Anhang

Anhang I: Eingabedateien für die *ab initio* Strukturvorhersage mit „GASBOR“

```
[Lauf 3-13]

U                   !! User mode (default)
hb_corr_gasbor3               !! Project name
hb_corr_gnom             !! Input data file (output from Gnom)
hb_corr_gasbor3 !!(project desctiption)
2                   !! Units
1.0                 !! Portion of the curve to fit
                    !! Initial file none (none)
P222                  !! No symmetry (default)
500                 !! Number of residues
15                  !! Fibonacci grid (for solvent molecules)
U                   !! Expected anisometry (unknown)


[Lauf 14-24]

E
gasbor_exp.log
hb_corr_gnom
gasbor_p222 10 2dums together
2 !!unit
1 !! curve protion
  !! number of knots
  !! no inital drm
P222  !! inital symmetry
500   !! residues per part
10 !! Fibonacci grid order
65 !! search radius
   !! hist pen
   !! bond pen
   !! disc pen
0.35 !! peripheral pen
U !! shape unknown
  !! hydration_layer cont
  !! no sequence file
  !! initial scale factor
  !! fix scael factor
  !! initial temp
  !! annealing schedule factor
2 !! string of indep atoms to modify
  !! max iterations
  !! max success
  !! min success
  !! max steps
```

```
[Lauf 25-35]

E
gasbor_exp.log
hb_corr_gnom
gasbor_p222 10 2dums together
2 !! unit
1 !! curve protion
  !! number of knots
  !! no inital drm
P222  !! inital symmetry
460   !! residues per part
12 !! Fibonacci grid order
70 !! search radius
   !! hist pen
   !! bond pen
   !! disc pen
0.15 !! peripheral pen
U !! shape unknown
  !! hydration_layer cont
  !! no sequence file
  !! initial scale factor
  !! fix scael factor
  !! initial temp
  !! annealing schedule factor
2 !! string of indep atoms to modify
  !! max iterations
  !! max success
  !! min success
  !! max steps
```

Anhang II: Kreuzkorrelationstabellen der NSD-Werte für die *ab initio* Strukturvorhersage mit „GASBOR“

[Lauf 4-24]

