

# Structure Factor Check

## 3SFE

Title: CRYSTAL STRUCTURE OF PORCINE MITOCHONDRIAL RESPIRATORY COMPL  
BOUND WITH OXALOACETATE AND THIABENDAZOLE  
Date: 13-JUN-11  
PDB code: 3SFE

### Crystal

Cell parameters:

a: 70.71 A    b: 83.42 A    c: 294.01 A  
 $\alpha$ : 90.00     $\beta$ : 90.00     $\gamma$ : 90.00

Space group: P 21 21 21

### Structure Factors

#### Input

Nominal resolution range: 45.2 – 2.81 A  
 Reflections in file: 43928  
 Unique reflections above 0: 34068  
 Reflections > 0: 9860

#### SFCHECK

Nominal resolution range: 45.2 – 2.81 A  
\05max. from input data, min. from author\05  
 Used reflections: 34067  
 Reflections out of resolution: 1  
 Completeness: 78.5 %  
 Anisotropic distribution of Structure Factors  
 ratio of eigen values: 0.8289 1.0000 0.8512  
 B\_overall (by Patterson): 45.A^2  
 Optical resolution: 2.08 A  
 Expected opt. resol. for complete data set: 2.08 A  
 Estimated minimal error: 0.028 A

### Model

8687 atoms (52 water molecules)

Number of chains: 15  
 Volume not occupied by model: 57.0 %  
 <B> (for atomic model): 56.5 A^2  
 $\sigma$ (B): 13.16 A^2  
 Matthews coefficient: 3.56  
 Corresponding solvent % : 65.23

### Model vs. Structure Factors

R-factor for all reflections: 0.274  
 Correlation factor: 0.829  
 R-factor: 0.285  
     for  $F > 2.0\sigma$   
         nom. resolution range: 50.00 – 2.81A  
         reflections used: 34067  
 Rfree: 0.327  
 Nfree: 1717  
 R-factor without free-refl.: 0.283  
 Non free-reflections: 32350  
 <u> (error in coords by Luzzati plot): 0.398 A  
 Estimated maximal error: 0.173 A  
 DPI: 0.415 A

#### Scaling

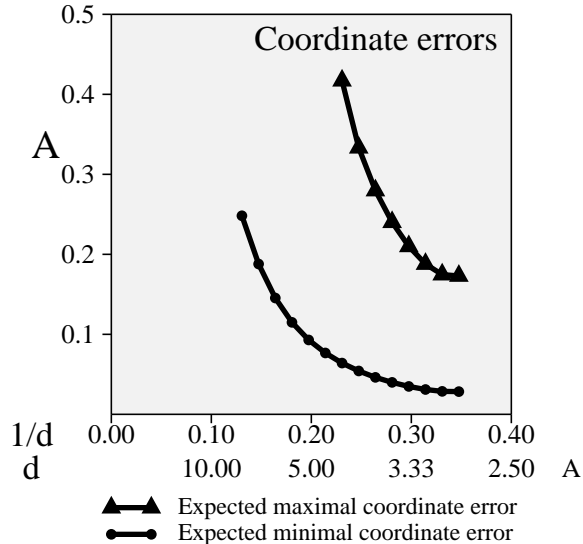
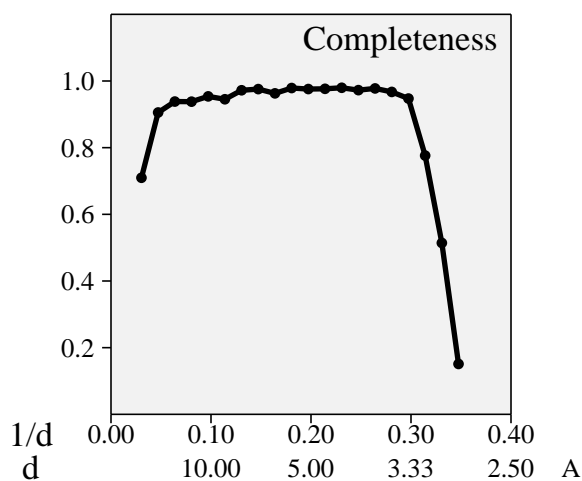
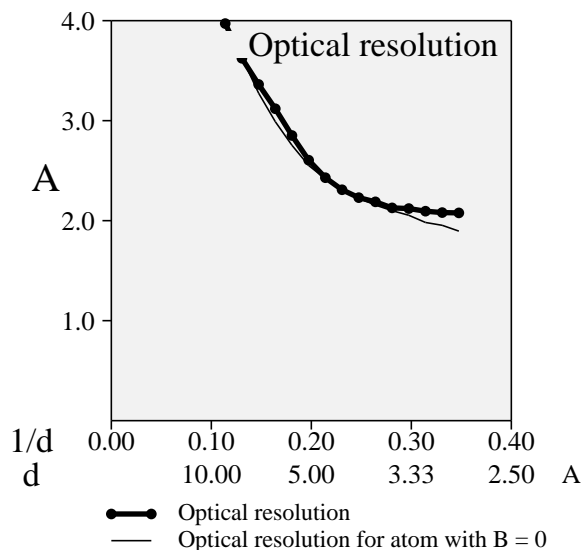
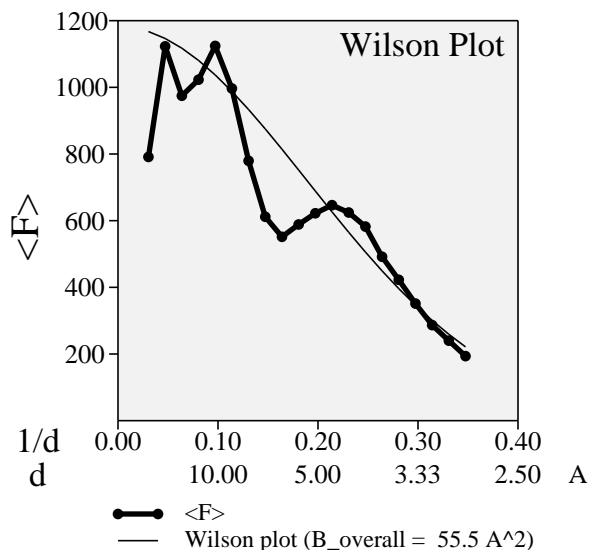
Scale: 0.893  
 Bdiff: -4.77  
 Anisothermal Scaling (Beta):  
 0.1084 1.9731 -0.2920 0.0000 0.0000 0.0000  
 Solvent correction – Ks,Bs: 0.808 250.036

