Section I Summary job-dir

RR Input T0951.rr.txt

PDB Input 5z82.pdb computed RR file

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

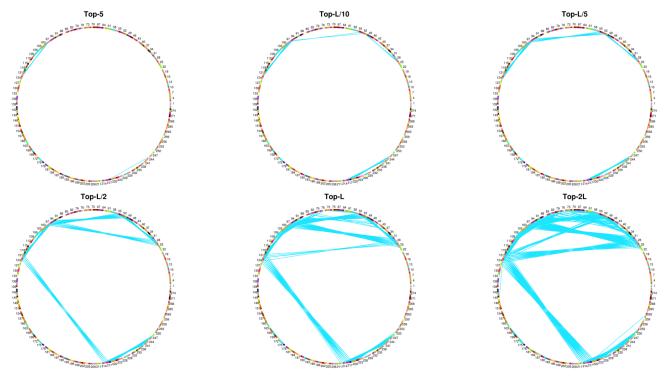
Contact Type ALL contacts with C β atoms within 8 Å with minimum 6 residues sequence separation

Section II Contact Count see description

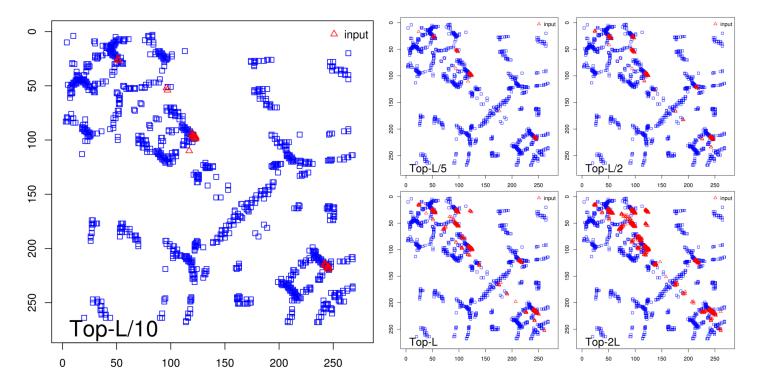
| | ALL Contacts | | | | | | L (= 268) from Native PDB (ignoring gaps) | | | | | |
|---------|--------------|------------------|-----------------|-------------|------------------|--------------------|---|-----------|-----------|------------|------------|------------|
| RR-File | Total | Not in Native | Remaining Total | Short-Range | Medium-Range | Long-Range | 5 | L/10 | L/5 | L/2 | L | 2L |
| all | 36315 | 2124 | <u>34191</u> | 1295 (4%) | <u>3006 (9%)</u> | <u>29890 (87%)</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>



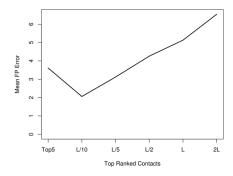
Section IV Contact Maps (with native in blue background)



Section V Precision see description



Section VI Mean False Positive Error see description

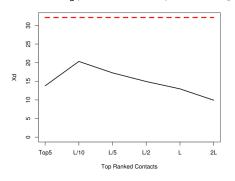


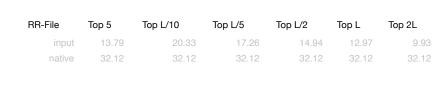


Section VII Coverage <u>see description</u>



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

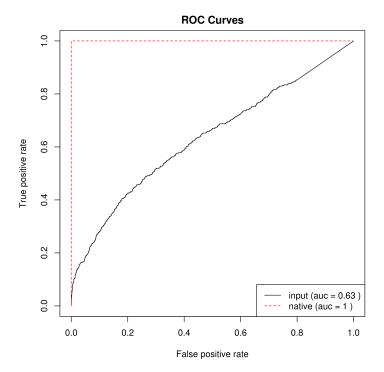




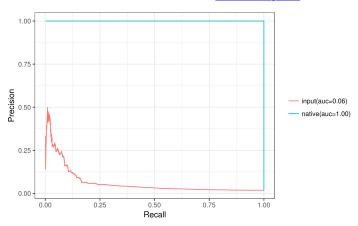
Section IX Spread <u>see description</u>



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]

 $--143 - 4766457633167 ****9766769175 - 274 - 26311899 ***7998666513 - 3511 - 2631722652344175 - 33 - 53599 **9*965777 \ [native: 633 pairs 235 residues]$

