SBML Level 3 Package: Layout ('layout')

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1 Introduction

With the development of the Systems Biology Markup Language (SBML), there now is a common standard for the exchange of dynamical models in systems biology. It has already been adopted by many applications in this field (Hucka et al., 2011, 2003; SBML Team, 2012).

In 2002, we worked on an automatic layout algorithm (Wegner and Kummer, 2005). This algorithm was based on the principle that, given an SBML file, the species and reactions should be placed automatically as a network. Since there was no way to save the final layout of the network, we started developing a layout extension for SBML. In 2003, the first draft was completed and presented at the SBML workshop in St. Louis in 2004. Based on the discussions in St. Louis, Ralph Gauges finalized a first specification and implementation for libSBML (Gauges et al., 2006). During the next several SBML meetings, the layout extension was discussed in depth and also challenged by other proposals, but due to the constant support from the community (e.g., Deckard et al., 2006), it was finally accepted as a package for SBML Level 3.

1.1 Proposal corresponding to this package specification

This specification for Layout in SBML Level 3 Version 1 is based on the proposal by the same authors, located at the following URL:

```
http://sbml.org/Community/Wiki/SBML_Level_3_Proposals/Layout
```

The version of the proposal used as the starting point for this specification is the version of April 2005. Previous versions of the current proposal are available from:

http://otto.bioquant.uni-heidelberg.de/sbml/

Details of earlier independent proposals are provided in Section 2.

1.2 Tracking number

The tracking number for Layout package activities in the SBML issue tracking system (SBML Team, 2010) is 233. The following is the direct link to the issue tracker for the SBML Level 3 Layout package:

http://sourceforge.net/p/sbml/sbml-specifications/233/.

1.3 Package dependencies

The Layout package adds classes to SBML Level 3 Version 1 Core and has no dependency on any other package.

1.4 Document conventions

Following the precedent set by the SBML Level 3 Version 1 Core specification document, we use UML 1.0 (Unified Modeling Language; Eriksson and Penker 1998; Oestereich 1999) class diagram notation to define the constructs provided by this package. We use color in the diagrams to carry additional information for the benefit of those viewing the document on media that can display color. The following are the colors used and what they represent:

- *Black*: Items colored black in the UML diagrams are components taken unchanged from their definition in the SBML Level 3 Version 1 Core specification document.
- *Green*: Items colored green are components that exist in SBML Level 3 Version 1 Core, but are extended by this package. Class boxes are also drawn with dashed lines to further distinguish them.

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■ *Blue*: Items colored blue are new components introduced in this package specification. They have no equivalent in the SBML Level 3 Version 1 Core specification.

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We also use the following typographical conventions to distinguish the names of objects and data types from other entities; these conventions are identical to the conventions used in the SBML Level 3 Version 1 Core specification document:

AbstractClass: Abstract classes are classes that are never instantiated directly, but rather serve as parents of other object classes. Their names begin with a capital letter and they are printed in a slanted, bold, sans-serif type-face. In electronic document formats, the class names defined within this document are also hyperlinked to their definitions; clicking on these items will, given appropriate software, switch the view to the section in this document containing the definition of that class. (However, for classes that are unchanged from their definitions in SBML Level 3 Version 1 Core, the class names are not hyperlinked because they are not defined within this document.)

Class: Names of ordinary (concrete) classes begin with a capital letter and are printed in an upright, bold, sansserif typeface. In electronic document formats, the class names are also hyperlinked to their definitions in this specification document. (However, as in the previous case, class names are not hyperlinked if they are for classes that are unchanged from their definitions in the SBML Level 3 Version 1 Core specification.)

SomeThing, otherThing: Attributes of classes, data type names, literal XML, and generally all tokens *other* than SBML UML class names, are printed in an upright typewriter typeface. Primitive types defined by SBML begin with a capital letter; SBML also makes use of primitive types defined by XML Schema 1.0 (Biron and Malhotra, 2000; Fallside, 2000; Thompson et al., 2000), but unfortunately, XML Schema does not follow any capitalization convention and primitive types drawn from the XML Schema language may or may not start with a capital letter.

The UML diagrams in this document show the name of the class on top. Below that are listed the attributes specific to that class. Optional attributes have some default value which may be NULL. Arrays are written in square brackets with the valid array length within those brackets. (For example, an array [2..] would mean that it can hold from 2 to ∞ number of objects.) For other matters involving the use of UML and XML, we follow the conventions used in the SBML Level 3 Version 1 Core specification document.

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2 Background and context

Currently, there is no official way of encoding the graphical layout of computational models in an SBML document. Software tools wishing to share this kind of data must use SBML annotations to store it in proprietary forms.

The Layout proposal was made in early 2003. It has been incorporated into libSBML (Gauges et al., 2006) and used by software applications (e.g., Bergmann and Sauro, 2006; Sahle et al., 2006) with SBML Levels 2 and 3. The overall structure of this proposal reflects design decisions detailed in this section. These decisions are mainly based on the discussion on the mailing list and during the workshop in St. Louis. For example, users requested that several layouts could be stored in one SBML file, and so the layout data is stored in a **ListOfLayouts** as a child of the **Model** element instead of being direct annotations on the **Model** constituents.

The layout of a reaction network diagram should be described as graphical representations of species and reactions (and not as arbitrary drawing or graph). This means that existing languages for the description of vector drawings (SVG) or general graphs cannot be used. While it may seem unnecessary to invent a new language when an existing one like SVG could in principle be used to describe the layout of a reaction network, there are good reasons to have a language tailored specifically for the layout of SBML models. Presumably, most programs that will use this SBML extension are primarily programs dealing with biochemical models. Internally, they will have data structures for species and reactions, so it will be natural for them to describe the layout of the reaction network also in terms of species and reactions (and not in terms of, e.g., polygons or splines). Thus, the **Layout** object has a similar structure like the SBML **Model** object and contains lists of graphical representations of compartments, species, and reactions (called **CompartmentGlyph**, **SpeciesGlyph**, and **ReactionGlyph** respectively). Additional layout elements and relationships can be represented by using the **GraphicalObject** and **GeneralGlyph** objects.

Another important question is the level of detail that the description should provide. For simplicity, only the layout (i.e., the position of the different graphical objects) of the diagram is encoded, not the details of how it should be rendered; the latter is left to the SBML Level 3 Render package. Figure 1 illustrates this distinction. All three diagrams could be renderings of the same layout and would be described by identical SBML files. No information about colors, line styles, fonts, etc., is present in the layout description.

The next question is how the relation between the model and the layout should be established. There seems to be a consensus that one model element can be represented by several layout elements. For example, it can be useful to have several representations of one species in the layout to avoid crossing lines. This can be accomplished if every layout element has a field that refers to the id of a model element.

There are also cases where a layout element does not correspondent to exactly one model element. One example is when a layout shows a simplified version of a model in which one reaction in the layout corresponds to several reactions and intermediate species in the model. This is the reason why the field in the layout elements that refers to the model elements is optional: to allow layout objects that do not have a specific counterpart in the SBML model.

The result of all this is a way to describe the graphical layout of a reaction network in biochemical terms. This layout can be closely tied to the model. A graphical editor, for example, would typically create a layout that is closely connected (by a one-to-several relation from the model

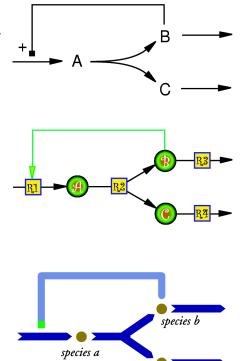


Figure 1: Examples of different renderings of the same layout.

species c

elements to the layout elements) to the model. A more general layout design program could create a layout that is not so closely tied to the model; for example, it could create a layout that shows a simplified version of the model.

3 Package syntax and semantics

In this section, we define the syntax and semantics of the Layout package for SBML Level 3 Version 1. We expound on the various data types and constructs defined in this package, then in Section 4 on page 21, we provide complete examples of using the constructs in an example SBML model.

3.1 Namespace URI and other declarations necessary for using this package

Every SBML Level 3 package is identified uniquely by an XML namespace URI. For an SBML document to be able to use a given SBML Level 3 package, it must declare the use of that package by referencing its URI. The following is the namespace URI for this version of the Layout package for SBML Level 3 Version 1:

```
"http://www.sbml.org/sbml/level3/version1/layout/version1"
```

In addition, SBML documents using a given package must indicate whether understanding the package is required for complete mathematical interpretation of a model, or whether the package is optional. This is done using the attribute required on the <sbml> element in the SBML document. For the Layout Package, the value of this attribute must be set to "false".

The following fragment illustrates the beginning of a typical SBML model using SBML Level 3 Version 1 and this version of the Layout package:

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core" level="3" version="1"
    xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1" layout:required="false">
```

Historically, the layout package has also been used to encode the layout of SBML Level 2 models, there the following namespace is to be used within an annotation:

```
"http://projects.eml.org/bcb/sbml/level2"
```

A minimal example would look like this:

3.2 Coordinate System and Size

All size information given for layout objects are understood to be in Point (pt), which is defined to be 1/72 of an inch (0.3527777778 mm) as in postscript.

The layout extension uses a Cartesian coordinate system. The origin of the coordinate system will be in the upper left corner of the screen. The positive x-axis runs from left to right, the positive y-axis run from top to bottom and the positive z-axis points into the screen. The reason for having the origin in the upper left corner of the screen is that most 2D packages do it that way. This coordinate system is also right handed just like the ones in OpenGL and Java3D, which should facilitate 3D implementations as well.

Section 3 Package syntax and semantics

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3.3 Primitive data types

Section 3.1 of the SBML Level 3 Version 1 Core specification defines a number of primitive data types and also uses a number of XML Schema 1.0 data types (Biron and Malhotra, 2000). Of the data types defined and referenced in SBML Level 3 Version 1 Core, the Layout package makes use of integer, double, string, SId, SIdRef and IDREF. The Layout package defines the additional primitive data type SpeciesReferenceRole (described below) and uses the xsi:type from the XML Schema instance (XSI) namespace.

The SId type is used as the data type for the identifiers of all layout classes. As such, the values of attributes of type SId have to be unique within the model and are not allowed to conflict with SId values from SBML elements or any package that use the same SId namespace.

3.3.1 Type SpeciesReferenceRole

The Layout package defines a new enumerated type **SpeciesReferenceRole** which represents the role that a species takes within a reaction. It can take only one of the following values:

| substrate | product |
|---------------|-------------|
| sidesubstrate | sideproduct |
| modifier | activator |
| inhibitor | undefined |

3.3.2 Type xsi:type

In order to easily differentiate between **LineSegment** and **CubicBezier** elements, the **xsi:type** attribute from the XML Schema instance (XSI) namespace is used. The namespace is:

