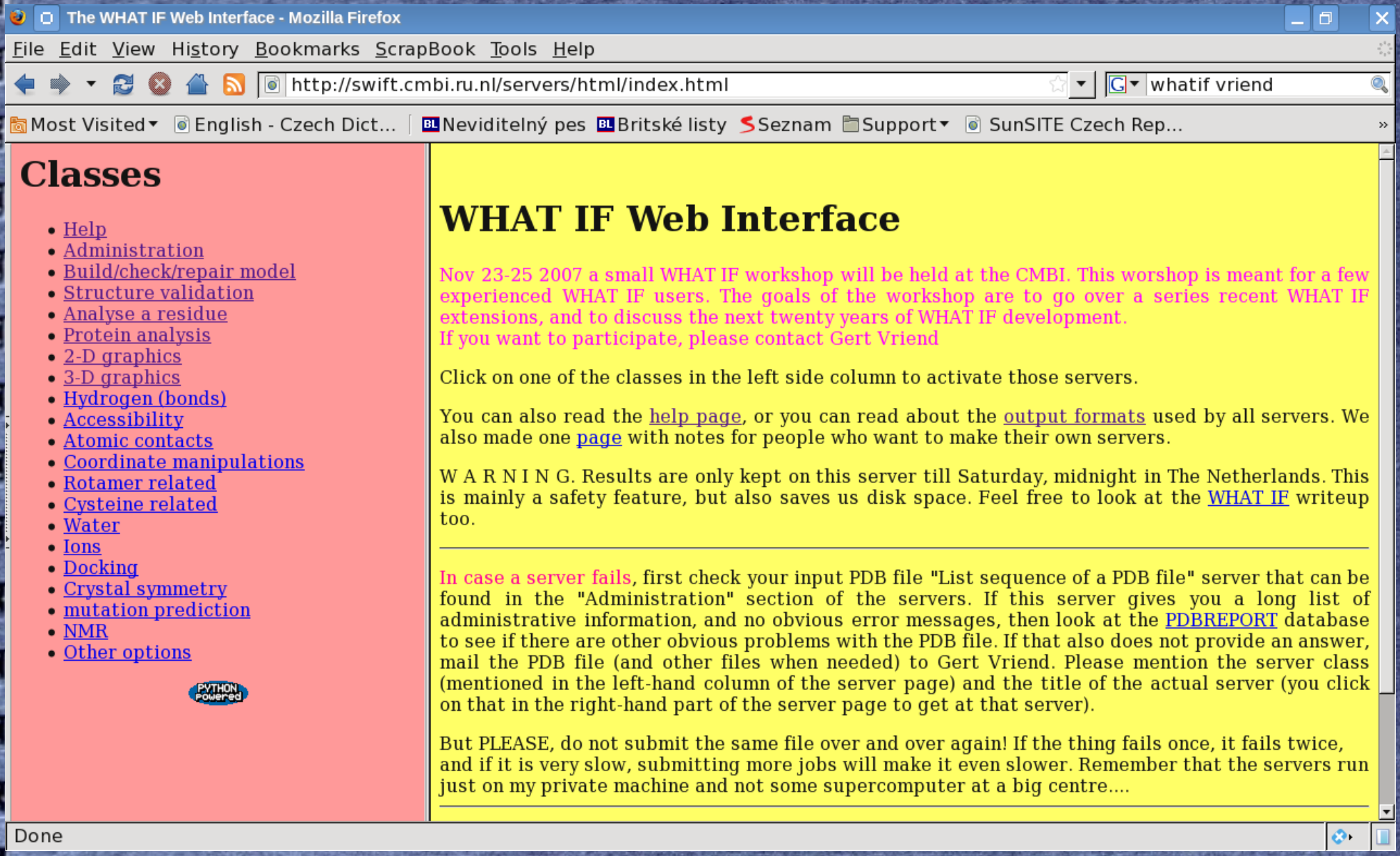
What If server

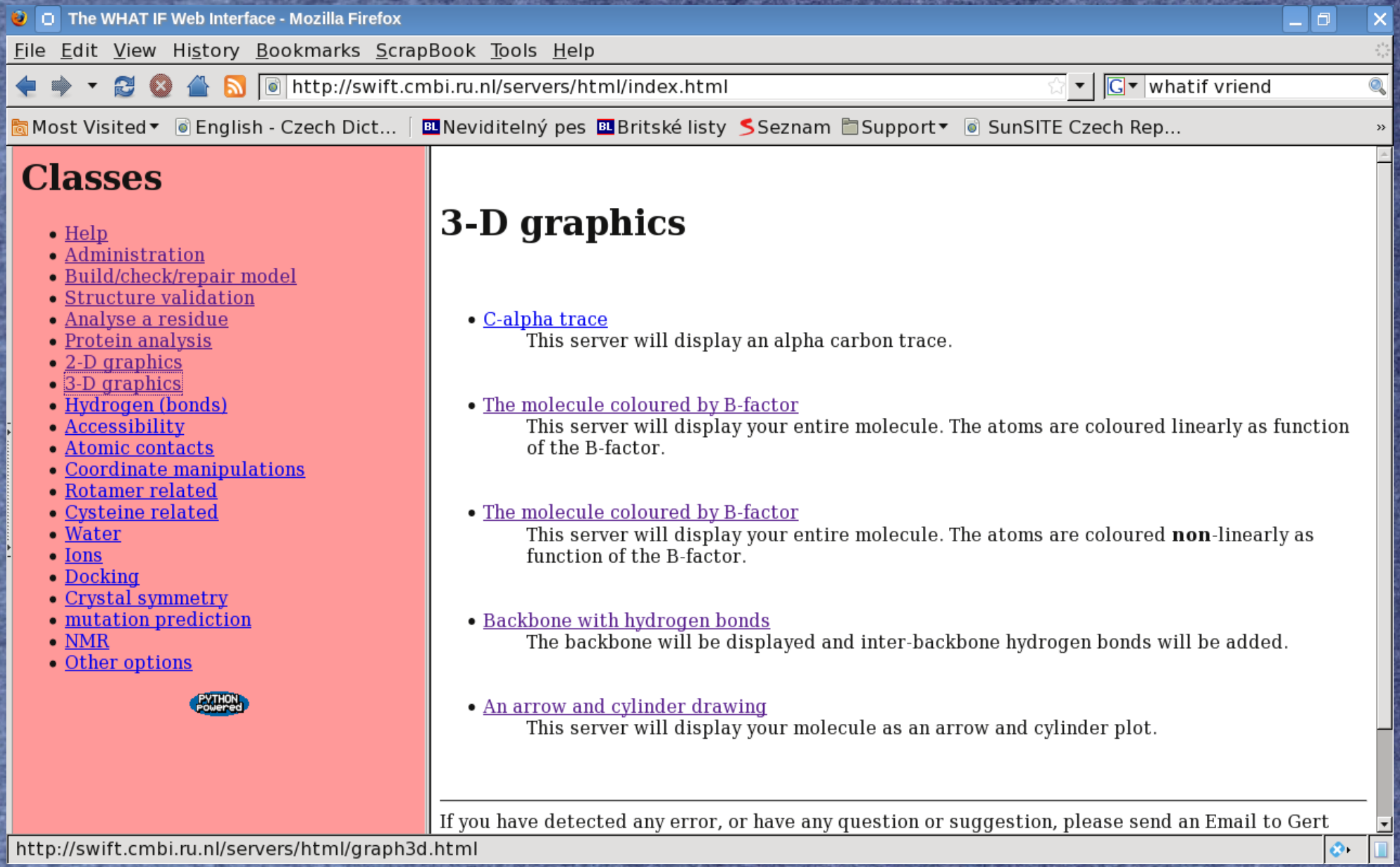
http://swift.cmbi.ru.nl/servers/html/index.html

Molekula pro analýzu – pdb kód 1PW2

What If server



3-D graphics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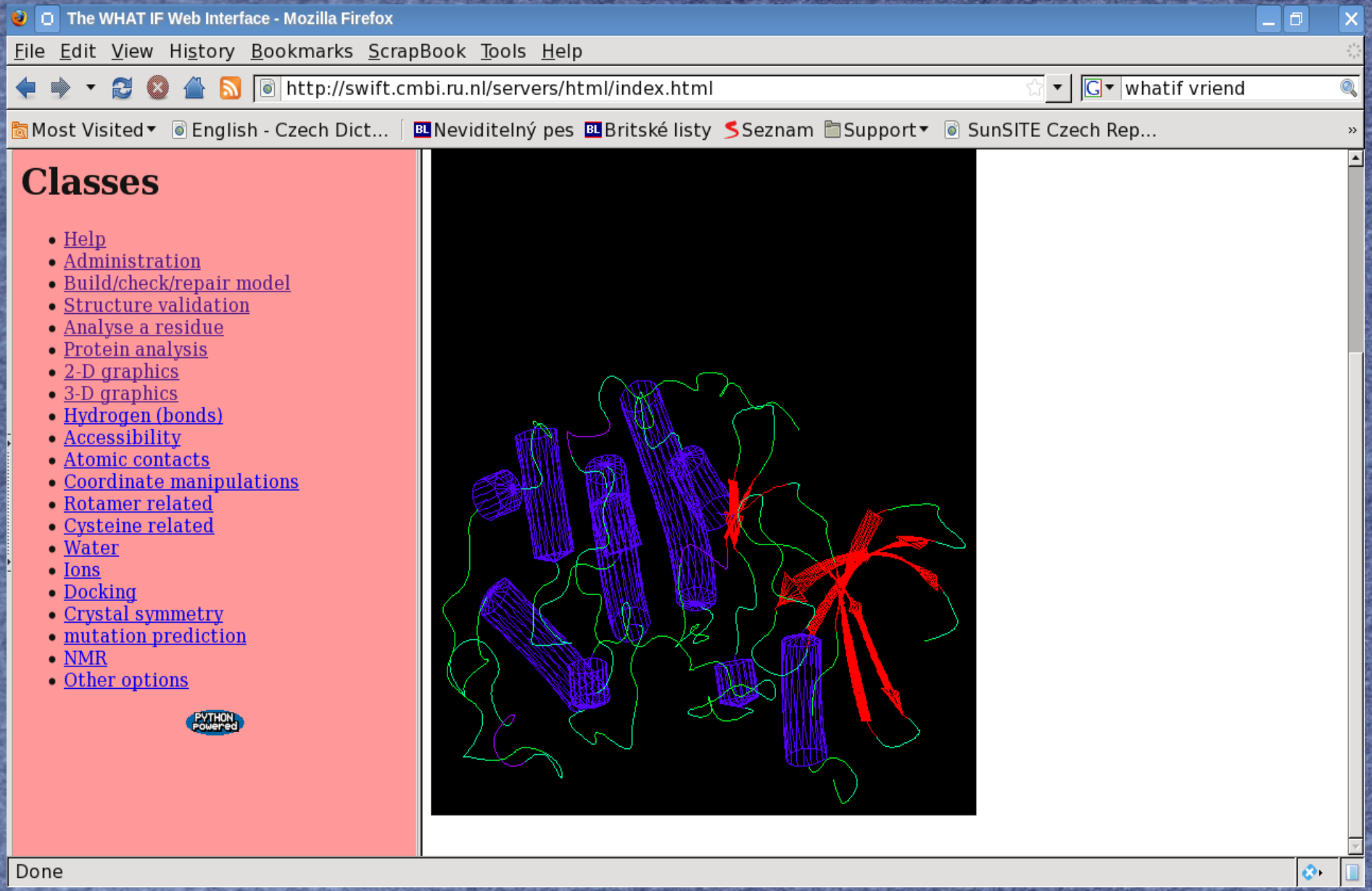
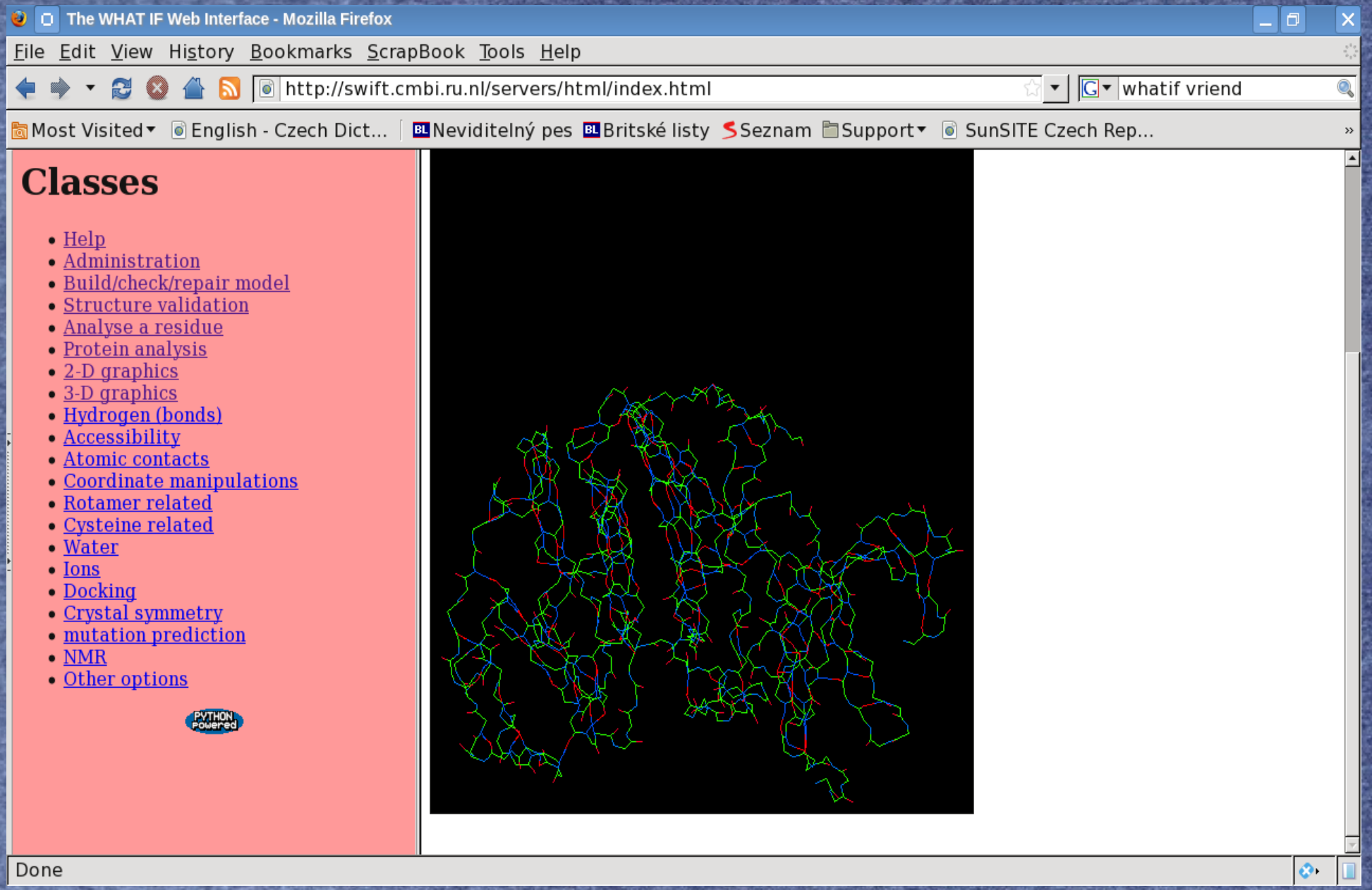
C-alpha trace
This server will display an alpha carbon trace.
The molecule coloured by B-factor
This server will display your entire molecule. The atoms are coloured linearly as function of the B-factor.
The molecule coloured by B-factor
This server will display your entire molecule. The atoms are coloured 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.
If you have detected any error, or have any question or suggestion, please send an Email to Gert
http://swift.cmbi.ru.nl/servers/html/graph3d.html

