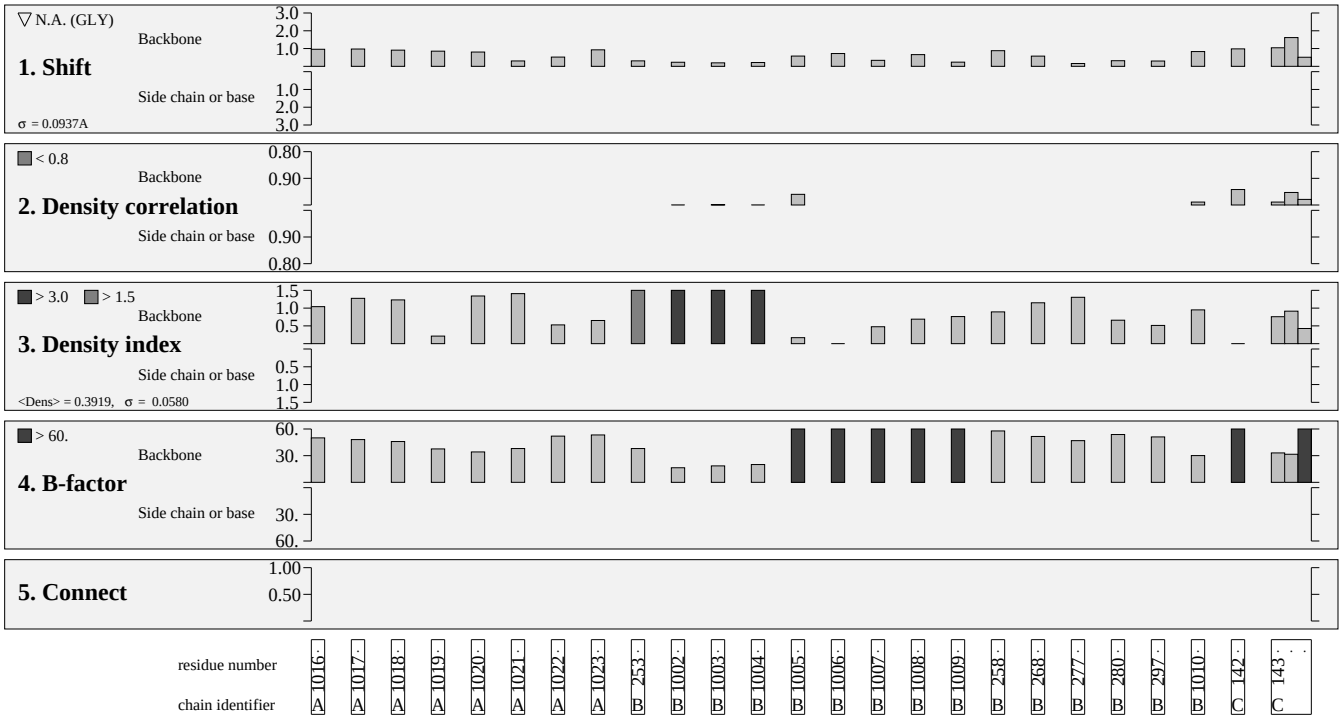


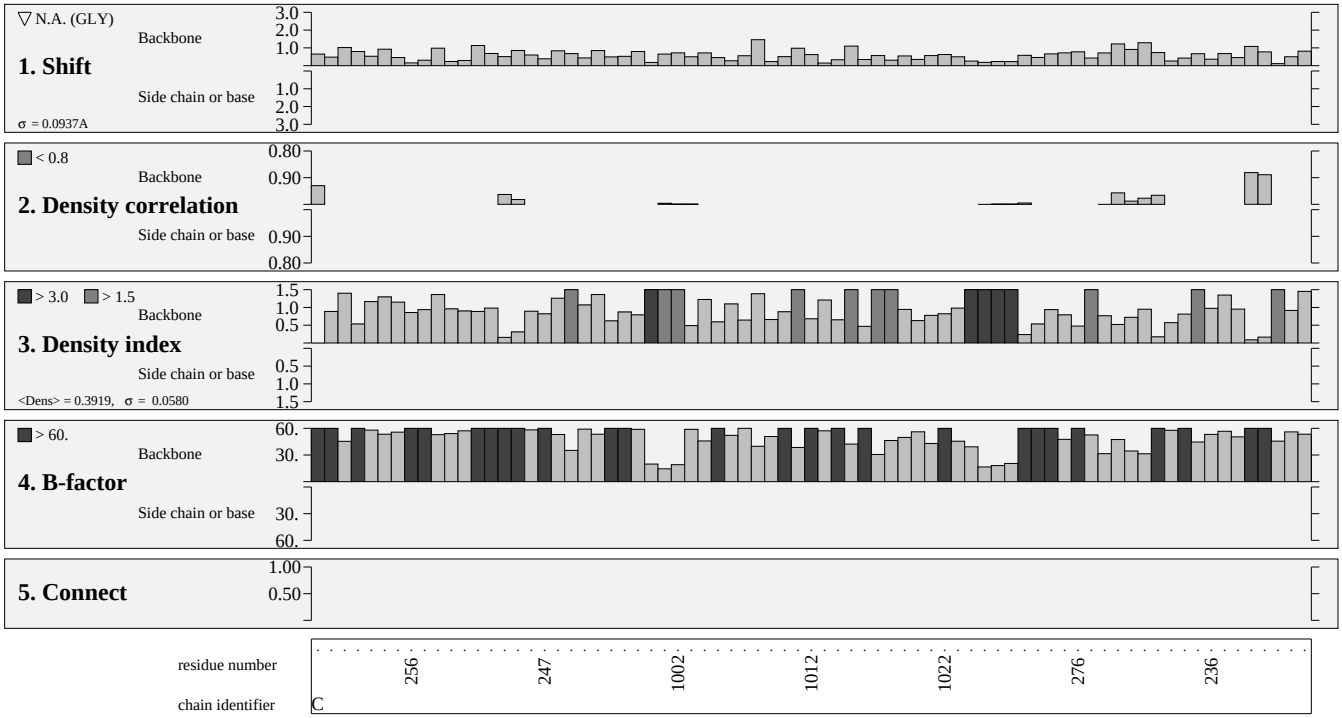
SFCHECK 7.03.16

Structure Factor Check

2FBW

Local estimation (16)





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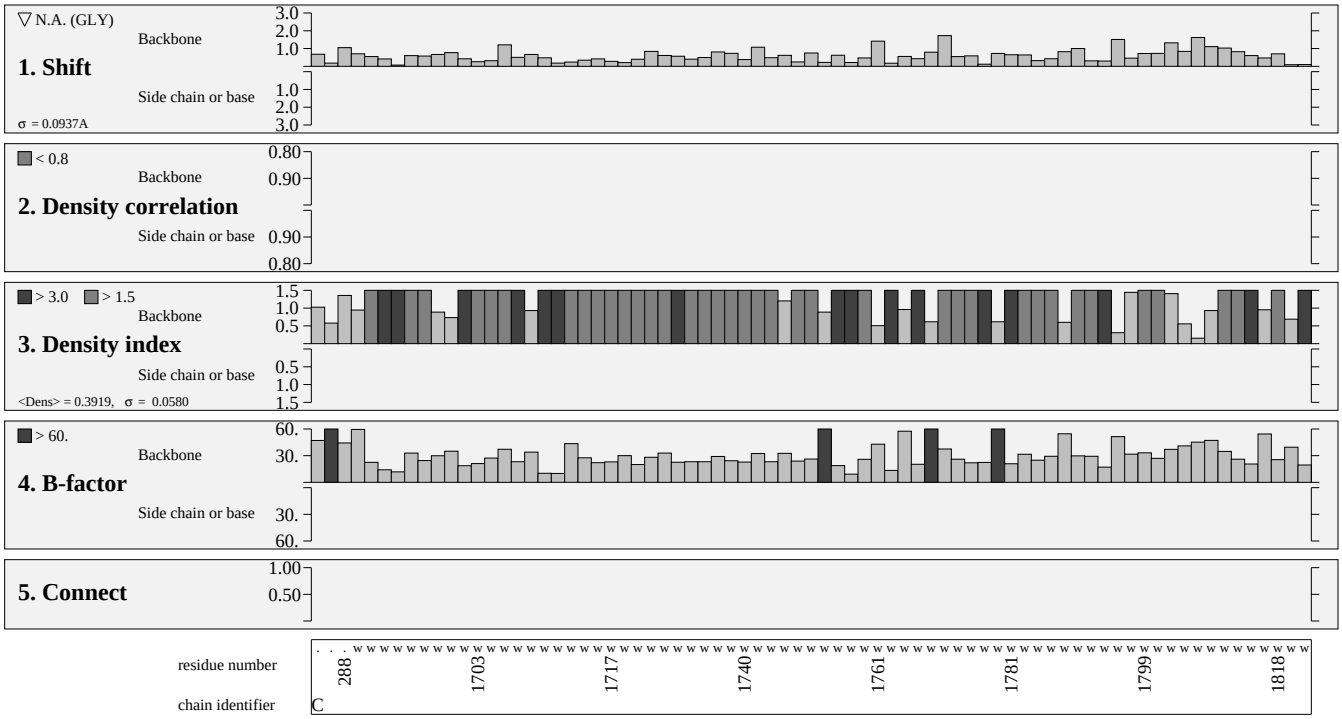
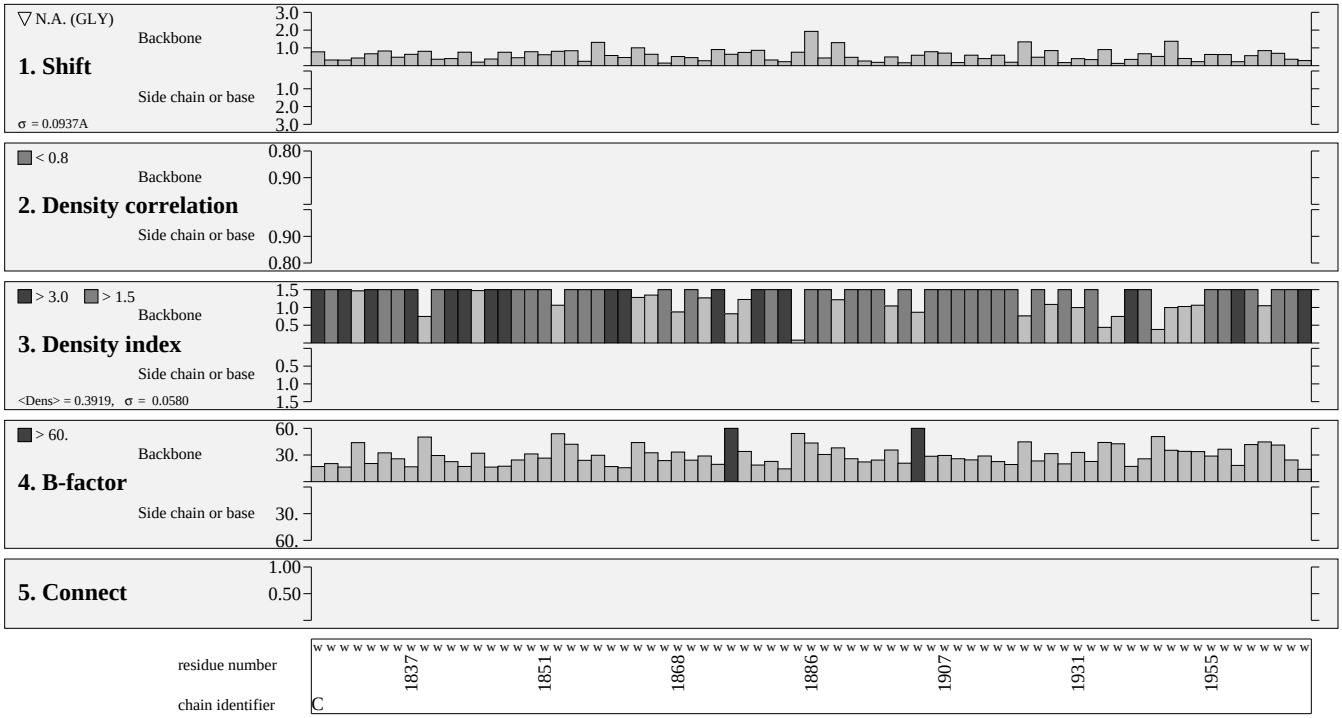
Structure Factor Check

