

Supplementary data



**Figure S1.** Protein reliability for ketohexokinase.

Protein Preparation - Problems

The following problems were found with this structure:

Atom Types Missing Atoms Overlapping Atoms Alternate Positions

Residues with missing atoms were detected. If the backbone is present and side chains are missing, Prime can be used to predict side chains using the button below:


Add Missing Side Chains

Residue	Type	Number of heavy atoms	Expected heavy atoms	Atoms missing
B:249	ARG	5	11	Side-chain only

Update

OK Help

**Figure S2.** Missing atoms, ARG-249 and several water molecules, including H<sub>2</sub>O-485, 487, 493, 495, 572, 579, 580, and 581, lacked hydrogen bond partners.


**Protein Preparation - Problems**
✕

The following problems were found with this structure:

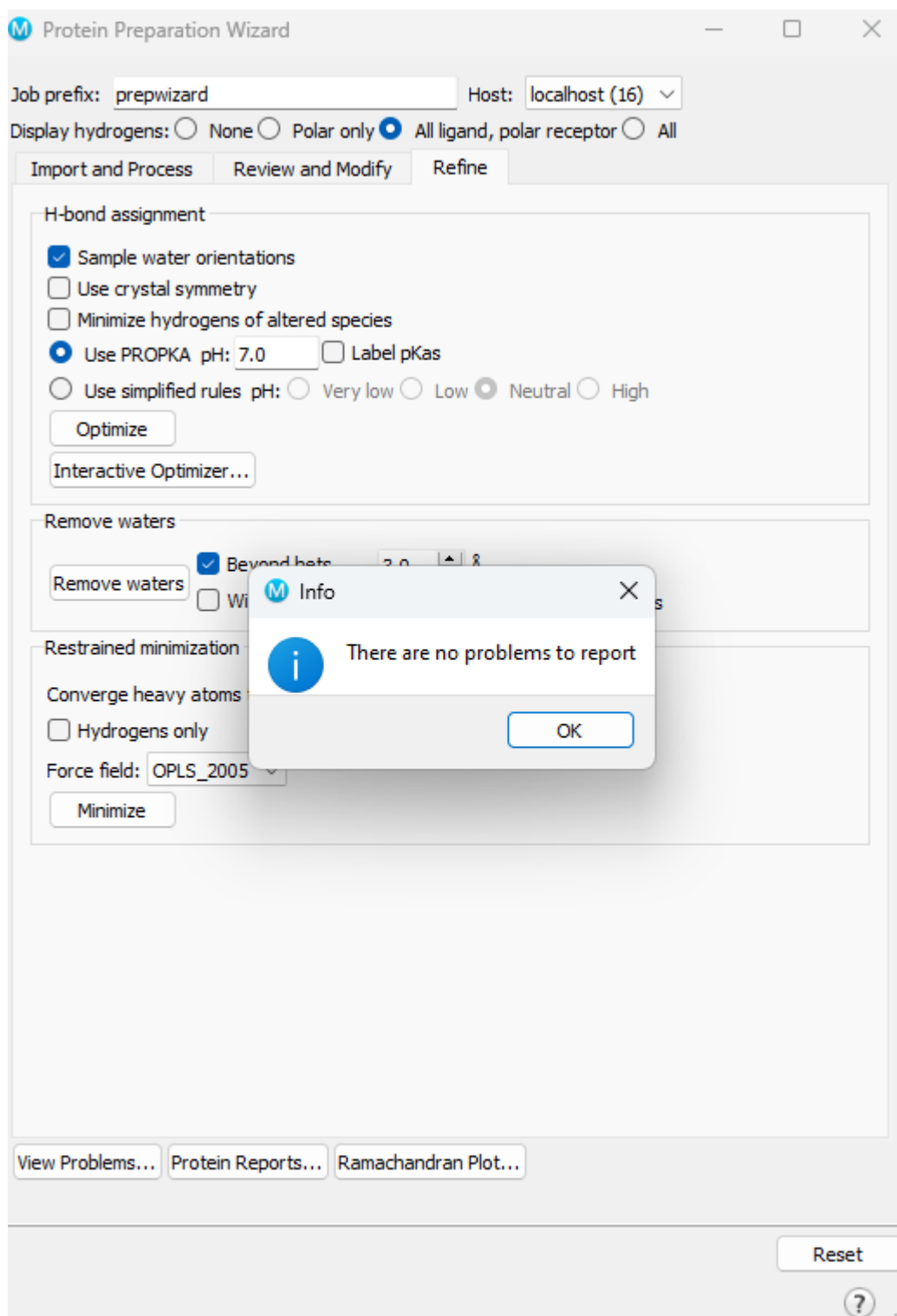
**Atom Types**
Missing Atoms
Overlapping Atoms
Alternate Positions

The following atoms have invalid atom types. This is often due to missing hydrogens or wrong number of bonds. Missing hydrogens can be added by checking "Add hydrogens" pre-processing step, and bonds can be fixed using the Build panel.