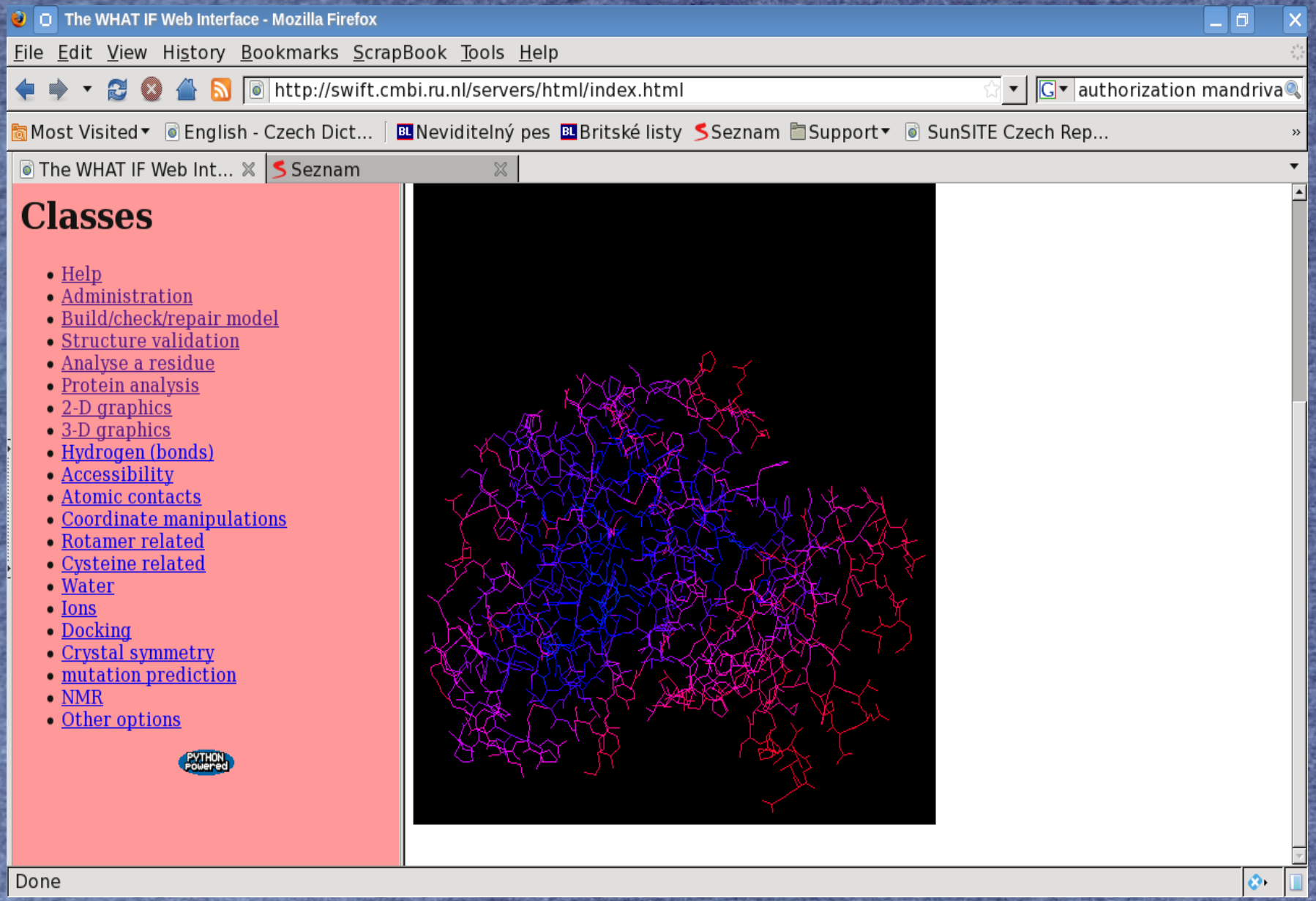
3-D graphics – arrows and cylinders



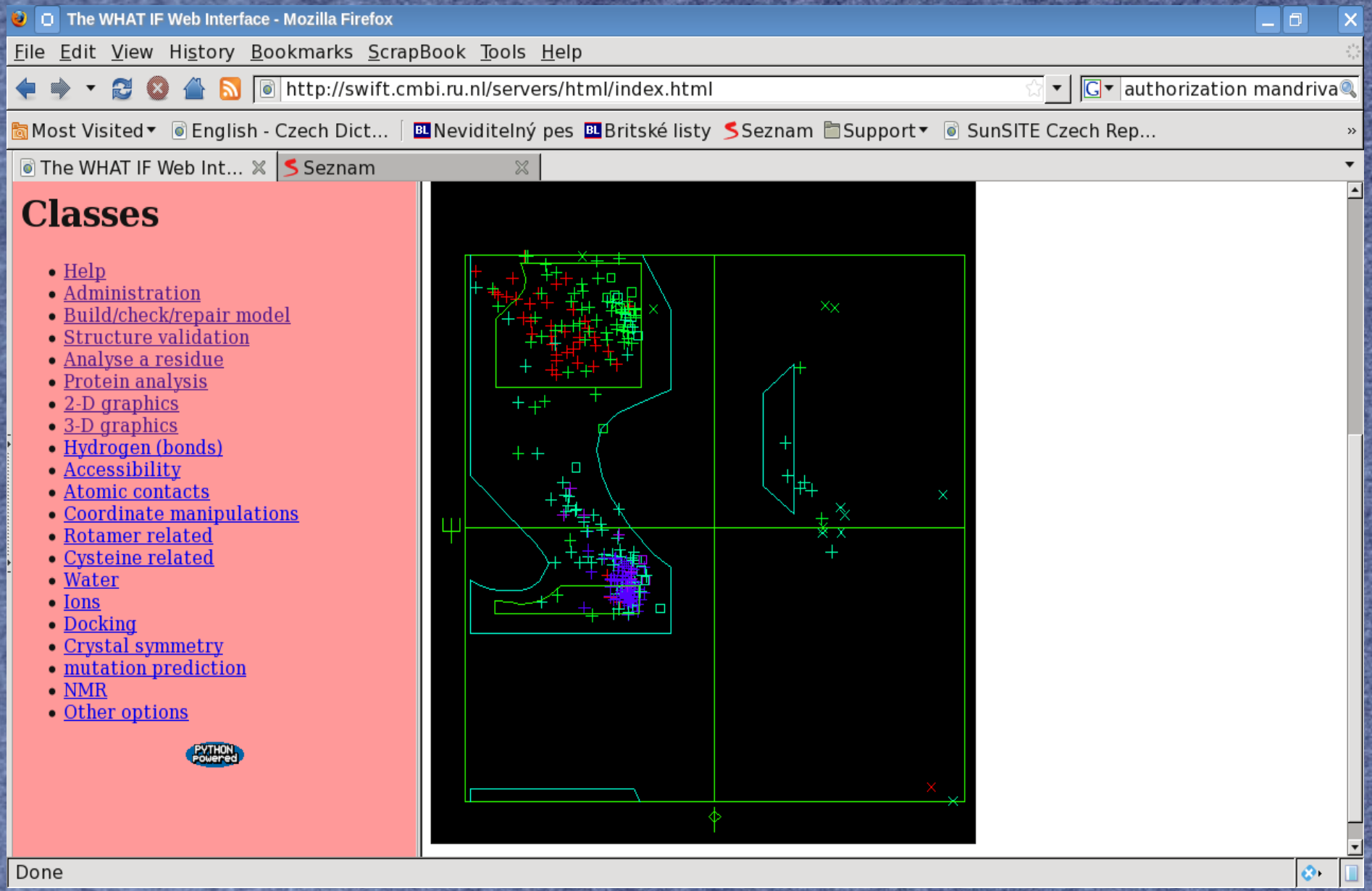
3-D graphics – backbone with H-bonds



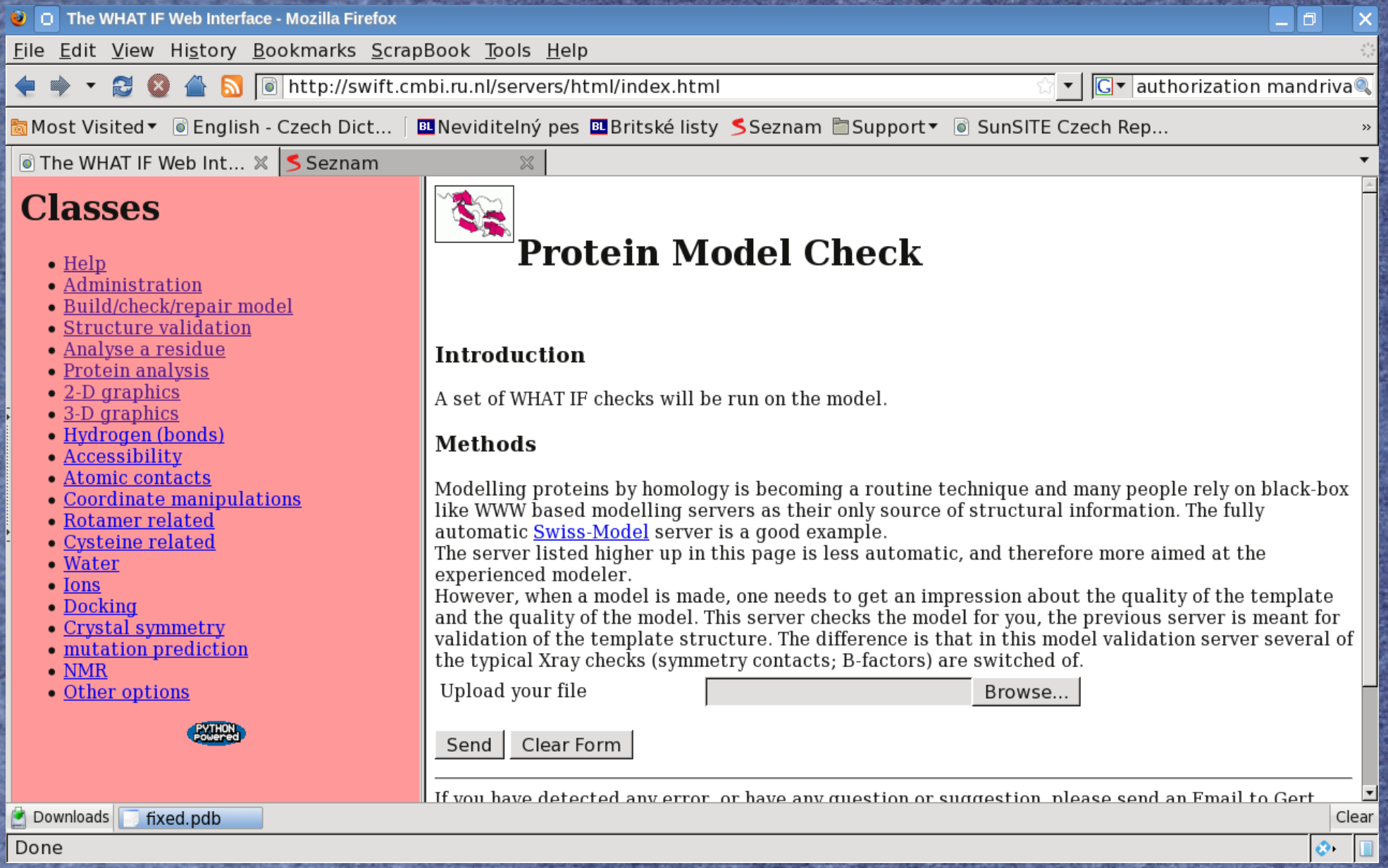
3-D graphics – B-factor coloring



2-D graphics – Ramachandran plot



Build, check, repair model



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 /home/zdenek/Desktop/1PW Browse...