### Refinement

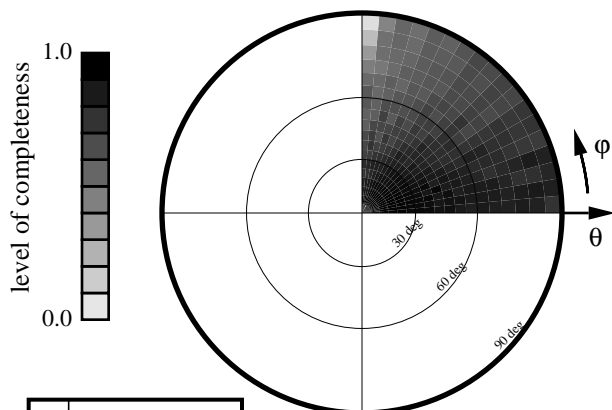
Program: REFMAC 5.5.0088  
 Nominal resolution range: 50.0 – 2.81 A  
 Reported R-factor: 0.214  
 Number of reflections used: 32353  
 Reported Rfree: 0.27  
 Sigma cut-off: N.A.

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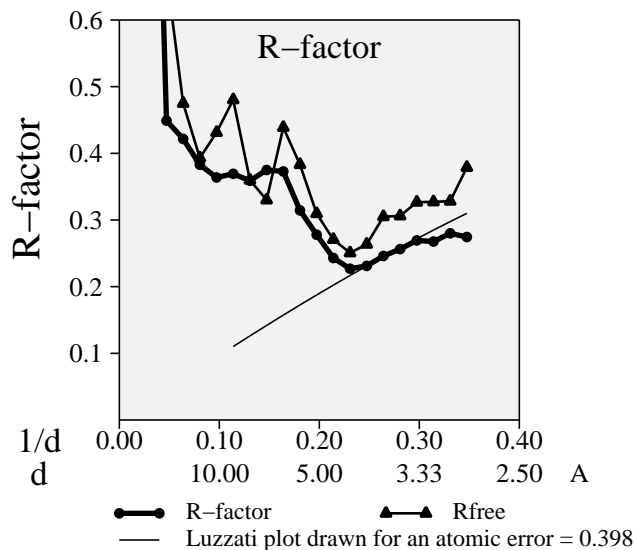