```
"http://www.w3.org/2001/XMLSchema-instance"
```

For this purpose, the attribute xsi:type is set to the following fixed values: "LineSegment" for line segments and "CubicBezier" for splines.

3.4 General features

This section describes the common classes **Point**, **Dimensions** and **BoundingBox** that are used by all other classes of this package. It also describes the representation of curves. Figure 8 on page 12 illustrates the relationships between these and other entities defined in the Layout package.

3.4.1 The Point class

A point is specified via the required attributes \mathbf{x} , \mathbf{y} and an optional attribute \mathbf{z} , all of which are of type **double**. If the attribute \mathbf{z} is not specified, the object is a two dimensional object. Figure 2 provides a UML diagram for the definition of **Point**.

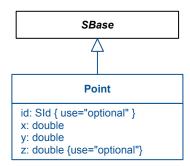


Figure 2: The definitions of the Point class.

The **Point** class also has an optional attribute **id** of type **SId**. While not used in the Layout package, it can be used by programs to refer to the elements.

3.4.2 The Dimensions class

A dimension is specified via the required attributes width, height and an optional attribute depth, all of which are of type double. If the attribute depth is not specified, the object is a two dimensional object. Figure 3 provides a UML diagram for the definition of Dimensions.

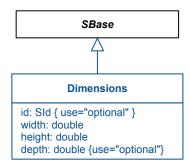


Figure 3: The definitions of the **Dimensions** class.

The width attribute of **Dimensions** specifies the size of the object in the direction of the positive x axis, the height attribute specifies the size of the object along the positive y axis and the depth attribute specifies the size of the object along the positive z axis. All sizes for **Dimensions** objects are positive values, and so the attributes are not allowed to take negative values.

The **Dimensions** class also has an optional attribute **id** of type **SId**. While not used in the Layout package, it can be used by programs to refer to the elements.

3.4.3 The BoundingBox class

A **BoundingBox** consists of the required elements **position** and **dimensions**. Figure 4 on the next page provides a UML diagram for the definition of **BoundingBox**; the **position** and **dimensions** elements are described in more detail below.

The **BoundingBox** class also has an optional attribute **id** of type **SId**. While not used in the Layout package, it can be used by programs to refer to the elements.

The position element

The position always specifies the upper left corner of the bounding box. The position is of type Point .

The dimensions element

The **dimensions** element is required and of type **Dimensions**. It represents the size of the bounding box. As can be seen in Figure 4 on the following page, the size is given in terms of width, height and depth.

3.4.4 The Curve class

The **Curve** class describes how to connect elements in a diagram defined with the use of the Layout package. The UML diagram defining **Curve** is shown in Figure 5 on page 10. A curve is fully specified by a mandatory listOfCurveSegments element and is used in four places in the Layout package:

SpeciesReferenceGlyph: Here it describes a curve from/to the center piece of the parent ReactionGlyph to/from the SpeciesGlyph it represents.

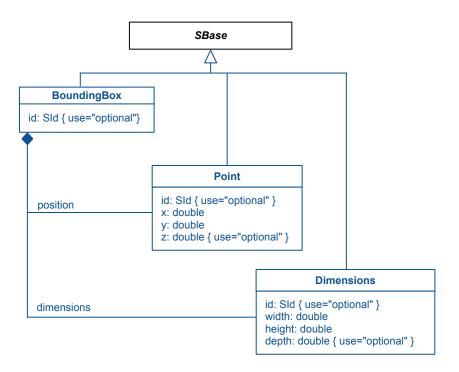


Figure 4: The definitions of the **BoundingBox** class.

- **ReactionGlyph**: Here it describes a curve for the center piece of a reaction.
- **ReferenceGlyph**: Here it describes a curve from/to the center piece of the parent **GeneralGlyph** to/from the glyph it represents.
- GeneralGlyph: Here it describes a curve for the center piece of an additional relationship.

In the text above, the term *center piece* refers to either the **Curve** element of a **ReactionGlyph**, or its **BoundingBox**.

The listOfCurveSegments element

The listOfCurveSegments contains an arbitrary number of curve segments that can be either of type LineSegment or of type CubicBezier.

3.4.5 The LineSegment class

The **LineSegment** class consists of the mandatory attribute **xsi:type** and two elements of type **Point**. One is called **start** and represents the starting point of the line, the other is called **end** and represents the endpoint of the line.

The xsi:type attribute

For straight line segments, the attribute xsi:type must have the value set to:

"LineSegment"

Note that the xsi:type is from the xsi namespace:

"http://www.w3.org/2001/XMLSchema-instance"

3.4.6 The CubicBezier class

In order to be able to represent smooth curves the Layout package defines the class **CubicBezier**. It represents a Bezier curve (Wikipedia, 2013), and is readily available in most graphics APIs.

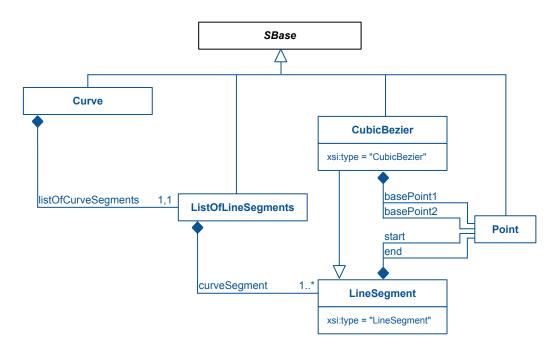


Figure 5: The definitions of the **Curve** class.

The class **CubicBezier** is derived from **LineSegment**. It consists of four elements: the two inherited elements **start** and **end**, which specify the starting point and the endpoint of the cubic bezier curve, and two elements **basePoint1** and **basePoint2**, which specify the two additional base points that are needed to describe a cubic bezier curve.

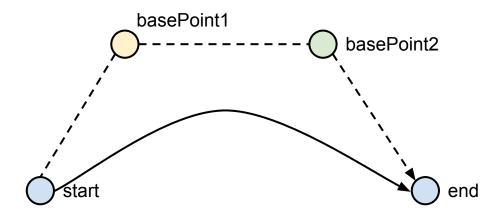


Figure 6: A depiction of a cubic bezier curve, including the points start, end as well as basePoint1 and basePoint2.

The basePoint1 element represents the base point closer to the start point and basePoint2 the base point closer to end point. This allows tools not able to render bezier curves to approximate them by directly connecting the four points (as visible in the dashed line of Figure 6).

The xsi:type attribute

For cubic bezier curves, the attribute xsi:type must have the value set to:

"CubicBezier"

Note that the xsi:type is from the xsi namespace:

"http://www.w3.org/2001/XMLSchema-instance"

3.5 The extended Model class

The Layout package extends the **SBML Model** class with the addition of one child element: the **listOfLayouts**. A **Model** may contain at most one such list. Figure 7 gives the definition of the extended **Model** class used in Layout.

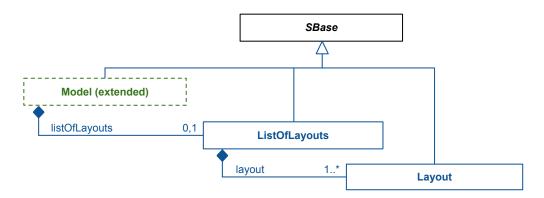


Figure 7: The definitions of the extended Model class.

The listOfLayouts class

As shown in Figure 7, the **ListOfLayouts** is derived from **SBase** and inherits the attributes **metaid** and **sboTerm**, as well as the subcomponents for **Annotation** and **Notes**. The **ListOfLayouts** must contain at least one Layout (defined in Section 3.6).

Should the Layout package be used in an **SBML** Level 2 model, the **ListOfLayouts** needs to be placed in an **Annotation** on the **Model** element. For a complete example that uses SBML Level 2, please see Section 4.6 on page 33.

3.6 The Layout class

The **Layout** class stores layout information for some or all elements of the SBML model as well as additional objects that need not be connected to the model. **Layout** is defined in Figure 8 on the following page.

The Layout has two attributes: id and name. Additionally, a Dimensions element specifies the size of the layout. The actual layout elements are contained in several lists, namely: a ListOfCompartmentGlyphs, a ListOfSpecies-Glyphs, a ListOfReactionGlyphs, a ListOfTextGlyphs, and a ListOfAdditionalGraphicalObjects. Each of these lists can only occur once, and, if present, is not allowed to be empty.

The id attribute

The id attributes takes a required value of type SId. The id which uniquely identifies the layout.

The name attribute

The name attribute takes an optional value of type string. It allows one to specify a human readable name for a **Layout** object.

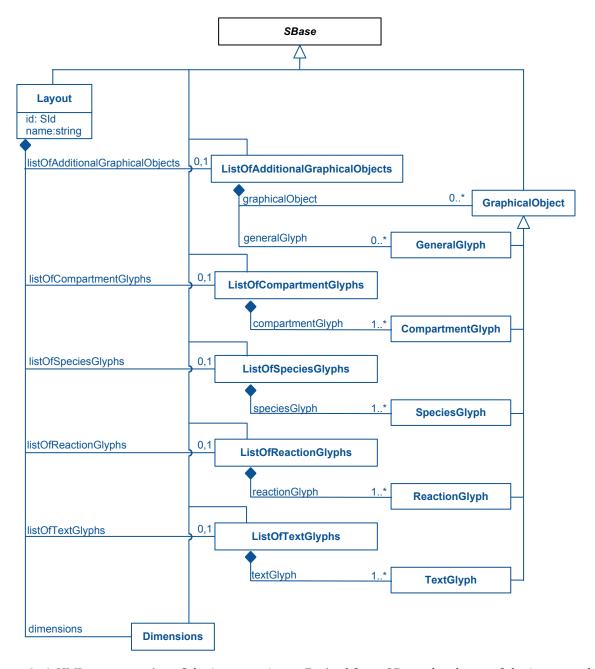


Figure 8: A UML representation of the Layout package. Derived from *SBase*, the classes of the Layout package inherit support for constructs such as SBML **Notes** and **Annotations**. See Section 1.4 on page 3 for an explanation of the conventions related to this figure. The individual classes shown in this diagram are discussed in the text.

The dimensions element

The **dimensions** element of type **Dimensions** specifies the dimensions of this layout. This element is required. It holds the dimensions of all layout elements (care should be taken when using cubic beziers (see Section 3.4.6), that the described curve also lies within the given dimensions).

The listOfCompartmentGlyphs element

The listOfCompartmentGlyphs, when present, must contain one or more CompartmentGlyph elements.

Note that not all **Compartment** elements have to be represented by a **CompartmentGlyph**. In fact quite often the compartment is omitted in a layout for a uni-compartmental network. (In which case the **ListOfCompartment-Glyphs** would be omitted altogether.)

The listOfSpeciesGlyphs element

The listOfSpeciesGlyphs, when present, must contain one or more SpeciesGlyph elements. Just as with CompartmentGlyph elements, not every Species of the model has to have a representation in this list.

The listOfReactionGlyphs element

The listOfReactionGlyphs, when present, must contain one or more ReactionGlyph elements. Again, not all reactions of the containing SBML model have to be included in the containing layout.

The listOfTextGlyphs element

The listOfTextGlyphs, when present, must contain one or more TextGlyph elements.

The listOfAdditionalGraphicalObjects element

Most objects for which layout information is to be included in an SBML file have a corresponding object in the SBML model. As there might be cases where the user wants to include object types in the layout that do fall in any of the other categories described below, we include a <code>listOfAdditionalGraphicalObjects</code> in each Layout object. This list holds an arbitrary number of <code>graphicalObject</code> elements. The <code>graphicalObject</code> only defines a bounding box in a specific place in the layout without giving additional information about its contents.

The listOfAdditionalGraphicalObjects, when present, must contain one or more of the following elements: GraphicalObject, GeneralGlyph.

When using a **GraphicalObject** it is recommended that some form of meta information is provided. For additional relationships such as SBML events or rules, the **GeneralGlyph** can be used, see Section 3.11.

3.7 The GraphicalObject class

All the more specific layout elements (CompartmentGlyph, GeneralGlyph, SpeciesGlyph, ReactionGlyph, Reference-Glyph, TextGlyph, and SpeciesReferenceGlyph) are derived from the class GraphicalObject. Each object of class GraphicalObject has a mandatory BoundingBox, which specifies the position and the size of the object. Figure 9 provides a UML diagram illustrating the definition of GraphicalObject.

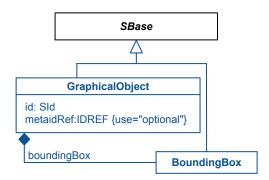


Figure 9: The definitions of the **GraphicalObject** class.

While **GraphicalObject** is the base class for most elements in the Layout package, it is **not** an abstract class. It can be instantiated when used in the **listOfAdditionalGraphicalObjects** to describe additional elements and relationships. Since it only describes a **BoundingBox**, programs are encouraged to add **Annotation** objects that

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describe program specific graphical information.

The id attribute

The GraphicalObject has a mandatory id attribute of type SId through which it can be identified.

The metaidRef attribute

The **GraphicalObject** has an optional **metaidRef** attribute of type **IDREF** that allows the object to uniquely reference elements in the **Model**. Wherever possible it is preferred that the more specific reference mechanisms are used.

3.8 The CompartmentGlyph class

The **CompartmentGlyph** class is derived from **GraphicalObject** and inherits its attributes. Additionally, it has two optional attributes: **compartment** and **order**. For an example, see Section 4.1 on page 21.

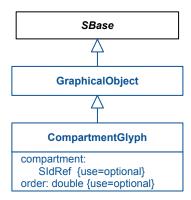


Figure 10: The definitions of the **CompartmentGlyph** class.

The compartment attribute

The compartment attribute is of type SIdRef. It is used to add a reference to the id of the corresponding compartment in the model. Since the compartment is optional, the user can specify compartments in the layout that are not part of the model.

If the **compartment** attribute is used together with the **metaidRef** attribute, they both need to refer to the same object in the **Model**.

The order attribute

The order attribute is an optional attribute of type double. It is there to handle the case where compartments in a layout overlap, and tools want to clearly disambiguate which CompartmentGlyph is on top of the other. The order attribute follows the coordinate system. There the z dimension points into the screen; thus, an element with a lower order value will be in front of elements with a higher value. If not specified, the order is undefined and tools are free to display the compartment glyphs in the order that best fits their needs.

Note: usually the **order** attribute is only used for two dimensional layouts since in three dimensional layouts the **z** coordinate can be used to easily distinguish **CompartmentGlyphs**. However, there may be uses for having the same **z** coordinate in three dimensional layouts, in which case, the **order** attribute can help to disambiguate the drawing order.

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3.9 The SpeciesGlyph class

In addition to the attributes from **GraphicalObject**, the **SpeciesGlyph** object has an optional **species** attribute. For an example, see Section 4.2 on page 22.

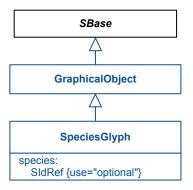


Figure 11: The definitions of the **SpeciesGlyph** class.

The species attribute

The species attribute of type SIdRef allows modelers to link the SpeciesGlyph to the id of the corresponding species object in the Model. The species attribute is optional to allow the program to specify species representations that do not have a direct correspondence in the model. This might be useful if some pathway has been collapsed, but is still treated by layout programs.

If the **species** attribute is used together with the **metaidRef** attribute, they both need to refer to the same object in the **Model**.

3.10 The ReactionGlyph class

The **ReactionGlyph** is used to represent **Reaction** elements in the layout. Analogous to how a **Reaction** object has to at least have one reactant or product, the **ReactionGlyph** has to at least have one **SpeciesReferenceGlyph** stored in the **ListOfSpeciesReferenceGlyphs**. Figure 12 on the following page provides the UML diagram for the class definition.

The ReactionGlyph inherits from GraphicalObject. In addition to the attributes inherited from GraphicalObject, the ReactionGlyph is described by an attribute reaction, a Curve element and a listOfSpeciesReferenceGlyphs element.

The **Curve** describes the center section of a **ReactionGlyph**. The center section is frequently used by tools to separate the point where substrates arcs come together, from the point where product arcs split off. The **Curve** is optional, and when not present the dimensions of the inherited **BoundingBox** describes the center section, by storing its position and dimension.

For an example of **ReactionGlyph**, see Section 4.3.

The reaction attribute

The **reaction** attribute of type **SIdRef** is used to specify the **id** of the corresponding **Reaction** in the model. This reference is optional.

If the reaction attribute is used together with the metaidRef, they need to refer to the same object in the Model.

Section 3 Package syntax and semantics

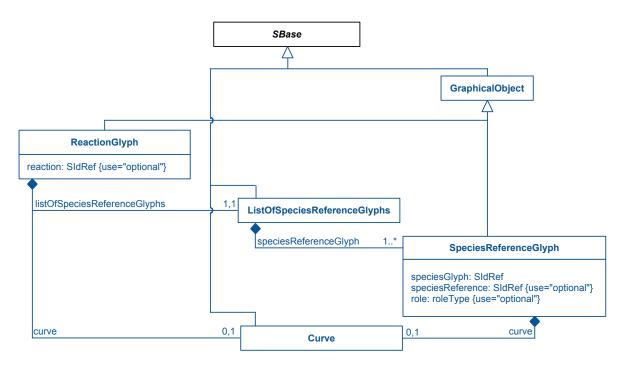


Figure 12: The definitions of the ReactionGlyph class.

The listOfSpeciesReferenceGlyphs element

Since a **Species** element can have several graphical representations in the layout there must be a way to specify which **SpeciesGlyph** should be connected to the **ReactionGlyph**. This is done using the **listOfSpeciesReference-Glyphs**.

The ListOfSpeciesReferenceGlyphs is mandatory, since every Reaction has to have at least one reactant or product.

The curve element

The optional **Curve** element (Section 3.4.4) can be used to describe a curve representation for the **ReactionGlyph**. If a **ReactionGlyph** specifies a curve, the bounding box is to be ignored.

3.10.1 The SpeciesReferenceGlyph class

The speciesReferenceGlyph element describes the graphical connection between a SpeciesGlyph and a Reaction-Glyph (which would be an arrow or some curve in most cases).

As can be seen in the diagram Figure 12, a **SpeciesReferenceGlyph** inherits from **GraphicalObject**. Additionally, it has a mandatory attribute **speciesGlyph** and two optional attributes **speciesReference** and **role**. Optionally, the **SpeciesReferenceGlyph** also has an element **curve**.

If the **curve** is specified, it overrides the inherited bounding box.

The speciesGlyph attribute

The speciesGlyph is of type SIdRef. It contains a reference to the id of a SpeciesGlyph object that is to be connected to the ReactionGlyph. This attribute is mandatory so as to ensure unambiguity about which SpeciesGlyph has to be connected with this ReactionGlyph.

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The speciesReference attribute

The role attribute

The speciesReference is an optional attribute of type SIdRef that allows modelers to connect the Species-Reference(or ModifierSpeciesReference) of the containing model.

If the **speciesReference** attribute is used together with the **metaidRef** attribute, they both need to refer to the same object in the **Model**.

Note: the id on a SpeciesReference and ModifierSpeciesReference was only introduced in SBML Level 3 Version 1 Core. In order to successfully use the speciesReference in prior Levels of SBML, the corresponding species reference has to be annotated with an identifier. The annotation would look like this:

