The TeXshade package[*]

Typesetting nucleotide and peptide alignments

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v1.29; 2025/10/16

Abstract

Setting alignments of nucleotides and peptides for publication or presentation purposes is usually a time consuming two-step process. First, a scientific software is used for the calculation of the alignment. This is done in a few minutes. Then, in order to highlight special sequence relationships and to label positions and regions of interest a second software with high quality output capability is needed. Manipulating sequence alignments with standard word processing or graphics programs takes its time—often several hours—and simple layout changes such as re-breaking lines, say from 50 to 40 residues per line, elongate the working time considerably.

TeXshade is an alignment shading software written in TeX/LaTeX which can process multiple sequence alignments in the MSF, ALN and FASTA file format. It provides in addition to common shading algorithms special shading modes featuring functional aspects, e. g. charge or hydropathy, and a plenitude of commands for handling shading colors, text styles, labels, legends and even allows the user to define completely new shading modes. TeXshade combines highest flexibility and the habitual TeX output quality—with reasonable time expenditure.

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Contents

1 Package Overview

After `texshade.ins` has been run through TeX the following files should appear in the directory:

`texshade.sty`	the style file with all TeXshade commands
`texshade.def`	an example parameter file with the standard parameter settings
`AQPDNA.MSF`	an example nucleotide alignment (MSF-format)
`AQPpro.MSF`	an example protein alignment (MSF-format)
`AQP_TC.asc`	an example T-Coffee shading file (`score_ascii`-format)
`AQP2spec.ALN`	a further protein alignment (minimal ALN-file)
`AQP1.phd`	secondary structure information (PHD-format)
`AQP1.top`	topology data extracted from `AQP1.phd`
`AQP1_HMM.sgl`	topology information (single line, HMMTOP-format)
`AQP1_HMM.ext`	topology information (extended, HMMTOP-format)
`AQP_sequence_logo_1FX8.cmd`	Chimera structure meme file
`AQP_subfamily_logo_1FX8.cmd`	Chimera structure meme file
`meme.eps`	structure meme example image
`frustr.txt`	local frustration example file
`bars.txt`	stacked bars example file
`standard.cod`	standard genetic code definitions
`ciliate.cod`	ciliate macronuclear genetic code

The alignment file examples as well as the topology data file are needed for TeXing this documentation and can serve as illustrations for the MSF and ALN file format.
The following subsections give an overview on the capabilities of the TeXshade package. All commands are described in detail later on.

1.1 Version History

v1.29 2025/10/16
Correction: corrected ruler position when names are hidden.
Introduction: new shadingmode `singleseq`; new commands `\shiftsingleseq`, `\keepsingleseqgaps`, and `\alignrightlabels'`; new featurestyles `stackedbars`, and `complement`; optional background color in features `complement`, `translate`, and `fill`; new featurestyle `frustratometer`; keyword `all` to select feature range.

v1.28 2024/01/10
Correction: Consensus export files can be in chimera or pymol format.
Introduction: Functional shading on DNA sequences was added.

v1.27 2024/01/06
Introduction: The possibility to show a second full ruler at the [top] or [bottom] was introduced plus the option to show ruler names by `\nameruler`. The `rulername` style can be adjusted using the common `setfamily` and `setsize` commands.

v1.26(a/b/c) 2021/04/01 (2022/08/29, 2023/05/28, 2023/06/04)
Corrections: Frames at line ends remain open to indicate continuity of the marked region, and `\par` line endings are now treated correctly. Motif labels were corrected.
Introductions: Chimera command file export option for 'structure memes' was introduced, i.e. mapping of sequence logo and subfamily logo data onto 3D protein structures. The new commands `\structurememe`, `\memeRed`, `\memeBlue`, `\memeYellow`, `\memeBlack`, `\memeWhite`, `\memeStandardcolors`, `\chimeraaxisdistance`, `\chimerachain`, `\chimeraballScale`, `\memelabelcutoff`, and `\echostructurefile` handle the new feature.

v1.25 2018/01/17
Corrections: Aligments with many seqs produced wrong calculation of threshold shading,[1] corrected; minor bug fixes.
Introduction: A new feature style `S-S` for disulfide bridges is implemented; hooks in top feature lines can be drawn down to alignment by adding an underscore in the definition, e.g. `{_,-,}`.

v1.24 2011/12/01
Introductions: The space between the ruler and the top or bottom sequence row can now be adjusted using `\rulerspace` and the textsize of the ruler numbering can be set with `\setsize` or `\rulerLarge` etc. Postscript color samples are shown in the manual next to the color names list.

v1.23 2011/05/13
Introductions: In diverse mode sequence positions where all residues match do not contain much information. A new command, `\hideallmatchpositions`,[2] will remove all such positions from the alignment and hence condense the output considerably.

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[1] Noted by Kathryn Parker.

[2] Requested by Matt Russell.

v1.22 2010/10/11
Introductions: Sets of shading colors can be defined and named using `\defshadingcolors` (p. 46) and different sets of colors can be selected for different sequence blocks by `\changeshadingcolors` (4.6.1).

v1.21 2010/03/01
Corrections: `\setdomain` now recognizes a changed `\startnumber`.
Introductions: (a) Sequence motifs (4.6.1) can be given as a selection pattern in sequence stretch labeling commands, such as `\shaderegion`, `\emphregion` or `\frameblock`, instead of numeral stretch definitions.
(b) A new type of sequence emphasis by lowercase letters was implemented: `\lowerregion` and `\lowerblock` (4.6.2).

v1.20a 2009/11/30
Corrections: Identity/similarity tables work now without having to set a conservation plot in the feature line.

v1.20 2009/10/05
Corrections: Landscape mode works now correctly. Annoying `Overfull \hbox ...` signals appearing after `\residuesperline*` commands are ignored; domains work now with frequency corrected sequence logos.
Introductions: (a) New commands for setting residue weight tables were introduced `\weighttable` (with parameters: `identity`, `structural`, `PAM250`, `PAM100`, and `BLOSUM62`), `\gappenalty`, and `\setweight`. (b) Similarity/identity percentage tables can be printed with `\similaritytable`[3] and values for specific sequence pairs can be utilized with `\percentsimilarity{`⟨*seqref1*⟩`}{`⟨*seqref2*⟩`}` and `\percentidentity{`⟨*seqref1*⟩`}{`⟨*seqref2*⟩`}`.

v1.19a 2009/06/11
Correction: Gaps are now treated correctly when setting domains.
Introduction: Stop-positions in protein sequences (`*` in the input file) can be indicated by a special character (`\stopchar`) in the alignment output.[4]

v1.19 2009/03/09
Correction: Logo characters are now horizontally scalable using `\charstretch`. Minor bugs were fixed.

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[3] Asked for by Giovanni M. Lesa.

[4] Suggestion by Yun He.

Introduction: (a) Selection of residue positions was enhanced (4.6.1) TeXshade can now select residues based on their 3D coordinates provided in a PDB structure file. 3D selection can be due to a certain distance around a point, along a line, or above and below a plane. It works with `\feature`, `\shaderegion`, `\shadeblock`, `\tintregion`, `\tintblock`, `\emphregion`, `\emphblock`, `\frameblock`. (b) The list of selected residues is printable with `\printPDBlist` or viewable during the TeX run with `\messagePDBlist`. (c) `\hideblock` and related commands were replaced by `\setdomain` (4.5.2). This command will display only selected residues in the alignment. Thickness and colors of a domain separator rule can be set using `\domaingaprule` and `\domaingapcolors`.

v1.18 2008/04/15

Correction: several bug fixed concerning featurename display, sequence ordering and numbering.

Introduction: (a) T-Coffee shading information can be loaded and put on the alignment.[5] The conservation data can also be displayed in the consensus as well as feature color scales and bar plots. (b) Two more feature lines were added on the top and at the bottom (`ttttop`, `tttop`, `bbbottom`, `bbbbottom`). (c) The `startnumber` and `setends` commands have been fused; either command can set both, a new start number as well as end definitions of the sequence section to be displayed.

v1.17 2007/06/19

Introduction:[6] (a) A second threshold percentage was introduced in order to label two levels of conservation in ‘identical’ and ‘similar’ mode. This is achieved by setting an optional parameter in `\threshold` or in `\allmatchspecial`, or by using a number as an optional parameter in `\shadingmode`. (b) The feature lines can be additionally labeled with a name left or right of the feature. This is handled using `\showfeaturename`, `\showfeaturestylename`, `\hidefeaturename`, `\hidefeaturestylename`, `\hidefeaturenames`, `\hidefeaturestylenames`. The color of such names can be changed with `\featurenamecolor`, `\featurestylenamecolor`, `\featurenamescolor`, `\featurestylenamescolor`, Font styles in feature names can be set as usual, e.g. `\setsize{featurenames}{large}` or `\featurestylenamesrm`.

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[5] Suggestion by Florian Mertes.

[6] Asked for by Marat Kazanov.

v1.16 2007/02/18

Correction: TeXshade crashed when calculating conservation using sequences with untypical residue characters, such as "X". Fixed. The reference sequence in diverse mode can now be shaded with `\conservedresidues` and, if active, `\allmatchresidues`.[7]

Introduction:[8] (a) A command was introduced, i.e. `\exportconsensus` which produces a pymol script file for coloring a 3D model according to TeXshade's conservation calculation. (b) With `namerulerpos` labels of the ruler can be exchanged by a string. (c) Various parts of the alignment can now be hidden by `\hideblock`.

New home: TeXshade, TeXtopo, and BioTeX have a new home: `www.pharmazie.uni-kiel.de/chem/Prof_Beitz/biotex.html`.

v1.15 2006/06/27

Correction: Sequence and subfamily logos can now be plotted with pdflatex; pstricks is not needed anymore.

v1.14 2006/05/11

Introduction: In order to better recognize relevant positions in a subfamily logo, a bit-value can now be set by `\relevance` above which a deviation is considered relevant. Such positions can be labeled with a symbol by `\showrelevance` and hidden by `\hiderelevance`.

v1.13 2006/02/23

Corrections: Helix symbols in feature lines were not drawn correctly if the standard Computer Modern Font was changed to another one, e.g. Palatino.[9] Fixed. Unintended gaps occurred due to numbers at the end of lines in Clustal W alignment files. Fixed. The limitations in the number of sequences per alignment have finally been overcome by a more restrictive use of counter variables.

Introductions: (a) The numbering can now be displayed—in addition to left or right—on both sides of the alignment with the optional parameter `{leftright}` in the `\shownumbering` command (p.59). (b) TeXshade tries to guess the sequence type, i. e. protein or nucleotide, if not defined by the user. (c) Plotting of sequence logos has been implemented (p.56). Logos can be shown in addition to or together with the consensus, or alone without any alignment sequences. (d) The ruler numbering can be rotated in order to make labeling of every

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[7] For this and suggesting `namerulerpos` credit to Marco Pasi.

[8] Both extensions were suggested by Phillip Hahn.

[9] Thanks to Markus Heller

position possible. (e) A new way to visualize subfamily characteristics has been implemented, i.e. subfamily logos (p.58).

v1.12 2005/09/20

Corrections: When regional labeling with `\shaderegion`, `\emphregion`, `\tintregion`, or `\frameblock` was combined with `\setends` incorrect output was produced lacking the labeling.[10] Other minor fixes.

Introductions: An additional optional parameter for setting consensus colors was implemented in the `\showconsensus` command (p.53). This even allows one to use color scales illustrating sequence conservation in the consensus line.

v1.11 2005/04/13

Corrections: Bounding boxes with `\frameblock` had a wrong height when `\separationline`s were used. Other minor fixes.

Introductions: (a) An additional parameter for setting individual bar and arrow thicknesses in feature lines has been introduced. (b) Additional parameters for setting the frame color and thickness of boxes in feature lines have been implemented. (c) Three more color scales have been defined: `RedBlue`, `RedGreen`, and `HotCold`. (d) Plotting of amino acid features (`hydrophobicity`, `molweight`, `charge`) as bar graphs or color scales. (e) Plotting of protein sequence `conservation` as bar graph or color scale[11]. (f) Color scales can be used for shading the consensus sequence according to protein sequence conservation. (g) Separate command for stretching color scales `\colorscalestretch`.

v1.10 2005/03/29

Corrections: Plotting of color scales and bar graphs has been sped up by more than a factor of 10.[12]

Introductions: (a) More colors have been introduced, i.e. even lighter versions of the existing PostScript colors 'LightLight' plus color name and 'LightLightLight' plus color name. (b) Sequence stretches and blocks can be tinted for labeling purposes `\tintreqion`, `\tintblock` and `\tintdefault`. (c) A new feature label style `{restriction}` has been introduced. (d) Java-typical 'NaN' values are now allowed in data files for bar graphs and color scales.

v1.9 2005/02/08

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[10] Discovered by Chris Page.

[11] Ahmad Mirza asked for (e) and (f), great suggestion!

[12] This and (d) I owe again to Christoph Gille.

Corrections: TeXshade version 1.8 introduced an incompatibility with TeX`topo`. This problem was identified by Meike Schmedt and has been fixed.
Introductions: (a) A short version of the figure caption can now be defined for display in the list of figures[13] `\shortcaption{`⟨*text*⟩`}`. (b) A colored frame can be drawn around a sequence block for labeling purposes with the command `\frameblock`.[14] (c) A new look for feature arrows has been implemented with scalable line thickness and a new end style 'ball'. (d) HMMTOP topology predictions can now be included for plotting feature lines with information on the location of the transmembrane domains.[15]

v1.8 2004/08/26

Corrections: Only minor bugs were fixed.
Introductions: (a) More colors have been designed, i.e. 'light' versions of the existing PostScript colors. (b) Three color ramps in 5% steps have been introduced: i) Blue-Red, ii) Green-Red and iii) Cold-Hot. (c) Two new feature label styles `bar` and `color` have been introduced which allow one to display number values as bar graphs or color scales along the alignment[16].

v1.7 2004/01/05

Corrections: Several bugs were fixed. In gaps the wrong character was plotted in 'donotshade' mode. Gaps were colored incorrectly when a single sequence was set as consensus. Another 'donotshade' problem was solved which led to a halt of the LaTeX run[17]. Due to several requests, the gap and match labels in `diverse` mode were switched ('`-`' in gaps; '`.`' at matching positions) in order to follow convention.
Introduction: TeXshade speaks Spanish (`\spanishlanguage`). Necessary translations were contributed by Mikel Egaña Aranguren. A new feature label style `helix` has been introduced.

v1.6 2002/03/26

Corrections: The unnecessary restriction to the DVIPS driver for `color.sty` has been removed[18]. Any color.sty compatible driver option can be given with the `\usepackage{texshade}` call and is then

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[13] Meike, here you go ...

[14] Alan Robinson, this is for you.

[15] Implemented after a request by Steffen Moeller.

[16] Inspired by Christoph Gille's `STRAP`

[17] Thanks to Jeferson J. Arenzon and Naomi Siew

[18] As suggested by Eckhart Guthöhrlein.

passed to the `color` package. The ‘`\namecolor`’ and ‘`\numbercolor`’ commands do now support sequence lists.[19]
Introductions: (a) The FASTA file format is supported by TeXshade as alignment inputs. (b) Two commands set the space between sequence blocks either to be flexible (as so far) ‘`\flexblockspace`’ or the be fixed ‘`\fixblockspace`’. (c) One can now refer to sequences by their name in addition to the number in the input file. (d) Using ‘`\firstcolumnDSSP`’ and ‘`\secondcolumnDSSP`’ one can choose which of the first to columns should refer to the sequence numbering (the second column remains default setting)[20].

v1.5a 2001/03/08

Corrections: ‘X’s in the alignment file caused a run-time error. Fixed.
Introductions: (a) The vertical space between feature lines can be controlled by four new commands: `\ttopspace`, `\topspace`, `\bottomspace` and `\bbottomspace`[21]. (b) It is now easily possible to add a caption to the alignment with the `\showcaption` command. (c) TeXshade stores the sequence lengths in the `.aux` file in order to have correct breaks of the gaps after the sequences.

v1.4&4a 2000/9/12 & 2000/10/3

Introductions: (a) The alignment legend can now be moved by the command ‘`\movelegend`’. (b) In commands with parameters that contain series of sequence numbers, e. g. `\orderseqs`, a dash can be used, e. g. `{1-3,6-4,7}` instead of `{1,2,3,6,5,4,7}`.

v1.3a&b 2000/7/28 & 2000/7/30

Introductions: (a) It is now possible to force TeXshade to display gap symbols before and after the actual sequence by the commands ‘`\showleadinggaps`’ and ‘`\hideleadinggaps`’ (4.5.1). (b) The sequence names input routine is now more tolerant concerning special characters.

v1.3 2000/3/3

Corrections: Line scrambling occured when features where set in the `ttop` row without a feature in the `top` row. Fixed. The incompatible command ‘`\language`’ with the `babel` package has been replaced by ‘`\germanlanguage`’ and ‘`\englishlanguage`’[22].

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[19] Thanks to Denys Bashtovyy.

[20] c and d were suggested by Christoph Gille.

[21] Suggested by Ulrike Folkers.

[22] Thanks to Eckhart Guthöhrlein.

Introductions: (a) Now, translations of sequence stretches are possible. Either nucleotide or amino acid sources can be translated. This is done by the new `{translate}` option for the feature command. (b) The codons are defined by the new command '`\codon`'. Complete codon sets can be loaded by '`\geneticcode`'. (c) Further, the size and style of the nucleotide triplets of backtranslations can be set by '`\backtranslabel`' and '`\backtranstext`'. (d) Two more feature counter styles were introduced: '`\Romancount`' and '`\romancount`'. (e) TeXshade is now compatible with TeX`topo`, a new TeX software for drawing and shading topology plots of membrane proteins.

v1.2a 1999/6/24 (not released)

Minor corrections: '`\namecolor`' and '`\numbercolor`' are now really correctly reordered. Brackets (and) are now allowed in sequence names. The option `{case}` in '`\funcshadingstyle`' works now.

v1.2 1999/6/12

Corrections: (a) Functional group definitions of more than seven groups produced an error when displaying group number eight. These residues where skipped in the alignment. Fixed.

Introductions: (a) Protein secondary structure files in the DSSP, STRIDE and PHD format can be included and displayed automatically within the alignment by '`\includeDSSP`' (and similar commands for STRIDE, PHDsec and PHDtopo, 4.6.4). (b) Which types of secondary structures are to be included or skipped in the alignment is chosen by '`\showonDSSP`' and '`\hideonDSSP`' (and respective commands for STRIDE, PHDsec and PHDtopo). (c) The appearance of the labels is defined by '`\appearance`'. (d) Internal counters for repeatedly occuring structure types can be activated by '`\numcount`', '`\alphacount`' and '`\Alphacount`'. All commands are described in 4.6.4.

v1.1 1999/5/26

Corrections: (a) The activation of '`emphregion`' lead to an emphasized following alignment. This has been corrected. (b) '`\namecolor`' and '`\numbercolor`' were not reordered with the command '`orderseqs`'. Fixed. (c) Sequence gaps at the beginning or the end of a sequence, i. e. before the first and after the last residue where labeled with the gap symbol. Now these positions are left blank.

Introductions: (a) In order to treat the preceeding and sequence following gaps correctly, TeXshade needs to know the length of the sequences. Therefore, the command '`\seqlength`' was introduced (4.5). (b) With '`\gapcolors`' (also 4.5) the color selection for gap symbols is independent from non-conserved residues. (c) The divisions of the ruler where so far fixed to 10. Now, this value is changeable by '`\rulersteps`' (again 4.5). (d) '`\hideresidues`' and '`\showresidues`' turn off or on the residue names, i. e. one can choose between a display of shaded boxes only or with letters in the boxes (4.5.3). (e) The changes (c) through (d) were necessary for the introduction of '`\fingerprint`'. This command allows one to display the complete sequence in one line for an easy survey of the alignment (4.5.5).

v1.0 1999/5/12
First release.

1.2 LaTeX basics

1.2.1 Typesetting documents using LaTeX

In order to use any of the macros provided by the BioTeX-project (TeXshade/TeXtopo) efficiently a basic understanding of the TeX typesetting system and its usage is required. Several books are available on this topic, but a rather quick and easy introduction is the *Not so short introduction to LaTeX*. This document is available from all Comprehensive TeX Archive Network (CTAN) servers, e. g. from `ftp://ftp.dante.de/pub/tex/documentation/lshort/`, in many different languages and formats besides LaTeX, such as PostScript and on-line viewable PDF. I also put a link from the BioTeX (TeXshade/TeXtopo) homepage to the document collection (`http://pharmazie.uni-kiel.de/chem/Prof_Beitz/BioTeX`).

1.2.2 Memory shortness when using TeXshade

If you are using TeXshade to align several large sequences (about 1000 residues/sequence), LaTeX will probably stop compiling and quit with one of the following messages:

```
!\ TeX capacity exceeded, sorry [main memory size=384000]
```

or

```
!\ TeX capacity exceeded, sorry [stack size=300].
```

TeX allocates space for different kinds of internal variables. Setting alignments needs lots of memory, usually more than for typesetting plain text. Thus, the parameter settings of a standard TeX installation might not be sufficient for certain projects. This manifests in TeX error messages about insufficient memory and the setting process is interrupted. There is no reason to be concerned. The parameters can be set by hand. Unfortunately, each TeX system hides its default parameter file in a different place in the system.

1.3 System requirements

TeXshade requires LaTeX 2$_\varepsilon$ with `color.sty` and `graphics.sty` for shading. For arrows in the feature line (p.70) the AMS Math style is needed. David Carlisle's `color.sty` is part of the Standard LaTeX 'Graphics Bundle' [1]. This and the other packages can be downloaded from any TeX archive, e.g. `ftp.dante.de`; usually they are included in a comprehensive TeX installation.

The `color` style allows one to use several `[`⟨*options*⟩`]`, e. g. `dvips`, `pdftex` or `dviwin`. These provide the commands which different devices/programs need to display colored output. It is advisable to make yourself familiar with the `color.sty` manual. You should define a default driver in the file `color.cfg`. Since there is no direct call of `color.sty` by the user, the option can be stated when TeXshade is loaded, see next subsection. If no option is stated the `DVIPS` driver will be loaded.

With the `[dvips]` option the output DVI-file can be converted to PostScript using the `DVIPS` program and can later be viewed or printed with the public domain GhostView program which is available for almost all computer platforms. Further, more and more standard TeX viewers are to a certain extent PostScript compatible.

1.4 The `texshade` environment

The commands provided by the TeXshade package are enabled by the following command in the document header section:

```
\usepackage[⟨option⟩]{texshade}
```

Make sure that the file '`texshade.sty`' is present in a directory searched by TeX (see the installation notes in the file '`texshade.txt`'). The ⟨*option*⟩ given here is passed to `color.sty` which handles the color commands for a particular output device, see previous subsection and the `color.sty` manual.

The TeXshade package provides only one single new environment: `texshade`. This environment has one mandatory and one optional argument, both of them designating file names which must be present in

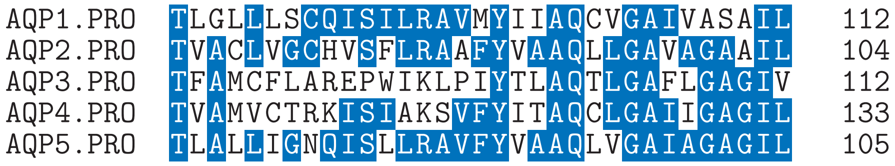
a directory searched by TeX. The required file ⟨*alignmentfile*⟩ contains the aligned nucleotide or peptide sequences (see section 2). This file is needed, because TeXshade does no alignment by itself, it has to take a preprocessed alignment as input. The optional file is a parameter file (section 3) with definitions for the customized calculation of the consensus, special sequence features or labels etc. In this parameter file all TeXshade commands which are allowed in the `texshade` environment can be used and are fully functional. Further commands can be given in the TeXshade environment to replace or complete settings from the parameter file.
Thus, setting an alignment with TeXshade is as simple as this:

> `\begin{texshade}[`⟨*parameterfile*⟩`]{`⟨*alignmentfile*⟩`}`
>
> *further* TeXshade *commands, if needed*
>
> `\end{texshade}`

1.5 Shading modes predefined in this package

1.5.1 Identity mode

This basic type of shading is provided by almost any alignment program. All identical residues at a position are shaded if the number of matching residues is higher than a given threshold (default is 50%).

