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 per model**

Distance violations per model
Calculated using sum over r^-6

0.1 - 0.2 Å	0.2 - 0.5 Å	> 0.5 Å
0.2	0	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, there are 4 cases that distance violations are between 0.1 and 0.2 Angstrom. Distance violations of 0.2-0.5 Angstrom and more than 0.5 Angstrom have no cases. It is good to see that there is no distance violations more than 0.5 Angstrom. If it is not zero, data needs to be checked if there is noise peaks or undetected peaks.

2. **Dihedral angle violations per model**

Dihedral angle violations per model

1 - 10 °	> 10 °
1.85	0

Dihedral angle violations are similar to distance ones. In this case, there are 37 cases over 20 models which dihedral angle violations are between 1-10 degree. And there is no cases more than 10 degree which is good.

3. **RPF Scores**

RPF Scores

Recall	Precision	F-measure	DP-score
0.929	0.947	0.938	0.838

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. If Recall is much lower than Precision score, there may be many noises in data; reversely, there may be not enough information from data. F-measure score considers contacts in models and in data simultaneously. The formula of the score is like some form of product of two kind of contacts. And according to Recall and Precision score, a best model (which has both best recall and precision scores) and a worst model (almost free random chain) are generated. In the range of expected F-measure scores given by these two models, former calculated 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 0.838 and other three scores are more than 0.9. So models are reliable. Using specific tools to determine quality of models are still necessary.

4. RMSD

RMSD	*All residues*	*Ordered residues*[2]	*Selected residues*[3]
All backbone atoms	0.2 Å	0.2 Å	0.2 Å
All heavy atoms	0.6 Å	0.6 Å	0.6 Å

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.

5. Ramachandran Plot Summary

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
95.4%	4.6%	0.0%	0.0%

Ramachandran Plot Summary for selected residues[3] from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
99.6%	0.4%	0%		

Screenshot above shows two ways to do Ramachandran Plot Summary. The second one is published later than the first one and is announced to be better choice to get Ramachandran Plot. It calculates psi and phi dihedral angles of each residue in models and plot them in a phi-psi chart. Most favoured regions are labeled in red. They represents most converged and low energy part in structures.

It is good to see most favoured regions have 95.4% (from Procheck) and 99.6% (from Richardson Lab's Molprobity) and nothing in Disallowed regions.

