

# SYSTEM SUPPORTING INFORMATION

## System No.

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```
0. 5NJY_pH70
1. 5NJY_F238L_pH70
2. 5NJY_I233T_pH70
3. 5NJY_F238LI233T_pH70
4. 5NJY_pH46
5. 5NJY_F238L_pH46
6. 5NJY_I233T_pH46
7. 5NJY_F238LI233T_pH46
8. 4HFI_pH46
9. 4HFI_F238L_pH46
10. 4HFI_I233T_pH46
11. 4HFI_F238LI233T_pH46
12. 4NPQ_pH70
13. 4NPQ_F238L_pH70
14. 4NPQ_I233T_pH70
15. 4NPQ_F238LI233T_pH70
16. 4HFI_pH70
17. 4NPQ_F238LI233T_pH46
18. 4NPQ_F238L_pH46
19. 4NPQ_pH46
20. 4NPQ_I233T_pH46
```

## Collective Variables

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'rmsd', 'wholepca_pc1', 'wholepca_pc2', 'ecd_pc1',
'tmd_pc1', 'domain twist', 'ecd_pc2', 'tmd_pc2',
'pore_profile_222', 'pore_profile_226', 'pore_profile_230',
'pore_profile_233', 'pore_profile_237',
'pore_profile_240', 'helix tilt angle',
'helix twist angle', 'hydration_data',
'beta_expansion', 'M2_radius', 'ECD_radius'
```

## Hydration Radius

Hydration is defined as the number of water molecules within the constriction region of the TMD pore—a cylinder of radius 7 Å, centered at resid 230, within  $\pm 10$  Å along principal axis z.

## **Domain Twist, Helix tilt, helix twist**

see <http://stb.proteinart.net/en/latest/analysis.html>

## **Pore profile of resid X**

The minimum distance between the heavy atoms of the residue X and the center of mass for these five residues X, then took average

## **Beta expansion**

A mean distance between Ca of resid D32 and R192

## **M2 radius**

Radii of gyration of M2 (Ca of resid 231 to 245)