Send Clear Form

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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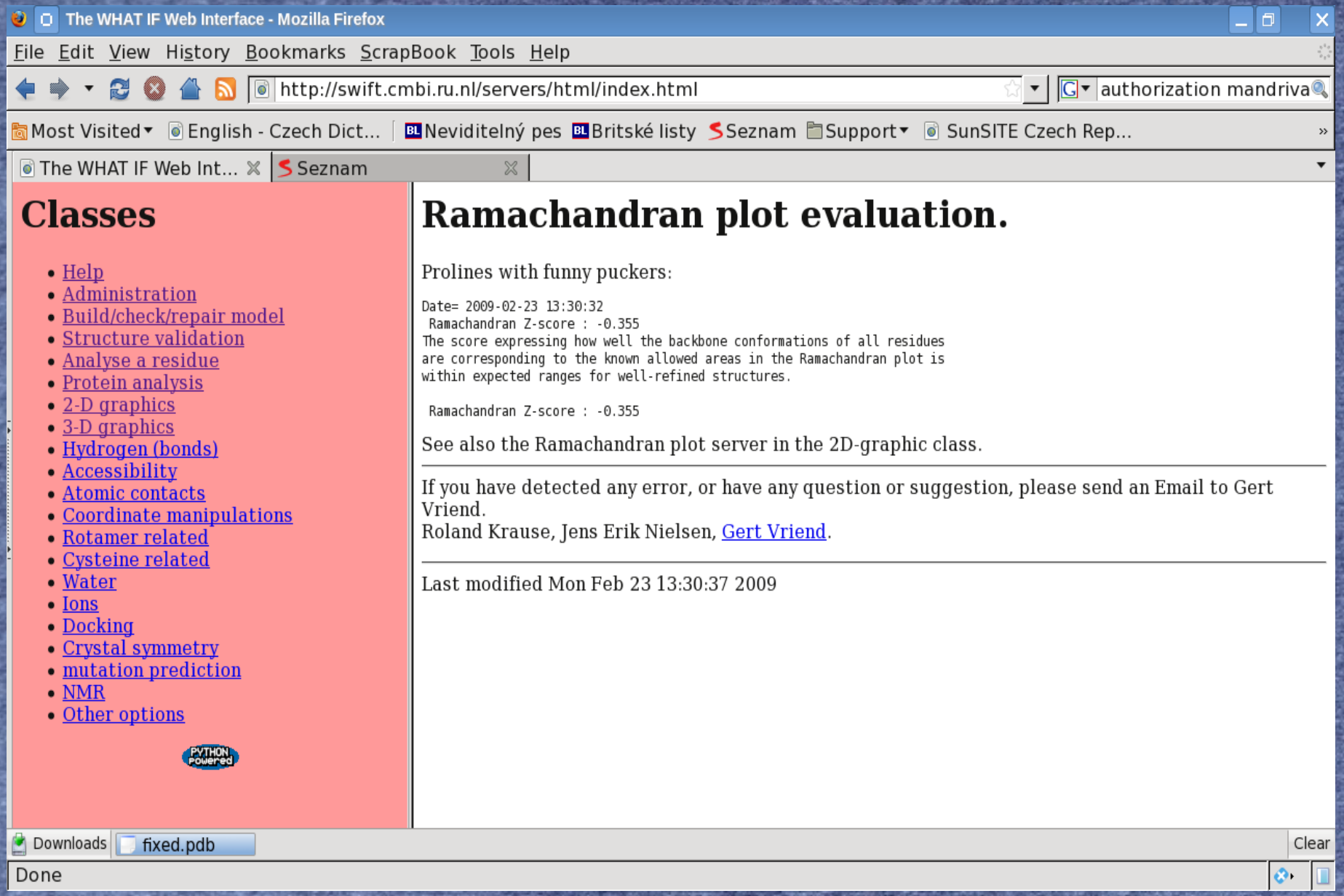
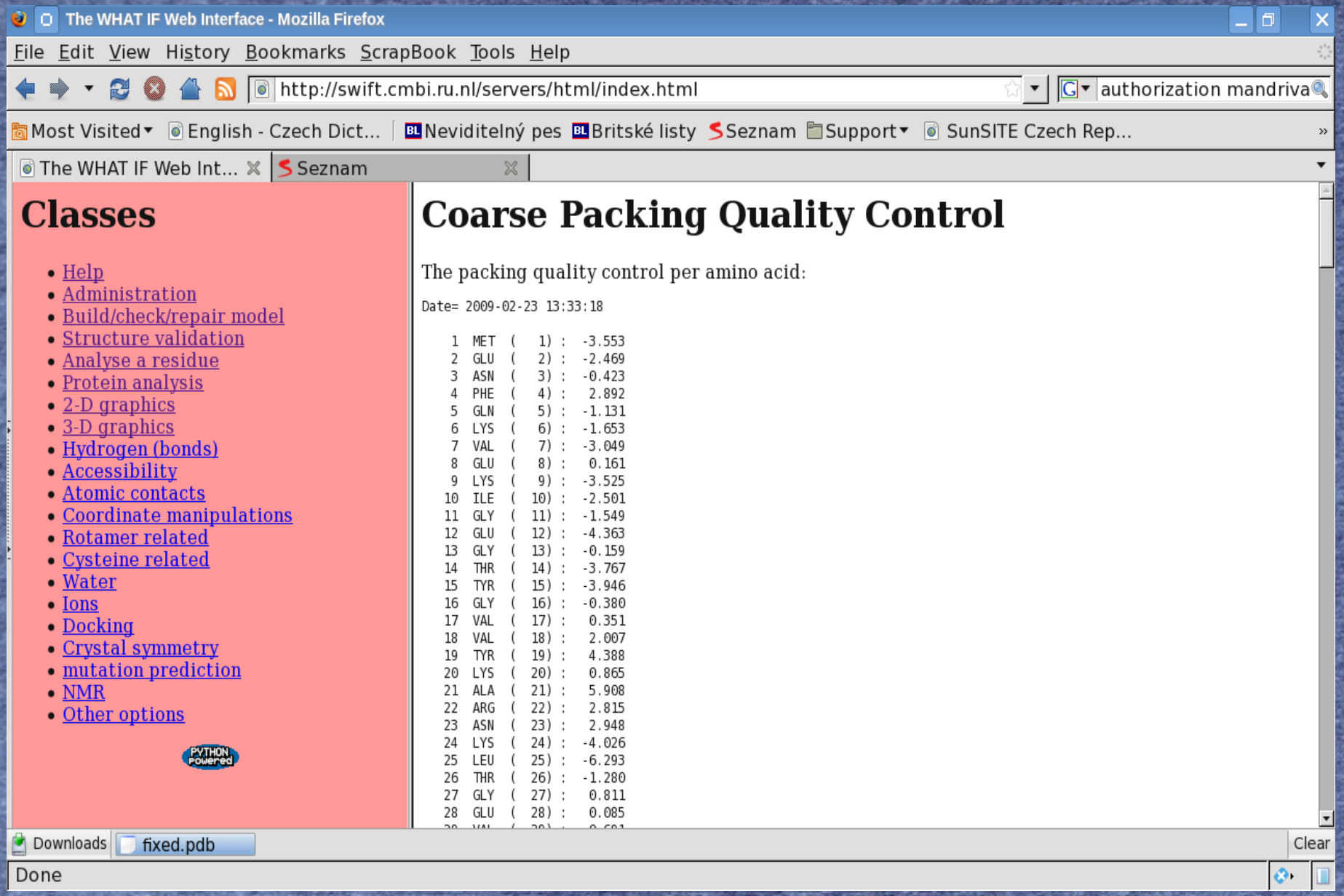
Done

Structure validation



Structure validation



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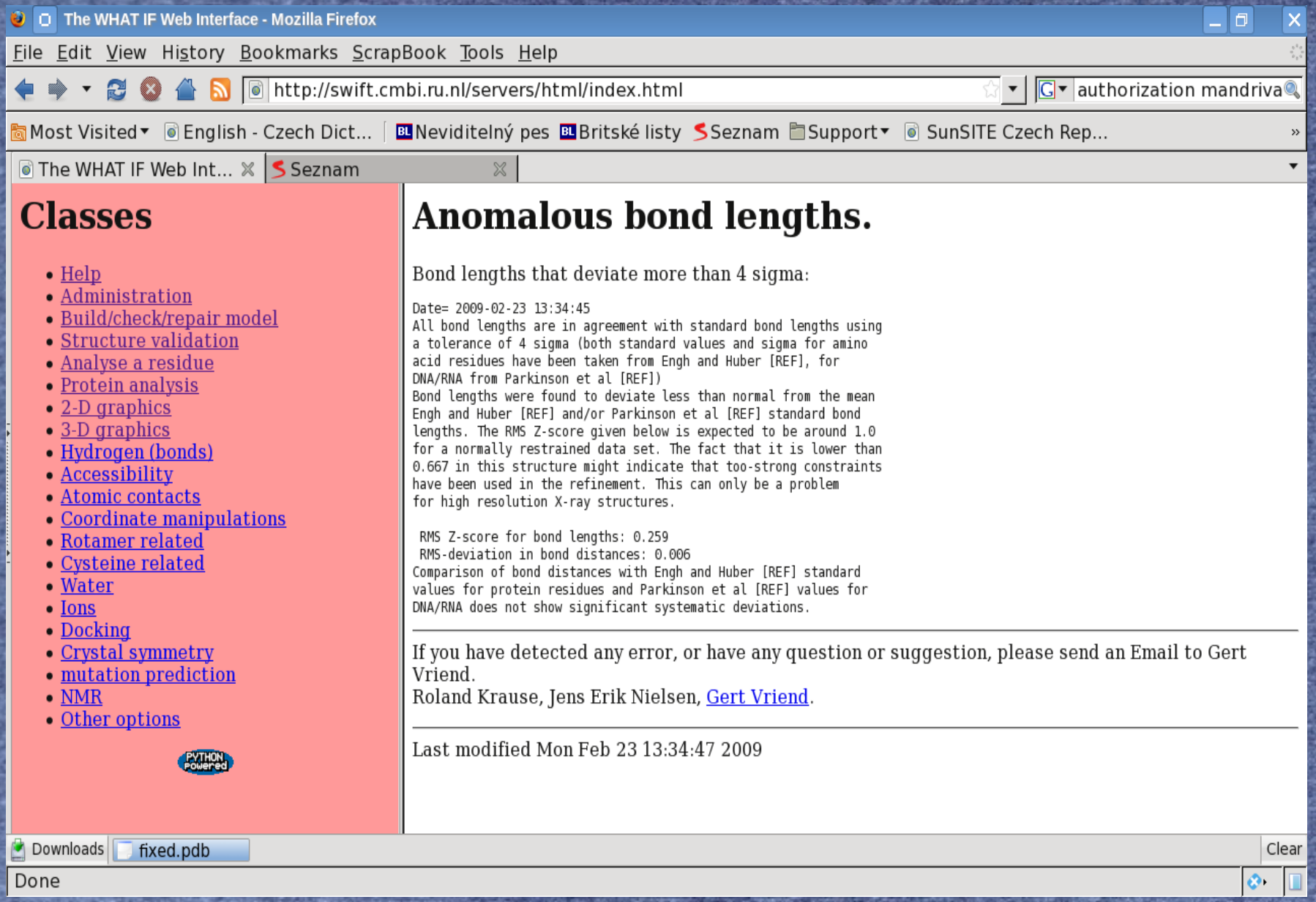

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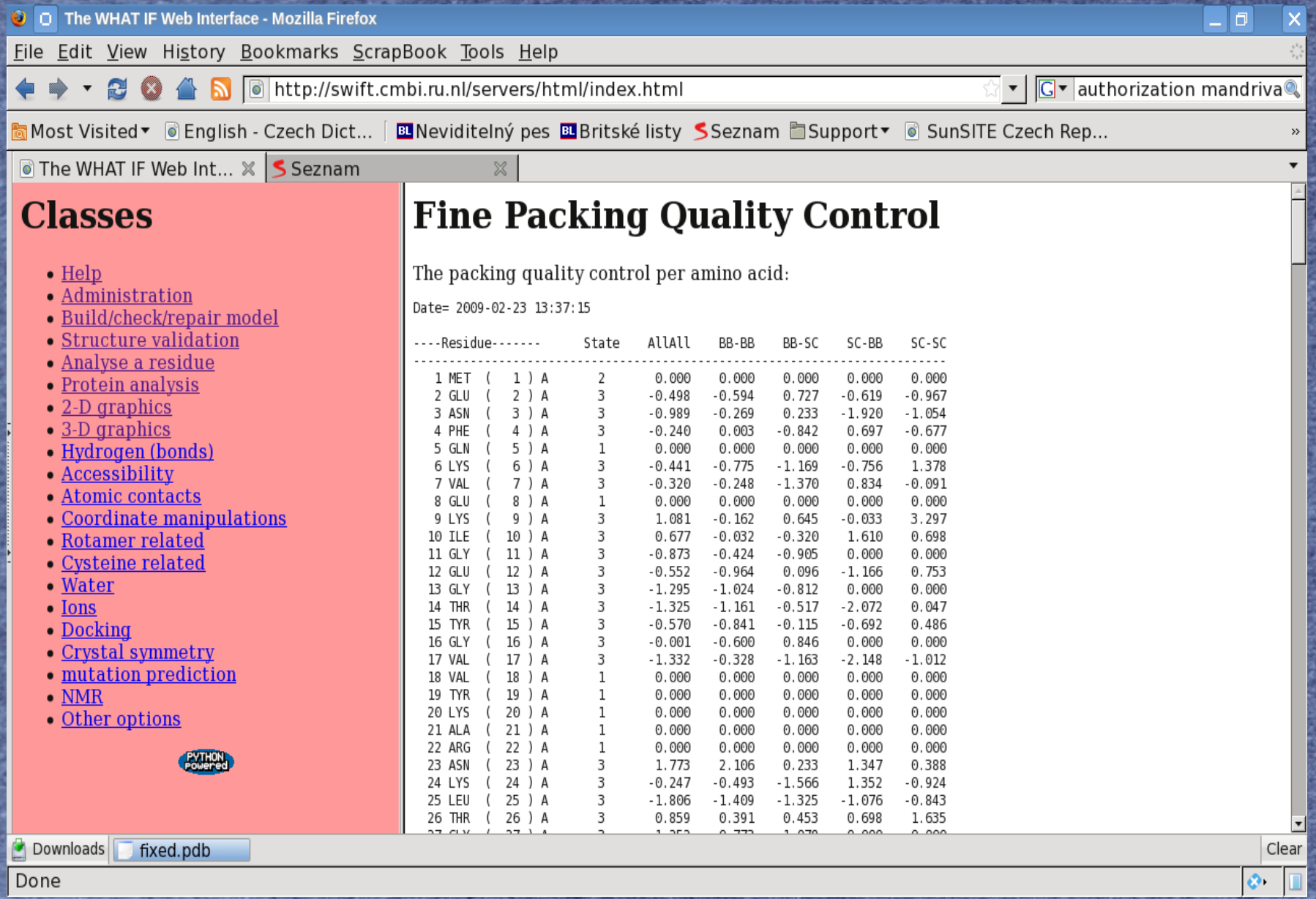
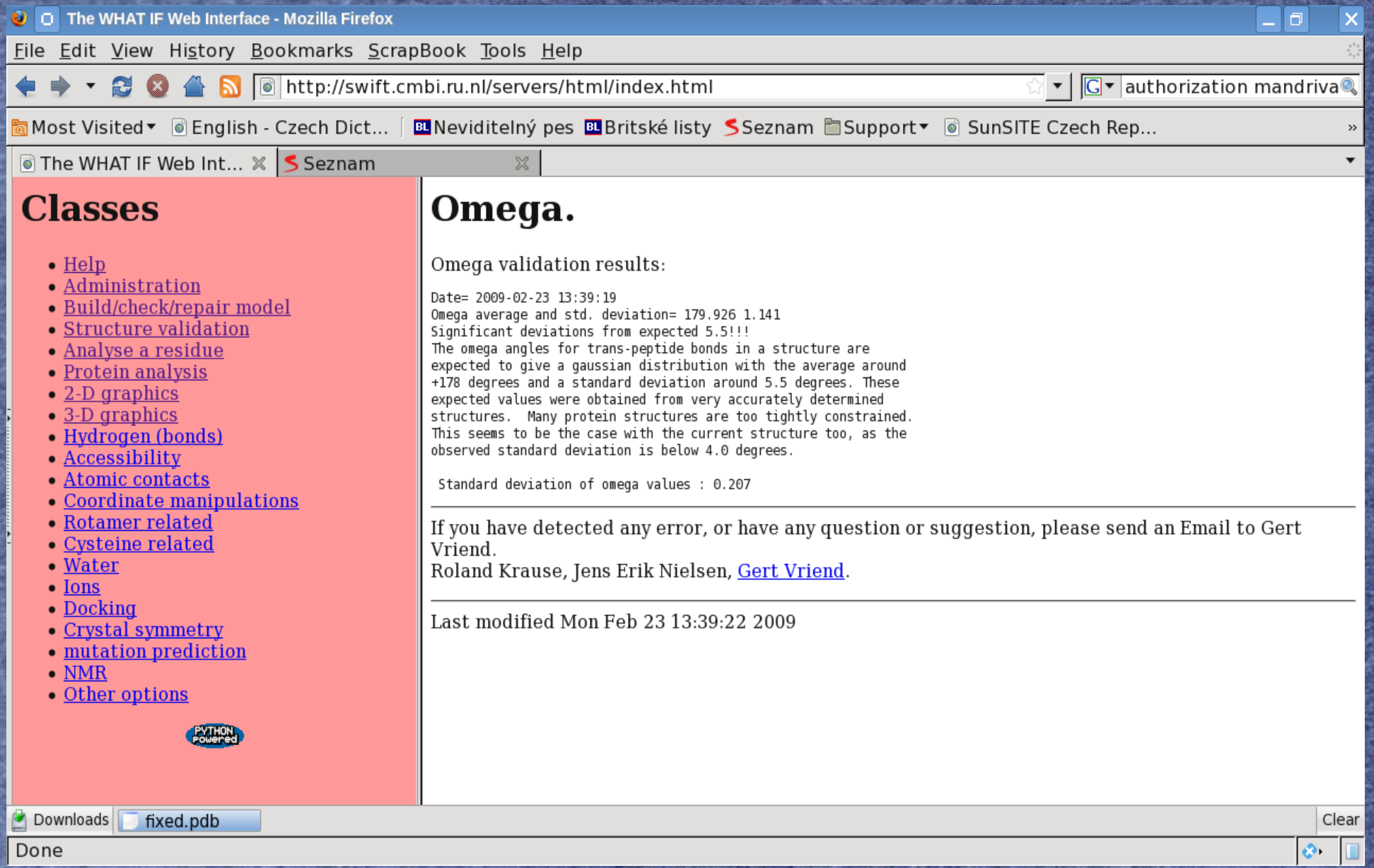
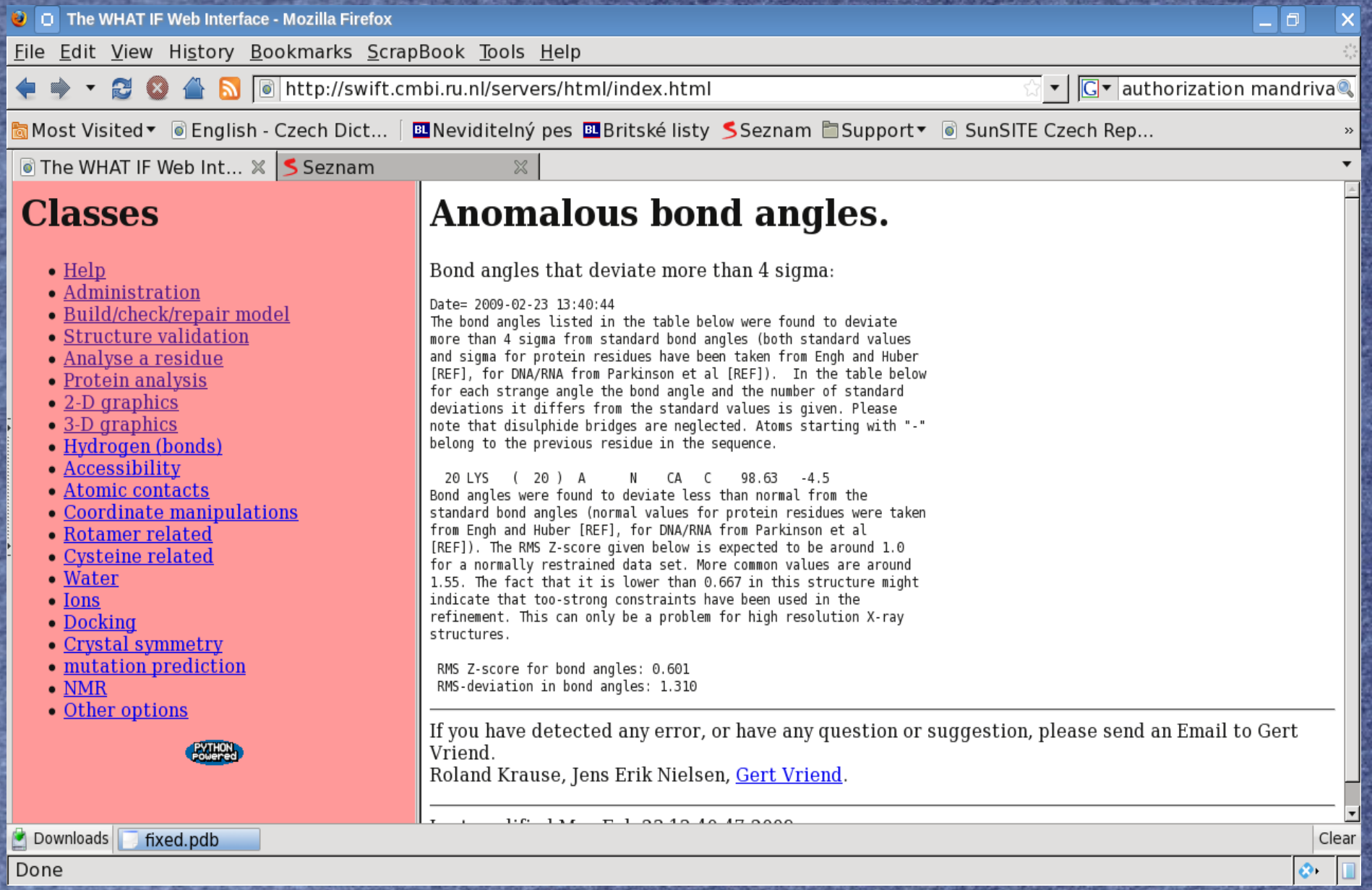


