

Overview

- MolTalk technix
 - object space
- iMolTalk server
 - tool-chains
- MolTalk advanced technix
- Perspectives

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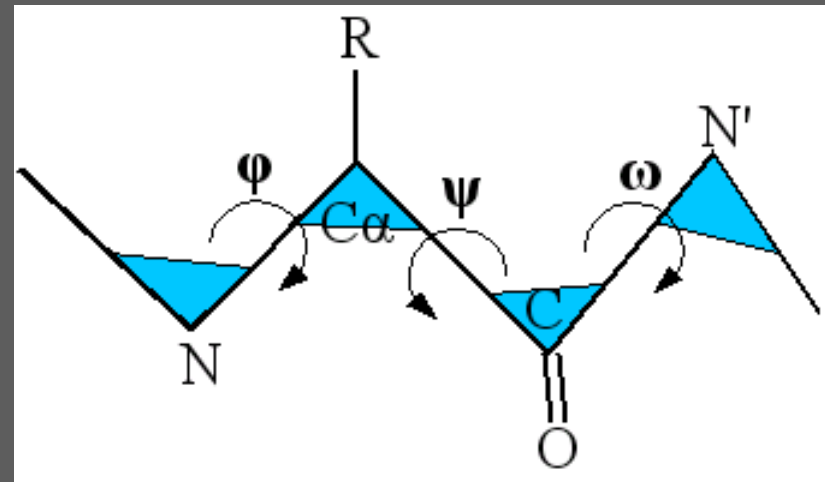


iMolTalk Aim and Scope

- *Paradigm:* it's easy to interpret sequences or MSAs but not 3D structures!
- *Need:* live repository of structural bioinformatics tools ready to serve recurrent analysis tasks in concert with and addition to visual inspection of structures.
- *Idea:* web-based, interactive server implemented in MolTalk, reporting in 1D or 2D
- *Action:* created and made available through <http://i.MolTalk.org>

iMolTalk quality check

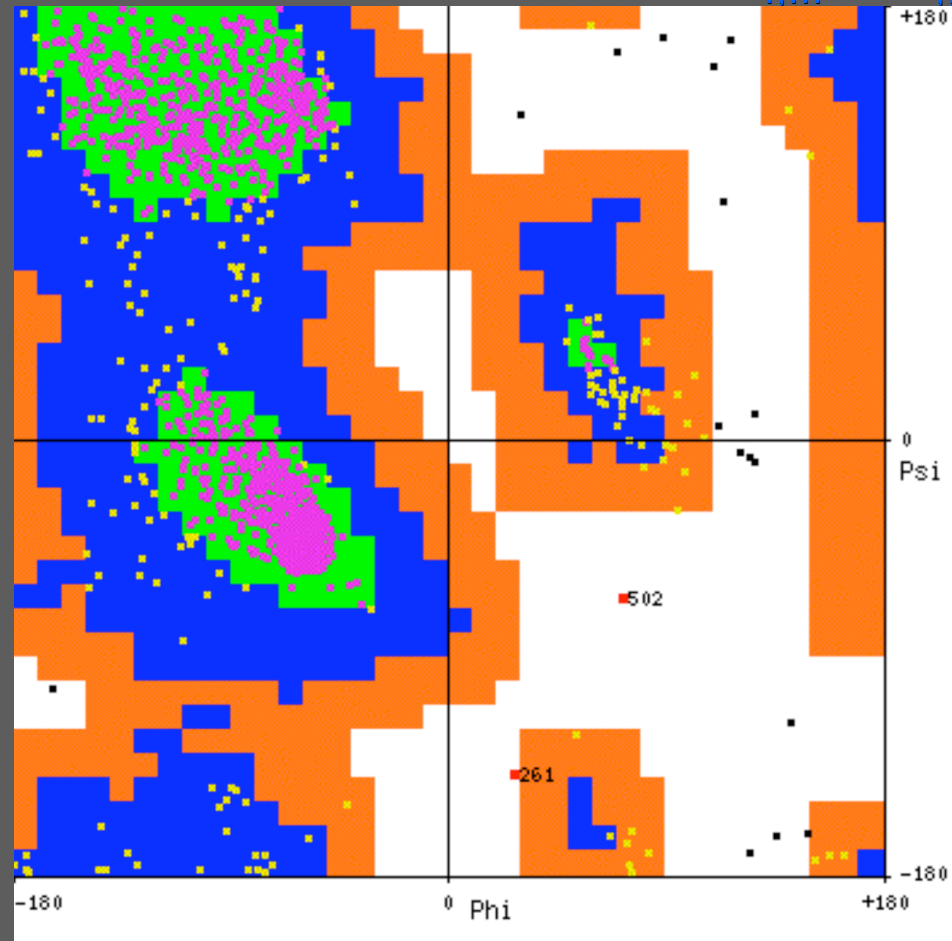
- Most important criteria:
Ramachandran plot as introduced in 1960's.
The observation that amino acids in protein structures prefer certain dihedral angles can be used in structure model assessment