```
<annotation>
    <layoutId xmlns="http://projects.eml.org/bcb/sbml/level2" id="theId"/>
</annotation>
```

This **id** has to be unique within the global **SId** namespace of the SBML model and can thus be used to reference a given species reference. For a complete example see also Section 4.3.2.

given species reference. For a complete example see also section 4.5.2.

The role attribute is of SpeciesReferenceRole (see Section 3.3.1) and is used to specify how the species reference should be displayed. Allowed values are "substrate", "product", "sidesubstrate", "sideproduct", "modifier", "activator", "inhibitor" and "undefined".

This attribute is optional and should only be necessary if the optional **speciesReference** attribute is not given or if the respective information from the model needs to be overridden.

- The values "substrate" and "product" are used if the species reference is a main product or substrate in the reaction.
- "sidesubstrate" and "sideproduct" are used for simple chemicals like ATP, NAD+, etc. This allows programs to render them as side reactions.
- "activator" and "inhibitor" are modifiers where their influence on the reaction is known and "modifier" is a more general term if the influence is unknown or changes during the course of the simulation.

To define more specific types of interactions, the recommended practice is to use the **sboTerm** attribute on the **SpeciesReference**. If both **role** and **sboTerm** are specified and they conflict, it is the **role** that takes precedence.

The curve element

The **curve** is an optional element of type **Curve**. When present, the glyphs bounding box (as inherited from the **GraphicalObject**) is to be disregarded.

So as to make the drawing of these curves as easy as possible, the line segments should be ordered depending on the role of the **SpeciesReferenceGlyph**. If no **role** attribute is defined, the role to be assumed is taken from the role that the **SpeciesReference** referenced via the attribute **speciesReference** has, otherwise it is "undefined".

- "product", "sideproduct", "substrate", "sidesubstrate", "undefined": The line segments have their start element at the ReactionGlyph and their end element at the SpeciesGlyph.
- "activator", "inhibitor", "modifier": The line segments have their start element at the SpeciesGlyph and their end element at the ReactionGlyph.

3.11 The GeneralGlyph class

The **GeneralGlyph** is used to facilitate the representation of elements other than **Compartment**, **Species** and **Reaction** and thus can be used for the display of relationships of **Rule** or elements defined by other SBML packages. It closely follows the structure of the **ReactionGlyph**.

As can be seen from the UML diagram of Figure 13, **GeneralGlyph** is defined to have an optional attribute reference as well as the elements curve, listOfReferenceGlyphs and listOfSubGlyphs.

For an example that uses the **GeneralGlyph** to represents a basic influence, see Section 4.7.

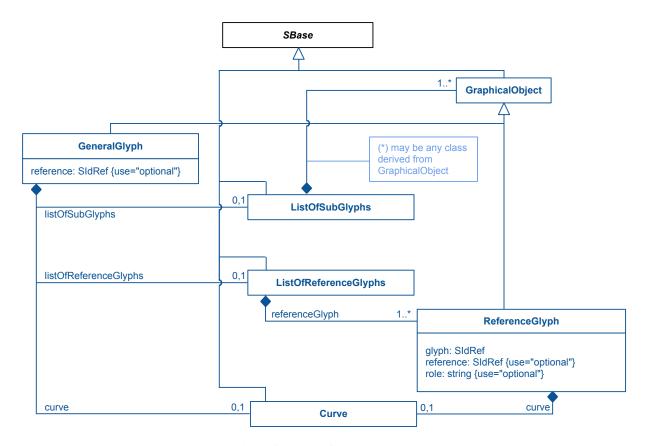


Figure 13: The definitions of the **GeneralGlyph** class.

The reference attribute

The optional **reference** attribute of type **SIdRef** that can be used to specify the **id** of the corresponding element in the model that is represented.

If the reference attribute is used together with the metaidRef, they need to refer to the same object in the Model.

The listOfSubGlyphs element

The **ListOfSubGlyphs** is an optional list that can contain sub glyphs of the **GeneralGlyph**. One example of its use could be a sub-module containing species glyphs and reaction glyphs that are not necessarily part of the enclosing **Model**. Another example is an **Event**, visualized with its **Trigger** and additional **GeneralGlyphs** for its **EventAssignments**. The **ListOfSubGlyphs** consists of **GraphicalObject** or derived classes. Thus, unlike the **ListOfAdditional-GraphicalObjects** (which may only contain **GraphicalObjects** or **GeneralGlyphs**), the **listOfSubGlyphs** may contain any derived class, such as for example **TextGlyph** elements.

The element names of the children of **ListOfSubGlyphs** are the de-capitalized forms of their class: **graphicalObject**, compartmentGlyph, generalGlyph, reactionGlyph, referenceGlyph, speciesGlyph, speciesReferenceGlyph, or textGlyph.

When present, the listOfSubGlyphs must contain at least one element.

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The listOfReferenceGlyphs element

The **ListOfReferenceGlyphs** is optional, since conceivably the **GeneralGlyph** could just contain a number of subglyphs. When present, it must include at least one **ReferenceGlyph**.

The curve element

The optional **Curve** element (Section 3.4.4) can be used to describe a curve representation for the **GeneralGlyph**.

If a GeneralGlyph specifies a curve, the bounding box is to be ignored.

3.11.1 The ReferenceGlyph class

The referenceGlyph element describes the graphical connection between an arbitrary **GraphicalObject** (or derived element) and a **GeneralGlyph** (which would be an arrow or some curve in most cases).

As can be seen in Figure 13 on the preceding page, a **ReferenceGlyph** inherits from **GraphicalObject**. Additionally it has a mandatory attribute **glyph** and two optional attributes **reference** and **role**. Optionally, the **ReferenceGlyph** also has an element **curve**.

The ReferenceGlyph should either contain a bounding box or a curve specification, if both are given, the bounding box should be ignored.

The glyph attribute

The glyph is of type SIdRef. It contains a reference to the id of a GraphicalObject (or derived) object that is to be connected to the GeneralGlyph.

This attribute is mandatory so as to ensure unambiguously which glyph has to be connected with this **General-Glyph**.

The reference attribute

The reference is an optional attribute of type SIdRef that is used to connect the ReferenceGlyph with an element of the containing SBML model.

The role attribute

The role attribute is of type string and is used to specify how the reference should be displayed.

While as a **string**, the value of the **role** attribute is unconstrained, current implementations use the same values as specified in Section 3.3.1.

The curve element

The **curve** is an optional element of type **Curve**. When present, the glyph's bounding box (as inherited from the **GraphicalObject**) is to be disregarded.

So as to make the drawing of these curves as easy as possible the line segments should be ordered depending on the role of the **ReferenceGlyph**:

- If the glyph represents a modification it should start at the glyph and end at the center of the GeneralGlyph.
- otherwise it should begin at the center section of the **GeneralGlyph** and end at the reference glyph.

3.12 The TextGlyph class

The **TextGlyph** class describes the position and dimension of text labels. It inherits from **GraphicalObject** and adds the attributes **graphicalObject**, **text** and **originOfText**.

For an example, see Section 4.4.

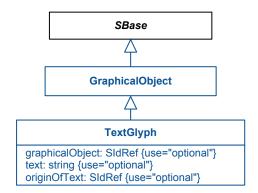


Figure 14: The definitions of the **TextGlyph** class.

The graphicalObject attribute

The attribute graphicalObject is of type SIdRef. It contains the id of any GraphicalObject and specifies that the TextGlyph should be considered to be a label to that object. This allows modelers to indicate that the label is to be moved together with the object.

If the **graphicalObject** attribute is used together with the **metaidRef** they need to refer to the same object in the **Layout**.

The text attribute

The optional text attribute is of type string. It facilitates adding of independent text, like a title or a comment to the diagram.

The originOfText attribute

Additionally the optional attribute originOfText of type SIdRef can hold the id of an entity in the SBML model. If it is specified, the text to be displayed is taken from the name attribute of the referenced object.

If both attributes originOfText and text are specified, the text attribute value overrides the value of originOfText.

4 Examples

4.1 CompartmentGlyph Example

Below a **CompartmentGlyph** is defined for the compartment **Yeast**. It is located at position x="5", y="5" and has dimensions width="390", height="220".

4.1.1 SBML Level 3 Version 1 Core using the Layout package

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core"</pre>
    xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1"
    level="3" version="1" layout:required="false" >
  <model id="TestModel_with_modifiers">
    <listOfCompartments>
      <compartment id="Yeast" spatialDimensions="3" constant="true"/>
    </listOfCompartments>
    <layout:listOfLayouts xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"</pre>
    xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1">
      <layout:layout layout:id="Layout_1">
        <layout:dimensions layout:width="400" layout:height="230"/>
        <layout:listOfCompartmentGlyphs>
          <layout:compartmentGlyph layout:id="CompartmentGlyph_1" layout:compartment="Yeast">
            <layout:boundingBox layout:id="bb1">
              <layout:position layout:x="5" layout:y="5"/>
              <layout:dimensions layout:width="390" layout:height="220"/>
            </layout:boundingBox>
          </layout:compartmentGlyph>
        </layout:listOfCompartmentGlyphs>
      </lavout:lavout>
    </layout:listOfLayouts>
 </model>
</sbml>
```

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4.1.2 SBML Level 2 Version 1 using the Annotation Scheme

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level2" level="2" version="1">
  <model id="TestModel_with_modifiers">
    <annotation>
     <listOfLayouts xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
              xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
      <layout id="Layout_1">
        <dimensions width="400" height="230"/>
        <listOfCompartmentGlyphs>
          <compartmentGlyph id="CompartmentGlyph_1" compartment="Yeast">
            <box><br/>dingBox id="bb1"></br>
              <position x="5" y="5"/>
              <dimensions width="390" height="220"/>
            </boundingBox>
          </compartmentGlyph>
        </listOfCompartmentGlyphs>
```

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4.2 SpeciesGlyph Example

Below a **SpeciesGlyph** is defined for the species **Glucose** at position x="105", y="20" with dimensions width="130", height="20".

4.2.1 SBML Level 3 Version 1 Core using the Layout package

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core"</pre>
    xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1"
    level="3" version="1" layout:required="false" >
  <model id="TestModel_with_modifiers">
    st0fSpecies>
      <species id="Glucose" compartment="Yeast" substanceUnits="substance"</pre>
      hasOnlySubstanceUnits="false" boundaryCondition="false" constant="false"/>
    </listOfSpecies>
    <layout:listOfLayouts xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"</pre>
    xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1">
      <layout:layout layout:id="Layout_1">
        <layout:dimensions layout:width="400" layout:height="230"/>
        <layout:listOfSpeciesGlyphs>
          <layout:speciesGlyph layout:id="SpeciesGlyph_Glucose" layout:species="Glucose">
            <layout:boundingBox layout:id="bb2">
              <layout:position layout:x="105" layout:y="20"/>
              <layout:dimensions layout:width="130" layout:height="20"/>
            </layout:boundingBox>
          </layout:speciesGlyph>
        </layout:listOfSpeciesGlyphs>
      </layout:layout>
    </layout:listOfLayouts>
  </model>
</sbml>
```

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4.2.2 SBML Level 2 Version 1 using the Annotation Scheme

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level2" level="2" version="1">
  <model id="TestModel_with_modifiers">
    <annotation>
     <listOfLayouts xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
              xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
      <layout id="Layout_1">
        <dimensions width="400" height="230"/>
        st0fSpeciesGlyphs>
          <speciesGlyph id="SpeciesGlyph_Glucose" species="Glucose">
            <boundingBox id="bb2">
              <position x="105" y="20"/>
              <dimensions width="130" height="20"/>
            </boundingBox>
          </speciesGlyph>
        </listOfSpeciesGlyphs>
      </layout>
      </list0fLayouts>
    </annotions>
    <listOfSpecies>
      <species id="Glucose" compartment="Yeast"/>
    </listOfSpecies>
 </model>
</sbml>
```

4.3 ReactionGlyph Example

The following defines a **ReactionGlyph** for reaction **Hexokinase** containing only a center segment represented as straight line.

4.3.1 SBML Level 3 Version 1 Core using the Layout package

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```
<layout:listOfLayouts xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"</pre>
    xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1">
      <layout:layout layout:id="Layout_1">
        <layout:dimensions layout:width="400" layout:height="230"/>
        <layout:listOfReactionGlyphs>
          <layout:reactionGlyph layout:id="glyph_Hexokinase" layout:reaction="Hexokinase">
            <layout:curve>
              <layout:listOfCurveSegments>
                <layout:curveSegment</pre>
          xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
          xsi:type="LineSegment">
                  <layout:start layout:x="170" layout:y="100"/>
                  <layout:end layout:x="170" layout:y="130"/>
                </layout:curveSegment>
              </layout:listOfCurveSegments>
            </layout:curve>
            <layout:listOfSpeciesReferenceGlyphs>
            </layout:listOfSpeciesReferenceGlyphs>
          </layout:reactionGlyph>
        </layout:listOfReactionGlyphs>
      </layout:layout>
    </layout:listOfLayouts>
  </model>
</sbml>
```

