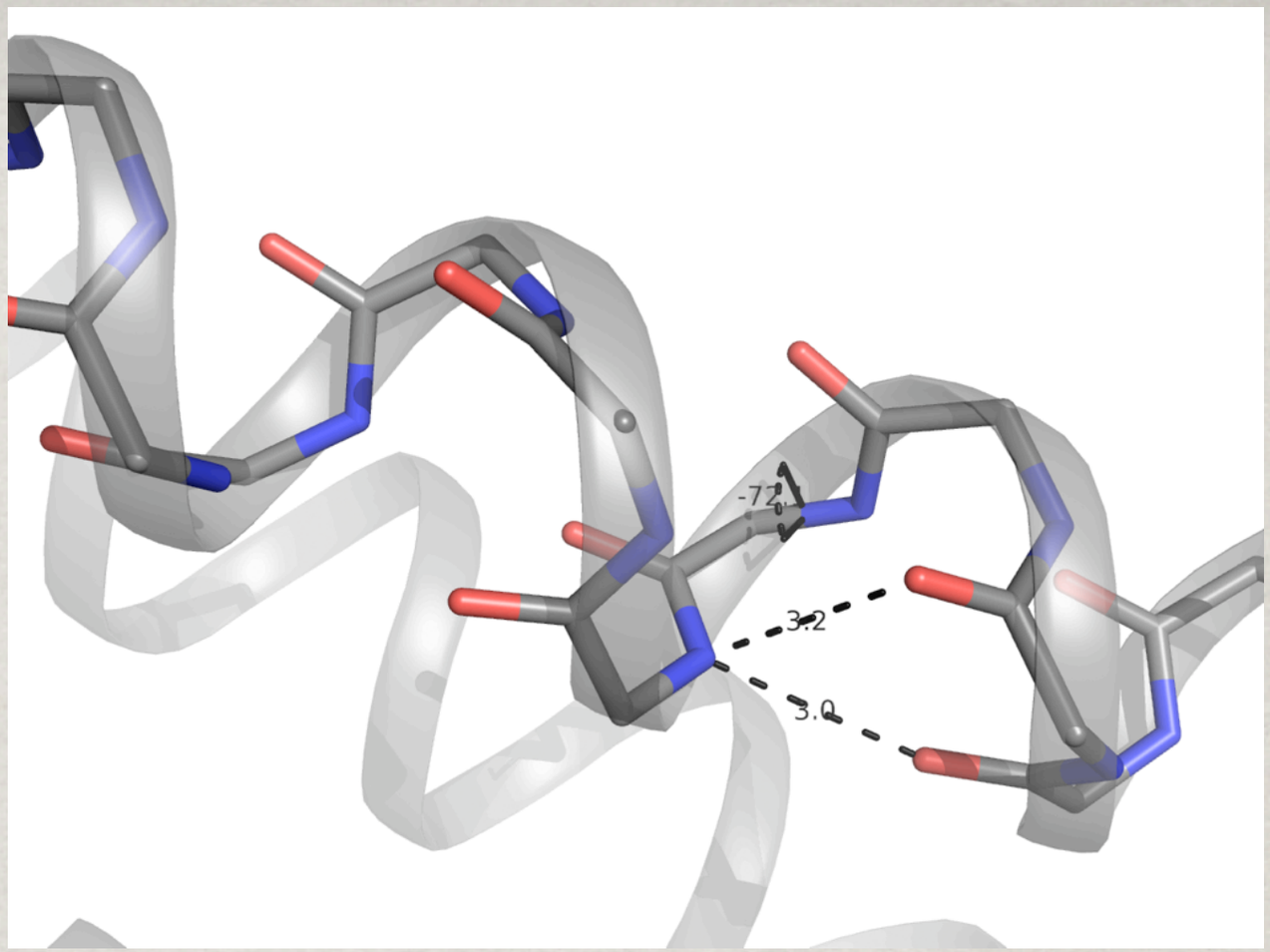
Force Field Improvements in Rosetta

Energy double-counting in statistics-based energy functions

Yifan Song
Baker Group
08.2009

score12:
fa_atr 0.8
fa_rep 0.44
fa_sol 0.65
fa_intra_rep 0.004
fa_pair 0.49
fa_plane 0
fa_dun 0.56
hbond_lr_bb 1.17
hbond_sr_bb 0.585
hbond_bb_sc 1.17
hbond_sc 1.1
p_aa_pp 0.320
rama 0.2
omega 0.5
...



