

# What If server

<http://swift.cmbi.ru.nl/servers/html/index.html>

Molekula pro analýzu – pdb kód 1PW2



# What If server

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## WHAT IF Web Interface

Nov 23-25 2007 a small WHAT IF workshop will be held at the CMBI. This workshop is meant for a few experienced WHAT IF users. The goals of the workshop are to go over a series recent WHAT IF extensions, and to discuss the next twenty years of WHAT IF development. If you want to participate, please contact Gert Vriend

Click on one of the classes in the left side column to activate those servers.

You can also read the [help page](#), or you can read about the [output formats](#) used by all servers. We also made one [page](#) with notes for people who want to make their own servers.

W A R N I N G. Results are only kept on this server till Saturday, midnight in The Netherlands. This is mainly a safety feature, but also saves us disk space. Feel free to look at the [WHAT IF](#) writeup too.

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**In case a server fails**, first check your input PDB file "List sequence of a PDB file" server that can be found in the "Administration" section of the servers. If this server gives you a long list of administrative information, and no obvious error messages, then look at the [PDBREPORT](#) database to see if there are other obvious problems with the PDB file. If that also does not provide an answer, mail the PDB file (and other files when needed) to Gert Vriend. Please mention the server class (mentioned in the left-hand column of the server page) and the title of the actual server (you click on that in the right-hand part of the server page to get at that server).

But PLEASE, do not submit the same file over and over again! If the thing fails once, it fails twice, and if it is very slow, submitting more jobs will make it even slower. Remember that the servers run just on my private machine and not some supercomputer at a big centre....

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# 3-D graphics

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## 3-D graphics

- [C-alpha trace](#)  
This server will display an alpha carbon trace.
- [The molecule coloured by B-factor](#)  
This server will display your entire molecule. The atoms are coloured linearly as function of the B-factor.
- [The molecule coloured by B-factor](#)  
This server will display your entire molecule. The atoms are coloured **non**-linearly as function of the B-factor.
- [Backbone with hydrogen bonds](#)  
The backbone will be displayed and inter-backbone hydrogen bonds will be added.
- [An arrow and cylinder drawing](#)  
This server will display your molecule as an arrow and cylinder plot.

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http://swift.cmbi.ru.nl/servers/html/graph3d.html



# 3-D graphics – arrows and cylinders

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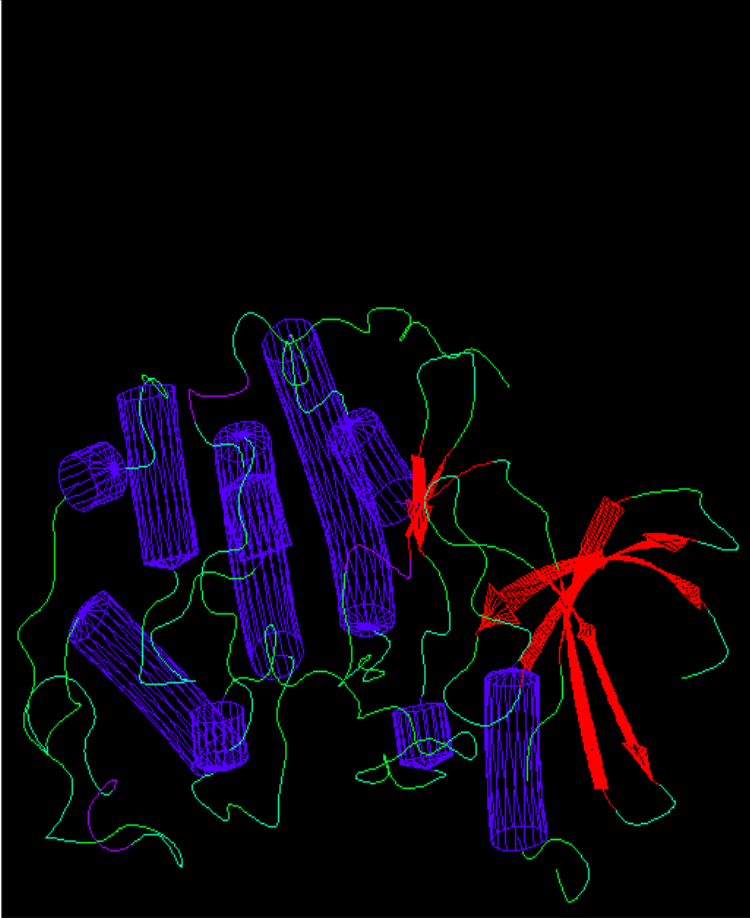
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# 3-D graphics – backbone with H-bonds

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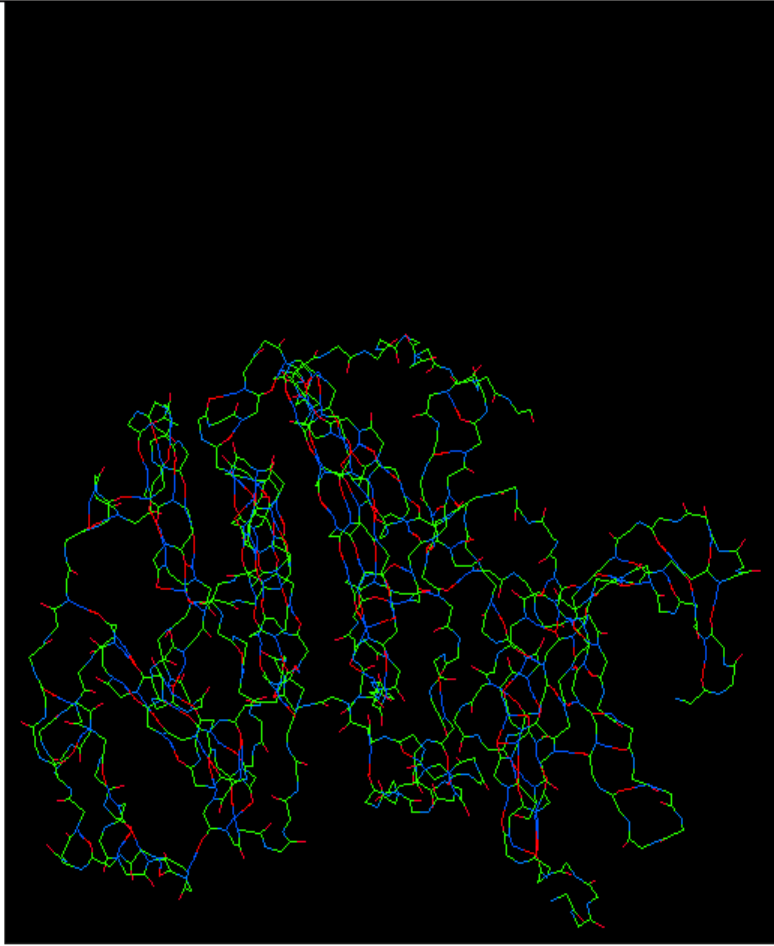
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# 3-D graphics – B-factor coloring

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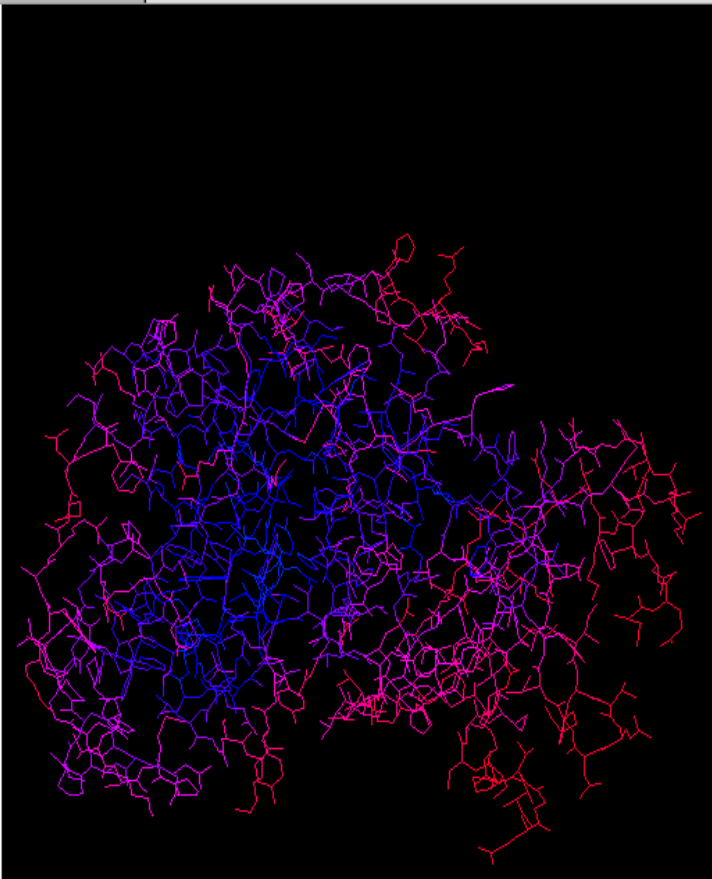
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# 2-D graphics – Ramachandran plot