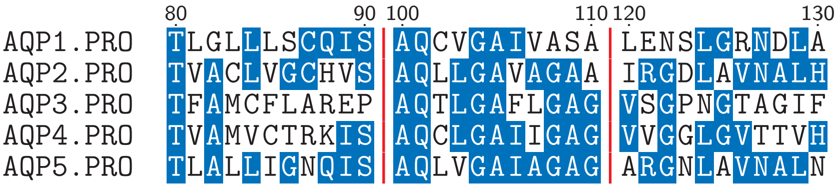


```
AQP1.PRO  TLGLLLSCQISILRAVMYIIAQCVGAIVASAIL  112
AQP2.PRO  TVACLVGCHVSFLRAAFYVAAQLLGAVAGAAIL  104
AQP3.PRO  TFAMCFLAREPWIKLPIYTLAQTLGAFLGAGIV  112
AQP4.PRO  TVAMVCTRKISIAKSVFYITAQCLGAIIGAGIL  133
AQP5.PRO  TLALLIGNQISLLRAVFYVAAQLVGAIAGAGIL  105
```

Code:

```
\begin{texshade}{AQPpro.MSF}
   \setends{1}{80..112}
   \hideconsensus
\end{texshade}
```

It is further possible to display only selected sequence domains, e. g. to eliminate uninteresting positions from the output (the following examples display additional TeXshade gimmicks such as rulers, shading, labels, color or bar graphs in order to illustrate the possibilities):

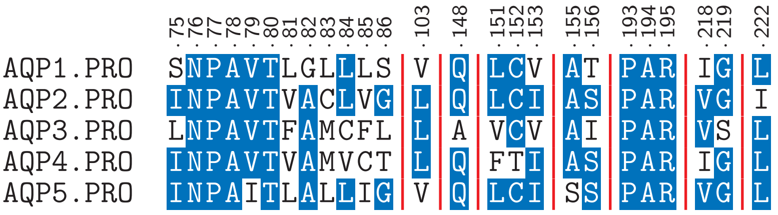


```
            80        90 100       110 120       130
AQP1.PRO    TLGLLLSCQIS | AQCVGAIVASA | LENSLGRNDLA
AQP2.PRO    TVACLVGCHVS | AQLLGAVAGAA | IRGDLAVNALH
AQP3.PRO    TFAMCFLAREP | AQTLGAFLGAG | VSGPNGTAGIF
AQP4.PRO    TVAMVCTRKIS | AQCLGAIIGAG | VVGGLGVTTVH
AQP5.PRO    TLALLIGNQIS | AQLVGAIAGAG | ARGNLAVNALN
```

Code:

```
\begin{texshade}{AQPpro.MSF}
   \setdomain{1}{80..90,100..110,120..130}
   \showruler{top}{1}
   \hidenumbering
   \hideconsensus
\end{texshade}
```

This goes even further. You can have TeXshade select positions based on the 3D coordinates provided by a PDB file, e. g. show all residues that are within an 8 Å radius around the α-carbon of the residue at position 81:

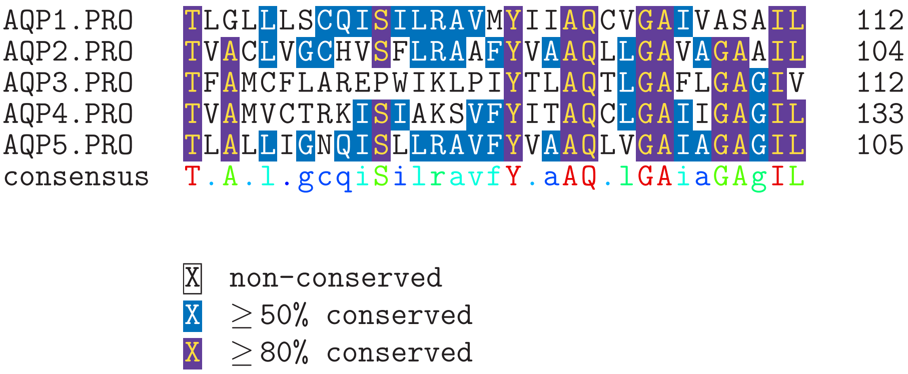


```
            75 76 77 78 79 80 81 82 83 84 85 86 | 103 | 148 | 151 152 153 | 155 156 | 193 194 195 | 218 219 | 222
AQP1.PRO    SNPAVTLGLLLS | V | Q | LCV | AT | PAR | IG | L
AQP2.PRO    INPAVTVACLVG | L | Q | LCI | AS | PAR | VG | I
AQP3.PRO    LNPAVTFAMCFL | L | A | VCV | AI | PAR | VS | L
AQP4.PRO    INPAVTVAMVCT | L | Q | FTI | AS | PAR | IG | L
AQP5.PRO    INPAITLALLIG | V | Q | LCI | SS | PAR | VG | L
```

Code:

```
\begin{texshade}{AQPpro.MSF}
   \setdomain{1}{point[8]:1J4N.pdb,81[CA]}
   \showruler{top}{1} \rulersteps{1}
   \hidenumbering
   \hideconsensus
\end{texshade}
```

If you like, positions where conservation is very high (here ≥ 80%) can be shaded in a special color and the consensus can be shown with or without shading according to the degree of conservation:



```
AQP1.PRO    TLGLLLSCQISILRAVMYIIAQCVGAIVASAIL    112
AQP2.PRO    TVACLVGCHVSFLRAAFYVAAQLLGAVAGAAIL    104
AQP3.PRO    TFAMCFLAREPWIKLPIYTLAQTLGAFLGAGIV    112
AQP4.PRO    TVAMVCTRKISIAKSVFYITAQCLGAIIGAGIL    133
AQP5.PRO    TLALLIGNQISLLRAVFYVAAQLVGAIAGAGIL    105
consensus   T.A.l.gcqiSilravfY.aAQ.lGAiaGAgIL
```

X non-conserved
X ≥ 50% conserved
X ≥ 80% conserved

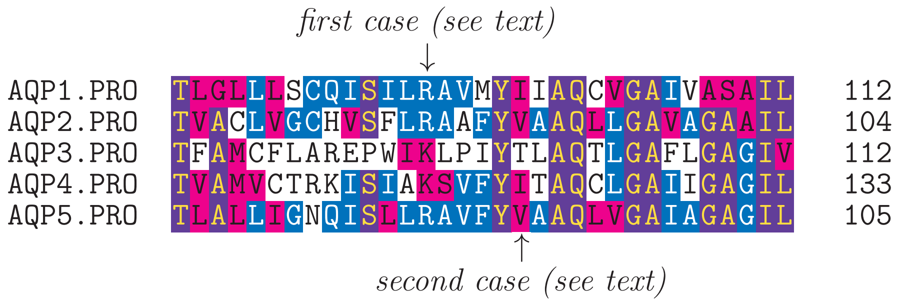
Code:

```
\begin{texshade}{AQPpro.MSF}
   \threshold[80]{50}
   \setends{1}{80..112}
   \showconsensus[ColdHot]{bottom}
   \defconsensus{.}{lower}{upper}
   \showlegend
\end{texshade}
```

1.5.2 Similarity mode

In many cases it is expedient—mostly when comparing protein sequences—to shade also residues which are not identical but similar to the consensus sequence. Consider a position where three out of five residues are basic arginines and two more residues are also basic but lysines (first case in figure below). In similarity mode TEXshade shades similar residues in a different color to distinguish them from the consensus residue. Even when none of the residues alone reaches the threshold but a group of similar residues does these are shaded in the 'similarity' color. This case is given for instance when at a position in a five sequence alignment two aliphatic valines and two also aliphatic isoleucins are present and the threshold is set to 50%. Neither residue exceeds this percentage but as a group of similars they do (second case below).

In grayscale printouts, some colors of the following alignment may appear undistinguishable. Don't worry if you usually use grayscale—all colors/grays can be selected freely (see 5).



```
AQP1.PRO   TLGLLLSCQISILRAVMYIIAQCVGAIVASAIL   112
AQP2.PRO   TVACLVGCHVSFLRAAFYVAAQLLGAVAGAAIL   104
AQP3.PRO   TFAMCFLAREPWIKLPIYTLAQTLGAFLGAGIV   112
AQP4.PRO   TVAMVCTRKISIAKSVFYITAQCLGAIIGAGIL   133
AQP5.PRO   TLALLIGNQISLLRAVFYVAAQLVGAIAGAGIL   105
```

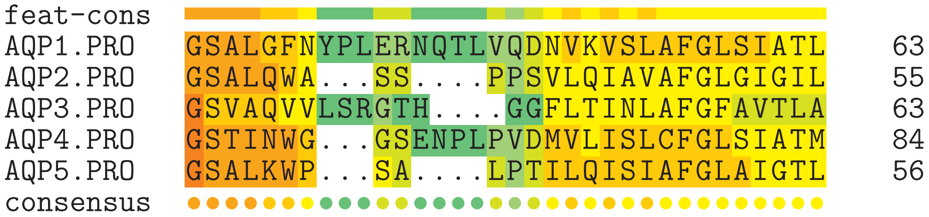
Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode{similar}
   \threshold[80]{50}
   \setends{1}{80..112}
   \hideconsensus
   \feature{top}{1}{93..93}{fill:$\downarrow$}{first case (see text)}
   \feature{bottom}{1}{98..98}{fill:$\uparrow$}{second case (see text)}
\end{texshade}
```

This kind of shading was introduced by the public domain program `BoxShade` by Kay Hofmann or from the Macintosh version `MacBoxShade` by Michael D. Barron. TeXshade provides the same functionality—and goes truly beyond—for the TeX community.

1.5.3 T-Coffee shading

TeXshade's capabilities of calculating alignment shadings are limited. `T-Coffee` (`www.tcoffee.org`) is a sophisticated alignment/shading software. You can apply shading from `T-Coffee` in TeXshade by loading the shading information file (`score_ascii`) generated by `T-Coffee`.



```
feat-cons
AQP1.PRO    GSALGFNYPLERNQTLVQDNVKVSLAFGLSIATL    63
AQP2.PRO    GSALQWA...SS....PPSVLQIAVAFGLGIGIL    55
AQP3.PRO    GSVAQVVLSRGTH....GGFLTINLAFGFAVTLA    63
AQP4.PRO    GSTINWG...GSENPLPVDMVLISLCFGLSIATM    84
AQP5.PRO    GSALKWP...SA....LPTILQISIAFGLAIGTL    56
consensus   ●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●
```

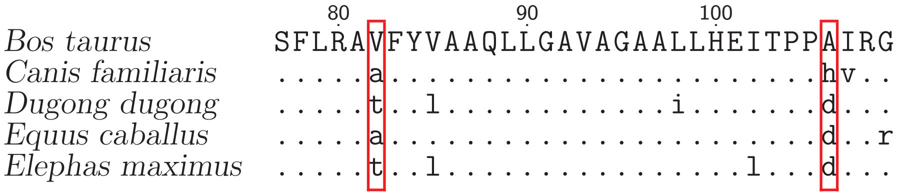
Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[AQP_TC.asc]{T-Coffee}
   \setends{1}{30..63}
   \feature{top}{1}{30..63}{color:conservation[T-Coffee]}{}
   \showfeaturestylename{top}{feat-cons}
   \showconsensus{bottom}
\end{texshade}
```

1.5.4 Diverse mode

Contrary to the above described modes this shading style displays sequence differences. Thus, it is most suitable for comparing very similar sequences, e. g. species variants of a protein.
One sequence is used as a reference. Matching residues in other sequences are blanked out, mismatches are shown in lowercase.

AQP2 species variants


80
90
100
Bos taurus SFLRAVFYVAAQLLGAVAGAALLHEITPPAIRG
Canis familiaris .....a.......................hv..
Dugong dugong .....t..l............i.......d...
Equus caballus .....a.......................d..r
Elephas maximus .....t..l................l...d...

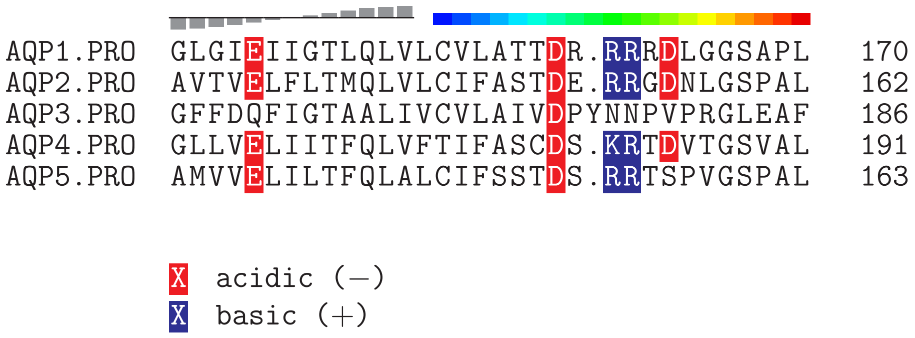
Code:

```
\begin{texshade}{AQP2spec.ALN}
   \shadingmode{diverse}
   \setends{1}{77..109}
   \featureslarge
   \feature{top}{1}{77..109}{}{AQP2 species variants}
   \namesrm\namessl
   \hidenumbering\showruler{top}{1}
   \shownames{left}
   \nameseq{1}{Bos taurus}
   \nameseq{2}{Canis familiaris}
   \nameseq{3}{Dugong dugong}
   \nameseq{4}{Equus caballus}
   \nameseq{5}{Elephas maximus}
   \frameblock{1}{82..82,106..106}{Red[1pt]}
\end{texshade}\label{frame}
```

1.5.5 Functional modes

Displaying functional peptide similarities is one of TeXshade's strong capabilities. Six functional shading modes are predefined; further user specific modes can easily be created. The examples may not look very impressive when printed in grayscale. Enjoy them on your screen or use color printouts. As mentioned before, all colors can be changed to others or to grays without restrictions (see chapter 5).

charge: residues which are charged at a physiological pH of 7.4 are shaded if their number at a position is higher than the threshold



```
AQP1.PRO  GLGIEIIGTLQLVLCVLATTDR.RRRDLGGSAPL   170
AQP2.PRO  AVTVELFLTMQLVLCIFASTDE.RRGDNLGSPAL   162
AQP3.PRO  GFFDQFIGTAALIVCVLAIVDPYNNPVPRGLEAF   186
AQP4.PRO  GLLVELIITFQLVFTIFASCDS.KRTDVTGSVAL   191
AQP5.PRO  AMVVELILTFQLALCIFSSTDS.RRTSPVGSPAL   163
```

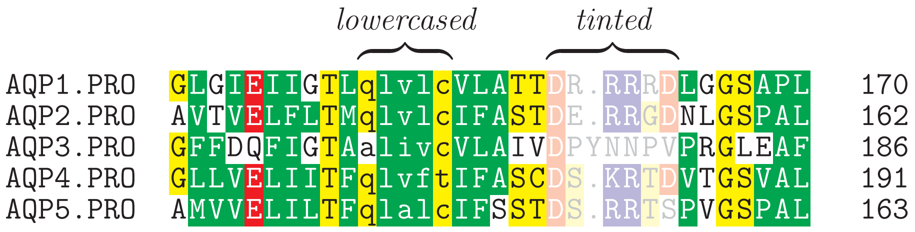
🟥 acidic (−)

🟦 basic (+)

Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[charge]{functional}
   \setends{1}{138..170}
   \feature{top}{3}{153..165}{bar[-50,50]:-50,-45,%
      -40,-30,-20,-10,0,10,20,30,40,45,50}{}
   \feature{top}{3}{167..186}{color:5,10,15,20,25,30,35,%
      40,45,50,55,60,65,70,75,80,85,90,95,100[ColdHot]}{}
   \showlegend
\end{texshade}
```

hydropathy: discrimination between acidic and basic, polar uncharged and hydrophobic nonpolar residues



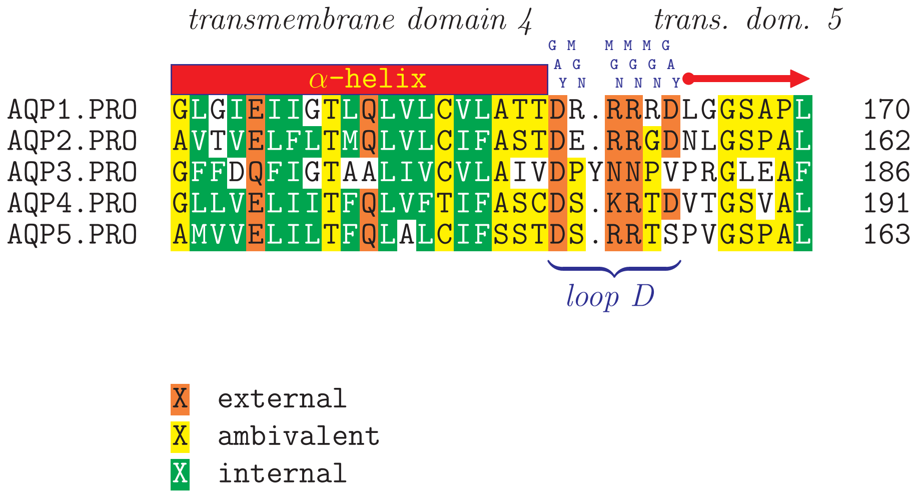
```
AQP1.PRO   GLGIEIIGTLqlvlcVLATTDR.RRRDLGGSAPL    170
AQP2.PRO   AVTVELFLTMqlvlcIFASTDE.RRGDNLGSPAL    162
AQP3.PRO   GFFDQFIGTAalivcVLAIVDPYNNPVPRGLEAF    186
AQP4.PRO   GLLVELIITFqlvftIFASCDS.KRTDVTGSVAL    191
AQP5.PRO   AMVVELILTFqlalcIFSSTDS.RRTSPVGSPAL    163
```

X acidic (−)
X basic (+)
X polar uncharged
X hydrophobic nonpolar

Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[hydropathy]{functional}
   \feature{top}{1}{158..163}{brace}{tinted}
   \tintblock{1}{158..163}
   \feature{top}{1}{QLVLC}{brace}{lowercased}
   \lowerblock{1}{QLVLC}
   \setends{1}{138..170}
   \showlegend
\end{texshade}
```

structure: displays the potential localization within the tertiary structure of the protein



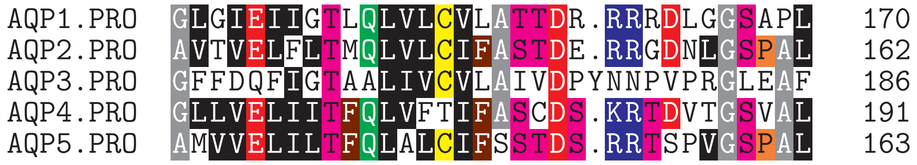
```
AQP1.PRO  GLGIEIIGTLQLVLCVLATTDR.RRRDLGGSAPL  170
AQP2.PRO  AVTVELFLTMQLVLCIFASTDE.RRGDNLGSPAL  162
AQP3.PRO  GFFDQFIGTAALIVCVLAIVDPYNNPVPRGLEAF  186
AQP4.PRO  GLLVELIITFQLVFTIFASCDS.KRTDVTGSVAL  191
AQP5.PRO  AMVVELILTFQLALCIFSSTDS.RRTSPVGSPAL  163
```

X external
X ambivalent
X internal

Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[structure]{functional}
   \setends{1}{138..170}
   \feature{top}{1}{138..157}{box[Blue,Red][0.5pt]: %
       $\alpha$-helix[Yellow]}{transmembrane domain 4}
   \feature{top}{1}{158..163}{translate[Blue]}{}
   \backtranslabel{oblique}
   \feature{bottom}{1}{[DE]RXXR[DE]}{brace[Blue]}{loop D [Blue]}
   \feature{top}{1}{164..170}{o->[Red]}{trans. dom. 5}
   \showlegend
\end{texshade}
```

chemical: residues are shaded due to chemical properties of their functional groups



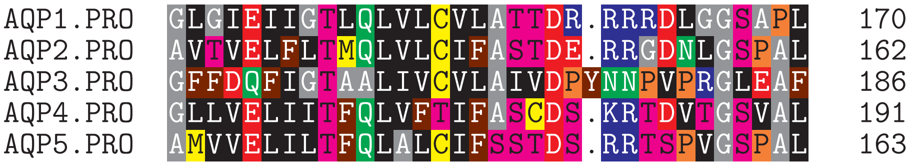
```
AQP1.PRO  GLGIEIIGTLQLVLCVLATTDR.RRRDLGGSAPL  170
AQP2.PRO  AVTVELFLTMQLVLCIFASTDE.RRGDNLGSPAL  162
AQP3.PRO  GFFDQFIGTAALIVCVLAIVDPYNNPVPRGLEAF  186
AQP4.PRO  GLLVELIITFQLVFTIFASCDS.KRTDVTGSVAL  191
AQP5.PRO  AMVVELILTFQLALCIFSSTDS.RRTSPVGSPAL  163
```

X acidic (−)
X aliphatic
X aliphatic (small)
X amide
X aromatic
X basic (+)
X hydroxyl
X imino
X sulfur

Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[chemical]{functional}
   \setends{1}{138..170}
   \showlegend
\end{texshade}
```

With `\shadeallresidues` the threshold is ignored and all residues are shaded due to their group assignment. This is *not* identical to a threshold of 0% where only the majority group would be shaded. See the difference:

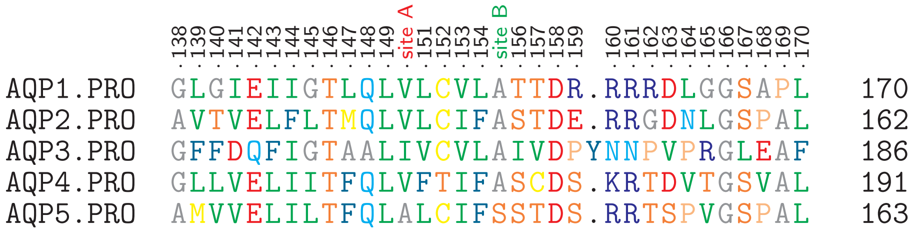


```
AQP1.PRO  GLGIEIIGTLQLVLCVLATTDR.RRRDLGGSAPL   170
AQP2.PRO  AVTVELFLTMQLVLCIFASTDE.RRGDNLGSPAL   162
AQP3.PRO  GFFDQFIGTAALIVCVLAIVDPYNNPVPRGLEAF   186
AQP4.PRO  GLLVELIITFQLVFTIFASCDS.KRTDVTGSVAL   191
AQP5.PRO  AMVVELILTFQLALCIFSSTDS.RRTSPVGSPAL   163
```

Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[chemical]{functional}
   \setends{1}{138..170}
   \shadeallresidues
\end{texshade}
```

rasmol: similar to `[chemical]` but with shading following the rasmol color scheme



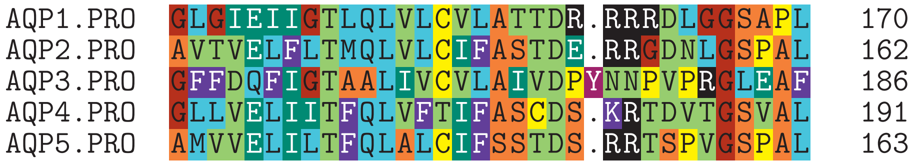
```
             .138 .139 .140 .141 .142 .143 .144 .145 .146 .147 .148 .149 site A .151 .152 .153 .154 site B .156 .157 .158 .159 .160 .161 .162 .163 .164 .165 .166 .167 .168 .169 .170
AQP1.PRO   GLGIEIIGTLQLVLCVLATTDR.RRRDLGGSAPL    170
AQP2.PRO   AVTVELFLTMQLVLCIFASTDE.RRGDNLGSPAL    162
AQP3.PRO   GFFDQFIGTAALIVCVLAIVDPYNNPVPRGLEAF    186
AQP4.PRO   GLLVELIITFQLVFTIFASCDS.KRTDVTGSVAL    191
AQP5.PRO   AMVVELILTFQLALCIFSSTDS.RRTSPVGSPAL    163
```

X Asp, Glu
X Arg, Lys, His
X Phe, Tyr, Trp
X Ala, Gly
X Cys, Met
X Ser, Thr
X Asn, Gln
X Leu, Val, Ile
X Pro

Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[rasmol]{functional}
   \setends{1}{138..170}
   \showruler{top}{1}
   \rulersteps{1}
   \namerulerpos{150}{site A[Red]}
   \namerulerpos{155}{site B[Green]}
   \shadeallresidues
   \showlegend
\end{texshade}
```

standard area: this shading displays the differences in the surface area of the different amino acid's sidechains



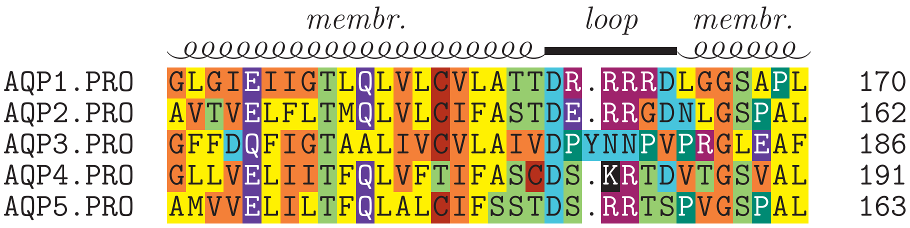
```
AQP1.PRO   GLGIEIIGTLQLVLCVLATTDR.RRRDLGGSAPL    170
AQP2.PRO   AVTVELFLTMQLVLCIFASTDE.RRGDNLGSPAL    162
AQP3.PRO   GFFDQFIGTAALIVCVLAIVDPYNNPVPRGLEAF    186
AQP4.PRO   GLLVELIITFQLVFTIFASCDS.KRTDVTGSVAL    191
AQP5.PRO   AMVVELILTFQLALCIFSSTDS.RRTSPVGSPAL    163
```

X 88.1 (G); Standard sidechain area (Å^2)
X 118.2 (A); 129.8 (S)
X 146.1 (C); 146.8 (P)
X 152.5 (T); 158.7 (D); 164.5 (V); 165.5 (N)
X 181.0 (I); 186.2 (E)
X 193.1 (L); 193.2 (Q); 202.5 (H); 203.3 (M)
X 222.8 (F); 225.8 (K)
X 238.8 (Y)
X 256.0 (R); 266.2 (W)

Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[standard area]{functional}
   \setends{1}{138..170}
   \showlegend
   \shadeallresidues
\end{texshade}
```

accessible area: here, the surface area which can be accessed by solvent molecules is used as a basis for shading; low accessibility means hydrophobic (i. e. strongly buried residues), whereas highly accessible sidechains are hydrophilic (compare to **hydropathy** and **structure**)



```
AQP1.PRO  GLGIEIIGTLQLVLCVLATTDR.RRRDLGGSAPL  170
AQP2.PRO  AVTVELFLTMQLVLCIFASTDE.RRGDNLGSPAL  162
AQP3.PRO  GFFDQFIGTAALIVCVLAIVDPYNNPVPRGLEAF  186
AQP4.PRO  GLLVELIITFQLVFTIFASCDS.KRTDVTGSVAL  191
AQP5.PRO  AMVVELILTFQLALCIFSSTDS.RRTSPVGSPAL  163
```

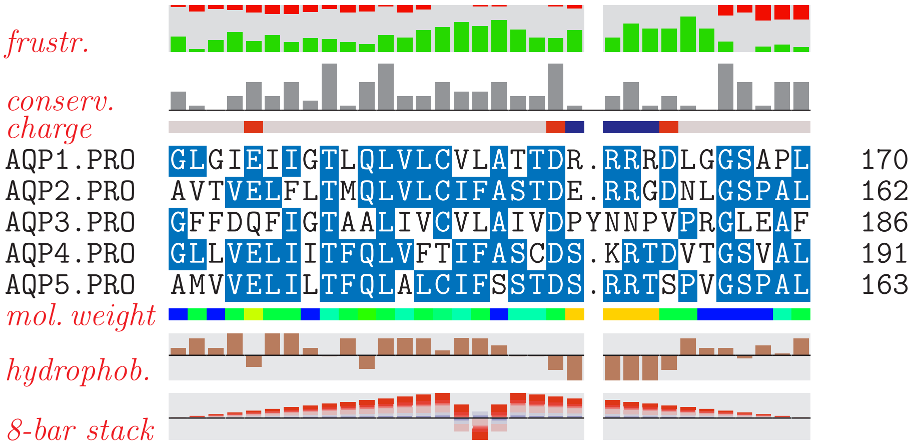
X 13.9 (C); Accessible sidechain area (Å^2)
X 23.0 (I); 23.5 (V); 25.2 (G)
X 28.7 (F); 29.0 (L); 30.5 (M); 31.5 (A)
X 41.7 (W); 44.2 (S); 46.0 (T); 46.7 (H)
X 53.7 (P)
X 59.1 (Y); 60.9 (D); 62.2 (N)
X 72.3 (E); 74.0 (Q)
X 93.8 (R)
X 110.3 (K)

Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[accessible area]{functional}
   \setends{1}{138..170}
   \showlegend
   \feature{top}{1}{138..157,164..170}{helix}{membr.}
   \feature{top}{1}{158..163}{---}{loop}
   \featurerule{1mm}
   \shadeallresidues
\end{texshade}
```

1.6 Bar graphs and color scales

Amino acid properties, such as hydrophobicity, molecular weight, or charge can be shown as bar graphs or color scales along the alignment. Further, the degree of protein sequence conservation can be indicated. As an example, in the following aquaporin alignment plots of residue conservation (bars, top), are shown as well as properties of the AQP1 sequence: charge (color scale, top), molecular weight (color scale, bottom), and hydrophobicity (bars, bottom). Local frustration data derived from the ‘frustratometer’ algorithm are displayed as triple bars; see page 76 for details.


frustr.
conserv.
charge
AQP1.PRO GLGIEIIGTLQLVLCVLATTDR.RRRDLGGSAPL 170
AQP2.PRO AVTVELFLTMQLVLCIFASTDE.RRGDNLGSPAL 162
AQP3.PRO GFFDQFIGTAALIVCVLAIVDPYNNPVPRGLEAF 186
AQP4.PRO GLLVELIITFQLVFTIFASCDS.KRTDVTGSVAL 191
AQP5.PRO AMVVELILTFQLALCIFSSTDS.RRTSPVGSPAL 163
mol. weight
hydrophob.
8-bar stack

Code:

```
\begin{texshade}{AQPpro.MSF}
   \residuesperline*{34} \setends{1}{138..170} \hideconsensus
   \feature{tttop}{1}{138..170}{frustratometer:frustr.txt}{}
   \showfeaturestylename{tttop}{frustr.}
   \tttopspace{-\baselineskip}
   \feature{ttop}{1}{138..170}{bar:conservation}{}
   \showfeaturestylename{ttop}{conserv.}
   \ttopspace{-1.2\baselineskip}
   \feature{top}{1}{138..170}{color:charge}{}
   \showfeaturestylename{top}{charge}
   \feature{bottom}{1}{138..170}{color:molweight[ColdHot]}{}
   \showfeaturestylename{bottom}{mol.\,weight}
   \bbottomspace{-0.8\baselineskip}
   \feature{bbottom}{1}{138..170}{bar:hydrophobicity[LightBrown,Gray10]}{}
   \showfeaturestylename{bbottom}{hydrophob.}
   \bbbottomspace{-1.4\baselineskip}
   \feature{bbbottom}{1}{138..170}{stackedbars:bars.txt[BlueRed,Gray10]}{}
   \showfeaturestylename{bbbottom}{8-bar stack}
   \bargraphstretch{2}
   \featurestylenamescolor{Red}
   \featurestylenamesrm  \featurestylenamesit
\end{texshade}
```

The degree of similarity and identity between all sequences in the alignment can be shown in a table using `\similaritytable` (4.10.2) outside the `texshade` environment:

	AQP1.PRO	AQP2.PRO	AQP3.PRO	AQP4.PRO	AQP5.PRO
AQP1.PRO	—	69.6	42.4	63.6	63.6
AQP2.PRO	48.4	—	36.3	66.6	75.7
AQP3.PRO	33.3	21.2	—	33.3	39.3
AQP4.PRO	45.4	54.5	24.2	—	75.7
AQP5.PRO	42.4	66.6	24.2	57.5	—

% similarity

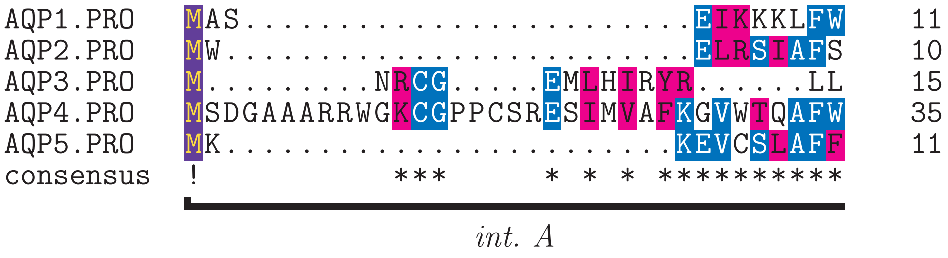
% identity

1.7 Secondary structures

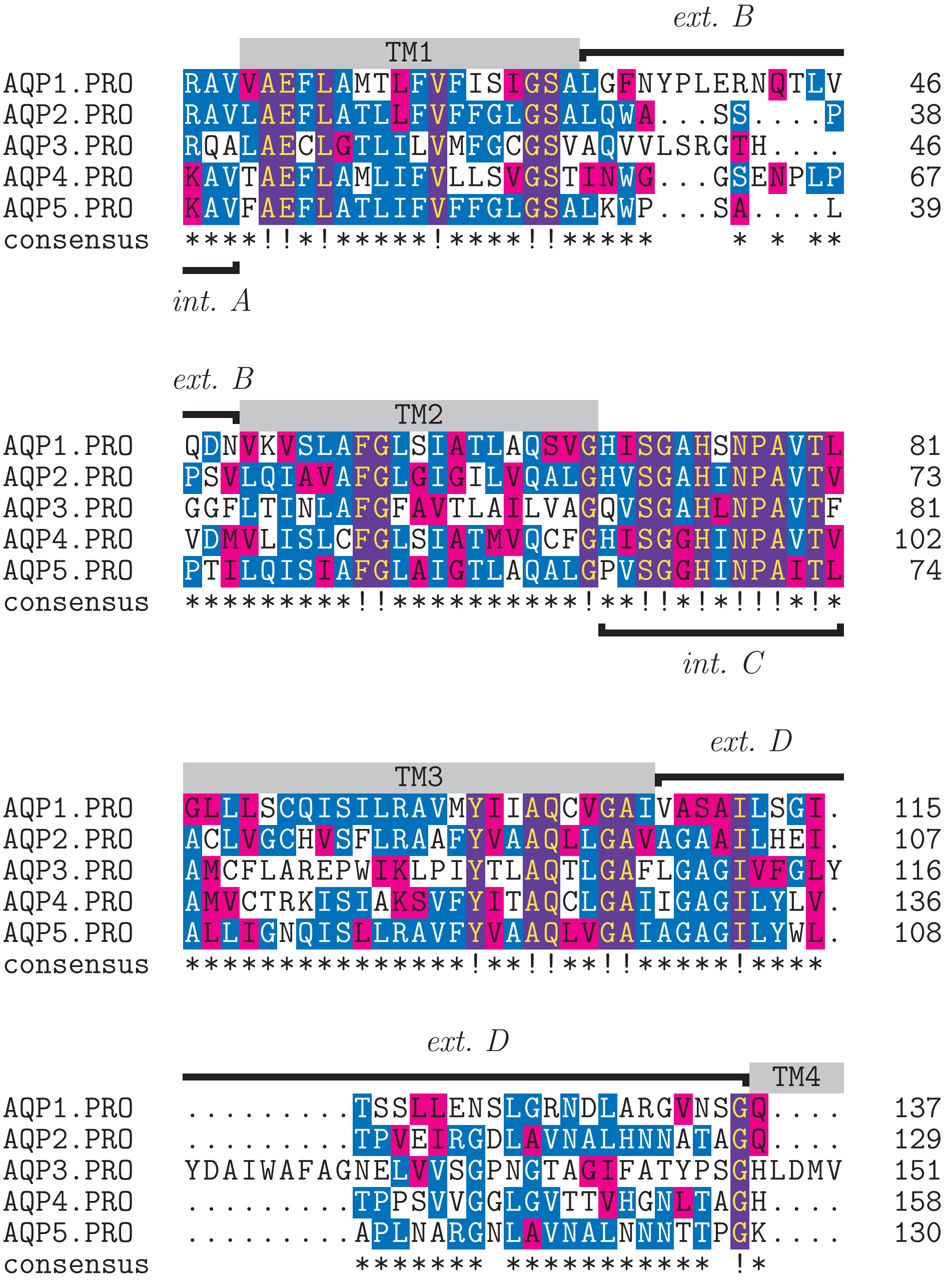
Predicted protein secondary structures in the DSSP, STRIDE PHD or HMMTOP file format can be included and displayed in the alignment. As an example, the following few commands show an aquaporin alignment with the PHD topology data for aquaporin type 1 (top sequence).

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[allmatchspecial]{similar}
   \includePHDtopo{1}{AQP1.phd}
\end{texshade}
```

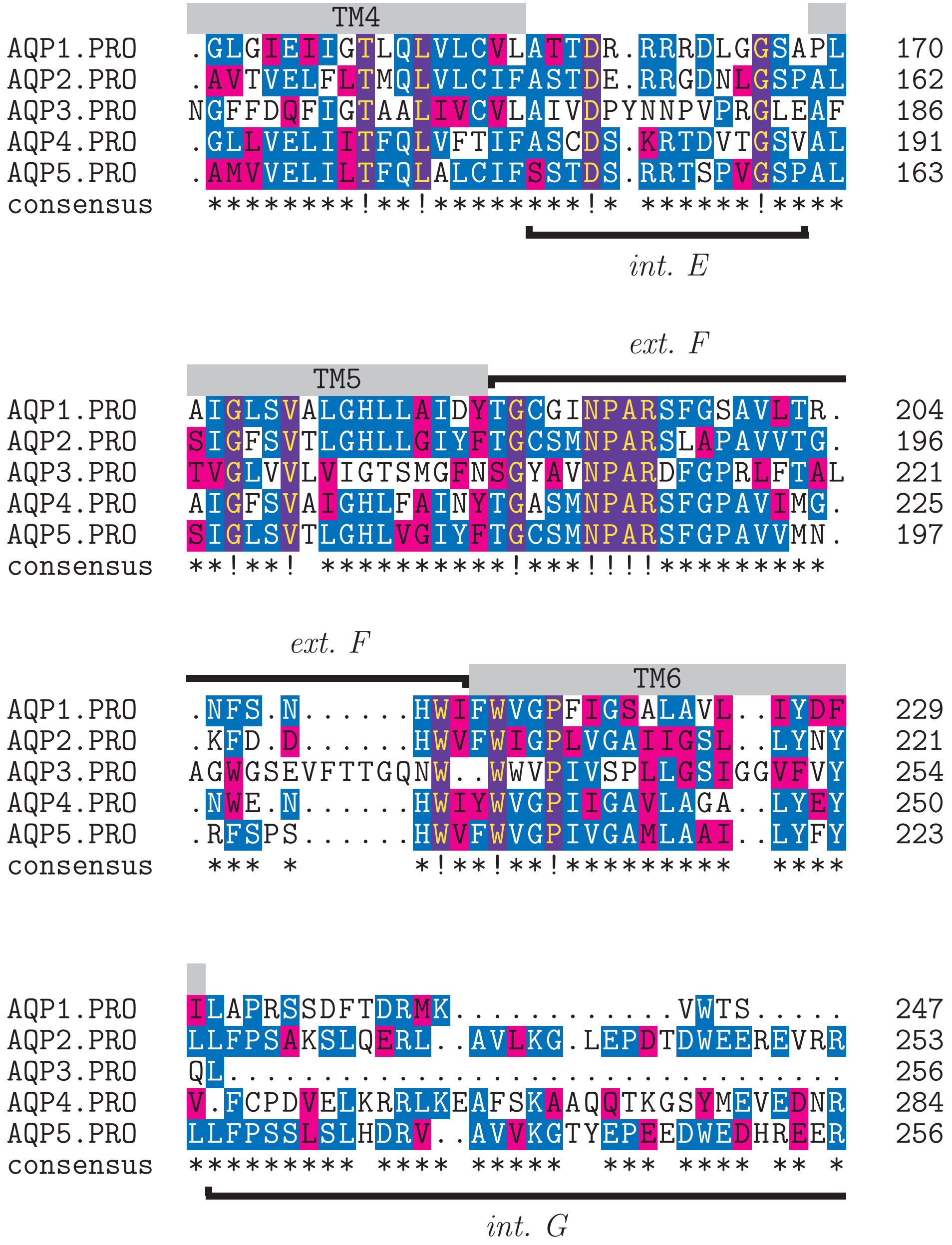
Abbr.: *int.* – internal; *ext.* – external; *TM* – transmembrane domain



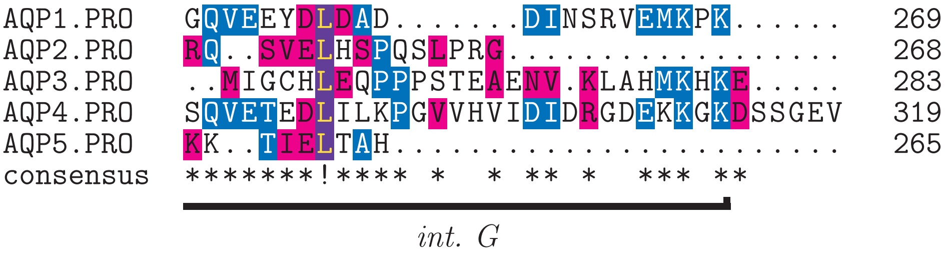
```
AQP1.PRO    MAS........................EIKKKLFW   11
AQP2.PRO    MW.........................ELRSIAFS   10
AQP3.PRO    M.........NRCG.....EMLHIRYR......LL   15
AQP4.PRO    MSDGAAARRWGKCGPPCSRESIMVAFKGVWTQAFW   35
AQP5.PRO    MK........................KEVCSLAFF   11
consensus   !          ***     * * * **********
```



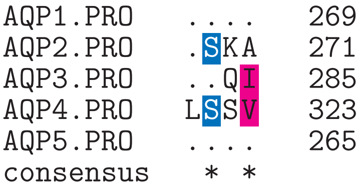
```
AQP1.PRO    RAVVAEFLAMTLFVFISIGSALGFNYPLERNQTLV     46
AQP2.PRO    RAVLAEFLATLLFVFFGLGSALQWA...SS....P     38
AQP3.PRO    RQALAECLGTLILVMFGCGSVAQVVLSRGTH....     46
AQP4.PRO    KAVTAEFLAMLIFVLLSVGSTINWG...GSENPLP     67
AQP5.PRO    KAVFAEFLATLIFVFFGLGSALKWP...SA....L     39
consensus   ****!!*!*****!****!!*****    * * **

AQP1.PRO    QDNVKVSLAFGLSIATLAQSVGHISGAHSNPAVTL     81
AQP2.PRO    PSVLQIAVAFGLGIGILVQALGHVSGAHINPAVTV     73
AQP3.PRO    GGFLTINLAFGFAVTLAILVAGQVSGAHLNPAVTF     81
AQP4.PRO    VDMVLISLCFGLSIATMVQCFGHISGGHINPAVTV    102
AQP5.PRO    PTILQISIAFGLAIGTLAQALGPVSGGHINPAITL     74
consensus   *********!!**********!**!!*!*!!!*!*

AQP1.PRO    GLLLSCQISILRAVMYIIAQCVGAIVASAILSGI.    115
AQP2.PRO    ACLVGCHVSFLRAAFYVAAQLLGAVAGAAILHEI.    107
AQP3.PRO    AMCFLAREPWIKLPIYTLAQTLGAFLGAGIVFGLY    116
AQP4.PRO    AMVCTRKISIAKSVFYITAQCLGAIIGAGILYLV.    136
AQP5.PRO    ALLIGNQISLLRAVFYVAAQLVGAIAGAGILYWL.    108
consensus   ***************!**!!**!!*****!****

AQP1.PRO    .........TSSLLENSLGRNDLARGVNSGQ....    137
AQP2.PRO    .........TPVEIRGDLAVNALHNNATAGQ....    129
AQP3.PRO    YDAIWAFAGNELVVSGPNGTAGIFATYPSGHLDMV    151
AQP4.PRO    .........TPPSVVGGLGVTTVHGNLTAGH....    158
AQP5.PRO    .........APLNARGNLAVNALNNNTTPGK....    130
consensus            ******* ***********  !*
```



```
AQP1.PRO    .GLGIEIIGTLQLVLCVLATTDR.RRRDLGGSAPL    170
AQP2.PRO    .AVTVELFLTMQLVLCIFASTDE.RRGDNLGSPAL    162
AQP3.PRO    NGFFDQFIGTAALIVCVLAIVDPYNNPVPRGLEAF    186
AQP4.PRO    .GLLVELIITFQLVFTIFASCDS.KRTDVTGSVAL    191
AQP5.PRO    .AMVVELILTFQLALCIFSSTDS.RRTSPVGSPAL    163
consensus    ********!**!********!* ******!****

AQP1.PRO    AIGLSVALGHLLAIDYTGCGINPARSFGSAVLTR.    204
AQP2.PRO    SIGFSVTLGHLLGIYFTGCSMNPARSLAPAVVTG.    196
AQP3.PRO    TVGLVVLVIGTSMGFNSGYAVNPARDFGPRLFTAL    221
AQP4.PRO    AIGFSVAIGHLFAINYTGASMNPARSFGPAVIMG.    225
AQP5.PRO    SIGLSVTLGHLVGIYFTGCSMNPARSFGPAVVMN.    197
consensus   **!**! **********!***!!!!*********

AQP1.PRO    .NFS.N......HWIFWVGPFIGSALAVL..IYDF    229
AQP2.PRO    .KFD.D......HWVFWIGPLVGAIIGSL..LYNY    221
AQP3.PRO    AGWGSEVFTTGQNW..WWVPIVSPLLGSIGGVFVY    254
AQP4.PRO    .NWE.N......HWIYWVGPIIGAVLAGA..LYEY    250
AQP5.PRO    .RFSPS......HWVFWVGPIVGAMLAAI..LYFY    223
consensus    *** *      *!**!**!*********  ****

AQP1.PRO    ILAPRSSDFTDRMK............VWTS.....    247
AQP2.PRO    LLFPSAKSLQERL..AVLKG.LEPDTDWEEREVRR    253
AQP3.PRO    QL.................................    256
AQP4.PRO    V.FCPDVELKRRLKEAFSKAAQQTKGSYMEVEDNR    284
AQP5.PRO    LLFPSSLSLHDRV..AVVKGTYEPEEDWEDHREER    256
consensus   ********* **** *****  *** **** ** *
```



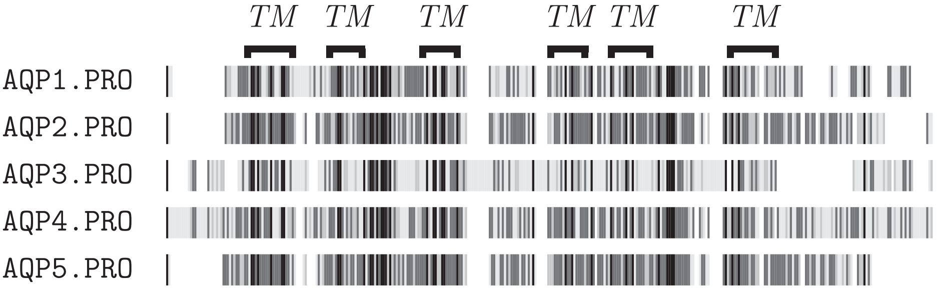
```
AQP1.PRO   GQVEEYDLDAD.......DINSRVEMKPK......   269
AQP2.PRO   RQ..SVELHSPQSLPRG.................   268
AQP3.PRO   ..MIGCHLEQPPPSTEAENV.KLAHMKHKE.....   283
AQP4.PRO   SQVETEDLILKPGVVHVIDIDRGDEKKGKDSSGEV   319
AQP5.PRO   KK..TIELTAH........................   265
consensus  *******!**** *  * ** *  *** **
```



```
AQP1.PRO   ....   269
AQP2.PRO   .SKA   271
AQP3.PRO   ..QI   285
AQP4.PRO   LSSV   323
AQP5.PRO   ....   265
consensus   * *
```

1.8 Sequence fingerprints

To gain a quick overview of sequence similarities or properties the `\fingerprint` command has been implemented. It can depict the complete sequence in one single line. The residues are presented as colored vertical lines. The implementation of this kind of output was inspired by a publication by Kai-Uwe Fröhlich [6].



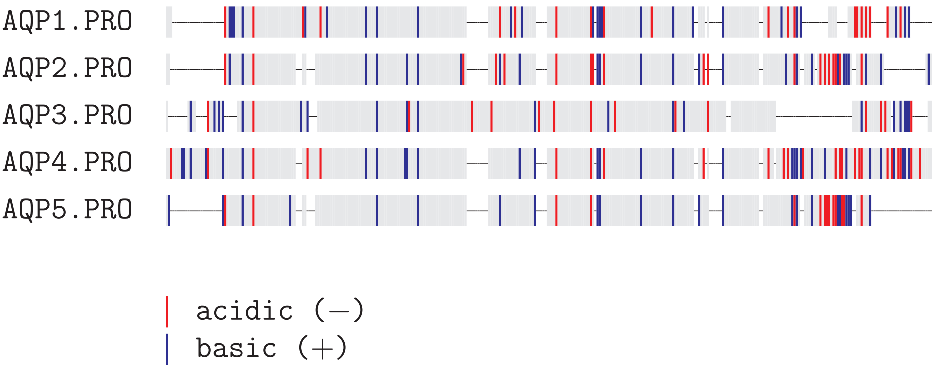
│ non-conserved
│ similar
│ ≥ 50% conserved
│ all match

Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[allmatchspecial]{similar}
   \shadingcolors{grays}
   \fingerprint{360}
   \showlegend
   \feature{top}{1}{13..36,51..68,94..112,138..156,%
                    165..185,211..232}{,-,}{TM}
\end{texshade}
```

The higher the similarity the darker the vertical lines. In this overview it becomes obvious that the transmembrane regions of the aquaporin isoforms are most conserved.

A fingerprint of charge distribution on different aquaporins is shown. below. Sequence gaps can be left blank (example above) or drawn as lines between the sequence blocks.

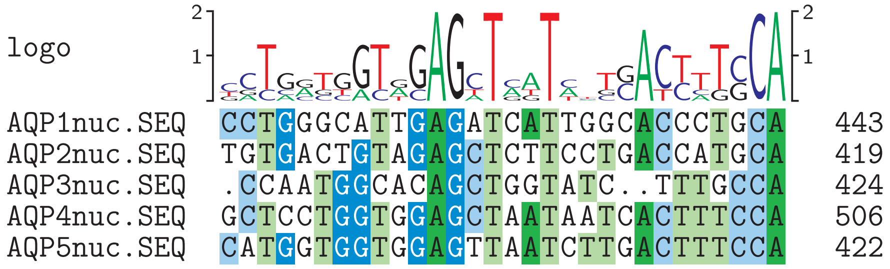


Code:

```
\begin{texshade}{AQPpro.MSF}
   \shadingmode[charge]{functional}
   \shadeallresidues
   \fingerprint{360}
   \gapchar{rule}
   \showlegend
\end{texshade}
```

1.9 Sequence logos

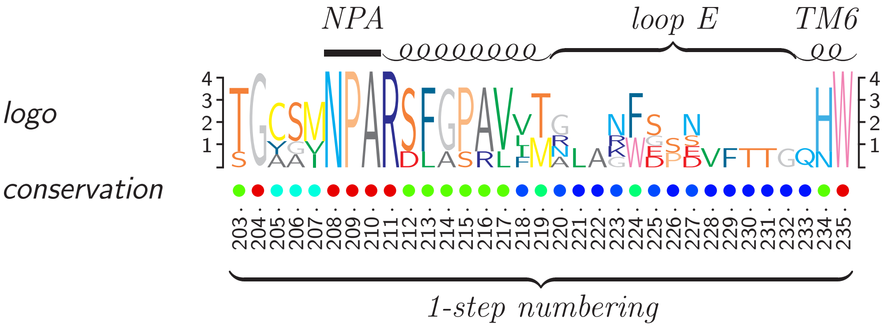
Sequence logos represent the information content of the aligned sequences at a position in bit (max. 2 bit for DNA, i. e. $\log_2 4$, and 4.322 bit for proteins, i. e. $\log_2 20$) and the relative frequency of a base or amino acid at this position. Thus, more information is contained in logos than in a standard consensus sequence. The example below shows a DNA sequence alignment with functional shading and the logo on the top (the logo colors can be set differently from the color set of the alignment, p.49).


logo
2
1
AQP1nuc.SEQ CCTGGGCATTGAGATCATTGGCACCCTGCA 443
AQP2nuc.SEQ TGTGACTGTAGAGCTCTTCCTGACCATGCA 419
AQP3nuc.SEQ .CCAATGGCACAGCTGGTATC..TTTGCCA 424
AQP4nuc.SEQ GCTCCTGGTGGAGCTAATAATCACTTTCCA 506
AQP5nuc.SEQ CATGGTGGTGGAGTTAATCTTGACTTTCCA 422

Code:

```
\begin{texshade}{AQPDNA.MSF}
   \setends{1}{414..443}
   \showsequencelogo{top}
   \shadingmode[DNA]{functional}
\end{texshade}
```

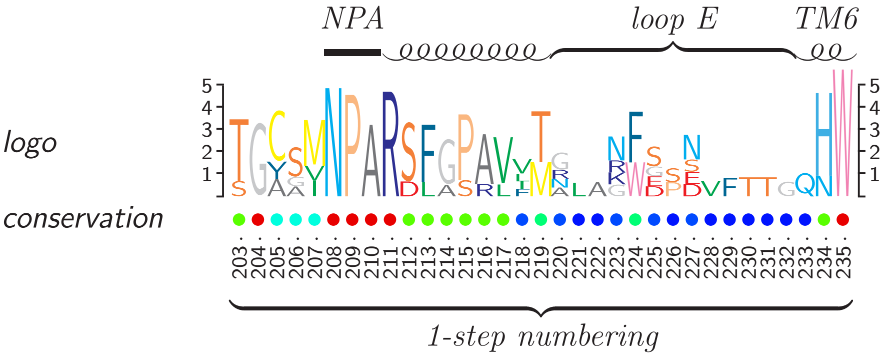
Next, the logo of a protein alignment is displayed without the actual sequences. The degree of sequence conservation is shown as a color scale in the consensus line. Note, that the full functionality of the feature lines remains.



Code:

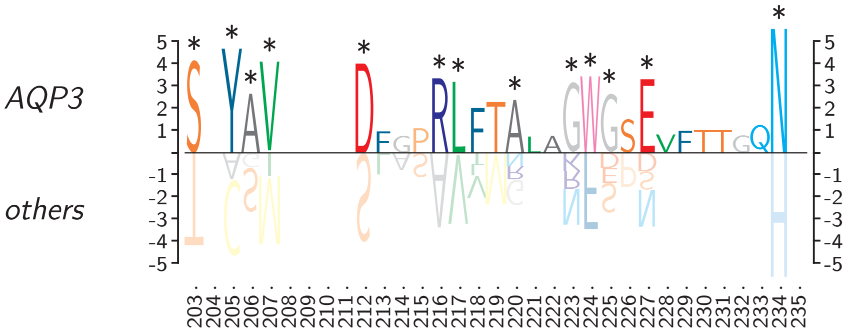
```
\begin{texshade}{AQPpro.MSF}
   \setends{AQP3.PRO}{203..235}
   \showsequencelogo{top} \showlogoscale{leftright}
   \hideseqs
   \residuesperline*{33}
   \defconsensus{{$\bullet$}}{{$\bullet$}}{{$\bullet$}}
   \showconsensus[ColdHot]{bottom}
   \nameconsensus{conservation} \namessf\namessl
   \showruler{bottom}{AQP3.PRO} \rulersteps{1}
   \feature{top}{AQP3.PRO}{208..210}{---}{NPA}
   \feature{top}{AQP3.PRO}{211..219}{helix}{}
   \feature{top}{AQP3.PRO}{220..232}{brace}{loop E}
   \feature{top}{AQP3.PRO}{233..235}{helix}{TM6}
   \feature{bottom}{AQP3.PRO}{203..235}{brace}{1-step numbering}
\end{texshade}
```

The same logo is shown below but with frequency correction turned on (`\dofrequencycorrection`), see p.56. This takes into account the difference between the amino acid distribution in the alignment and an equal distribution of 5% for each residue.



1.10 Subfamily logos

The following output is derived from the calculation of a subfamily logo. Such logos display relevant deviations of a subfamily compared to the remaining set of sequences. Here, typical residues of AQP3 are shown (upright) which deviate from the remaining four aquaporins of this alignment (upside-down). The output can be directly compared to the sequence logo above, which displays the same section of the alignment. Note, that five sequences are far too few to obtain meaningful results with this method. This is just to illustrate the approach.



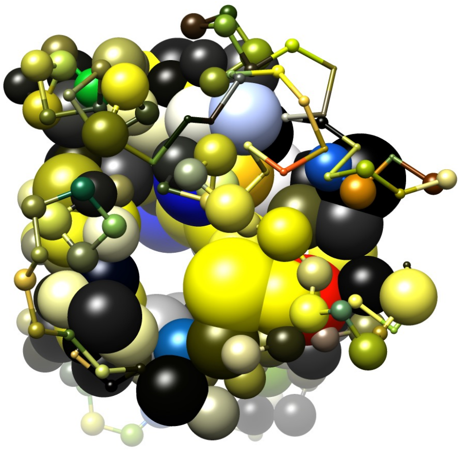
Code:

```
\begin{texshade}{AQPpro.MSF}
   \setends{AQP3.PRO}{203..235}
   \residuesperline*{33}
   \setsubfamily{3}
   \showsubfamilylogo{top} \showlogoscale{leftright}
   \namesubfamilylogo[others]{AQP3}
   \namessf \namessl
   \showruler{bottom}{AQP3.PRO} \rulersteps{1}
   \hideseqs
   \hideconsensus
   \dofrequencycorrection
\end{texshade}
```

1.11 Structure memes

The calculated sequence logo and subfamily logo data can be used to generate *Structure memes*. This a type of 3D protein display that visualizes the residue composition, their frequency, and the information content of each sequence position. Therefore, in the structure file, a red-yellow-blue plus black and white color code is projected onto a sphere at the α-carbon position, which is scaled according to the information content. TeXshade generates an output file for the molecular structure display software Chimera. Use the files

`AQP_sequence_logo_1FX8.cmd` and `AQP_subfamily_logo_1FX8.cmd` generated from `texshade.dtx` to test it out in Chimera.
The structure meme example below shows an aquaporin protomer in top down view with projected sequence logo information. The image was made with Chimera from `AQP_sequence_logo_1FX8.cmd` using *E. coli* GlpF aquaglyceroporin structure data (PDB no. 1FX8). The standard residue colors are `CGNQST` (yellow), `HKR` (blue), `DE` (red), `APV` (white), and `FILMW` (black).