----Residue-------	State	AllAll	BB-BB	BB-SC	SC-BB	SC-SC
1 MET (1) A	2	0.000	0.000	0.000	0.000	0.000
2 GLU (2) A	3	-0.498	-0.594	0.727	-0.619	-0.967
3 ASN (3) A	3	-0.989	-0.269	0.233	-1.920	-1.054
4 PHE (4) A	3	-0.240	0.003	-0.842	0.697	-0.677
5 GLN (5) A	1	0.000	0.000	0.000	0.000	0.000
6 LYS (6) A	3	-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

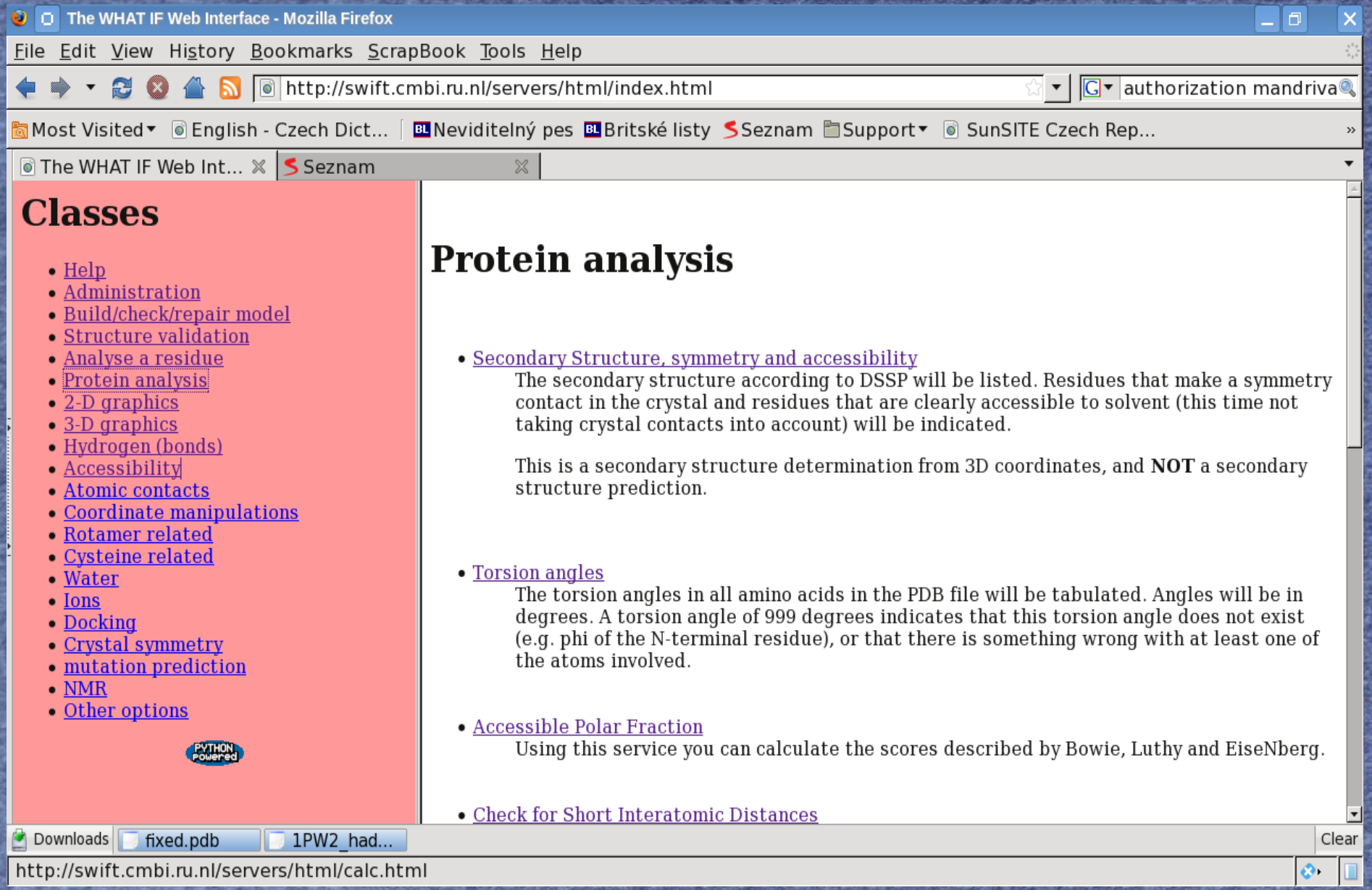
Structure validation



Structure validation



Protein analysis



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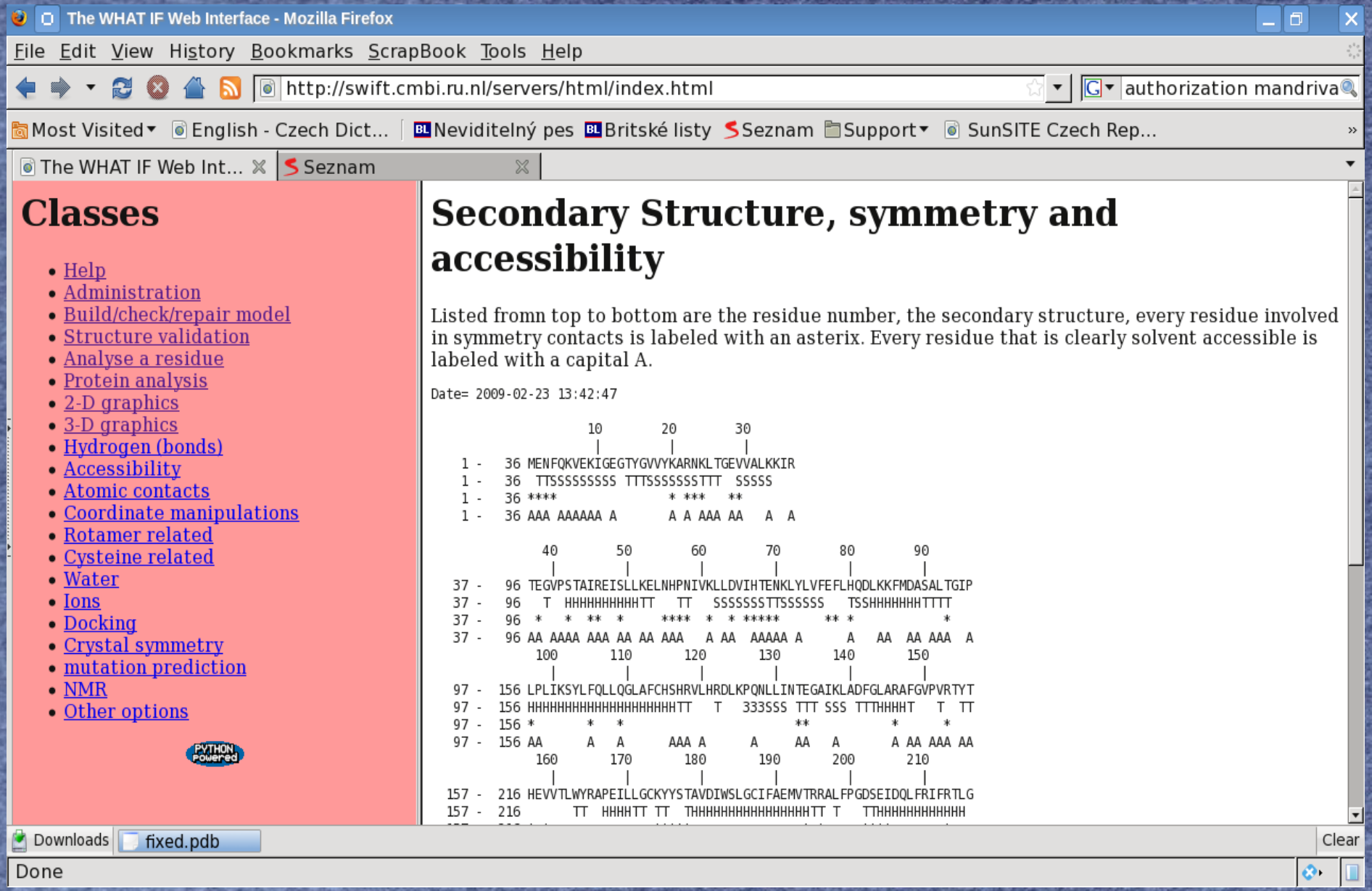

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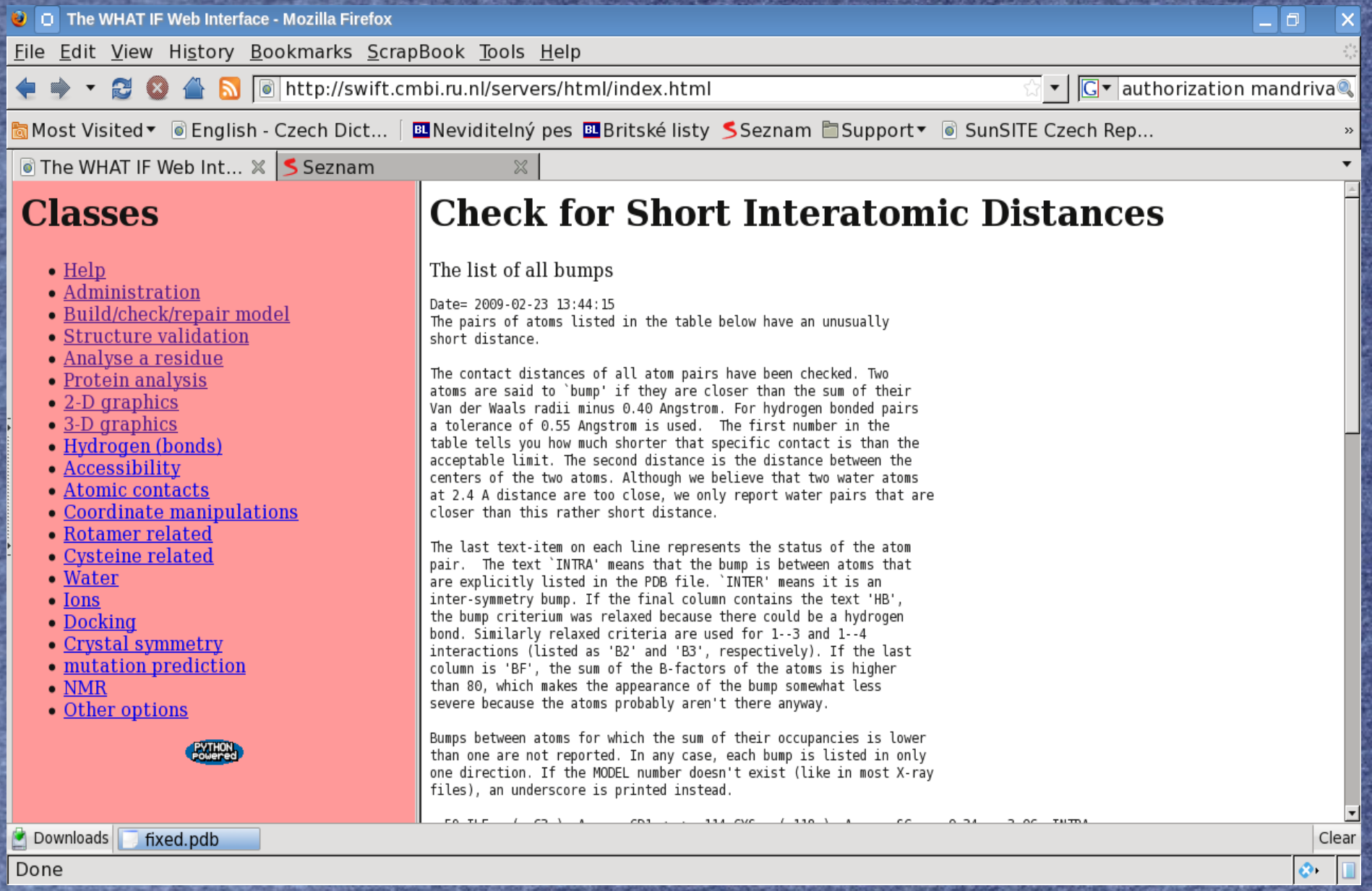