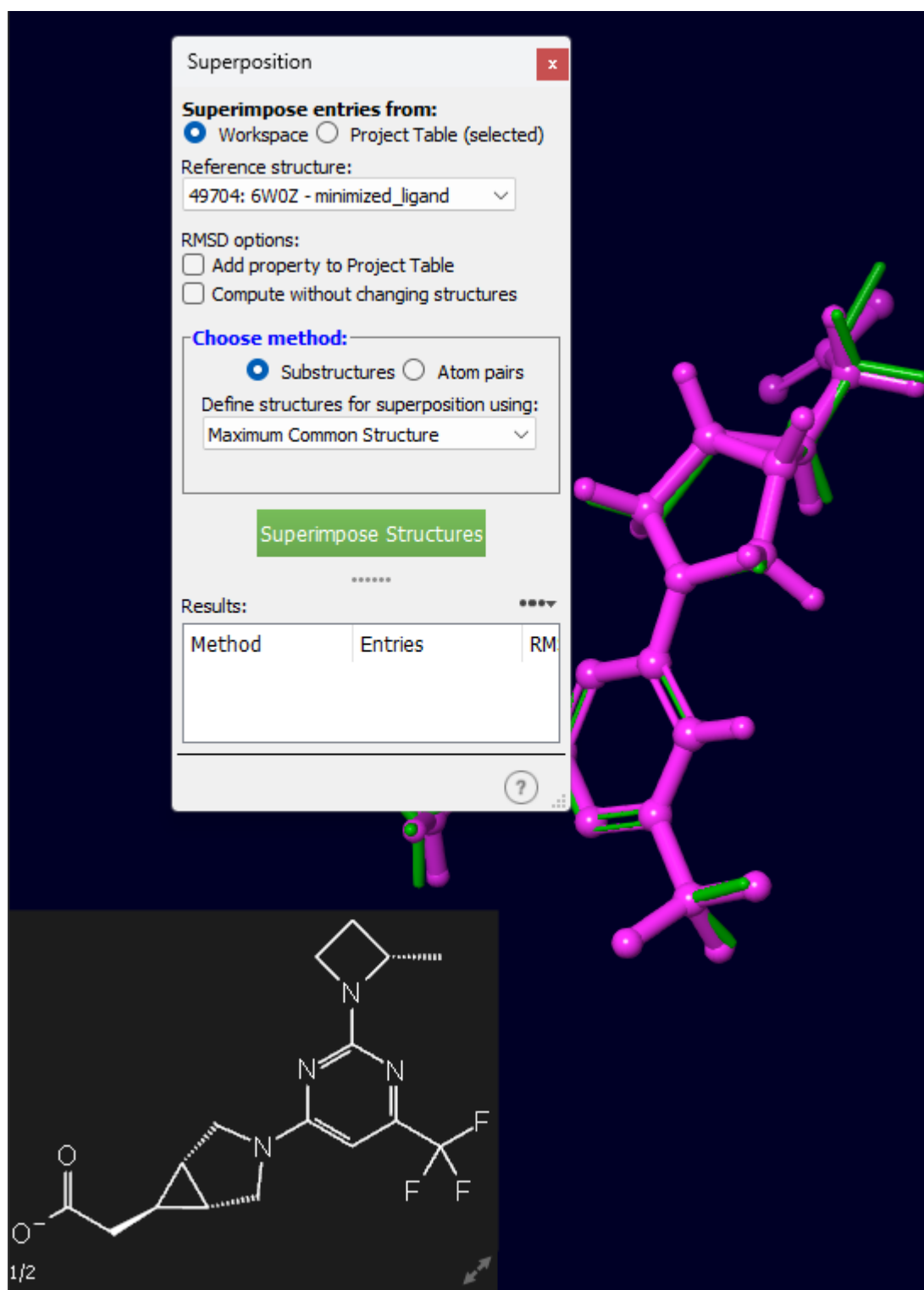
Atom	Residue	Atom type	Expected bond count	Actual bond count
1 (N)	A:3	NB (28)	3	1
2 (C)	A:3	CB (5)	4	2
5 (N)	A:4	NC (29)	3	2
6 (C)	A:4	CA (4)	4	3
9 (C)	A:4	CB (5)	4	2
10 (O)	A:4	OA (17)	2	1
11 (N)	A:5	NC (29)	3	2
12 (C)	A:5	CA (4)	4	3
15 (C)	A:5	CB (5)	4	2
16 (C)	A:5	CB (5)	4	2
19 (N)	A:5	ND (30)	3	1
20 (N)	A:6	NC (29)	3	2
21 (C)	A:6	CA (4)	4	3
24 (C)	A:6	CA (4)	4	3

Update
OK
Help

**Figure S3.** Invalid atom types with missing hydrogen atoms or wrong number of bonds.



**Figure S4.** All issues for ketohexokinase crystal structure were addressed, and no further problems were reported.



**Figure S5.** Alignment of the predicted lowest energy conformation of the target with its corresponding co-crystalline ligand.