Code to generate the respective Chimera command file:

```
\begin{texshade}{AQPall.aln}
   \seqtype{P}
   \showsequencelogo{top}
   \hideseqs
   \structurememe[AQP_sequence_logo_1FX8.cmd]{14}
\end{texshade}
```

1.12 Displaying a single sequence

Due to several requests a 'single-sequence'-mode has been implemented. The sequence of interest can be provided in form of a file that holds a single sequence, or it can be taken from a multiple sequence alignment. In either case, gaps in the sequence will be removed for a coherent display (can be turned off if desired). Adding labels or shading to the output is fully supported in 'single-sequence'-mode. Sequence stretches can be translated or nucleotide complements can be displayed. The starting position within the first line can be adjusted. The following example shows 5'- and 3'-UTR in lower case with the reverse strand (complement, light blue), a sequence translation (red), and shading of a poly-Arg region (white on blue). The first line is shifted to align the open reading frame to the beginning of a new line.

```
 -84                                      atggccagcgaaatcaagaagaag   -61
                                          taccggtcgctttagttcttcttc

 -60  ctcttctggagggctgtggtggctgagttcctggccatgaccctcttcgtcttcatcagc    -1
      gagaagacctcccgacaccaccgactcaaggaccggtactgggagaagcagaagtagtcg

   1  ATGGGTTCTGCCCTAGGCTTCAATTACCCACTGGAGAGAAACCAGACGCTGGTCCAGGAC    60
       M  G  S  A  L  G  F  N  Y  P  L  E  R  N  Q  T  L  V  Q  D

  61  AATGTGAAGGTGTCACTGGCCTTTGGTCTGAGCATCGCTACTCTGGCCCAAAGTGTGGGT   120
       N  V  K  V  S  L  A  F  G  L  S  I  A  T  L  A  Q  S  V  G

 121  CACATCAGTGGTGCTCACTCCAACCCAGCGGTCACACTGGGGCTTCTGCTCAGCTGTCAG   180
       H  I  S  G  A  H  S  N  P  A  V  T  L  G  L  L  L  S  C  Q

 181  ATCAGCATCCTCCGGGCTGTCATGTATATCATCGCCCAGTGTGTGGGAGCCATCGTTGCC   240
       I  S  I  L  R  A  V  M  Y  I  I  A  Q  C  V  G  A  I  V  A

 241  TCCGCCATCCTCTCCGGCATCACCTCCTCCCTGCTCGAGAACTCACTTGGCCGAAATGAC   300
       S  A  I  L  S  G  I  T  S  S  L  L  E  N  S  L  G  R  N  D

 301  CTGGCTCGAGGTGTGAACTCCGGCCAGGGCCTGGGCATTGAGATCATTGGCACCCTGCAG   360
       L  A  R  G  V  N  S  G  Q  G  L  G  I  E  I  I  G  T  L  Q

 361  CTGGTGCTGTGCGTTCTGGCTACCACTGACCGGAGGCGCCGAGACTTAGGTGGCTCAGCC   420
       L  V  L  C  V  L  A  T  T  D  R  R  R  R  D  L  G  G  S  A
                                         poly-Arg
 421  CCACTTGCCATTGGCTAGtctgtggctcttggacacctgctggccattgactacactggc   480
       P  L  A  I  G  . agacaccgagaacctgtggacgaccggtaactgatgtgaccg

 481  tgtgggatcaaccctgcccggtcatttggctctgctgtgctcacc                  525
      acaccctagttgggacgggccagtaaaccgagacgacacgagtgg
```

Code:

```
\begin{texshade}{AQPDNA.MSF}
   \shadingmode[1]{singleseq}
   \shiftsingleseq
   \setends[-84]{1}{-84..525}
   \lowerregion{1}{-84..-1,439..525}
   \feature{bottom}{1}{-84..-1,424..525}{complement[LightBlue][lower]}{}
   \feature{bottom}{1}{1..390,403..438}{translate[Red]}{}
   \feature{bottom}{1}{390..402}{translate[White,Blue]}{poly-Arg}
   \setsize{all}{footnotesize}\noblockskip
\end{texshade}
```

1.13 Customization of the alignment output

Extensive possibilities are given to the user to customize the final output of an alignment (see section 4). Several examples are shown in the previous figures. Thus, all parameters defining the appearance of letters can be changed individually for sequence residues, names and numbering or the describing feature texts. Additional manual shading can be applied to any region or block of residues. Sequences are easily re-ordered, separated, hidden or blanked out without recalculation of the entire alignment; sections of the alignment can also be shown. Numbering and rulers can be displayed and set to any value. A powerful tool is the `\feature` command which allows one to label stretches of residues with bars, arrows, braces or any fill character and describing text. Legends are set automatically if desired, but user commands are also provided to build individual legends.

2 Format of alignment input files

TeXshade can handle two common alignment input formats, i. e. the MSF format (multiple sequence format) and the ALN format (alignment format). The MSF format is used by `PILEUP` of the Unix GCG sequence analysis package[23]. Files in the ALN format are produced by `CLUSTAL` which is available for free for Unix, DOS and Macintosh. Further, upon request, the FASTA format is supported since version 1.6. In addition to the mentioned software many alignment

---

[23] For a description see `http://gene.md.huji.ac.il/Computer/GCG9doc`

programs have export filters for the MSF, ALN or FASTA format, e. g. `MACAW` produces ALN files. If you are not sure whether your favorite sequence aligner produces one of the required formats compare its output to the following examples. TeXshade determines the format from the internal file structure, thus extensions like MSF, ALN or FASTA are not required. If you can choose the alignment format MSF is recommended, because this format gives information about the sequence type, i. e. peptide or nucleotide sequences, and length (for the correct setting of gaps at the sequence end).

2.1 The MSF file format

Files of this type are divided into a header section and the multiple sequence alignment. The header may contain the following components:

File Type: (optional) The first header line reads for nucleic acids alignments `!!NA_MULTIPLE_ALIGNMENT 1.0` and for amino acid sequences `!!AA_MULTIPLE_ALIGNMENT 1.0` (all uppercase).

Description: (optional) Informative text describing what is in the file.

Dividing line: (required!) Must include the following attributes:

- `MSF`: Displays the number of bases or residues in the multiple sequence alignment.
- `Type`: Displays the sequence type, ‘P’ for a peptide and ‘N’ for a nucleotide alignment.
- `Checksum`: Displays an integer value that characterizes the contents of the file.
- `..` The two periods act as a divider between the descriptive information and the following sequence information.

Name/Weight: (required!) Must include the name of each sequence included in the alignment, as well as its length, checksum and weight.

Two slashes (`//`): (required!) This separating line divides the name/weight information from the sequence alignment

The alignment section consists of sequence blocks divided by an empty line. Each sequence line starts out with the sequence name. An example file is shown here:

```
AQP.MSF  MSF: 87  Type: P  May 1st, 1998 Check: 2586 ..
Name: AQP1.PRO  Len: 66  Check:  1367    Weight: 1.00
Name: AQP2.PRO  Len: 58  Check:  2176    Weight: 1.00
Name: AQP3.PRO  Len: 83  Check:  1893    Weight: 1.00
Name: AQP4.PRO  Len: 63  Check:  3737    Weight: 1.00
Name: AQP5.PRO  Len: 59  Check:  3413    Weight: 1.00
//
          1                                           45
AQP1.PRO  MAS........................EIKKKLFWRAVVAEFLAM
AQP2.PRO  MW.........................ELRSIAFSRAVLAEFLAT
AQP3.PRO  M.........NRCG.....EMLHIRYR......LLRQALAECLGT
AQP4.PRO  MSDGAAARRWGKCGPPCSRESIMVAFKGVWTQAFWKAVTAEFLAM
AQP5.PRO  MK........................KEVCSLAFFKAVFAEFLAT

          45                                        87
AQP1.PRO  TLFVFISIGSALGFNYPLERNQTLVQDNVKVSLAFGLSIATL
AQP2.PRO  LLFVFFGLGSALQWA...SS....PPSVLQIAVAFGLGIGIL
AQP3.PRO  LILVMFGCGSVAQVVLSRGTHGGF....LTINLAFGFAVTLA
AQP4.PRO  LIFVLLSVGSTINWG...GSENPLPVDMVLISLCFGLSIATM
AQP5.PRO  LIFVFFGLGSALKWP...SA....LPTILQISIAFGLAIGTL
```

TeXshade extracts only the information from the file it really needs. So, do not mind all the checksums listed in the file—TeXshade does not either. The same is true for `Weight`. Required are the string `MSF:` for the identification of the file format and `Type:` for the determination of the sequence type (both in the dividing line), further all `Name:` definitions and finally `//`. The MSF format allows one to comment out sequences. This is done by putting an exclamation point directly infront of the respective `Name`. These sequences are neither displayed nor used for the calculation of the consensus. This works for TeXshade, too. To comment out sequences without changing the input file use the TeXshade command `\killseq{`⟨*seqref*⟩`}` (4.5.3).

```
AQP.MSF  MSF: 87  Type: P  May 1st, 1998 Check: 2586 ..
Name: AQP1.PRO  Len: 66  Check:  1367    Weight: 1.00
!Name: AQP2.PRO  Len: 58  Check:  2176    Weight: 1.00
!Name: AQP3.PRO  Len: 83  Check:  1893    Weight: 1.00
Name: AQP4.PRO  Len: 63  Check:  3737    Weight: 1.00
Name: AQP5.PRO  Len: 59  Check:  3413    Weight: 1.00
//
          1                                           45
AQP1.PRO  MAS........................EIKKKLFWRAVVAEFLAM
AQP2.PRO  MW.........................ELRSIAFSRAVLAEFLAT
AQP3.PRO  M.........NRCG.....EMLHIRYR......LLRQALAECLGT
AQP4.PRO  MSDGAAARRWGKCGPPCSRESIMVAFKGVWTQAFWKAVTAEFLAM
AQP5.PRO  MK........................KEVCSLAFFKAVFAEFLAT

          45                                       87
AQP1.PRO  TLFVFISIGSALGFNYPLERNQTLVQDNVKVSLAFGLSIATL
AQP2.PRO  LLFVFFGLGSALQWA...SS....PPSVLQIAVAFGLGIGIL
AQP3.PRO  LILVMFGCGSVAQVVLSRGTHGGF....LTINLAFGFAVTLA
AQP4.PRO  LIFVLLSVGSTINWG...GSENPLPVDMVLISLCFGLSIATM
AQP5.PRO  LIFVFFGLGSALKWP...SA....LPTILQISIAFGLAIGTL
```

The sequence lengths given after `Len:` are not used by TeXshade. Due to the fact that most alignment programms calculate the sequence length by summing up residues and additionally gaps which is not really correct. In order to have the sequence break right after the last residue without printing further gap symbols TeXshade counts the number of residues by itself. You can also use the command `\seqlength` in the TeXshade environment to set the values manually if you do not trust a machine.

2.2 The ALN file format

ALN files are quite similar to the above described MSF files. They simply lack a defined header section. Nevertheless, describing text is allowed before the alignment part. TeXshade determines the number of sequences and their names from the last sequence block—so, no further text lines are allowed after this block! Due to a lacking declaration in the file the sequence type has to be set in the `texshade` environment by `\seqtype{`⟨*type*⟩`}` with 'P' for peptide and 'N' for nucleotide sequences; for the example below: `\seqtype{P}`. If no `\seqtype` command is used TeXshade assumes a nucleotide sequence.

```
              profalign  May 1st, 1998, 16:58

of AQPpro.MSF{}

Muliple alignment parameter:

Gap Penalty (fixed):           10.00
Gap Penalty (varying):         .05
Gap separation penalty range:  8
Percent. identity for delay:   0%
List of hydrophilic residue:   GPSNDQEKRH
Protein Weight Matrix:         blosom

                  10        20        30        40
                   .         .         .         .
AQP1.PRO  MAS........................EIKKKLFWRAVVAEFLAM
AQP2.PRO  MW.........................ELRSIAFSRAVLAEFLAT
AQP3.PRO  M.........NRCG.....EMLHIRYR......LLRQALAECLGT
AQP4.PRO  MSDGAAARRWGKCGPPCSRESIMVAFKGVWTQAFWKAVTAEFLAM
AQP5.PRO  MK........................KEVCSLAFFKAVFAEFLAT
          *                                  .   ** *.

AQP1.PRO  TLFVFISIGSALGFNYPLERNQTLVQDNVKVSLAFGLSIATL
AQP2.PRO  LLFVFFGLGSALQWA...SS....PPSVLQIAVAFGLGIGIL
AQP3.PRO  LILVMFGCGSVAQVVLSRGTHGGF....LTINLAFGFAVTLA
AQP4.PRO  LIFVLLSVGSTINWG...GSENPLPVDMVLISLCFGLSIATM
AQP5.PRO  LIFVFFGLGSALKWP...SA....LPTILQISIAFGLAIGTL
          .. *   .**                    .   **  .
```

The minimal contents of an ALN file are shown below; this is fully sufficient. Many sequence alignment programs can produce such an output. Have a look at `seqpup` by DON GILBERT if you need a comprehensive conversion program[24].

---

[24] Sorry, `seqpup` is much more!

```
AQP1.PRO  MAS........................EIKKKLFWRAVVAEFLAM
AQP2.PRO  MW.........................ELRSIAFSRAVLAEFLAT
AQP3.PRO  M.........NRCG.....EMLHIRYR......LLRQALAECLGT
AQP4.PRO  MSDGAAARRWGKCGPPCSRESIMVAFKGVWTQAFWKAVTAEFLAM
AQP5.PRO  MK........................KEVCSLAFFKAVFAEFLAT

AQP1.PRO  TLFVFISIGSALGFNYPLERNQTLVQDNVKVSLAFGLSIATL
AQP2.PRO  LLFVFFGLGSALQWA...SS....PPSVLQIAVAFGLGIGIL
AQP3.PRO  LILVMFGCGSVAQVVLSRGTHGGF....LTINLAFGFAVTLA
AQP4.PRO  LIFVLLSVGSTINWG...GSENPLPVDMVLISLCFGLSIATM
AQP5.PRO  LIFVFFGLGSALKWP...SA....LPTILQISIAFGLAIGTL
```

2.3 The FASTA file format

In FASTA files each sequence is led by a single description line starting with a '`>`'. TeXshade uses the first word delimited by the leading '`>`' and a space as the sequence name. If no descriptive text is present TeXshade generates a sequence name consisting of '`seq`' plus a consecutive number. The lines following the description line contain the sequence.

```
>AQP1.PRO
MAS........................EIKKKLFWRAVVAEFLAM
TLFVFISIGSALGFNYPLERNQTLVQDNVKVSLAFGLSIATL

>AQP2.PRO
MW.........................ELRSIAFSRAVLAEFLAT
LLFVFFGLGSALQWA...SS....PPSVLQIAVAFGLGIGIL

>AQP3.PRO
M.........NRCG.....EMLHIRYR......LLRQALAECLGT
LILVMFGCGSVAQVVLSRGTHGGF....LTINLAFGFAVTLA

>AQP4.PRO
MSDGAAARRWGKCGPPCSRESIMVAFKGVWTQAFWKAVTAEFLAM
LIFVLLSVGSTINWG...GSENPLPVDMVLISLCFGLSIATM

>AQP5.PRO
MK........................KEVCSLAFFKAVFAEFLAT
LIFVFFGLGSALKWP...SA....LPTILQISIAFGLAIGTL
```

3 Processes in the TeXshade environment and parameter files

Five steps are executed by TeXshade when processing the `texshade` environment:

`\begin{texshade}[⟨parameterfile⟩]{⟨alignmentfile⟩}`

1. Analysis of the ⟨*alignmentfile*⟩; determination of the number of sequences and sequence names
2. Setting parameters to default
3. Setting parameters to the definitions of the ⟨*parameterfile*⟩, if existent
4. Execution of further TeXshade commands within the evironment, if existent

`\end{texshade}`

5. Loading and setting the alignment on a line by line basis

Using predefined parameter files for repeatedly occuring situations can save a lot of typing and makes the output throughout a publication or presentation more consistent. Further, such files are an easy way to exchange self-defined shading modes or new color schemes with other users.
No special file format is required for parameter files. TeXshade simply calls the file using the `\input` command right after resetting all parameters to default. An example parameter file is present containing the standard parameters of TeXshade called `texshade.def`. This file can be changed freely and can be used as a template for the creation of personal parameter files.

4 `texshade` user commands

The TEXshade package must be loaded by the `\usepackage` command in the document header section.

`\usepackage[`⟨*option*⟩`]{texshade}`

Then, the `texshade` environment is ready to use as described in 1.4. See also section 3 for a description of the optional parameter file. All other commands provided by TEXshade (except `\shadebox` [4.7], `\molweight` and `\charge` [4.10.1], and `\percentsimilarity`, `\percentidentity` and `\similaritytable` [4.10.2]) must be used within the `texshade` environment.

4.1 Using predefined shading modes

If no `\shadingmode` command is given in the `texshade` environment the default shading mode (*identical*, see 1.5.1) is active. For the selection of one of the other predefined shading modes the following command is provided.

`\shadingmode[`⟨*option*⟩`]{`⟨*mode*⟩`}`

You can choose from six shading modes and declare one option which depends on the selected mode.

1. `\shadingmode[`⟨*allmatchspecial/number*⟩`]{identical}`

   See 1.5.1 for examples. Use the option `allmatchspecial` to shade positions with a special color where all residues are identical. Or use a percentage number (0–100) as an option to set an additional threshold for highly conserved residues, e. g. `\shadingmode[90]{identical}`. `\allmatchspecial` can also be used as a command with or without an optional parameter for setting the high conservation threshold. As both, option or command, `allmatchspecial` is only active in the *identical* and *similar* shading modes.

   One can choose from five predefined shading color schemes with the command `\shadingcolors{`⟨*scheme*⟩`}`. The sets are named 'blues' (used in the example, 1.5.1), 'reds', 'greens', 'grays' and 'black'. Default is `\shadingcolors{blues}`. Further, the colors for the non matching, the conserved and all matching (or highly conserved) residues can be set individually plus the letter case (lower or upper) or any character can be chosen:

```
\nomatchresidues{⟨res.col.⟩}{⟨shad.col.⟩}{⟨case⟩}{⟨style⟩}
\conservedresidues{⟨res.col.⟩}{⟨shad.col.⟩}{⟨case⟩}{⟨style⟩}
\allmatchresidues{⟨res.col.⟩}{⟨shad.col.⟩}{⟨case⟩}{⟨style⟩}
```

For how to handle colors for the foreground ⟨*res.col.*⟩ and the background ⟨*shad.col.*⟩ see section 5. The third parameter ⟨*case*⟩ tells TeXshade to print the corresponding residue as a lowercase or an uppercase letter or even to print any other character. Finally, the ⟨*style*⟩ parameter tells TeXshade which shape to use for the letters. Use one of the following styles for ⟨*style*⟩.

⟨*style*⟩	*effect*
`bf`	bold face series
`md`	normal series
`up`	upright shape (normal shape)
`it`	italics shape
`sl`	slanted shape
`rm`	modern roman family
`sf`	sans serif family
`tt`	typewriter family

In order to change only some of the parameters it is sufficient to declare these and use empty braces for the others. Examples:

`\conservedresidues{White}{Blue}{upper}{bf}` (the conserved residues are printed as bold face white uppercase letters on blue)

`\nomatchresidues{}{}{{$\bullet$}}{}` (instead of the non matching residues a '•' is printed. The colors and style are not changed; note the double curly braces which make TeXshade interpret this complex symbol description as one single character)

Once a set of shading colors is redefined, it can be saved using `\defshadingcolors{⟨name⟩}` for later use in the document (see 4.6.1).

2. `\shadingmode[`*⟨allmatchspecial/number⟩*`]{similar}`

   See 1.5.2 for an example output and an explanation of the shading. In addition to the described commands for changing shading colors this shading mode provides the command `\similarresidues`. Use it in analogy to the commands above.

   How does TeXshade know which residues are considered to be similar? These definitions are set by two command couples, i. e. `\pepsims`,`\pepgroups` for peptides and `\DNAsims`,`\DNAgroups` for nucleotides. With `\pepsims` and `\DNAsims` residues are defined which are similar to the consensus residue. Examples:

   `\pepsims{S}{TA}` If a serine is the consensus residue then all threonins and alanines at this position are shaded in the color for similars. This definition does *not* imply that threonine and alanine are similar to each other! This becomes obvious when you inspect the next definition:

   `\pepsims{T}{S}` Serine but not alanine is declared to be similar to threonine.

   What happens if there is no consensus residue? How does TeXshade decide if a group of similars is greater than the threshold? For this, groups are pre-defined:

   `\pepgroups{FYW,ILVM,RK,DE,GA,ST,NQ}` This command allows one to define up to nine groups of similars, separated by commas. Each residue can belong to only one group. If one residue is assigned to several groups only the last assignment will be used.

   `\DNAgroups{GAR,CTY}` This command is used in analogy to the amino acid groups. Here, two ambiguity codes ('R' for purine base and 'Y' for pyrimidine base) are assigned in addition.

   Residues which do not appear in any of the four commands are considered not to belong to a group. The default settings for similars are listed below:

```
\pepgroups{FYW,ILVM,RK,DE,GA,ST,NQ}

\pepsims{F}{YW}  % Y and W are similar to F
\pepsims{Y}{WF}  % W and F are similar to Y
\pepsims{W}{YF}  % Y and F are similar to W
```

```
\pepsims{I}{LVM} % L, V and M are similar to I
\pepsims{L}{VMI} % V, M and I are similar to L
\pepsims{V}{MIL} % M, I and L are similar to V

\pepsims{R}{KH}  % K and H are similar to R
\pepsims{K}{HR}  % H and R are similar to K
\pepsims{H}{RK}  % R and K are similar to H

\pepsims{A}{GS}  % G and S are similar to A
\pepsims{G}{A}   % A (but not S) is similar to G

\pepsims{S}{TA}  % T and A are similar to S
\pepsims{T}{S}   % S (but not A) is similar to T

\pepsims{D}{EN}  % E and N (but not Q) are similar to D
\pepsims{E}{DQ}  % D and Q (but not N) are similar to E
\pepsims{N}{QD}  % Q and D (but not E) are similar to N
\pepsims{Q}{NE}  % N and E (but not D) are similar to Q

\DNAgroups{GAR,CTY}

\DNAsims{A}{GR}  % G and R are similar to A
\DNAsims{G}{AR}  % A and R are similar to G
\DNAsims{R}{AG}  % A and G are similar to R

\DNAsims{C}{TY}  % T and Y are similar to C
\DNAsims{T}{CY}  % C and Y are similar to T
\DNAsims{Y}{CT}  % C and T are similar to Y
```

3. `\shadingmode[`⟨*filename*⟩`]{T-Coffee}`

   Enter a ⟨*filename*⟩ to load the shading information from a `T-Coffee score_ascii` file (`www.tcoffee.org`); see example in 1.5.3. Make sure that the alignment file specified in the `\texshade` environment command and the `T-Coffee` shading file correspond to each other.

   If you do not enter a ⟨*filename*⟩ here, a separate command `\includeTCoffee{`⟨*filename*⟩`}` must be used.

   `T-Coffee` shading can also be used in the consensus (p. 53) and in the feature lines, in particular color scales and bar plots (p. 74), for the display of shading information.

4. `\shadingmode[`⟨*seqref*⟩`]{diverse}`

   1.5.4 depicts an example alignment. Choose the number or the name of the sequence ⟨*seqref*⟩ which will be treated as the reference and to which the other sequences are compared. If no ⟨*seqref*⟩ is declared the first sequence is used as a reference (⟨*seqref*⟩ = 1).

   Standard definitions for `diverse` mode are:

   ```
   \nomatchresidues{Black}{White}{lower}{up}
   \similarresidues{Black}{White}{lower}{up}
   \conservedresidues{Black}{White}{{.}}{up}
   \allmatchresidues{Black}{White}{{.}}{up}
   \gapchar{-}
   ```

   After calling `\shadingmode{diverse}` these commands can be used to redefine the `diverse` mode settings (mind the double curly braces around the dot-symbol!).

   Since alignment positions where all residues match may not contain much information, those sites can be blanked out using `\hideallmatchpositions`. The resulting break in the alignment is indicated by a gap and a vertical line. See the `\setdomain` command (4.5.2) for further information on how to change the gap and ruler colors. A single-stepped ruler is also recommended (4.5.1). `\hideallmatchpositions` can be combined with `\setends` (4.5.2).

5. `\shadingmode[`⟨*type*⟩`]{functional}` There are seven different functional shading types available for peptide sequences, and one for DNA sequences. Five of TeXshade's functional shading types correspond to the four 'alphabets' employed by Karlin and Ghandour for peptide alignments [2] or by the rasmol software. Additional 'alphabets' to the standard 20-letter array of amino acids can highlight peptide similarities which were otherwise not visible. For the 'alphabet' definitions see below:

   - ⟨*type*⟩ = `charge` Acidic (D, E) and basic (H, K, R).
   - ⟨*type*⟩ = `hydropathy` Acidic and basic (as above), polar uncharged (C, G, N, Q, S, T, Y) and hydrophobic nonpolar (A, F, I, L, M, P, V, W), see also Kyte & Doolittle [3].

- ⟨*type*⟩ = `structure` External (D, E, H, K, N, Q, R), internal (F, I, L, M, V) and ambivalent (A, C, G, P, S, T, W, Y).
- ⟨*type*⟩ = `chemical` Acidic (D, E), aliphatic (I, L, V), aliphatic (small) (A, G), amide (N, Q), aromatic (F, W, Y), basic (H, K, R), hydroxyl (S, T), imino (P) and sulfur (C, M).
- ⟨*type*⟩ = `rasmol` (D, E), (K, R, H), (F, Y, W), (A, G), (C, M), (S, T), (N, Q), (I, L, V), (P).

The two types described below highlight sidechain sizes and hydrophobicity, respectively, according to ROSE *et al.* [4, 5]. Standard area stands for the surface area of the residue in Å^2, i. e. it is a measure for the size of a residue's sidechain. The accessible area value (also in Å^2) gives information about the size of the surface area which is typically accessible by solvent molecules within the folded protein. A very small area means that the residue is strongly buried and is thus very hydrophobic. Hydrophilic residues in turn possess large accessible areas due to their preferred location at the protein surface. Therefore, this type of functional shading provides an additional method to `hydropathy` and `structure` for the visualization of structural protein properties.

- ⟨*type*⟩ = `standard area` for the area values see legend of the alignment in 1.5.5
- ⟨*type*⟩ = `accessible area` for values see 1.5.5

Functional shading can also be shown for DNA sequences using:

- ⟨*type*⟩ = `DNA`

If no ⟨*type*⟩ or an unknown ⟨*type*⟩ is designated as option all functional groups and shading colors are cleared. This is also achieved by the command `\clearfuncgroups`. With all groups cleared one can start to build new shading modes from scratch. How to do this is explained in the next section.

In order to exchange the colors but to keep the group definitions and descriptions the command `\funcshadingstyle` can be employed. Usage:

```
\funcshadingstyle{⟨residue⟩}{⟨res.col.⟩}{⟨shad.col.⟩}
                                          {⟨case⟩}{⟨style⟩}
```

⟨*residue*⟩ is one representative of the whole amino acid group. The colors which are declared by the next four parameters are used for all residues in this group. ⟨*case*⟩ and ⟨*style*⟩ are as described for example in `\nomatchresidues`.

With `\shadeallresidues` the threshold is ignored and all residues are shaded due to their group assignment.

6. `\shadingmode[`⟨*seqref*⟩`]{singleseq}`

   Use `singleseq` mode in order to display a single sequence rather than a sequence alignment in a formatted way with all kinds of shadings and labels, see example in 1.12.

   Both, nulceotide and protein sequences can be set. The sequence is derived from a file holding a single sequence or a multiple sequence alignment using ⟨*seqref*⟩. Sequence gaps present in the file due the alignment procedure are removed during loading. In order to keep the gaps use `\keepsingleseqgaps`.

   Standard-wise, the sequence name is not displayed (but can be turned on, 4.5.1), the numbering is shown left and right (can be changed, 4.5.1). Rulers (4.5.1), shading (4.6.1), emphasization (4.6.2), and sequence features (4.6.3), including translations or complements, etc. can be shown.