4.3.2 SBML Level 2 Version 1 using the Annotation Scheme

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level2" level="2" version="1">
  <model id="TestModel_with_modifiers">
     <listOfLayouts xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
              xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
      <layout id="Layout_1">
        <dimensions width="400" height="230"/>
        <listOfReactionGlyphs>
          <reactionGlyph id="glyph_Hexokinase" reaction="Hexokinase">
            <curve>
              <listOfCurveSegments>
                <curveSegment xsi:type="LineSegment">
                  <start x="170" y="100"/>
                  <end x="170" y="130"/>
                </curveSegment>
              </list0fCurveSegments>
            </curve>
            <listOfSpeciesReferenceGlyphs>
            </listOfSpeciesReferenceGlyphs>
          </reactionGlyph>
        </listOfReactionGlyphs>
```

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The following adds a **SpeciesReferenceGlyph** and demonstrates adding an **id** to a **SpeciesReference** in SBML Level 2 Version 1. This is not necessary in SBML Level 3 Version 1 Core, as there **SpeciesReference** elements have an **id** attribute.

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level2" level="2" version="1">
  <model id="TestModel_with_modifiers">
    <annotation>
     <listOfLayouts xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
              xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
      <layout id="Layout_1">
        <dimensions width="400" height="230">
        </dimensions>
        <listOfReactionGlyphs>
          <reactionGlyph id="glyph_Hexokinase" reaction="Hexokinase">
            <listOfSpeciesReferenceGlyphs>
              <speciesReferenceGlyph id="SpeciesReferenceGlyph_Glucose"</pre>
                   speciesReference="SpeciesReference_Glucose"
                   speciesGlyph="SpeciesGlyph_Glucose" role="substrate">
                <curve>
                  <listOfCurveSegments>
                    <curveSegment xsi:type="LineSegment">
                      <start x="170" y="100">
                      </start>
                      <end x="170" y="50">
                      </end>
                    </curveSegment>
                  </list0fCurveSegments>
                </curve>
              </speciesReferenceGlyph>
            </listOfSpeciesReferenceGlyphs>
          </reactionGlyph>
        </listOfReactionGlyphs>
```

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```
</layout>
    </list0fLayouts>
    </annotation>
    <listOfReactions>
      <reaction id="Hexokinase" reversible="false">
        <listOfReactants>
          <speciesReference species="Glucose">
            <annotation>
              <layoutId xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
                        id="SpeciesReference_Glucose"/>
            </annotation>
          </speciesReference>
        </list0fReactants>
      </reaction>
    </listOfReactions>
 </model>
</sbml>
```

4.4 TextGlyph Example

The following defines a **TextGlyph** with id="TextGlyph_Glucose" that is connected to a **SpeciesGlyph** "SpeciesGlyph_Glucose" and retrieves the text to display from the **Species** with id="Glucose".

4.4.1 SBML Level 3 Version 1 Core using the Layout package

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core"</pre>
    xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1"
    level="3" version="1" layout:required="false" >
  <model id="TestModel_with_modifiers">
    <listOfSpecies>
      <species id="Glucose" compartment="Yeast" substanceUnits="substance"</pre>
      hasOnlySubstanceUnits="false" boundaryCondition="false" constant="false"/>
    </listOfSpecies>
    <layout:listOfLayouts xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"</pre>
    xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1">
      <layout:layout layout:id="Layout_1">
        <layout:dimensions layout:width="400" layout:height="230"/>
        <layout:listOfSpeciesGlyphs>
          <layout:speciesGlyph layout:id="SpeciesGlyph_Glucose" layout:species="Glucose">
            <layout:boundingBox layout:id="bb2">
              <layout:position layout:x="105" layout:y="20"/>
              <layout:dimensions layout:width="130" layout:height="20"/>
```

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```
</layout:boundingBox>
          </layout:speciesGlyph>
        </layout:listOfSpeciesGlyphs>
        <layout:listOfTextGlyphs>
          <layout:textGlyph layout:id="TextGlyph_Glucose"</pre>
      layout:originOfText="Glucose"
      layout:graphicalObject="SpeciesGlyph_Glucose">
            <layout:boundingBox layout:id="bbA">
              <layout:position layout:x="115" layout:y="20"/>
              <layout:dimensions layout:width="110" layout:height="20"/>
            </layout:boundingBox>
          </layout:textGlyph>
        </layout:listOfTextGlyphs>
      </layout:layout>
    </layout:listOfLayouts>
  </model>
</sbml>
```

4.4.2 SBML Level 2 Version 1 using the Annotation Scheme

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level2" level="2" version="1">
  <model id="TestModel_with_modifiers">
    <annotation>
     <listOfLayouts xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
              xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
      <layout id="Layout_1">
        <dimensions width="400" height="230"/>
        <listOfSpeciesGlyphs>
          <speciesGlyph id="SpeciesGlyph_Glucose" species="Glucose">
            <boundingBox id="bb2">
              <position x="105" y="20"/>
              <dimensions width="130" height="20"/>
            </boundingBox>
          </speciesGlyph>
        </listOfSpeciesGlyphs>
        <listOfTextGlyphs>
          <textGlyph id="TextGlyph_Glucose" graphicalObject="SpeciesGlyph_Glucose"</pre>
                     originOfText="Glucose">
            <box id="bbA">
              <position x="115" y="20">
              </position>
              <dimensions width="110" height="20">
              </dimensions>
            </boundingBox>
          </textGlyph>
        </listOfTextGlyphs>
      </layout>
     </list0fLayouts>
    </annotation>
```

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4.5 Complete Example using SBML Level 3 Version 1

Here a small complete example to illustrate and complement the paragraphs above. The model consists of the Hexokinase reaction.

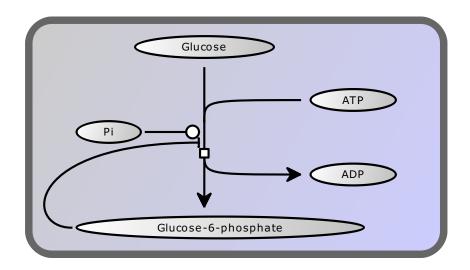


Figure 15: One possible rendering of the example layout.

This reaction has a feedback inhibition by glucose-6-phosphate and it is activated by free organic phosphate. These two relations are represented by species reference glyphs and a corresponding role attribute. We did not include any coordinates in the third dimension.

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core"</pre>
    xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1"
    level="3" version="1" layout:required="false" >
  <model id="TestModel_with_modifiers" timeUnits="time">
    <listOfUnitDefinitions>
      <unitDefinition id="volume">
        tofUnits>
          <unit kind="litre" exponent="1" scale="0" multiplier="1"/>
        </listOfUnits>
      </unitDefinition>
      <unitDefinition id="substance">
        tofUnits>
          <unit kind="mole" exponent="1" scale="0" multiplier="1"/>
        </listOfUnits>
      </unitDefinition>
```

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```
<unitDefinition id="time">
    tofUnits>
      <unit kind="second" exponent="1" scale="0" multiplier="1"/>
    </listOfUnits>
  </unitDefinition>
</list0fUnitDefinitions>
<listOfCompartments>
  <compartment id="Yeast" spatialDimensions="3" units="volume" constant="true"/>
</list0fCompartments>
Species>
  <species id="Glucose" compartment="Yeast" substanceUnits="substance"</pre>
 hasOnlySubstanceUnits="false" boundaryCondition="false" constant="false"/>
  <species id="G6P" name="Glucose-6-phosphate" compartment="Yeast"</pre>
                                                                                                              13
 substanceUnits="substance" hasOnlySubstanceUnits="false"
boundaryCondition="false" constant="false"/>
                                                                                                              14
                                                                                                              15
  <species id="ATP" compartment="Yeast" substanceUnits="substance"</pre>
                                                                                                              16
 hasOnlySubstanceUnits="false" boundaryCondition="false" constant="false"/>
 <species id="ADP" compartment="Yeast" substanceUnits="substance"</pre>
                                                                                                              18
 hasOnlySubstanceUnits="false" boundaryCondition="false" constant="false"/>
<species id="Pi" compartment="Yeast" substanceUnits="substance"
                                                                                                              19
                                                                                                              20
 hasOnlySubstanceUnits="false" boundaryCondition="false" constant="false"/>
                                                                                                              21
</listOfSpecies>
                                                                                                              22
<listOfReactions>
                                                                                                              23
  <reaction id="Hexokinase" reversible="false" fast="false">
                                                                                                              24
    1istOfReactants>
      <speciesReference id="SpeciesReference_Glucose" species="Glucose"</pre>
  stoichiometry="1" constant="true"/>
                                                                                                              27
      <speciesReference id="SpeciesReference_ATP" species="ATP"</pre>
  stoichiometry="1" constant="true"/>
                                                                                                              29
    </listOfReactants>
                                                                                                              30
    <speciesReference id="SpeciesReference_G6P" species="G6P"</pre>
                                                                                                              32
  stoichiometry="1" constant="true"/>
                                                                                                              33
      <speciesReference id="SpeciesReference_ADP" species="ADP"</pre>
 stoichiometry="1" constant="true"/>
                                                                                                              35
    </listOfProducts>
                                                                                                              36
    <listOfModifiers>
                                                                                                              37
      <modifierSpeciesReference id="ModifierSpeciesReference_G6P" species="G6P"/>
                                                                                                              38
      <modifierSpeciesReference id="ModifierSpeciesReference_Pi" species="Pi"/>
                                                                                                              39
    </listOfModifiers>
  </reaction>
                                                                                                              41
</listOfReactions>
                                                                                                              42
<layout:listOfLayouts xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"</pre>
                                                                                                              43
xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1">
                                                                                                              44
  <layout:layout layout:id="Layout_1">
    <layout:dimensions layout:width="400" layout:height="230"/>
                                                                                                              46
    <layout:listOfCompartmentGlyphs>
                                                                                                              47
      <layout:compartmentGlyph layout:id="CompartmentGlyph_1" layout:compartment="Yeast">
        <layout:boundingBox layout:id="bb1">
                                                                                                              49
          <layout:position layout:x="5" layout:y="5"/>
                                                                                                              50
          <layout:dimensions layout:width="390" layout:height="220"/>
                                                                                                              51
        </layout:boundingBox>
                                                                                                              52
      </layout:compartmentGlyph>
                                                                                                              53
    </layout:listOfCompartmentGlyphs>
    <layout:listOfSpeciesGlyphs>
                                                                                                              55
      <layout:speciesGlyph layout:id="SpeciesGlyph_Glucose" layout:species="Glucose">
                                                                                                              56
        <layout:boundingBox layout:id="bb2">
          <layout:position layout:x="105" layout:y="20"/>
                                                                                                              58
          <layout:dimensions layout:width="130" layout:height="20"/>
                                                                                                              59
        </layout:boundingBox>
      </layout:speciesGlyph>
                                                                                                              61
      <layout:speciesGlyph layout:id="SpeciesGlyph_G6P" layout:species="G6P">
                                                                                                              62
        <layout:boundingBox layout:id="bb5">
                                                                                                              63
          <layout:position layout:x="50" layout:y="190"/>
                                                                                                              64
          <layout:dimensions layout:width="270" layout:height="20"/>
                                                                                                              65
        </layout:boundingBox>
```

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58

59

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65

```
</layout:speciesGlyph>
  <layout:speciesGlyph layout:id="SpeciesGlyph_ATP" layout:species="ATP">
    <layout:boundingBox layout:id="bb3">
      <layout:position layout:x="270" layout:y="70"/>
      <layout:dimensions layout:width="80" layout:height="20"/>
    </layout:boundingBox>
  </layout:speciesGlyph>
  <layout:speciesGlyph layout:id="glyph_ADP" layout:species="ADP">
    <layout:boundingBox layout:id="bb4">
      <layout:position layout:x="270" layout:y="140"/>
      <layout:dimensions layout:width="80" layout:height="20"/>
    </layout:boundingBox>
  </layout:speciesGlyph>
  <layout:speciesGlyph layout:id="SpeciesGlyph_Pi" layout:species="Pi">
    <layout:boundingBox layout:id="bb6">
      <layout:position layout:x="50" layout:y="100"/>
      <layout:dimensions layout:width="60" layout:height="20"/>
    </layout:boundingBox>
  </layout:speciesGlyph>
</layout:listOfSpeciesGlyphs>
<layout:listOfReactionGlyphs>
  <layout:reactionGlyph layout:id="glyph_Hexokinase" layout:reaction="Hexokinase">
    <layout:curve>
      <layout:listOfCurveSegments>
        <layout:curveSegment</pre>
 xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
 xsi:type="LineSegment">
          <layout:start layout:x="170" layout:y="100"/>
          <layout:end layout:x="170" layout:y="130"/>
        </layout:curveSegment>
      </layout:listOfCurveSegments>
    </layout:curve>
    <layout:listOfSpeciesReferenceGlyphs>
      <layout:speciesReferenceGlyph layout:id="SpeciesReferenceGlyph_Glucose"</pre>
layout:speciesReference="SpeciesReference_Glucose"
layout:speciesGlyph="SpeciesGlyph_Glucose"
layout:role="substrate">
        <lavout:curve>
          <layout:listOfCurveSegments>
            <layout:curveSegment</pre>
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
    xsi:type="LineSegment">
              <layout:start layout:x="170" layout:y="100"/>
              <layout:end layout:x="170" layout:y="50"/>
            </layout:curveSegment>
          </layout:listOfCurveSegments>
        </layout:curve>
      </layout:speciesReferenceGlyph>
      <layout:speciesReferenceGlyph layout:id="SpeciesReferenceGlyph_ATP"</pre>
layout:speciesReference="SpeciesReference_ATP"
layout:speciesGlyph="SpeciesGlyph_ATP"
layout:role="sidesubstrate">
        <layout:curve>
          <layout:listOfCurveSegments>
            <layout:curveSegment</pre>
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
    xsi:type="CubicBezier">
              <layout:start layout:x="170" layout:y="100"/>
              <layout:end layout:x="260" layout:y="80"/>
              <layout:basePoint1 layout:x="170" layout:y="80"/>
              <layout:basePoint2 layout:x="170" layout:y="80"/>
            </lavout:curveSeament>
          </layout:listOfCurveSegments>
        </layout:curve>
      </layout:speciesReferenceGlyph>
      <layout:speciesReferenceGlyph layout:id="SpeciesReferenceGlyph_G6P_1"</pre>
```

