BINF 731

Protein Structure Analysis

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Structure verification and validation

Biotech Validation Suite
ERRAT
Verify3D
Procheck

Procheck programs

CLEAN - cleaning PDF file
SECSTR - assigning secondary structure
NB - identifying non-bonded interactions
ANGLEN - calculating bond lengths and bond angles
TPLOT, PPLOT, BPLOT - graphical output

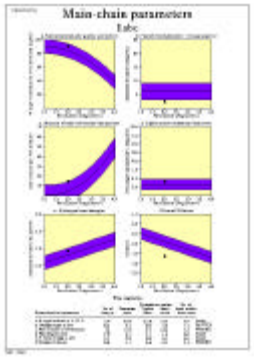
Bond lengths (Procheck)

Bond	labeling		Value	sigma
C-N	C-NH1	(except Pro)	1.329	0.014
	C-N	(Pro)	1.341	0.016
C-O	C-O		1.231	0.020
Calpha-C	CH1E-C	(except Gly)	1.525	0.021
	CH2G*-C	(Gly)	1.516	0.018
Calpha-Cbeta	CH1E-CH3E	(Ala)	1.521	0.033
	CH1E-CH1E	(Ile,Thr,Val)	1.540	0.027
	CH1E-CH2E	(the rest)	1.530	0.020
N-Calpha	NH1-CH1E	(except Gly,Pro)	1.458	0.019
	NH1-CH2G*	(Gly)	1.451	0.016
	N-CH1E	(Pro)	1.466	0.015

Bond angles (Procheck)

Angle	labeling		Value	sigma
C-N-Calpha	C-NH1-CH1E	(except Gly,Pro)	121.7	1.8
	C-NH1-CH2G*	(Gly)	120.6	1.7
	C-N-CH1E	(Pro)	122.6	5.0
Calpha-C-N	CH1E-C-NH1	(except Gly,Pro)	116.2	2.0
	CH2G*-C-NH1	(Gly)	116.4	2.1
	CH1E-C-N	(Pro)	116.9	1.5
Calpha-C-O	CH1E-C-O	(except Gly)	120.8	1.7
	CH2G*-C-O	(Gly)	120.8	2.1

Procheck output



a. Ramachandran plot quality - **percentage** of the protein's residues that are in the **core** regions of the Ramachandran plot.

b. Peptide bond planarity - **standard deviation** of the protein structure's **omega** torsion angles.

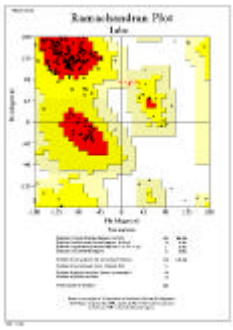
c. Bad non-bonded interactions - **number of bad contacts** per **100** residues.

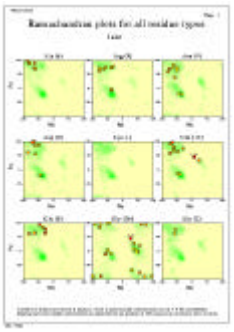
d. C$_\alpha$ tetrahedral distortion - **standard deviation** of the **z torsion angle** (**C$_\alpha$**, **N**, **C**, and **C$_\beta$**).

e. Main-chain hydrogen bond energy - **standard deviation** of the **hydrogen bond energies** for **main-chain hydrogen bonds**.

f. Overall G-factor - average of different G-factors for each residue in the structure.

Procheck output





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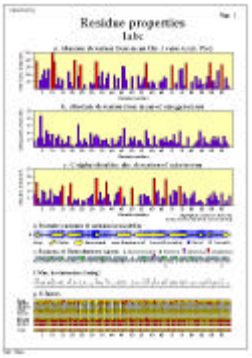
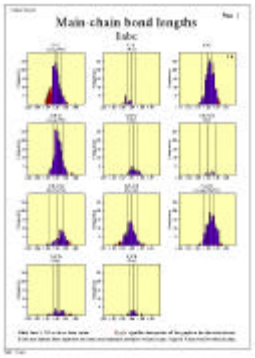
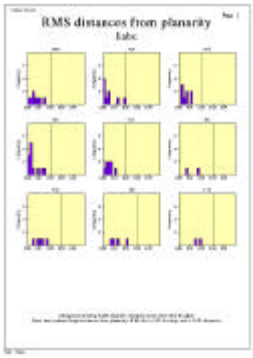
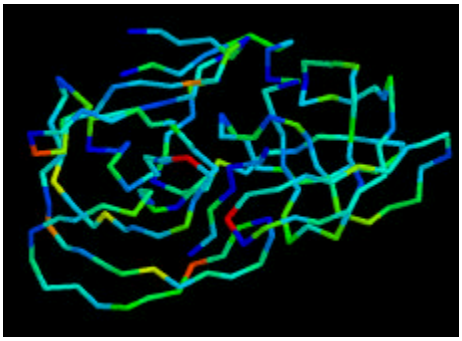




Procheck output



Procheck output - backbone G factors



Procheck output - all atom G factors