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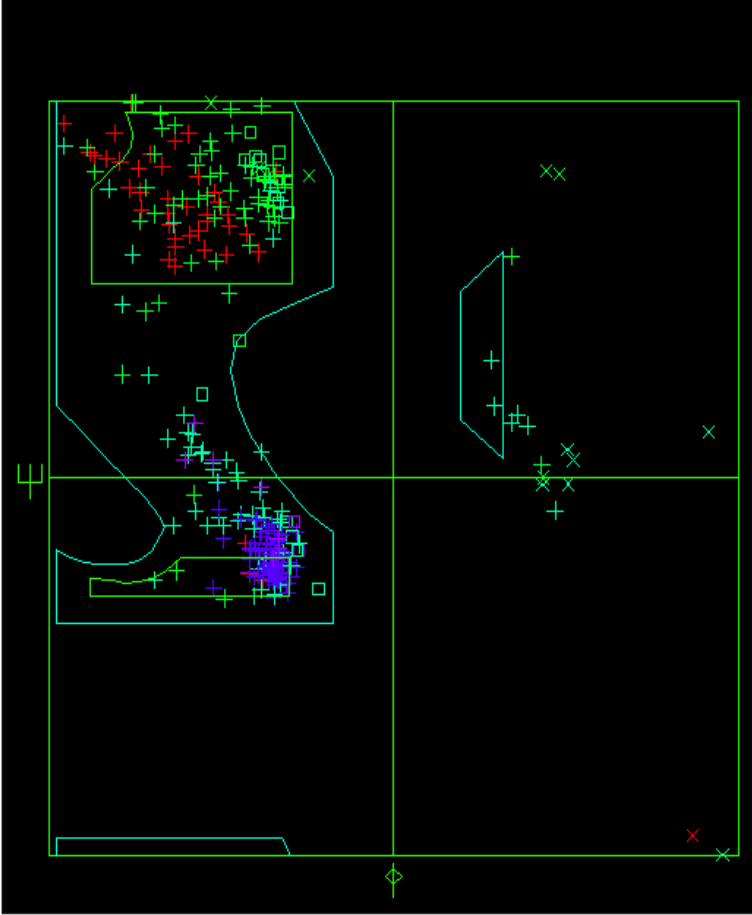
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# Build, check, repair model

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## Protein Model Check

### Introduction

A set of WHAT IF checks will be run on the model.

### Methods

Modelling proteins by homology is becoming a routine technique and many people rely on black-box like WWW based modelling servers as their only source of structural information. The fully automatic [Swiss-Model](#) server is a good example. The server listed higher up in this page is less automatic, and therefore more aimed at the experienced modeler. However, when a model is made, one needs to get an impression about the quality of the template and the quality of the model. This server checks the model for you, the previous server is meant for validation of the template structure. The difference is that in this model validation server several of the typical Xray checks (symmetry contacts; B-factors) are switched of.

Upload your file

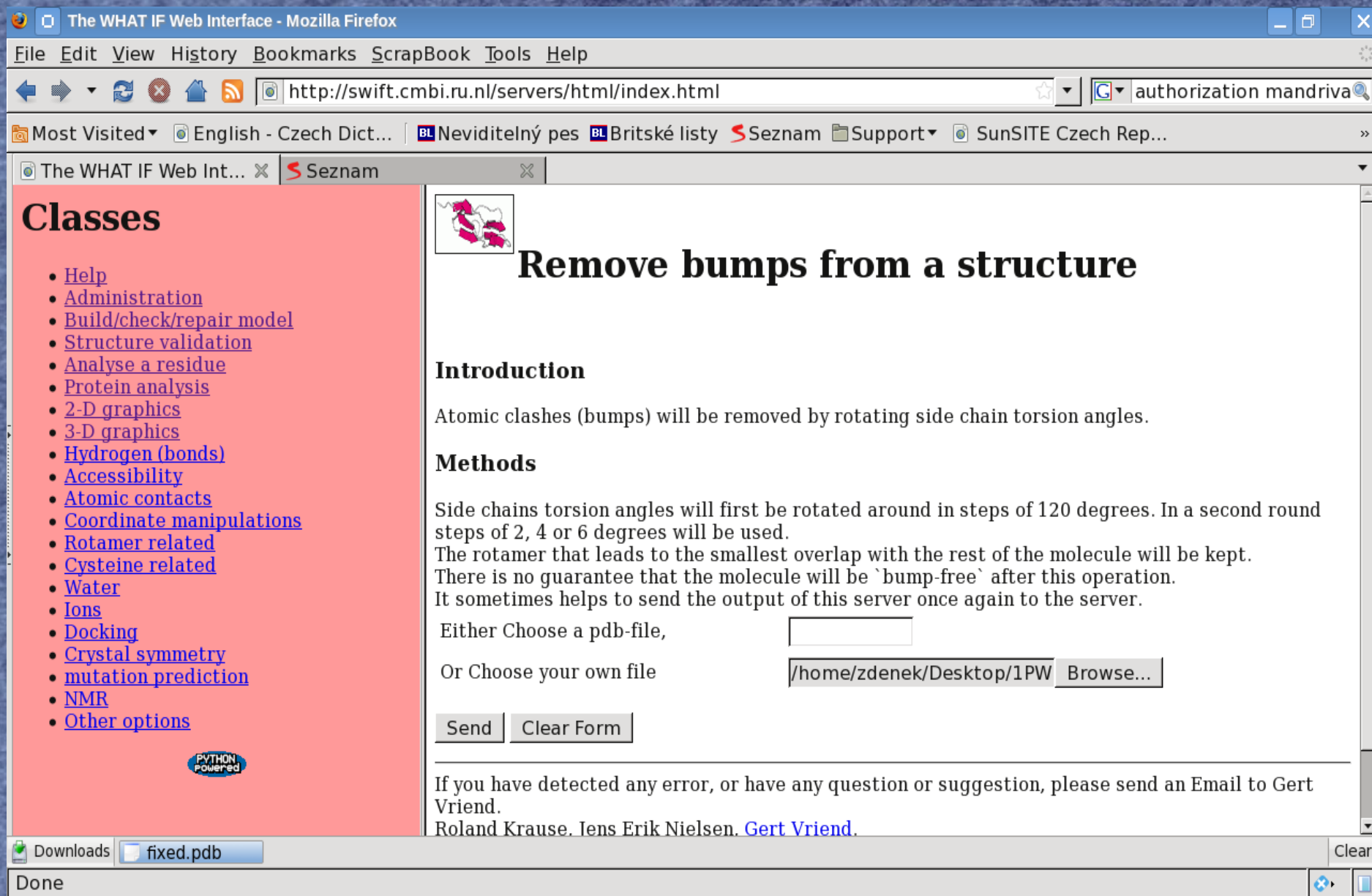
If you have detected any error or have any question or suggestion, please send an Email to Gert

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# Build, check, repair model



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## Remove bumps from a structure

### Introduction

Atomic clashes (bumps) will be removed by rotating side chain torsion angles.

