BINF 731

Protein Structure Analysis

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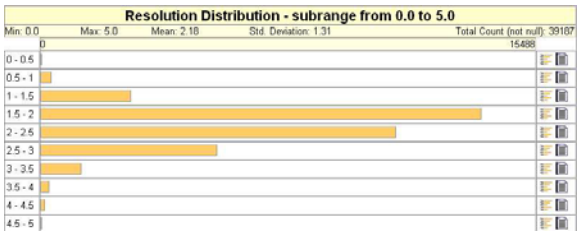
wwPDB statistics

Year	Total Depositions	Deposited To			Processed By		
		RCSB	PDBj	EBI	RCSB	PDBj	EBI
2000	2983	2445	10	528	2294	161	528
2001	3286	2673	118	495	2407	384	495
2002	3563	2769	289	505	2401	657	505
2003	4830	3488	673	669	3135	1026	669
2004	5508	3796	900	812	3083	1613	812
2005	6678	4507	1166	1005	3563	2110	1005
2006	7282	5145	1052	1085	4252	1945	1085
2007	6045	3872	1373	800	3575	1670	800
TOTAL	40175	28695	5581	5899	24714	9562	5899

PDB resolutions



PDB redundancy

Method	Description	# of Clusters
blast	95% identity (one chain)	17575
blast	90% identity (one chain)	16853
blast	70% identity (one chain)	15114
blast	50% identity (one chain)	12886
blast	40% identity (one chain)	11218
blast	30% identity (one chain)	9294

PDB ambiguities

Table 1 The number of PDB structures retrieved by ambiguous chemical component codes

Code	Name	Number of PDB structures[a]
SUL	Sulfate anion	156 (3.6%)
SO4	Sulfate ion	4083 (96.4%)
SUL and SO4	Sulfate anion and sulfate ion	1 (0.03%)
NET	Tetraethylammonium ion	9 (90%)
E4N	Tetraethylammonium ion	1 (10%)
MMC	Methyl mercury ion	8 (66.66%)
HGC	Methyl mercury ion	4 (33.33%)

[a]Percentages of the total number of structures with the chemical component are shown in brackets. Search carried out August 2006.

Schierz et al., Nature Biotechnology 25:437

Structure verification and validation

Biotech Validation Suite
ERRAT
Verify3D
Procheck

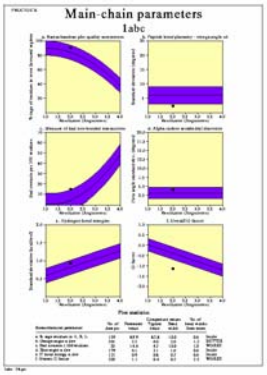
Bond lengths (Procheck)

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.

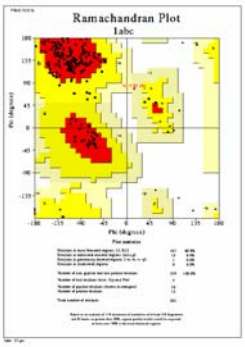
c. Bad non-bonded interactions - number of bad contacts per 100 residues.

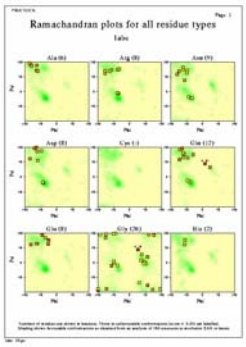
d. Cα tetrahedral distortion - standard deviation of the ζ torsion angle (Cα, N, C, and Cβ).

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

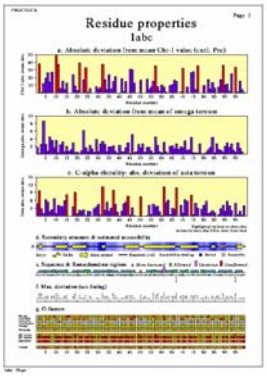
f. Overall G-factor - average of different G-factors for each residue in the structure.