2FBW

Local estimation (17)





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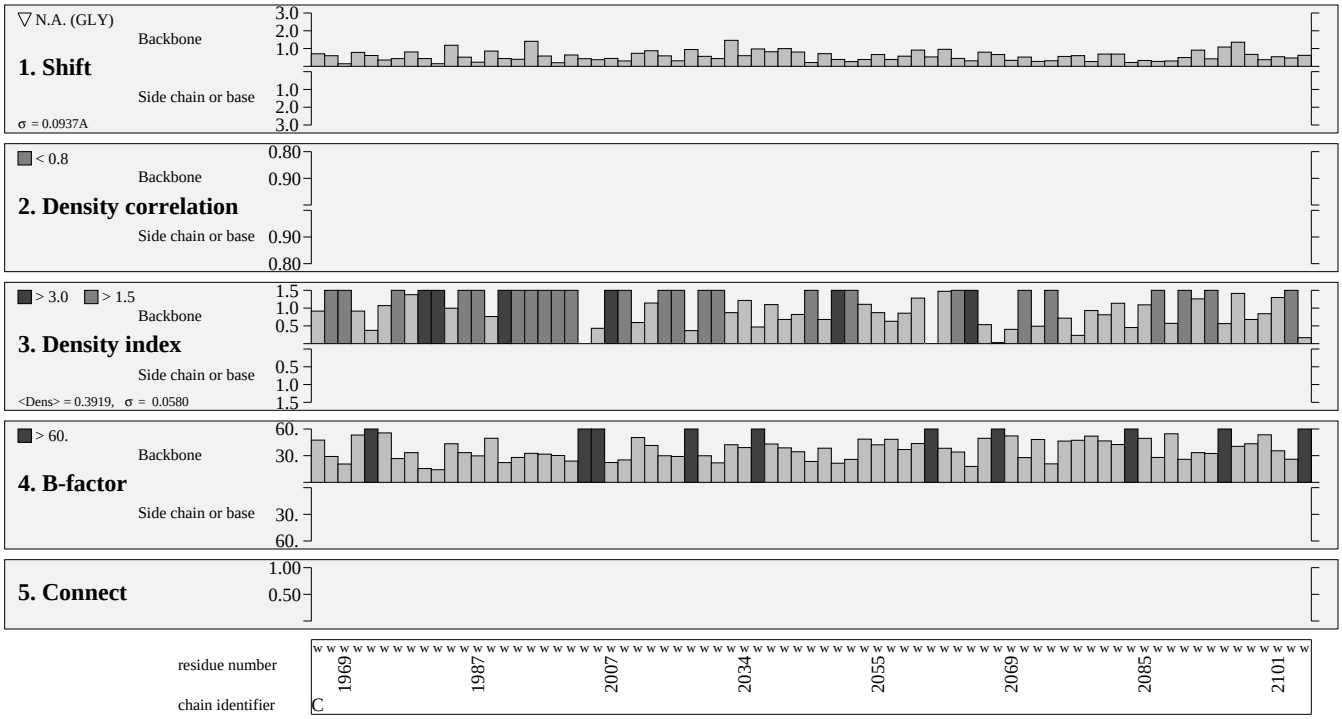
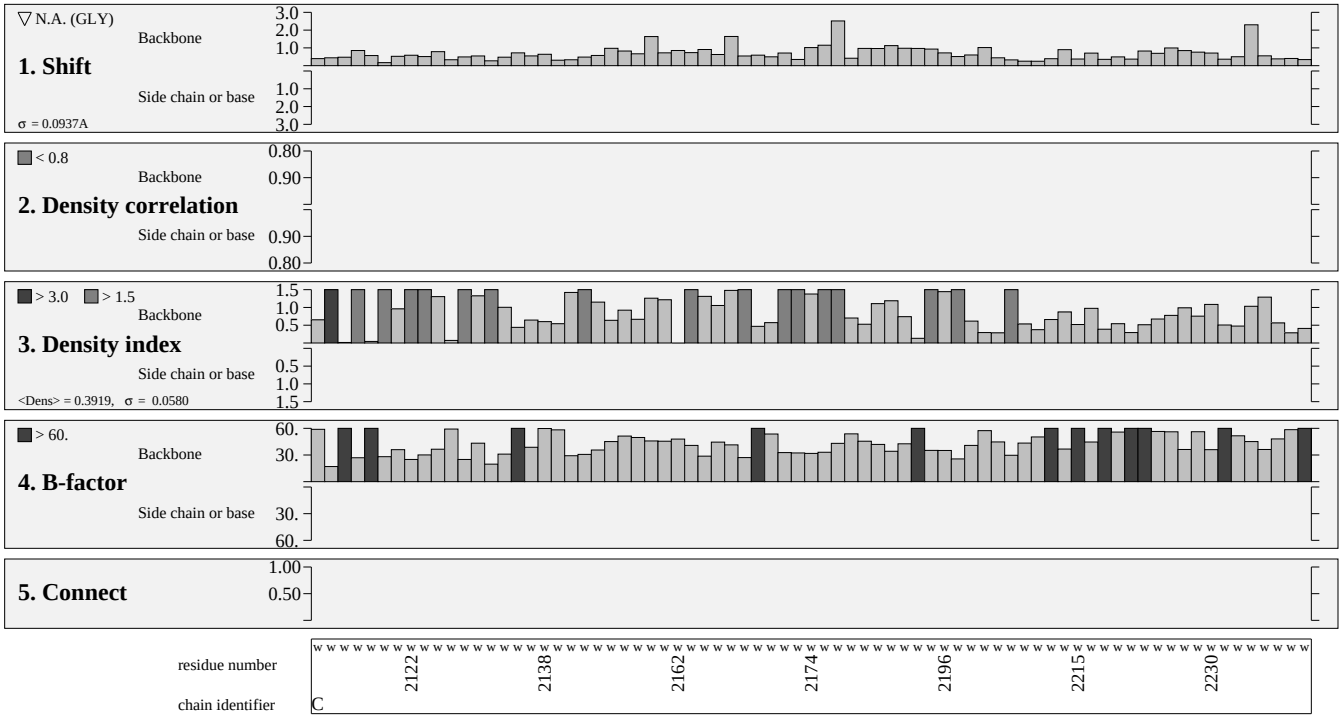
Structure Factor Check

2FBW

Local estimation (18)





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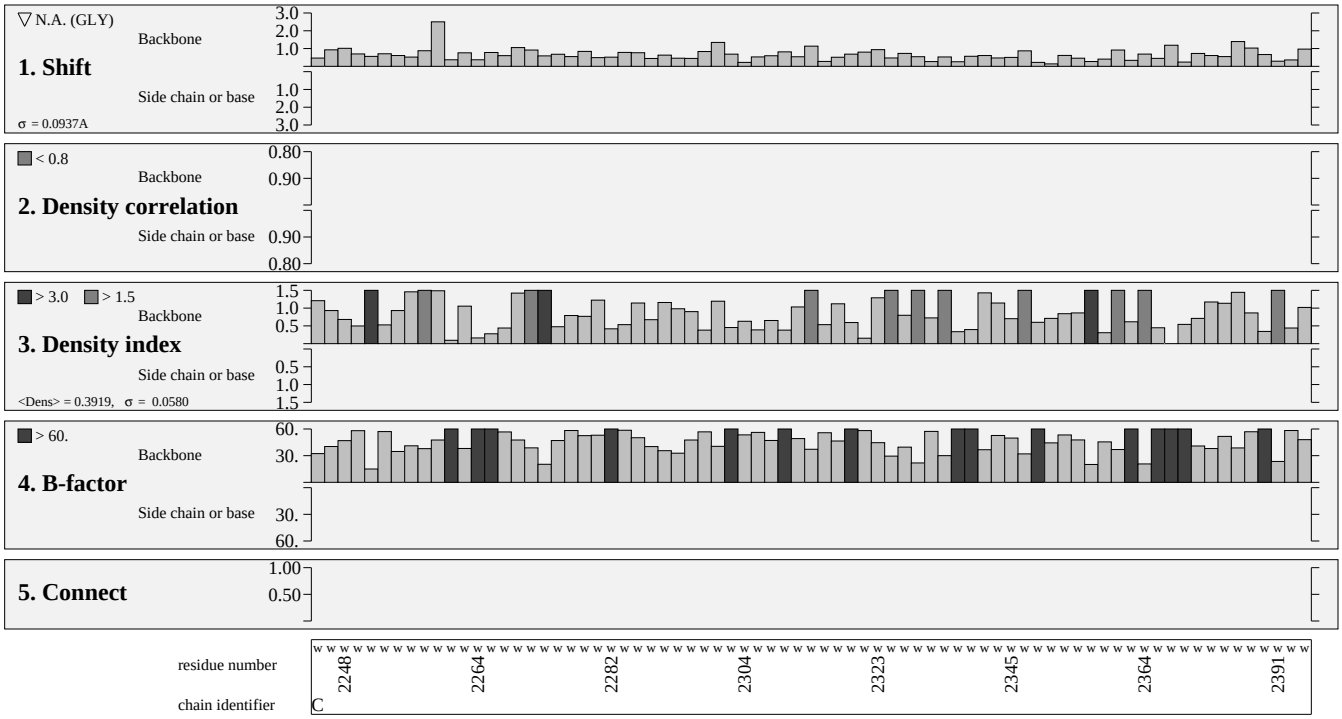
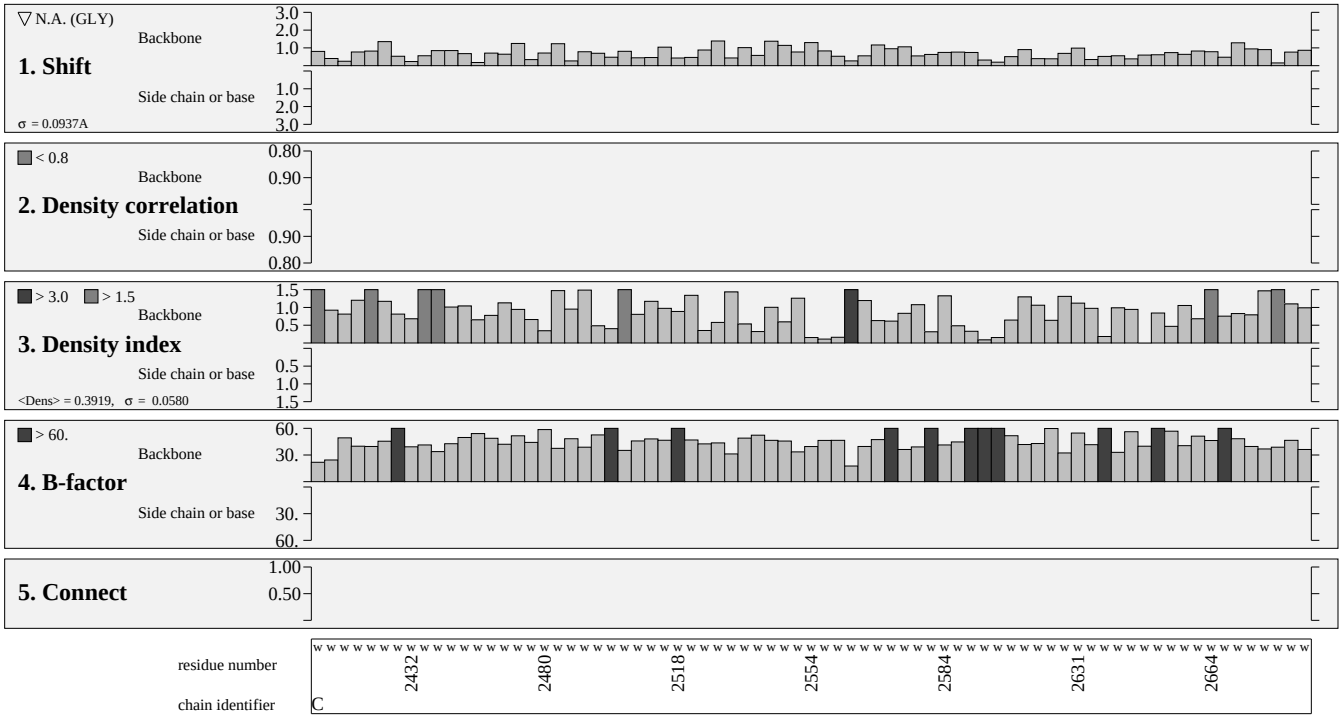
Structure Factor Check