### Methods

Side chains torsion angles will first be rotated around in steps of 120 degrees. In a second round steps of 2, 4 or 6 degrees will be used. The rotamer that leads to the smallest overlap with the rest of the molecule will be kept. There is no guarantee that the molecule will be `bump-free` after this operation. It sometimes helps to send the output of this server once again to the server.

Either Choose a pdb-file,

Or Choose your own file

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## Ramachandran plot evaluation.

Prolines with funny puckers:

Date= 2009-02-23 13:30:32  
Ramachandran Z-score : -0.355  
The score expressing how well the backbone conformations of all residues are corresponding to the known allowed areas in the Ramachandran plot is within expected ranges for well-refined structures.

Ramachandran Z-score : -0.355

See also the Ramachandran plot server in the 2D-graphic class.

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## Coarse Packing Quality Control

The packing quality control per amino acid:

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1	MET	( 1 )	: -3.553
2	GLU	( 2 )	: -2.469
3	ASN	( 3 )	: -0.423
4	PHE	( 4 )	: 2.892
5	GLN	( 5 )	: -1.131
6	LYS	( 6 )	: -1.653
7	VAL	( 7 )	: -3.049
8	GLU	( 8 )	: 0.161
9	LYS	( 9 )	: -3.525
10	ILE	( 10 )	: -2.501
11	GLY	( 11 )	: -1.549
12	GLU	( 12 )	: -4.363
13	GLY	( 13 )	: -0.159
14	THR	( 14 )	: -3.767
15	TYR	( 15 )	: -3.946
16	GLY	( 16 )	: -0.380
17	VAL	( 17 )	: 0.351
18	VAL	( 18 )	: 2.007
19	TYR	( 19 )	: 4.388
20	LYS	( 20 )	: 0.865
21	ALA	( 21 )	: 5.908
22	ARG	( 22 )	: 2.815
23	ASN	( 23 )	: 2.948
24	LYS	( 24 )	: -4.026
25	LEU	( 25 )	: -6.293
26	THR	( 26 )	: -1.280
27	GLY	( 27 )	: 0.811
28	GLU	( 28 )	: 0.085
29	VAL	( 29 )	: 0.603

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# Structure validation

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## Anomalous bond lengths.

Bond lengths that deviate more than 4 sigma:

Date= 2009-02-23 13:34:45

All bond lengths are in agreement with standard bond lengths using a tolerance of 4 sigma (both standard values and sigma for amino acid residues have been taken from Engh and Huber [REF], for DNA/RNA from Parkinson et al [REF])

Bond lengths were found to deviate less than normal from the mean Engh and Huber [REF] and/or Parkinson et al [REF] standard bond lengths. The RMS Z-score given below is expected to be around 1.0 for a normally restrained data set. The fact that it is lower than 0.667 in this structure might indicate that too-strong constraints have been used in the refinement. This can only be a problem for high resolution X-ray structures.

RMS Z-score for bond lengths: 0.259  
RMS-deviation in bond distances: 0.006

Comparison of bond distances with Engh and Huber [REF] standard values for protein residues and Parkinson et al [REF] values for DNA/RNA does not show significant systematic deviations.

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## Fine Packing Quality Control

The packing quality control per amino acid:

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---Residue---	State	AllAll	BB-BB	BB-SC	SC-BB	SC-SC
1 MET ( 1 ) A	2	0.000	0.000	0.000	0.000	0.000
2 GLU ( 2 ) A	3	-0.498	-0.594	0.727	-0.619	-0.967
3 ASN ( 3 ) A	3	-0.989	-0.269	0.233	-1.920	-1.054
4 PHE ( 4 ) A	3	-0.240	0.003	-0.842	0.697	-0.677
5 GLN ( 5 ) A	1	0.000	0.000	0.000	0.000	0.000
6 LYS ( 6 ) A	3	-0.441	-0.775	-1.169	-0.756	1.378
7 VAL ( 7 ) A	3	-0.320	-0.248	-1.370	0.834	-0.091
8 GLU ( 8 ) A	1	0.000	0.000	0.000	0.000	0.000
9 LYS ( 9 ) A	3	1.081	-0.162	0.645	-0.033	3.297
10 ILE ( 10 ) A	3	0.677	-0.032	-0.320	1.610	0.698
11 GLY ( 11 ) A	3	-0.873	-0.424	-0.905	0.000	0.000
12 GLU ( 12 ) A	3	-0.552	-0.964	0.096	-1.166	0.753
13 GLY ( 13 ) A	3	-1.295	-1.024	-0.812	0.000	0.000
14 THR ( 14 ) A	3	-1.325	-1.161	-0.517	-2.072	0.047
15 TYR ( 15 ) A	3	-0.570	-0.841	-0.115	-0.692	0.486
16 GLY ( 16 ) A	3	-0.001	-0.600	0.846	0.000	0.000
17 VAL ( 17 ) A	3	-1.332	-0.328	-1.163	-2.148	-1.012
18 VAL ( 18 ) A	1	0.000	0.000	0.000	0.000	0.000
19 TYR ( 19 ) A	1	0.000	0.000	0.000	0.000	0.000
20 LYS ( 20 ) A	1	0.000	0.000	0.000	0.000	0.000
21 ALA ( 21 ) A	1	0.000	0.000	0.000	0.000	0.000
22 ARG ( 22 ) A	1	0.000	0.000	0.000	0.000	0.000
23 ASN ( 23 ) A	3	1.773	2.106	0.233	1.347	0.388
24 LYS ( 24 ) A	3	-0.247	-0.493	-1.566	1.352	-0.924
25 LEU ( 25 ) A	3	-1.806	-1.409	-1.325	-1.076	-0.843
26 THR ( 26 ) A	3	0.859	0.391	0.453	0.698	1.635
27 GLY ( 27 ) A	3	1.353	0.773	1.070	0.000	0.000

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## Omega.

Omega validation results:

Date= 2009-02-23 13:39:19  
Omega average and std. deviation= 179.926 1.141  
Significant deviations from expected 5.5!!!  
The omega angles for trans-peptide bonds in a structure are expected to give a gaussian distribution with the average around +178 degrees and a standard deviation around 5.5 degrees. These expected values were obtained from very accurately determined structures. Many protein structures are too tightly constrained. This seems to be the case with the current structure too, as the observed standard deviation is below 4.0 degrees.

Standard deviation of omega values : 0.207

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## Anomalous bond angles.

Bond angles that deviate more than 4 sigma:

Date= 2009-02-23 13:40:44

The bond angles listed in the table below were found to deviate more than 4 sigma from standard bond angles (both standard values and sigma for protein residues have been taken from Engh and Huber [REF], for DNA/RNA from Parkinson et al [REF]). In the table below for each strange angle the bond angle and the number of standard deviations it differs from the standard values is given. Please note that disulphide bridges are neglected. Atoms starting with "-" belong to the previous residue in the sequence.

20 LYS ( 20 ) A N CA C 98.63 -4.5

Bond angles were found to deviate less than normal from the standard bond angles (normal values for protein residues were taken from Engh and Huber [REF], for DNA/RNA from Parkinson et al [REF]). The RMS Z-score given below is expected to be around 1.0 for a normally restrained data set. More common values are around 1.55. The fact that it is lower than 0.667 in this structure might indicate that too-strong constraints have been used in the refinement. This can only be a problem for high resolution X-ray structures.

RMS Z-score for bond angles: 0.601  
RMS-deviation in bond angles: 1.310

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Roland Krause, Jens Erik Nielsen, [Gert Vriend](#).

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# Protein analysis

The screenshot shows a Mozilla Firefox browser window with the title 'The WHAT IF Web Interface - Mozilla Firefox'. The address bar contains the URL 'http://swift.cmbi.ru.nl/servers/html/index.html'. The browser's menu bar includes 'File', 'Edit', 'View', 'History', 'Bookmarks', 'ScrapBook', 'Tools', and 'Help'. The browser's toolbar shows navigation buttons and a search box containing 'authorization mandriva'. The browser's status bar at the bottom shows 'Downloads' with files 'fixed.pdb' and '1PW2\_had...'. The address bar at the bottom of the page shows 'http://swift.cmbi.ru.nl/servers/html/calc.html'.

