

From the PSVS Results Report, we could know that there are 20 models generated by CYANA. And main analyses that the report shows are Distance Violations per Model, Dihedral Angle Violations per Model, RPF Scores, RMSD, Ramachandran Plot Summary, Global Quality Scores and Visual tools.

### 1. Distance violations and dihedral angle violations per model

#### Distance violations per model

Calculated using average  $r^{-6}$

0.1 - 0.2 Å	0.2 - 0.5 Å	> 0.5 Å
28	69.1	173

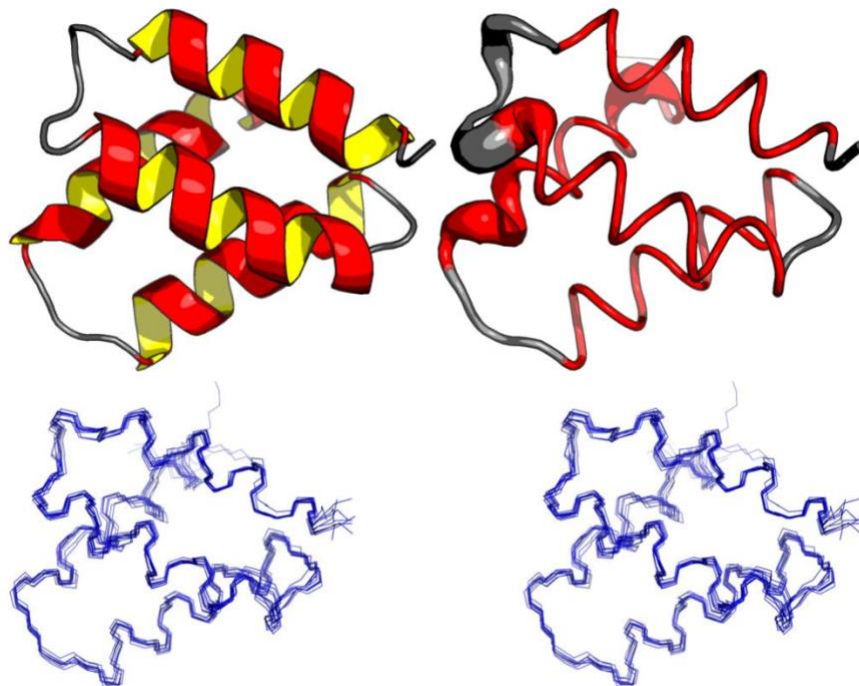
#### Dihedral angle violations per model

1 - 10 °	> 10 °
3.9	0

Experimental data determine the upper limit of distance. After calculation using sum of minus six square of limits (base values), PSVS will give number of distances (which are 0.1 - 0.2 Angstrom more, 0.2 - 0.5 Angstrom more and > 0.5 Angstrom more than base values) over number of models. Here, all cases are between 0.1-0.2 Angstrom which is optimal.

Dihedral angle violations are similar to distance ones. In this case, all models which dihedral angle violations are between 1-10 degree. And there is no cases more than 10 degree which is good.

### 2. Simulated model



### 3. Several scores

## RPF Scores

Recall	Precision	F-measure	DP-score
0.908	0.922	0.915	0.796

RMSD	All residues	Ordered residues <sup>2</sup>	Selected residues <sup>3</sup>
All backbone atoms	0.7 Å	0.4 Å	0.4 Å
All heavy atoms	1.2 Å	0.9 Å	0.9 Å

## Ramachandran Plot Summary for selected residues<sup>3</sup> from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
97.0%	3.0%	0.0%	0.0%

## Ramachandran Plot Summary for selected residues<sup>3</sup> from Richardson Lab's Molprobability

Most favoured regions	Allowed regions	Disallowed regions	<a href="#">View plot</a>	<a href="#">View model summary</a>
99.9%	0.1%	0%		

## Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) <sup>3</sup>	Procheck (all) <sup>3</sup>	MolProbability Clashscore
-Raw score	0.35	1.04	0.24	-0.29	29.00
Z-score <sup>1</sup>	-1.77	1.61	1.26	-1.71	-3.45

RPF Scores are scores to analyze the comparison between models and experiments data. Recall score is used to calculate how many contacts are matched with real contacts in data. Precision score is used to calculate how many real contacts that appear in expected contacts of models. The good result is, these two scores are comparable. F-measure score considers contacts in models and in data simultaneously. F-measure score is normalized into this range and turn out to be a new score which is called DP-score. DP-score is what we usually looks at to determine the quality of models. Generally speaking, DP-score > 0.7 and other three scores > 0.9 are expected. In this case, DP-score is 0.796 and other three scores are more than 0.9. So models are reliable. Using specific tools to determine quality of models are still necessary.