2FBW

Local estimation (19)



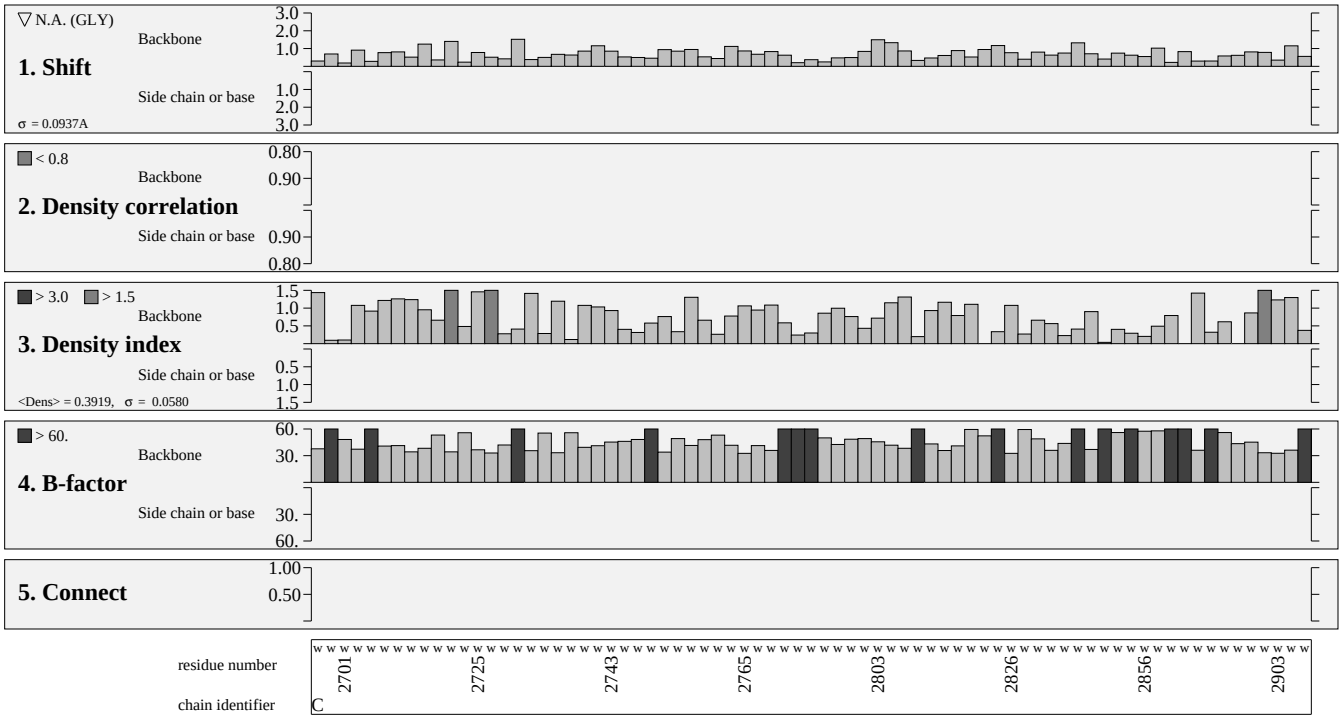


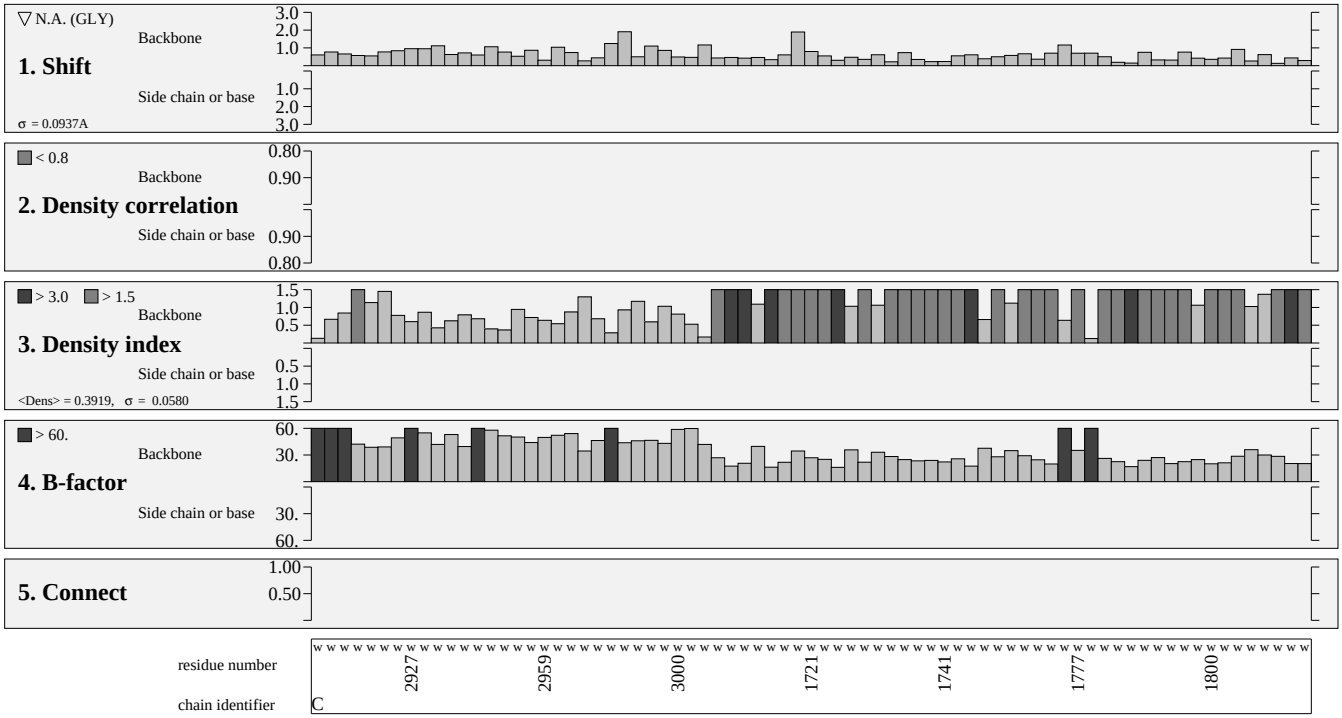
SFCHECK 7.03.16

Structure Factor Check

2FBW

Local estimation (20)



