

Results (the output file)

In this chapter the comments are written with Times New Roman font.

The output file parts are written with Courier New. The values of the output files corresponding to the particular example are written with blue.

1st part

The parameters given by the user.

Example:

Water mapping on the file C:\WaterMap\testmol.pdb

```
No-water atom to Water oxygen Tight distance : 2.8
No-water atom to Water oxygen Medium distance : 4
No-water atom to Water oxygen Loose distance : 5.2
Water oxygen to Water oxygen Tight distance : 3.5
Water oxygen to Water oxygen Medium distance : 4.5
Water oxygen to Water oxygen Loose distance : 5.2
    No-water atom to layers distance : 4
        Inlayer max distance : 3.5
No-water atom to cluster distance : 4
    Incluster max distance : 5.2
        Noise filter distance : 3
```

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2nd part

The numbers of the water oxygens and the no-water atoms connected with waters in the PDB file.

Example:

488 H2O in the PDB file.

1175 non-water atoms (O, N or S) possible interfere with water according to the user defined criteria.

List of the no-water atoms (O, N and S) that are closer (or in equal proximity) than the “no-water atom to water oxygen Loose distance” to any water oxygen, together with these water oxygens.

AtoID, AtNa, RNa, C, ReID : The records of the atom’s serial number, name, residue name, chain and residue serial number as mentioned in the PDB file.

Layer, Clust, Subclusters : The layer, cluster and subcluster(s) in which each water oxygen belongs.

N : “n” stands if the water is less than the “Noise filter distance” from any of the O, N and S no-water atoms.

Bond Dist : the distance between the two atoms.

Bond Prop : “**” stands if the distance is less (or equal) than the “no-water atom to water oxygen Tight distance”.

“*” stands if the distance is bigger than the “no-water atom to water oxygen Tight distance” and less (or equal) than the “no-water atom to water oxygen Medium distance”.

Example:

| NO-WATER ATOMS RANK --> | | | | | WATER OXYGENS | | SUBRANK | | | | | Bond | |
|-------------------------|------|-----|---|------|---------------|---|---------|-------|-------|---|-------------|------|------|
| No-water atom | | | | | Water Oxygen | | | | | | | | |
| AtoID | AtNa | RNa | C | ReID | AtoID | C | ReID | Layer | Clust | N | Subclusters | Dist | Prop |
| 1 | N | LYS | | 1 | 4146 | | 94 | 1 | 12 | 1 | | 3.43 | * |
| | | | | | 4148 | | 96 | 1 | 29 | n | 1 | 4.79 | |
| 9 | NZ | LYS | | 1 | 4147 | | 95 | 1 | | | | 3.77 | * |
| | | | | | 4146 | | 94 | 1 | 12 | 1 | | 4.88 | |
| ... | | | | | | | | | | | | | |
| ===== | | | | | | | | | | | | | |

3rd part

This list includes the same data as the previous, but sorted according to all water oxygens present in the PDB file.

AtoID, AtNa, RNa, C, ReID : The records of the atom’s serial number, name, residue name, chain and residue serial number as mentioned in the PDB file.

Layer, Clust, Subclusters : The layer, cluster and subcluster(s) in which each water oxygen belongs.

N : “n” stands if the water is closer (or in equal proximity) than the “noise filter distance” to any of the O, N and S no-water atoms.

Bond Dist : the distance between the two atoms.

Bond Prop : “**” stands if the distance is less (or equal) than the “no-water atom to water oxygen Tight distance”.

“*” stands if the distance is bigger than the “no-water atom to water oxygen Tight distance” and less (or equal) than the “no-water atom to water oxygen Medium distance”.

Example:

| WATER OXYGENS RANK --> NO-WATER ATOMS SUBRANK | | | | | | | | | | | | |
|---|---|------|-------|-------|---------------|---------------|------|-----|---|------|------|------|
| Water Oxygen | | | | | | No-water atom | | | | Bond | | |
| AtoID | C | ReID | Layer | Clust | N Subclusters | AtoID | AtNa | RNa | C | ReID | Dist | Prop |
| 4053 | | 1 | 1 | 0 | n | 1699 | OD1 | ASP | | 212 | 2.37 | ** |
| 4055 | | 3 | 2 | 4 | 1 | 765 | OD1 | ASP | | 95 | 4.20 | |
| | | | | | | 1018 | O | VAL | | 127 | 4.29 | |
| | | | | | | 1015 | N | VAL | | 127 | 4.44 | |

...

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4th part

List of all the water oxygen pairs with distance less (or equal) than the “water oxygen to water oxygen Loose distance”.

AtoID, C, ReID : The records of the oxygen’s serial number, chain and residue serial number as mentioned in the PDB file.

Layer, Clust, Subclusters : The layer, cluster and subcluster(s) in which the water oxygen belongs.

N : “n” stands if the water is less than the “Noise filter distance” from any of the O, N and S no-water atoms.

Bond Dist : the distance between the two oxygens.

Bond Prop : “**” stands if the distance is less (or equal) than the “water oxygen to water oxygen Tight distance”.

“*” stands if the distance is bigger than the “water oxygen to water oxygen Tight distance” and less (or equal) than “water oxygen to water oxygen Medium distance”.