Cross-correlation NSD table by SUPCOMB

File	Aver	r10	r11	r12	r13	r14	r15	r16	r17	r18	r19	r20	r21	r22	r23	r24	or3	or4	or5	or6	or7	or8	or9
gasbor	1.34	0.00	1.39	1.46	1.18	1.30	1.23	1.57	1.47	1.89	1.19	1.34	1.17	1.45	1.19	1.48	1.18	1.33	1.24	1.68	1.09	1.08	1.21
gasbor	1.47	1.39	0.00	1.14	1.77	1.57	1.52	1.13	1.18	1.03	1.55	1.70	1.52	1.45	1.58	1.20	1.68	1.52	1.55	1.07	1.95	1.56	1.72
gasbor	1.33	1.46	1.14	0.00	1.47	1.56	1.22	1.14	1.11	1.22	1.50	1.49	1.41	1.30	1.42	1.03	1.27	1.10	1.64	0.95	1.55	1.51	1.47
gasbor	1.34	1.18	1.77	1.47	0.00	1.24	1.27	1.65	1.54	1.52	1.14	1.08	1.31	1.30	1.28	1.58	1.24	1.46	1.21	1.49	1.13	1.19	1.14
gasbor	1.40	1.30	1.57	1.56	1.24	0.00	1.29	1.61	1.60	1.60	1.17	1.30	1.48	1.72	1.32	1.58	1.44	1.19	1.09	1.54	1.33	1.21	1.31
gasbor	1.30	1.23	1.52	1.22	1.27	1.29	0.00	1.56	1.24	1.48	1.39	1.16	1.30	1.32	1.32	1.25	1.24	1.14	1.18	1.32	1.38	1.37	1.19
gasbor	1.46	1.57	1.13	1.14	1.65	1.61	1.56	0.00	1.10	1.10	1.85	1.63	1.57	1.40	1.63	1.18	1.51	1.30	1.60	1.12	1.80	1.67	1.63
gasbor	1.35	1.47	1.18	1.11	1.54	1.60	1.24	1.10	0.00	1.20	1.79	1.28	1.44	1.22	1.43	1.07	1.32	1.25	1.59	1.09	1.54	1.58	1.36
gasbor	1.47	1.89	1.03	1.22	1.52	1.60	1.48	1.10	1.20	0.00	1.56	1.62	1.48	1.40	1.84	1.25	1.72	1.54	1.50	1.20	1.50	1.63	1.70
gasbor	1.39	1.19	1.55	1.50	1.14	1.17	1.39	1.85	1.79	1.56	0.00	1.30	1.39	1.64	1.31	1.57	1.36	1.26	1.11	1.53	1.13	1.10	1.27
gasbor	1.34	1.34	1.70	1.49	1.08	1.30	1.16	1.63	1.28	1.62	1.30	0.00	1.31	1.26	1.18	1.48	1.23	1.29	1.35	1.58	1.27	1.29	1.08
gasbor	1.36	1.17	1.52	1.41	1.31	1.48	1.30	1.57	1.44	1.48	1.39	1.31	0.00	1.35	1.33	1.39	1.19	1.40	1.49	1.34	1.16	1.33	1.28
gasbor	1.41	1.45	1.45	1.30	1.30	1.72	1.32	1.40	1.22	1.40	1.64	1.26	1.35	0.00	1.42	1.29	1.22	1.39	1.73	1.37	1.50	1.48	1.34
gasbor	1.35	1.19	1.58	1.42	1.28	1.32	1.32	1.63	1.43	1.84	1.31	1.18	1.33	1.42	0.00	1.41	1.14	1.23	1.31	1.62	1.20	1.21	1.08
gasbor	1.35	1.48	1.20	1.03	1.58	1.58	1.25	1.18	1.07	1.25	1.57	1.48	1.39	1.29	1.41	0.00	1.28	1.12	1.66	1.04	1.53	1.55	1.48
gasbor	1.30	1.18	1.68	1.27	1.24	1.44	1.24	1.51	1.32	1.72	1.36	1.23	1.19	1.22	1.14	1.28	0.00	1.10	1.25	1.43	1.13	1.30	1.08
gasbor	1.28	1.33	1.52	1.10	1.46	1.19	1.14	1.30	1.25	1.54	1.26	1.29	1.40	1.39	1.23	1.12	1.10	0.00	1.12	1.22	1.30	1.51	1.20
gasbor	1.36	1.24	1.55	1.64	1.21	1.09	1.18	1.60	1.59	1.50	1.11	1.35	1.49	1.73	1.31	1.66	1.25	1.12	0.00	1.61	1.14	1.11	1.19
gasbor	1.38	1.68	1.07	0.95	1.49	1.54	1.32	1.12	1.09	1.20	1.53	1.58	1.34	1.37	1.62	1.04	1.43	1.22	1.61	0.00	1.69	1.52	1.62
gasbor	1.35	1.09	1.95	1.55	1.13	1.33	1.38	1.80	1.54	1.50	1.13	1.27	1.16	1.50	1.20	1.53	1.13	1.30	1.14	1.69	0.00	1.05	1.09
gasbor	1.35	1.08	1.56	1.51	1.19	1.21	1.37	1.67	1.58	1.63	1.10	1.29	1.33	1.48	1.21	1.55	1.30	1.51	1.11	1.52	1.05	0.00	1.18
gasbor	1.31	1.21	1.72	1.47	1.14	1.31	1.19	1.63	1.36	1.70	1.27	1.08	1.28	1.34	1.08	1.48	1.08	1.20	1.19	1.62	1.09	1.18	0.00
Aver	1.37	1.34	1.47	1.33	1.34	1.40	1.30	1.46	1.35	1.47	1.39	1.34	1.36	1.41	1.35	1.35	1.30	1.28	1.36	1.38	1.35	1.35	1.31

[Lauf 25-35]