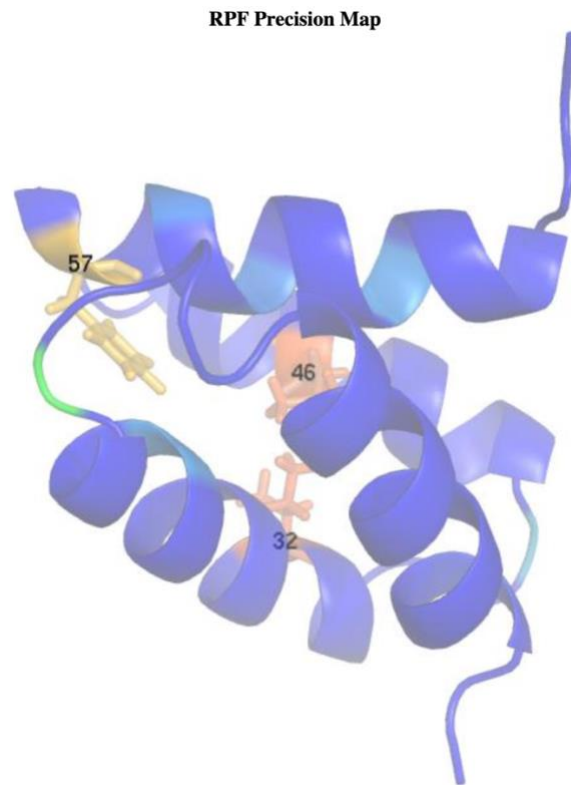
This part is calculation of RMSD of either backbone or heavy atoms. The reason that RMSD of all heavy atoms are more than that of backbone atoms is, heavy atoms also appear in side chains which may not converge. Since PSVS calculates mean values of RMSD of 20 models, RMSD will much low. The expectation of these two is, RMSD of all backbone atoms is less than 0.7~0.8 Angstrom and RMSD of all heavy atoms is less than 1.5 Angstrom.

It is good to see in Ramachandran Plot Summary, most favoured regions have 97% (from Procheck) and 99.9% (from Richardson Lab's Molprobability) and nothing in Disallowed regions.

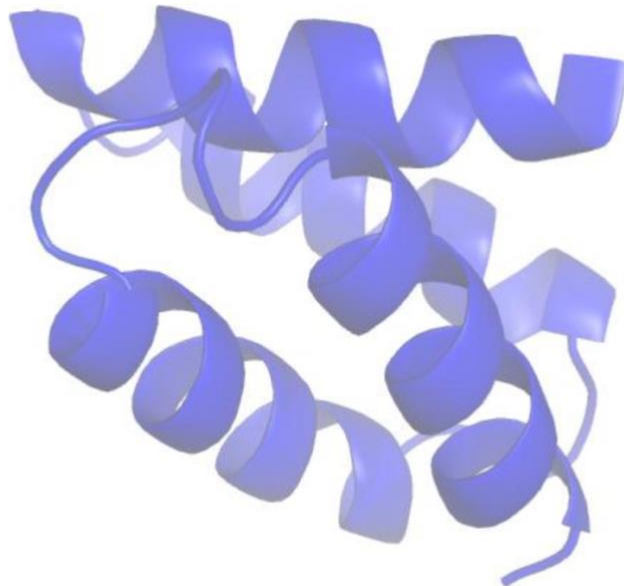
There are 5 programs to calculate different quality scores. In the table shown above, raw scores are calculated directly from programs. Z-score is a measure of how many standard deviations below or above the population mean a raw score is. Therefore, the best Z-score is more than 0. However, since experimental data is not very perfect, the expected raw score is more than -0.5 and Z-score is more than -3. Generally, scores from MolProbability Clashscore (which is also calculated from Richardson Lab's Molprobability) and Procheck will be not so good if structures are from CYANA. In this

case, we could see that Clashscore not good which means data still can be improved. Then we could use other visual tools to determine which part is more possible to be improved.

#### 4. Visual Plots



It is RPF score of each residue. Bluer means higher score and redder means low score. In this case, light blue parts could be checked with data again to see if there is any improvement that could be done. The analysis of the plot below is similar.



**Residue Plot of Ramachandran anlysis(based on data from Richardson Lab's Molprobit)**