The main content area is divided into two columns. The left column has a pink background and is titled 'Classes'. It contains a list of links: [Help](#), [Administration](#), [Build/check/repair model](#), [Structure validation](#), [Analyse a residue](#), [Protein analysis](#), [2-D graphics](#), [3-D graphics](#), [Hydrogen \(bonds\)](#), [Accessibility](#), [Atomic contacts](#), [Coordinate manipulations](#), [Rotamer related](#), [Cysteine related](#), [Water](#), [Ions](#), [Docking](#), [Crystal symmetry](#), [mutation prediction](#), [NMR](#), and [Other options](#). A 'PYTHON Powered' logo is visible at the bottom of this column.

The right column has a white background and is titled 'Protein analysis'. It contains a list of links: [Secondary Structure, symmetry and accessibility](#), [Torsion angles](#), [Accessible Polar Fraction](#), and [Check for Short Interatomic Distances](#).

**Secondary Structure, symmetry and accessibility**  
The secondary structure according to DSSP will be listed. Residues that make a symmetry contact in the crystal and residues that are clearly accessible to solvent (this time not taking crystal contacts into account) will be indicated.

This is a secondary structure determination from 3D coordinates, and **NOT** a secondary structure prediction.

**Torsion angles**  
The torsion angles in all amino acids in the PDB file will be tabulated. Angles will be in degrees. A torsion angle of 999 degrees indicates that this torsion angle does not exist (e.g. phi of the N-terminal residue), or that there is something wrong with at least one of the atoms involved.

**Accessible Polar Fraction**  
Using this service you can calculate the scores described by Bowie, Luthy and Eisenberg.



# Protein analysis

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## Secondary Structure, symmetry and accessibility

Listed from top to bottom are the residue number, the secondary structure, every residue involved in symmetry contacts is labeled with an asterisk. Every residue that is clearly solvent accessible is labeled with a capital A.

Date= 2009-02-23 13:42:47

```
          10      20      30
1 - 36  MENFQKVEKIGEGTYGVVYKARNKL TGEVVALKKIR
1 - 36  TTSSSSSSSS TTTSSSSSSSTT SSSSS
1 - 36  ****          * *** **
1 - 36  AAA AAAAA A      A A AAA AA  A  A

          40      50      60      70      80      90
37 - 96  TEGVPS TAIREISLLKELNHPNIVKLLDVIHTENKLYLVFEFLHQDLKKFMDASAL TGIP
37 - 96  T HHHHHHHHHHTT TT SSSSSSTTSSSSSS TSSHHHHHHHTTT
37 - 96  * * * * * **** * * ***** ** *
37 - 96  AA AAAA AAA AA AA AAA A AA AAAAA A      A AA AA AAA A
          100     110     120     130     140     150
97 - 156 LPLIKSYL FOLLQGLAFCHSHRVLHRDLKPQMLL INTEGAIKLADFLGARA FGVPRTYT
97 - 156 HHHHHHHHHHHHHHHHHHTT T 333SSS TTT SSS TTHHHHT T TT
97 - 156 * * * * * ** * * *
97 - 156 AA A A AAA A A AA A A AA AAA AA
          160     170     180     190     200     210
157 - 216 HEVVTLYRAPEILLGCKYYSTAVDIWSLGCIFAEMVTRRAL FPGDSEIDQL FRI FRTL G
157 - 216 TT HHHHTT TT THHHHHHHHHHHHHHHTT T TTHHHHHHHHHHH
```

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# Protein analysis

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## Check for Short Interatomic Distances

The list of all bumps

Date= 2009-02-23 13:44:15  
The pairs of atoms listed in the table below have an unusually short distance.

The contact distances of all atom pairs have been checked. Two atoms are said to 'bump' if they are closer than the sum of their Van der Waals radii minus 0.40 Angstrom. For hydrogen bonded pairs a tolerance of 0.55 Angstrom is used. The first number in the table tells you how much shorter that specific contact is than the acceptable limit. The second distance is the distance between the centers of the two atoms. Although we believe that two water atoms at 2.4 A distance are too close, we only report water pairs that are closer than this rather short distance.

The last text-item on each line represents the status of the atom pair. The text 'INTRA' means that the bump is between atoms that are explicitly listed in the PDB file. 'INTER' means it is an inter-symmetry bump. If the final column contains the text 'HB', the bump criterium was relaxed because there could be a hydrogen bond. Similarly relaxed criteria are used for 1--3 and 1--4 interactions (listed as 'B2' and 'B3', respectively). If the last column is 'BF', the sum of the B-factors of the atoms is higher than 80, which makes the appearance of the bump somewhat less severe because the atoms probably aren't there anyway.

Bumps between atoms for which the sum of their occupancies is lower than one are not reported. In any case, each bump is listed in only one direction. If the MODEL number doesn't exist (like in most X-ray files), an underscore is printed instead.

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## Torsion angles

Torsion angles in degrees (phi,psi,omega and chi1 till chi5)

Date= 2009-02-23 13:46:03

Amino acid	Int.	Phi	Psi	Omega	Chi1-5
1 MET ( 1 ) A		999.9	177.6	-179.3	-176.7 178.0 -102.5
2 GLU ( 2 ) A		-74.0	-17.8	-179.5	-54.0 67.6 63.8
3 ASN ( 3 ) A		-81.1	-1.3	-179.2	-69.8 -64.2
4 PHE ( 4 ) A		-132.2	136.6	178.0	-57.0 79.6
5 GLN ( 5 ) A		-102.2	117.6	-179.5	63.7 156.3 -55.2
6 LYS ( 6 ) A		-70.9	107.7	179.9	-66.6 -175.2 -64.2 -178.8
7 VAL ( 7 ) A		-68.5	-48.5	180.0	175.4
8 GLU ( 8 ) A		-172.5	169.0	179.5	74.2 -170.3 -52.2
9 LYS ( 9 ) A		-85.8	120.4	179.8	-179.3 169.3 -64.0 -178.3
10 ILE ( 10 ) A		-77.5	-31.0	179.8	-76.2 -179.5
11 GLY ( 11 ) A		156.0	-170.6	179.7	
12 GLU ( 12 ) A		-97.6	125.4	179.7	-42.4 -67.0 -48.8
13 GLY ( 13 ) A		-95.5	179.1	179.6	
14 THR ( 14 ) A		-67.1	-38.7	-177.7	-62.6
15 TYR ( 15 ) A		-103.6	-16.0	-179.4	-50.2 -67.0
16 GLY ( 16 ) A		171.6	-179.8	-179.4	
17 VAL ( 17 ) A		-61.5	146.5	178.9	-169.8
18 VAL ( 18 ) A		-118.3	126.4	-179.4	179.5
19 TYR ( 19 ) A		-120.9	148.8	174.9	-73.4 -64.9
20 LYS ( 20 ) A		-91.6	131.9	-179.3	175.5 173.4 -173.5 177.3
21 ALA ( 21 ) A		-145.8	164.6	-179.9	
22 ARG ( 22 ) A		-118.2	133.4	178.9	-175.0 -174.8 -53.4 -74.0
23 ASN ( 23 ) A		-76.8	116.6	-178.9	-172.3 -46.7
24 LYS ( 24 ) A		-69.1	12.4	179.6	-62.2 178.5 -176.9 -179.8
25 LEU ( 25 ) A		-124.7	-48.5	179.0	-78.7 174.2
26 THR ( 26 ) A		-91.5	-18.7	-179.9	59.5

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# Protein analysis

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## Accessible Polar Fraction

This is the WHAT\_IF output

Date= 2009-02-23 13:47:50

Accessible Polar Fraction Score. For a reference see:  
A Method to Identify Protein Sequences That Fold into a Known  
Three-Dimensional Structure. Science, Vol 253, pp 164-170, (1991).  
For every residue you this polar fraction score is shown.