Stereographic projection of the averaged radial completeness



	$\theta$	$\phi$
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

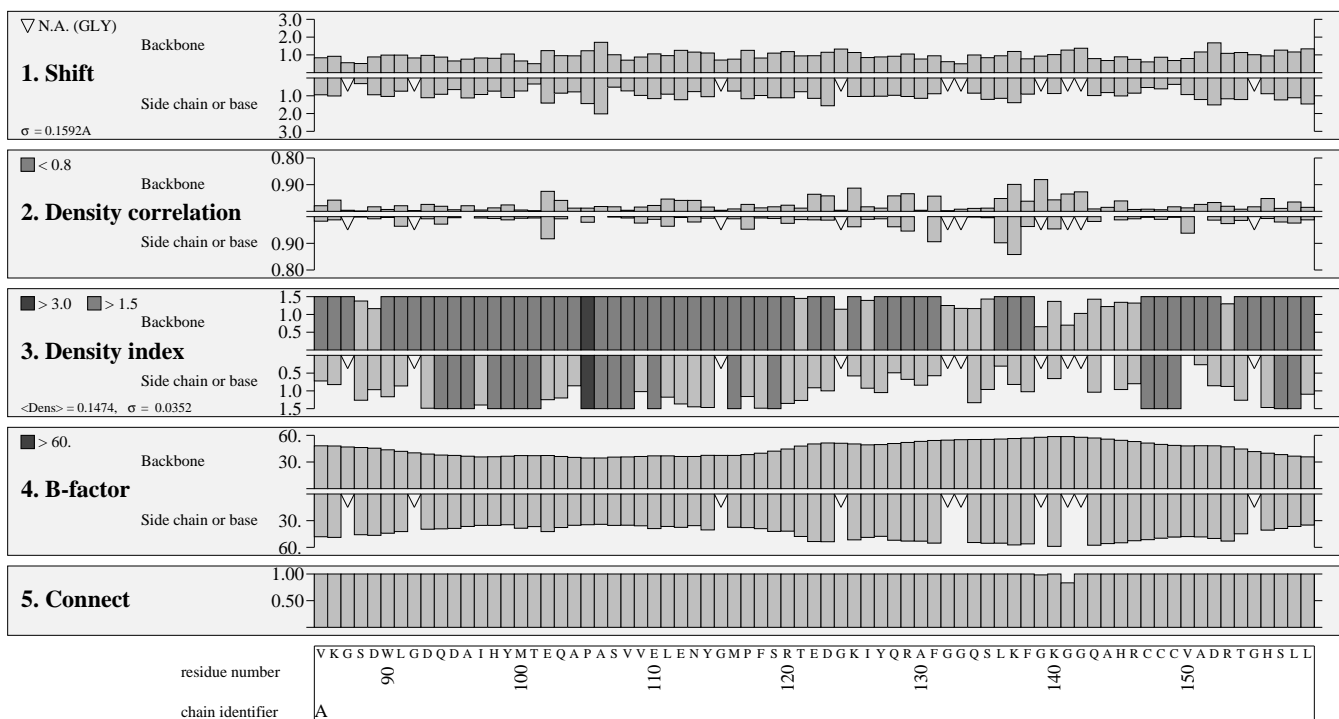
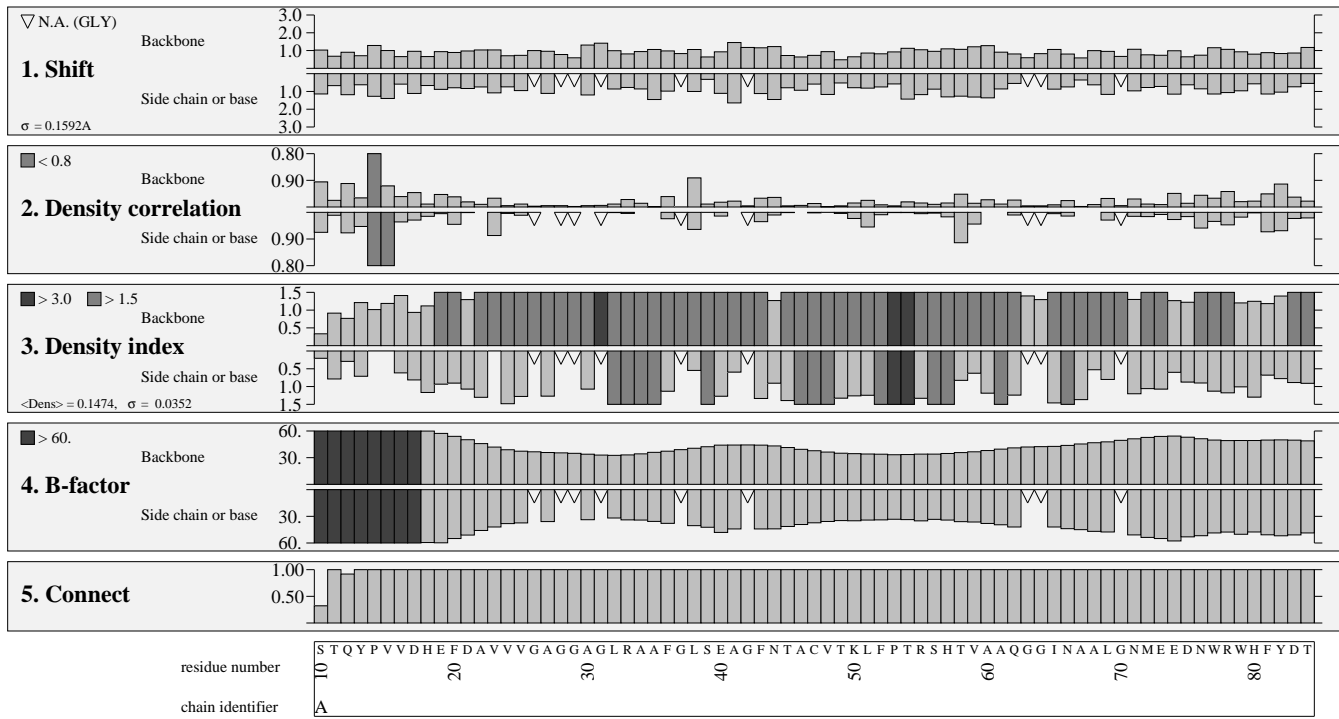
polar coordinates of the crystallographical axes