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```
layout:speciesReference="SpeciesReference_G6P"
layout:speciesGlyph="SpeciesGlyph_G6P"
layout:role="product">
        <lavout:curve>
          <layout:listOfCurveSegments>
            <layout:curveSegment</pre>
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
    xsi:type="LineSegment">
               <layout:start layout:x="170" layout:y="130"/>
               <layout:end layout:x="170" layout:y="180"/>
             </layout:curveSegment>
          </layout:listOfCurveSegments>
        </layout:curve>
                                                                                                        13
      </layout:speciesReferenceGlyph>
                                                                                                        14
      <layout:speciesReferenceGlyph layout:id="SpeciesReferenceGlyph_ADP"</pre>
                                                                                                        15
layout:speciesReference="SpeciesReference_ADP"
                                                                                                        16
layout:speciesGlyph="glyph_ADP"
layout:role="sideproduct">
                                                                                                        18
        <layout:curve>
                                                                                                        19
          <layout:listOfCurveSegments>
                                                                                                        20
            <layout:curveSegment</pre>
                                                                                                        21
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
                                                                                                        22
    xsi:type="CubicBezier">
                                                                                                        23
               <layout:start layout:x="170" layout:y="130"/>
                                                                                                        24
               <layout:end layout:x="260" layout:y="150"/>
               <layout:basePoint1 layout:x="170" layout:y="150"/>
                                                                                                        26
               <layout:basePoint2 layout:x="170" layout:y="150"/>
                                                                                                        27
             </layout:curveSegment>
          </layout:listOfCurveSegments>
                                                                                                        29
        </layout:curve>
                                                                                                        30
      </layout:speciesReferenceGlyph>
      <layout:speciesReferenceGlyph layout:id="SpeciesReferenceGlyph_G6P_2"</pre>
                                                                                                        32
layout:speciesReference="ModifierSpeciesReference_G6P"
                                                                                                        33
layout:speciesGlyph="SpeciesGlyph_G6P"
                                                                                                        34
layout:role="inhibitor">
                                                                                                        35
        <layout:curve>
                                                                                                        36
          <layout:listOfCurveSegments>
                                                                                                        37
            <layout:curveSegment</pre>
                                                                                                        38
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
                                                                                                        39
    xsi:type="CubicBezier">
               <layout:start layout:x="45" layout:y="200"/>
                                                                                                        41
               <layout:end layout:x="165" layout:y="120"/>
                                                                                                        42
               <layout:basePoint1 layout:x="0" layout:y="200"/>
                                                                                                        43
               <layout:basePoint2 layout:x="0" layout:y="120"/>
                                                                                                        44
             </layout:curveSegment>
          </layout:listOfCurveSegments>
                                                                                                        46
        </layout:curve>
                                                                                                        47
      </layout:speciesReferenceGlyph>
      <layout:speciesReferenceGlyph layout:id="SpeciesReferenceGlyph_PI"</pre>
                                                                                                        49
layout:speciesReference="ModifierSpeciesReference_Pi"
                                                                                                        50
layout:speciesGlyph="SpeciesGlyph_Pi"
                                                                                                        51
layout:role="activator">
                                                                                                        52
        <layout:curve>
                                                                                                        53
          <layout:listOfCurveSegments>
            <layout:curveSegment</pre>
                                                                                                        55
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
                                                                                                        56
    xsi:type="CubicBezier">
               <layout:start layout:x="115" layout:y="110"/>
                                                                                                        58
               <layout:end layout:x="165" layout:y="110"/>
                                                                                                        59
               <layout:basePoint1 layout:x="140" layout:y="110"/>
               <layout:basePoint2 layout:x="140" layout:y="110"/>
                                                                                                        61
             </lavout:curveSeament>
                                                                                                        62
          </layout:listOfCurveSegments>
        </layout:curve>
                                                                                                        64
      </layout:speciesReferenceGlyph>
                                                                                                        65
    </layout:listOfSpeciesReferenceGlyphs>
```

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```
</layout:reactionGlyph>
        </layout:listOfReactionGlyphs>
        <layout:listOfTextGlyphs>
          <layout:textGlyph layout:id="TextGlyph_Glucose"</pre>
      layout:originOfText="Glucose"
      layout:graphicalObject="SpeciesGlyph_Glucose">
            <layout:boundingBox layout:id="bbA">
              <layout:position layout:x="115" layout:y="20"/>
              <layout:dimensions layout:width="110" layout:height="20"/>
            </layout:boundingBox>
          </layout:textGlyph>
          <layout:textGlyph layout:id="TextGlyph_G6P"</pre>
      layout:originOfText="G6P"
      layout:graphicalObject="SpeciesGlyph_G6P">
            <layout:boundingBox layout:id="bbD">
              <layout:position layout:x="60" layout:y="190"/>
              <layout:dimensions layout:width="250" layout:height="20"/>
            </layout:boundingBox>
          </layout:textGlyph>
          <layout:textGlyph layout:id="TextGlyph_ATP"</pre>
      layout:originOfText="ATP"
      layout:graphicalObject="SpeciesGlyph_ATP">
            <layout:boundingBox layout:id="bbB">
              <layout:position layout:x="280" layout:y="70"/>
              <layout:dimensions layout:width="60" layout:height="20"/>
            </layout:boundingBox>
          </layout:textGlyph>
          <layout:textGlyph layout:id="TextGlyph_ADP"</pre>
      layout:originOfText="ADP"
      layout:graphicalObject="glyph_ADP">
            <layout:boundingBox layout:id="bbC">
              <layout:position layout:x="280" layout:y="140"/>
              <layout:dimensions layout:width="60" layout:height="20"/>
            </layout:boundingBox>
          </layout:textGlyph>
          <layout:textGlyph layout:id="TextGlyph_PI"</pre>
      layout:originOfText="Pi"
      layout:graphicalObject="SpeciesGlyph_Pi">
            <layout:boundingBox layout:id="bbE">
              <layout:position layout:x="60" layout:y="100"/>
              <layout:dimensions layout:width="40" layout:height="20"/>
            </layout:boundingBox>
          </layout:textGlyph>
        </layout:listOfTextGlyphs>
      </layout:layout>
    </layout:listOfLayouts>
  </model>
</sbml>
```

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4.6 Complete Example using SBML Level 2 Version 1

As mentioned before, the Layout package has been used since 2003 in **SBML** Level 2 documents. Whereas the previous example used the Level 3 package, here we are using the **SBML** annotations.

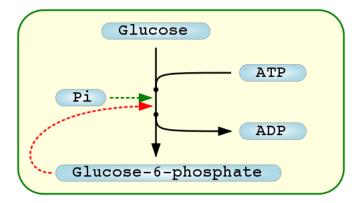


Figure 16: Another possible rendering of the example layout.

In order to use the Layout package in **SBML** Level 2 documents, all that is needed is to use the Level 2 Namespace (see Section 3.1) and move the **ListOfLayouts** into the **Model annotation** element.

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level2" level="2" version="1">
  <model id="TestModel_with_modifiers">
    <annotation>
     <listOfLayouts xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
               xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
      <layout id="Layout_1">
        <dimensions width="400" height="230"/>
        <listOfCompartmentGlyphs>
          <compartmentGlyph id="CompartmentGlyph_1" compartment="Yeast">
             <box><box<br/>dingBox<br/>id="bb1"></br>
               <position x="5" y="5"/>
               <dimensions width="390" height="220"/>
             </boundingBox>
          </compartmentGlyph>
        </list0fCompartmentGlyphs>
        <listOfSpeciesGlyphs>
          <speciesGlyph id="SpeciesGlyph_Glucose" species="Glucose">
             <box><br/>boundingBox id="bb2"></br>
               <position x="105" y="20"/>
               <dimensions width="130" height="20"/>
             </boundingBox>
          </speciesGlyph>
          <speciesGlyph id="SpeciesGlyph_G6P" species="G6P">
             <box><box<br/>dingBox<br/>id="bb5"></br>
               <position x="50" y="190"/>
               <dimensions width="270" height="20"/>
             </boundingBox>
          </speciesGlyph>
          <speciesGlyph id="SpeciesGlyph_ATP" species="ATP">
             <box><box<br/>dingBox<br/>id="bb3"></br>
               cposition x="270" y="70"/>
               <dimensions width="80" height="20"/>
             </boundingBox>
          </speciesGlyph>
          <speciesGlyph id="glyph_ADP" species="ADP">
             <boundingBox id="bb4">
```

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```
<position x="270" y="140"/>
      <dimensions width="80" height="20"/>
    </boundingBox>
  </speciesGlyph>
  <speciesGlyph id="SpeciesGlyph_Pi" species="Pi">
    <box><br/>d="bb6"></br>
      <position x="50" y="100"/>
      <dimensions width="60" height="20"/>
    </boundingBox>
  </speciesGlyph>
</listOfSpeciesGlyphs>
<listOfReactionGlyphs>
  <reactionGlyph id="glyph_Hexokinase" reaction="Hexokinase">
                                                                                                        13
      <listOfCurveSegments>
        <curveSegment xsi:type="LineSegment">
                                                                                                        16
          <start x="170" y="100"/>
          <end x="170" y="130"/>
                                                                                                        18
        </curveSegment>
                                                                                                        19
      </listOfCurveSegments>
                                                                                                        20
    </curve>
                                                                                                        21
    <listOfSpeciesReferenceGlyphs>
                                                                                                        22
      <speciesReferenceGlyph id="SpeciesReferenceGlyph_Glucose"</pre>
                     speciesReference="SpeciesReference_Glucose"
                                                                                                        24
                     speciesGlyph="SpeciesGlyph_Glucose" role="substrate">
        <curve>
          <listOfCurveSegments>
                                                                                                        27
            <curveSegment xsi:type="LineSegment">
              <start x="170" y="100"/>
                                                                                                        29
              <end x="170" y="50"/>
                                                                                                        30
            </curveSegment>
          <le></listOfCurveSegments>
                                                                                                        32
        </curve>
                                                                                                        33
      </speciesReferenceGlyph>
      <speciesReferenceGlyph id="SpeciesReferenceGlyph_ATP"</pre>
                                                                                                        35
                     speciesReference="SpeciesReference_ATP"
                                                                                                        36
                     speciesGlyph="SpeciesGlyph_ATP" role="sidesubstrate">
                                                                                                        37
        <curve>
                                                                                                        38
          <listOfCurveSegments>
                                                                                                        39
            <curveSegment xsi:type="CubicBezier">
              <start x="170" y="100"/>
                                                                                                        41
              <end x="260" y="80"/>
                                                                                                        42
              <basePoint1 x="170" y="80"/>
                                                                                                        43
              <basePoint2 x="170" y="80"/>
                                                                                                        44
            </curveSegment>
          </list0fCurveSegments>
                                                                                                        46
        </curve>
                                                                                                        47
      </speciesReferenceGlyph>
      <speciesReferenceGlyph id="SpeciesReferenceGlyph_G6P_1"</pre>
                                                                                                        49
                       speciesReference="SpeciesReference_G6P"
                                                                                                        50
                       speciesGlyph="SpeciesGlyph_G6P" role="product">
                                                                                                        51
        <curve>
                                                                                                        52
          <listOfCurveSegments>
                                                                                                        53
            <curveSegment xsi:type="LineSegment">
              <start x="170" y="130"/>
                                                                                                        55
              <end x="170" y="180"/>
                                                                                                        56
            </curveSegment>
          </listOfCurveSegments>
                                                                                                        58
        </curve>
                                                                                                        59
      </speciesReferenceGlyph>
      <speciesReferenceGlyph id="SpeciesReferenceGlyph_ADP"</pre>
                                                                                                        61
                     speciesReference="SpeciesReference_ADP"
                                                                                                        62
                     speciesGlyph="glyph_ADP" role="sideproduct">
        <curve>
                                                                                                        64
          <listOfCurveSegments>
                                                                                                        65
            <curveSegment xsi:type="CubicBezier">
```

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```
<start x="170" y="130"/>
              <end x="260" y="150"/>
              <basePoint1 x="170" y="150"/>
              <basePoint2 x="170" y="150"/>
             </curveSegment>
          </listOfCurveSegments>
        </curve>
      </speciesReferenceGlyph>
      <speciesReferenceGlyph id="SpeciesReferenceGlyph_G6P_2"</pre>
              speciesReference="ModifierSpeciesReference_G6P"
              speciesGlyph="SpeciesGlyph_G6P" role="inhibitor">
          <listOfCurveSegments>
             <curveSegment xsi:type="CubicBezier">
              <start x="45" y="200"/>
              <end x="165" y="120"/>
              <basePoint1 x="0" y="200"/>
              <basePoint2 x="0" y="120"/>
            </curveSegment>
          </listOfCurveSegments>
        </curve>
      </speciesReferenceGlyph>
      <speciesReferenceGlyph id="SpeciesReferenceGlyph_PI"</pre>
            speciesReference="ModifierSpeciesReference_Pi"
            speciesGlyph="SpeciesGlyph_Pi" role="activator">
        <curve>
          <listOfCurveSegments>
            <curveSegment xsi:type="CubicBezier">
              <start x="115" y="110"/>
              <end x="165" y="110"/>
              <basePoint1 x="140" y="110"/>
              <basePoint2 x="140" y="110"/>
            </curveSeament>
          </list0fCurveSegments>
        </curve>
      </speciesReferenceGlyph>
    </listOfSpeciesReferenceGlyphs>
  </reactionGlyph>
</listOfReactionGlyphs>
<listOfTextGlyphs>
  <textGlyph id="TextGlyph_Glucose" graphicalObject="SpeciesGlyph_Glucose"</pre>
             originOfText="Glucose">
    <box><box<br/>d="bbA"></br>
      <position x="115" y="20"/>
      <dimensions width="110" height="20"/>
    </boundingBox>
  </textGlyph>
  <textGlyph id="TextGlyph_G6P" graphicalObject="SpeciesGlyph_G6P"</pre>
             originOfText="G6P">
    <box><br/>d="bbD"></br>
      <position x="60" y="190"/>
      <dimensions width="250" height="20"/>
    </boundingBox>
  </textGlyph>
  <textGlyph id="TextGlyph_ATP" graphicalObject="SpeciesGlyph_ATP"</pre>
             originOfText="ATP">
    <box>
<br/>boundingBox id="bbB"></br>
      <position x="280" y="70"/>
      <dimensions width="60" height="20"/>
    </boundingBox>
  </textGlyph>
  <textGlyph id="TextGlyph_ADP" graphicalObject="glyph_ADP"</pre>
             originOfText="ADP">
    <box><box<br/>d="bbC"></br>
      <position x="280" y="140"/>
<dimensions width="60" height="20"/>
```

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```
</boundingBox>
      </textGlyph>
      <textGlyph id="TextGlyph_PI" graphicalObject="SpeciesGlyph_Pi"</pre>
                  originOfText="Pi">
        <box><br/>boundingBox id="bbE"></br>
          <position x="60" y="100"/>
          <dimensions width="40" height="20"/>
        </boundingBox>
      </textGlyph>
    </listOfTextGlyphs>
   </layout>
</list0fLayouts>
</annotation>
                                                                                                               13
<listOfCompartments>
                                                                                                               14
  <compartment id="Yeast"/>
</listOfCompartments>
                                                                                                               16
Species>
  <species id="Glucose" compartment="Yeast"/>
                                                                                                               18
 <species id="G6P" name="Glucose-6-phosphate" compartment="Yeast"/>
<species id="ATP" compartment="Yeast"/>
                                                                                                               19
                                                                                                               20
 <species id="ADP" compartment="Yeast"/>
                                                                                                               21
  <species id="Pi" compartment="Yeast"/>
                                                                                                               22
</listOfSpecies>
                                                                                                               23
24
  <reaction id="Hexokinase" reversible="false">
    <listOfReactants>
      <speciesReference species="Glucose">
                                                                                                               27
        <annotation>
          <layoutId xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
                                                                                                               29
                     id="SpeciesReference_Glucose"/>
                                                                                                               30
        </annotation>
      </speciesReference>
                                                                                                               32
      <speciesReference species="ATP">
                                                                                                               33
        <annotation>
                                                                                                               34
          <layoutId xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
                                                                                                               35
                     id="SpeciesReference_ATP"/>
                                                                                                               36
        </annotation>
                                                                                                               37
      </speciesReference>
                                                                                                               38
    </list0fReactants>
                                                                                                               39
    tofProducts>
      <speciesReference species="G6P">
                                                                                                               41
        <annotation>
                                                                                                               42
          <layoutId xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
                                                                                                               43
                     id="SpeciesReference_G6P"/>
                                                                                                               44
        </annotation>
      </speciesReference>
                                                                                                               46
      <speciesReference species="ADP">
                                                                                                               47
        <annotation>
          <layoutId xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
                                                                                                               49
                     id="SpeciesReference_ADP"/>
                                                                                                               50
        </annotation>
                                                                                                               51
      </speciesReference>
                                                                                                               52
    </list0fProducts>
                                                                                                               53
    <listOfModifiers>
      <modifierSpeciesReference species="G6P">
                                                                                                               55
        <annotation>
                                                                                                               56
          <layoutId xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
                     id="ModifierSpeciesReference_G6P"/>
                                                                                                               58
        </annotation>
                                                                                                               59
      </modifierSpeciesReference>
      <modifierSpeciesReference species="Pi">
                                                                                                               61
        <annotation>
                                                                                                               62
          <layoutId xmlns="http://projects.eml.org/bcb/sbml/level2"</pre>
                                                                                                               63
                     id="ModifierSpeciesReference_Pi"/>
                                                                                                               64
        </annotation>
                                                                                                               65
      </modifierSpeciesReference>
```