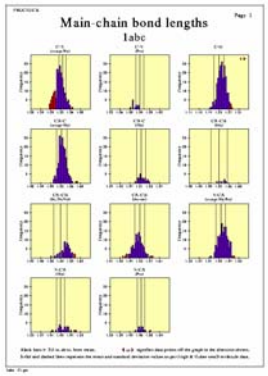
Procheck output



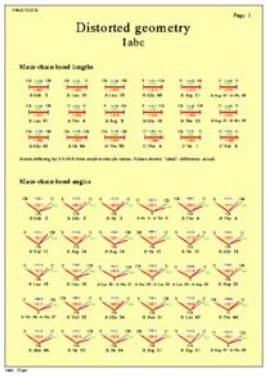


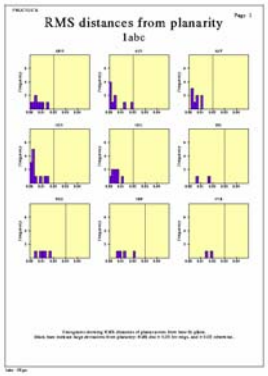
Procheck output



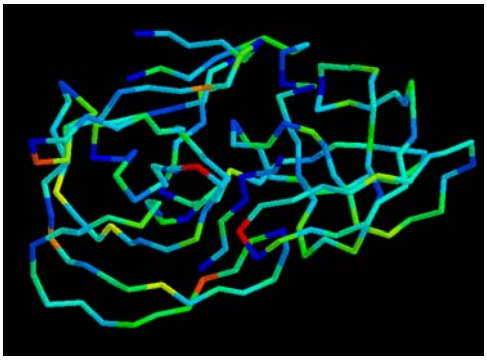


Procheck output

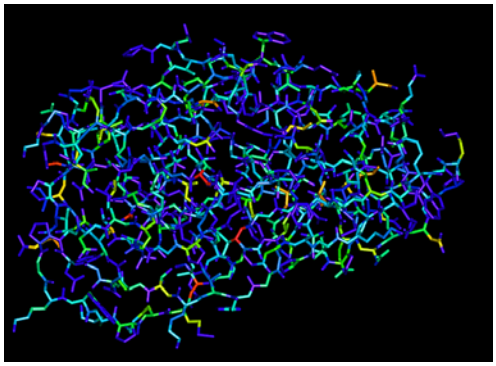




Procheck output - backbone G factors



Procheck output - all atom G factors



Root mean square deviation

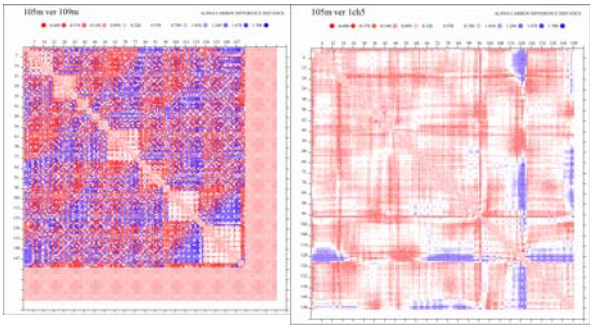
Coordinate based RMSD

$$RMSd(A,B) = \min_T \sqrt{\sum_{i=1}^{n} (A_i - TB_i)^2}$$

Distance based RMSD

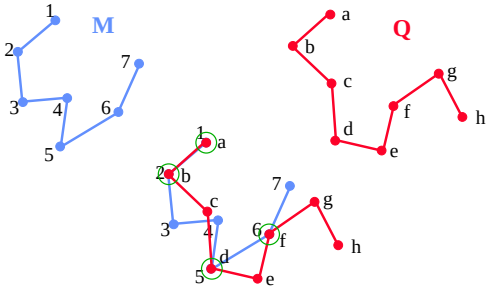
$$RMSd_D(A,B) = \frac{1}{m}\sqrt{\sum_{i=1}^{m}\sum_{j=1}^{m}\left(d_{ij}^A - d_{ij}^B\right)^2}$$

Difference Distance Matrix Plot (DDMP)



Geometric Hashing

Find common subsets, invariant under rotation and translation in two point sets M (model) and Q (query).



Finding the maximum coincidence set is an NP-hard problem

Geometric Hashing

Reference frames

- Two points (basis pair) define a reference frame
- The coordinates of all points are computed in the reference frame (reference frame system)
- There will be pairs of points (from M and Q) with the same coordinates
- The number of such pairs depends on selection of reference frame and reference frame system resolution

Geometric Hashing Algorithm

Preprocessing

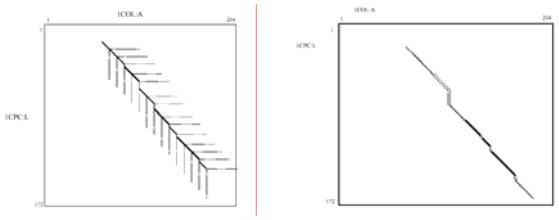
Hash table H is created. It has a bin for each cell in the frame systems. The coordinates of all points in each model frame system are calculated. If there is a point in the cell (p,q) in the frame system with basis (a_i,a_k), then (a_i,a_k) is placed in the bin H(p,q)

Recognition

A pair of points in the query is chosen as basis, and the coordinates of the other points are calculated. These coordinates are used as indices for H, and for each cell being indexed, a vote is given for the (model) basis pairs in the cell. The number of votes for a model basis pair is the number of coinciding points to the query (using the specified query basis pair)

Combinatorial Extension (CE) Algorithm

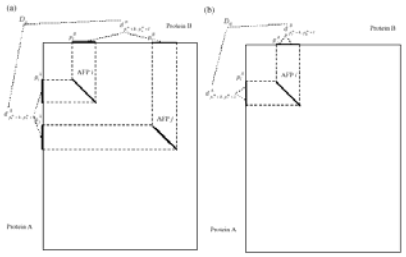
Structure alignment of phycocyanin (1CPC:L) to colicin A (1COL:A).



The solid line represents the optimal path built from AFPs. The dotted line represents the search area at every step of path extension.

The thick solid line represents alignment overlap both before and after optimization.

Combinatorial Extension (CE) Algorithm



Calculation of distance

Dij for two AFPs *i* and *j* from the path

Dii for single AFP *i* from the path.