   The sequence start position in the first line can be shifted by a certain number of residue positions `\shiftsingleseq[`⟨*num*⟩`]`. If no ⟨*num*⟩ is stated the sequence will be automatically shifted so that position 1 is at the start of a new line.

4.2 Creating new functional shading types

The grouping of amino acids due to other properties can make sense as suggested by KARLIN and GHANDOUR [2], e. g. physical properties (molecular weight, shape), kinetic properties (reaction velocity, Michaelis-Menton constant), or structure (α-helices, β-sheets, turns). New amino acid groups are defined with the `\funcgroup` command. This command needs six parameters:

```
\funcgroup{⟨descr⟩}{⟨residues⟩}{⟨res.col.⟩}{⟨shad.col.⟩}
                                          {⟨case⟩}{⟨style⟩}
```

⟨*descr*⟩ contains descriptive text which is displayed in the legend. The second parameter ⟨*residues*⟩ holds the amino acids to be grouped. The colors for the foreground and background are set with the following two parameters, the case and style is declared by the last parameters. The example below defines a funcional group named ‘acidic (−)’ containing the amino acids aspartic and glutamic acid with white letters on a red background:

```
\funcgroup{acidic ($-$)}{DE}{White}{Red}{upper}{up}
```

For the usage of colors see section 5. Up to nine individual groups can be defined. New groups are simply added to the already existing groups, i. e. if an extension of the group definitions of an existing shading mode is desired there is no need to clear these groups und re-define them again. Just add the new groups with the `\funcgroup` command. To create completely new modes use the command `\shadingmode{functional}` without an option *before* setting the new groups. The new definitions are active only in the functional shading mode—so be sure to have it switched on before setting the new groups. Remember, `\shadingmode{functional}` without an optional parameter clears all groups defined before, see above. The following example shows the definitions needed to produce an output which is identical to the functional mode ‘charge’:

```
\begin{texshade}{⟨alignmentfile⟩}

  \shadingmode{functional}
  \funcgroup{acidic ($-$)}{DE}{White}{Red}{upper}{up}
  \funcgroup{basic ($+$)}{HKR}{White}{Blue}{upper}{up}

\end{texshade}
```

4.3 Appearance of the consensus line

An important parameter for the calculation of the consensus is the threshold percentage. Default setting is 50%, i. e. to become the consensus residue more than half of the residues at this position must be identical or similar, depending on the shading mode. Any percentage between 0 and 100 is allowed and can be set with `\threshold{⟨percentage⟩}`, e. g. `\threshold{50}`.
Additionally, an optional parameter can be set, e. g. `\threshold[90]{50}`, to label residues that are highly conserved in a special color (see example on page 15).

Another possibility is to set one sequence of the alignment as a reference and compare the other sequences to this one. Therefore, the command `\constosingleseq{⟨seqref⟩}` is provided. The ⟨*seqref*⟩ selects the sequence to be used as reference (numbering according to the appearance in the alignment file; top sequence is number 1, or use the sequence name). Nevertheless, the threshold percentage is also taken into account, i. e. with a threshold of 50% half of the sequences must be identical or similar compared to the specified reference sequence in order to be shaded. With `\constoallseqs` the consensus is calculated considering all sequences (the case described in the paragraph above). Consensus lines are displayed either on the top or at the bottom of the alignment by calling

`\showconsensus[⟨color/scale⟩[,⟨color/scale⟩]]{⟨position⟩}`

with ⟨*scale*⟩ `BlackWhite`, `WhiteBlack`, `BlueRed`, `RedBlue`, `GreenRed`, `RedGreen`, `ColdHot` (recommended), `HotCold`, or `T-Coffee` (see 1.5.3), and ⟨*position*⟩ `top` or `bottom`.
The first color defines the foreground, i.e. the letters, the second color—if specified—defines the background. If a color scale is named the consensus will be shaded according to the level of sequence conservation (see section 4.3.1 on residue weight tables below). For an example output see page 16. You can find more information on color scales on page 74. The calculated consensus colors can be exported as a Pymol [7] script or Chimera command file (default) by `\exportconsensus[⟨pymol/chimera⟩]{⟨seqref⟩}{⟨filename⟩}`. The generated file can be opened in Pymol or Chimera, resp., in order to shade a 3D model of the sequence ⟨*seqref*⟩.
To hide the consensus use `\hideconsensus`. The consensus line is named ‘consensus’ in english texts, ‘consenso’ in spanish or ‘Konsensus’ if the `german.sty` is used. With `\nameconsensus{⟨name⟩}` any name can be set.
You can tell TeXshade which symbols or letters to use in the consensus line for different matching qualities by

`\defconsensus{⟨symbol1⟩}{⟨symbol2⟩}{⟨symbol3⟩}`.

The following parameters are allowed for symobols 1–3:

1. ⟨*symbol1*⟩ = no match symbol (if below threshold)

    - any character or letter

  - `{}` (empty braces) for blank space

2. ⟨*symbol2*⟩ = conserved symbol (if threshold is exceeded)
   - `upper` (prints the consensus residue in uppercase)
   - `lower` (prints the consensus residue in lowercase)
   - any character or letter
   - `{}` (empty braces) for blank space
3. ⟨*symbol3*⟩ = highly conserved symbol (if `\allmatchspecial` is active)
   - see ⟨*symbol2*⟩

Example: `\defconsensus{{}}{*}{upper}` does not show non matching residues in the consensus line, marks conserved residues with '`*`', and displays the uppercase letter of the consensus residue at positions with high conservation.
Finally, the colors of the above defined symbols are adjustable by the command:

```
\consensuscolors{⟨res.col.1⟩}{⟨shad.col.1⟩}
                {⟨res.col.2⟩}{⟨shad.col.2⟩}
                {⟨res.col.3⟩}{⟨shad.col.3⟩}
```

The color definitions are in the same order as in the `\defconsensus` command:

1. ⟨*res.col.1*⟩ = no match residue color (if below threshold)
   ⟨*shad.col.1*⟩ = no match background color
2. ⟨*res.col.2*⟩ = conserved residue color (if threshold is exceeded)
   ⟨*shad.col.2*⟩ = conserved background color
3. ⟨*res.col.3*⟩ = highly conserved residue color (if `\allmatchspecial` is active)
   ⟨*shad.col.3*⟩ = highly conserved background color

For colors which are not to be changed empty braces can be used. Example:

```
\consensuscolors{}{}{Blue}{White}{Red}{Green}
```

Non matching symbol colors are not changed, conserved residues are displayed blue on white and highly conserved residues appear as red symbols on a green background in the consensus line.

4.3.1 Residue weight tables

The degree of similarity between two amino acid residues is defined using so-called *residue weight tables*. The values usually range roughly from -10 to 10, with positive values denoting similarity and negative values dissimilarity. The most simple table sets pairs of identical residues to a value of 10 and all others to 0, i.e. the `identity` matrix. Several more matrices based on extensive protein alignments exist and can be used, e.g. `PAM250` (`Point Accepted Mutations`), `PAM100`, or `BLOSUM62` (`BLOcks of amino acid SUbstitution Matrix`); for details see respective sources and section 6.3. TeXshade further contains a `structural` matrix where similarity is defined on simple comparisons of the sidechain properties with respect to volume and hydropathy.

For calculation of the consensus color shading or for bar graphs or color scales in the `\feature` lines (4.6.3), a residue weight table can be selected by `\weighttable{`⟨*table*⟩`}` with ⟨*table*⟩ being `identity`, `structural`, `PAM250`, `PAM100`, or `BLOSUM62` (default is `identity`). Which matrix suits the analysis best needs to be decided case by case. Due to the all-positive values of the `structural` matrix (section 6.3) the similarity level appears usually very high; the `identity` matrix simply represents the number of identical residues at each position. The `PAM` and `BLOSUM` matrices provide more differentiated results. One can change individual values or even define a new weight table using the command `\setweight{`⟨*res.1*⟩`}{`⟨*res.2*⟩`}{`⟨*value*⟩`}`, e.g. `\setweight{E}{Q}{2}` or `\setweight{K}{C}{-5}`. A full table, thus, needs 200 entries $(20 * 20/2)$. A value for the gap penalty is set with `\gappenalty{`⟨*value*⟩`}`.

4.4 Display of logos

4.4.1 Sequence logos

In a sequence logo [8], the information content $I(P_i)$ of each alignment position i is defined as

$$I(P_i) = \log_2 |\Sigma| + \sum P_{ij} \cdot \log_2 P_{ij}$$

with $|\Sigma|$ being the cardinality of the used alphabet, i. e. 4 for DNA and 20 for protein sequences, and P_{ij} being the frequency of residue j at this position. Each position is displayed as a stack of residue symbols whose heights represent their proportion of the information content (example on p.33).
The display of sequence logos can be either on the top or at the bottom of a nucleotide or protein alignment. Logos will be shown after the command: `\showsequencelogo[`⟨*colorset*⟩`]{`⟨*top/bottom*⟩`}`. If no optional ⟨*colorset*⟩ is selected the residues will be shaded as follows:

- Nucleotide sequences

  G : Black
  A : Green
  T,U : Red
  C : Blue

- Protein sequences (similar to rasmol)

  D,E : Red
  C,M : Yellow
  K,R : Blue
  S,T : Orange
  F,Y : MidnightBlue
  N,Q : Cyan
  G : LightGray
  L,V,I : Green
  A : DarkGray
  W : CarnationPink

H : CornflowerBlue
P : Apricot
B,Z : LightMagenta

Optional color sets correspond to the functional shading modes `chemical`, `rasmol`, `hydropathy`, `structure`, `standard area`, `accessible area`, `DNA` (see p.49). The `\showsequencelogo` command can be reversed by `\hidesequencelogo`.

Logo colors can be turned to 'Black' with the command `\clearlogocolors[⟨color⟩]` with the optional parameter not set. The optional parameter can be used to set all residue colors to ⟨*color*⟩, e.g. `\clearlogocolors[Blue]`. User specific logo color sets are defined by using `\logocolor{⟨residues⟩}{⟨color⟩}`, e.g. `\logocolor{DE}{Red}` `\logocolor{CM}{Yellow}` etc.

It is common practice for protein sequence logos to correct amino acid frequencies to the background frequency in the alignment, which usually differs from the equal distribution of 5% for each residue. Frequency correction can be turned on by `\dofrequencycorrection` and off by `\undofrequencycorrection`.

The vertical extent of the logo can be changed by `\logostretch{⟨factor⟩}`, e.g. `\logostretch{1.5}`. The width of the logo characters is dependent on the character width set for the alignment, see `\charstretch` on p.65.

Finally, the bit-scale can be turned off and on using `\hidelogoscale` and `\showlogoscale[⟨color⟩]{⟨position⟩}`, respectively, with ⟨*position*⟩ `left`, `right`, or `leftright` and an optional ⟨*color*⟩. A name for the sequence logo can be set, which is displayed next to the scale by `\namesequencelogo{⟨name⟩}`.

4.4.2 Subfamily logos

Subfamily logos provide a novel tool to visualize subfamily-specific sequence deviations at alignment positions with a high information content in an intuitive way [9].

This is achieved by subtracting from the frequency of a residue within a pre-defined subset of sequences, i. e. a subfamily, the frequency of this residue in the remaining set of sequences. The difference is then weighted by the information content, see above section on sequence logos. An example is shown on p.34.

Subtraction of frequencies produces values from -1 to 1. Positive values correspond to residues which are characteristic for the subfamily (shown upright in the output), negative values to those that are typical for the remaining sequences (shown upside-down). Positions with an equal distribution of the residue result in a zero value.

Subfamily logos are displayed analogous to sequence logos by the command `\showsubfamilylogo[⟨colorset⟩]{⟨top/bottom⟩}` and hidden by `\hidesubfamilylogo`. To calculate a subfamily logo, it is further required to define a subfamily within the alignment by `\setsubfamily{⟨seqrefs⟩}`, e.g. `\setsubfamily{1-10,20,AQP3}`.

For coloring residues, display/stretching of the scales, and frequency correction the same commands as for sequence logos apply with two exceptions. First, subfamily logos contain negative values, which can be displayed `\shownegatives[⟨weak, medium, strong⟩]` or hidden `\hidenegatives`. Without the optional parameter negative residues will be tinted by 50%, i.e. `medium`. This greatly improves readability. Second, a name for the subfamily logo is set by `\namesubfamilylogo[⟨neg.name⟩]{⟨pos.name⟩}` with a required name for the positive part of the logo and an optional name for the negative part.

In order to better recognize relevant positions in the subfamily logo, a bit-value can be set above which the deviation is considered relevant by the command `\relevance{⟨bit-value⟩}`. If this command is not given 2.321 bit is assumed for proteins, i. e. $\log_2 5$, and 1 bit for DNA, i. e. $\log_2 2$. Such positions will be labeled by `\showrelevance[⟨color⟩]{⟨symbol⟩}`, e. g. `\showrelevance[Blue]{$\nabla$}`. The symbol will be hidden with `\hiderelevance`.

4.4.3 Structure memes

Structure memes combine sequence logo and subfamily logo information with 3D protein structure data [11]. TeXshade generates a 'command file' output that can be loaded into the molecular structure display software Chimera.

A sequence logo or subfamily logo must be calculated as described in the two subsections above. Then, the command `\structurememe[⟨seqref⟩]{⟨filename⟩}` generates an Chimera output file (use the ending `.cmd` or `.com`) with ⟨*seqref*⟩ as the reference sequence for which a protein structure file must be available for display. Two example files are distributed with this TeXshade version to load into Chimera; the PDB file 1FX8 must be used for the structure meme. The `\memeStandardcolors` are: `DE` (Red), `CGNQSTY` (Yellow), `HKR`

(Blue), `APV` (White), `FILMW` (Black).
The color grouping can be changed using `\memeRed{`⟨*residues*⟩`}`, and accordingly `\memeYellow`, `\memeBlue`, `\memeWhite`, and `\memeBlack`. If a 3D structure file contains more than one chain, the structure meme display can be restricted to one chain using `\chimerachain{`⟨*chainlabel*⟩`}` with ⟨*chainlabel*⟩ typically being a letter e.g. `{A}`. For the radius of the α-carbon spheres the logo information bit-value is used, which can be scaled using `\chimeraballScale{`⟨*factor*⟩`}` with ⟨*factor*⟩ from 0–1. The residue composition at a sequence position is stored in a name label of the command file and will be visible in Chimera when pointing to it. To eliminate irrelevant residues a cut-off bit-value can be set `\memelabelcutoff{`⟨*bit-value*⟩`}`. The symbols `>` `:` and `.` indicate the 3, 2, and 1 bit levels.
Structure memes from subfamily logos will duplicate the structure model and shift it by 40 Å along the x-axis to achieve a side-by-side arrangement. The translational direction can be changed using `\chimeraxisdistance{`⟨*x-dist*⟩`}{`⟨*y-dist*⟩`}{`⟨*z-dist*⟩`}` in Ångstrøm.
Eventually, with `\echostructurefile{`⟨*strucref*⟩`}` a reference to a suitable structure file, e.g. from the PDB, can be named, which will be put into the command file and which will appear when Chimera asks for a structure file in a load dialog window.

4.5 Appearance of the sequence lines

4.5.1 Names, numbers and gaps

Many parameters that influence the appearance of the actual sequence lines can be changed for customization. Thus, the sequence names can be shown colored via ⟨*color*⟩ either left or right by

`\shownames[`⟨*color*⟩`]{`⟨*position*⟩`}`

with ⟨*position*⟩ set to `left` or `right`. The numbering can be displayed either left or right and even on both sides by

`\shownumbering[`⟨*color*⟩`]{`⟨*position*⟩`}`

with ⟨*position*⟩ `left`, `right` or `leftright`. Both, names and numbering can be displayed on the same side. The colors can also be set with `\namescolor{`⟨*color*⟩`}` and `\numberingcolor{`⟨*color*⟩`}`, respectively. Names and numbering of the last alignment block can either be displayed right next to the sequences or aligned right with the previous labels: `\alignrightlabels` (undo with `\unalignrightlabels`).

TeXshade uses the sequence names from the alignment input file. This can cause some problems during the TeX-run when special characters are present in those names! TeXshade does not accept the following characters in sequence names: `\ { } @` spaces and the tilde. Those have to be replaced in the input file. The characters `#` and `%` can only be used with a leading backslash, e. g. `\#`. This must also be changed in the input file. All other special characters should be displayed properly.

Sequence names that are accepted by TeXshade can further be changed in the `texshade` environment:

`\nameseq{`⟨*seqref*⟩`}{`⟨*name*⟩`}`

⟨*seqref*⟩ selects the sequence whose name is to be changed. The basis for the ⟨*seqref*⟩ is the appearance in the alignment input file with the top sequence = 1, or the old name. In order to change the colors only of some sequence names or numbers the commands `\namecolor{`⟨*seq1*⟩`, ... ,`⟨*seq n*⟩`}{`⟨*color*⟩`}` and `\numbercolor{`⟨*seq1*⟩`, ... ,`⟨*seq n*⟩`}{`⟨*color*⟩`}` are provided.

In order to hide all names or the numbering use the command `\hidenames` or `\hidenumbering`. If only the names or numbers of some sequences should be hidden apply
`\hidename{`⟨*seq1*⟩`, ... ,`⟨*seq n*⟩`}` or
`\hidenumber{`⟨*seq1*⟩`, ... ,`⟨*seq n*⟩`}`, respectively.

In some situations, e. g. when only sections of sequences are displayed, one may not want to have the residue numbering start out with number 1. The command `\startnumber[`⟨*start..stop*⟩`]{`⟨*seqref*⟩`}{`⟨*startnumber*⟩`}` allows one to set the starting number of any sequence to any value incl. negative values but except ‘0’ which is not usually used in sequence numbering (the transition from negative to positive values is like this: $\ldots\ -2, -1, 1, 2 \ldots$). If, however, the use of the number ‘0’ is wanted as sometimes in sequence logos this can be turned on by `\allowzero` and off with `\disallowzero`. The optional parameter can be used to truncate the sequence display to a certain section (see also `\setends` below).

TeXshade needs to know the correct length of the sequences to be able to break them right after the last residue. If MSF files are used as an input the length is already given but the calculation is usually wrong because the gaps are also counted. Thus, TeXshade counts the number of residues during each run by itself and stores the values in the `.aux` file. That means that it needs two runs to get the numbers right. Again, this is only important if the gap symbol after the sequence end should be suppressed, see below (`\hideleadinggaps`). If you know the correct length of the sequences you can use the command

```
\seqlength{⟨seqref⟩}{⟨length⟩}
```

in order to set the values by hand and have the gaps break properly already in the first TEX run.

Example: `\seqlength{1}{346}` means that sequence no. 1 is 346 residues long.
Another possibility to label sequence positions is to switch on a ruler on the top or at the bottom of the sequence block using `\showruler[⟨color⟩]{⟨top/bottom⟩}{⟨seqref⟩}`. The residue ruler of one sequence ⟨*seqref*⟩ or the consensus (declare '`consensus`' as ⟨*seqref*⟩) can be displayed at `top` or `bottom`. A ruler is hidden with `\hideruler[⟨top/bottom⟩]`. When `[⟨top/bottom⟩]` is omitted, both rulers are addressed. The steps between two numbers are set by `\rulersteps[⟨top/bottom⟩]{⟨number⟩}`. If the steps are set to be very close (< 4) or when every position is numbered, the numbering is automatically rotated by 90°. Using `\rotateruler` and `\unrotateruler` this can be done and undone manually, again with the `[⟨top/bottom⟩]` option. In order to change the ruler color use the optional parameter or the command `\rulercolor[⟨top/bottom⟩]{⟨color⟩}`. Also, the label and its color at individual ruler numbers can be changed by the user to a string using `\namerulerpos[⟨top/bottom⟩]{⟨number⟩}{⟨text⟩[⟨color⟩]}` (see example on p. 23). To adjust the distance between the ruler and the top or bottom sequence row use `\rulerspace[⟨top/bottom⟩]{⟨length⟩}`, e. g. `\rulerspace{1mm}`. Finally, ruler names can be displayed using `\nameruler[⟨top/bottom⟩]{⟨name⟩}` with `\setfamily`, `\setsize`, and `\rulernamecolor[⟨top/bottom⟩]{⟨color⟩}` for further adjustments.
Further, the symbol which is displayed in sequence gaps is freely selectable with `\gapchar{⟨symbol⟩}`. ⟨*symbol*⟩ can be any character or symbol. If math symbols are to be used math mode must be activated by `$` characters, i. e. `\gapchar{{$\triangle$}}`. Note the double curly braces in the last command. Everytime a 'complex' character is used, i. e. a character definition consisting of more than one letter, it must be braced in order to be interpreted as one character. One exception is `\gapchar{rule}`; with this parameter

lines are drawn in the sequence gaps with a certain thickness defined by `\gaprule{⟨thickness⟩}`, e. g. `\gaprule{1.5pt}`. The colors of the gaps and gap symbols are set by `\gapcolors{⟨symbol color⟩}{⟨background color⟩}`.

There are some discussions whether or not to display gap symbols before and after the actual sequence. Since v1.3a one can control the appearance of those gap symbols by the commands `\showleadinggaps` and `\hideleadinggaps`. By default, leading gaps are indicated by symbols despite my personal thinking that it could suggest that there are some not displayed residues upstream resp. downstream of the gap.

At certain instances a protein alignment input file may contain stop positions, e. g. due to frame shifts in the underlying DNA sequence. If such positions are labeled in the input with an `*` this will be shown in the output as well as an asterisk, i. e. distinguishable from a normal gap symbol. The character shown at stop positions can be changed by `\stopchar{⟨symbol⟩}`.

4.5.2 Displaying selected residues in the alignment

TeXshade can display a section of the complete alignment without the need to edit the alignment input file or even to re-calculate the entire alignment. This allows one to use one single alignment of the full length proteins or open reading frames for multiple visualizations of different sections in a document as done in this manual. Thus, the file `AQPpro.MSF` contains the full-length multiple protein alignment of five aquaporins but only sections are displayed as examples in 1.5.1 through 1.5.5. The definition of a section is done by

`\setends[⟨startnumber⟩]{⟨seqref⟩}{⟨start..stop⟩}`.

Again, ⟨*seqref*⟩ is the sequence number based on the appearance in the alignment file, or the name; further, in order to use the consensus as a measure for the sequence section the string '`consensus`' as ⟨*seqref*⟩ is accepted. The specified sequence is truncated at positions ⟨*start*⟩ and ⟨*stop*⟩. All other sequences are cut accordingly. If the number of the first residue in the sequence is set to a new value with the `\startnumber` command (s. a.) this is taken into account. The ⟨*startnumber*⟩ can be set as an optional parameter directly in the `\setends` command as well.

Some examples:

a) `\setends{1}{21..100}`

b) `\startnumber{1}{101} \setends{1}{121..200}`

Both commands select the same sequence section from the alignment but numbering for sequence 1 starts at position 21 in the first example and at position 121 in the latter.

c) `\setends[101]{1}{121..200}` equals example b.

d) `\startnumber[121..200]{1}{101}` also equals example b.

e) `\setends{consensus}{21..100}`

This may describe a very different section of the multiple sequence alignment because the consensus counts every position including gaps. The output can be even further restricted to individually selected residues, e.g. to eliminate uninteresting alignment stretches or to condense the output, by:

`\setdomain{`⟨*seqref*⟩`}{`⟨*selection*⟩`}`

Here, ⟨*seqref*⟩ denotes the reference sequence by its number or name. This sequence is used to define the alignment positions ⟨*selection*⟩ to be shown. ⟨*selection*⟩ can have two different formats depending on whether (a) the user wants to select the positions manually or (b) TeXshade is supposed to select the residues based on 3D coordinates provided by a PDB file.
To select the residues manually, the user provides a position list of the following format:

`{`⟨*start1*⟩..⟨*stop1*⟩`,`⟨*start2*⟩..⟨*stop2*⟩`,`...`,`⟨*start n*⟩..⟨*stop n*⟩`}`

For how to select positions by 3D coordinates provided by a PDB file, see 4.6.1.

Examples (see also p. 15ff):

```
\setdomain{1}{20..80}
\setdomain{consensus}{20..80,100..150,200..220}
\setdomain{AQP1}{point[6]:1FX8.pdb,173[side]}
\setdomain{3}{plane[0.5]:1JN4.pdb,66[CA],73[side],199[CA]}
```

It is helpful to show a ruler (e.g. single-stepped, see p. 61) to label the residue positions.
The resulting gaps between sequence stretches are marked by a vertical rule, which can be changed in thickness by

`\domaingaprule{`⟨*thickness*⟩`}`, e. g. `\domaingaprule{1pt}`.

Also, the colors can be set by

`\domaingapcolors{⟨foreground⟩}{⟨background⟩}`

e. g. `\domaingapcolors{Blue}{Yellow}`.

4.5.3 Hiding, killing, separating and ordering

If one or more sequences from the alignment input file should be used for the calculation of the consensus but it is desired not to display these sequences in the final output use the command `\hideseq{⟨seq1⟩,⟨seq2⟩,...,⟨seq n⟩}`. For consecutive sequence numbers a dash can be used, e. g. `\hideseq{1-3}` instead of `\hideseq{1,2,3}`. Decending series are also permitted, e. g. `\hideseq{3-1}`. This command allows one for example to hide the sequence which has been defined as the consensus sequence with `\constosingleseq`. When all sequences should be hidden, e.g. to show a sequence logo alone, one can simply say `\hideseqs`. This command is reversed by `\showseqs`.

In order to completely exclude sequences the command `\killseq{⟨seq1⟩,⟨seq2⟩,...,⟨seq n⟩}` is provided. Again, for number series the dash can be used (s. a.). The designated sequences are neither displayed nor considered for the calculation of the consensus. This is another possibility to comment out sequences in addition to the use of an exclamation point infront of the `Name:` definition in an MSF-file (see figure on page 41).

The command `\donotshade{⟨seq1⟩,⟨seq2⟩...,⟨seq n⟩}` makes one or more sequences (remember the dash, s. a.) appear unshaded in black letters on white background. This does not influence any other sequences or the consensus calculation.

If a very graphical output of the sequences is desired, the residue symbols or letters can be blanked out by `\hideresidues`. Now, only the shaded boxes are printed. In combination with `\gapchar{rule}` one obtains alignments in a style à la Mondrian. The residues reappear with `\showresidues`.

If an alignment contains members of several subgroups of a protein or a gene family it may be rather helpful to visualize the group divisions by a separation line. Therefore, the command `\separationline{⟨seqref⟩}` is applicable. This command inserts vertical space after the sequence which is refered to by ⟨*seqref*⟩. How much space is inserted is defined by one of the following commands: `\smallsep`, `\medsep` (default) or `\bigsep`. These lengths corre-

spond to the known `\small-`, `\med-` and `\bigskip` commands. With `\vsepspace{`⟨*length*⟩`}` any length with any TeX unit can be assigned, e. g. `\vsepspace{2mm}`.
The sequence order given by the alignment input file is easily reorganized by `\orderseqs{`⟨*seq1*⟩`,`⟨*seq2*⟩`,`. . . `,`⟨*seq n*⟩`}` without the need for editing the alignment input file (which would be a big copy'n'paste job). Make sure that all sequences are assigned in this command. If there are more sequences present than numbers or names in the command an error message will occur. Here also, the dash can be used for sequence number series. Example: `\orderseqs{1-3,6-4,7}` is equivalent to `\orderseqs{1,2,3,6,5,4,7}`. Reordering of sequences only changes the output; all commands using the parameter ⟨*seqref*⟩ are not influenced, because ⟨*seqref*⟩ always corresponds to the appearance in the alignment file. Thus, to completely reverse the order of a five sequence alignment simply type `\orderseqs{5-1}`.