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4.7 Example using the GeneralGlyph

Here a small complete example that shows how to draw a basic influence diagram, where **Node0** negatively influences **Node1**.

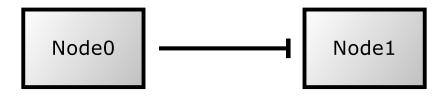


Figure 17: One possible rendering of an influence diagram.

In this example we have a simple SBML model that contains two species, Node0 and Node1. For both of them there are species glyph elements and associated Text labels. A **GeneralGlyph** then represents the influence.

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core"</pre>
     xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1"
    level="3" version="1" layout:required="false" >
 <model id="GeneralGlyphExample" >
 <listOfCompartments>
      <compartment id="compartment"</pre>
    spatialDimensions="3" size="1" constant="true"/>
    </listOfCompartments>
  Species>
      <species sboTerm="SBO:0000395" id="Node0"</pre>
      compartment="compartment" initialConcentration="0"
      hasOnlySubstanceUnits="false" boundaryCondition="false" constant="false"/>
      <species sboTerm="SBO:0000395" id="Node1"</pre>
      compartment="compartment" initialConcentration="0"
      hasOnlySubstanceUnits="false" boundaryCondition="false" constant="false"/>
    </listOfSpecies>
    <layout:listOfLayouts</pre>
     xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
     xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1">
      <layout:layout layout:id="example">
        <layout:dimensions layout:width="239.037328720093" layout:height="76.5"/>
    <layout:listOfSpeciesGlyphs>
          <layout:speciesGlyph layout:id="sGlyph_0" layout:species="Node0" >
            <layout:boundingBox>
              <layout:position layout:x="16" layout:y="18"/>
              <layout:dimensions layout:width="62" layout:height="40"/>
            </layout:boundingBox>
          </layout:speciesGlyph>
          <layout:speciesGlyph layout:id="sGlyph_1" layout:species="Node1" >
            <layout:boundingBox>
              <layout:position layout:x="161" layout:y="18"/>
```

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```
<layout:dimensions layout:width="62" layout:height="40"/>
            </layout:boundingBox>
          </layout:speciesGlyph>
        </layout:listOfSpeciesGlyphs>
    <layout:listOfAdditionalGraphicalObjects>
          <layout:generalGlyph layout:id="rGlyph_0" layout:reference="sGlyph_0">
        <!-- unused bounding box -->
            <layout:boundingBox>
              <layout:position layout:x="0" layout:y="0"/>
              <layout:dimensions layout:width="0" layout:height="0"/>
            </layout:boundingBox>
            <layout:listOfReferenceGlyphs>
        <!-- reference glyph representing the inhibited species -->
              <layout:referenceGlyph</pre>
            layout:id="SpeciesReference_J0_0"
          layout:reference="Node1"
          layout:glyph="sGlyph_1"
          layout:role="inhibitor">
                <layout:curve>
                  <layout:listOfCurveSegments>
                    <layout:curveSegment</pre>
            xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
            xsi:type="LineSegment">
                      <layout:start layout:x="86" layout:y="38"/>
                      <layout:end layout:x="153" layout:y="38"/>
                    </layout:curveSegment>
                  </layout:listOfCurveSegments>
                </layout:curve>
              </layout:referenceGlyph>
            </layout:listOfReferenceGlyphs>
          </layout:generalGlyph>
        </layout:listOfAdditionalGraphicalObjects>
    <layout:listOfTextGlyphs>
          <layout:textGlyph layout:id="tGlyph_0" layout:text="Node0"</pre>
           layout:graphicalObject="sGlyph_0">
            <layout:boundingBox>
              <layout:position layout:x="16" layout:y="18"/>
              <layout:dimensions layout:width="62" layout:height="40"/>
            </layout:boundingBox>
          </layout:textGlyph>
          <layout:textGlyph layout:id="tGlyph_1" layout:text="Node1"</pre>
                         layout:graphicalObject="sGlyph_1">
            <layout:boundingBox>
              <layout:position layout:x="161" layout:y="18"/>
              <layout:dimensions layout:width="62" layout:height="40"/>
            </layout:boundingBox>
          </layout:textGlyph>
        </layout:listOfTextGlyphs>
      </layout:layout>
    </layout:listOfLayouts>
  </model>
</sbml>
```

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A Validation of SBML documents

A.1 Validation and consistency rules

This section summarizes all the conditions that must (or in some cases, at least *should*) be true of an SBML Level 3 Version 1 model that uses the Layout package. We use the same conventions as are used in the SBML Level 3 Version 1 Core specification document. In particular, there are different degrees of rule strictness. Formally, the differences are expressed in the statement of a rule: either a rule states that a condition *must* be true, or a rule states that it *should* be true. Rules of the former kind are strict SBML validation rules—a model encoded in SBML must conform to all of them in order to be considered valid. Rules of the latter kind are consistency rules. To help highlight these differences, we use the following three symbols next to the rule numbers:

- ✓ A checked box indicates a *requirement* for SBML conformance. If a model does not follow this rule, it does not conform to the Layout specification. (Mnemonic intention behind the choice of symbol: "This must be checked.")
- A triangle indicates a *recommendation* for model consistency. If a model does not follow this rule, it is not considered strictly invalid as far as the Layout specification is concerned; however, it indicates that the model contains a physical or conceptual inconsistency. (Mnemonic intention behind the choice of symbol: "This is a cause for warning.")
- ★ A star indicates a strong recommendation for good modeling practice. This rule is not strictly a matter of SBML encoding, but the recommendation comes from logical reasoning. As in the previous case, if a model does not follow this rule, it is not strictly considered an invalid SBML encoding. (Mnemonic intention behind the choice of symbol: "You're a star if you heed this.")

The validation rules listed in the following subsections are all stated or implied in the rest of this specification document. They are enumerated here for convenience. Unless explicitly stated, all validation rules concern objects and attributes specifically defined in the Layout package.

For convenience and brevity, we use the shorthand "layout:x" to stand for an attribute or element name x in the namespace for the Layout package, using the namespace prefix layout. In reality, the prefix string may be different from the literal "layout" used here (and indeed, it can be any valid XML namespace prefix that the modeler or software chooses). We use "layout:x" because it is shorter than to write a full explanation everywhere we refer to an attribute or element in the Layout package namespace.

General rules about this package

layout-10101 ✓ To conform to the Layout package specification for SBML Level 3 Version 1, an SBML document must declare the use of the following XML Namespace:

"http://www.sbml.org/sbml/level3/version1/layout/version1".

(References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.1 on page 6.)

Wherever they appear in an SBML document, elements and attributes from the Layout package must be declared either implicitly or explicitly to be in the XML namespace "http://www.sbml.org/sbml/level3/version1/layout/version1".

(References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.1 on page 6.)

General rules about identifiers

layout-10301

✓ (Extends validation rule #10301 in the SBML Level 3 Version 1 Core specification.) Within a Model the values of the attributes id and layout:id on every instance of the following classes of objects must be unique across the set of all id and layout:id attribute values of all such objects in a model: the Model itself, plus all contained FunctionDefinition, Compartment, Species, Reaction, SpeciesReference, ModifierSpeciesReference, Event, and Parame-

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| | objects defined by the Layout package. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.3 on page 7.) |
|-------------------|---|
| layout-10302 | The value of the <code>layout:id</code> attribute must always conform to the syntax of the SBML data type SId. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.3 on page 7.) |
| General rules ab | out xsi:type |
| layout-10401 ☑ | The attribute xsi:type must be present on all LineSegment and CubicBezier objects. It is not permitted on any other element from the SBML Level 3 Layout namespace. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.3 on page 7.) |
| layout-10402 ☑ | The value of the xsi:type attribute must be either "LineSegment" or "CubicBezier" appropriate to the object where it is located. No other values are permitted. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.3 on page 7.) |
| Rules for the ext | ended SBML class |
| layout-20101 ✓ | In all SBML documents using the Layout package, the SBML object must include a value for the attribute layout:required attribute. (References: SBML Level 3 Version 1 Core, Section 4.1.2.) |
| layout-20102 ✓ | The value of attribute <code>layout:required</code> on the <code>SBML</code> object must be of the data type <code>boolean</code> . (References: SBML Level 3 Version 1 Core, Section 4.1.2.) |
| layout-20103 ✓ | The value of attribute layout:required on the SBML object must be set to "false". (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.1 on page 6.) |
| Rules for extend | ed Model object |
| layout-20201 ☑ | There may be at most one instance of ListOfLayouts element within a Model object using Layout. No other elements from the Layout package are allowed. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.5 on page 11.) |
| layout-20202 ✓ | The ListOfLayouts within a Model object is optional, but if present, must not be empty. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.5 on page 11.) |
| layout-20203 ✓ | Apart from the general notes and annotation subobjects permitted on all SBML objects, a ListOfLayouts container object may only contain Layout objects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.5 on page 11.) |
| layout-20204 ✓ | A ListOfLayouts object may have the optional metaid and sboTerm defined by SBML Level 3 Core. No other attributes from the SBML Level 3 Core namespace or the Layout namespace are permitted on a ListOfLayouts object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.5 on page 11.) |
| Rules for the Lay | vout object |
| layout-20301 ☑ | A Layout object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core namespace are permitted on a Layout . (References: SBML Level 3 Version 1 Core, Section 3.2.) |
| layout-20302 ✓ | A Layout object may have the optional SBML Level 3 Core attributes metaid and sboTerm . No other attributes from the SBML Level 3 Core namespace are permitted on a Layout . (Ref- |

erences: SBML Level 3 Version 1 Core, Section 3.2.)

ter objects, plus the BoundingBox, CompartmentGlyph, GeneralGlyph, GraphicalObject, Layout, SpeciesGlyph, SpeciesReferenceGlyph, ReactionGlyph, ReferenceGlyph, and TextGlyph

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There may be at most one instance of each of the following ListOf kinds of objects within a Layout object: ListOfCompartmentGlyphs, ListOfSpeciesGlyphs, ListOfReactionGlyphs, List-OfTextGlyphs, ListOfAdditionalGraphicalObjects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 11.) layout-20304

✓ The various ListOf... subobjects within a Layout object are optional, but if present, these container object must not be empty. Specifically, if any of the following classes of objects are present on the Layout, it must not be empty: ListOfCompartmentGlyphs, ListOfSpecies-Glyphs, ListOfReactionGlyphs, ListOfTextGlyphs, ListOfAdditionalGraphicalObjects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 11.) layout-20305

✓ A Layout object must have the required attribute layout:id and may have the optional attribute layout: name. No other attributes from the SBML Level 3 Layout namespace are permitted on a Layout object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 11.) layout-20306

✓ The attribute layout:name of a Layout must be of the data type string. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 11.) layout-20307
✓ A ListOfCompartmentGlyphs object may have the optional attributes metaid and sboTerm defined by SBML Level 3 Core. No other attributes from the SBML Level 3 Core namespace or the Layout namespace are permitted on a **ListOfCompartmentGlyphs** object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 12.) layout-20308 V Apart from the general notes and annotation subobjects permitted on all SBML objects, a ListOfCompartmentGlyphs container object may only contain CompartmentGlyph objects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 12.) layout-20309

✓ A ListOfSpeciesGlyphs object may have the optional attributes metaid and sboTerm defined by SBML Level 3 Core. No other attributes from the SBML Level 3 Core namespace or the Layout namespace are permitted on a ListOfSpeciesGlyphs object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 13.) layout-20310 **☑** Apart from the general notes and annotation subobjects permitted on all SBML objects, a ListOfSpeciesGlyphs container object may only contain SpeciesGlyph objects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 13.) A ListOfReactionGlyphs object may have the optional attributes metaid and sboTerm defined by SBML Level 3 Core. No other attributes from the SBML Level 3 Core namespace or the Layout namespace are permitted on a ListOfReactionGlyphs object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 13.) layout-20312 ✓ Apart from the general notes and annotation subobjects permitted on all SBML objects, a ListOfReactionGlyphs container object may only contain ReactionGlyph objects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 13.) layout-20313