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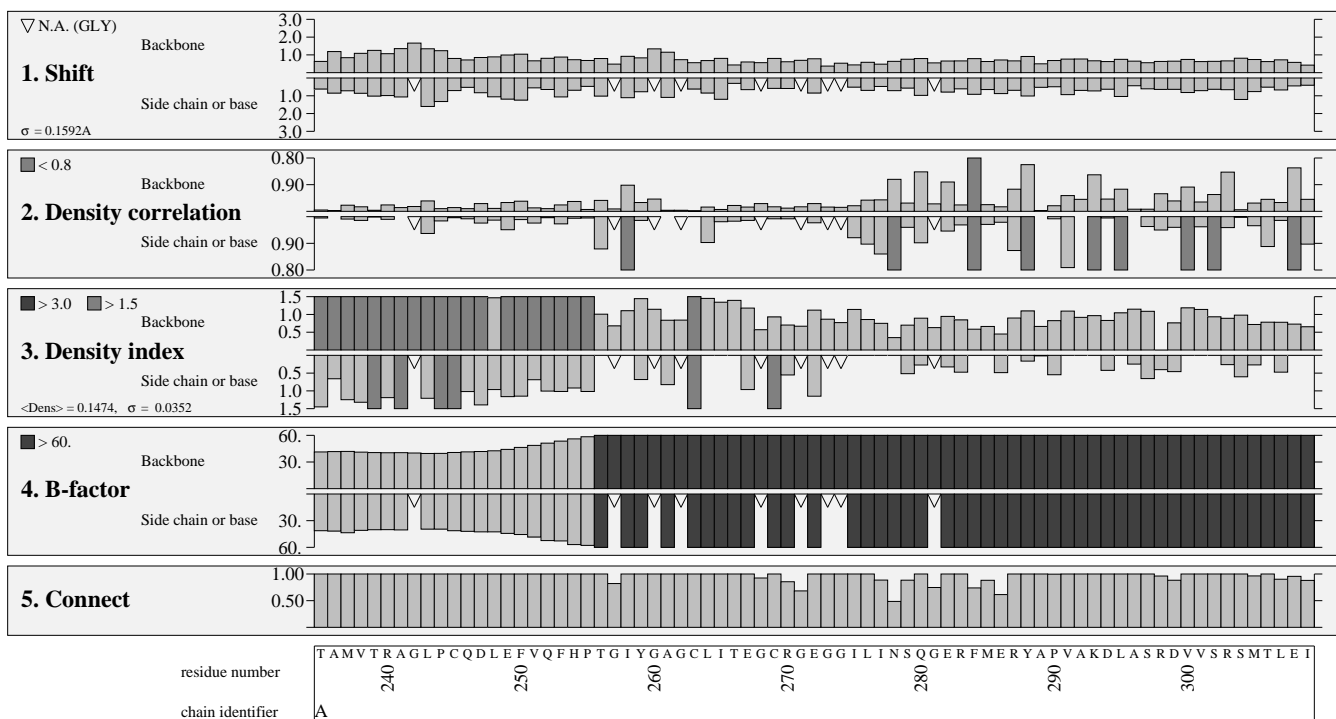
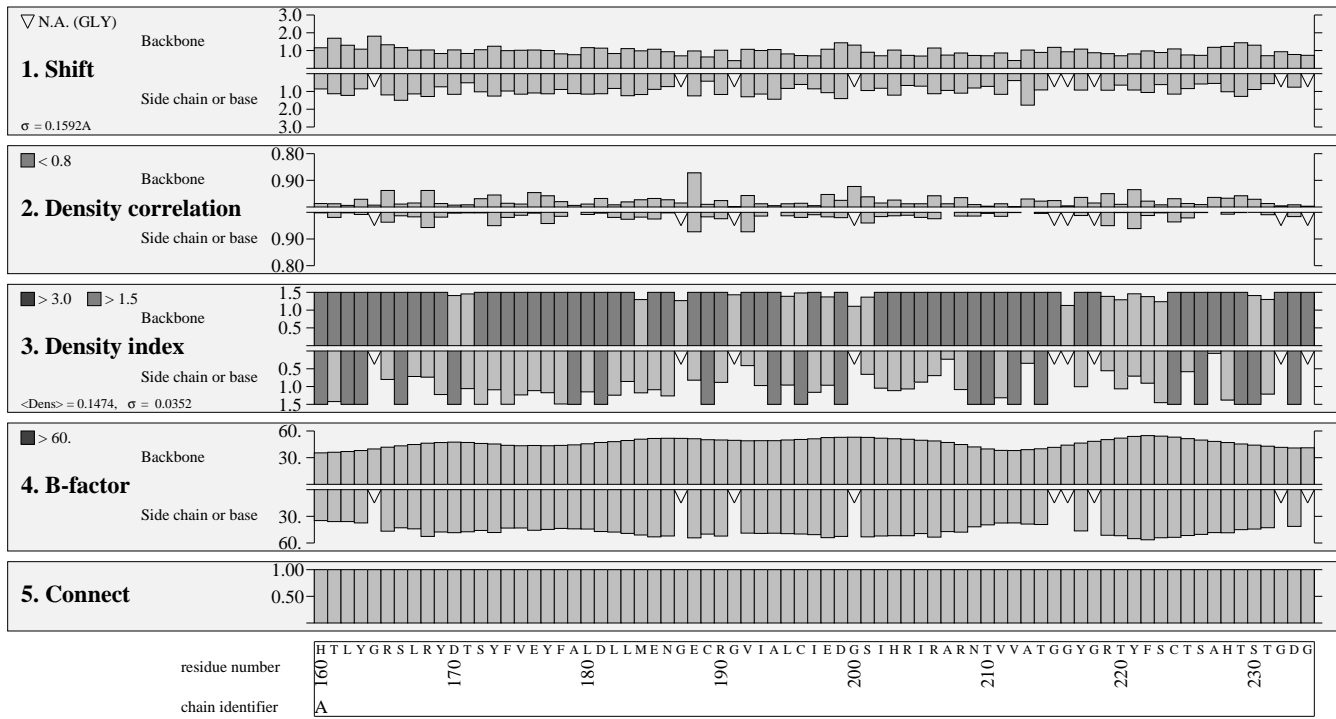
### Local estimation



