

# Package: xvm (via r-universe)

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**Title** Read, Parse and Visualize 'XVG'/'XPM' Files from Molecular Dynamics

**Version** 0.0.2

**Description** Provides tools for reading, parsing and visualizing simulation data stored in 'xvg'/'xpm' file formats (commonly generated by 'GROMACS' molecular dynamics software). Streamlines post-processing and analysis of molecular dynamics ('MD') simulation outputs, enabling efficient exploration of molecular stability and conformational changes. Supports import of trajectory metrics ('RMSD', energy, temperature) and creation of publication-ready visualizations through integration with 'ggplot2'.

**URL** <https://github.com/RightSZ/xvm>, <https://rightsz.github.io/xvm/>

**BugReports** <https://github.com/RightSZ/xvm/issues>

**Encoding** UTF-8

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**Imports** ggplot2, tidyr, ggnewscale, plotly

**Suggests** knitr, rmarkdown, ggpubr, stringr

**VignetteBuilder** knitr

**License** GPL (>= 3)

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**Repository** <https://rightsz.r-universe.dev>

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## Contents

export_xvg	2
plot_xpm	3
plot_xpm_3d	4
plot_xpm_facet	4
plot_xvg	5
read_xpm	6
read_xvg	7
summary_xvg	8
<b>Index</b>	<b>9</b>

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export_xvg	<i>export xvg data object</i>
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## Description

write the data component of an `xvg_data` object (or multiple objects) to a delimited text file, controlled via the `sep` parameter rather than file extension detection.

## Usage

```
export_xvg(xvg_data, file, sep = "\t", row.names = FALSE, merge = FALSE, ...)
```

## Arguments

<code>xvg_data</code>	An object of class <code>xvg_data</code> , or a list of <code>xvg_data</code> objects, as returned by <code>read_xvg()</code> .
<code>file</code>	Path to the output file (any extension is acceptable).
<code>sep</code>	Field separator (e.g., <code>"\t"</code> for TSV, <code>","</code> for CSV). Default is <code>"\t"</code> .
<code>row.names</code>	Logical, whether to write row names. Default is <code>FALSE</code> .
<code>merge</code>	Logical, whether to merge multiple <code>xvg_data</code> objects before exporting. Default is <code>FALSE</code> .
<code>...</code>	Additional arguments passed to <code>write.table()</code> .

## Value

Invisibly returns the path to the written file.

**Examples**

```
## Not run:
xvg <- read_xvg(system.file("extdata/rmsd.xvg", package = "xvm"))
# Export as TSV
export_xvg(xvg, "rmsd.tsv", sep = "\t")
# Export as CSV
export_xvg(xvg, "rmsd.csv", sep = ",")

## End(Not run)
```

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plot\_xpm

*plot xpm data*

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**Description**

plot xpm data using ggplot2

**Usage**

```
plot_xpm(xpm_data, interpolate = FALSE)
```

**Arguments**

xpm\_data        a xpm object returned by read\_xpm

interpolate    logical indicating whether to use raster interpolation (TRUE) or discrete tiles (FALSE). Default is FALSE.

**Value**

a ggplot2 object

**Examples**

```
library(xvm)
xpm_file_path <- system.file("extdata/gibbs.xpm", package = "xvm")
xpm_data <- read_xpm(xpm_file_path)
plot_xpm(xpm_data) # plot the xpm data using plot_xpm() function
```

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plot_xpm_3d	<i>generate 3d scatter plot from xpm data</i>
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**Description**

creates 3d visualization of xpm data with scatter plot.

**Usage**

```
plot_xpm_3d(xpm_data, reversescale = FALSE, point_size = 2)
```

**Arguments**

xpm_data	a xpm object (from <code>read_xpm()</code> ) or list containing parsed objects.
reversescale	whether to reverse the color scale; default is FALSE
point_size	the size of the points in the scatter plot; default is 2

**Value**

a plotly object

**Examples**

```
library(xvm)
xpm_file_path <- system.file("extdata/gibbs.xpm", package = "xvm")
xpm_data <- read_xpm(xpm_file_path)
plot_xpm_3d(xpm_data) # plot 3D scatter plot from xpm file
```

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plot_xpm_facet	<i>generate faceted plots from xpm data</i>
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**Description**

creates dual-panel visualizations of xpm data with scatter or area plots.

**Usage**

```
plot_xpm_facet(xpm_data, plot_type = "scatter")
```

**Arguments**

xpm_data	a xpm object (from <code>read_xpm()</code> ) or list containing parsed objects.
plot_type	visualization type: "scatter" (default) or "area".

