Section I Summary job-dir

PDB Input 5z82.pdb computed RR file

Sequence Length RR - 276 , Native - 270 <u>sequence comparison!</u>

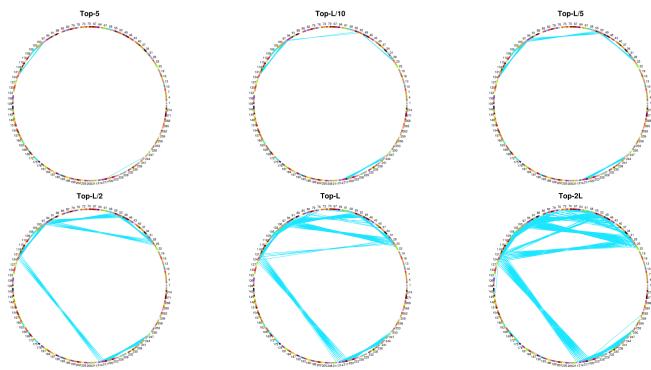
Contact Type ALL contacts with Cβ atoms within 8 Å with minimum 6 residues sequence separation

Section II Contact Count see description

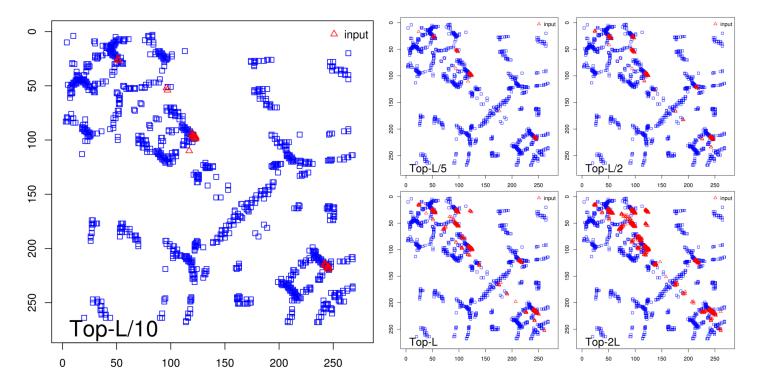
	ALL Contacts							L (= 268) from Native PDB (ignoring gaps)					
RR-File	Total	Not in Native	Remaining Total	Short-Range	Medium-Range	Long-Range	5	L/10	L/5	L/2	L	2L	
all	27600	1306	<u>26294</u>	966 (4%)	<u>2314 (9%)</u>	<u>23014(88%)</u>	<u>5</u>	<u>27</u>	<u>54</u>	<u>134</u>	<u>268</u>	<u>536</u>	

How to visualize these contacts in UCSF Chimera?

Section III Chord Diagrams <u>see description</u>



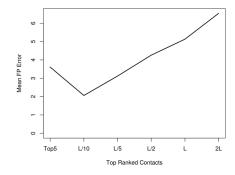
Section IV Contact Maps (with native in blue background)



Section V Precision see description



Section VI Mean False Positive Error see description

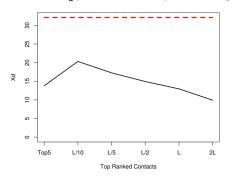


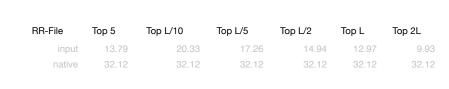


Section VII Coverage <u>see description</u>



Section VIII X_d (Distance distribution) <u>see description</u>

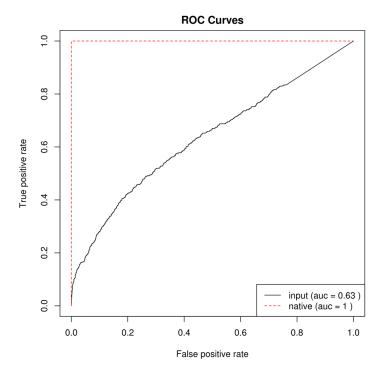




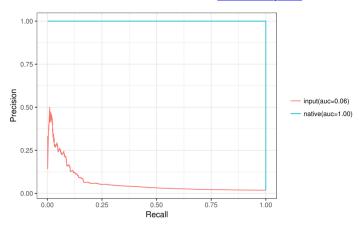
Section IX Spread <u>see description</u>



Section X ROC Curves and AUC see description



Section XI Precision-Recall Curves and AUC-PR $\underline{\mathtt{see}}$ $\underline{\mathtt{description}}$



Section XII Matthew's Correlation Coefficient (MCC) see description

RR-File	TP	FP	TN	FN	MCC
input	86	677	33143	547	0.11
native	633	0	33820	0	1.00

Section XIII Coordination Numbers see description

Top-5 Top-L/10 Top-L/5 Top-L/2 Top-L Top-2L 10 20 30 50 70 80 90 100 GPLGSMSSIGLAHNVTILGSGETTVVLGHGYGTDQSVWKLLVPYLVDDYKVLLYDHMGAGTTNPDYFDFDRYSSLEGYSYDLIAILEEFQVSKCIYVGHS [sequence] -----2543----18*******99213-19--16-131-59******9554541-----234558*--5*-2*7-47--4-69******* [input: 536 pairs 162 residues] --143-4766457633167****9766769175-274-26311899***7998666513-3511-2631722652344175-33-53599**9*965777 [native: 633 pairs 235 residues]