# Structure Factor Check

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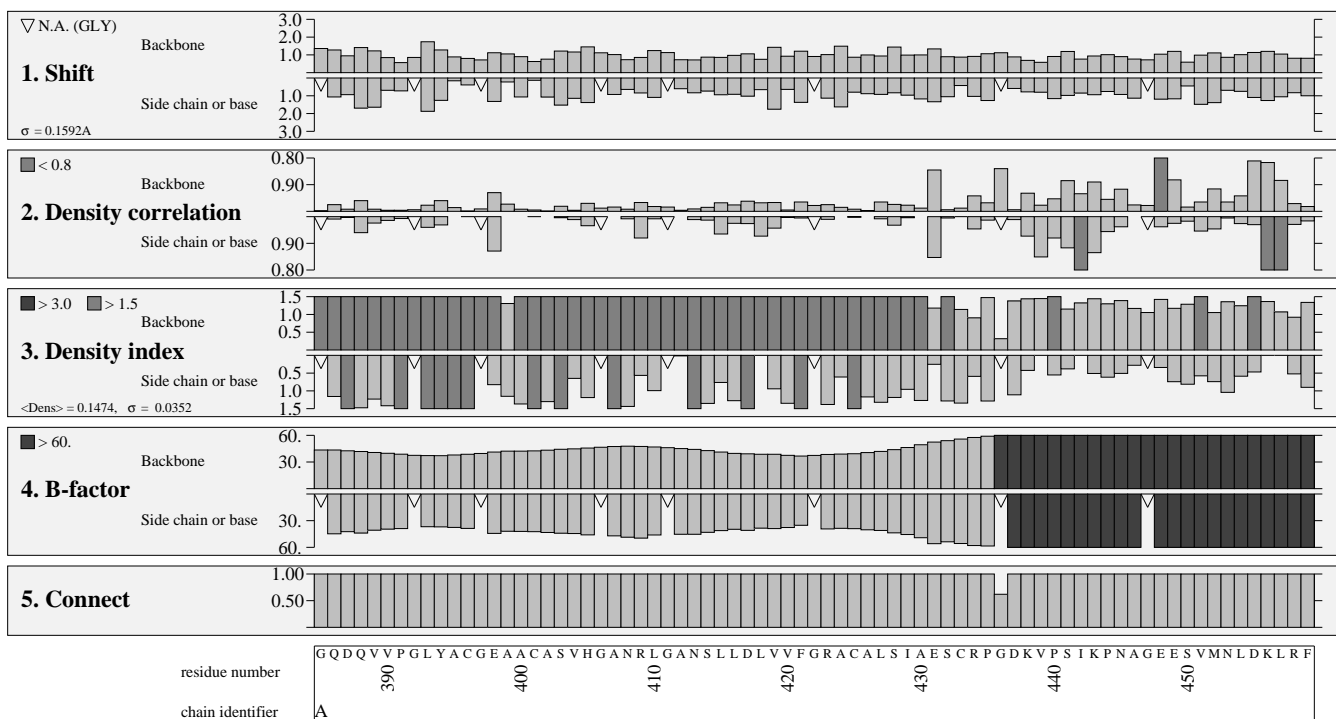
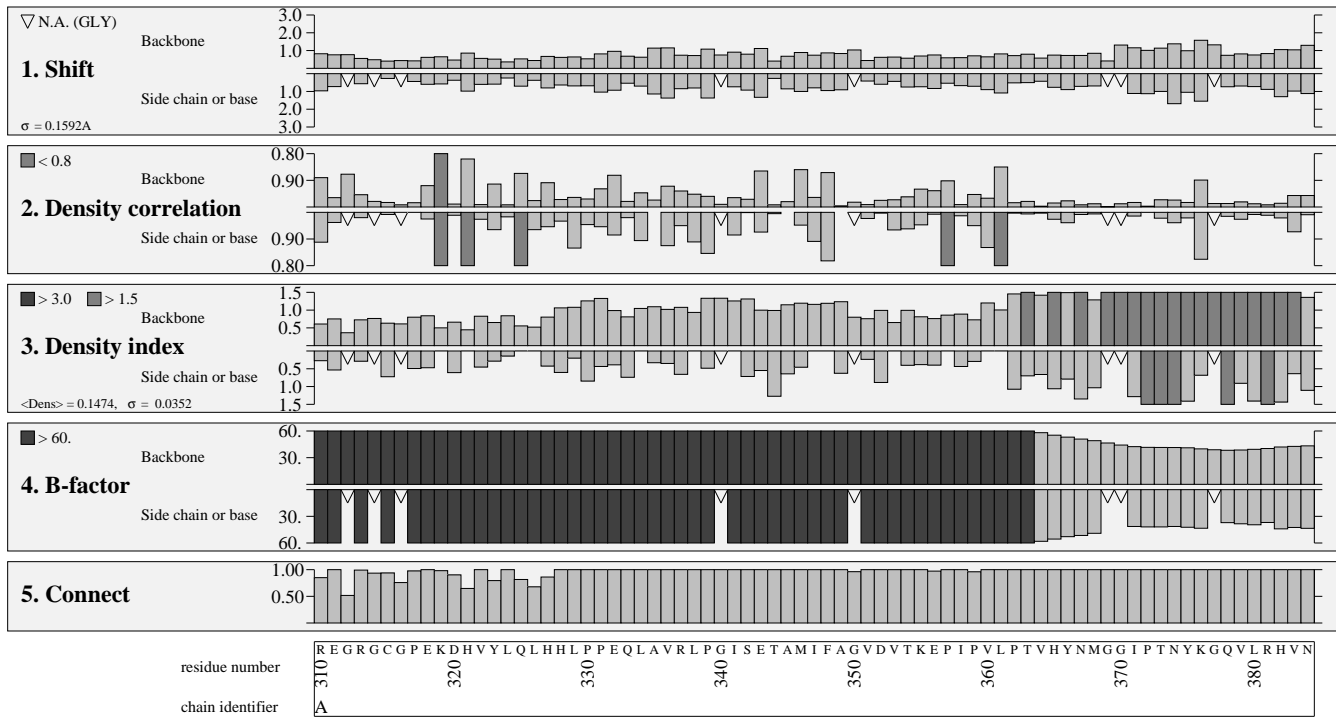
### Local estimation (2)