Ramachandran et al., 1963

iMolTalk quality check

- 4 regions defined:
 - CORE
 - ALLOWED
 - GENEROUS
 - DISALLOWED



Morris et al., 1992

iMolTalk 2ndary structure

Computational assignment of secondary structure based on prior knowledge

STRIDE knows several types, in iMolTalk supported:

- α helix
- 3-10 helix
- strand
- turn

iMolTalk residue contacts

Given a Structure, a residue or heterogeneous

- search for all close contacts of residue's atoms with their environment
- infer bonding type for every close contact:
 - hydrogen bond
 - salt bridge
 - other, unspecified

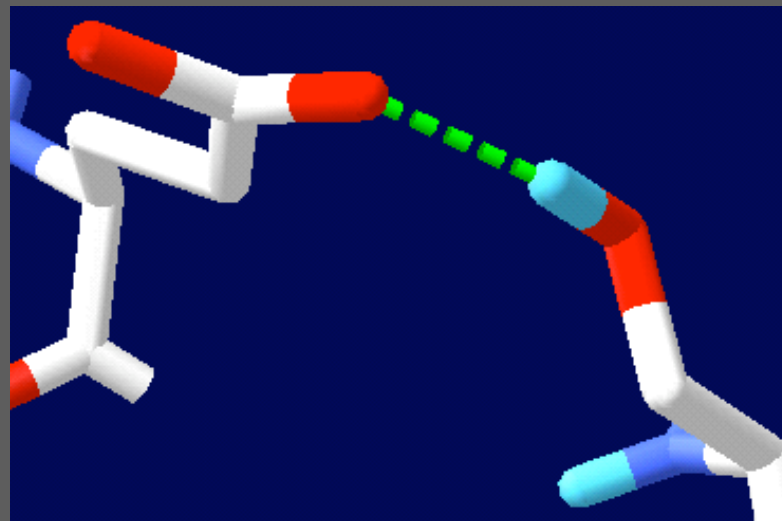
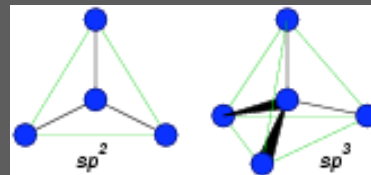
iMolTalk residue contacts

Molecular contacts of Heterogen Residue 258 in Chain: 'A' / #65 Structure: 7AAT

chain1	res1/atm1	distance	res2/atm2	chain2	H-bonding	Charge interaction
7AATA	PLP258(OP1)	2.53	TYR70(OH)	7AATB	H-bond [D-A-AA]:105.9° [A-D-DD]:142.4° a_planarity:-32.6°	O[]...O[]
7AATA	PLP258(OP3)	2.58	SER107(OG)	7AATA	H-bond [D-A-AA]:102.4° [A-D-DD]:119.2°	O[]...O[]
7AATA	PLP258(OP3)	2.79	GLY108(N)	7AATA	H-bond [D-A-AA]:121.4° [A-D-DD]:105.1° d_planarity:-15.4°	O[]...N[]
7AATA	PLP258(OP2)	2.88	THR109(N)	7AATA	H-bond [D-A-AA]:123.0° [A-D-DD]:107.0° d_planarity:-14.2°	O[]...N[]
7AATA	PLP258(OP2)	2.58	THR109(OG1)	7AATA	H-bond [D-A-AA]:106.4° [A-D-DD]:136.9°	O[]...O[]
7AATA	PLP258(O3)	2.92	ASN194(ND2)	7AATA	H-bond [D-A-AA]:137.1° [A-D-DD]:130.6° d_planarity:-7.5°	O[]...N[]
7AATA	PLP258(N1)	2.69	ASP222(OD2)	7AATA	H-bond [D-A-AA]:115.0° [A-D-DD]:123.1° d_planarity:-19.1° a_planarity:-32.2°	N[]...O[-]
7AATA	PLP258(O3)	2.49	TYR225(OH)	7AATA	H-bond [D-A-AA]:111.2° [A-D-DD]:133.2° a_planarity:30.9°	O[]...O[]
7AATA	PLP258(OP3)	2.71	SER255(OG)	7AATA	H-bond [D-A-AA]:112.4° [A-D-DD]:142.0°	O[]...O[]
7AATA	PLP258(C3)	3.08	LYS258(NZ)	7AATA		C[]...N[+]
7AATA	PLP258(C4)	2.33	LYS258(NZ)	7AATA		C[]...N[+]
7AATA	PLP258(C4A)	2.48	LYS258(CE)	7AATA		C[]...C[]
7AATA	PLP258(C4A)	1.29	LYS258(NZ)	7AATA		C[]...N[+]
7AATA	PLP258(OP1)	3.06	ARG266(NH1)	7AATA	H-bond [D-A-AA]:105.5° [A-D-DD]:113.5° d_planarity:3.5°	O[]...N[+]