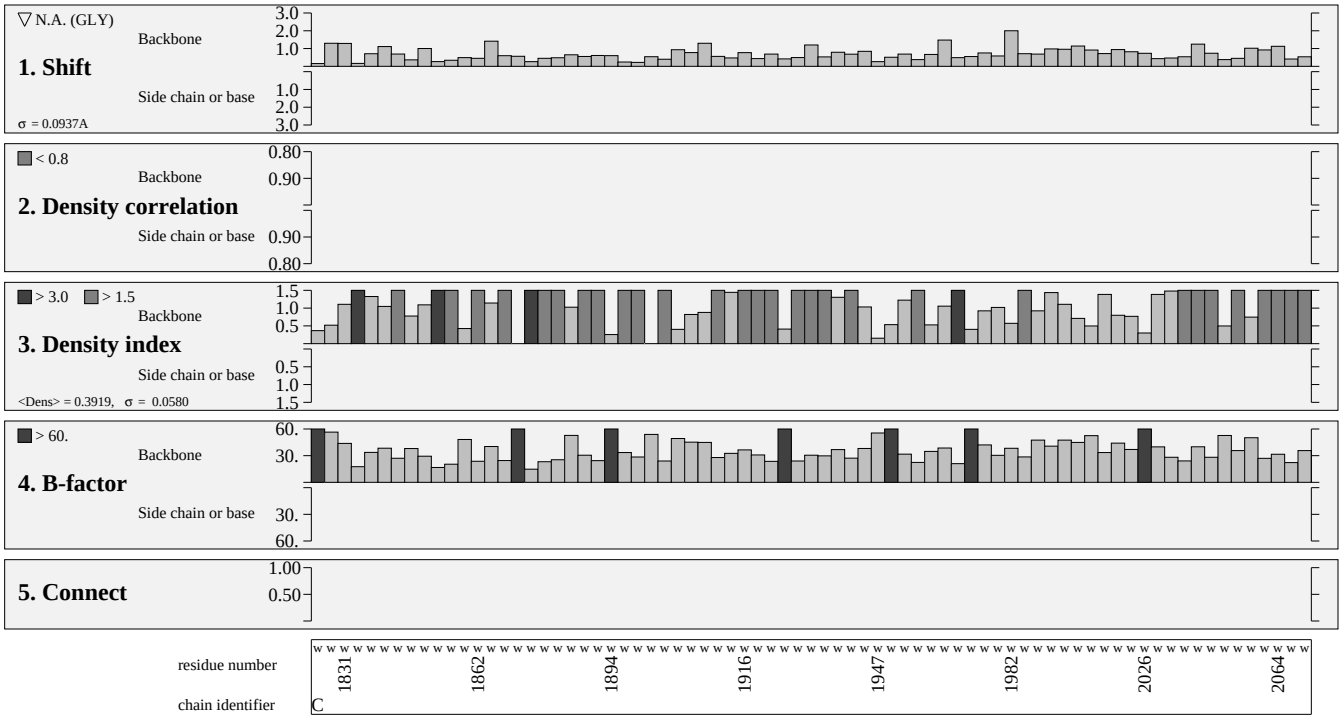


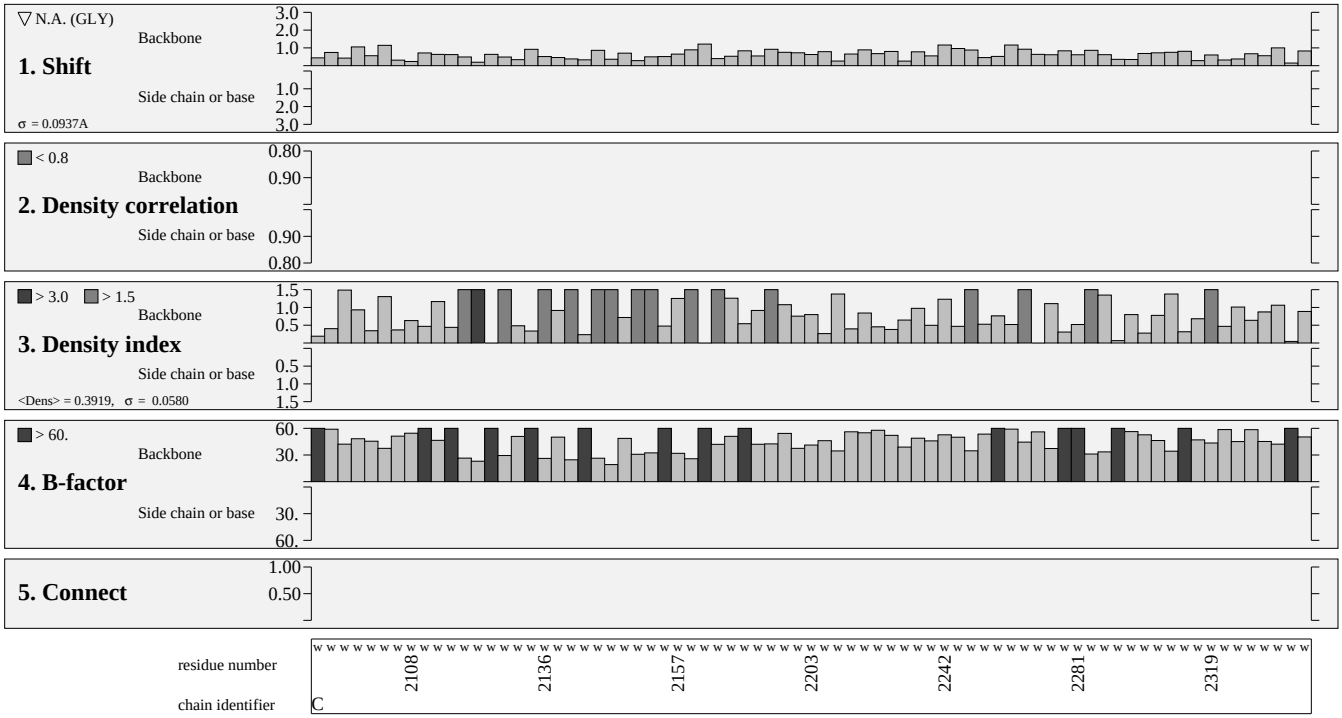
SFCHECK 7.03.16

Structure Factor Check

2FBW

Local estimation (21)

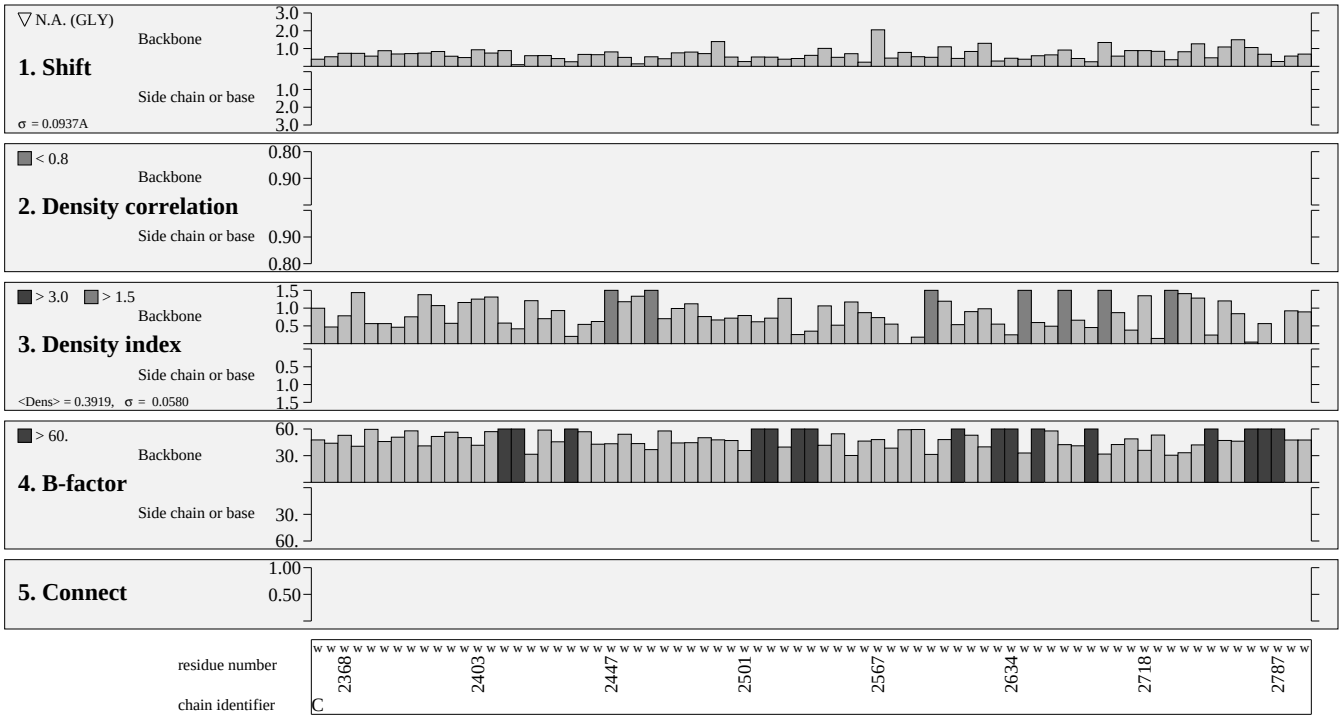


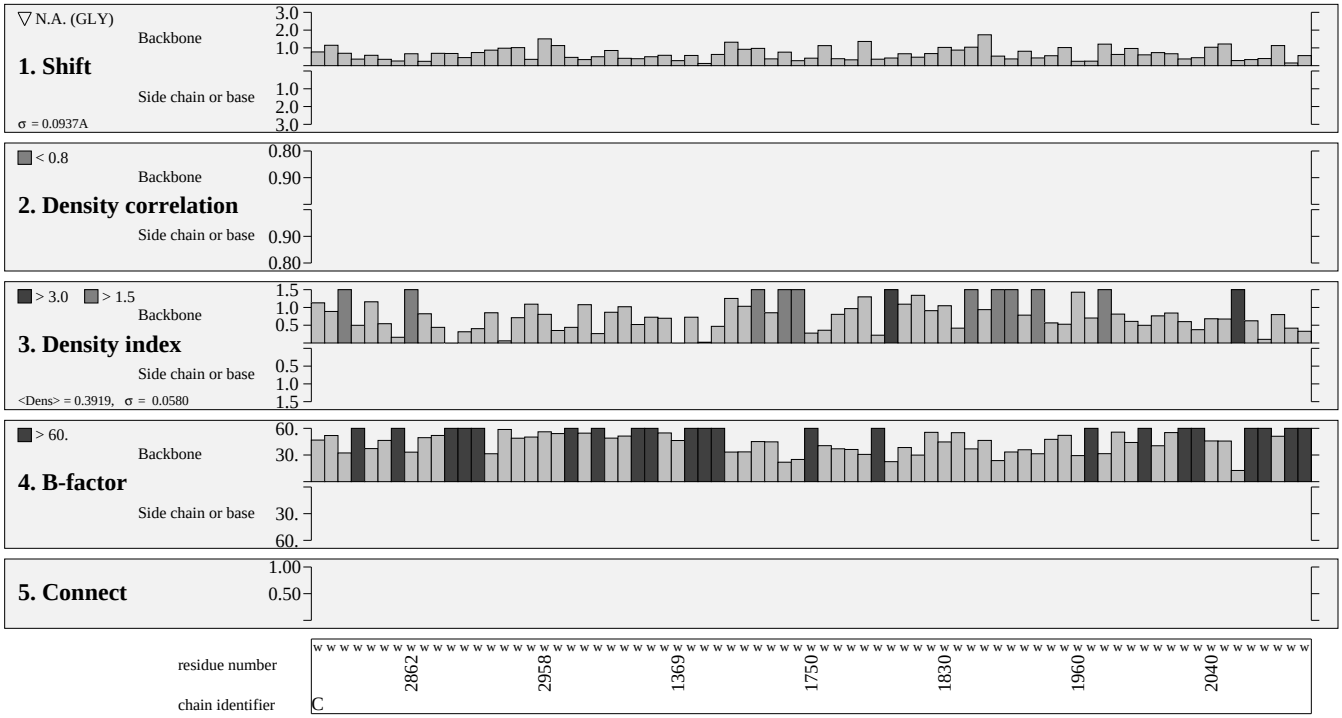


Structure Factor Check

2FBW

Local estimation (22)