# Structure Factor Check

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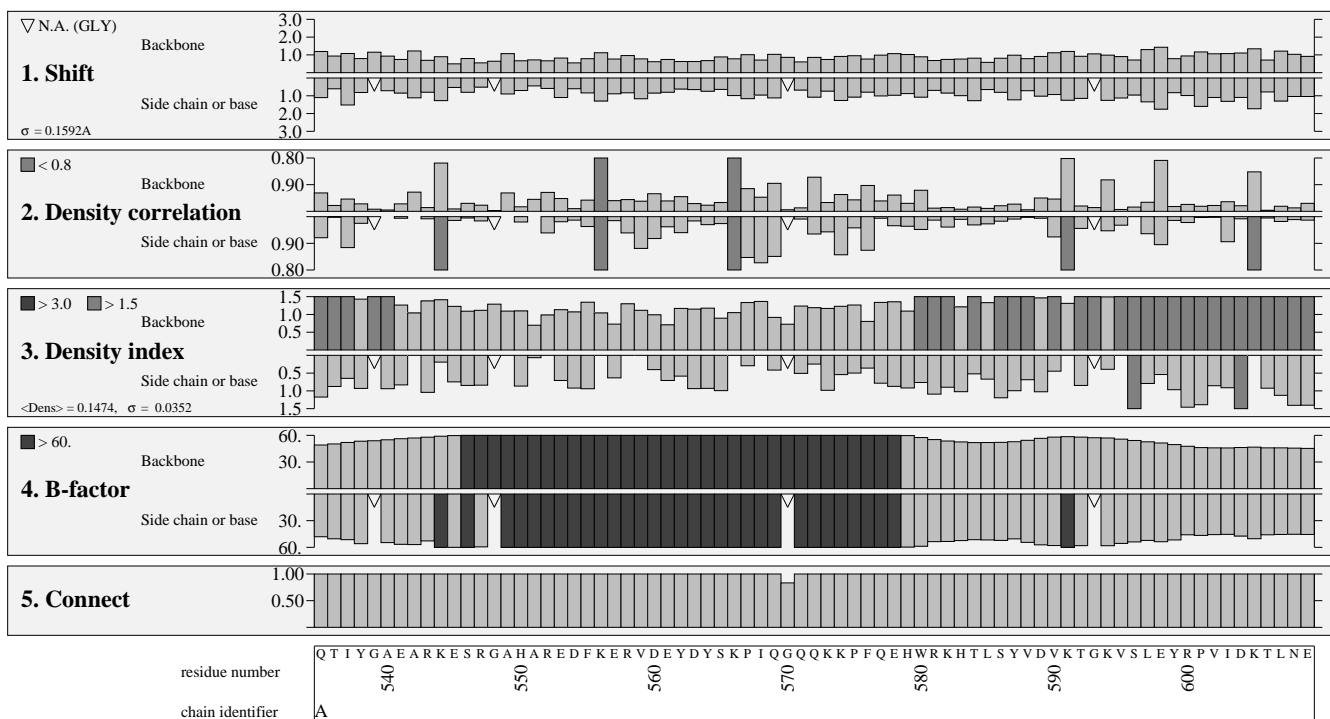
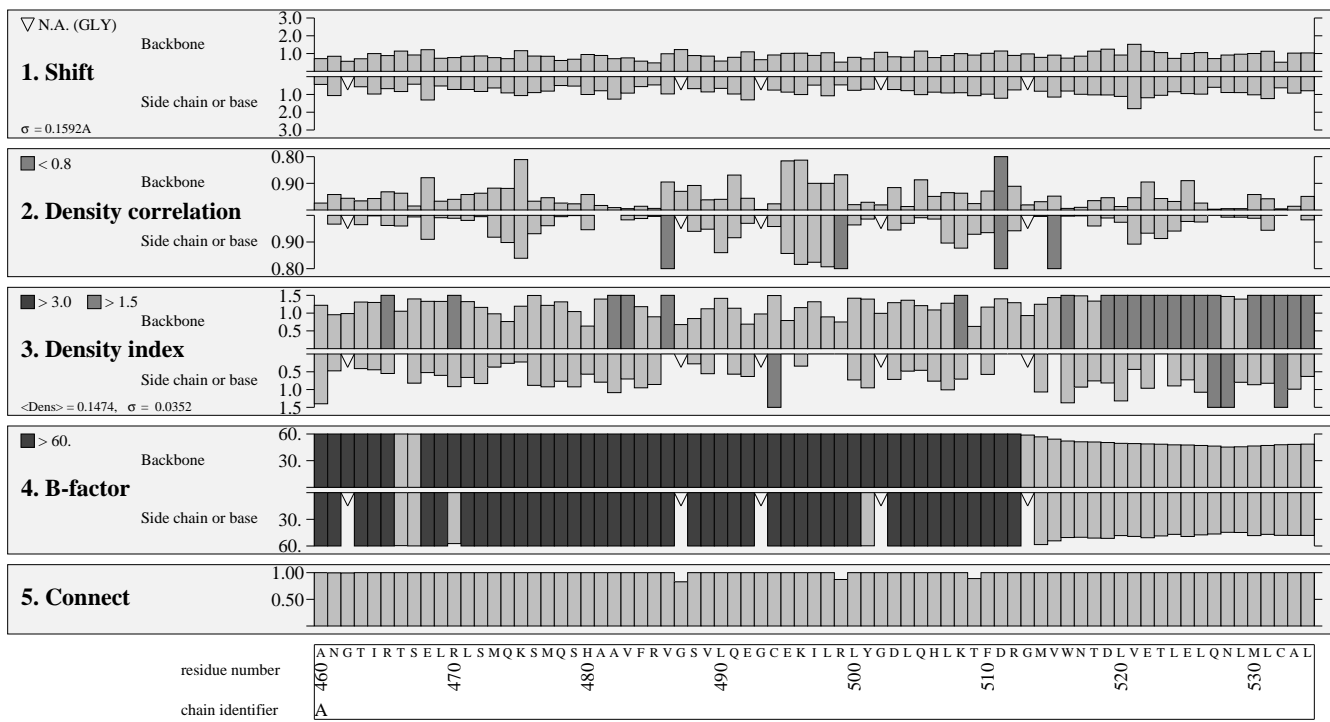
### Local estimation (3)



# Structure Factor Check

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### Local estimation (4)