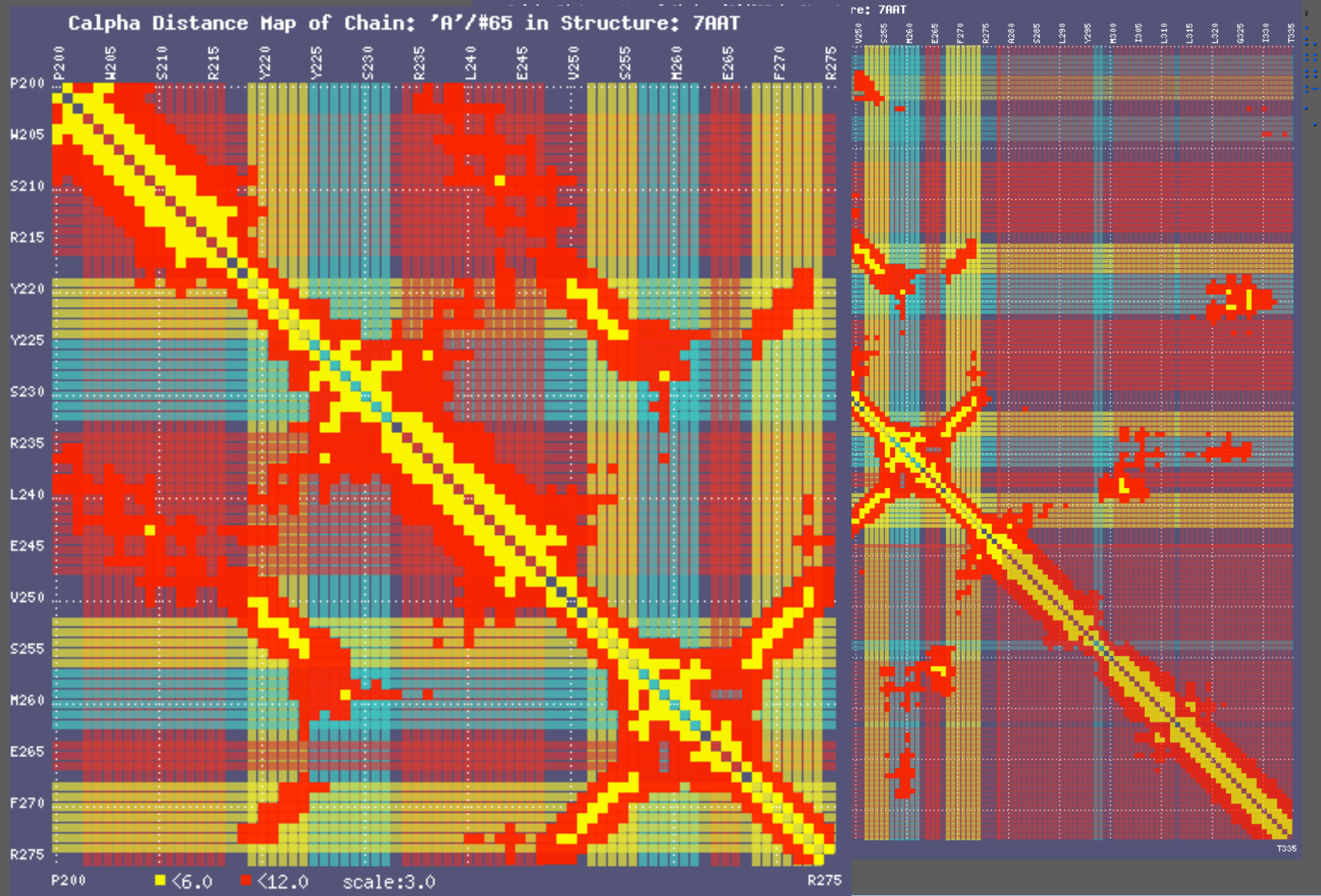
iMolTalk bond inference

- H-bonds (directed)
 - mainchain NH(D) - CO(A)
 - sidechain D – Acheck distance, angles (sp^2 , sp^3) and planarity (sp^2)
- Salt-bridges (undirected)
 - sidechain cation(+) - anion(-)
 - (R, K, D, E)



Baker & Hubbard, 1984; Stickle et al., 1992

iMolTalk distmap



MolTalk technix II

- Scripting language (SmallTalk)
- Programming Library (Objective-C)
- XMLRPC
- CORBA

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Conclusions and Outlook

- MolTalk has been successfully deployed in bioinformatics projects:
 - PDBChainSaw
 - iMolTalk
- MolTalk is OpenSource and licensed under the GNU General Public License
- iMolTalk can be used in structural analyses alone or in concert with a structure viewer

Acknowledgements

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Cedric Notredame

ISB-SIB

Holger Scheib