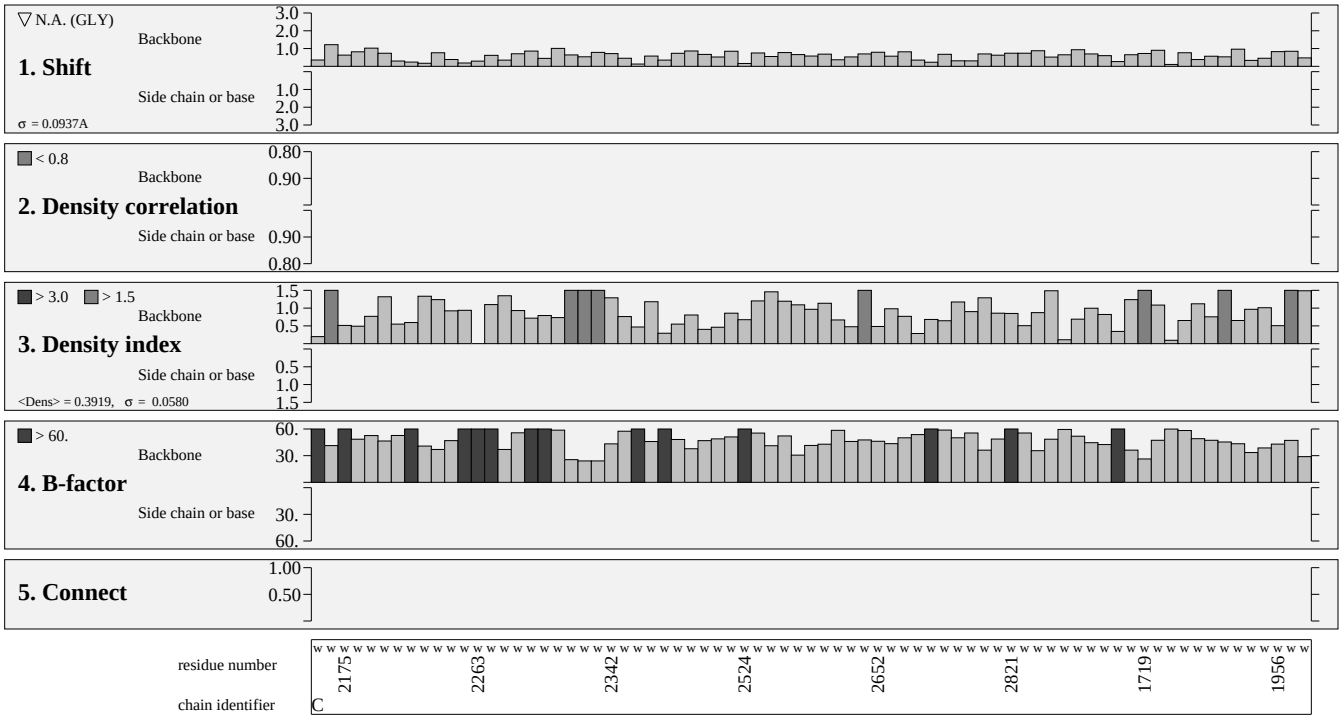


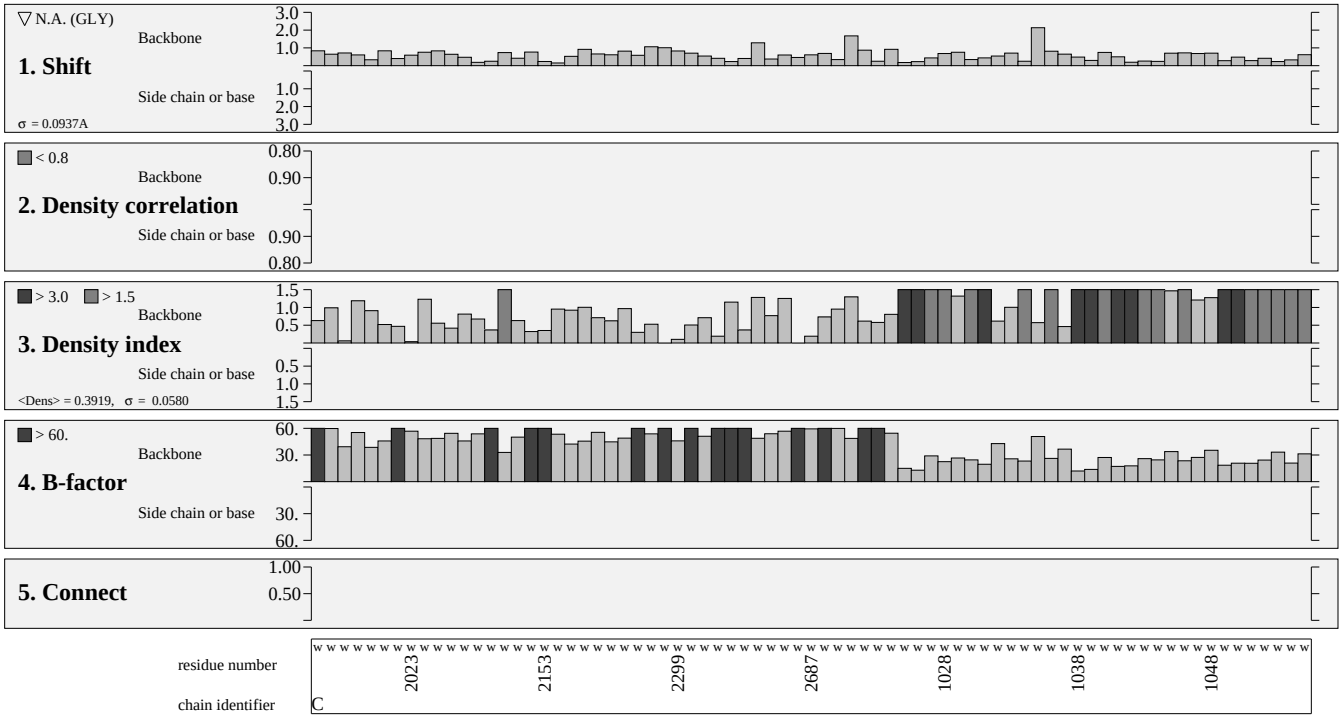
SFCHECK 7.03.16

Structure Factor Check

2FBW

Local estimation (23)



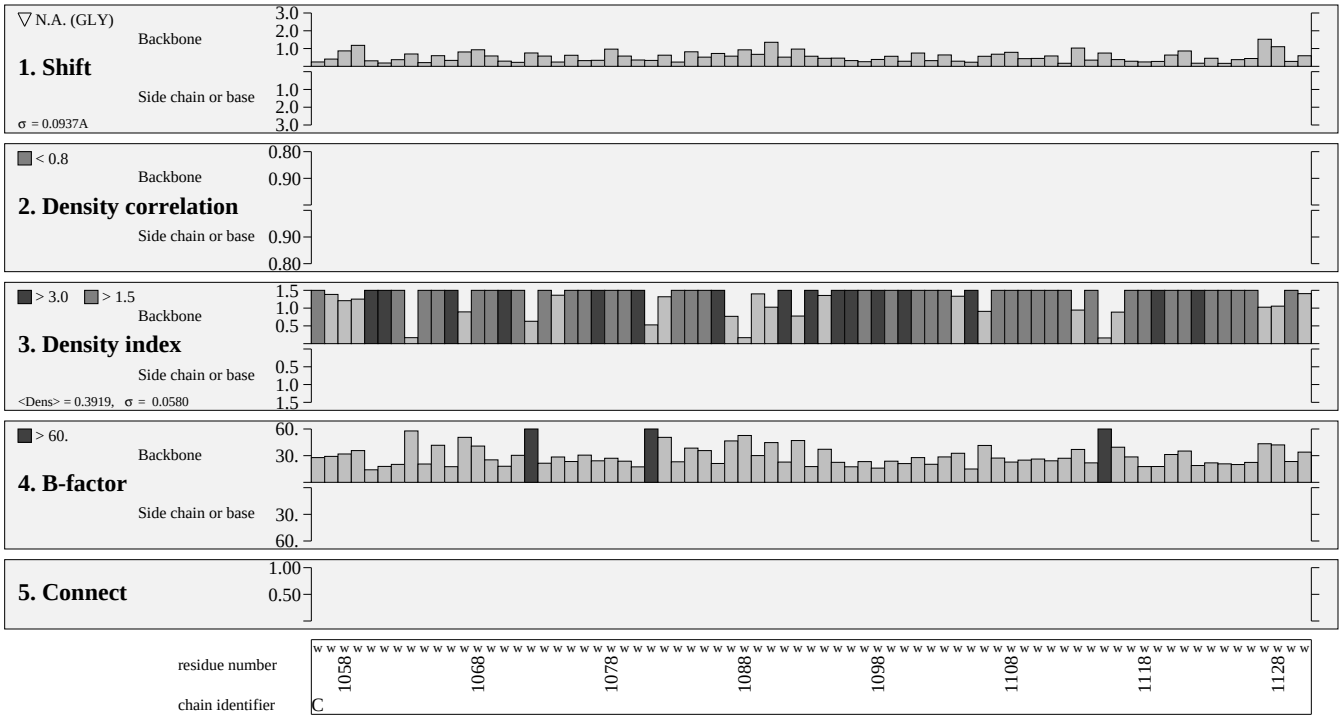


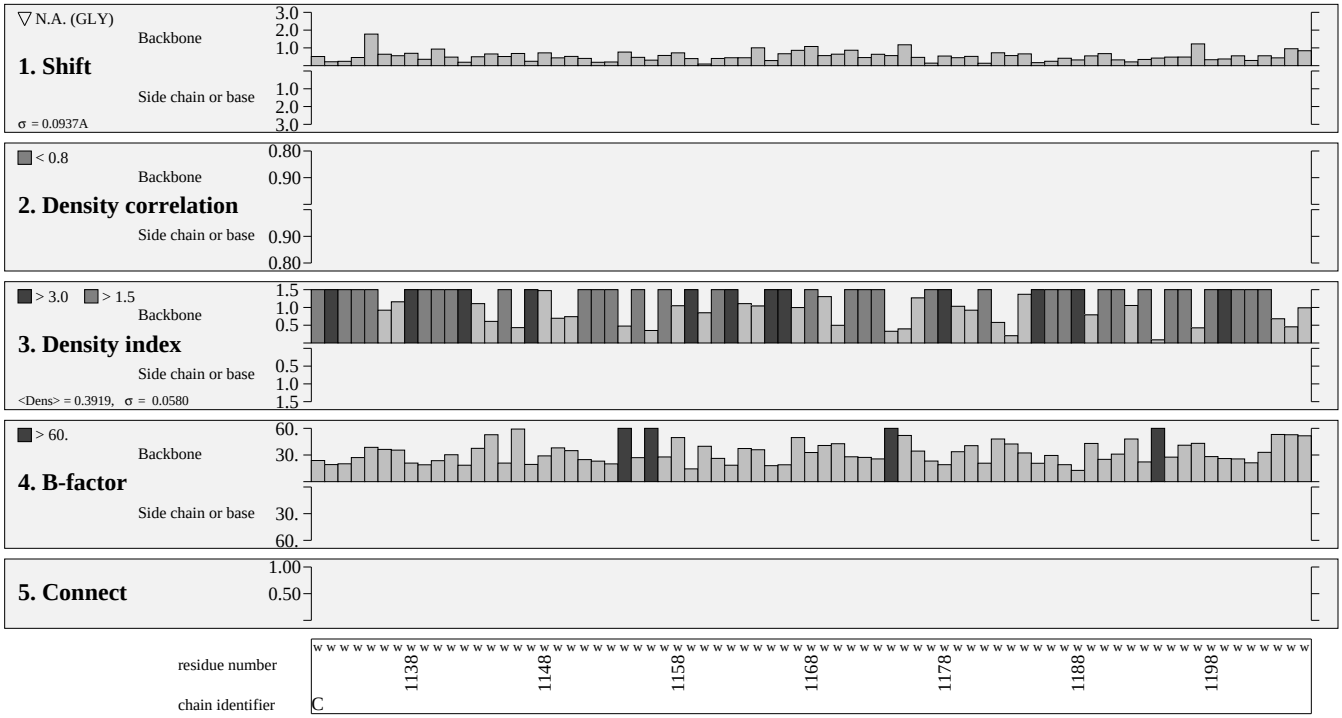
SFCHECK 7.03.16

Structure Factor Check

2FBW

Local estimation (24)