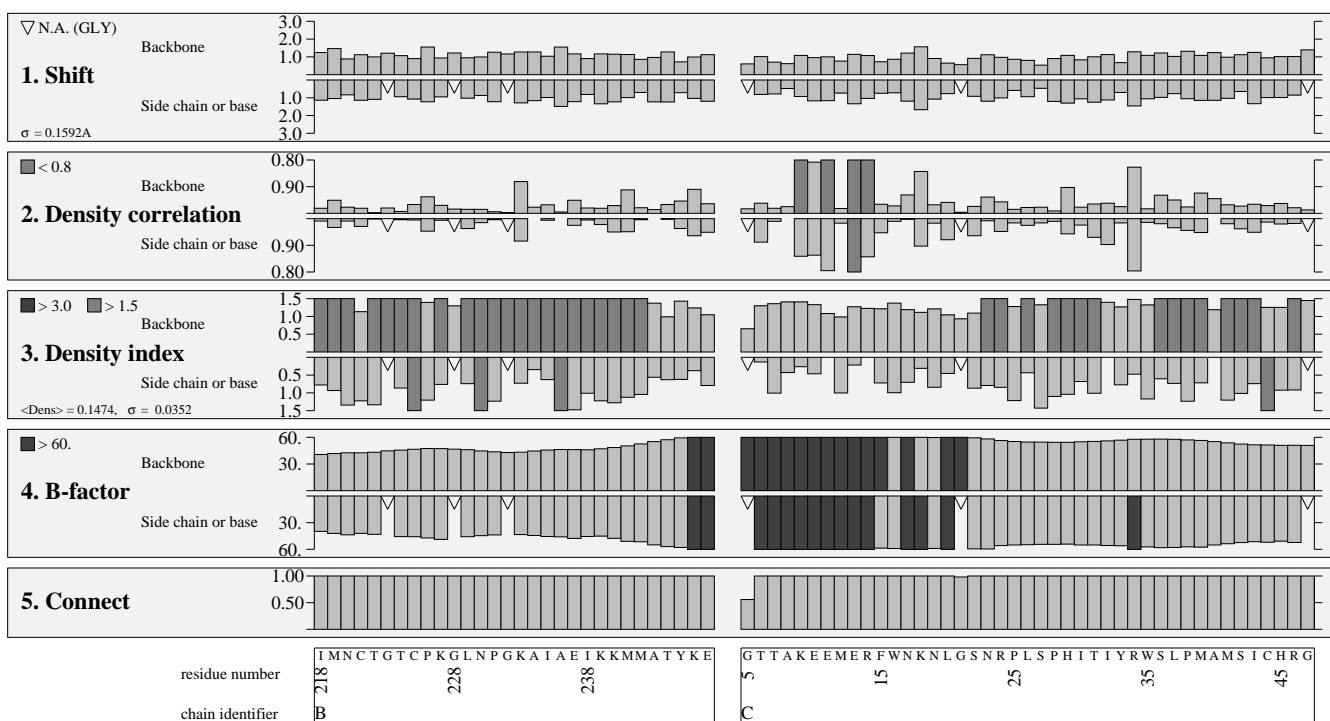
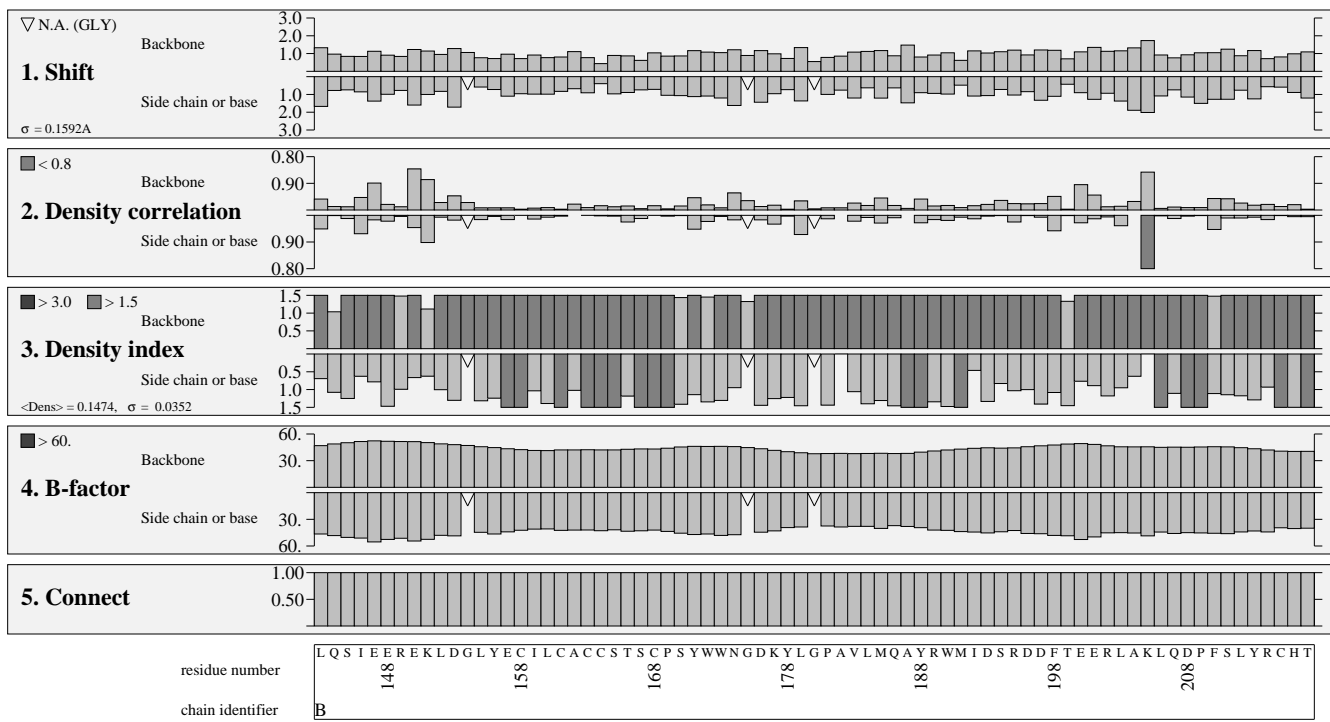




# Structure Factor Check

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### Local estimation (6)





# Structure Factor Check

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### Local estimation (7)