1	MET	( 1 )	A	0.6242
2	GLU	( 2 )	A	0.8312
3	ASN	( 3 )	A	0.5041
4	PHE	( 4 )	A	0.2965
5	GLN	( 5 )	A	0.5905
6	LYS	( 6 )	A	0.6705
7	VAL	( 7 )	A	0.7225
8	GLU	( 8 )	A	0.7162
9	LYS	( 9 )	A	0.7429
10	ILE	( 10 )	A	0.5934
11	GLY	( 11 )	A	0.6857
12	GLU	( 12 )	A	0.7614
13	GLY	( 13 )	A	0.5546
14	THR	( 14 )	A	0.3814
15	TYR	( 15 )	A	0.3816
16	GLY	( 16 )	A	0.6335
17	VAL	( 17 )	A	0.4608
18	VAL	( 18 )	A	0.4523
19	TYR	( 19 )	A	0.5387
20	LYS	( 20 )	A	0.4752
21	ALA	( 21 )	A	0.4010
22	ARG	( 22 )	A	0.7417
23	ASN	( 23 )	A	0.6368
24	LYS	( 24 )	A	0.8151
25	LEU	( 25 )	A	0.9561
26	THR	( 26 )	A	0.8367

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## Accessible Molecular Surface

Accessibility values and some statistics as function of the amino acid distribution

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When applicable, O, B, or OB is added at the end of the line to indicate that the residue contains atoms with an occupancy (O) lower than 0.5, or a B-factor (B) higher than 80.0.

Res# Number of the residue  
Res Residue type  
PDB# Name of the residue in the PDB file  
Tot.Acc. Total accessibility of the residue  
Back. Accessibility of the backbone of this residue  
Side. Accessibility of the sidechain of this residue  
(Back. + Side. = Tot.Acc.)!

Res#	Res	PDB#	Tot. Acc.	Back.	Side.
1	MET ( 1 )	A	21.4092	10.6593	10.7499
2	GLU ( 2 )	A	38.6979	4.5239	34.1741
3	ASN ( 3 )	A	16.8788	0.3495	16.5294
4	PHE ( 4 )	A	5.7514	2.4313	3.3201
5	GLN ( 5 )	A	22.0947	1.3979	20.6968
6	LYS ( 6 )	A	37.0271	8.2075	28.8196
7	VAL ( 7 )	A	19.7610	8.2280	11.5330
8	GLU ( 8 )	A	26.0431	3.1454	22.8978
9	LYS ( 9 )	A	31.9067	6.8889	25.0179
10	ILE ( 10 )	A	22.4232	8.7932	13.6299
11	GLY ( 11 )	A	7.3392	7.3392	0.0000
12	GLU ( 12 )	A	18.0983	5.0185	13.0798
13	GLY ( 13 )	A	3.4949	3.4949	0.0000
14	THR ( 14 )	A	6.6742	2.7349	3.9393
15	TYR ( 15 )	A	9.1675	2.0958	7.0717
16	GLY ( 16 )	A	0.7346	0.7346	0.0000
17	VAL ( 17 )	A	2.6686	0.8888	1.7798

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# Hydrogen (bonds)

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## Hydrogen (bonds)

- [Hydrogen bonded pairs in DNA/RNA](#)  
This server lists the pairs of nucleic acids that are connected by hydrogen bonds.
- [Potential Hydrogen Bonds](#)  
This module computes all possible hydrogen bonds in your molecule. It will not determine which bonds would be most favorable; you can use the "Optimal Hydrogen Bonds" server for that purpose.
- [Optimal Hydrogen Bonding Network](#)  
This server will compute the best possible hydrogen bond network.
- [Add Protons to the Structure](#)  
All missing protons will be added to the structure.
- [IUPAC atom name validation](#)  
This server will read your PDB file, list all atoms and indicate deviations from the IUPAC nomenclature rules. A PDB file with the corrected nomenclature will be made.

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## Potential Hydrogen Bonds

For each hydrogen bond the four geometric parameters will be shown, together with the corresponding hydrogen coordinates.

WARNING. These are not the hydrogen bonds in the molecule(s), but the hydrogen bonds that could potentially be observed. Some of these hydrogen bonds only exist for a very small fraction of the time, or contribute only minimally to the stability of the molecule. The 'best' hydrogen bonds, i.e., the ones that we believe are there most of the time, and that contribute to the stability of the (macro) molecule are determined by another server.

Date= 2009-02-23 14:02:27

Hydrogen bond related parameters  
Maximal donor - acceptor distance ..... 3.50  
Maximal hydrogen - acceptor distance ..... 2.50  
Maximal angular error donor - H - acceptor ... 60.00  
Maximal angular error H - acceptor - xxx ..... 90.00

```
4 PHE ( 4 ) A      N <--> 1 MET ( 1 ) A      0
D(DA)= 3.40 D(HA)= 2.44 A(H)= 19.5 A(A)= 71.9 H= 23.38 59.44 21.62
3 ASN ( 3 ) A      ND2 <--> 1 MET ( 1 ) A      SD
D(DA)= 3.08 D(HA)= 2.23 A(H)= 38.5 A(A)= 34.9 H= 26.77 58.18 17.88
24 LYS ( 24 ) A     N <--> 3 ASN ( 3 ) A      0
D(DA)= 2.96 D(HA)= 1.98 A(H)= 11.3 A(A)= 31.5 H= 20.19 60.89 18.28
5 GLN ( 5 ) A      N <--> 22 ARG ( 22 ) A     0
D(DA)= 3.07 D(HA)= 2.09 A(H)= 16.1 A(A)= 35.7 H= 19.05 60.08 22.22
22 ARG ( 22 ) A     N <--> 5 GLN ( 5 ) A      0
D(DA)= 3.05 D(HA)= 2.11 A(H)= 23.9 A(A)= 44.6 H= 16.80 58.67 22.44
7 VAL ( 7 ) A      N <--> 20 LYS ( 20 ) A     0
D(DA)= 2.75 D(HA)= 1.98 A(H)= 47.9 A(A)= 45.5 H= 15.72 57.71 26.04
8 GLU ( 8 ) A      N <--> 20 LYS ( 20 ) A     0
D(DA)= 2.33 D(HA)= 2.27 A(H)= 30.1 A(A)= 43.8 H= 14.54 56.27 28.01
```

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# Hydrogen (bonds)

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## Add Protons to the Structure

### Introduction

All missing protons will be added to the structure.

### Methods

The protons will be placed such that an optimal hydrogen bonding network will result.  
WARNING. When using files with many waters, please be prepared for a loooooong waiting time.

Either Choose a pdb-file,

Or Choose your own file

---

If you have detected any error, or have any question or suggestion, please send an Email to Gert Vriend.  
Roland Krause, Jens Erik Nielsen, [Gert Vriend](#).

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## Optimal Hydrogen Bonding Network

This is the WHAT\_IF output. See: *Positioning hydrogen atoms by optimizing hydrogen-bond networks in protein structures.*  
R.W.W.Hoof, C.Sander, G.Vriend, **PROTEINS** (1996) 26, 363-376.  
for an explanation of the scores and penalties used.