4.5.4 Residues per line and further format settings

By default TeXshade puts the highest possible by five divisible number of residues in one line depending on the document's `\linewidth`. With `\residuesperline{`⟨*number*⟩`}` a new value can be set. If this value exceeds the highest possible number of residues per line it is ignored; lower values are accepted of course. But also in the latter case the number of residues printed per line is rounded such to be divisible by five. To force TeXshade to set lines with exactly the desired number of residues use the asterisk-extended command `\residuesperline*{`⟨*number*⟩`}`. You have to take care yourself of the alignment width after this command, because in this mode TeXshade does not check the length of the lines any more.
TeXshade calculates the dimensions of a shaded box from the width and height of the uppercase letter 'M' and the depth of the lowercase 'g'. Depending on the font used for the sequence residues the box dimensions might not be fully satisfactory. With `\charstretch{`⟨*factor*⟩`}` and `\linestretch{`⟨*factor*⟩`}` the width and height/depth, respectively, of the boxes can be multiplied individually by a ⟨*factor*⟩ to stretch (> 1) or shrink (< 1) the dimensions.
The reserved space for the sequence numbering is set by the command `\numberingwidth{`⟨*n digits*⟩`}`. Here, the default setting is four-digit numbering, i. e. -999 through 9999. If this range is to be changed assign the desired number as parameter ⟨*n digits*⟩, e. g. `\numberingwidth{111111}` reserves space for 6 digit numbering.

The vertical space between the sequence blocks can be controlled by the commands `\smallblockskip`, `\medblockskip` (default setting), `\bigblockskip` or `\noblockskip`. Further, the command `\vblockspace{`⟨*length*⟩`}` allows one to set a defined space length using any TeX unit, e. g. `\vblockspace{0.4in}`.
Two more commands set the space between the sequence blocks to be flexible (`\flexblockspace`) (default) or fixed (`\fixblockspace`). Flexible means, that only the vertical white space between the blocks is kept to the settings by e. g. `\medblockskip`. This results in flexible space between the actual blocks depending on the presence of feature lines. When switching to fixed space the distance of the blocks is kept constant by using more white space between blocks without feature lines. Thus, a difference between flexible and fixed space will only be noticeable when features are used.
The position of the output can be aligned left, right or centered on the page by `\alignment{`⟨*position*⟩`}` with the ⟨*position*⟩ parameter `left`, `center` or `right`.

4.5.5 Fingerprinting

An easy way to gain an overview on complete alignments is provided by displaying a so called alignment 'fingerprint'. In this style the whole sequence can be shown in one line. Due to the lacking space the residue names are hidden and the shaded boxes are reduced to thin vertical colored lines. The command `\fingerprint{`⟨*res. per line*⟩`}` takes one argument stating the desired number of residues per line, e. g. `\fingerprint{1000}`. All TeXshade commands are compatible with `\fingerprint`, i. e. all shading modes are applicable for displaying overviews on similarity or every functional aspect. Also, all kinds of labeling—as described in the following—work with this command.

4.6 Individual shading and labeling of sequence stretches

Computer calculated conservation shading is informative—but even more information can be visualized by additional labeling of positions and regions of interest with different colors, text styles or graphical marks and descriptive text. This is provided by the following TeXshade commands.

4.6.1 Shading of regions and blocks

Besides the shading calculated by TeXshade any region can be additionally shaded with a color specified by the user. This is very useful to highlight secondary protein modification sites such as phosphorylation or glycosylation sites, or longer motifs for example protein/protein interaction sites or protein domains. This is done with the following command:

```
\shaderegion{⟨seqref⟩}{⟨selection⟩}{⟨res.col.⟩}{⟨shad.col.⟩}
```

Here, ⟨*seqref*⟩ refers to the sequence by its name or number within the alignment. The foreground and background colors can be set with the last two parameters. ⟨*selection*⟩ can have three different formats depending on whether (a) the user wants to select the positions manually, (b) the selection should be based on a sequence motif to be found by TeXshade, or (c) TeXshade is supposed to select the residues based on 3D coordinates provided by a PDB file.

(a) To select the residues manually, the user provides a position list of the following format:

```
{⟨start1⟩..⟨stop1⟩,⟨start2⟩..⟨stop2⟩,...,⟨start n⟩..⟨stop n⟩}
```

In order to shade residue number 13 and the region 20–30 of sequence number 1 in red letters on a green background type the following command:

```
\shaderegion{1}{13..13,20..30}{Red}{Green}
```

If the consensus is to be shaded use `consensus` as ⟨*seqref*⟩.

(b) A sequence motif can be given, which will be found and labeled. A simple example selecting all sequence motifs 'NNAD' in sequence '1' would be:

```
\shaderegion{1}{NNAD}{Red}{Green}
```

The definition can further include 'X' for any residue and groups of residues in brackets at uncertain positions. The example below will find all motifs in sequence '1' that start with an asparagine, followed by any two residues, an acidic, a basic residue, again any two residues and finally a glutamine.

```
\shaderegion{1}{NXX[DE][KR]XXQ}{Red}{Green}
```

(c) In order to select positions based on the 3D structure a PDB structure file is required. TeXshade can select residues within a given distance in Å around a point, along a line, or above and below a plane, which are defined by one to three residues. The points can be further specified to be the α-carbon atom, i. e. the protein backbone, or the most distant atom of the sidechain. Accordingly, ⟨*selection*⟩ has one of the formats:

```
{point[⟨dist⟩]:⟨file⟩,⟨num⟩[CA/side]}
{line[⟨dist⟩]:⟨file⟩,⟨num1⟩[CA/side],⟨num2⟩[CA/side]}
{plane[⟨dist⟩]:⟨file⟩,⟨num1⟩[CA/side],⟨num2⟩[CA/side],
                                              ⟨num3⟩[CA/side]}
```

Example: in order to select and shade as above all residues that are within an 8 Å sphere around the α-carbon of residue 81 and the data are provided in the PDB file `1J4N.pdb`, type:

```
\shaderegion{1}{point[8]:1J4N.pdb,81[CA]}{Red}{Green}
```

Example: two points denote a line, hence, give two residues to select everything within 1 Å along the line between the α-carbon of residue 81 and the sidechain of residue 168 with:

```
\shaderegion{1}{line[1]:1J4N.pdb,81[CA],168[side]}
                                                {Red}{Green}
```

Definition of a plane follows the same format but requires three points. If the optional parameters `[\meta{dist}]` and `[CA/side]` are not given, TeXshade assumes `[1]` and `[side]`, respectively.

In case one needs the position numbers of the selected residues for usage in other applications, those can be either printed in the TeX document with `\printPDBlist{`⟨*selection*⟩`}` or shown during the TeX run with `\messagePDBlist{`⟨*selection*⟩`}`. The commands can be used outside of the TeXshade environment.

Both selection formats, i. e. a manually given list and the 3D selection, can be used with `\shadeblock` (see below), `\tintregion`, `\tintblock`, `\emphregion`, `\emphblock`, `\lowerregion`, `\lowerblock`, `\frameblock` (all in 4.6.2), and `\feature` (4.6.3).

In analogy to `\shaderegion` which is restricted to a single sequence, `\shadeblock` shades the corresponding region in all other sequences as well except the consensus. If also the consensus is to be shaded define the region using `consensus` as ⟨*seqref*⟩.

```
\shadeblock{⟨seqref⟩}{⟨selection⟩}{⟨res.col.⟩}{⟨shad.col.⟩}
```

Another option is to change the whole set of shading colors for certain sequence blocks, e. g. from `blues` to `reds` or self-defined color sets (see 4.1). Therefore, the following command was implemented:

`\changeshadingcolors{`⟨*seqref*⟩`}{`⟨*selection*⟩`}{`⟨*name*⟩`}`

Examples:

`\changeshadingcolors{1}{10..50}{reds}`

`\changeshadingcolors{AQP1}{[AS]NKD}{my_set}`

etc.

4.6.2 Emphasizing, tinting, lowercasing, and framing

If it is preferred to keep the calculated shading colors but distinct regions or blocks are yet to be emphasized one can use the following commands to change the font style of such regions:

`\emphregion{`⟨*seqref*⟩`}{`⟨*selection*⟩`}`

and

`\emphblock{`⟨*seqref*⟩`}{`⟨*selection*⟩`}`

For the format possibilities of the ⟨*selection*⟩ parameter please see 4.6.1.
Which style TeXshade uses for emphasizing regions is defined by `\emphdefault{`⟨*style*⟩`}`. Default setting is the *italics* font shape (set by `\emphdefault{it}`). In order to change this setting choose one of the styles `bf, md, up, it, sl, rm, sf, tt`.
Example: `\emphdefault{bf}`

Further, it is possible to tint the region or block in question or to switch the characters to lowercase by using the commands (for example see hydropathy-figure on page 21):

`\tintregion{`⟨*seqref*⟩`}{`⟨*selection*⟩`}`

and

`\tintblock{`⟨*seqref*⟩`}{`⟨*selection*⟩`}`

The level of tinting in the region in question can be set by `\tintdefault{`⟨*level*⟩`}` with `weak`, `normal`, and `strong` as possible ⟨*level*⟩s.

`\lowerregion{`⟨*seqref*⟩`}{`⟨*selection*⟩`}`

and

`\lowerblock{⟨seqref⟩}{⟨selection⟩}`

Another option is to draw a bounding box around the sequence block in question (for an example see diversity mode-figure on page 19) with the command:[25]

`\frameblock{⟨seqref⟩}{⟨selection⟩}{⟨color⟩[⟨length⟩]}`

With the optional parameter the default line thickness of the frame can be changed, example: `\frameblock{1}{10..20,50..70}{Red[2pt]}`

4.6.3 Graphical labeling of sequence features

The `\feature` command is designed to fulfill most needs for the graphical labeling of sequence stretches and the setting of descriptive text. It needs five parameters:

`\feature{⟨position⟩}{⟨seqref⟩}{⟨selection⟩}{⟨labelstyle⟩}{⟨text⟩}`

In the following paragraphs all possible parameter settings of this rather complex but mighty command are discussed in detail. The parameter ⟨*position*⟩ tells TeXshade where to display the feature label, i. e. on the top of the alignment (`top`), or at the bottom (`bottom`). Further, there can be three more feature lines ontop of the top feature line (`ttop`, `tttop`, and `ttttop`) or below the bottom feature line (`bbottom`, `bbbottom`, `bbbbottom`). Thus, up to eight features overlapping in eight different lines may be displayed. Depending on the content of the feature lines the gaps between them might be not satisfactory. Therefore, eight separate commands can be employed to change the space below `ttttop`, `tttop`, `ttop`, or `top` (`\topspace{⟨length⟩}` etc.), and above `bottom`, `bbottom`, `bbbottom`, or `bbbbottom` (`\bottomspace{⟨length⟩}` etc.). Use positive values to further separate the lines, e. g. `\ttopspace{3mm}` or negative values to reduce the space, e. g. `\bottomspace{-0.1in}`.

The argument ⟨*seqref*⟩ and the third parameter containing the ⟨*selection*⟩ of the specified residues are identical to the ones described before in several commands, e. g. `\shaderegion` (4.6.1).

The fourth parameter holds the definition of the label style. There are many possibilities like braces, helices, boxes, arrows, bars, any fill character, bar graphs, color scales or translations of the specified regions.

Braces:

In order to display an over- or underbrace as a label use the parameter

---

[25] Thanks to Alan Robinson for inspiration.

`{brace}`. Depending on the ⟨*position*⟩ (`ttttop`, `tttop`, `ttop`, `top`, `bottom`, `bbottom`, `bbbottom`, or `bbbbottom`) the respective brace is displayed. The standard color of braces is black. It can be changed by an optional parameter directly after the definition of the symbol, e. g. `{brace[Red]}`.

Protein α-Helices:
The parameter `{helix}` will plot a symbolized α-helix as a label. The standard color of the helix spiral is black. It can be changed by an optional parameter directly after the definition of the symbol, e. g. `{helix[Red]}`.

Filling a stretch with a symbol:
A region can be filled with any character for labeling purposes using the parameter `{fill:`⟨*symbol*⟩`}`. The ⟨*symbol*⟩ is freely selectable; the usage is like in `\gapchar` (4.5.1). Do not use spaces before or after the expression ⟨*symbol*⟩; this will shift the symbols to the respective direction. The standard color of the fill symbol is black. The textcolor and optionally the background can be changed by a parameter directly after the definition of the symbol, e. g. `{fill:$\bullet$[Red,LightGray]}` for a red symbol on a light gray background.
Special non-text mode characters, e. g. `\dag`, can be used in the `\feature` command by using the math version of those symbols between `$`-signs. The following quite common symbols have a math equivalent[26]:

symbol	*command*	*description*
†	`$\dagger$`	dagger
‡	`$\ddagger$`	double dagger
¶	`$\mathparagraph$`	paragraph mark
§	`$\mathsection$`	section mark
$	`$\mathdollar$`	dollar
{	`$\lbrace$`	left brace
}	`$\rbrace$`	right brace

Labeling restriction or protease cutting sites:
If a label is needed that points between two residues, e. g. for showing restriction sites, use the feature style `{restriction[`⟨*color*⟩`]}`. This will show a filled triangle with

---

[26] Thanks to Darrell Conklin for reporting this problem

the tip placed at the right edge of the stated residue position, e. g. `\feature{top}{1}{25..25}{restriction[Blue]}{EcoR I}`.

Boxes:
Boxed text is printed using the parameter `{box:`⟨*text*⟩`}`. By default black letters in a white framed box are displayed. In order to change these colors optional parameters can be included in the argument:

`{box[`⟨*framecolor,boxcolor*⟩`][`⟨*length*⟩`]:`⟨*text*⟩`[`⟨*textcolor*⟩`]}`.

If the box frame and fill colors are the same it is sufficient to use only this one color as an argument in the command. The optional parameter ⟨*length*⟩ defines the thickness of the box frame. If this parameter is not set in the command the value from the `\featurerule{`⟨*length*⟩`}` command (see below) is used.

Examples:

```
{box[Blue]:$\alpha$-helix[Yellow]}
{box[Blue,Red]:$\alpha$-helix[Yellow]}
{box[Blue,Red][2pt]:$\alpha$-helix[Yellow]}
```

Horizontal bars and arrows:
For displaying bars and arrows a selection scheme consisting of three consecutive characters is used as the ⟨*labelstyle*⟩ parameter. Each bar or arrow is defined by its left end, the center part, and the right end. The following table gives some examples for the construction of arrows and bars.

center left end ↓ right end	
`---`	plain bar
`===`	double bar
`-->`	right arrow
`'->`	right arrow with up hook
`<-|`	left *maps to* arrow
`<-o`	left arrow with ball at right end
`<=>`	double arrow, two heads
`,-,`	plain bar with down hooks
`|=|`	double bar with vertical ends
`S-S`	labels disulfide bridges

Combinations of the left-end-characters (`-=<',|o`), the center-characters (`-=`), and the right-end-characters (`-=>',|o`) are allowed

and produce the desired arrow or bar. Adding an underscore in the definition for top feature hooks, e.g. `{_,-,}` makes the hooks fully reach down to the alignment. The color is changed as described above. The thickness can be generally set by the separate command `\featurerule{`⟨*length*⟩`}` with any TeX measure as ⟨*length*⟩, e. g. `\featurerule{3pt}`. This value is then used for all arrows, bars, and boxes (see above) throughout the alignment. If an individual thickness for a particular arrow should be set one can add an optional parameter to the ⟨*labelstyle*⟩ parameter, e.g. `{o->[Red][1mm]}`. Similar to the boxes described above, a text can be put on the arrow or bar, e. g. `{<->[Red][1mm]:$\beta$-sheet[Blue]}`.
In very old TeXshade versions before v1.9, the original LaTeX-arrows were used. These have been replaced by more modern looking arrows with scalable line thickness. If the classical look is requested, use `v` instead of `<` or `>` in the arrow definition, e. g. `{--v}`, to get them back. The new arrow style makes use of of the AMS math symbol font (amssymb.sty). Thus, in order to display the arrow heads correctly make sure that this style is present on your system (usually it is in a common LaTeX installation).

Sequence translations:
With the option `{translate}`, sequence stretches can be translated from nucleotide to peptide sequences as well as backtranslations from peptide to nucleotide sequences are possible. An optional color can be stated; for translated peptide sequences a background color can be set in addition `[textcolor(,bgcolor)]`.
Default setting for the translations is the standard genetic code. The codons can be re-defined by `\codon{`⟨*amino acid*⟩`}{`⟨*triplet1, . . . , triplet n*⟩`}`. Replace ⟨*amino acid*⟩ by the single letter code of the amino acid to be defined and add a list of triplets for this residue. Example definition for the amino acid *alanine*:

```
\codon{A}{GCA,GCG,GCC,GCT,GCU,GCN}
```

Note the last triplet in the list. It contains an ambiguity code `N` which stands for *any* nucleotide. This triplet has been added at the last position because the last triplet is used for the generation of the backtranslated nucleotide sequence from a peptide. Two files are included in the TeXshade distribution as examples (`standard.cod, ciliate.cod`). If you want to define a new genetic code store your commands in a file like the examples. Such files with the suffix `.cod` can be loaded in the TeXshade environment by `\geneticcode{`⟨*filename*⟩`}`, e. g. `\geneticcode{ciliate}`. Do not designate the suffix `.cod` in

⟨*filename*⟩. Please note, when inspecting the example files, that only the exchanges compared to the standard code need to be defined in a new genetic code file.
When DNA sequences are translated to protein the resulting amino acids are aligned to the second nucleotide of each triplet. It is more difficult to produce a satisfactory display of backtranslated nucleotide sequences due to the lack of space. You need thrice as much space than the original peptide sequence, because single letter amino acid code is translated to a triplet code. Therefore, the user can choose from five display styles for backtranslations depending on personal preferences:

`\backtranslabel[`⟨*size*⟩`]{`⟨*style*⟩`}`, with

`{`⟨*style*⟩`}` = `{horizontal}`
= `{alternating}`
= `{zigzag}`
= `{oblique}`
= `{vertical}`

⟨*size*⟩ can be any TeX size from `tiny` up to `Huge`, but `tiny` is recommended (and default setting). Translations can be colored as all other labels, see above.

Sequence complement:
Similar to translations above for nucleotide sequences the complement sequence can be displayed using `[complement]` as a feature option. Text and background colors can be set by the optional parameter `[textcolor(,bgcolor)]`. The complement sequence can be switched to lower case by a second optional parameter `[lower]`, e.g. `\feature{bottom}{1}{1..99}{complement[Blue,Red][lower]}{}`.

Bar graphs and color scales:
Sequence related numeral data, such as hydropathy or solvent accessibility data etc., can be shown in a feature line as simple bar graphs, '`bar[`⟨*min*⟩`,`⟨*max*⟩`]:`', stacked bars '`stackedbars[`⟨*min*⟩`,`⟨*max*⟩`]:`', or color scales '`color[`⟨*min*⟩`,`⟨*max*⟩`]:`'. The data are (a) pre-defined or calculated by TeXshade due to amino acid properties or conservation, (b) are provided in a separate file or (c) may be entered by hand in the `\feature` command.
(a) Currently, three different properties can be plotted, i.e. `hydrophobicity`, `molweight`, and `charge`. Further, the level of sequence conservation at the given protein sequence stretch can be

shown (`conservation`). See 4.3.1 for selecting an appropriate *residue weight table.*
(b) The format of a data file for simple (single) bar graphs or color scales must contain one value per line. For stacked bars, a series of comma-separated values must appear in each line; for the latter, a residue number can be assigned as the first number in each line followed by a colon, e.g.:

```
    45: 62.2, -34, -21, 55, 25.4
```

See provided example file `bars.txt`. Numbers and the Java-typical 'NaN' for 'Not a Number' are permitted. Comments are allowed, because TeXshade ignores all lines starting with a letter except 'NaN' lines (avoid '`-`' as the first character of a comment line as this is interpreted as a negative number). TeXshade will read this file and determine the minimal and maximal values. These data are then normalized for plotting. Due to TeX's limited calculation capabilities no values above 10 737 are allowed and the difference between minimum and maximum must not exceed this very number. Values below 0.001 may be susceptible to major rounding errors. Thus, try to provide your data already normalized to moderate scales, e.g. $0.0-1.0$ or $-100-100$.
(c) Data can be entered directly in the `\feature` command. For simple bars, this is a comma-separated series of values; for stacked bars, values of a stack must appear in parantheses, e.g. `(43.3,11.9,-0.8,2.9)`. Make sure that each stack of bars contains the same number of values.
For (b) and (c), the range to be plotted can be set by hand as an optional parameter in the `\feature` command. This can be necessary when the data file contains values between e.g. -0.44 and 0.87. Without help TeXshade will assume -0.44 as minimum and 0.87 as maximum. But if the actual range to be plotted should be -1.0 to 1.0, this needs to be set manually, see examples below. Be aware of the fact, that if you define a scale by hand, which is more narrow than the values of the input, this will stretch the bars accordingly. It is not recommended to use this method for stretching bars vertically. Instead another command has been introduced. The plotted bars can be stretched by a factor if the appearance is not as desired: `\bargraphstretch[`⟨*position*⟩`]{`⟨*factor*⟩`}`. Here, the factor is multiplied with the bar length, e.g `\bargraphstretch{2}` will double the height of all bar graphs, `\bargraphstretch[top]{0.5}` will make the one in the `top` feature row half as high. Similarly, color scales can be stretched vertically with `\colorscalestretch[`⟨*position*⟩`]{`⟨*factor*⟩`}`.

The default color of bar graphs is gray and can be changed by an optional parameter at the end of the `label` definition. Further, an optional background color can be chosen for the bars. Doing so will visualize the maximal bar extension.
Default for color scales is a 5% gray scale from very light gray to black (`WhiteBlack`). More colorful scales have been implemented, i.e. `BlueRed`, `RedBlue`, `GreenRed`, `RedGreen`, `ColdHot` and `HotCold`, the latter two being particularly useful for ranges from negative to positive values. Further, a scale called `T-Coffee` is available if `T-Coffee` shading information has been imported as the `\shadingmode` 4.1.
The general format of these feature label definitions are as follows:

`{bar[`⟨*min*⟩`,`⟨*max*⟩`]:`⟨*properties/file/data*⟩`[`⟨*color(,bgcolor)*⟩`]}`
`{stackedbars[`⟨*min*⟩`,`⟨*max*⟩`]:`⟨*file/data*⟩`[`⟨*colors/scale(,bgcolor)*⟩`]}`
`{color[`⟨*min*⟩`,`⟨*max*⟩`]:`⟨*properties/file/data*⟩`[`⟨*scale*⟩`]}`

Some examples:

```
{bar:conservation}
{bar:conservation[T-Coffee]}
{bar:hydrophobicity}
{bar:charge[Red]}
{bar:molweight[Red,Gray10]}
{bar:10,20,30,40,50[Red]}
{bar[-20,40]:-10,0,10,20,30[Red,Gray10]}
{bar:data.txt}
{bar[-10,10]:data.txt[Red,Gray10]}
{stackedbars[-20,40]:(-10,-5,1),(0,5,30),(8,20,4)[Red,Blue,Green]}
{stackedbars:data.txt}
{stackedbars[-10,10]:data.txt[HotCold,Gray10]}
{color:conservation[BlueRed]}
{color:conservation[T-Coffee]}
{color:hydrophobicity[GreenRed]}
{color:charge}
{color:molweight}
{color[-0.5,1]:0.4,0.2,-0.3,-0.1,0.9,0,8,-0.5[RedBlue]}
{color[-10,10]:data.txt[ColdHot]}
{color[-0.1,0.1]:otherdata.txt[ColdHot]}
```

See also the example output in section 1.6 on page 26.

Plotting 'frustratometer' data

From the abstract by Parra *et al.* [10]: "The protein frustratometer is

an energy landscape theory-inspired algorithm that aims at localizing and quantifying the energetic frustration present in protein molecules. Frustration is a useful concept for analyzing proteins' biological behavior. It compares the energy distributions of the native state with respect to structural decoys. The network of minimally frustrated interactions encompasses the folding core of the molecule. Sites of high local frustration often correlate with functional regions such as binding sites and regions involved in allosteric transitions."
The 'frustrometer' server provides several types of data as an output. The ASCII-files ending with '`_adens`' can be used by TeXshade for plotting relative values for minimally, neutrally and maximally frustrated densities. Have a look at the paper and the provided sample file 'frustr.txt'. The data will be displayed within a `\feature` line by using the style:

`{frustratometer:`⟨*filename*⟩`}` (see example on p. 26)

Standard colors for the bars are green/gray/red but can be changed by adding an optional argument in the style definition:

`[`⟨*mincolor*⟩`,`⟨*neutralcolor*⟩`,`⟨*maxcolor*⟩`]`

The residue numbers are listed in the first column of the data files and are used by TeXshade for assigning the frustration values to the alignment.

No graphical label
If no graphical label is wanted the fourth parameter of `\feature` can be empty braces.

Label description
Finally, the fifth parameter of the `\feature` command contains the descriptive text for the labeled region. The text can contain symbols and math chars. Again, the color can be set by an optional parameter appended to the text. For how to change the font size of text or symbols in the feature style line (`featurestyles`) or the in descriptive text line (`features`) see section 4.9.1, page 83.

Naming the feature lines
Names can be shown for each row of the top/bottom feature lines and descriptive texts, which is printed together with the sequence names at the left or right side of the alignment, i. e.

`\showfeaturename{`⟨*ttttop...bbbbottom*⟩`}{`⟨*name*⟩`}`,

`\showfeaturestylename{`⟨*ttttop...bbbbottom*⟩`}{`⟨*name*⟩`}`

`\hidefeaturename{`⟨*ttttop...bbbbottom*⟩`}`

`\hidefeaturestylename{`⟨*ttttop...bbbbottom*⟩`}`

`\hidefeaturenames`, and `\hidefeaturestylenames`.

Using `\showfeaturename` will print the name in the same line as the descriptive text of the feature whereas `\showfeaturestylename` will put the name in the same line as the feature symbols.
The color of such names can be generally changed with

`\featurenamescolor{`⟨*color*⟩`}` and

`\featurestylenamescolor{`⟨*color*⟩`}`

or individually with

`\featurenamecolor{`⟨*ttttop...bbbbottom*⟩`}{`⟨*color*⟩`}` and

`\featurestylenamecolor{`⟨*ttttop...bbbbottom*⟩`}{`⟨*color*⟩`}`

See section 5 for how to select colors in TEXshade. Font styles can be set as usual (see section 4.9.1), e. g.

`\setsize{featurenames}{large}` or `\featurestylenamesrm` etc.

Examples for the appearance of features are given in the overview section (1), see:

similarity mode (1.5.2): fill-character; here, only one position is labeled. It is also possible to label a longer stretch, then, the character is printed several times to fill the specified region.

```
\feature{top}{1}{93..93}{fill:$\downarrow$}{first...}
\feature{bottom}{1}{98..98}{fill:$\uparrow$}{second...}
```

T-Coffee mode (1.5.3): `T-Coffee` color scale

```
\feature{top}{1}{30..63}{color:conservation[T-Coffee]}{}
\showfeaturestylename{bottom}{cons}
```

diversity mode (1.5.4): frames, text only

```
\feature{top}{1}{77..109}{}{AQP2 species variants}
\frameblock{1}{82..82,106..106}{Red[1pt]}
```

functional mode (1.5.5): bar graph, color scale, tinting, box, arrow, translation, brace, helix

```
\feature{top}{3}{153..165}
        {bar[-50,50]:-50,-45,-40,...,40,45,50}{}
```

```
\feature{top}{3}{167..186}
        {color:5,10,15,...,90,95,100[ColdHot]}{}
```

```
\feature{top}{1}{158..163}{brace}{tinted}
```

```
\tintblock{1}{158..163}

\feature{top}{1}{138..157}
        {box[Blue,Red][0.5pt]:$\alpha$-helix[Yellow]}
        {transmembrane domain 4}
\feature{top}{1}{164..170}{o->[Red]}{trans. dom. 5}
\feature{top}{1}{158..163}{translate[Blue]}{}
\backtranslabel{oblique}
\feature{bottom}{1}{-83..-1,424..525}
        {complement[LightBlue][lower]}{}
\feature{bottom}{1}{158..163}
        {brace[Blue]}{loop D[Blue]}

\feature{top}{1}{138..157,164..170}{helix}{membr.}
\feature{top}{1}{158..163}{---}{loop}
\featurerule{1mm}
```

bar graphs and color scales (1.6): local frustration, sequence conservation, charge, molecular weight, hydrophobicity, stacked bars

```
\feature{tttop}{1}{138..170}{frustratometer:frustr.txt}{}
\feature{ttop}{1}{138..170}{bar:conservation}{}
\feature{top}{1}{138..170}{color:charge}{}
\feature{bottom}{1}{138..170}{color:molweight[ColdHot]}{}
\feature{bbottom}{1}{138..170}{bar:hydrophobicity[LightBrown,Gray10]}{}
\feature{bbbottom}{1}{138..170}{stackedbars:bars.txt[BlueRed,Gray10]}{}
```

4.6.4 Including secondary structure information

The DSSP [12], STRIDE [13], PHD [14] and HMMTOP [15] algorithms produce secondary protein structure predictions. PHD files contain both, secondary structure information and topology data. This information can be displayed in an alignment by one of the commands:

`\includeDSSP`	sec. structure calculated by DSSP
`\includeSTRIDE`	sec. structure calculated by STRIDE
`\includePHDsec`	sec. structure calculated by PHD
`\includePHDtopo`	topology data calculated by PHD
`\includeHMMTOP`	topology data calculated by HMMTOP

The syntax is `\includeDSSP{`⟨*seqref*⟩`}{`⟨*filename*⟩`}`, with `seqref` indicating the number or name of the sequence for which the secondary structure data is calculated and `filename` designating the corresponding structure file to be included.