Example:

| WATER OXYGENS RANK --> WATER OXYGENS SUBRANK | | | | | | | | | | | | | |
|--|---|------|-------|-------|---------------|--------------|---|------|-------|-------|---------------|------|------|
| Water Oxygen | | | | | | Water Oxygen | | | | | | Bond | |
| AtoID | C | ReID | Layer | Clust | N Subclusters | AtoID | C | ReID | Layer | Clust | N Subclusters | Dist | Prop |
| 4054 | | 2 | 2 | 2 | 1 | 4446 | | 394 | 3 | 2 | 1 | 3.10 | ** |

| | | | | | | | | | | | |
|------|---|---|---|---|------|-----|---|---|-----|------|----|
| 4055 | 3 | 2 | 2 | 1 | 4520 | 468 | 1 | 2 | 1 | 3.41 | ** |
| | | | | | 4522 | 470 | 1 | 2 | n 1 | 2.35 | ** |
| ... | | | | | | | | | | | |

5th part

The layers of the water oxygens.

Example:

```

WATER LAYERS & WATER to ANY NO-WATER MINIMUM DISTANCE
  4 water layers are defined with  484 H2O within
  427 H2O in the 1st layer
  57 H2O in all the other layers
  4 H2O unassigned

```

List of the water oxygen atoms and data of the layer and cluster and subcluster(s) in which they belong.

AtoID, C, ReID : The records of the oxygen's serial number, chain and residue serial number as mentioned in the PDB file.

Dist : The minimum distance from water oxygen to any no-water atom.

Layer, Clust, Subclusters : The layer, cluster and subcluster(s) in which the water oxygen belongs.

N : "n" stands if the water oxygen is less than the "Noise filter distance" from any of the O, N and S no-water atoms.

Example:

| AtoID | C | ReID | Dist | Layer | Clust | N | Subclusters |
|-------|---|------|------|-------|-------|---|-------------|
| 4053 | | 1 | 2.67 | 1 | | n | |
| 4054 | | 2 | 2.85 | 2 | 2 | 1 | |
| 4055 | | 3 | 3.01 | 2 | 2 | 1 | |
| ... | | | | | | | |

The layers of the water and after that a list of the oxygens that can not be assigned in layers.

Example:

Distribution of water oxygens (their residue IDs) in the layers :

Layer 1

1 4 5 6 7 8 9 10 11 12 13 14 15 16 17
18 19 20 21 22 23 24 25 26 27 28 29 30 31 32
...

Unassigned

281 296 482 486 ...
4 water oxygens

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6th part

The clusters of the water oxygens.

Example:

WATER CLUSTERS

Number of clusters: 49 Water oxygens in clusters: 458 Water Os out of clusters: 30

The data of each cluster and the data of the no-water atoms that are closer (or in equal proximity) than the “no-water atom to cluster distance” to any water oxygen of the cluster.

AtOID, AtNa, RNa, C, ReID : The records of the atom’s serial number, name, residue name, chain and residue serial number as mentioned in the PDB file.

Water(s) (res. IDs) in contact : The residue IDs of the water oxygens (as mentioned in the PDB file).

Example:

Cluster 1
Water oxygens in the cluster: 209 Number of contacts between the waters: 425
 25 subclusters in the cluster
Chains of the no-water atoms in contact with the cluster : A
Number of no-water atoms in contact with the cluster : 297
The water residues IDs :
 4 7 9 11 12 13 14 15 16 17 18 19 20 21 22 ...

The no-water atoms in contact with the cluster :
AtOID AtNa RNA C ReID Water(s) (res. IDs) in contact
 43 OH TYR 5 17
 55 OG SER 7 107
 59 O GLU 8 18
 63 OE1 GLU 8 17 108
...

The residue IDs (as mentioned in the PDB file) of the water oxygen atoms that do not forms or participate in clusters.

Example:

Waters (residues ID) that do not participate in clusters :
 1 5 6 8 10 46 57 76 80 84 86 90 91 95 137
 199 201 225 227 246 252 258 283 318 376 396 437 457 459 484
...
=====

7th part

The subclusters of the water oxygens.

Example:

```

WATER SUBCLUSTERS
                Total number of subclusters:      81
    Water oxygens out of the noise area, in subclusters: 205
        Water Os in the noise area, in subclusters: 182
            Total number of water oxygens, in subclusters: 387
                Total number of water Os, in the noise area: 275
    Water Os in the noise area, not belonging in clusters: 22
    Water Os in clusters, out of subclusters (obligate in the noise area): 71

```

Data of each one of the subclusters belonging to each cluster.

Waters : The number of the water oxygen atoms in the whole subcluster, in the core (main) and in the noise area of the subcluster.

Bonds : The number of the water atom pairs with a distance between them less (or equal) than the “incluster max distance” (water to water distance cut off), in the whole subcluster and in its core area.

A list of the residue IDs of the water oxygens (as mentioned in the PDB file) in the core and in the noise areas of the subcluster.

The chains in which all the no-water atoms, in contact with the subcluster (these are the atoms that come next), belong.

The residue IDs of the no-water atoms (as mentioned in the PDB file) that are closer (or in equal proximity) than the “no-water atom to cluster distance” to any water oxygen of the cluster.

AtoID, AtNa, RNa, C, ReID : The records of the atom’s serial number, name, residue name, chain and residue serial number as mentioned in the PDB file.

Water(s) (res. IDs) in contact : The residue IDs of the water oxygens (as mentioned in the PDB file).

The residue IDs of the water oxygen atoms (as mentioned in the PDB file) of the cluster, that are not arranged in subclusters.

Example:

```

CLUSTER      1  contains      25  subclusters

Subcluster   1
  Whole      No-noise      Noise area
Waters :     30             14             16
Bonds :     67             21
The subcluster's waters (res. IDs) (main & in noise):
  88  133  134  135  229  230  231  232  233  234  235  325  326  479

```