✓ A ListOfAdditionalGraphicalObjects object may have the optional attributes metaid and sboTerm defined by SBML Level 3 Core. No other attributes from the SBML Level 3 Core namespace or the Layout namespace are permitted on a ListOfAdditionalGraphicalObjects object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 13.) layout-20314 ✓ Apart from the general notes and annotation subobjects permitted on all SBML objects, a ListOfAdditionalGraphicalObjects container object may only contain GeneralGlyph and GraphicalObject objects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 13.)

layout-20315 ✓ A Layout object must contain exactly one Dimensions object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.6 on page 11.) A **ListOfTextGlyphs** object may have the optional attributes metaid and sboTerm defined by layout-20316 🗹 SBML Level 3 Core. No other attributes from the SBML Level 3 Core namespace or the Layout namespace are permitted on a ListOfTextGlyphs object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.12 on page 19.) Apart from the general notes and annotation subobjects permitted on all SBML objects, a layout-20317 ✓ **ListOfTextGlyphs** container object may only contain **TextGlyph** objects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.12 on page 19.) Rules for the GraphicalObject class layout-20401
✓ A GraphicalObject object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core namespace are permitted on a GraphicalObject. (References: SBML Level 3 Version 1 Core, Section 3.2.) A GraphicalObject object may have the optional SBML Level 3 Core attributes metaid and 14 sboTerm. No other attributes from the SBML Level 3 Core namespace are permitted on a **GraphicalObject.** (References: SBML Level 3 Version 1 Core, Section 3.2.) There may be at most one instance of a **BoundingBox** object on a **GraphicalObject**. No other layout-20403

✓ elements from the Layout namespace are permitted on a GraphicalObject. (References: SBML 18 Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) layout-20404

✓ A GraphicalObject object must have the required attribute layout:id and may have the optional attribute layout:metaidRef. No other attributes from the SBML Level 3 Layout 21 namespace are permitted on a GraphicalObject object. (References: SBML Level 3 Package 22 Specification for Layout, Version 1, Section 3.7 on page 13.) The attribute layout:metaidRef of a GraphicalObject must be of the data type IDREF. (Reflayout-20405

✓ erences: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) layout-20406

✓ The value of a layout:metaidRef attribute of a GraphicalObject must be of the metaid of an 26 existing element in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) layout-20407

✓ A GraphicalObject object must contain exactly one BoundingBox object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) 30 Rules for the CompartmentGlyph object layout-20501 \(\sqrt{20} \) A CompartmentGlyph object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core namespace are permitted on a CompartmentGlyph. (References: SBML Level 3 Version 1 Core, Section 3.2.) A CompartmentGlyph object may have the optional SBML Level 3 Core attributes metaid and sboTerm. No other attributes from the SBML Level 3 Core namespace are permitted on a 36 CompartmentGlyph. (References: SBML Level 3 Version 1 Core, Section 3.2.) There may be at most one instance of an **BoundingBox** object on a **CompartmentGlyph**. No other elements from the Layout namespace are permitted on a CompartmentGlyph. (Refer-39 ences: SBML Level 3 Package Specification for Layout, Version 1, Section 3.8 on page 14.)

> A CompartmentGlyph object must have the required attribute layout:id and may have the optional attributes layout:metaidRef, layout:compartment or layout:order. No other

layout-20504

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| | attributes from the SBML Level 3 Layout namespace are permitted on a CompartmentGlyph object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.8 on page 14.) | 1 2 3 |
|----------------------|---|----------------------|
| layout-20505 ✓ | The attribute layout:metaidRef of a CompartmentGlyph must be of the data type IDREF. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) | 4 |
| layout-20506 ☑ | The value of a layout:metaidRef of a CompartmentGlyph must be of the metaid of an existing element in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) | 6 7 8 |
| layout-20507 ✓ | The attribute <code>layout:compartment</code> of a <code>CompartmentGlyph</code> must be of the data type <code>SIdRef</code> . (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.8 on page 14.) | 9 |
| layout-20508 | The value of the layout:compartment attribute of a CompartmentGlyph must be of the id of an existing Compartment in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.8 on page 14.) | 11 12 13 |
| layout-20509 ✓ | If both attributes layout:compartment and layout:metaidRef are specified on a CompartmentGlyph they have to reference the same Compartment of the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.8 on page 14.) | 14 15 16 |
| layout-20510 ✓ | The attribute layout: order of a CompartmentGlyph must be of the data type double. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.8 on page 14.) | 17 18 |
| Rules for the Spe | eciesGlyph object | 19 |
| layout-20601 ☑ | A SpeciesGlyph object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core namespace are permitted on a SpeciesGlyph . (References: SBML Level 3 Version 1 Core, Section 3.2.) | 20 21 22 |
| layout-20602 ✓ | A SpeciesGlyph object may have the optional SBML Level 3 Core attributes metaid and sboTerm . No other attributes from the SBML Level 3 Core namespace are permitted on a SpeciesGlyph . (References: SBML Level 3 Version 1 Core, Section 3.2.) | 23 24 25 |
| layout-20603 ✓ | There may be at most one instance of an BoundingBox object on a SpeciesGlyph . No other elements from the Layout namespace are permitted on a SpeciesGlyph . (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.9 on page 15.) | 26 27 28 |
| layout-20604 ☑ | A SpeciesGlyph object must have the required attribute layout:id and may have the optional attribute layout:metaidRef or layout:species . No other attributes from the SBML Level 3 Layout namespace are permitted on a SpeciesGlyph object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.9 on page 15.) | 29 30 31 32 |
| layout-20605 ✓ | The attribute layout:metaidRef of a SpeciesGlyph must be of the data type IDREF. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) | 33 34 |
| layout-20606 ☑ | The value of a layout:metaidRef of a SpeciesGlyph must be of the metaid of an existing element in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) | 35 36 37 |
| layout-20607 ✓ | The attribute layout: species of a SpeciesGlyph must be of the data type SIdRef. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.9 on page 15.) | 38 39 |
| layout-20608 ✓ | The value of a layout: species of a SpeciesGlyph must be of the id of an existing Species in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.9 on page 15.) | 40 41 42 |

they have to reference the same **Species** of the **Model**. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.9 on page 15.) Rules for the ReactionGlyph object layout-20701
A ReactionGlyph object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core namespace are permitted on a **ReactionGlyph.** (References: SBML Level 3 Version 1 Core, Section 3.2.) layout-20702 **☑** A ReactionGlyph object may have the optional SBML Level 3 Core attributes metaid and sboTerm. No other attributes from the SBML Level 3 Core namespace are permitted on a 9 ReactionGlyph. (References: SBML Level 3 Version 1 Core, Section 3.2.) layout-20703

✓ There may be at most one instance of each of the following kinds of objects within a Reaction-Glyph object: BoundingBox and Curve and there must be one instance of ListOfSpecies-ReferenceGlyphs. No other elements from the Layout namespace are permitted on a Reaction-Glyph. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.10 on 14 page 15.) layout-20704

✓ A ReactionGlyph object must have the required attribute layout:id and may have the optional attribute layout:metaidRef or layout:reaction. No other attributes from the SBML Level 3 Layout namespace are permitted on a **ReactionGlyph** object. (References: SBML 18 Level 3 Package Specification for Layout, Version 1, Section 3.10 on page 15.) 19 The attribute layout:metaidRef of a ReactionGlyph must be of the data type IDREF. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) The value of a layout: metaidRef of a ReactionGlyph must be of the metaid of an existing element in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, 23 Section 3.7 on page 13.) layout-20707

✓ The attribute layout:reaction of a ReactionGlyph must be of the data type SIdRef. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.10 on page 15.) layout-20708 V The value of a layout:reaction of a ReactionGlyph must be of the id of an existing Reaction in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.10 on page 15.) If both attributes layout:reaction and layout:metaidRef are specified on a Reaction-Glyph they have to reference the same Reaction of the Model. (References: SBML Level 3 31 Package Specification for Layout, Version 1, Section 3.10 on page 15.) layout-20710 ✓ Apart from the general notes and annotation subobjects permitted on all SBML objects, a 33 ListOfSpeciesReferenceGlyphs container object may only contain SpeciesReferenceGlyph objects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.10 on page 15.) layout-20711 ✓ A ListOfSpeciesReferenceGlyphs object may have the optional metaid and sboTerm defined by SBML Level 3 Core. No other attributes from the SBML Level 3 Core namespace or the 38 Layout namespace are permitted on a **ListOfSpeciesReferenceGlyphs** object. (References: 39 SBML Level 3 Package Specification for Layout, Version 1, Section 3.10 on page 15.) A ListOfSpeciesReferenceGlyphs container object must not be empty. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.10 on page 15.) 42

If both attributes layout: species and layout: metaidRef are specified on a SpeciesGlyph

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Rules for the GeneralGlyph object

- layout-20801 ✓ A GeneralGlyph object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core namespace are permitted on a GeneralGlyph. (References: SBML Level 3 Version 1 Core, Section 3.2.)
- layout-20802 ✓ A GeneralGlyph object may have the optional SBML Level 3 Core attributes metaid and sboTerm. No other attributes from the SBML Level 3 Core namespace are permitted on a GeneralGlyph. (References: SBML Level 3 Version 1 Core, Section 3.2.)
- layout-20803 ✓ There may be at most one instance of each of the following kinds of objects within a General-Glyph object: BoundingBox, Curve, ListOfReferenceGlyphs and ListOfSubGlyphs. No other elements from the Layout namespace are permitted on a GeneralGlyph. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11 on page 17.)
- layout-20804 ✓ A GeneralGlyph object must have the required attribute layout:id and may have the optional attribute layout:metaidRef or layout:reference. No other attributes from the SBML Level 3 Layout namespace are permitted on a GeneralGlyph object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11 on page 17.)
- layout-20805

 ✓ The attribute layout:metaidRef of a GeneralGlyph must be of the data type IDREF. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.)
- layout-20806 ✓ The value of a layout:metaidRef of a GeneralGlyph must be of the metaid of an existing element in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.)
- layout-20807

 ✓ The attribute layout:reference of a GeneralGlyph must be of the data type SIdRef. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11 on page 17.)
- layout-20808

 ✓ The value of a layout:reference of a GeneralGlyph must be of the id of an existing element in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11 on page 17.)
- layout-20809
 ✓ If both attributes layout:reference and layout:metaidRef are specified on a General-Glyph they have to reference the same element of the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11 on page 17.)
- layout-20810 ✓ Apart from the general notes and annotation subobjects permitted on all SBML objects, a ListOfReferenceGlyphs container object may only contain ReferenceGlyph objects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11 on page 17.)
- layout-20811 ✓ A ListOfReferenceGlyphs object may have the optional metaid and sboTerm defined by SBML Level 3 Core. No other attributes from the SBML Level 3 Core namespace or the Layout namespace are permitted on a ListOfReferenceGlyphs object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11 on page 17.)
- layout-20812 ✓ Apart from the general notes and annotation subobjects permitted on all SBML objects, a ListOfSubGlyphs container object may only contain CompartmentGlyph, SpeciesGlyph, ReactionGlyph, GeneralGlyph, GraphicalObject, TextGlyph,

 SpeciesReferenceGlyph and ReferenceGlyph objects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11 on page 17.)
- layout-20813 ✓ A ListOfSubGlyphs object may have the optional metaid and sboTerm defined by SBML Level 3 Core. No other attributes from the SBML Level 3 Core namespace or the Layout namespace are permitted on a ListOfSubGlyphs object.
 (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11 on page 17.)

Rules for the TextGlyph object

- layout-20901 ✓ A TextGlyph object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core namespace are permitted on a TextGlyph. (References: SBML Level 3 Version 1 Core, Section 3.2.)
- layout-20902 ✓ A TextGlyph object may have the optional SBML Level 3 Core attributes metaid and sboTerm. No other attributes from the SBML Level 3 Core namespace are permitted on a TextGlyph. (References: SBML Level 3 Version 1 Core, Section 3.2.)
- layout-20903 ✓ A TextGlyph object must contain exactly one BoundingBox object. No other elements from the Layout namespace are permitted on a TextGlyph. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.12 on page 19.)
- layout-20904 ✓ A TextGlyph object must have the required attribute layout:id and may have the optional attributes layout:metaidRef, layout:graphicalObject, layout:text and layout:originOfText. No other attributes from the SBML Level 3 Layout namespace are permitted on a TextGlyph object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.12 on page 19.)
- layout-20905

 ✓ The attribute layout:metaidRef of a TextGlyph must be of the data type IDREF. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.)
- layout-20906 ✓ The value of a layout:metaidRef of a TextGlyph must be of the metaid of an existing element in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.)
- layout-20907

 The attribute layout:originOfText of a TextGlyph must be of the data type SIdRef. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.12 on page 19.)
- layout-20908

 ✓ The value of a layout:originOfText of a TextGlyph must be of the id of an existing element in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.12 on page 19.)
- layout-20909
 ✓ If both attributes layout:originOfText and layout:metaidRef are specified on a Text-Glyph they have to reference the same element of the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.12 on page 19.)
- layout-20910

 The attribute layout:graphicalObject of a TextGlyph must be of the data type SIdRef.

 (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.12 on page 19.)
- layout-20911 ✓ The value of a layout:graphicalObject of a TextGlyph must be of the id of an existing GraphicalObject (or derived) element in the Layout. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.12 on page 19.)
- layout-20912

 ✓ The attribute layout:text of a TextGlyph must be of the data type string. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.12 on page 19.)

Rules for the SpeciesReferenceGlyph object

- layout-21001
 ✓ A SpeciesReferenceGlyph object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core namespace are permitted on a SpeciesReferenceGlyph. (References: SBML Level 3 Version 1 Core, Section 3.2.)
- layout-21002 ☑ A SpeciesReferenceGlyph object may have the optional SBML Level 3 Core attributes metaid and sboTerm. No other attributes from the SBML Level 3 Core namespace are permitted on a SpeciesReferenceGlyph. (References: SBML Level 3 Version 1 Core, Section 3.2.)