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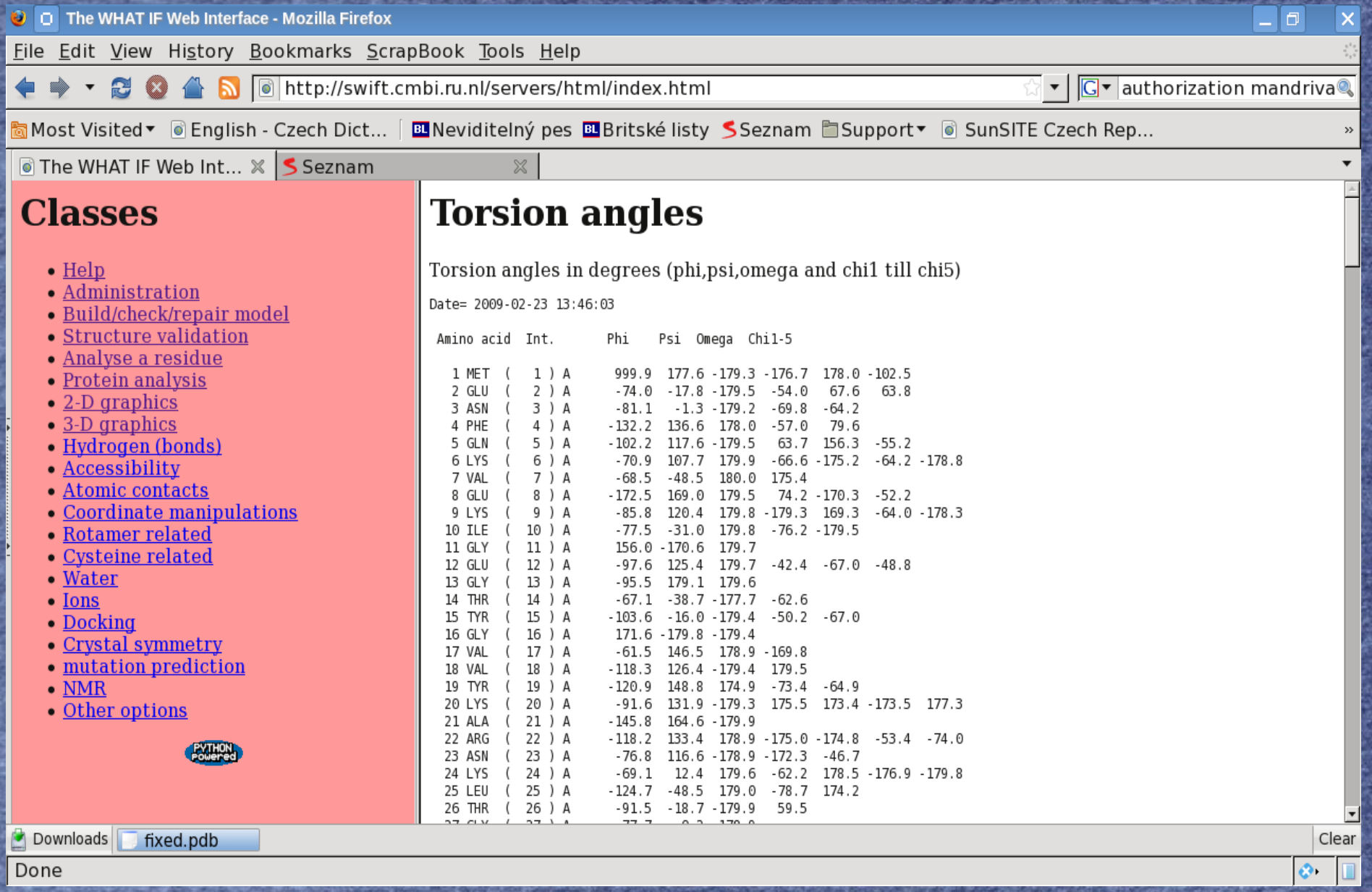

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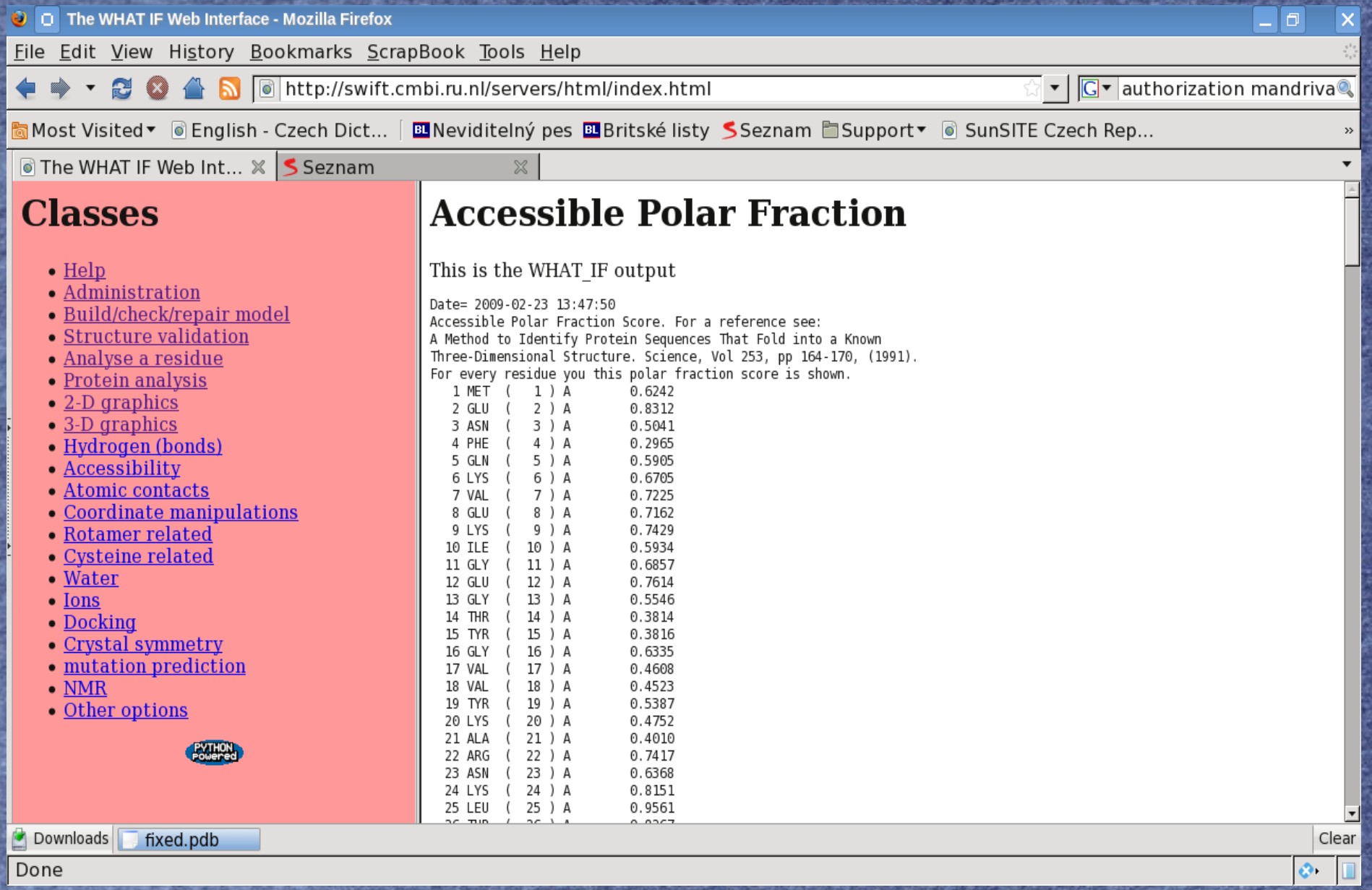

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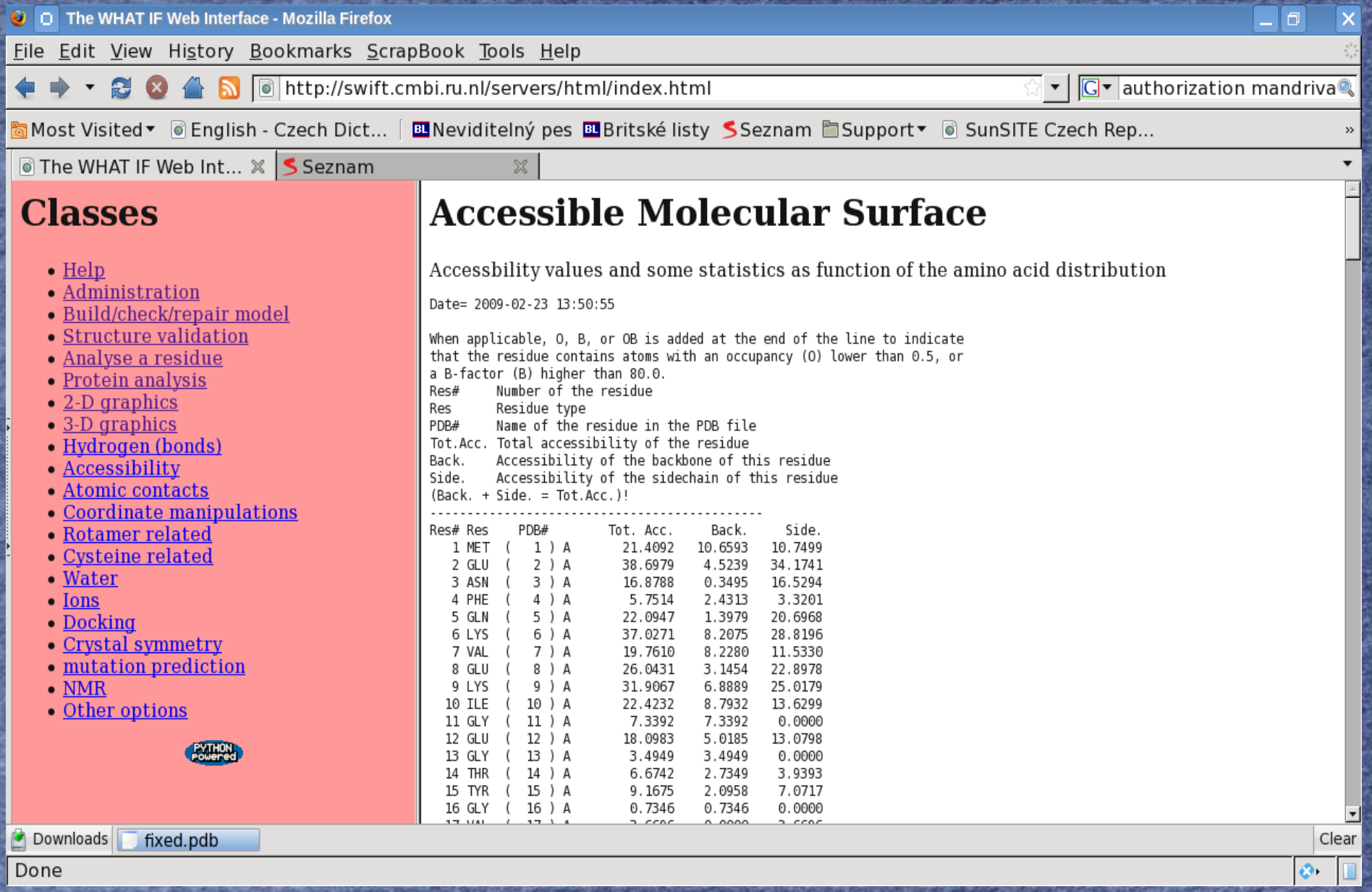
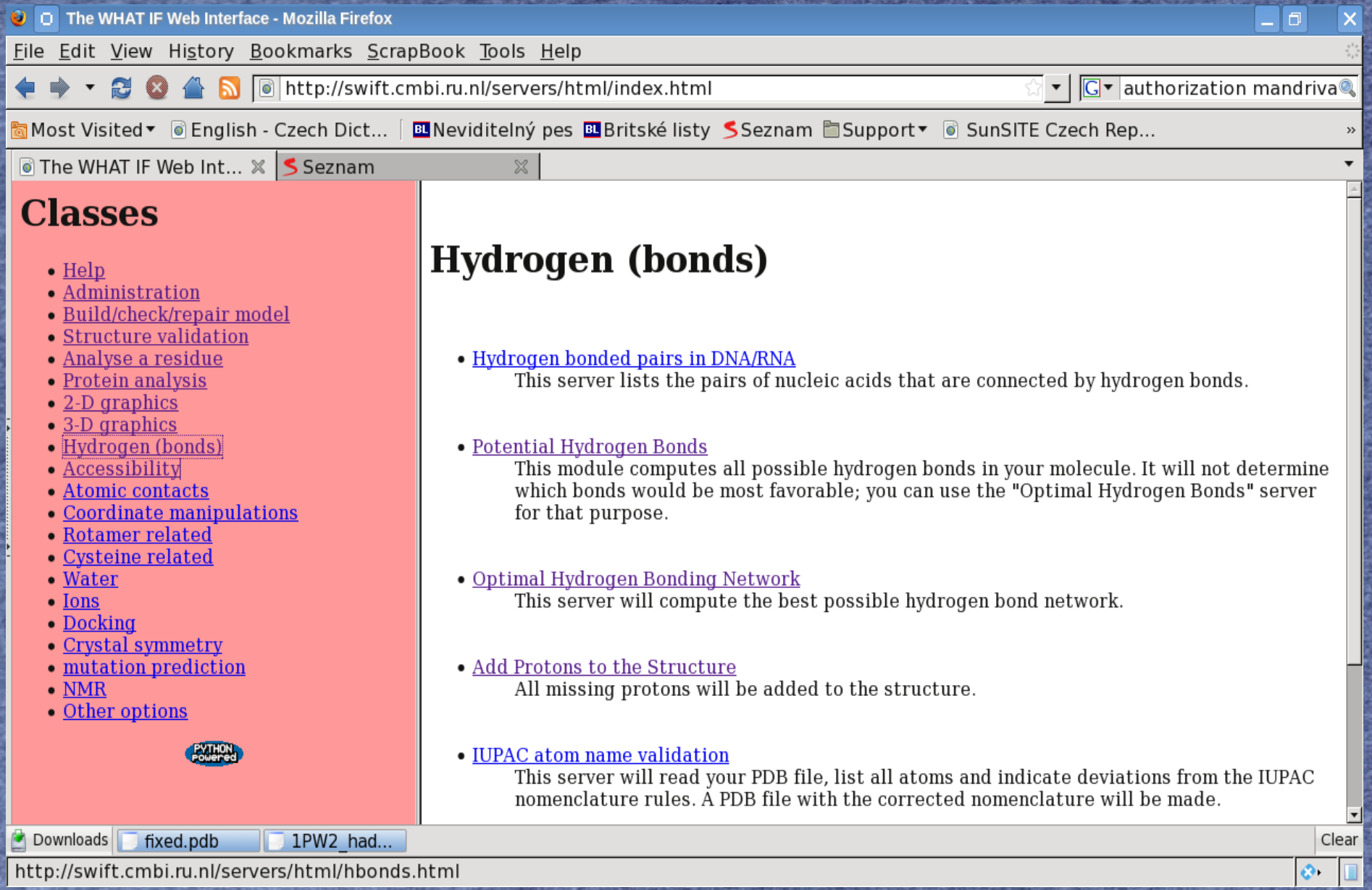
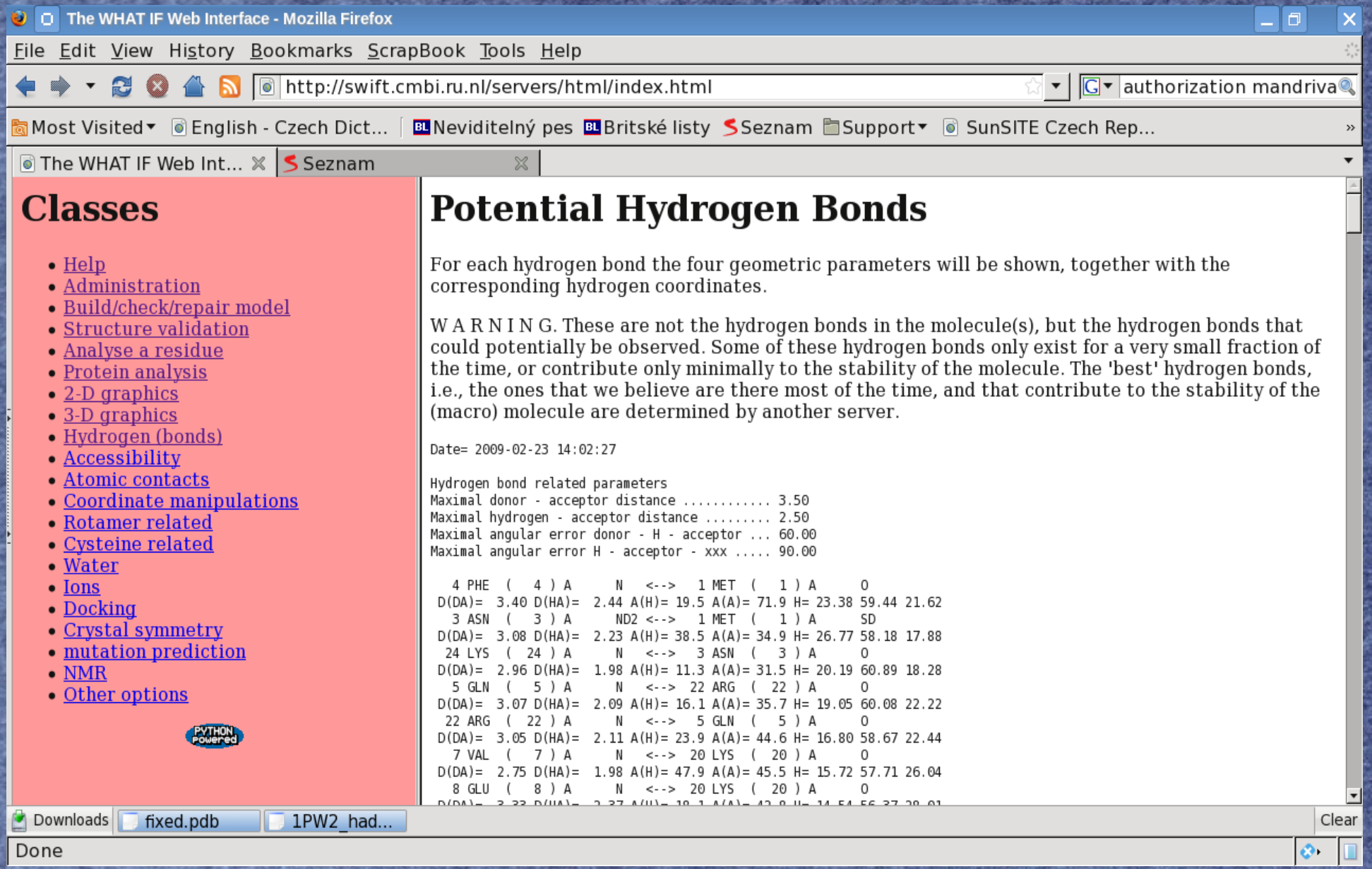