Date= 2009-02-23 13:58:35

3 ASN ( 3 ) A	ND2 ->	1 MET ( 1 ) A	SD Sym=	1 Val= 0.107	DA= 3.08	DHA= 38.50
4 PHE ( 4 ) A	N ->	1 MET ( 1 ) A	0 Sym=	1 Val= 0.479	DA= 3.40	DHA= 19.46
5 GLN ( 5 ) A	N ->	22 ARG ( 22 ) A	0 Sym=	1 Val= 0.772	DA= 3.07	DHA= 16.09
7 VAL ( 7 ) A	N ->	20 LYS ( 20 ) A	0 Sym=	1 Val= 0.584	DA= 2.75	DHA= 47.92
7 VAL ( 7 ) A	N ->	5 GLN ( 5 ) A	0 Sym=	1 Val= 0.269	DA= 3.08	DHA= 81.44
8 GLU ( 8 ) A	N ->	20 LYS ( 20 ) A	0 Sym=	1 Val= 0.663	DA= 3.33	DHA= 18.12
10 ILE ( 10 ) A	N ->	18 VAL ( 18 ) A	0 Sym=	1 Val= 0.560	DA= 2.75	DHA= 37.97
11 GLY ( 11 ) A	N ->	18 VAL ( 18 ) A	0 Sym=	1 Val= 0.522	DA= 3.35	DHA= 26.58
13 GLY ( 13 ) A	N ->	16 GLY ( 16 ) A	0 Sym=	1 Val= 0.469	DA= 2.85	DHA= 45.73
15 TYR ( 15 ) A	OH ->	148 PHE ( 152 ) A	0 Sym=	1 Val= 0.561	DA= 2.96	DHA= 24.80
18 VAL ( 18 ) A	N ->	11 GLY ( 11 ) A	0 Sym=	1 Val= 0.614	DA= 2.99	DHA= 22.32
19 TYR ( 19 ) A	N ->	32 LEU ( 32 ) A	0 Sym=	1 Val= 0.783	DA= 2.84	DHA= 6.83
20 LYS ( 20 ) A	N ->	8 GLU ( 8 ) A	0 Sym=	1 Val= 0.714	DA= 2.80	DHA= 13.03
21 ALA ( 21 ) A	N ->	30 VAL ( 30 ) A	0 Sym=	1 Val= 0.745	DA= 2.93	DHA= 13.91
22 ARG ( 22 ) A	N ->	5 GLN ( 5 ) A	0 Sym=	1 Val= 0.645	DA= 3.05	DHA= 23.91
22 ARG ( 22 ) A	NE ->	5 GLN ( 5 ) A	OE1 Sym=	1 Val= 0.090	DA= 3.37	DHA= 62.67
22 ARG ( 22 ) A	NH1 ->	27 GLY ( 27 ) A	0 Sym=	1 Val= 0.474	DA= 3.22	DHA= 33.44
23 ASN ( 23 ) A	N ->	28 GLU ( 28 ) A	0 Sym=	1 Val= 0.770	DA= 2.82	DHA= 9.43
24 LYS ( 24 ) A	N ->	3 ASN ( 3 ) A	0 Sym=	1 Val= 0.706	DA= 2.96	DHA= 11.26
25 LEU ( 25 ) A	N ->	23 ASN ( 23 ) A	OD1 Sym=	1 Val= 0.644	DA= 2.79	DHA= 43.06
26 THR ( 26 ) A	N ->	26 THR ( 26 ) A	OG1 Sym=	1 Val= 0.257	DA= 2.90	DHA= 82.32
26 THR ( 26 ) A	N ->	23 ASN ( 23 ) A	OD1 Sym=	1 Val= 0.212	DA= 3.32	DHA= 20.88
27 GLY ( 27 ) A	N ->	23 ASN ( 23 ) A	0 Sym=	1 Val= 0.509	DA= 2.72	DHA= 48.58
28 GLU ( 28 ) A	N ->	26 THR ( 26 ) A	OG1 Sym=	1 Val= 0.765	DA= 3.36	DHA= 13.02

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## Accessibility

- [Accessibility](#)  
Calculate the accessible molecular surface. Output per atom.
- [Buried surface.](#)  
Calculate the surface buried relative to the residue in vacuum.
- [Accessible Molecular Surface](#)  
Calculate the accessible molecular surface. Output per residue.
- [Relative Surface exposure.](#)  
Often normal accessibility calculations exaggerate things. This server calculates for every residue what its accessibility would be if you would have mutated it into an alanine.
- [Surface buried by a ligand.](#)  
This server calculates the molecular surface area that is buried because a ligand is bound to a macromolecule.

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## Accessibility

This is the WHAT\_IF output:

Date= 2009-02-23 14:11:43

Residue: 1 MET ( 1 ) A (Prp= 0.00)

Atom	X	Y	Z	Acc	B	WT	VdW	Colr	AtOK	Val	
N	25.6	56.2	23.7	5.6	66.5	1.0	1.7	340	+	37.00	N
CA	26.6	57.1	23.0	1.9	65.8	1.0	1.8	240	+	40.00	CA
C	26.0	58.6	22.9	1.2	63.8	1.0	1.8	240	+	31.00	C
O	24.9	58.8	23.4	1.9	64.8	1.0	1.4	120	+	30.00	O
CB	26.8	56.6	21.6	0.5	67.1	1.0	1.8	240	+	37.00	CB
CG	27.8	57.5	20.8	0.3	69.4	1.0	1.8	240	+	33.00	CG
SD	28.1	56.9	19.1	3.2	72.8	1.0	2.0	180	+	34.00	SD
CE	29.7	56.1	19.3	6.6	70.7	1.0	1.8	240	+	27.00	CE

Residue: 2 GLU ( 2 ) A (Prp= 0.00)

Atom	X	Y	Z	Acc	B	WT	VdW	Colr	AtOK	Val	
N	26.8	59.5	22.4	0.0	62.3	1.0	1.7	340	+	31.00	N
CA	26.4	60.9	22.3	2.4	60.1	1.0	1.8	240	+	32.00	CA
C	25.3	61.1	21.2	0.2	58.4	1.0	1.8	240	+	37.00	C
O	24.6	62.1	21.2	1.9	57.7	1.0	1.4	120	+	31.00	O
CB	27.6	61.7	21.9	7.3	60.1	1.0	1.8	240	+	24.00	CB
CG	28.8	61.6	22.8	11.4	60.6	1.0	1.8	240	+	17.00	CG
CD	29.4	60.2	22.7	3.3	61.4	1.0	1.8	240	+	19.00	CD
OE1	29.9	59.9	21.6	5.6	60.8	1.0	1.4	120	+	16.00	OE1
OE2	29.4	59.5	23.7	6.6	62.1	1.0	1.4	120	+	16.00	OE2

Residue: 3 ASN ( 3 ) A (Prp= 0.00)

Atom	X	Y	Z	Acc	B	WT	VdW	Colr	AtOK	Val	
N	25.1	60.1	20.3	0.0	55.8	1.0	1.7	340	+	40.00	N
CA	24.1	60.2	19.3	0.3	54.0	1.0	1.8	240	+	48.00	CA
C	22.7	59.8	19.8	0.0	53.0	1.0	1.8	240	+	50.00	C
O	21.7	59.8	19.8	0.0	53.0	1.0	1.4	120	+	44.00	O

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## Buried surface.

This is the WHAT\_IF output:

Date= 2009-02-23 14:06:53

Residue: 1 MET ( 1 ) A (Prp= 0.00)  
Phi= 999.9 Psi= 177.6 Omega=-179.3

Atom	X	Y	Z	Acc	B	WT	VdW	Colr	OK	Use	Vac.	%
N	25.6	56.2	23.7	5.6	66.5	1.0	1.7	340	+	-	16.7	33.6
CA	26.6	57.1	23.0	1.9	65.8	1.0	1.8	240	+	-	4.2	45.8
C	26.0	58.6	22.9	1.2	63.8	1.0	1.8	240	+	-	1.9	63.6
O	24.9	58.8	23.4	1.9	64.8	1.0	1.4	120	+	-	6.6	29.0
CB	26.8	56.6	21.6	0.5	67.1	1.0	1.8	240	+	-	7.0	7.5
CG	27.8	57.5	20.8	0.3	69.4	1.0	1.8	240	+	-	3.3	10.5
SD	28.1	56.9	19.1	3.2	72.8	1.0	2.0	180	+	-	19.4	16.7
CE	29.7	56.1	19.3	6.6	70.7	1.0	1.8	240	+	-	21.7	30.6
				21.4							80.7	26.5