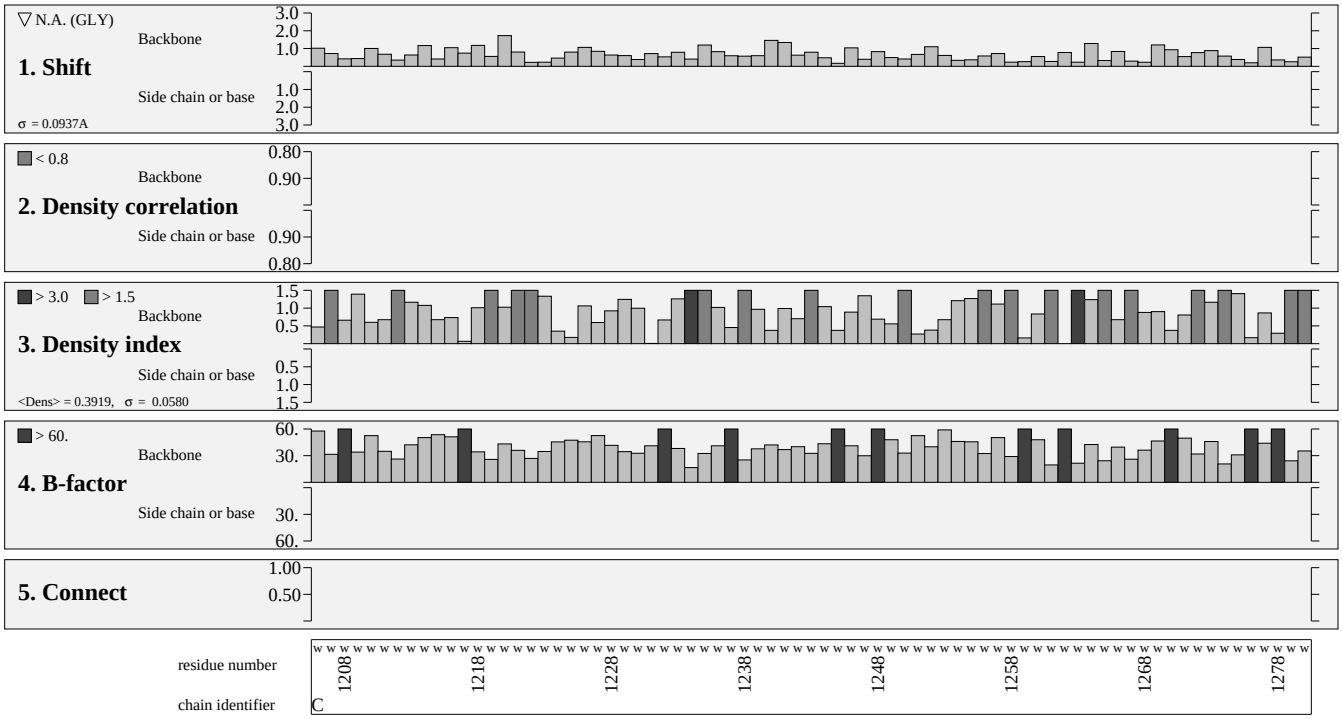


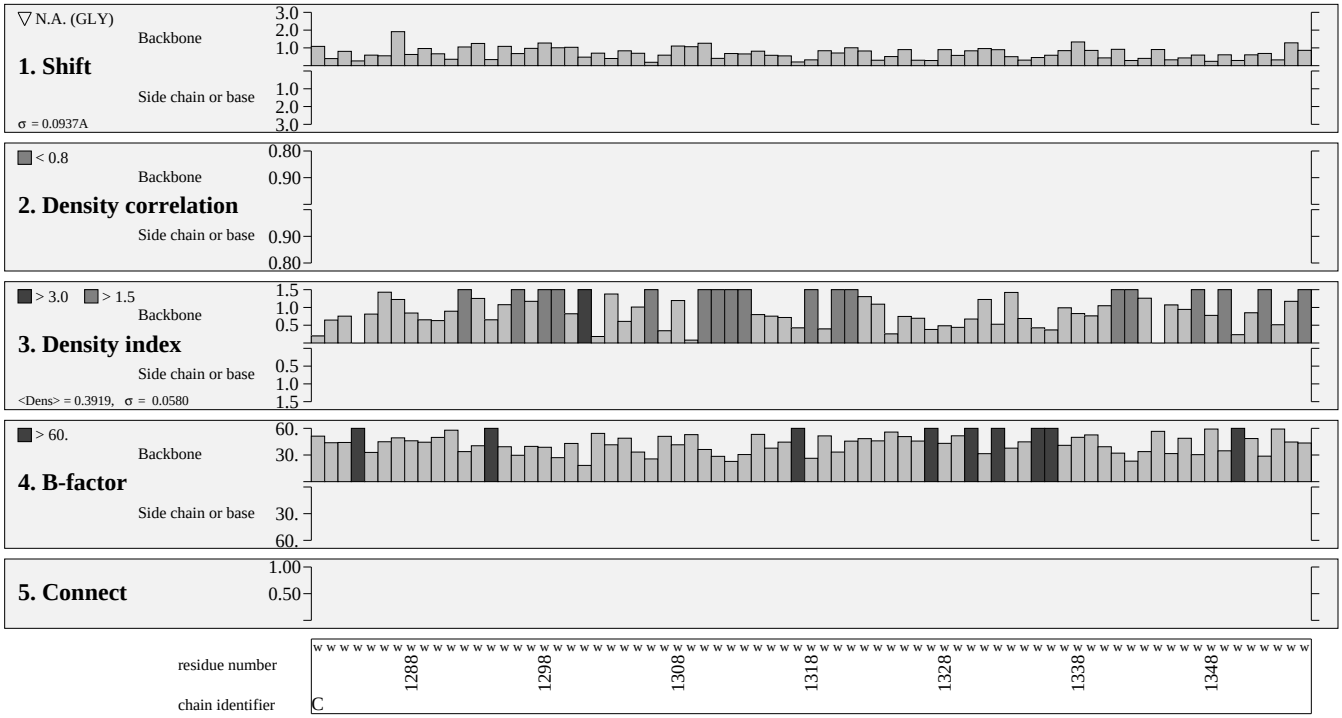


Structure Factor Check

2FBW

Local estimation (25)