Hydrogen (bonds)



Hydrogen (bonds)



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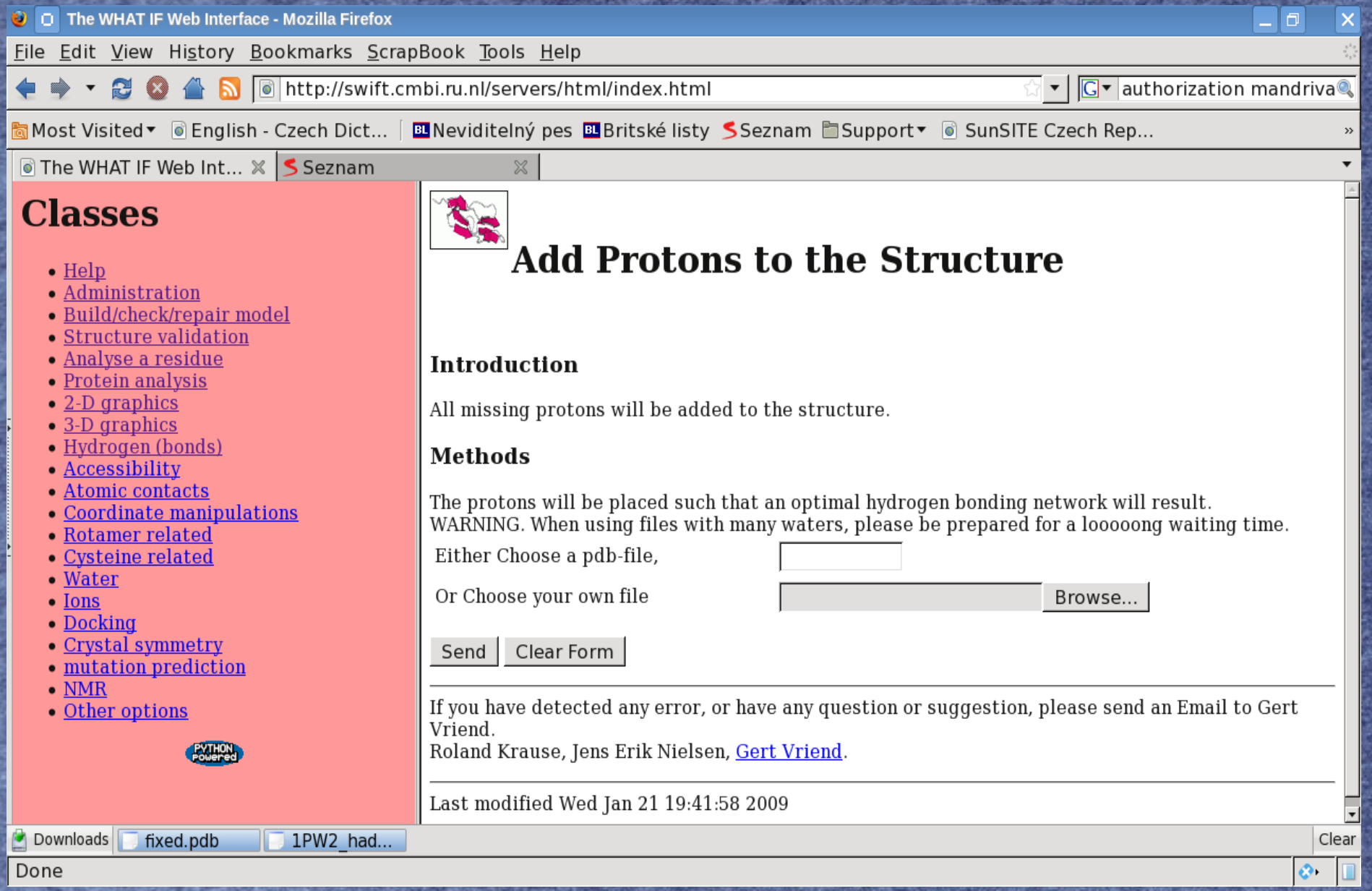

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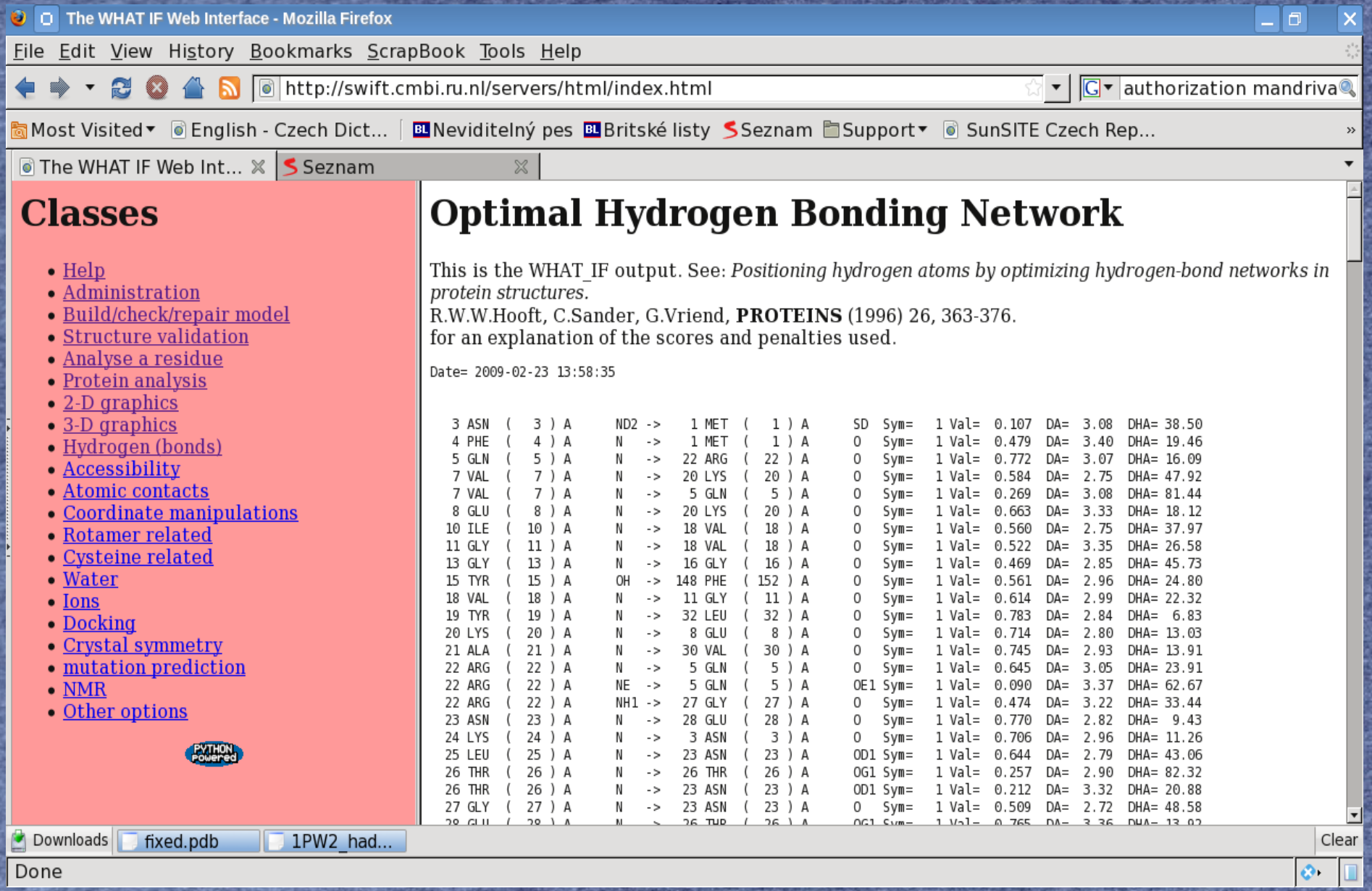

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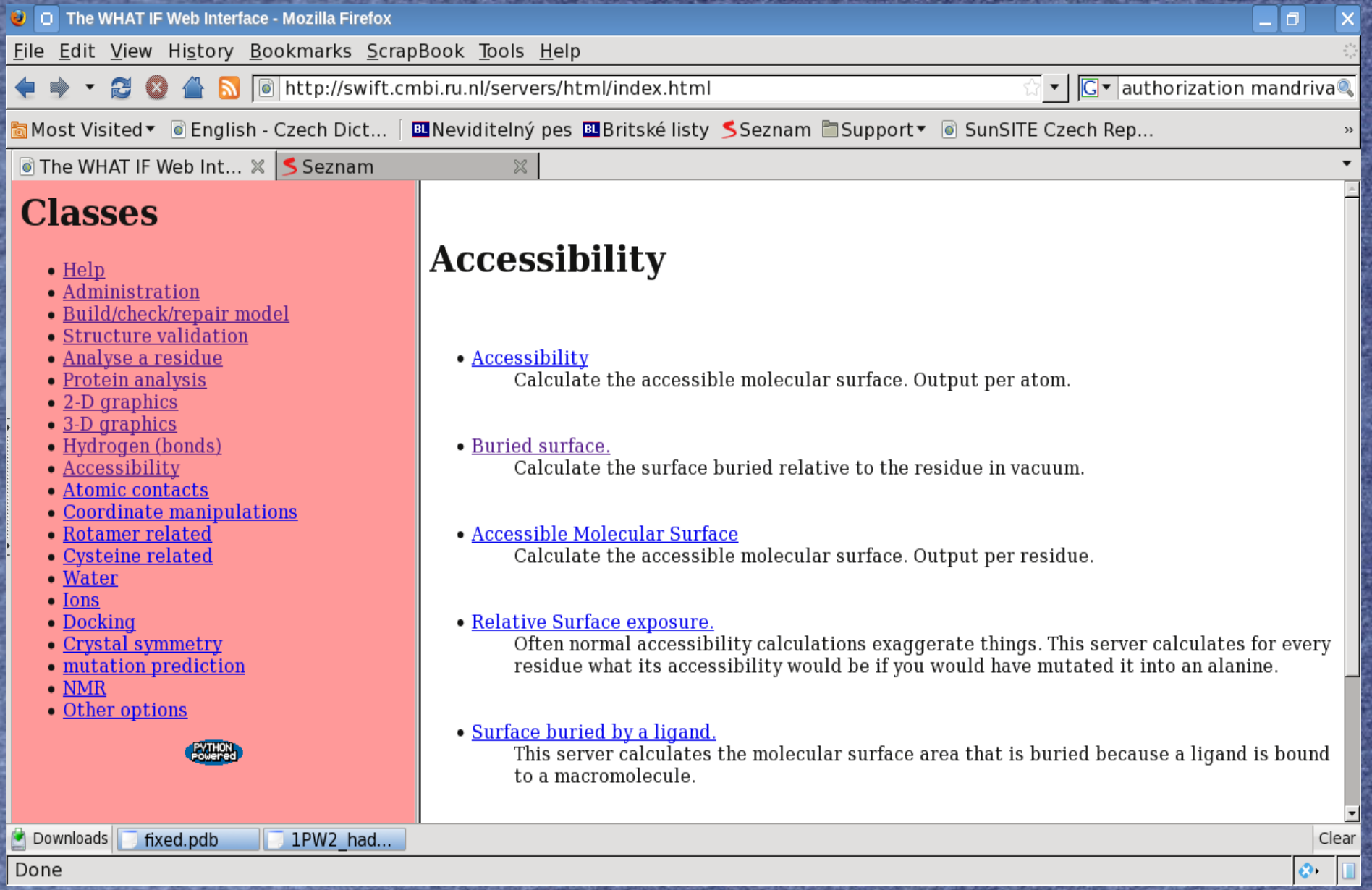