Residue: 2 GLU ( 2 ) A (Prp= 0.00)  
Phi= -74.0 Psi= -17.8 Omega=-179.5

Atom	X	Y	Z	Acc	B	WT	VdW	Colr	OK	Use	Vac.	%
N	26.8	59.5	22.4	0.0	62.3	1.0	1.7	340	+	-	0.5	0.0
CA	26.4	60.9	22.3	2.4	60.1	1.0	1.8	240	+	-	2.6	93.3
C	25.3	61.1	21.2	0.2	58.4	1.0	1.8	240	+	-	0.9	20.0
O	24.6	62.1	21.2	1.9	57.7	1.0	1.4	120	+	-	7.4	25.7
CB	27.6	61.7	21.9	7.3	60.1	1.0	1.8	240	+	-	8.2	89.4
CG	28.8	61.6	22.8	11.4	60.6	1.0	1.8	240	+	-	11.4	100.0
CD	29.4	60.2	22.7	3.3	61.4	1.0	1.8	240	+	-	3.3	100.0
OE1	29.9	59.9	21.6	5.6	60.8	1.0	1.4	120	+	-	9.2	60.9
OE2	29.4	59.5	23.7	6.6	62.1	1.0	1.4	120	+	-	6.7	98.4
				38.7							50.1	77.2

Residue: 3 ASN ( 3 ) A (Prp= 0.00)  
Phi= 81.1 Psi= 1.2 Omega=179.3

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# Atomic contacts

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## Atomic contacts

- [Interatomic bumps.](#)  
Check for (too) short interatomic distances (bumps).
- [Residue contact diagonal plot](#)  
A two dimensional plot is generated. The sequence is placed along each of the axes. Little squares indicate that the corresponding residues on the two axes make at least one atomic contact in the PDB file.
- [Interatomic contacts.](#)  
This server calculates contacts between all atoms in your PDB file, including water. All contacts are listed only once. Symmetry contacts are excluded. Contact distance 0.25 Ångstrom.
- [Interatomic contacts.](#)  
This server calculates contacts between all atoms in your PDB file, including water. All contacts are listed only once. Symmetry contacts are excluded. Contact distance 1.0 Ångstrom.

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# Atomic contacts

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## Interatomic contacts.

The list of contacting atom pairs:

Date= 2009-02-23 14:41:21

Calculate contacts 1 - 295 -> 1 - 295 d= 0.250

1	1 MET ( 1 ) A	C	↔	3 ASN ( 3 ) A	N	D= 3.17	H-ene= -- 0	Sym= (B-B)
2	1 MET ( 1 ) A	SD	↔	3 ASN ( 3 ) A	ND2	D= 3.08	H-ene= 0.11	Sym= (S-S)
3	1 MET ( 1 ) A	CE	↔	66 ILE ( 70 ) A	CG2	D= 3.68	H-ene= -- 0	Sym= (S-S)
4	2 GLU ( 2 ) A	C	↔	4 PHE ( 4 ) A	N	D= 3.16	H-ene= -- 0	Sym= (B-B)
5	2 GLU ( 2 ) A	O	↔	4 PHE ( 4 ) A	N	D= 3.35	H-ene= -- 0	Sym= (B-B)
6	3 ASN ( 3 ) A	O	↔	24 LYS ( 24 ) A	N	D= 2.96	H-ene= 0.71	Sym= (B-B)
7	3 ASN ( 3 ) A	CG	↔	295 HOH ( 635 ) -	O	D= 3.32	H-ene= -- 0	Sym= (S-W)
8	3 ASN ( 3 ) A	ND2	↔	295 HOH ( 635 ) -	O	D= 2.80	H-ene= 0.68	Sym= (S-W)
9	4 PHE ( 4 ) A	CA	↔	22 ARG ( 22 ) A	O	D= 3.34	H-ene= -- 0	Sym= (B-B)
10	4 PHE ( 4 ) A	CB	↔	32 LEU ( 32 ) A	CD1	D= 3.62	H-ene= -- 0	Sym= (S-S)
11	4 PHE ( 4 ) A	CG	↔	32 LEU ( 32 ) A	CD1	D= 3.84	H-ene= -- 0	Sym= (S-S)
12	4 PHE ( 4 ) A	CE1	↔	66 ILE ( 70 ) A	CD1	D= 3.57	H-ene= -- 0	Sym= (S-S)
13	5 GLN ( 5 ) A	C	↔	7 VAL ( 7 ) A	N	D= 3.57	H-ene= -- 0	Sym= (B-B)
14	5 GLN ( 5 ) A	O	↔	7 VAL ( 7 ) A	N	D= 3.08	H-ene= 0.27	Sym= (B-B)
15	5 GLN ( 5 ) A	O	↔	21 ALA ( 21 ) A	CA	D= 3.22	H-ene= -- 0	Sym= (B-B)
16	5 GLN ( 5 ) A	O	↔	21 ALA ( 21 ) A	CB	D= 3.32	H-ene= -- 0	Sym= (B-S)
17	5 GLN ( 5 ) A	N	↔	22 ARG ( 22 ) A	O	D= 3.07	H-ene= 0.77	Sym= (B-B)
18	5 GLN ( 5 ) A	O	↔	22 ARG ( 22 ) A	N	D= 3.05	H-ene= 0.64	Sym= (B-B)
19	5 GLN ( 5 ) A	CG	↔	22 ARG ( 22 ) A	CB	D= 3.50	H-ene= -- 0	Sym= (S-S)
20	5 GLN ( 5 ) A	OE1	↔	22 ARG ( 22 ) A	CD	D= 3.32	H-ene= -- 0	Sym= (S-S)
21	5 GLN ( 5 ) A	CB	↔	24 LYS ( 24 ) A	CE	D= 3.68	H-ene= -- 0	Sym= (S-S)
22	6 LYS ( 6 ) A	C	↔	8 GLU ( 8 ) A	N	D= 3.46	H-ene= -- 0	Sym= (B-B)
23	6 LYS ( 6 ) A	CD	↔	19 TYR ( 19 ) A	CG	D= 3.79	H-ene= -- 0	Sym= (S-S)
24	6 LYS ( 6 ) A	CD	↔	19 TYR ( 19 ) A	CD2	D= 3.47	H-ene= -- 0	Sym= (S-S)
25	6 LYS ( 6 ) A	CD	↔	19 TYR ( 19 ) A	CE2	D= 3.65	H-ene= -- 0	Sym= (S-S)
26	7 VAL ( 7 ) A	N	↔	20 LYS ( 20 ) A	O	D= 2.75	H-ene= 0.58	Sym= (B-B)
27	7 VAL ( 7 ) A	CB	↔	20 LYS ( 20 ) A	O	D= 3.36	H-ene= -- 0	Sym= (S-B)

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# Coordinate manipulation

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## Coordinate manipulations

- [Center a structure](#)  
Put the center of gravity of a structure in the origin.
- [Center of a structure](#)  
Determines the center of gravity.

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If you have detected any error, or have any question or suggestion, please send an Email to Gert Vriend.  
Roland Krause, Jens Erik Nielsen, [Gert Vriend](#).

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Last modified Wed Jan 21 19:41:58 2009

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# Crystal symmetry

The screenshot shows a Mozilla Firefox browser window with the address bar at <http://swift.cmbi.ru.nl/servers/html/index.html>. The page content is as follows:

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## Crystal symmetry

- [Contacts with symmetry related molecules in a crystal](#)  
This server calculates contacts between pairs of atoms. Pairs of atoms are analysed only if both atoms sit in different asymmetric units. The contact cutoff is 0.5 Ångstrom.
- [Contacts with symmetry related molecules in a crystal](#)  
This server calculates contacts between pairs of atoms. Pairs of atoms are analysed only if both atoms sit in different asymmetric units. The contact cutoff is 2.5 Ångstrom.
- [Contacts with symmetry related molecules in a crystal](#)  
This server calculates contacts between pairs of atoms. Pairs of atoms are analysed only if both atoms sit in different asymmetric units. The contact cutoff is 5.0 Ångstrom.
- [Add shell of symmetry related residues](#)  
This server will add a 1.0 Ångstrom shell of symmetry related residues around the molecule read from the PDB file.
- [Add shell of symmetry related residues](#)  
This server will add a 5.0 Ångstrom shell of symmetry related residues around the molecule read from the PDB file.

The browser's address bar at the bottom shows <http://swift.cmbi.ru.nl/servers/html/symmetry.html>.



