# JSON Types and Parameters

The software Olga and the library avtraj use text files in JavaScript Object Notation (JSON) as exchange data format (**Fig. 1**). These JSON files

1. define all necessary parameters for the calculation of accessible volumes (AVs)
2. store experimental data to validate models against experimentally determined distances
3. store information on necessary pre-processing of structural models for successful calculations of accessible volumes
4. instruct the software Olga to actions, e.g., saving accessible volumes to later visualization

{  
 "Distances": {  
 "344-496": {  
 "Forster\_radius": 52,  
 "distance": 54.8,  
 "distance\_type": "RDAMean",  
 "error\_neg": 6.3,  
 "error\_pos": 5.5,  
 "position1\_name": "344A",  
 "position2\_name": "496D"  
 }  
 },  
 "Positions": {  
 "344A": {  
 "chain\_identifier": "A",  
 "residue\_seq\_number": 344,  
 "atom\_name": "CB",  
 "linker\_length": 20.0,  
 "linker\_width": 1.5,  
 "radius1": 3.5,  
 "strip\_mask": "MDTraj: residue 344 and not (name CA or name C or name N or name O)",  
 "contact\_volume\_thickness": 0.0,  
 "contact\_volume\_trapped\_fraction": 0.8,  
 "simulation\_type": "AV1",  
 "simulation\_grid\_resolution": 0.5,  
 "label\_interaction\_sites": [  
 {  
 "selection": "MDTraj: resSeq 344",  
 "weight": 1.0,  
 "radius": 6.0  
 }  
 ]  
 },

"496D": {  
 "chain\_identifier": "A",  
 "residue\_seq\_number": 496,  
 "atom\_name": "CB",  
 "linker\_length": 20.0,  
 "linker\_width": 1.5,  
 "radius1": 3.5,  
 "strip\_mask": "MDTraj: residue 496 and not (name CA or name C or name N or name O)",  
 "contact\_volume\_thickness": 0.0,  
 "contact\_volume\_trapped\_fraction": 0.8,  
 "simulation\_type": "AV1",  
 "simulation\_grid\_resolution": 0.5,  
 "label\_interaction\_sites": [  
 {  
 "selection": "MDTraj: resSeq 344",  
 "weight": 1.0,  
 "radius": 6.0  
 }  
 ]  
 }  
 }  
}

**Figure 1.** Content of a JSON file for Olga or avtraj

The top-level of these JSON files is a dictionary where the most relevant keys are

1. “Distances”
2. “Positions”.

Via the keys “Positions” and “Distances” dictionaries can be accessed, which store the necessary information to simulate and compare simulated and experimental distances, respectively (**Fig. 1.**).

The keys of the “Positions” dictionary serve as identifier of the labeling positions, which are referred to be the position names in the “Distances” dictionary.

## Distances

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | | | | **Support** | | |
| **Parameter (type), optional (yes/no)** | **Options** | **Description** | **Example** | **FPS** | **Olga** | **avtraj** |
| distance\_type (string), mandatory | “RDAMean“, “RDAMeanE”, “Rmp”, “Efficiency” | The type of distance that is calculated between for the set of labeling positions. | “RDAMean“ | same distance type for all distances | + | + |
| position1\_name (string), mandatory |  | The name of the first position. This name refers to the entry defined in the dictionary of labeling positions | “Labeling\_site\_A” | + | + | + |
| position2\_name (string), mandatory |  | The name of the second position. This name refers to the entry defined in the dictionary of labeling positions | “LP123” | + | + | + |
| distance (float), mandatory |  | The reference distance (typically the experimental distance). | 45.5 | + | + | + |
| error\_neg (float), mandatory |  | Parameter to weight the deviation between the model (the distance calculated for the pair of accessible volumes) and the data (provided by the parameter “distance”). The deviation is weighted by “error\_neg” if Model – Data < 0. | 1.2 | + | + | + |
| error\_pos (float), mandatory |  | “error\_pos” applies if Model – Data > 0 (see description “error\_neg”). | 1.4 | + | + | + |
| Forster\_radius (float), mandatory for the distance\_type options “Efficiency” and “RDAMeanE” |  | The Förster radius of the dye pair selected by position1\_name and position2\_name. | 51.5 | same Forster radius for all distances | + | + |
| distance\_samples (int), optional |  | Optional parameter to set the number of random distance samples to calculate the distance between the two positions. Default value 200000 | 10000 | same for all distances  (default 200.000) | + | + |
| distance\_sampling\_method (string), optional | “sobol\_sequence”,  “random” (default), “weighted\_random” | “random”: Takes random points with densities bigger than zero in each accessible volume and calculates the distance between the points and the weights according to the density of the points. The random points are NOT taken according to the weights of the points. The number of distance samples is defined by the option “distance\_samples” (see above)  “sobol”: Calculates for grid points taken from a six-dimensional Sobol-sequence with a length of “distance\_samples” distances and weights  “weighted\_random”: takes random samples |  | - | - | + |