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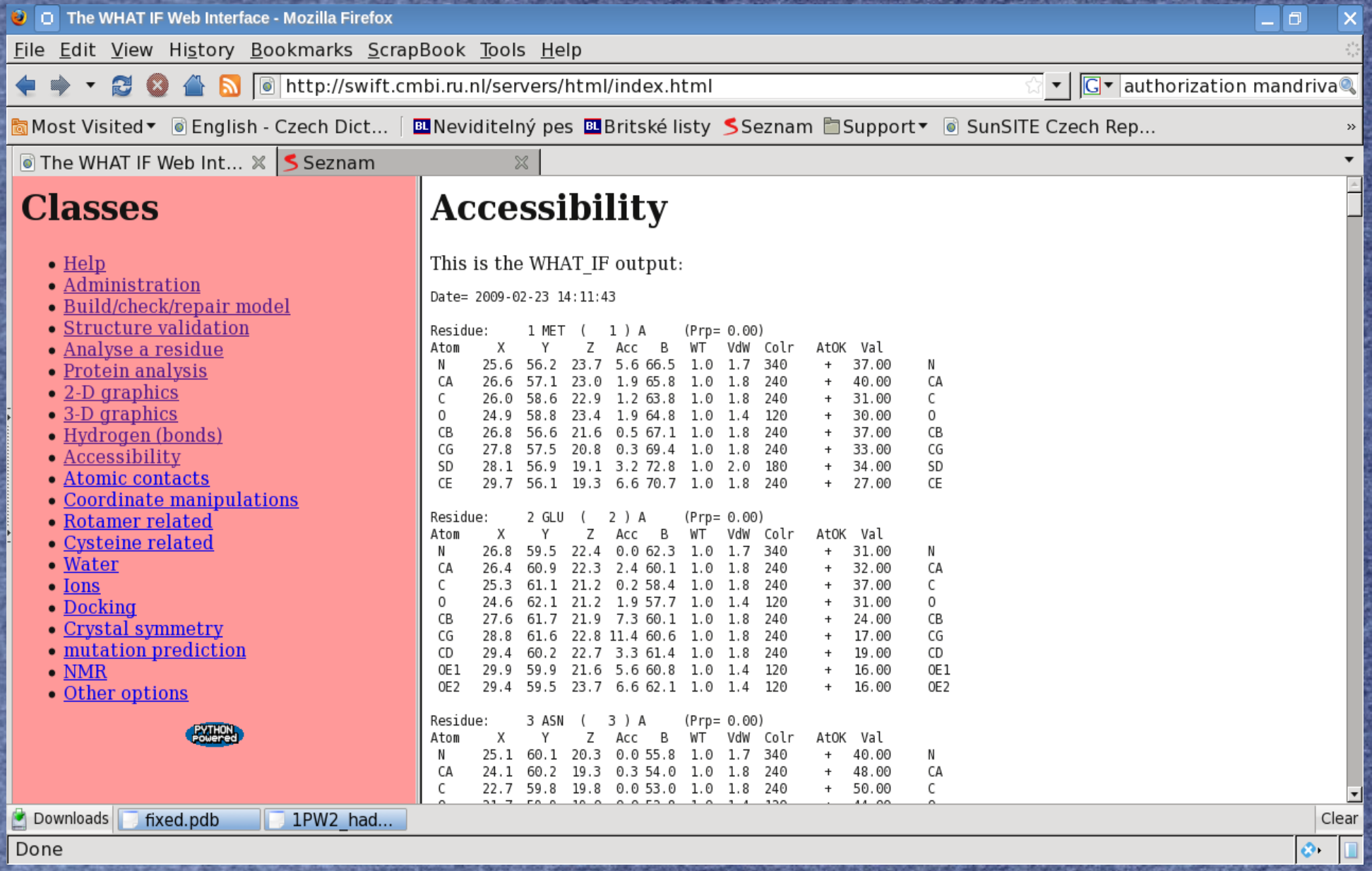

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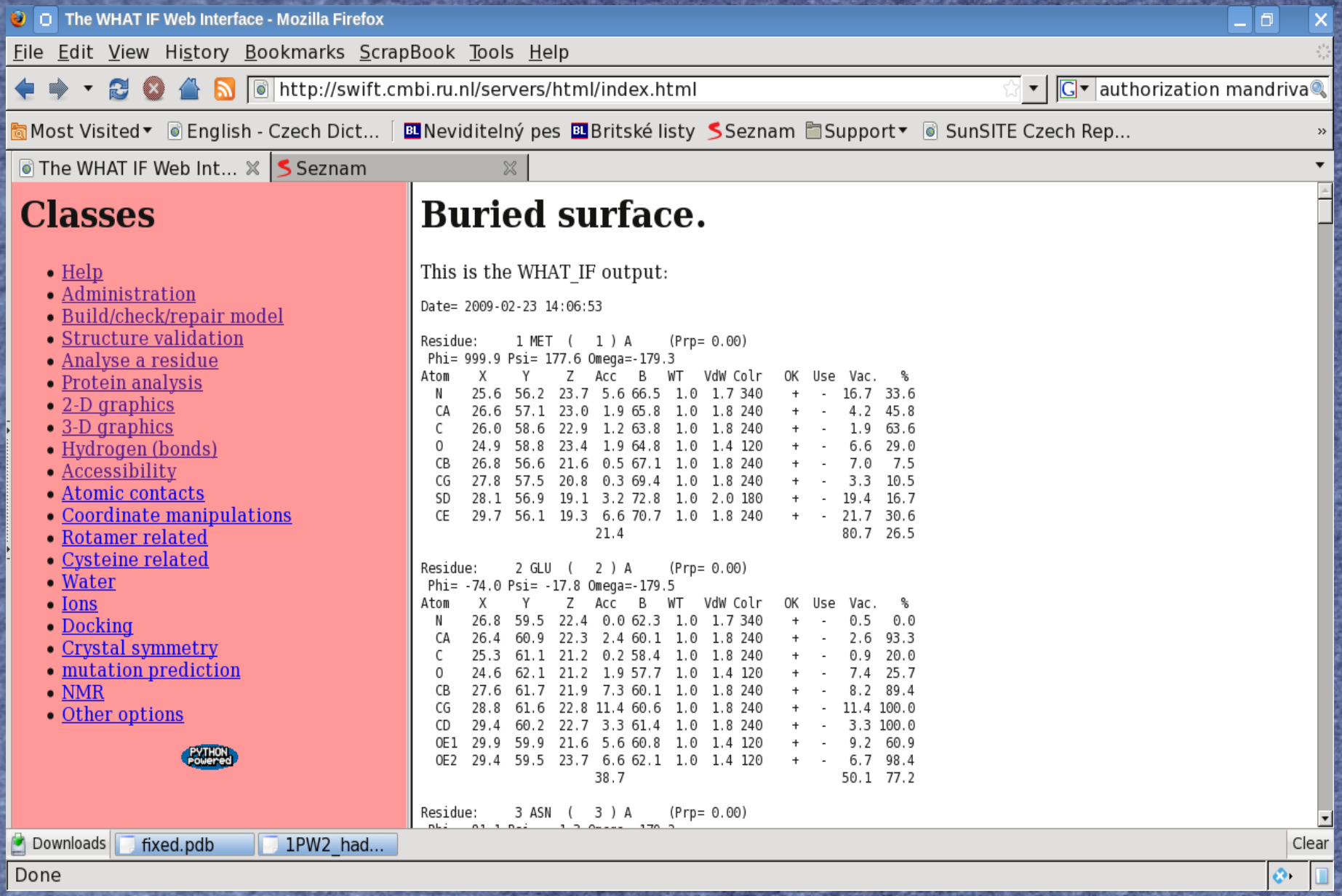
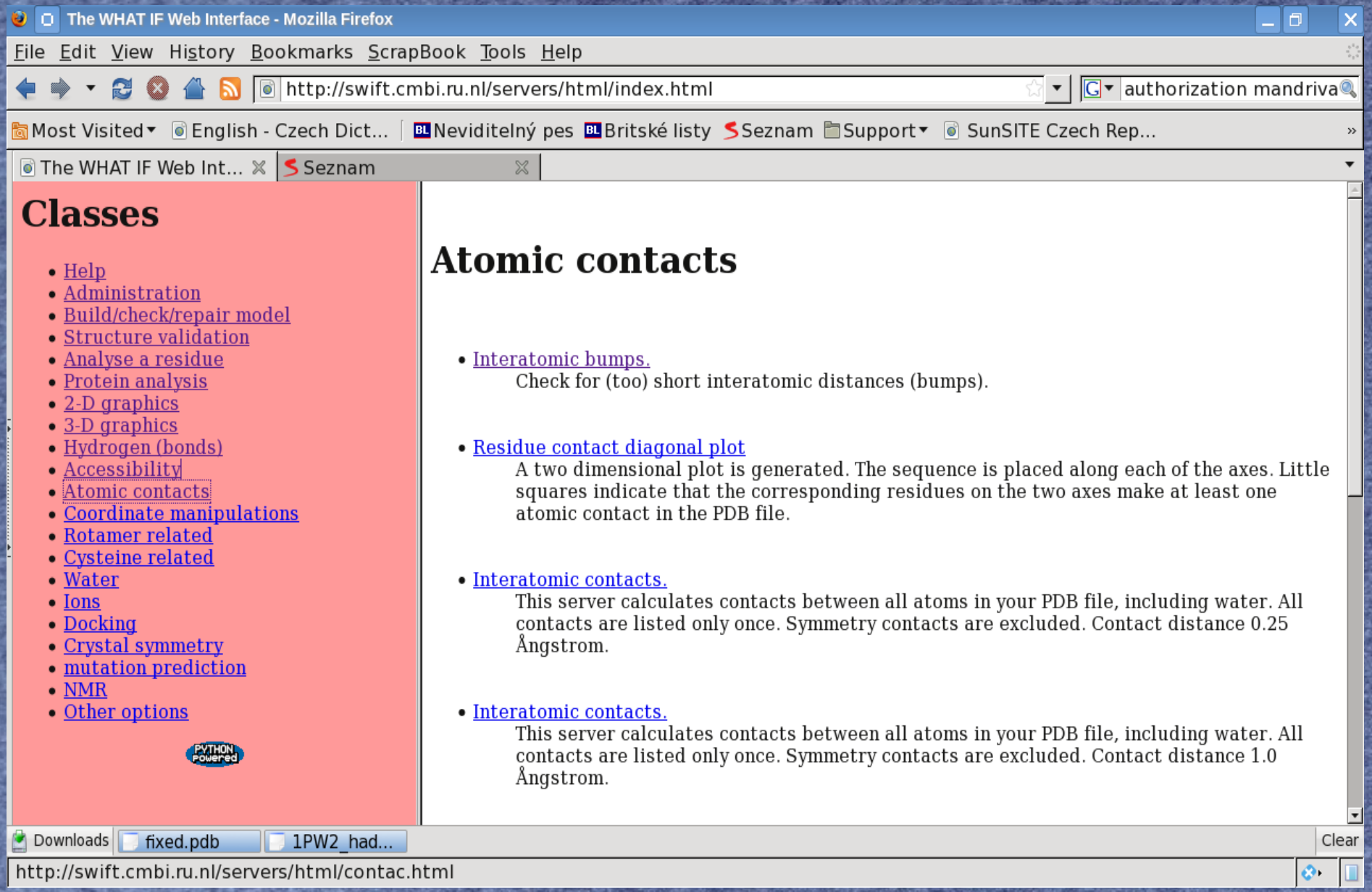