Several types of secondary structures are predicted by these programs; in order to designate them in TeXshade use the names from the right column:

secondary structure	designation
DSSP and STRIDE	
4-helix (α-helix)	`alpha`
isolated β-bridge	`bridge`
extended strand (β-strand)	`beta`
3-helix (3_{10}-helix)	`3-10`
5-helix (π-helix)	`pi`
H-bonded turn	`turn`
PHDsec	
helix	`alpha`
sheet	`beta`
PHDtopo and HMMTOP	
internal region	`internal`
external region	`external`
transmembrane domain	`TM`

By default all three types of helices and the strands are displayed whereas turns and bridges are skipped. If it is desired to shown them as well, call for example `\shownonDSSP{bridge,turn}`. In analogy to this example all structure features can be activated in DSSP, STRIDE, PHDsec, PHDtopo and HMMTOP. In order to hide certain structure types use for example `\hideonDSSP{3-10,pi}`.

The DSSP format has two columns of sequence numberings. The first column is consecutive, whereas the second column contains the actual sequence numbering. This can be different from the first column when sequence parts are missing in the DSSP file. One can choose which column will be read by TeXshade by ‘`\firstcolumnDSSP`’ and `\secondcolumnDSSP`’. The second column is still default.

The HMMTOP algorithm can present its results as plain text or as HTML—plain text needs to be selected here. Further, the output can be formatted in a single line or in an extended form (see the HMMTOP documentation). Both can be read and interpreted by TeXshade. Importantly, HMMTOP files can contain topology predictions of multiple sequences. TeXshade tries to find the correct data based on the respective sequence name. If the sequence name is not found in the file, the first topology data is used. Using an optional parameter (number of the prediction in the file or name) one can define which data from the file is to be used:

`\includeHMMTOP{`⟨*seqref in texshade*⟩`[`⟨*seqref in file*⟩`]}{`⟨*filename*⟩`}`

PHD predictions: when starting the PHD software do not restrict the prediction to secondary structure or topology alone. This leads to changes in the PHD output file which are not correctly interpretable by TeXshade due to ambiguities. There is no way around it—thus, run the full prediction.

Now, some information on how TeXshade extracts and displays secondary structure features. In short, it is a two step process. First, TeXshade analyzes the secondary structure file and extracts all necessary data. This data is converted into a format which is readable and processable by TeXshade using the `feature` command (see 4.6.3). This command allows one to label sequence stretches graphically. For a detailed explanation see the indicated reference. A list of feature commands is saved in a file with the ending '`.sec`' for DSSP, STRIDE and PHDsec or '`.top`' for PHDtopo. Then, in a second step, this file is loaded again and executed. When TeXshade encouters this file a second time, i. e. in a second TeX run, it uses the already existing file for the output. The advantage of this method is its flexibility because the feature file can be edited in the meantime. Thus, the user has the ability to change the computer-generated file according to his personal needs. On the other hand, one can force TeXshade to write a new file every time by the optional argument `[make new]` in the include command, e. g. `\includePHDsec[make new]{1}{AQP.phd}`.

Finally, the appearance of the feature labels can be assigned by the command

`\appearance{`⟨*filetype*⟩`}{`⟨*type*⟩`}{`⟨*position*⟩`}{`⟨*labelstyle*⟩`}{`⟨*text*⟩`}`.

Here, ⟨*filetype*⟩ stands for one of the following secondary structure file types: `DSSP`, `STRIDE`, `PHDsec`, `PHDtopo` or `HMMTOP` and ⟨*type*⟩ designates the secondary structure type as shown in the right column of the table above. The other arguments ⟨*position*⟩, ⟨*labelstyle*⟩ and ⟨*text*⟩ are almost as described in 4.6.3. One further possibility is to include internal counters for each secondary structure type. Just add one of the following commands to the text in the feature description.

counter	*display*
`\numcount`	1, 2, 3 . . .
`\alphacount`	a, b, c . . .
`\Alphacount`	A, B, C . . .
`\romancount`	i, ii, iii . . .
`\Romancount`	I, II, III . . .

Examples:

```
\appearance{DSSP}{alpha}{ttop}
          {-->}{$\alpha$-helix~\Alphacount}
\appearance{PHDtopo}{TM}{bottom}
          {box[Blue]:TM\numcount[Yellow]}{}
```

4.7 Displaying and building legends

For each predefined shading mode TeXshade can print an appropriate legend to explain the used shading colors. The commands `\showlegend` and `\hidelegend` display or clear the legend at the end of the alignment. The legend is displayed by default beneath the first residue of the last alignment line. The location can be changed by `\movelegend{`⟨*x-offset*⟩`}{`⟨*y-offset*⟩`}`. Both parameters require a TeX length, e. g. `\movelegend{5cm}{-2cm}` moves the legend 5 cm to the right and 2 cm up.

The language for the descriptions is english by default; if the `\german.sty` package is active legend texts are in german. So far, german, spanish and english are implemented. With the commands `\germanlanguage`, `\spanishlanguage` and `\englishlanguage` switching between the languages is made possible. For the addition of other languages contact me. Finally, the color of the describing legend texts can be set with the command `\legendcolor{`⟨*color*⟩`}`.

User defined legends are easily built with the following command `\shadebox{`⟨*color*⟩`}`. Use this command outside the TeXshade environment, e. g. in the text or in the caption. As ⟨*color*⟩ any color can be designated (see section 5) or one of the following parameters:

- `nomatch` = the color used for nonmatching residues
- `similar` = the color used for similar residues
- `conserved` = the color used for conserved residues

- `allmatch` = the color used for highly conserved residues (if `\allmatchspecial` is active)

The command simply prints a shaded box in the specified color then a describing text can be appended. Examples:

```
\shadebox{nomatch}---nonmatching residues
\shadebox{similar}: similar residues
\shadebox{conserved}~conserved residues
\shadebox{Yellow}\quad PKA phosphorylation sites
```

4.8 Adding captions to the alignment

Since TeXshade v1.5 captions can be added to the alignment. So far, captions were difficult to use when the alignment was bigger than one page and therefore did not fit into a figure environment. The TeXshade captions behave exactly as normal figure captions. They adopt their style, use the figure counter number and appear in the list of figures as any other figure.
The usage is slightly different from normal captions but intuitive:

```
\showcaption[⟨position⟩]{⟨text⟩}
```

The optional ⟨*position*⟩ tells TeXshade to put the caption on `top` or at the `bottom` of the alignment. If nothing is stated here the caption will appear at the bottom. The parameter ⟨*text*⟩ just holds the caption text as in the normal `\caption`. The command can be used at any position within the `texshade` environment. A simple example would be:

```
\showcaption{A beautiful \TeXshade{} alignment.}
```

In order to show a short version of the caption in the "List of Figures" the `\shortcaption{`⟨*short caption text*⟩`}` command can be used.

4.9 Font handling

4.9.1 Changing font styles

The font styles for the numbering, the sequence names, the sequence residues, the descriptive feature texts and the legends can be changed by several commands.

```
\setfamily{⟨text⟩}{⟨family⟩}
\setseries{⟨text⟩}{⟨series⟩}
```

```
\setshape{⟨text⟩}{⟨shape⟩}
\setsize{⟨text⟩}{⟨size⟩}
```

Possible ⟨*text*⟩ parameters are `numbering`, `names`, `residues`, `features`, `featurestyles`, `hideblock`, `ruler`, and `legend`. To address all characters in the output use `all`, e.g. `\setsize{all}{small}` sets the character sizes of the residues, names, numbering, features, etc. to `small`.

The style is set by the second parameter:

command	⟨*2. parameter*⟩	
`\setfamily`	`rm`	modern roman font family
	`sf`	sans serif font family
	`tt`	typewriter font family
`\setseries`	`bf`	bold face series
	`md`	normal series
`\setshape`	`it`	italics shape
	`sl`	slanted shape
	`sc`	small capitals shape
	`up`	upright shape
`\setsize`	`tiny`	the known TEX sizes
	`scriptsize`	
	`footnotesize`	
	`small`	
	`normalsize`	
	`large`	
	`Large`	
	`LARGE`	
	`huge`	
	`Huge`	

Example: `\setfamily{features}{it} \setseries{features}{bf}`

With `\setfont{⟨text⟩}{⟨family⟩}{⟨series⟩}{⟨shape⟩}{⟨size⟩}`

all four font attributes of one ⟨*text*⟩ can be changed simultaneously. The order of the parameters is as indicated.

Example: `\setfont{features}{rm}{it}{bf}{normalsize}`

Short commands are provided to change single font attributes quickly:

```
\featuresrm   \featurestiny
\featuressf   \featuresscriptsize
\featurestt   \featuresfootnotesize
```

```
\featuresbf   \featuressmall
\featuresmd   \featuresnormalsize
\featuresit   \featureslarge
\featuressl   \featuresLarge
\featuressc   \featuresLARGE
\featuresup   \featureshuge
              \featuresHuge
```

Corresponding sets are provided for the numbering (`\numberingrm` etc.), featurestyles (`featurestylesrm` etc.), names (`\namesrm` etc.), featurenames (`\featurenamesrm` etc.), featurestylenames (`\featurestylenames` etc.), residues (`\residuesrm` etc.), hideblock labels (`hideblockrm` etc.), rulers (`\rulerrm` etc.), and rulernames (`\rulernamerm` etc.), and legend texts (`legendrm` etc.).

4.9.2 Using PostScript fonts

As already mentioned TeXshade makes intensive use of PostScript for shading. Now, that PostScript output is active anyway, including PostScript fonts is very easy. Just declare in the document header

`\usepackage{`⟨*PS-font*⟩`}`.

The typewriter font of TeX is always a topic of discussions. By including the package `\usepackage{courier}` TeX's typewriter font is replaced by the widely accepted Courier. Have a look into the directory `..texinputs:latex:psnfss`; there, some styles are located which exchange the common TeX fonts by PostScript fonts, e. g. `avant.sty`, `bookman.sty`, `chancery.sty`, `courier.sty`, `helvet.sty` or `utopia.sty`. Depending on the style used the `\rmdefault`-, `\sfdefault`-, and `\ttdefault` fonts are substituted partly or completely. Thus, `courier.sty` for instance exchanges only the typewriter font, whereas `bookman.sty` sets Bookman as `\rmdefault`, Avantgarde as `\sfdefault` and Courier as `\ttdefault`.
For further information see Tomas Rokicki's `dvips` manual [16].

4.10 Goodies

The following commands give information on sequence properties, such as molecular weight, charge or similarity data. They can be used outside the `texshade` environment directly in the document or in a caption text.

4.10.1 Molweight and charge

During the process of sequence setting TeXshade sums up the molecular weight and charge of the aligned proteins. This data can be accessed by the following commands.

`\molweight{`⟨*seqref*⟩`}{`⟨*Da/kDa*⟩`}`
`\charge{`⟨*seqref*⟩`}{`⟨*i/o/N/C*⟩`}`

The first parameter ⟨*seqref*⟩ selects the sequence. The second parameter in the `\molweight` command allows one to switch the units between Dalton (`Da`) and kilo-Dalton (`kDa`). The `\charge` command needs the second parameter for the correct consideration of the charged protein termini. Thus, '`i`' refers to internal sequences (omitting the charged N- and C-termini), '`o`' to the overall charge (including the termini), '`N`' to N-terminal sequence parts, and '`C`' to the C-terminal end of a protein.

Example: Charge: `\charge{1}{o}`; Weight: `\molweight{1}{Da}`

4.10.2 Similarity/identity data and tables

The degree of similarity and identity in percent for any two sequences in the displayed alignment section can be read out with the commands `\percentsimilarity{`⟨*seqref1*⟩`}{`⟨*seqref2*⟩`}` and `\percentidentity{`⟨*seqref1*⟩`}{`⟨*seqref2*⟩`}`.
Using the example alignment on page 28 and typing outside the `texshade` environment in the document text the following phrase:

```
AQP1 and AQP2 share a sequence similarity
of \percentsimilarity{AQP1.pro}{AQP2.pro}\%
```

will result in the text:

AQP1 and AQP2 share a sequence similarity of 69.6%

Likewise, `\percentidentity{1}{2}` will give the value `48.4`; note that sequences can be referred to by their number or their assigned name. The percent value is calculated by dividing the number of identical or similar positions, respectively, by the total of non-gap positions shared by both sequences. Here, only the part of the alignment is taken into account that is actually displayed. Two residues are considered similar when this is defined by the command `\pepsims` (see page 47).

A full similarity/identity table showing values for all sequences of the alignment can be set using `\similaritytable`. The labels and number format will be adjusted according to the language settings (4.7).

Example (see page 28):

```
\begin{center}

  \similaritytable

\end{center}
```

The command generates a valid LaTeX `tabular` environment, which can be embedded into a `table` environment, e.g.

```
\begin{table}[htdp]
\caption{Text ...}
\begin{center}

  \similaritytable

\end{center}
\end{table}
```

5 The PostScript color selection scheme

PostScript provides 64 standard colors. All these colors are predefined in the `color.sty`. Each color has a pictorial name such as `Bittersweet` and a distinct composition, e. g. 0% cyan + 75% magenta + 100% yellow + 24% black—the so-called CMYK scheme. TeXshade enhances this color scheme by gray scales in 5% steps. The following colors and grays can be used in TeXshade by simply declaring the name of the color in the respective command, e. g. `\consensuscolors`:

name	*CMYK*	*name*	*CMYK*
●GreenYellow	0.15,0,0.69,0	●Yellow	0,0,1,0
●Goldenrod	0,0.10,0.84,0	●Dandelion	0,0.29,0.84,0
●Apricot	0,0.32,0.52,0	●Peach	0,0.50,0.70,0
●Melon	0,0.46,0.50,0	●YellowOrange	0,0.42,1,0
●Orange	0,0.61,0.87,0	●BurntOrange	0,0.51,1,0
●Bittersweet	0,0.75,1,0.24	●RedOrange	0,0.77,0.87,0
●Mahagony	0,0.85,0.87,0.35	●Maroon	0,0.87,0.68,0.32
●BrickRed	0,0.89,0.94,0.28	●Red	0,1,1,0
●OrangeRed	0,1,0.50,0	●RubineRed	0,1,0.13,0
●WildStrawberry	0,0.96,0.39,0	●Salmon	0,0.53,0.38,0
●CarnationPink	0,0.63,0,0	●Magenta	0,1,0,0
●VioletRed	0,0.81,0,0	●Rhodamine	0,0.82,0,0
●Mulberry	0.34,0.90,0,0.02	●RedViolet	0.07,0.90,0,0.34
●Fuchsia	0.47,0.91,0,0.08	●Lavender	0,0.48,0,0
●Thistle	0.12,0.59,0,0	●Orchid	0.32,0.64,0,0
●DarkOrchid	0.40,0.80,0.20,0	●Purple	0.45,0.86,0,0
●Plum	0.50,1,0,0	●Violet	0.79,0.88,0,0
●RoyalPurple	0.75,0.90,0,0	●BlueViolet	0.86,0.91,0,0.04
●Periwinkle	0.57,0.55,0,0	●CadetBlue	0.62,0.57,0.23,0
●CornflowerBlue	0.65,0.13,0,0	●MidnightBlue	0.98,0.13,0,0.43
●NavyBlue	0.94,0.54,0,0	●RoyalBlue	1,0.50,0,0
●Blue	1,1,0,0	●Cerulean	0.94,0.11,0,0
●Cyan	1,0,0,0	●ProcessBlue	0.96,0,0,0
●SkyBlue	0.62,0,0.12,0	●Turquoise	0.85,0,0.20,0
●TealBlue	0.86,0,0.34,0.02	●Aquamarine	0.82,0,0.30,0
●BlueGreen	0.85,0,0.33,0	●Emerald	1,0,0.50,0
●JungleGreen	0.99,0,0.52,0	●SeaGreen	0.69,0,0.50,0
●Green	1,0,1,0	●ForestGreen	0.91,0,0.88,0.12
●PineGreen	0.92,0,0.59,0.25	●LimeGreen	0.50,0,1,0
●YellowGreen	0.44,0,0.74,0	●SpringGreen	0.26,0,0.76,0
●OliveGreen	0.64,0,0.95,0.40	●RawSienna	0,0.72,1,0.45
●Sepia	0,0.83,1,0.70	●Brown	0,0.81,1,0.60
●Tan	0.14,0.42,0.56,0		
White (Gray0)	0,0,0,0	●Black (Gray100)	0,0,0,1
●Gray5	0,0,0,0.05	●Gray10	0,0,0,0.10
●Gray15	0,0,0,0.15	●Gray20	0,0,0,0.20

●Gray25	0,0,0,0.25	●Gray30	0,0,0,0.30
●LightGray	0,0,0,0.33	●Gray35	0,0,0,0.35
●Gray40	0,0,0,0.40	●Gray45	0,0,0,0.45
●Gray50	0,0,0,0.50	●Gray	0,0,0,0.50
●Gray55	0,0,0,0.55	●Gray60	0,0,0,0.60
●Gray65	0,0,0,0.65	●DarkGray	0,0,0,0.66
●Gray70	0,0,0,0.70	●Gray75	0,0,0,0.75
●Gray80	0,0,0,0.80	●Gray85	0,0,0,0.85
●Gray90	0,0,0,0.90	●Gray95	0,0,0,0.95
●LightGreenYellow	0.08,0,0.35,0	●LightYellow	0,0,0.50,0
●LightGoldenrod	0,0.05,0.42,0	●LightDandelion	0,0.15,0.42,0
●LightApricot	0,0.16,0.26,0	●LightPeach	0,0.25,0.35,0
●LightMelon	0,0.23,0.25,0	●LightYellowOrange	0,0.21,0.50,0
●LightOrange	0,0.31,0.44,0	●LightBurntOrange	0,0.26,0.50,0
●LightBittersweet	0,0.38,0.50,0.12	●LightRedOrange	0,0.39,0.44,0
●LightMahagony	0,0.43,0.44,0.18	●LightMaroon	0,0.44,0.34,0.16
●LightBrickRed	0,0.45,0.47,0.14	●LightRed	0,0.50,0.50,0
●LightOrangeRed	0,0.50,0.25,0	●LightRubineRed	0,0.50,0.07,0
●LightWildStrawberry	0,0.48,0.20,0	●LightSalmon	0,0.27,0.19,0
●LightCarnationPink	0,0.32,0,0	●LightMagenta	0,0.50,0,0
●LightVioletRed	0,0.40,0,0	●LightRhodamine	0,0.41,0,0
●LightMulberry	0.17,0.45,0,0.01	●LightRedViolet	0.04,0.45,0,0.17
●LightFuchsia	0.24,0.46,0,0.04	●LightLavender	0,0.24,0,0
●LightThistle	0.06,0.30,0,0	●LightOrchid	0.16,0.32,0,0
●LightDarkOrchid	0.20,0.40,0.10,0	●LightPurple	0.23,0.43,0,0
●LightPlum	0.25,0.50,0,0	●LightViolet	0.40,0.44,0,0
●LightRoyalPurple	0.38,0.45,0,0	●LightBlueViolet	0.43,0.46,0,0.02
●LightPeriwinkle	0.29,0.28,0,0	●LightCadetBlue	0.31,0.29,0.12,0
●LightCornflowerBlue	0.33,0.07,0,0	●LightMidnightBlue	0.49,0.07,0,0.22
●LightNavyBlue	0.47,0.27,0,0	●LightRoyalBlue	0.50,0.25,0,0
●LightBlue	0.50,0.50,0,0	●LightCerulean	0.47,0.06,0,0
●LightCyan	0.50,0,0,0	●LightProcessBlue	0.48,0,0,0
●LightSkyBlue	0.31,0,0.06,0	●LightTurquoise	0.43,0,0.10,0
●LightTealBlue	0.43,0,0.17,0.01	●LightAquamarine	0.41,0,0.15,0
●LightBlueGreen	0.43,0,0.17,0	●LightEmerald	0.50,0,0.25,0
●LightJungleGreen	0.50,0,0.26,0	●LightSeaGreen	0.35,0,0.25,0
●LightGreen	0.50,0,0.50,0	●LightForestGreen	0.46,0,0.44,0.06
●LightPineGreen	0.46,0,0.30,0.13	●LightLimeGreen	0.25,0,0.50,0
●LightYellowGreen	0.22,0,0.37,0	●LightSpringGreen	0.13,0,0.38,0
●LightOliveGreen	0.32,0,0.48,0.20	●LightRawSienna	0,0.36,0.50,0.23
●LightSepia	0,0.44,0.50,0.35	●LightBrown	0,0.41,0.50,0.30
●LightTan	0.07,0.21,0.28,0		

LightLight- and LightLightLight-versions were derived by dividing all values from Light-color definitions by 2 and 4, respectively.

name	*RGB*	*name*	*RGB*
●WhiteBlack5	0,0,0,0.05	●WhiteBlack10	0,0,0,0.10
●WhiteBlack15	0,0,0,0.15	●WhiteBlack20	0,0,0,0.20
●WhiteBlack25	0,0,0,0.25	●WhiteBlack30	0,0,0,0.30
●WhiteBlack35	0,0,0,0.35	●WhiteBlack40	0,0,0,0.40
●WhiteBlack45	0,0,0,0.45	●WhiteBlack50	0,0,0,0.50
●WhiteBlack55	0,0,0,0.55	●WhiteBlack60	0,0,0,0.60
●WhiteBlack65	0,0,0,0.65	●WhiteBlack70	0,0,0,0.70
●WhiteBlack75	0,0,0,0.75	●WhiteBlack80	0,0,0,0.80
●WhiteBlack85	0,0,0,0.85	●WhiteBlack90	0,0,0,0.90
●WhiteBlack95	0,0,0,0.95	●WhiteBlack100	0,0,0,1.00
●BlueRed5	0.15,0.17,0.55	●BlueRed10	0.20,0.23,0.57
●BlueRed15	0.24,0.29,0.60	●BlueRed20	0.33,0.35,0.64
●BlueRed25	0.43,0.43,0.68	●BlueRed30	0.52,0.52,0.73
●BlueRed35	0.60,0.60,0.78	●BlueRed40	0.70,0.70,0.84
●BlueRed45	0.80,0.80,0.85	●BlueRed50	0.86,0.82,0.82
●BlueRed55	0.87,0.73,0.73	●BlueRed60	0.89,0.64,0.64
●BlueRed65	0.90,0.55,0.55	●BlueRed70	0.91,0.47,0.46
●BlueRed75	0.91,0.39,0.37	●BlueRed80	0.90,0.33,0.28
●BlueRed85	0.89,0.25,0.20	●BlueRed90	0.88,0.23,0.14
●BlueRed95	0.87,0.21,0.09	●BlueRed100	0.87,0.16,0.04
●GreenRed5	0,1,0	●GreenRed10	0.05,0.95,0
●GreenRed15	0.10,0.90,0	●GreenRed20	0.15,0.85,0
●GreenRed25	0.20,0.80,0	●GreenRed30	0.25,0.75,0
●GreenRed35	0.30,0.70,0	●GreenRed40	0.35,0.65,0
●GreenRed45	0.40,0.60,0	●GreenRed50	0.45,0.55,0
●GreenRed55	0.50,0.50,0	●GreenRed60	0.55,0.45,0
●GreenRed65	0.60,0.40,0	●GreenRed70	0.65,0.35,0
●GreenRed75	0.70,0.30,0	●GreenRed80	0.75,0.25,0
●GreenRed85	0.80,0.20,0	●GreenRed90	0.85,0.15,0
●GreenRed95	0.90,0.10,0	●GreenRed100	0.95,0.05,0
●ColdHot5	0,0.08,1	●ColdHot10	0,0.29,1
●ColdHot15	0,0.49,1	●ColdHot20	0,0.70,1
●ColdHot25	0,0.90,1	●ColdHot30	0,1,0.87
●ColdHot35	0,1,0.68	●ColdHot40	0,1,0.46
●ColdHot45	0,1,0.25	●ColdHot50	0,1,0.04
●ColdHot55	0.16,1,0	●ColdHot60	0.35,1,0
●ColdHot65	0.56,1,0	●ColdHot70	0.79,1,0
●ColdHot75	0.98,1,0	●ColdHot80	1,0.82,0
●ColdHot85	1,0.60,0	●ColdHot90	1,0.40,0
●ColdHot95	1,0.20,0	●ColdHot100	0.91,0,0

and reverse definitions: `BlackWhite`, `RedBlue`, `RedGreen`, `HotCold`.

Type the color names with the upper case letters exactly as described above. For the definition of new colors use one of the `color.sty` commands:

```
  \definecolor{⟨name⟩}{cmyk}{⟨C,M,Y,K⟩}
  \definecolor{⟨name⟩}{rgb}{⟨R,G,B⟩}
```

The ⟨*name*⟩ can be chosen freely, the values for the color composition must be in the range 0–1, i e. 0–100% of the respective component (‘C’ – cyan, ‘M’ – magenta, ‘Y’ – yellow, ‘K’ – black; or ‘R’ – red, ‘G’ – green, ‘Blue’ – blue) separated by commas.

Examples:

```
\definecolor{Salmon}{cmyk}{0,0.53,0.38,0}
\definecolor{ColdHot15}{rgb}{0,0.49,1}
```

6 Listing of the `texshade` default settings

6.1 Standard definitions

The file `texshade.def` mirrors all commands which are carried out at the beginning of the `texshade` environment. Short comments are also included, thus, it is refered to this file for further information.