Helix geometry

- Angular dependence of short-range backbone hydrogen bond (Helix)
- Ramachandran potential
- Non-polar hydrogen bond

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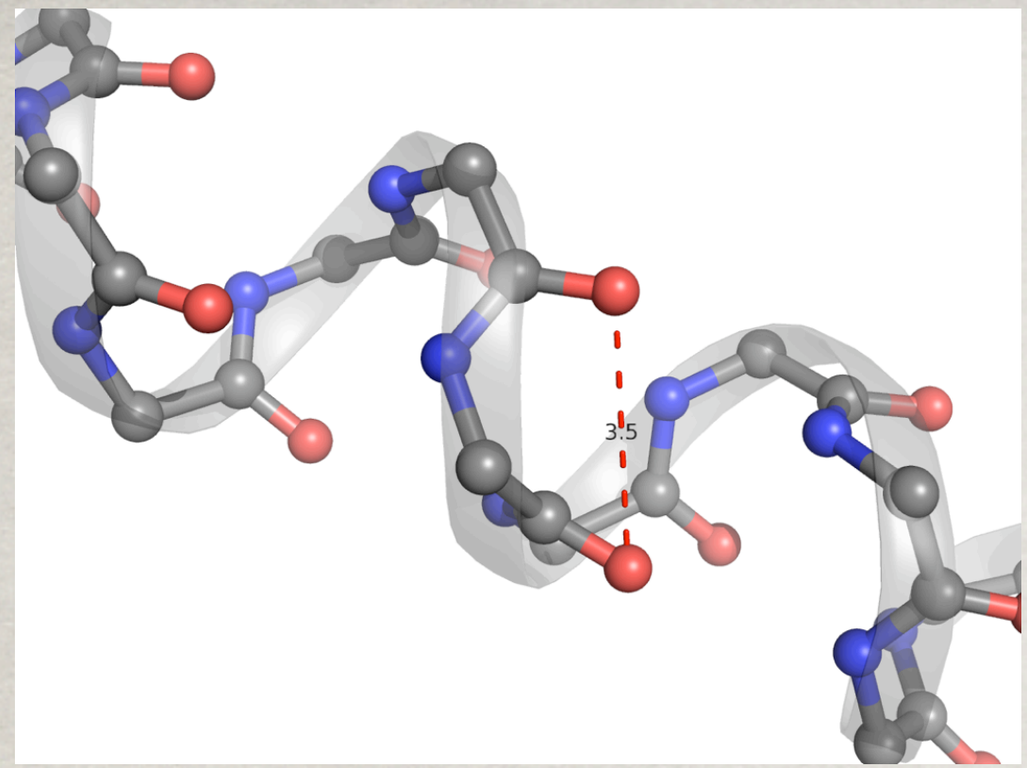