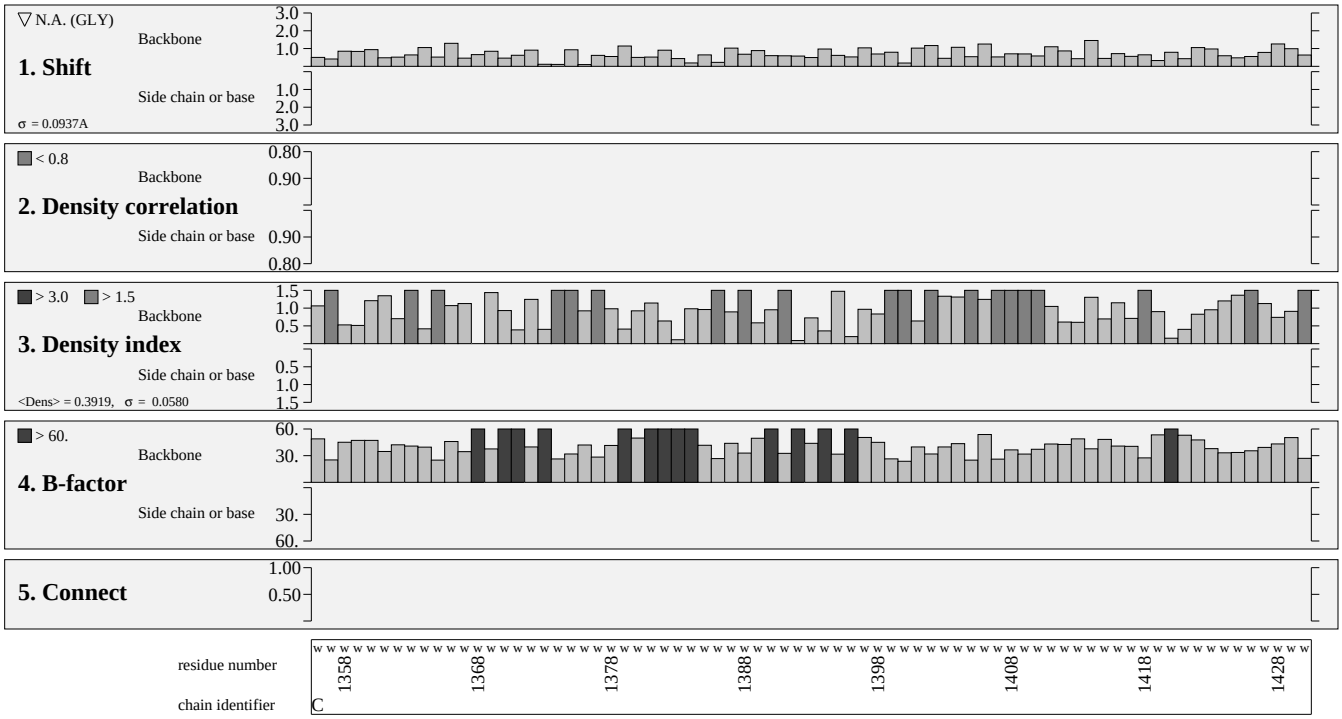


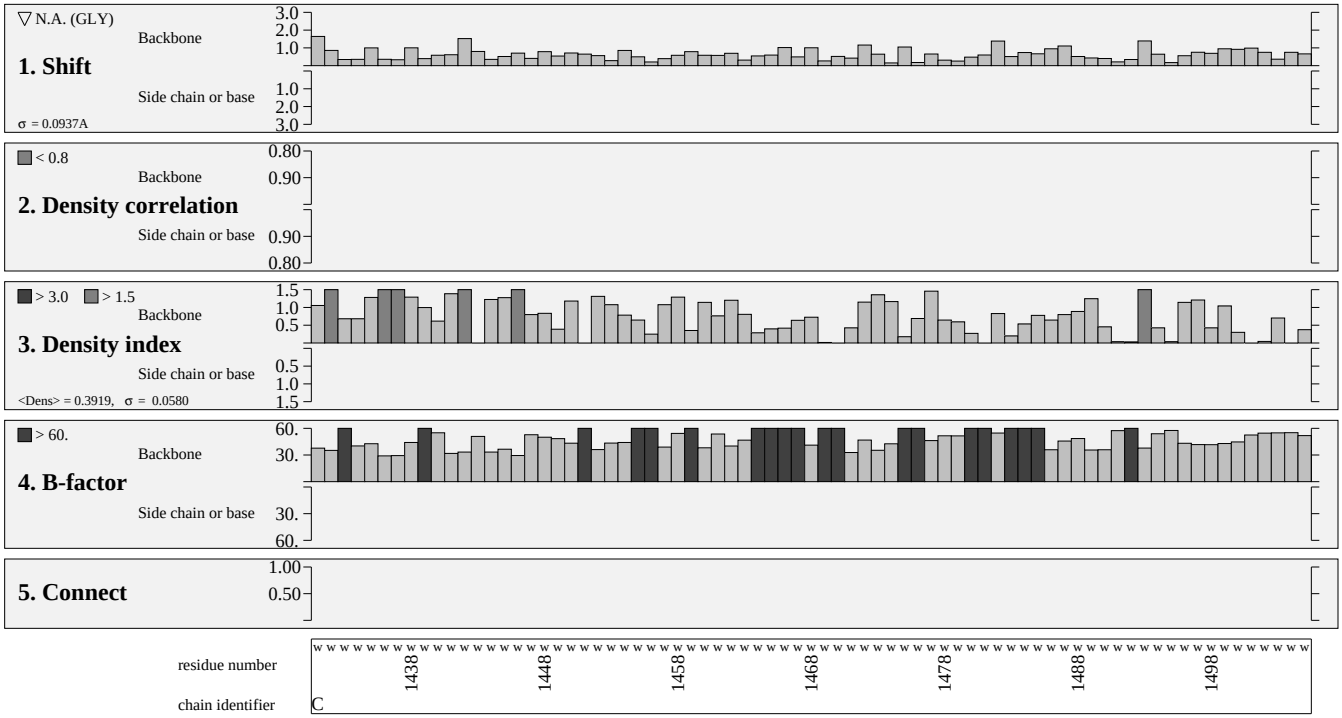
SFCHECK 7.03.16

Structure Factor Check

2FBW

Local estimation (26)



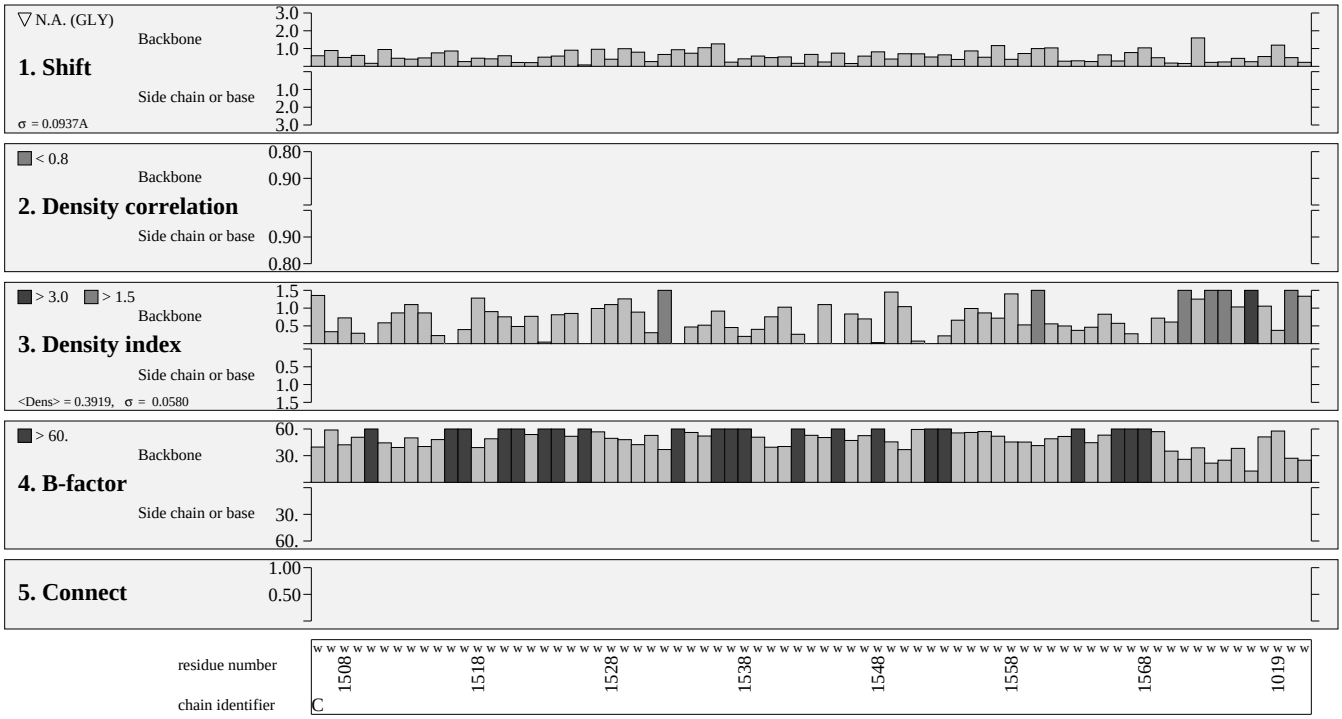


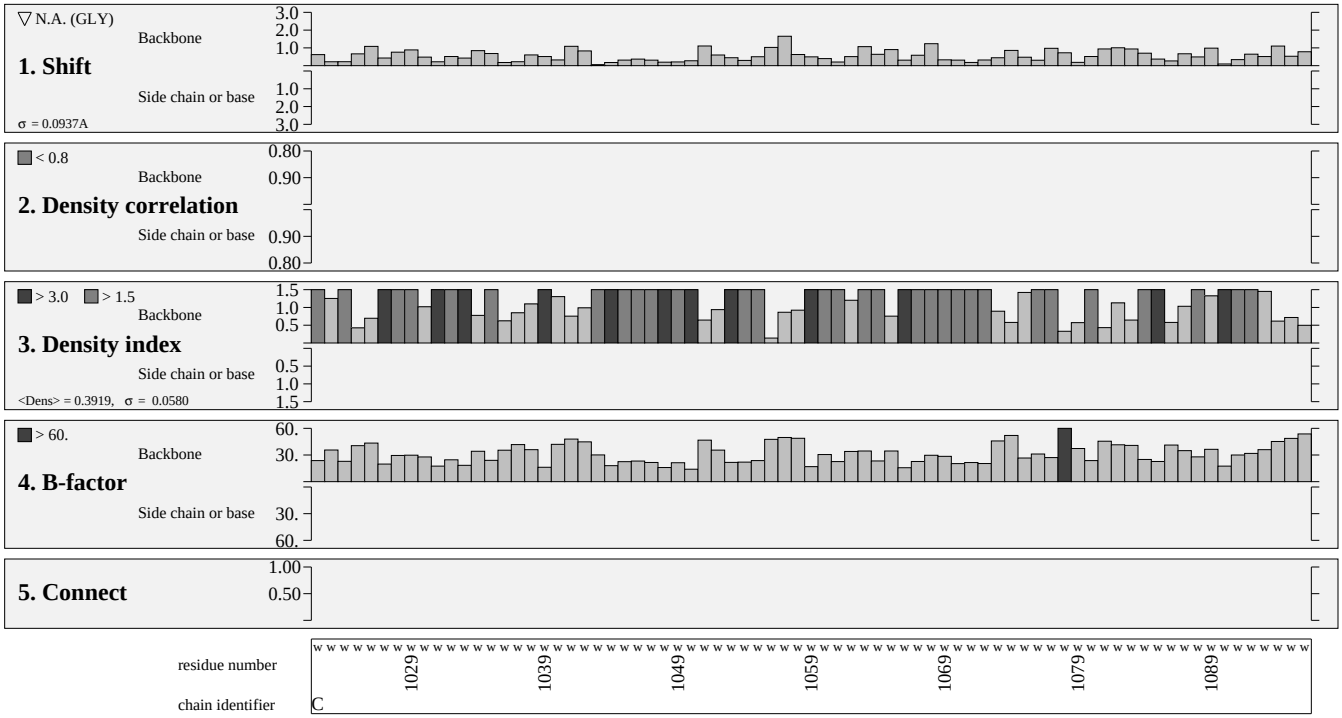
SFCHECK 7.03.16

Structure Factor Check

2FBW

Local estimation (27)