# Crystal symmetry

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## Contacts with symmetry related molecules in a crystal

The list of contacting atom pairs:

Date= 2009-02-23 15:26:00

You are prompted for the first range

Calculate contacts 1 - 295 -> 1 - 295 d= 2.500

1	1 MET ( 1 ) A	CG	<>	175 TYR ( 179 ) A	CB	D= 5.39	H-ene= -- 0	Sym= 9 (S-S)
2	1 MET ( 1 ) A	CG	<>	175 TYR ( 179 ) A	CG	D= 5.72	H-ene= -- 0	Sym= 9 (S-S)
3	1 MET ( 1 ) A	CG	<>	175 TYR ( 179 ) A	CD1	D= 5.68	H-ene= -- 0	Sym= 9 (S-S)
4	1 MET ( 1 ) A	SD	<>	175 TYR ( 179 ) A	N	D= 5.94	H-ene= -- 0	Sym= 9 (S-B)
5	1 MET ( 1 ) A	SD	<>	175 TYR ( 179 ) A	CA	D= 4.62	H-ene= -- 0	Sym= 9 (S-B)
6	1 MET ( 1 ) A	SD	<>	175 TYR ( 179 ) A	C	D= 4.84	H-ene= -- 0	Sym= 9 (S-B)
7	1 MET ( 1 ) A	SD	<>	175 TYR ( 179 ) A	O	D= 5.34	H-ene= -- 0	Sym= 9 (S-B)
8	1 MET ( 1 ) A	SD	<>	175 TYR ( 179 ) A	CB	D= 3.64	H-ene= -- 0	Sym= 9 (S-S)
9	1 MET ( 1 ) A	SD	<>	175 TYR ( 179 ) A	CG	D= 4.15	H-ene= -- 0	Sym= 9 (S-S)
10	1 MET ( 1 ) A	SD	<>	175 TYR ( 179 ) A	CD1	D= 4.37	H-ene= -- 0	Sym= 9 (S-S)
11	1 MET ( 1 ) A	SD	<>	175 TYR ( 179 ) A	CD2	D= 5.05	H-ene= -- 0	Sym= 9 (S-S)
12	1 MET ( 1 ) A	SD	<>	175 TYR ( 179 ) A	CE1	D= 5.39	H-ene= -- 0	Sym= 9 (S-S)
13	1 MET ( 1 ) A	SD	<>	175 TYR ( 179 ) A	CE2	D= 5.96	H-ene= -- 0	Sym= 9 (S-S)
14	1 MET ( 1 ) A	SD	<>	175 TYR ( 179 ) A	CZ	D= 6.10	H-ene= -- 0	Sym= 9 (S-S)
15	1 MET ( 1 ) A	CE	<>	175 TYR ( 179 ) A	CA	D= 5.10	H-ene= -- 0	Sym= 9 (S-B)
16	1 MET ( 1 ) A	CE	<>	175 TYR ( 179 ) A	C	D= 4.85	H-ene= -- 0	Sym= 9 (S-B)
17	1 MET ( 1 ) A	CE	<>	175 TYR ( 179 ) A	O	D= 4.98	H-ene= -- 0	Sym= 9 (S-B)
18	1 MET ( 1 ) A	CE	<>	175 TYR ( 179 ) A	CB	D= 4.19	H-ene= -- 0	Sym= 9 (S-S)
19	1 MET ( 1 ) A	CE	<>	175 TYR ( 179 ) A	CG	D= 5.10	H-ene= -- 0	Sym= 9 (S-S)
20	1 MET ( 1 ) A	CE	<>	175 TYR ( 179 ) A	CD1	D= 5.69	H-ene= -- 0	Sym= 9 (S-S)
21	1 MET ( 1 ) A	CE	<>	175 TYR ( 179 ) A	CD2	D= 5.83	H-ene= -- 0	Sym= 9 (S-S)
22	1 MET ( 1 ) A	CG	<>	176 TYR ( 180 ) A	O	D= 5.23	H-ene= -- 0	Sym= 9 (S-B)
23	1 MET ( 1 ) A	SD	<>	176 TYR ( 180 ) A	N	D= 5.00	H-ene= -- 0	Sym= 9 (S-B)
24	1 MET ( 1 ) A	SD	<>	176 TYR ( 180 ) A	CA	D= 5.77	H-ene= -- 0	Sym= 9 (S-B)
25	1 MET ( 1 ) A	SD	<>	176 TYR ( 180 ) A	C	D= 5.18	H-ene= -- 0	Sym= 9 (S-B)

Done

# Other options

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## Average B factors

Residue with secondary structure, averaged B factor for backbone, side chain, and all (heavy) atoms:

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B-factors averaged over:

Residue	Chain	Backbone	Side chain	All
1 MET ( 1 )	A	64.9725	69.7275	67.4750
2 GLU ( 2 )	A T	59.3700	60.7980	60.2744
3 ASN ( 3 )	A T	53.6350	52.0100	52.9475
4 PHE ( 4 )	A S	50.3975	42.3129	45.3436
5 GLN ( 5 )	A S	50.3000	59.4240	55.4800
6 LYS ( 6 )	A S	48.8750	50.7200	50.0111
7 VAL ( 7 )	A S	47.7400	45.4633	46.9071
8 GLU ( 8 )	A S	46.2275	50.8820	48.9244
9 LYS ( 9 )	A S	47.0050	49.6160	48.5667
10 ILE ( 10 )	A S	48.0375	47.0900	47.6888
11 GLY ( 11 )	A S	47.5375	-1.0000	47.5375
12 GLU ( 12 )	A S	45.4225	53.7880	50.1811
13 GLY ( 13 )	A	38.9275	-1.0000	38.9275
14 THR ( 14 )	A T	35.6600	37.1467	36.4400
15 TYR ( 15 )	A T	31.0475	32.5175	32.1108
16 GLY ( 16 )	A T	27.7700	-1.0000	27.7700
17 VAL ( 17 )	A S	28.6475	32.2900	30.3514
18 VAL ( 18 )	A S	27.0100	26.8700	27.0929
19 TYR ( 19 )	A S	25.7900	45.1838	38.8025
20 LYS ( 20 )	A S	24.5725	25.5140	25.2067
21 ALA ( 21 )	A S	26.4075	25.9700	26.5200
22 ARG ( 22 )	A S	32.2350	35.0171	34.0964
23 ASN ( 23 )	A S	41.6075	43.5675	42.7125
24 LYS ( 24 )	A T	48.5050	47.2500	47.9189
25 LEU ( 25 )	A T	52.7225	55.7525	54.3625
26 THR ( 26 )	A T	50.7900	52.4533	51.6457

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# Residue contacts

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## Residue contact diagonal plot

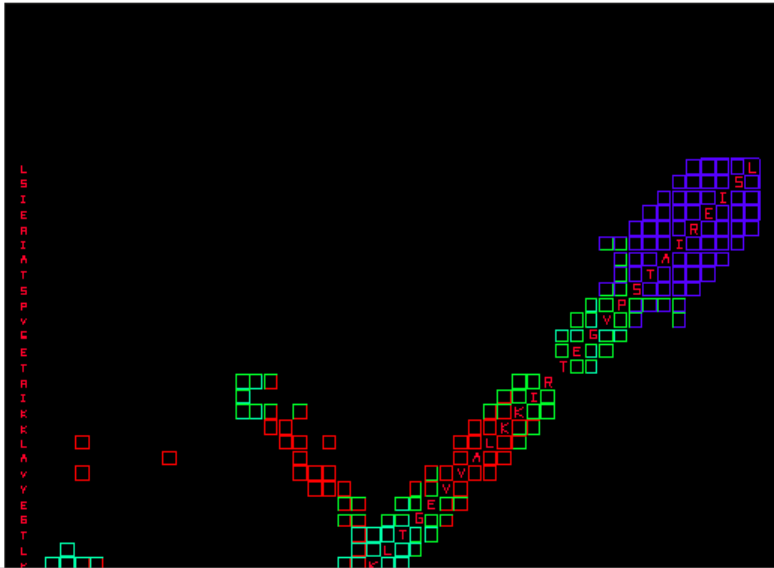
Residue-residue contact plot.

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If you have detected any error, or have any question or suggestion, please send an Email to Gert Vriend.

Roland Krause, Jens Erik Nielsen, [Gert Vriend](#).

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