## Labeling position

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  | **Support** | | |
| **Parameter (type)** | **Options** | **Description** | **Example** | **FPS** | **Olga** | **avtraj** |
| chain\_identifier (string), mandatory |  | Chain identifier like in PDB format: A, B, C, etc.  single letter uppercase | “A” | - |  |  |
| residue\_seq\_number (int),  mandatory |  | Actual residue number as in the PDB NOT the residue index! | 10 | - |  |  |
| residue\_name (string), optional |  | As in PDB, e.g., three letter code for aa (all uppercase) | CYS | - |  |  |
| atom\_name (string),  mandatory |  |  | CA, CB, H, N | - |  |  |
| simulation\_type (string),  mandatory | AV1,  AV3,  ATOM | AV1:  AV3:  ATOM: AV consists of one point (the center of the attachment atom) |  | + |  |  |
| strip\_mask (string),  optional | string,  VMD or MDTraj selection syntax | This defines a strip mask. All atoms selected by the strip mask are not considered as clashed for the calculation of an AV.  The characters till the colon define the selection syntax that is used (see example) | “VMD: resid 1 to 100“  “MDTraj: resSeq 1 to 100“ | - |  |  |
| allowed\_sphere\_radius (float),  optional |  | Excludes atoms within this radius around the attachment point | 2.0 | + |  |  |
| anchor\_atoms  (string) | selection mask  (see strip\_mask) | Anchor atoms for FRET restrained MDs (selection mask) VMD syntax | name CA and resid 89 to 93  this selects all C-alphas of the residues 89 to 93 as anchor points for FRET restrained MDs | - | - | - |
| simulation\_grid\_resolution (float) |  | The resolution of the grid used for the AV simulations (default value 0.4) | 0.4 | + | + | + |
| linker\_length  (float) |  | The length of the linker connecting the dye moiety. The linker length is the maximum distance from the attachment point to the center of the dye moity. | 20.5 | + | + | + |
| linker\_width  (float) |  | The width of the linker connecting the dye moiety. | 2.0 | + | + | + |
| radius1 (float),  mandatory |  | A radius of the dye moiety. This parameter is used for the "AV1" and the "AV3" calculations. | 3.5 | + | + | + |
| radius2 (float),  mandatory for “simulation\_type” option “AV3) |  | A radius of the dye moiety. For "AV3" calculations this parameter needs to be specified. | 1.5 | + | + | + |
| radius3 (float),  mandatory for “simulation\_type” option “AV3) |  | A radius of the dye moiety. For "AV3" calculations this parameter needs to be specified. | 7.0 | + | + | + |
| min\_sphere\_volume\_fraction (float),  optional | The float should be in the range between 0.0 and 1.0 | If AV is smaller than this fraction in Volume from complete sphere then AV is NAN (default 0%, recommended 10%) | 0.2 | - | + | + |
| contact\_volume\_thickness (float),  optional |  | Parameter defining the thickness of the contact volume. All grid points which are closer to the molecular van der Waals surface than "contact\_volume\_thickness" are considered as parts of the contact volume.  Example: For an atom with a vdW radius of 1.3 A and contact\_volume\_thickness of 2.7 A all grid points which are closer that atom than 4.0 A are considered as a part of the contact volume. | 3.0 | - | + | + |
| contact\_volume\_trapped\_fraction (float),  optional, deprecated | In the range between 0.0 and 1.0 | The fraction of dyes located in the contact volume.  Example: 0.3 means that for an ensemble of dye positions 30% of the dyes are within the contact volume. | 0.3 | - | + | + |
| label\_interaction\_sites (string, JSON),  optional | list of dictionaries defining selection and weights. For selections see:“strip\_mask” description. | The selection mask defines which atoms contribute with the specified weight to the ACV. The corresponding weights are intended for future use. The key “radius” defines the interaction radius for the selection added to the vdW radius of the corresponding atoms.  Currently the ACV will be uniformly weighted according to contact\_volume\_trapped\_fraction. | [  {  “selection”: “MDTraj: resSeq 11”,  “weight”: 0.2,  “radius”: 4.0  },  {  “selection”: “MDTraj: resSeq 11”,  “weight”: 0.8,  “radius”: 2.0  }  ] | - | - | + |

## AV File

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Parameter (type)** | **Options** | **Description** | **Example** | **FPS** | **Olga** | **avtraj** |
| position\_name (string) |  | Refers to an existing Labeling position name | “LP123” |  |  |  |
| write\_dir (string) | Vaild directory | The directory where the AV file is saved. | "AV File": {  "LP123\_AV": {  "only\_shell": false,  "openDX": false,  "position\_name": "LP123",  "write\_dir": ""  }  }  This saves the labeling position “LP123” to the file “LP123\_AV.xyz” |  |  |  |
| only\_shell (bool) | true,  false | If true only the outer layer of the AV is saved to the file. | true |  |  |  |
| filename  (string)  optional | “” | The “av\_filename” key specifies the filename of the saved AV. If no “av\_filename” is specified, the key of the “AV File” entry is used as a filename. The suffix “.xxx” of the filename is automatically added to correspond to the filetype. | “my\_favorite\_av” | - | - | + |
| openDX  (bool) | true,  false | If true, the output file is an openDX of the AV grid containing the densities of the AV. Otherwise, an xyz file is saved with all AV points with a density bigger than 0.0 | false |  |  |  |

# Future

Future: Definition of dye-groups (extend to multiple pair FRET)