6. Global quality scores

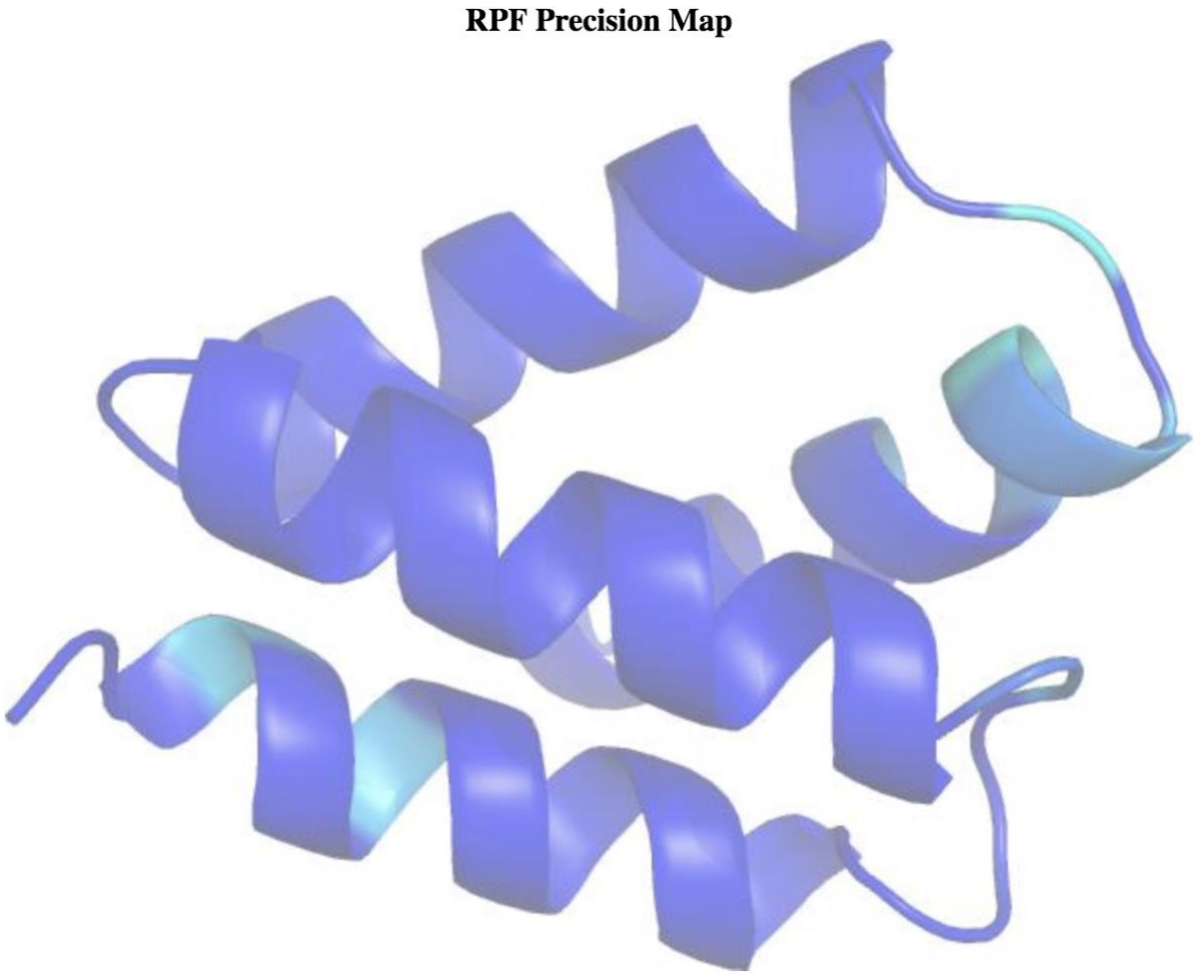
Global quality scores

Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*[3]	*Procheck (all)*[3]	*MolProbity Clashscore*
-Raw score	0.36	1.07	-0.01	-0.27	26.53
Z-score[1]	-1.61	1.74	0.28	-1.60	-3.03

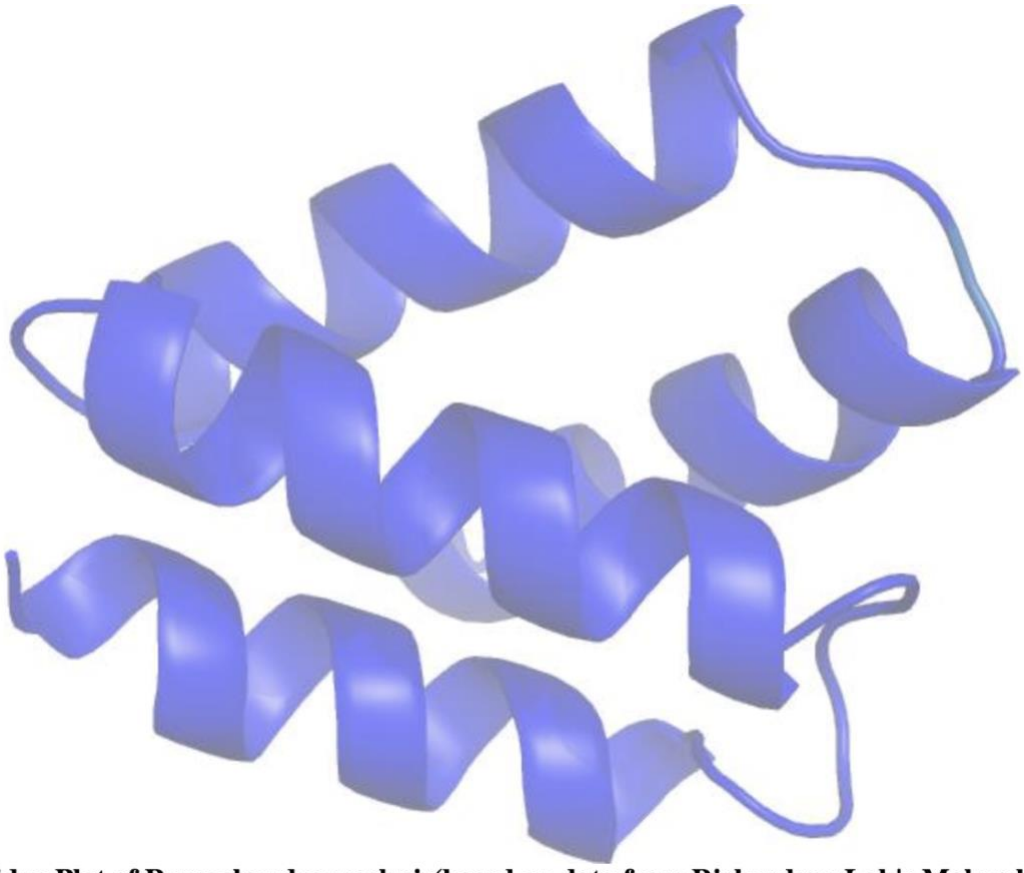
There are 5 programs to calculate different quality scores. In the table shown above, raw scores are calculated directly from programs. Z-score is a measure of how many standard deviations below or above the population mean a raw score is. Therefore, the best Z-score is more than 0. However, since experimental data is not very perfect, the expected raw score is more than -0.5 and Z-score is

more than -3. Generally, scores from MolProbity Clashscore (which is also calculated from Richardson Lab's Molprobity) 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.

7. 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 Molprobity)