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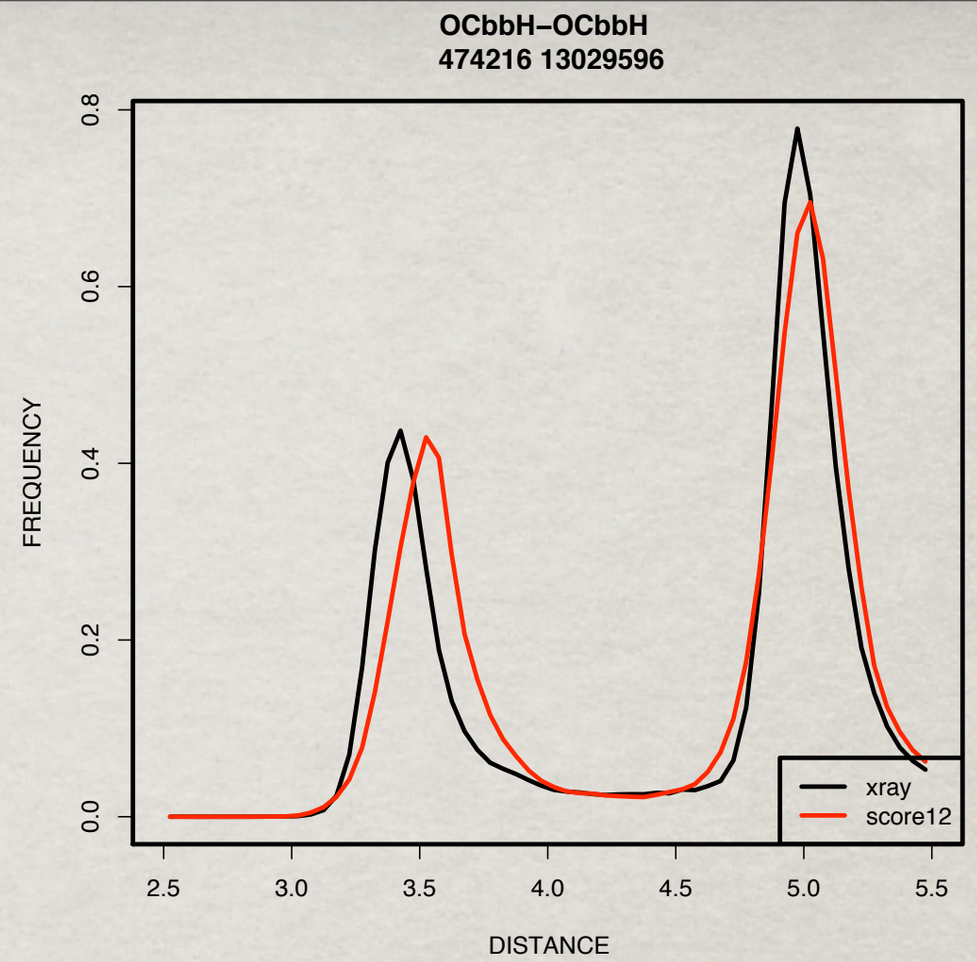
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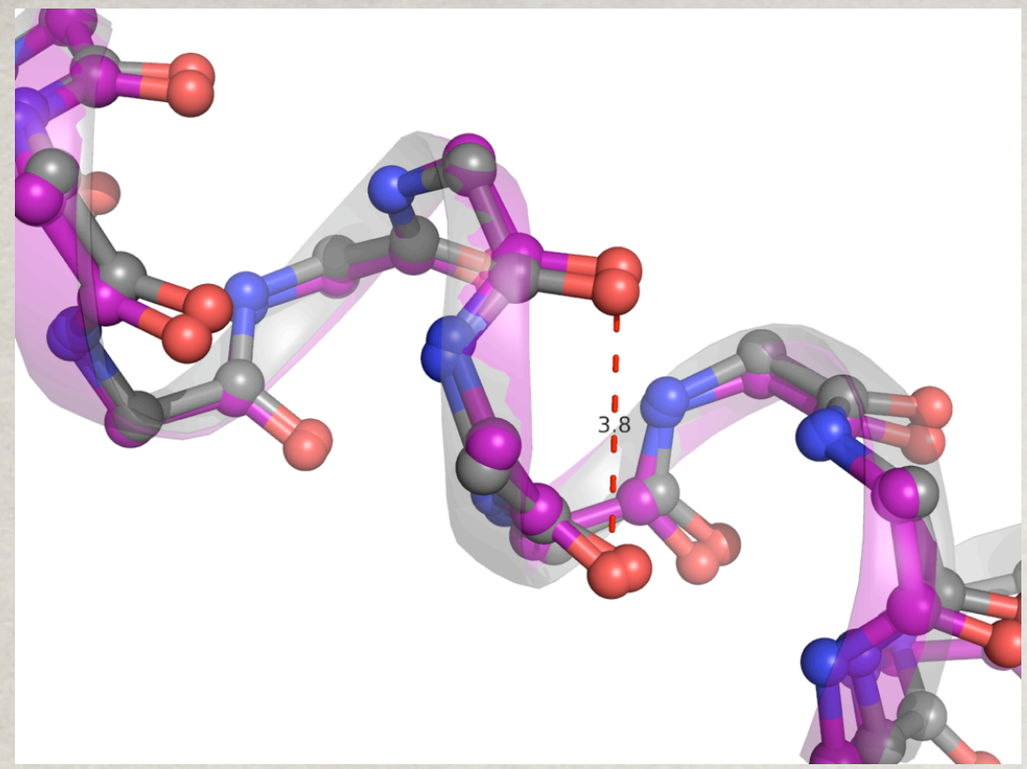
474216 13029596
FREQUENCY
0.0
0.2