**Value**

a ggplot2 object with:

- Dual facets showing x/y axis relationships
- Automatic data transformation for visualization
- NULL if invalid plot\_type specified

**Examples**

```
library(xvm)
xpm_file_path <- system.file("extdata/gibbs.xpm", package = "xvm")
xpm_data <- read_xpm(xpm_file_path)
plot_xpm_facet(xpm_data) # plot pseudo-3D from xpm file
```

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plot\_xvg

*plot xvg data*

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**Description**

plot xvg data using ggplot2

**Usage**

```
plot_xvg(
  xvg_data,
  merge = FALSE,
  title = NULL,
  subtitle = NULL,
  use_color_scale = NULL,
  ...
)
```

**Arguments**

xvg_data	xvg data object returned by read_xvg
merge	logical; if TRUE and multiple datasets provided, merge them (default: FALSE)
title	chart title (default uses xvg file's title)
subtitle	chart subtitle (default uses xvg file's subtitle)
use_color_scale	custom color scale function (e.g., ggsci::scale_color_bmj) to override default colors
...	additional parameters passed to ggplot2::geom_line

**Value**

a ggplot2 object

## Examples

```
library(xvm)
rmsd_file_path <- system.file("extdata/rmsd.xvg", package = "xvm")
rmsd_data <- read_xvg(rmsd_file_path)
plot_xvg(rmsd_data) # plot the xvg data using plot_xvg() function
```

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read\_xpm

*read xpm files*

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## Description

This function reads xpm (X PixMap) files, validates their existence, and returns parsed data structures in a list format.

## Usage

```
read_xpm(xpm_files)
```

## Arguments

`xpm_files` a character vector containing paths to one or more xpm files.

## Details

The function performs the following operations:

1. Validates input type (must be character vector)
2. Checks for file existence and filters missing files with warnings
3. Reads valid files and parses them using [parse\\_xpm\(\)](#)
4. Returns aggregated results in a named list

## Value

list with the following components:

- `data` - Data frame containing matrix values with coordinates
- `title` - Chart title extracted from xpm
- `legend` - Legend text extracted from xpm
- `x_label` - X-axis label extracted from xpm
- `y_label` - Y-axis label extracted from xpm
- `color_map` - Named list mapping color codes to hex values
- `color_values` - Named list mapping color codes to numeric values

**Examples**

```
library(xvm)
# Retrieve the path to the example file included in the package
xpm_file_path <- system.file("extdata/gibbs.xpm", package = "xvm")
xpm_data <- read_xpm(xpm_file_path) # read the xpm file using read_xpm() function
names(xpm_data)
```

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read_xvg	<i>read xvg files</i>
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**Description**

read one or more GROMACS-generated xvg files

**Usage**

```
read_xvg(xvg_files, skip_comments = TRUE)
```

**Arguments**

xvg\_files      character vector of xvg file paths  
skip\_comments   logical indicating whether to skip comment lines (default: TRUE)

**Value**

Named list containing xvg data, using filenames (without extension) as keys

**Examples**

```
library(xvm)
# Retrieve the path to the example file included in the package:
rmsd_file_path <- system.file("extdata/rmsd.xvg", package = "xvm")
rmsd_data <- read_xvg(rmsd_file_path) # read the xvg file using read_xvg() function
names(rmsd_data)
```

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summary_xvg	<i>summarize xvg data</i>
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### Description

compute basic summary statistics (mean, sd, min, median, max) for each variable in one or more xvg\_data objects.

### Usage

```
summary_xvg(xvg_data, merge_results = FALSE)
```

### Arguments

**xvg\_data** a list of class 'xvg\_data' or a list containing multiple 'xvg\_data' objects, as returned by read\_xvg().

**merge\_results** logical, whether to combine results from multiple objects (default: FALSE). When TRUE, results will include a 'group' column identifying the source.

### Value

a data.frame with columns:

**group** (Optional) Source identifier when processing multiple objects with merge\_results=TRUE.

**variable** Name of the variable (column) in the xvg data.

**mean** Arithmetic mean of that variable.

**sd** Standard deviation.

**min** Minimum value.

**median** Median value.

**max** Maximum value.

### Examples

```
path <- system.file("extdata/rmsd.xvg", package = "xvm")
xvg <- read_xvg(path)
summary_xvg(xvg)
```

# Index

`export_xvg`, 2

`parse_xpm()`, 6

`plot_xpm`, 3

`plot_xpm_3d`, 4

`plot_xpm_facet`, 4

`plot_xvg`, 5

`read_xpm`, 6

`read_xpm()`, 4

`read_xvg`, 7

`summary_xvg`, 8