Cross-correlation NSD table by SUPCOMB

File	Aver	r25	r26	r27	r28	r29	r30	r31	r32	r33	r34	r35
gasbor	1.45	0.00	1.18	1.34	1.54	1.56	1.39	1.76	1.38	1.49	1.37	1.45
gasbor	1.38	1.18	0.00	1.19	1.42	1.59	1.34	1.65	1.22	1.37	1.45	1.43
gasbor	1.48	1.34	1.19	0.00	1.62	1.71	1.42	1.61	1.37	1.33	1.62	1.57
gasbor	1.42	1.54	1.42	1.62	0.00	1.24	1.61	1.25	1.48	1.40	1.38	1.25
gasbor	1.46	1.56	1.59	1.71	1.24	0.00	1.63	1.18	1.59	1.56	1.32	1.24
gasbor	1.50	1.39	1.34	1.42	1.61	1.63	0.00	1.73	1.17	1.47	1.55	1.65
gasbor	1.52	1.76	1.65	1.61	1.25	1.18	1.73	0.00	1.68	1.56	1.42	1.38
gasbor	1.44	1.38	1.22	1.37	1.48	1.59	1.17	1.68	0.00	1.40	1.58	1.55
gasbor	1.47	1.49	1.37	1.33	1.40	1.56	1.47	1.56	1.40	0.00	1.50	1.63
gasbor	1.46	1.37	1.45	1.62	1.38	1.32	1.55	1.42	1.58	1.50	0.00	1.35
gasbor	1.45	1.45	1.43	1.57	1.25	1.24	1.65	1.38	1.55	1.63	1.35	0.00
Aver	1.46	1.45	1.38	1.48	1.42	1.46	1.50	1.52	1.44	1.47	1.46	1.45

Lebenslauf

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Geburtsdatum	12.01.1974
Geburtsort	Göttingen
Familienstand	ledig, ein Kind

Schulausbildung:

Grundschule	Grundschule Angerstein, Nörten-Hardenberg 1980-1984
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Gymnasium	Max-Planck-Gymnasium, Göttingen 1986-1993 Abitur im Mai 1993

Universitäre Ausbildung:

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Okt. - Dez. 1996	Wissenschaftl. Hilfskraft am Inst. für Pflanzenbiochemie, Tübingen
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seit Nov. 1999	Arbeit an der vorliegenden Promotion unter der Anleitung von Prof. Dr. W. Saenger am Institut für Chemie/Kristallographie der Freien Universität Berlin

Publikationen und Vorträge

Publikationen:

Maier, T., Strater, N., Schuette, C.G., Klingenstein, R., Sandhoff, K. und Saenger, W. (2003) The X-ray crystal structure of human beta-hexosaminidase B provides new insights into Sandhoff disease. *J. Mol. Biol.*, **328**, 669-681

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Niere, M., Dettloff, M., Maier, T., Ziegler, M. und Wiesner, A. (2001) Insect immune activation by apolipophorin III is correlated with the lipid-binding properties of this protein. *Biochemistry*, **40**, 11502-11508

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Publikationen in Vorbereitung:

Maier, T., Przylas, I., Strater, N., Herdewijn, P. und Saenger, W. Reinforced backbone hydration in the X-ray crystal structure of a decameric HNA/RNA hybrid.

Maier, T., Rossokha, M., Klingenstein, R., Sandhoff, K. und Saenger, W. Recombinant expression in *Pichia pastoris* and crystallization of human SapC.

Maier, T., Rossokha, M., Remmel, N., Sandhoff, K. und Saenger, W. Expression, purification and crystallization of human SapD.

Maier, T., Rossokha, M., Remmel, N., Sandhoff, K. und Saenger, W. The crystal structure of SapD suggests a novel site of primary phospholipid-interaction.

Posterbeiträge:

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Maier, T., Strater, N., Schuette, C.G., Klingenstein, R., Sandhoff, K. und Saenger, W. (2003) The crystal structure of human beta-hexosaminidase B - New insights into Sandhoff disease. Enzyme Mechanism – A structural perspective, 12.01.-14.01.2003, St. Andrews, Scotland, Great Britain

Maier, T., Saenger, W., Lodge, J.A., und Strater, N. (2002) Protein crystallography at BESSY-II: Determination of two new protein structures. Bessy User's Meeting 2002, 5.12-6.12. 2002, Berlin, Germany

Vorträge:

Maier, T., Strater, N., Schuette, C.G., Klingenstein, R., Sandhoff, K. und Saenger, W. (2003) The crystal structure of human beta-hexosaminidase B - New insights into Sandhoff disease. 5th Heart of Europe Bio-Crystallography Meeting, 25.09-27.09.2002, Goslar, Germany