0.4
0.6
0.8
2.5
3.0
3.5
4.0
4.5
5.0
5.5
DISTANCE
xray
score12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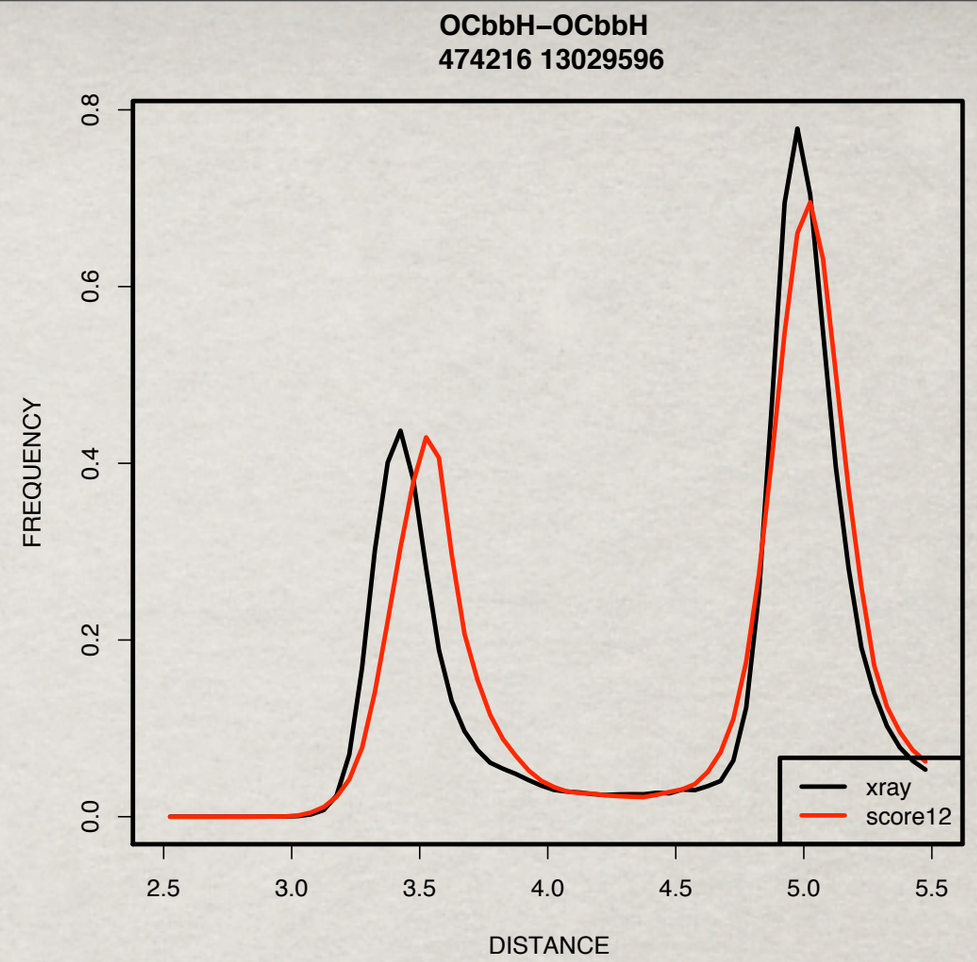
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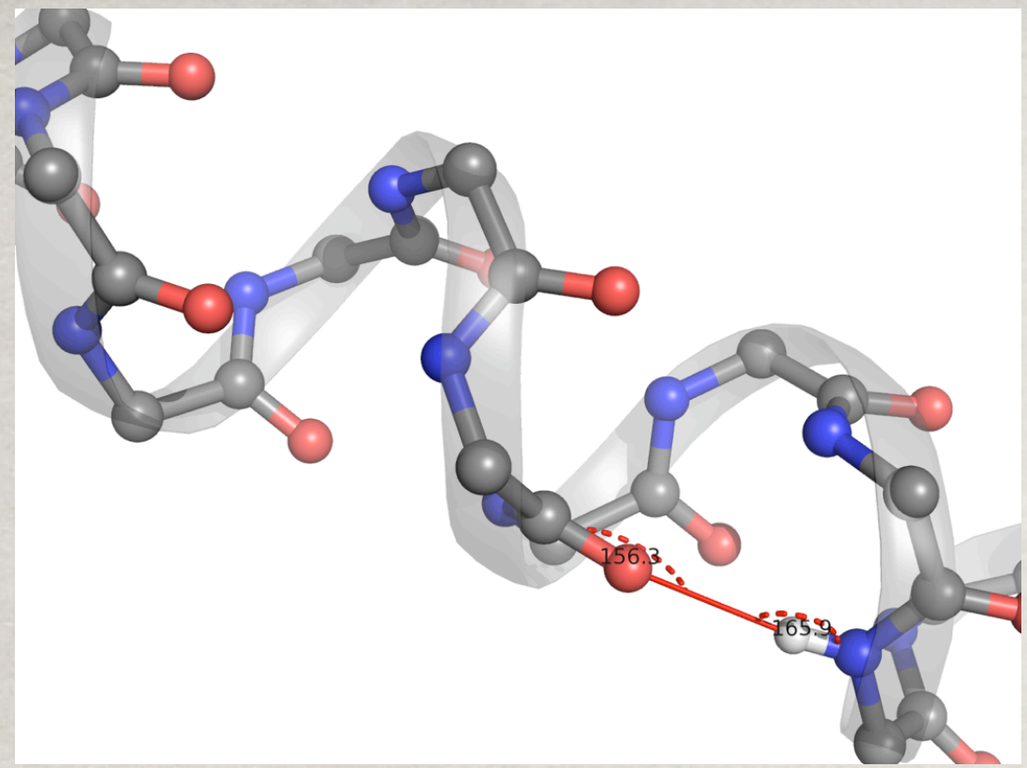