Atomic contacts



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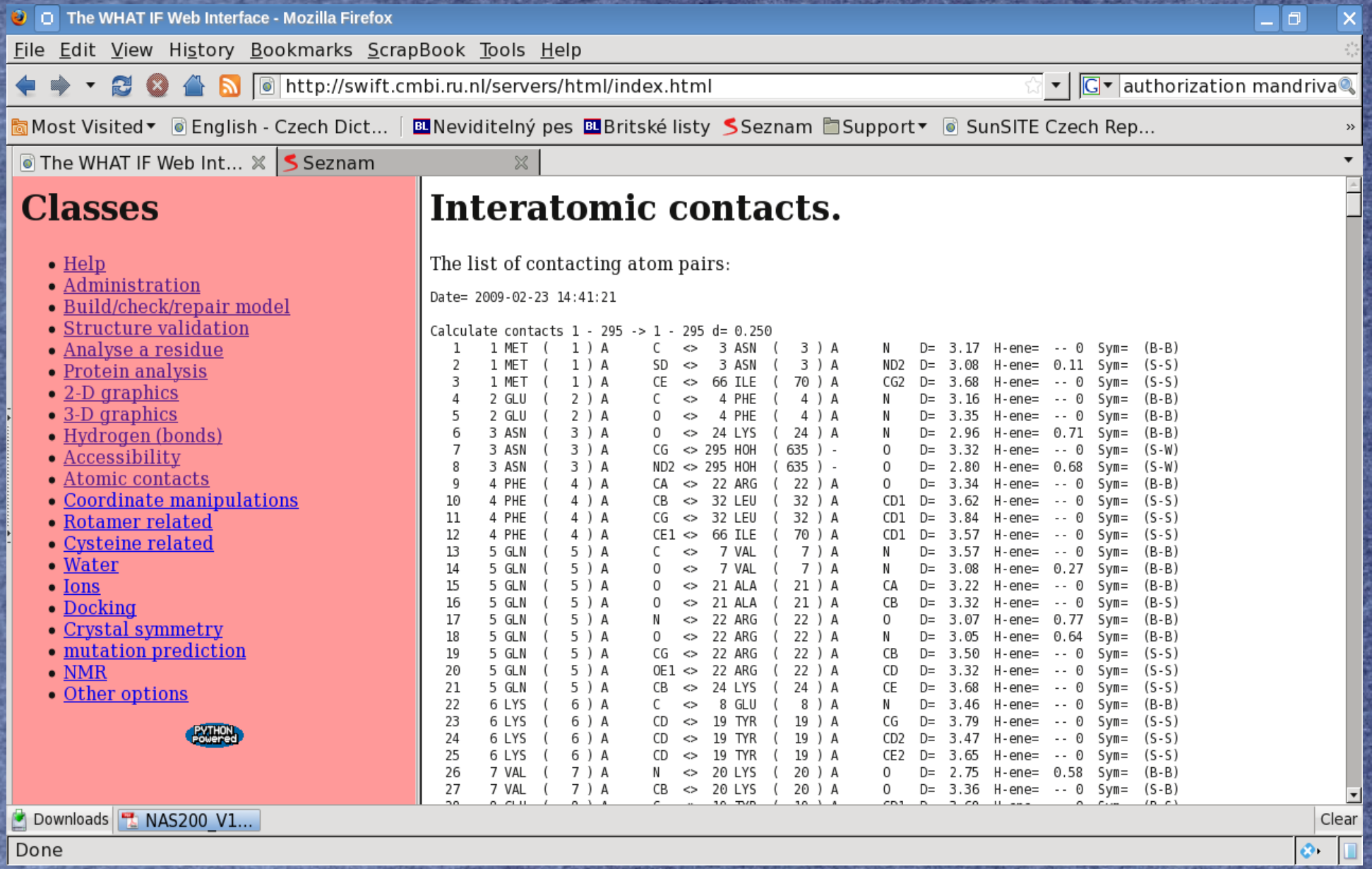
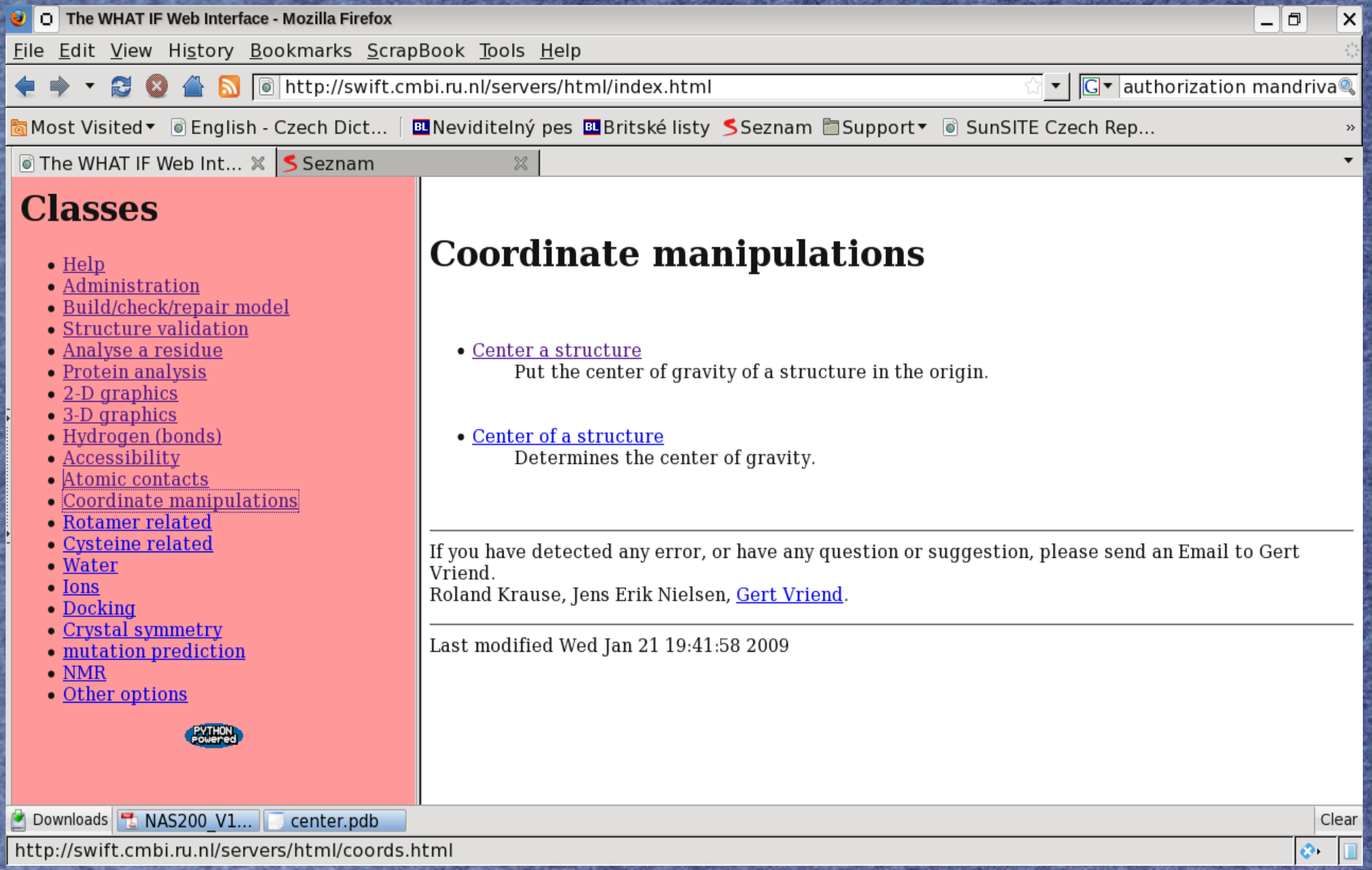
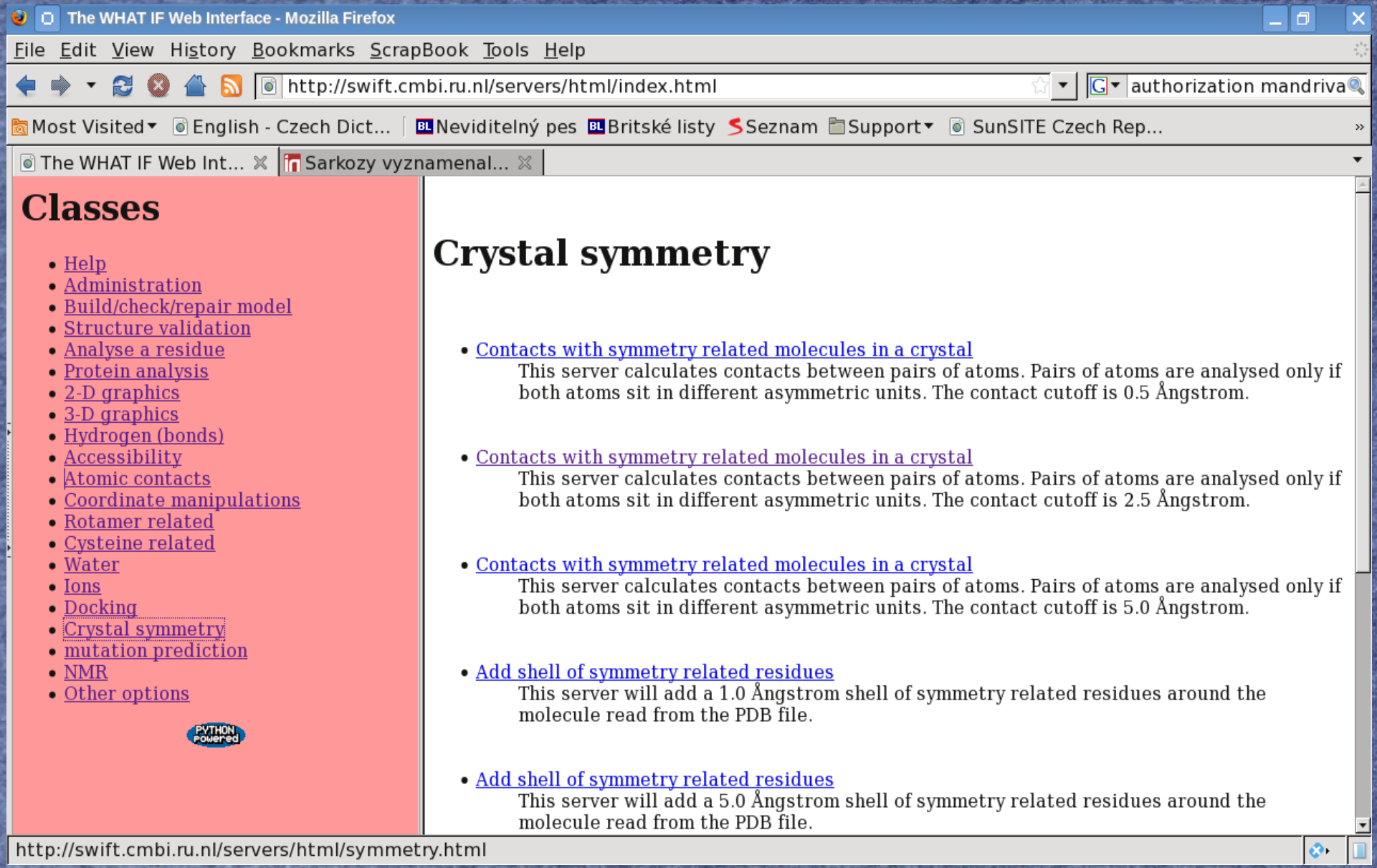


Coordinate manipulation



Crystal symmetry



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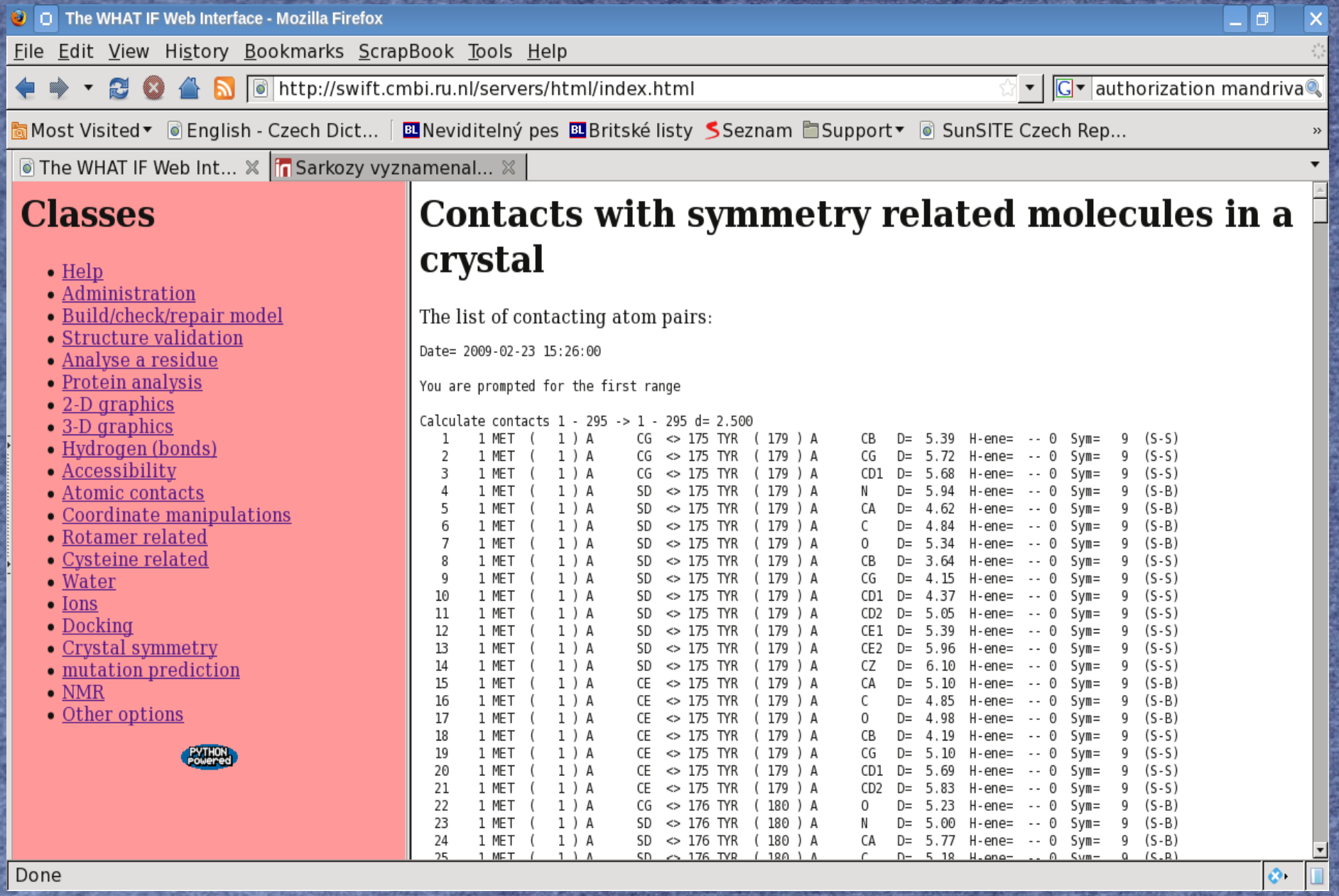

Other options

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Average B factors

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

Date= 2009-02-23 14:55:20

Residue	Chain		B-factors averaged over: 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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PYTHON Powered

Residue contact diagonal plot

Residue-residue contact plot.

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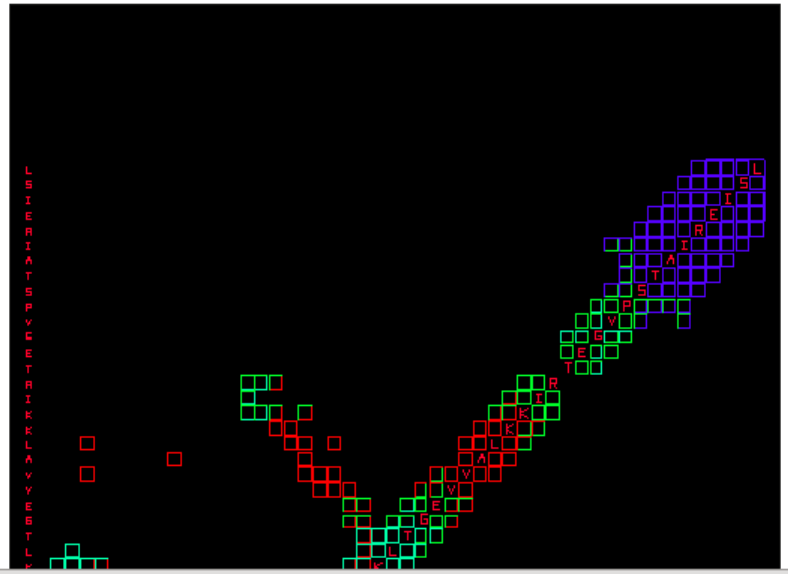
Roland Krause, Jens Erik Nielsen, Gert Vriend.

Last modified Mon Feb 23 14:38:58 2009



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