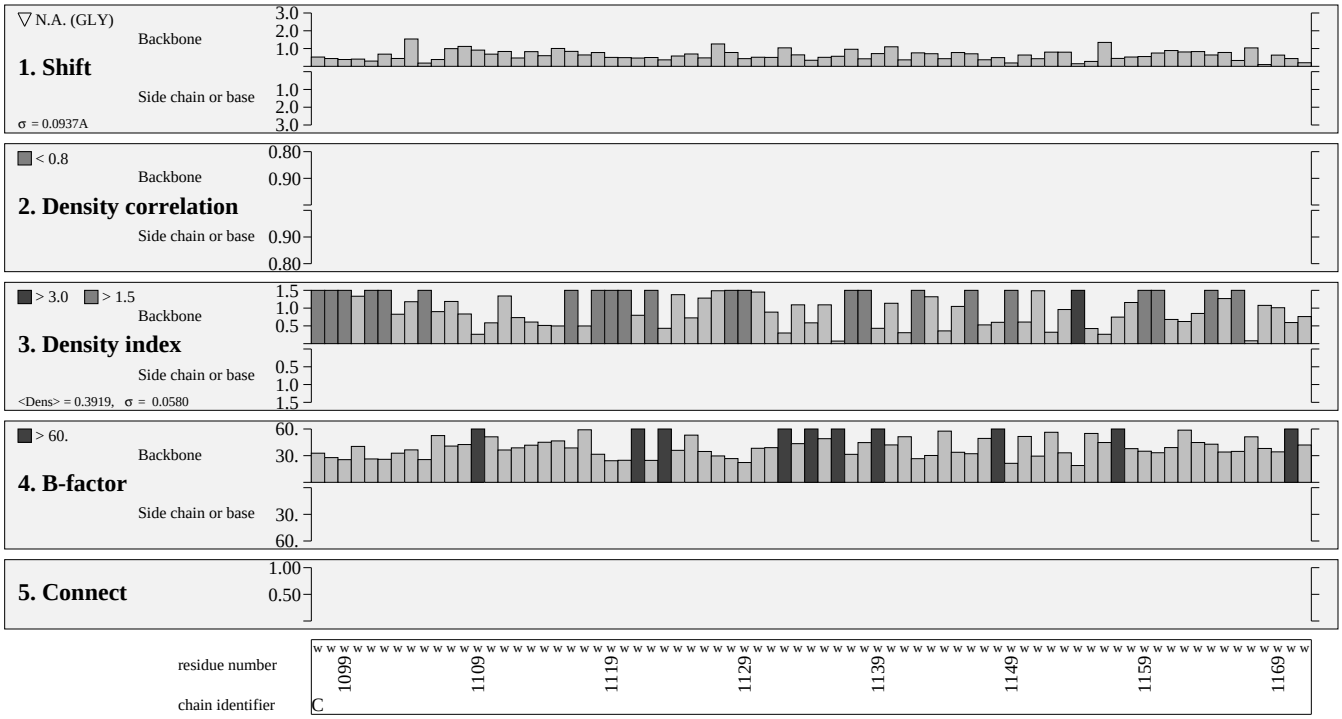


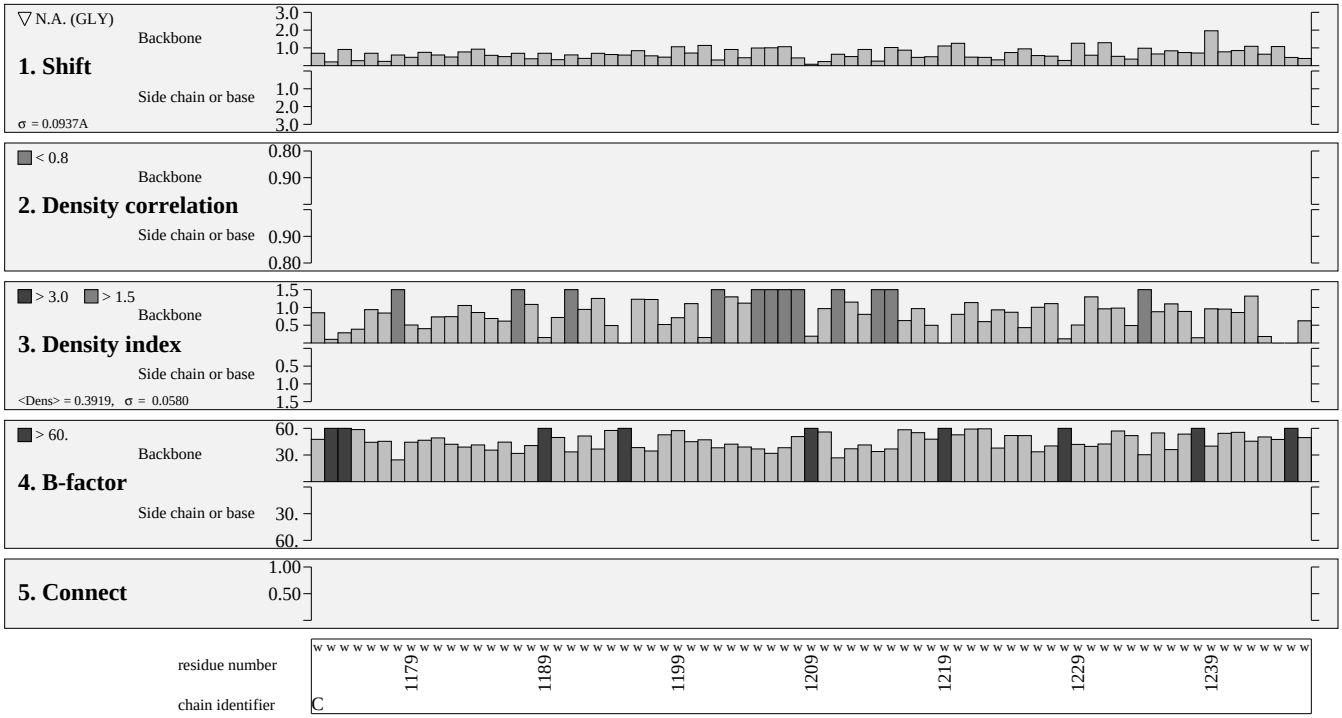
SFCHECK 7.03.16

Structure Factor Check

2FBW

Local estimation (28)



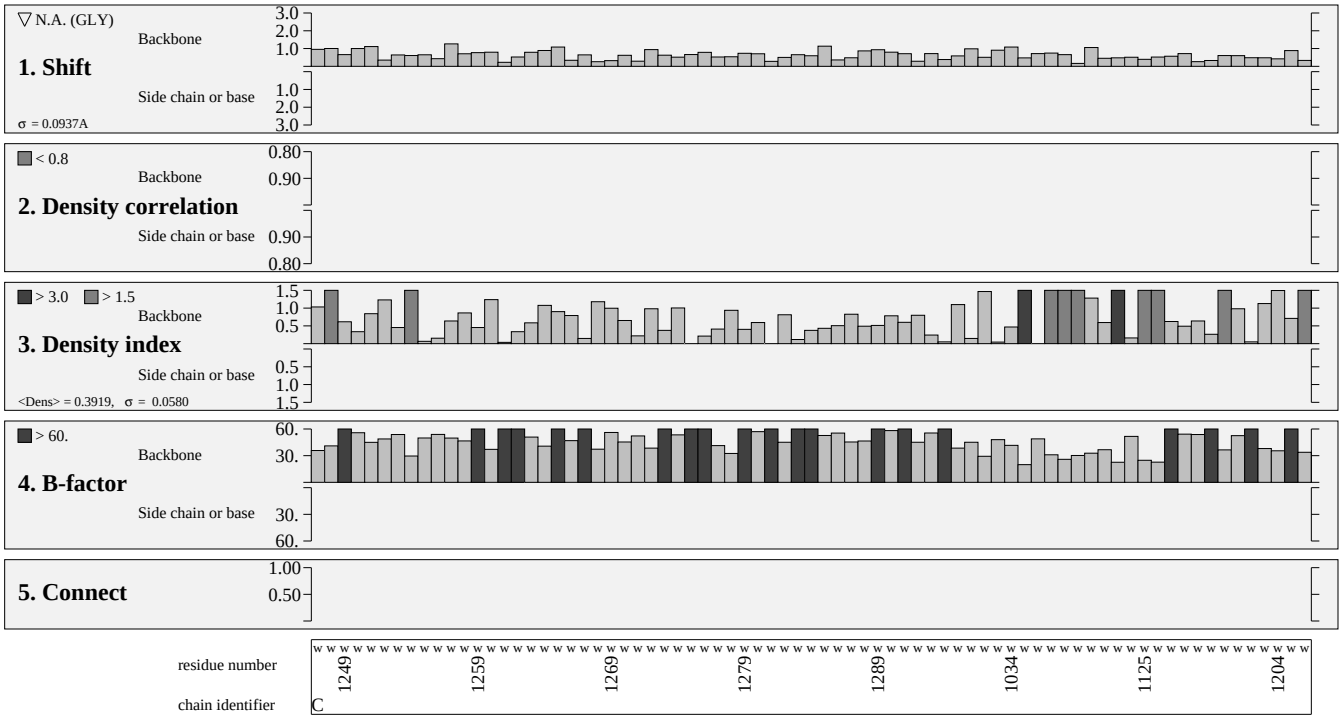


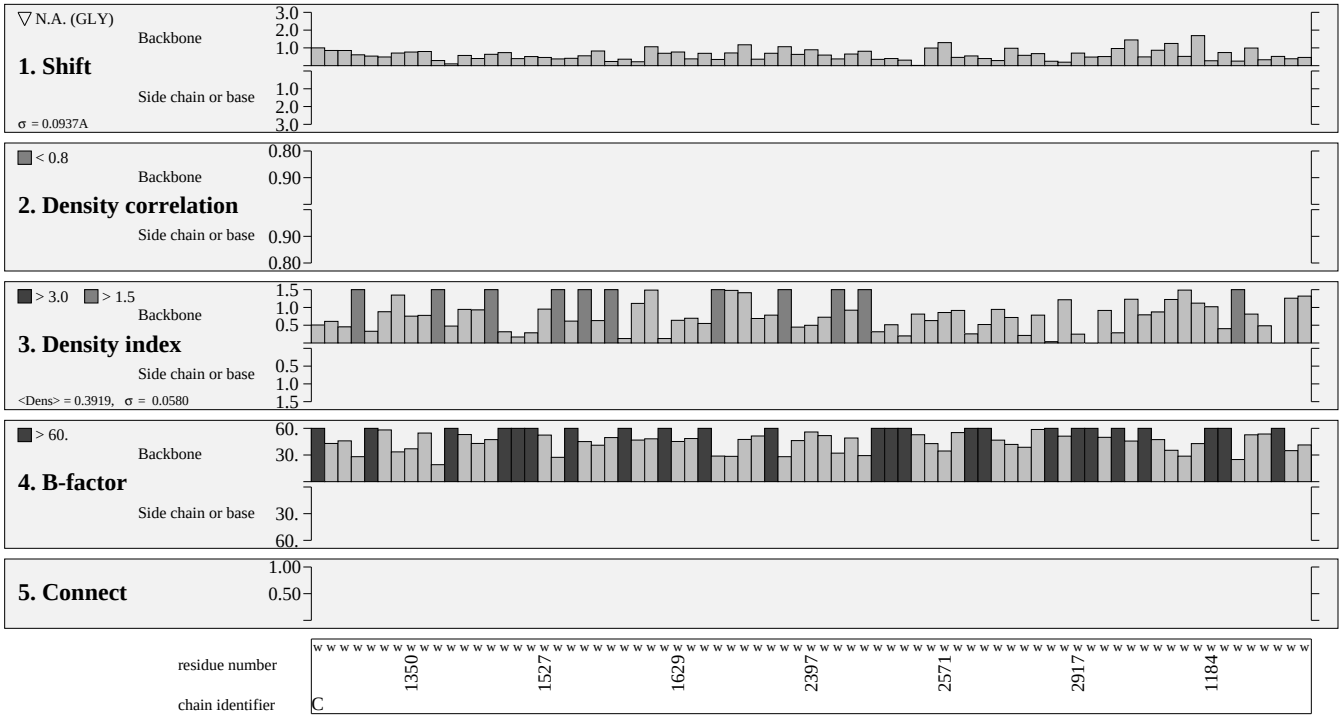
SFCHECK 7.03.16

Structure Factor Check

2FBW

Local estimation (29)





SFCHECK 7.03.16

Structure Factor Check

2FBW

Local estimation (30)