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layout-21003

✓ A SpeciesReferenceGlyph may have at most one instance of a BoundingBox and Curve object. No other elements from the Layout namespace are permitted on a SpeciesReference-Glyph. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.10.1 on page 16.) layout-21004

✓ A Species Reference Glyph object must have the required attributes layout: id and layout:speciesGlyph and may have the optional attribute layout:metaidRef or layout:species-Reference and layout:role. No other attributes from the SBML Level 3 Layout namespace are permitted on a SpeciesReferenceGlyph object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.10.1 on page 16.) The attribute layout:metaidRef of a SpeciesReferenceGlyph must be of the data type IDREF. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) layout-21006

✓ The value of a layout:metaidRef of a SpeciesReferenceGlyph must be of the metaid of an existing element in the Model. (References: SBML Level 3 Package Specification for Layout, 13 Version 1, Section 3.7 on page 13.) The attribute layout: speciesReference of a SpeciesReferenceGlyph must be of the data type SIdRef. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.10.1 on page 16.) layout-21008 🗹 The value of a layout: speciesReference of a SpeciesReferenceGlyph must be of the id of an existing SpeciesReference in the Model. (References: SBML Level 3 Package Specification 19 for Layout, Version 1, Section 3.10.1 on page 16.) If both attributes layout: speciesReference and layout: metaidRef are specified on a Species Reference Glyph they have to reference the same Species Reference of the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.10.1 on page 16.) 23 The attribute layout: speciesGlyph of a SpeciesReferenceGlyph must be of the data type layout-21010 🗹 SIdRef. (References: SBML Level 3 Package Specification for Layout, Version 1, 25 Section 3.10.1 on page 16.) 26 The value of a layout:speciesGlyph of a SpeciesReferenceGlyph must be of the id of an layout-21011 ✓ existing SpeciesGlyph in the Layout. (References: SBML Level 3 Package Specification for 28 Layout, Version 1, Section 3.10.1 on page 16.) The attribute layout:role of a SpeciesReferenceGlyph must be of the data type Specieslayout-21012 ReferenceRole, i.e. it must have one of the following values: substrate, product, side-31 substrate, sideproduct, modifier, activator, inhibitor or undefined. (References: 32 SBML Level 3 Package Specification for Layout, Version 1, Section 3.10.1 on page 16.) Rules for the ReferenceGlyph object layout-21101 ✓ A ReferenceGlyph object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core namespace are permitted on a 36 **ReferenceGlyph.** (References: SBML Level 3 Version 1 Core, Section 3.2.) A ReferenceGlyph object may have the optional SBML Level 3 Core attributes metaid and layout-21102 🗹 sboTerm. No other attributes from the SBML Level 3 Core namespace are permitted on a 39 **ReferenceGlyph.** (References: SBML Level 3 Version 1 Core, Section 3.2.) There may be at most one instance of an BoundingBox and Curve object on a Referencelayout-21103 ✓ Glyph. No other elements from the Layout namespace are permitted on a ReferenceGlyph. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11.1 on page 19.)

| layout-21104 ☑ | A ReferenceGlyph object must have the required attributes layout:id and layout:glyph and may have the optional attribute layout:metaidRef or layout:reference and layout:role. No other attributes from the SBML Level 3 Layout namespace are permitted on a ReferenceGlyph object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11.1 on page 19.) | 1 2 3 4 5 |
|-------------------|---|-----------|
| layout-21105 ✓ | The attribute layout:metaidRef of a ReferenceGlyph must be of the data type IDREF. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) | 6 |
| layout-21106 ☑ | The value of a layout:metaidRef of a ReferenceGlyph must be of the metaid of an existing element in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) | 5 |
| layout-21107 ✓ | The attribute layout:reference of a ReferenceGlyph must be of the data type SIdRef. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11.1 on page 19.) | 1 |
| layout-21108 ☑ | The value of a layout:reference of a ReferenceGlyph must be of the id of an existing element in the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11.1 on page 19.) | 1 |
| layout-21109 | If both attributes layout:reference and layout:metaidRef are specified on a Reference-Glyph they have to reference the same element of the Model. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11.1 on page 19.) | 1 |
| layout-21110 ✓ | The attribute layout:glyph of a ReferenceGlyph must be of the data type SIdRef. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11.1 on page 19.) | 1 |
| layout-21111 ☑ | The value of a layout:glyph of a ReferenceGlyph must be of the id of an existing Graphical-Object (or derived) element in the Layout. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11.1 on page 19.) | 2 |
| layout-21112 ✓ | The attribute layout:role of a ReferenceGlyph must be of the data type string. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.11.1 on page 19.) | 2 |
| Rules for the Poi | int class | 2 |
| layout-21201 ✓ | A Point object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core or Layout namespace are permitted on a Point . (References: SBML Level 3 Version 1 Core, Section 3.2.) | 2 |
| layout-21202 ✓ | A Point object may have the optional SBML Level 3 Core attributes metaid and sboTerm . No other attributes from the SBML Level 3 Core namespace are permitted on a Point . (References: SBML Level 3 Version 1 Core, Section 3.2.) | 3 |
| layout-21203 ✓ | A Point object must have the required attributes <code>layout:x</code> and <code>layout:y</code> and may have the optional attributes <code>layout:id</code> and <code>layout:z</code> . No other attributes from the SBML Level 3 Layout namespace are permitted on a Point object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.1 on page 7.) | 3 |
| layout-21204 ✓ | The attributes layout:x, layout:y and layout:z of a Point element must be of the data type double. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.1 on page 7.) | 3 |
| Rules for the Box | undingBox class | 4 |

layout-21301

✓ A BoundingBox object may have the optional SBML Level 3 Core subobjects for notes and

BoundingBox. (References: SBML Level 3 Version 1 Core, Section 3.2.)

annotations. No other elements from the SBML Level 3 Core namespace are permitted on a

| layout-21302 ✓ | A BoundingBox object may have the optional SBML Level 3 Core attributes metaid and sboTerm . No other attributes from the SBML Level 3 Core namespace are permitted on a BoundingBox . (References: SBML Level 3 Version 1 Core, Section 3.2.) | 1 2 3 |
|--------------------|--|----------------------|
| layout-21303 ✓ | There must be exactly one instance of a Point and a Dimensions object on a BoundingBox . No | 4 |
| | other elements from the Layout namespace are permitted on a BoundingBox . (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.3 on page 8.) | 5 |
| layout-21304 ✓ | A BoundingBox object may have the optional attribute layout:id . No other attributes from the SBML Level 3 Layout namespace are permitted on a BoundingBox object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.3 on page 8.) | 7 8 9 |
| layout-21305 ✓ | If the layout:z attribute of a Point element on a BoundingBox is not specified, the attribute layout:depth of its Dimensions object must also not be specified. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.7 on page 13.) | 10 11 12 |
| Rules for the Cur | rve class | 13 |
| layout-21401 ✓ | A Curve object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core namespace are permitted on a Curve . (References: SBML Level 3 Version 1 Core, Section 3.2.) | 14 15 |
| layout-21402 ✓ | A Curve object may have the optional SBML Level 3 Core attributes metaid and sboTerm . No | 17 |
| , | other attributes from the SBML Level 3 Core namespace are permitted on a Curve . (References: SBML Level 3 Version 1 Core, Section 3.2.) | 18 19 |
| layout-21403 ✓ | There must be exactly one instance of a ListOfCurveSegments object on a Curve . No other elements from the Layout namespace are permitted on a Curve . (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.4 on page 8.) | 20 21 22 |
| layout-21404 ✓ | No attributes from the SBML Level 3 Layout namespace are permitted on a Curve object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.4 on page 8.) | 23 24 |
| layout-21405 ✓ | A ListOfCurveSegments object may have the optional metaid and sboTerm defined by SBML Level 3 Core. No other attributes from the SBML Level 3 Core namespace or the Layout namespace are permitted on a ListOfCurveSegments object. (References: SBML Level 3 | 25 26 27 |
| | Package Specification for Layout, Version 1, Section 3.4.4 on page 9.) | 28 |
| layout-21406 ✓ | Apart from the general notes and annotation subobjects permitted on all SBML objects, a ListOfCurveSegments container object may only contain LineSegment and CubicBezier objects. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.4 on page 9.) | 29 30 31 32 |
| layout-21407 ✓ | The ListOfCurveSegments container object may not be empty. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.4 on page 9.) | 33 34 |
| Rules for the Line | eSegment class | 35 |
| layout-21501 ☑ | A LineSegment object may have the optional SBML Level 3 Core subobjects for notes and | 36 |
| | annotations. No other elements from the SBML Level 3 Core namespace are permitted on a LineSegment . (References: SBML Level 3 Version 1 Core, Section 3.2.) | 37 38 |
| layout-21502 ✓ | A LineSegment object may have the optional SBML Level 3 Core attributes metaid and sboTerm . No other attributes from the SBML Level 3 Core namespace are permitted on a | 39 40 |

LineSegment. (References: SBML Level 3 Version 1 Core, Section 3.2.)

layout-21503
A LineSegment must specify the two Point elements start and end. No other elements from the Layout namespace are permitted on a LineSegment. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.5 on page 9.) layout-21504 **☑** No attributes from the SBML Level 3 Layout namespace are permitted on a LineSegment object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.5 on page 9.) Rules for the CubicBezier class layout-21601
✓ A CubicBezier object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core namespace are permitted on a **CubicBezier**. (References: SBML Level 3 Version 1 Core, Section 3.2.) layout-21602 ✓ A CubicBezier object may have the optional SBML Level 3 Core attributes metaid and sboTerm. No other attributes from the SBML Level 3 Core namespace are permitted on a CubicBezier. (References: SBML Level 3 Version 1 Core, Section 3.2.) layout-21603 ✓ A CubicBezier must specify the four Point elements start, basePoint1, basePoint2 and end. No other elements from the Layout namespace are permitted on a CubicBezier. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.6 on page 9.) No attributes from the SBML Level 3 Layout namespace are permitted on a CubicBezier oblayout-21604 **☑** ject. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.6 on 18 page 9.) Rules for the Dimensions class layout-21701 \(\text{ A Dimensions} \) object may have the optional SBML Level 3 Core subobjects for notes and annotations. No other elements from the SBML Level 3 Core or Layout namespace are permitted on a **Dimensions**. (References: SBML Level 3 Version 1 Core, Section 3.2.) A Dimensions object may have the optional SBML Level 3 Core attributes metaid and sboTerm. No other attributes from the SBML Level 3 Core namespace are permitted on a 25 **Dimensions.** (References: SBML Level 3 Version 1 Core, Section 3.2.) A Dimensions object must have the required attributes layout:width and layout:height and may have the optional attributes layout:id and layout:depth. No other attributes from the SBML Level 3 Layout namespace are permitted on a **Dimensions** object. (References: SBML Level 3 Package Specification for Layout, Version 1, Section 3.4.2 on page 8.) layout-21704 **☑** The attributes layout:width, layout:height and layout:depth of a Dimensions object must be of the data type double. (References: SBML Level 3 Package Specification for Layout, 32 Version 1, Section 3.4.2 on page 8.)

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References

Bergmann, F. T. and Sauro, H. M. (2006). SBW – a modular framework for systems biology. In *Proceedings of the 38th conference on Winter simulation*, WSC '06, pages 1637–1645. Winter Simulation Conference.

Biron, P. V. and Malhotra, A. (2000). XML Schema part 2: Datatypes (W3C candidate recommendation 24 October 2000). Available via the World Wide Web at http://www.w3.org/TR/xmlschema-2/.

Deckard, A., Bergmann, F. T., and Sauro, H. M. (2006). Supporting the SBML layout extension. *Bioinformatics*, 22(23):2966–2967.

Eriksson, H.-E. and Penker, M. (1998). UML Toolkit. John Wiley & Sons, New York.

Fallside, D. C. (2000). XML Schema part 0: Primer (W3C candidate recommendation 24 October 2000). Available via the World Wide Web at http://www.w3.org/TR/xmlschema-0/.

Gauges, R., Rost, U., Sahle, S., and Wegner, K. (2006). A model diagram layout extension for SBML. *Bioinformatics*, 22(15):1879–1885.

Hucka, M., Bergmann, F. T., Hoops, S., Keating, S. M., Sahle, S., and Wilkinson, D. J. (2011). Available via the World Wide Web at http://sbml.org/Documents/Specifications.

Hucka, M., Finney, A., Sauro, H., Bolouri, H., Doyle, J., Kitano, H., Arkin, A., Bornstein, B., Bray, D., Cornish-Bowden, A., Cuellar, A., Dronov, S., Gilles, E., Ginkel, M., Gor, V., Goryanin, I., Hedley, W., Hodgman, T., Hofmeyr, J., Hunter, P., Juty, N., Kasberger, J., Kremling, A., Kummer, U., Novère, N. L., Loew, L., Lucio, D., Mendes, P., Minch, E., Mjolsness, E., Nakayama, Y., Nelson, M., Nielsen, P., Sakurada, T., Schaff, J., Shapiro, B., shimizu, T., Spence, H., Stelling, J., Takahashi, K., Tomita, M., Wagner, J., and Wang, J. (2003). The Systems Biology Markup Language (SBML): a medium for representation and exchange of biochemical network models. *Bioinformatics*, 19(4):524–31.

Oestereich, B. (1999). *Developing Software with UML: Object-Oriented Analysis and Design in Practice*. Addison-Wesley.

Sahle, S., Gauges, R., Pahle, J., Simus, N., Kummer, U., Hoops, S., Lee, C., Singhal, M., Xu, L., and Mendes, P. (2006). Simulation of biochemical networks using COPASI: a complex pathway simulator. In *Proceedings of the 38th conference on Winter simulation*, WSC '06, pages 1698–1706. Winter Simulation Conference.

SBML Team (2010). The SBML Issue Tracker. Available via the World Wide Web at http://sourceforge.net/p/sbml/sbml-specifications/.

SBML Team (2012). Sbml: the System Biology Markup Language. Available via the World Wide Web at http://www.sbml.org/.

Thompson, H. S., Beech, D., Maloney, M., and Mendelsohn, N. (2000). XML Schema part 1: Structures (W3C candidate recommendation 24 October 2000). Available online via the World Wide Web at the address http://www.w3.org/TR/xmlschema-1/.

Wegner, K. and Kummer, U. (2005). A new dynamical layout algorithm for complex biochemical reaction networks. *BMC Bioinformatics*, 6(1):212.

Wikipedia (2013). Bèzier curve — Wikipedia, the free encyclopedia. Available via the World Wide Web at http://en.wikipedia.org/wiki/B%C3%A9zier_curve. [Online; accessed 5-May-2013].

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