6.2 Colors used in the different shading modes

Color scheme *blues*:

res.color	*shad.color*	*residues*
Black	White	no match
Black	Magenta	similar
White	RoyalBlue	identical
Goldenrod	RoyalPurple	all match

Color scheme *greens*:

res.color	*shad.color*	*residues*
Black	White	no match
Black	GreenYellow	similar
White	PineGreen	identical
YellowOrange	OliveGreen	all match

Color scheme *reds*:

res.color	*shad.color*	*residues*
Black	White	no match
Black	YellowOrange	similar
White	BrickRed	identical
YellowGreen	Mahagony	all match

Color scheme *grays*:

res.color	*shad.color*	*residues*
Black	White	no match
Black	LightGray	similar
White	DarkGray	identical
White	Black	all match

Color scheme *black*:

res.color	*shad.color*	*residues*
Black	White	no match
Black	White	similar
White	Black	identical
White	Black	all match

Functional mode *charge*:

res.color	*shad.color*	*residues*
Black	White	no match
White	Red	acidic
White	Blue	basic

Functional mode *hydropathy*:

res.color	*shad.color*	*residues*
Black	White	no match
White	Red	acidic
White	Blue	basic
Black	Yellow	polar uncharged
White	Green	hydrophobic nonpolar

Functional mode *chemical*:

res.color	*shad.color*	*residues*
Black	White	no match
White	Red	acidic
White	Black	aliphatic
White	Gray	aliphatic (small)
White	Green	amide
White	Brown	aromatic
White	Blue	basic
Black	Magenta	hydroxyl
Black	Orange	imino
Black	Yellow	sulfur

Functional mode *rasmol*:

res.color	*shad.color*	*residues*
Black	White	no match
Red	White	Asp, Glu
Blue	White	Arg, Lys, His
MidnightBlue	White	Phe, Tyr, Trp
Gray	White	Ala, Gly
Yellow	White	Cys, Met
Orange	White	Ser, Thr
Cyan	White	Asn, Gln
Gree	White	Leu, Val, Ile
Apricot	White	Pro

Functional mode *structure*:

res.color	*shad.color*	*residues*
Black	White	no match
Black	Orange	external
Black	Yellow	ambivalent
White	Green	internal

Functional mode *standard area*:

res.color	*shad.color*	*residues*
Black	White	no match
Black	BrickRed	G
Black	Orange	A, S
Black	Yellow	C, P
Black	YellowGreen	T, D, V, N
White	PineGreen	I, E
Black	SkyBlue	L, Q, H, M
White	RoyalPurple	F, K
White	RedViolet	Y
White	Black	R, W

Functional mode *accessible area*:

res.color	*shad.color*	*residues*
Black	White	no match
Black	BrickRed	C
Black	Orange	I, V, G
Black	Yellow	F, L, M, A
Black	YellowGreen	W, S, T, H
White	PineGreen	P
Black	SkyBlue	Y, D, N
White	RoyalPurple	E, Q
White	RedViolet	R
White	Black	K

6.3 Residue weight tables

`identity`

```
C  10
S   0  10
T   0   0  10
P   0   0   0  10
A   0   0   0   0  10
G   0   0   0   0   0  10
N   0   0   0   0   0   0  10
D   0   0   0   0   0   0   0  10
E   0   0   0   0   0   0   0   0  10
Q   0   0   0   0   0   0   0   0   0  10
H   0   0   0   0   0   0   0   0   0   0  10
R   0   0   0   0   0   0   0   0   0   0   0  10
K   0   0   0   0   0   0   0   0   0   0   0   0  10
M   0   0   0   0   0   0   0   0   0   0   0   0   0  10
I   0   0   0   0   0   0   0   0   0   0   0   0   0   0  10
L   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  10
V   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  10
F   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  10
Y   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  10
W   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  10

    C   S   T   P   A   G   N   D   E   Q   H   R   K   M   I   L   V   F   Y   W
```

structural

C	10																			
S	6	10																		
T	3	8	10																	
P	3	6	6	10																
A	3	8	8	8	10															
G	5	8	6	6	8	10														
N	3	8	6	3	5	5	10													
D	1	6	5	5	6	6	8	10												
E	0	5	5	5	6	6	6	8	10											
Q	1	5	5	5	5	3	5	6	6	10										
H	3	5	3	5	3	1	6	5	3	6	10									
R	3	5	5	5	3	5	5	3	5	5	6	10								
K	0	5	6	3	5	3	6	5	6	6	5	8	10							
M	3	5	5	3	5	1	1	3	3	3	3	3	3	10						
I	3	3	5	3	3	3	3	1	1	1	3	3	3	6	10					
L	3	3	3	5	3	3	1	1	1	3	5	3	3	8	8	10				
V	3	6	6	6	8	6	3	5	6	3	1	3	5	6	3	3	10			
F	5	5	3	5	5	3	3	1	3	1	3	1	1	5	6	6	6	10		
Y	5	5	3	3	3	3	5	3	1	3	5	1	1	3	5	5	5	8	10	
W	5	3	1	3	3	5	0	0	1	1	1	3	1	5	5	6	5	5	5	10
	C	S	T	P	A	G	N	D	E	Q	H	R	K	M	I	L	V	F	Y	W

PAM250

C	4																			
S	0	3																		
T	-2	1	3																	
P	-3	1	0	6																
A	-2	1	1	1	2															
G	-3	1	0	-1	1	5														
N	-4	1	0	-1	0	0	2													
D	-5	0	0	-1	0	1	2	4												
E	-5	0	0	-1	0	0	1	3	4											
Q	-5	-1	-1	0	0	-1	1	2	2	4										
H	-3	-1	-1	0	-1	-2	2	1	1	3	6									
R	-4	0	-1	0	-2	-3	0	-1	-1	1	2	6								
K	-5	0	0	-1	-1	-2	1	0	0	1	0	3	5							
M	-5	-2	-1	-2	-1	-3	-2	-3	-2	-1	-2	0	0	6						
I	-2	-1	0	-2	-1	-3	-2	-2	-2	-2	-2	-2	-2	2	5					
L	-6	-3	-2	-3	-2	-4	-3	-4	-3	-2	-2	-3	-3	4	2	6				
V	-2	-1	0	-1	0	-1	-2	-2	-2	-2	-2	-2	-2	2	4	2	4			
F	-4	-3	-2	-5	-4	-5	-4	-6	-5	-5	-2	-4	-5	0	1	2	-1	9		
Y	0	-3	-3	-5	-3	-5	-2	-4	-4	-4	0	-4	-4	-2	-1	-1	-2	7	10	
W	-8	-2	-5	-6	-6	-7	-4	-7	-7	-5	-3	2	-3	-4	-5	-2	-6	0	0	17
	C	S	T	P	A	G	N	D	E	Q	H	R	K	M	I	L	V	F	Y	W

PAM100

C	14																			
S	-1	6																		
T	-5	2	7																	
P	-6	1	-1	10																
A	-5	2	2	1	6															
G	-8	1	-3	-3	1	8														
N	-8	2	0	-3	-1	-1	7													
D	-11	-1	-2	-4	-1	-1	4	8												
E	-11	-2	-3	-3	0	-2	1	5	8											
Q	-11	-3	-3	-1	-2	-5	-1	1	4	9										
H	-6	-4	-5	-2	-5	-7	2	-1	-2	4	11									
R	-6	-1	-4	-2	-5	-8	-3	-6	-5	1	1	10								
K	-11	-2	-1	-4	-4	-5	1	-2	-2	-1	-3	3	8							
M	-11	-4	-2	-6	-3	-8	-5	-8	-6	-2	-7	-2	1	13						
I	-5	-4	-1	-6	-3	-7	-4	-6	-5	-5	-7	-4	-4	2	9					
L	-12	-7	-5	-5	-5	-8	-6	-9	-7	-3	-5	-7	-6	4	2	9				
V	-4	-4	-1	-4	0	-4	-5	-6	-5	-5	-6	-6	-6	1	5	1	8			
F	-10	-5	-6	-9	-7	-8	-6	-11	-11	-10	-4	-7	-11	-2	0	0	-5	12		
Y	-2	-6	-6	-11	-6	-11	-3	-9	-7	-9	-1	-10	-10	-8	-4	-5	-6	6	13	
W	-13	-4	-10	-11	-11	-13	-8	-13	-14	-11	-7	1	-9	-11	-12	-7	-14	-2	-2	19
	C	S	T	P	A	G	N	D	E	Q	H	R	K	M	I	L	V	F	Y	W

BLOSUM62

C	9																			
S	-1	4																		
T	-1	1	4																	
P	-3	-1	1	7																
A	0	1	-1	-1	4															
G	-3	0	1	-2	0	6														
N	-3	1	0	-2	-2	0	6													
D	-3	0	1	-1	-2	-1	1	6												
E	-4	0	0	-1	-1	-2	0	2	5											
Q	-3	0	0	-1	-1	-2	0	0	2	5										
H	-3	-1	0	-2	-2	-2	1	1	0	0	8									
R	-3	-1	-1	-2	-1	-2	0	-2	0	1	0	5								
K	-3	0	0	-1	-1	-2	0	-1	1	1	-1	2	5							
M	-1	-1	-1	-2	-1	-3	-2	-3	-2	0	-2	-1	-1	5						
I	-1	-2	-2	-3	-1	-4	-3	-3	-3	-3	-3	-3	-3	1	4					
L	-1	-2	-2	-3	-1	-4	-3	-4	-3	-2	-3	-2	-2	2	2	4				
V	-1	-2	-2	-2	0	-3	-3	-3	-2	-2	-3	-3	-2	1	3	1	4			
F	-2	-2	-2	-4	-2	-3	-3	-3	-3	-3	-1	-3	-3	0	0	0	-1	6		
Y	-2	-2	-2	-3	-2	-3	-2	-3	-2	-1	2	-2	-2	-1	-1	-1	-1	3	7	
W	-2	-3	-3	-4	-3	-2	-4	-4	-3	-2	-2	-3	-3	-1	-3	-2	-3	1	2	11
	C	S	T	P	A	G	N	D	E	Q	H	R	K	M	I	L	V	F	Y	W

7 Quick Reference

The TeXshade logo

`\TeXshade`

The TeXshade environment (14 ff.)

```
\begin{texshade}[⟨parameterfile⟩] {⟨alignmentfile⟩}
  further TeXshade commands, if needed
\end{texshade}
```

Predefined shading modes

`\seqtype{⟨type⟩}`	(`P` – peptide, `N` – nucleotide)	[41]
`\shadingmode[⟨option⟩]{⟨mode⟩}`		[45]

⟨*mode*⟩	⟨*option*⟩	
`identical`	`allmatchspecial/number`	
`similar`	`allmatchspecial/number`	
`T-Coffee`	⟨*filename*⟩	
`diverse`	⟨*seqref*⟩	
`functional`	⟨*type*⟩	`charge`
		`hydropathy`
		`structure`
		`chemical`
		`rasmol`
		`standard area`
		`accessible area`
		`DNA`
`singleseq`	⟨*seqref*⟩	

`\allmatchspecial[⟨percentage⟩]`	[45]
`\hideallmatchpositions`	[49]
`\shadeallresidues`	[51]
`\shiftsingleseq[⟨num⟩]`	[51]
`\keepsingleseqgaps`	[51]

Shading colors (45 ff.)

`\shadingcolors{⟨scheme⟩}` (`blues`, `reds`, `greens`, `grays`, `black`)	
`\nomatchresidues{⟨res.col.⟩}{⟨shad.col.⟩}{⟨case⟩}{⟨style⟩}`	
`\similarresidues{⟨res.col.⟩}{⟨shad.col.⟩}{⟨case⟩}{⟨style⟩}`	
`\conservedresidues{⟨res.col.⟩}{⟨shad.col.⟩}{⟨case⟩}{⟨style⟩}`	
`\allmatchresidues{⟨res.col.⟩}{⟨shad.col.⟩}{⟨case⟩}{⟨style⟩}`	
`\defshadingcolors{⟨name⟩}`	
`\funcshadingstyle{⟨residue⟩}{⟨res.col.⟩}{⟨shad.color⟩}{⟨case⟩}{⟨style⟩}`	[50]

Residue grouping

`\pepsims{⟨residue⟩}{⟨similars⟩}`	[47]
`\pepgroups{⟨group1⟩,⟨group2⟩, ... , ⟨groupn⟩}`	[47]
`\DNAsims{⟨residue⟩}{⟨similars⟩}`	[47]
`\DNAgroups{⟨group1⟩,⟨group2⟩, ... , ⟨groupn⟩}`	[47]

Definition of new functional shading modes

`\clearfuncgroups`	[50]
`\funcgroup{⟨descr⟩}{⟨residues⟩}{⟨res.col.⟩}{⟨shad.col.⟩}{⟨case⟩}{⟨style⟩}`	[51]

Appearance of the consensus line

`\threshold[⟨percentage⟩]{⟨percentage⟩}`	[52]
`\constosingleseq{⟨seqref⟩}`	[52]
`\showconsensus[⟨color/scale⟩[,⟨color/scale⟩]]{⟨top/bot.⟩}`	[53]
`\exportconsensus[⟨pymol/chimera⟩]{⟨seqref⟩}{⟨filename⟩}`	[53]
`\hideconsensus`	[53]
`\nameconsensus{⟨name⟩}`	[53]
`\defconsensus{⟨symbol1⟩}{⟨symbol2⟩}{⟨symbol3⟩}`	[53]
`\consensuscolors{⟨res.col.1⟩}{⟨shad.col.1⟩}{⟨res.col.2⟩}{⟨shad.col.2⟩}{⟨res.col.3⟩}{⟨shad.col.3⟩}`	[54]

`\weighttable{⟨table⟩}`	[55]
`\setweight{⟨res.1⟩}{⟨res.2⟩}{⟨value⟩}`	[55]
`\gappenalty{⟨value⟩}`	[55]

Sequence logos

`\showsequencelogo[⟨colorset⟩]{⟨top/bottom⟩}`	[56]
`\hidesequencelogo`	[56]
`\clearlogocolors[⟨color⟩]`	[57]
`\logocolor{⟨residues⟩}{⟨color⟩}`	[57]
`\showlogoscale[⟨color⟩]{⟨left/right/leftright⟩}`	[57]
`\hidelogoscale`	[57]
`\logostretch{⟨factor⟩}`	[57]
`\namesequencelogo{⟨name⟩}`	[57]
`\dofrequencycorrection`	[57]
`\undofrequencycorrection`	[57]

Subfamily logos

`\showsubfamilylogo[⟨colorset⟩]{⟨top/bottom⟩}`	[58]
`\hidesubfamilylogo`	[58]
`\setsubfamily{⟨seqrefs⟩}`	[58]
`\shownegatives[⟨weak, medium, strong⟩]`	[58]
`\hidenegatives`	[58]
`\namesubfamilylogo[⟨neg.name⟩]{⟨name⟩}`	[58]
`\relevance{⟨bit-value⟩}`	[58]
`\showrelevance[⟨color⟩]{⟨symbol⟩}`	[58]
`\hiderelevance`	[58]

Structure memes

`\structurememe[⟨seqref⟩]{⟨filename⟩}`	[58]
`\memeStandardcolors`	[58]
`\memeRed{⟨residues⟩}`	[58]
`\memeYellow{⟨residues⟩}`	[58]
`\memeBlue{⟨residues⟩}`	[58]
`\memeWhite{⟨residues⟩}`	[58]
`\memeBlack{⟨residues⟩}`	[58]
`\chimerachain{⟨chainlabel⟩}`	[58]
`\chimeraballScale{⟨factor⟩}`	[58]
`\memelabelcutoff{⟨bit-value⟩}`	[58]
`\chimeraxisdistance{⟨x-dist⟩}{⟨y-dist⟩}{⟨z-dist⟩}`	[58]
`\echostructurefile{⟨strucref⟩}`	[58]

Appearance of the sequence lines

`\shownames[⟨color⟩]{⟨left/right⟩}`	[59]

\shownumbering[⟨*color*⟩]{⟨*left/right/leftright*⟩}	[59]
\alignrightlabels, \unalignrightlabels	[59]
\nameseq{⟨*seqref*⟩}{⟨*name*⟩}	[59]
\namescolor{⟨*color*⟩}	[59]
\namecolor{⟨*seq1*⟩, ... ,⟨*seq n*⟩}{⟨*color*⟩}	[60]
\hidenames	[60]
\hidename{⟨*seq1*⟩, ... ,⟨*seq n*⟩}	[60]
\numberingcolor{⟨*color*⟩}	[59]
\numbercolor{⟨*seq1*⟩, ... ,⟨*seq n*⟩}{⟨*color*⟩}	[60]
\hidenumbering	[60]
\hidenumber{⟨*seq1*⟩, ... ,⟨*seq n*⟩}	[60]
\hideresidues	[64]
\showresidues	[64]
\startnumber[⟨*start..stop*⟩]{⟨*seqref*⟩}{⟨*startnumber*⟩}	[60]
\allowzero	[60]
\disallowzero	[60]
\seqlength{⟨*seqref*⟩}{⟨*length*⟩}	[60]
\showruler[⟨*color*⟩]{⟨*top/bottom*⟩}{⟨*seqref*⟩}	[61]
\rulersteps[⟨*top/bottom*⟩]{⟨*number*⟩}	[61]
\rulercolor[⟨*top/bottom*⟩]{⟨*color*⟩}	[61]
\hideruler[⟨*top/bottom*⟩]	[61]
\rotateruler[⟨*top/bottom*⟩]	[61]
\unrotateruler[⟨*top/bottom*⟩]	[61]
\namerulerpos[⟨*top/bottom*⟩]{⟨*number*⟩}{⟨*text*⟩[⟨*color*⟩]}	[61]
\nameruler[⟨*top/bottom*⟩]{⟨*name*⟩]}	[61]
\rulernamecolor[⟨*top/bottom*⟩]{⟨*color*⟩]}	[61]
\rulerspace[⟨*top/bottom*⟩]{⟨*length*⟩}	[61]
\gapchar{⟨*symbol*⟩} (incl. rule)	[61]
\gapcolors{⟨*symbol color*⟩}{⟨*background color*⟩}	[61]
\showleadinggaps	[62]
\hideleadinggaps	[62]
\stopchar{⟨*symbol*⟩}	[62]
\fingerprint{⟨*res. per line*⟩}	[66]

Displaying selected residues in the alignment

\setends[⟨*startnumber*⟩]{⟨*seqref*⟩}{⟨*start..stop*⟩}	[62]
\setdomain{⟨*seqref*⟩}{⟨*selection*⟩} (see \shaderegion p. 67)	[63]
\domaingaprule{⟨*thickness*⟩}	[63]
\domaingapcolors{⟨*foreground*⟩}{⟨*background*⟩}	[63]

Hiding, killing, separating and ordering

\hideseq{⟨*seq1*⟩,⟨*seq2*⟩,...,⟨*seq n*⟩}	[64]
\hideseqs	[64]
\showseqs	[64]
\killseq{⟨*seq1*⟩,⟨*seq2*⟩,...,⟨*seq n*⟩}	[64]
\donotshade{⟨*seq1*⟩,⟨*seq2*⟩,...,⟨*seq n*⟩}	[64]
\separationline{⟨*seqref*⟩}	[64]
\smallsep	[64]
\medsep	[64]
\bigsep	[64]
\vsepspace{⟨*length*⟩}	[64]
\orderseqs{⟨*seq1*⟩,⟨*seq2*⟩,...,⟨*seq n*⟩}	[65]

Residues per line and further format settings

\residuesperline{⟨*number*⟩}	[65]
\residuesperline*{⟨*number*⟩}	[65]
\charstretch{⟨*factor*⟩}	[65]
\linestretch{⟨*factor*⟩}	[65]
\numberingwidth{⟨*n digits*⟩}	[65]
\smallblockskip	[66]
\medblockskip	[66]
\bigblockskip	[66]
\noblockskip	[66]
\vblockspace{⟨*length*⟩}	[66]
\flexblockspace	[66]
\fixblockspace	[66]
\alignment{⟨*left/center/right*⟩}	[66]

Individual shading and labeling of sequence stretches

\shaderegion{⟨*seqref*⟩}{⟨*selection*⟩}{⟨*res.col.*⟩}{⟨*shad.col.*⟩}	[67]

{⟨*selection*⟩} =

{⟨*start1*⟩..⟨*stop1*⟩,⟨*start2*⟩..⟨*stop2*⟩,...,⟨*start n*⟩..⟨*stop n*⟩}

{point[⟨*dist*⟩]:⟨*file*⟩,⟨*num*⟩[CA/side]}

{line[⟨*dist*⟩]:⟨*file*⟩,⟨*num1*⟩[CA/side],⟨*num2*⟩[CA/side]}

{plane[⟨*dist*⟩]:⟨*file*⟩,⟨*num1*⟩[CA/side],⟨*num2*⟩[CA/side],
⟨*num3*⟩[CA/side]}

\printPDBlist{⟨*selection*⟩}	\messagePDBlist{⟨*selection*⟩}	[68]
\shadeblock{⟨*seqref*⟩}{⟨*selection*⟩}{⟨*res.col.*⟩}{⟨*shad.col.*⟩}		[68]
\changeshadingcolors{⟨*seqref*⟩}{⟨*selection*⟩}{⟨*name*⟩}		[69]
\emphregion{⟨*seqref*⟩}{⟨*selection*⟩}		[69]
\emphblock{⟨*seqref*⟩}{⟨*selection*⟩}		[69]
\emphdefault{⟨*style*⟩}		[69]
\tintregion{⟨*seqref*⟩}{⟨*selection*⟩}		[69]
\tintblock{⟨*seqref*⟩}{⟨*selection*⟩}		[69]
\tintdefault{⟨*effect*⟩}	weak, normal, strong	[69]
\lowerregion{⟨*seqref*⟩}{⟨*selection*⟩}		[69]
\lowerblock{⟨*seqref*⟩}{⟨*selection*⟩}		[69]
\frameblock{⟨*seqref*⟩}{⟨*selection*⟩}{⟨*color*⟩[⟨*length*⟩]}		[70]

\feature{⟨*position*⟩}{⟨*seqref*⟩}{⟨*selection*⟩}
{⟨*labelstyle*⟩}{⟨*text*⟩}
		[70]

{⟨*labelstyle*⟩} = {brace[⟨*color*⟩]}
= {fill:⟨*symbol*⟩[⟨*textcolor(,bgcolor)*⟩]}
= {restriction[⟨*color*⟩]}
= {helix[⟨*helixcolor*⟩]}
= {box[⟨*framecolor,boxcolor*⟩][⟨*length*⟩]:
⟨*text*⟩[⟨*textcolor*⟩]}
= {S-S}
= arrows and bars (-=<',|o)(-=)(-=>',|o)
= {translate[⟨*color(,bgcolor)*⟩]}
= {complement[⟨*textcolor(,bgcolor)*⟩][lower]}
(only for nucleotide sequences)
= {bar[⟨*min*⟩,⟨*max*⟩]:
⟨*property/file/data*⟩[⟨*color(,bgcolor)*⟩]}
= {color[⟨*min*⟩,⟨*max*⟩]:
⟨*property/file/data*⟩[⟨*color scale*⟩]
⟨*properties*⟩: hydrophobicity, charge,
molweight, conservation
⟨*col.scales*⟩: BlueRed, RedBlue,
GreenRed, RedGreen,
ColdHot, HotCold,
WhiteBlack, BlackWhite,
T-Coffee}
= {stackedbars[⟨*min*⟩,⟨*max*⟩]:
⟨*file/data*⟩[⟨*colors/scale(,bgcolor)*⟩]}
= {frustratometer:
⟨*file*⟩[⟨*mincolor*⟩,⟨*neutralcolor*⟩,⟨*maxcolor*⟩]}

\ttttopspace{⟨*length*⟩}	[70]
\tttopspace{⟨*length*⟩}	[70]
\ttopspace{⟨*length*⟩}	[70]
\topspace{⟨*length*⟩}	[70]
\bottomspace{⟨*length*⟩}	[70]
\bbottomspace{⟨*length*⟩}	[70]
\bbbottomspace{⟨*length*⟩}	[70]
\bbbbottomspace{⟨*length*⟩}	[70]
\featurerule{⟨*length*⟩}	[73]
\bargraphstretch[⟨*position*⟩]{⟨*factor*⟩}	[75]
\colorscalestretch{⟨*factor*⟩}	[75]
\codon{⟨*amino acid*⟩}{⟨*triplet1,. . . , triplet n*⟩}	[73]
\geneticcode{⟨*filename*⟩}	[73]
\backtranslabel[⟨*size*⟩]{⟨*style*⟩}	[74]
\backtranstext[⟨*size*⟩]{⟨*style*⟩}	[**??**]

{⟨*style*⟩} = {horizontal}
= {alternating}
= {zigzag}
= {oblique}
= {vertical}

\showfeaturename{⟨*ttttop...bbbbottom*⟩}{⟨*name*⟩}	[77]
\showfeaturestylename{⟨*ttttop...bbbbottom*⟩}{⟨*name*⟩}	[77]
\hidefeaturename{⟨*ttttop...bbbbottom*⟩}	[77]
\hidefeaturestylename{⟨*ttttop...bbbbottom*⟩}	[77]
\hidefeaturenames	[77]
\hidefeaturestylenames	[77]
\featurenamescolor{⟨*color*⟩}	[78]
\featurestylenamescolor{⟨*color*⟩}	[78]
\featurenamecolor{⟨*ttttop...bbbbottom*⟩}{⟨*color*⟩}	[78]
\featurestylenamecolor{⟨*ttttop...bbbbottom*⟩}{⟨*color*⟩}	[78]

Including secondary structure information

\includeDSSP[make new]{⟨*seqref*⟩}{⟨*filename*⟩}	[79]
\includeSTRIDE[make new]{⟨*seqref*⟩}{⟨*filename*⟩}	[79]
\includePHDsec[make new]{⟨*seqref*⟩}{⟨*filename*⟩}	[79]
\includePHDtopo[make new]{⟨*seqref*⟩}{⟨*filename*⟩}	[79]

\includeHMMTOP[make new]{⟨*seqref*⟩[⟨*seqref*⟩]}{⟨*filename*⟩}	[79]
\showonDSSP{⟨*structures*⟩}	[80]
\showonSTRIDE{⟨*structures*⟩}	[80]
\showonPHDsec{⟨*structures*⟩}	[80]
\showonPHDtopo{⟨*structures*⟩}	[80]
\showonHMMTOP{⟨*structures*⟩}	[80]
\hideonDSSP{⟨*structures*⟩}	[80]
\hideonSTRIDE{⟨*structures*⟩}	[80]
\hideonPHDsec{⟨*structures*⟩}	[80]
\hideonPHDtopo{⟨*structures*⟩}	[80]
\hideonHMMTOP{⟨*structures*⟩}	[80]
\appearance{⟨*type*⟩}{⟨*position*⟩}{⟨*labelstyle*⟩}{⟨*text*⟩}	[81]
\numcount	[81]
\alphacount	[81]
\Alphacount	[81]
\romancount	[81]
\Romancount	[81]
\firstcolumnDSSP	[80]
\secondcolumnDSSP	[80]

Displaying and building legends

\showlegend	[82]
\hidelegend	[82]
\movelegend{⟨*x-offset*⟩}{⟨*y-offset*⟩}	[82]
\germanlanguage, \spanishlanguage, \englishlanguage	[82]
\legendcolor{⟨*color*⟩}	[82]
\shadebox{⟨*color*⟩}	[82]

Adding captions to the alignment

\showcaption[⟨*top/bottom*⟩]{⟨*text*⟩}	[83]
\shortcaption{⟨*text*⟩}	[83]

Font handling

\setfamily{⟨*text*⟩}{⟨*family*⟩}	[83]
\setseries{⟨*text*⟩}{⟨*series*⟩}	[83]
\setshape{⟨*text*⟩}{⟨*shape*⟩}	[83]
\setsize{⟨*text*⟩}{⟨*size*⟩}	[83]
\setfont{⟨*text*⟩}{⟨*family*⟩}{⟨*series*⟩}{⟨*shape*⟩}{⟨*size*⟩}	[84]

```
\featuresrm   \featurestiny                                 [84]
\featuressf   \featuresscriptsize
\featurestt   \featuresfootnotesize
\featuresbf   \featuressmall
\featuresmd   \featuresnormalsize
\featuresit   \featureslarge
\featuressl   \featuresLarge
\featuressc   \featuresLARGE
\featuresup   \featureshuge
              \featuresHuge
```

Corresponding sets are provided for the numbering (`\numberingrm` etc.), featurestyles (`featurestylesrm` etc.), names (`\namesrm` etc.), featurenames (`\featurenamesrm` etc.), featurestylenames (`\featurestylenames` etc.), residues (`\residuesrm` etc.), hideblock labels (`hideblockrm` etc.), rulers (`\rulerrm` etc.), and legend texts (`legendrm` etc.).

Goodies—molweight and charge

```
\molweight{⟨seqref⟩}{⟨Da/kDa⟩}                               [86]
\charge{⟨seqref⟩}{⟨i/o/N/C⟩}                                 [86]
\percentsimilarity{⟨seqref1⟩}{⟨seqref2⟩}                     [86]
\percentidentity{⟨seqref1⟩}{⟨seqref2⟩}                       [86]
\similaritytable                                             [87]
```

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