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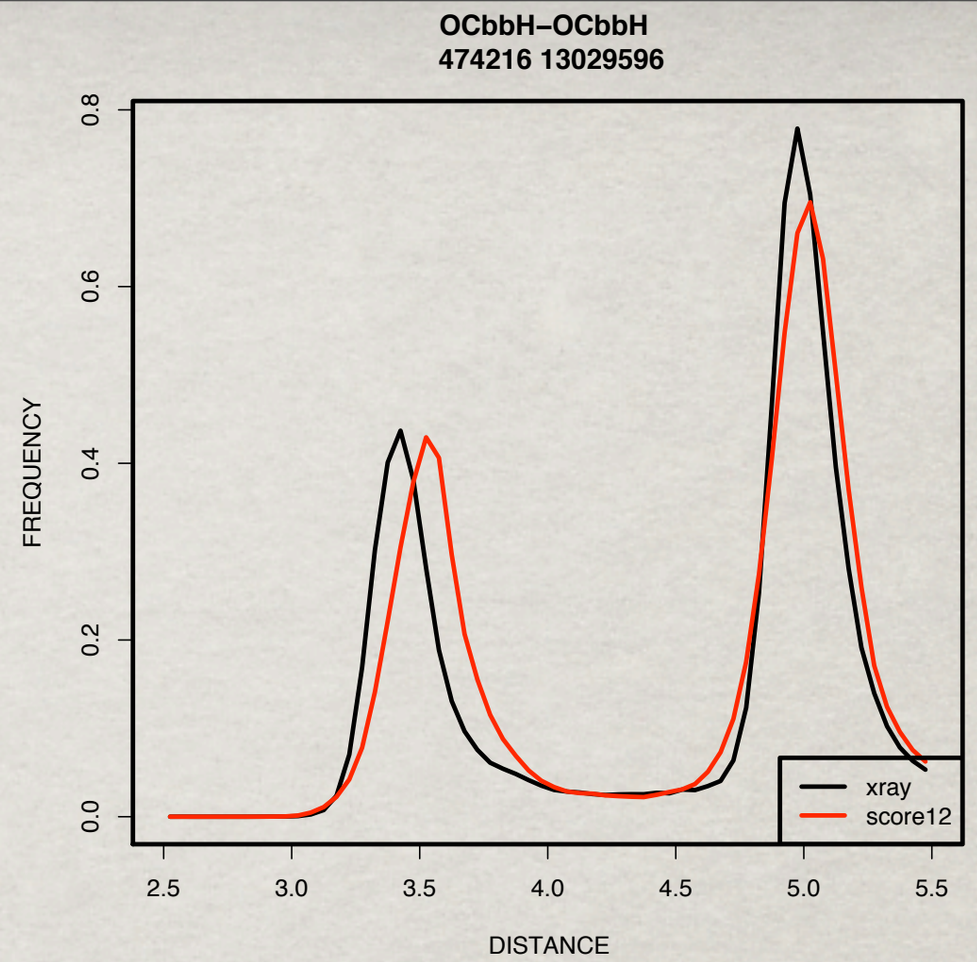
165.9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2.5
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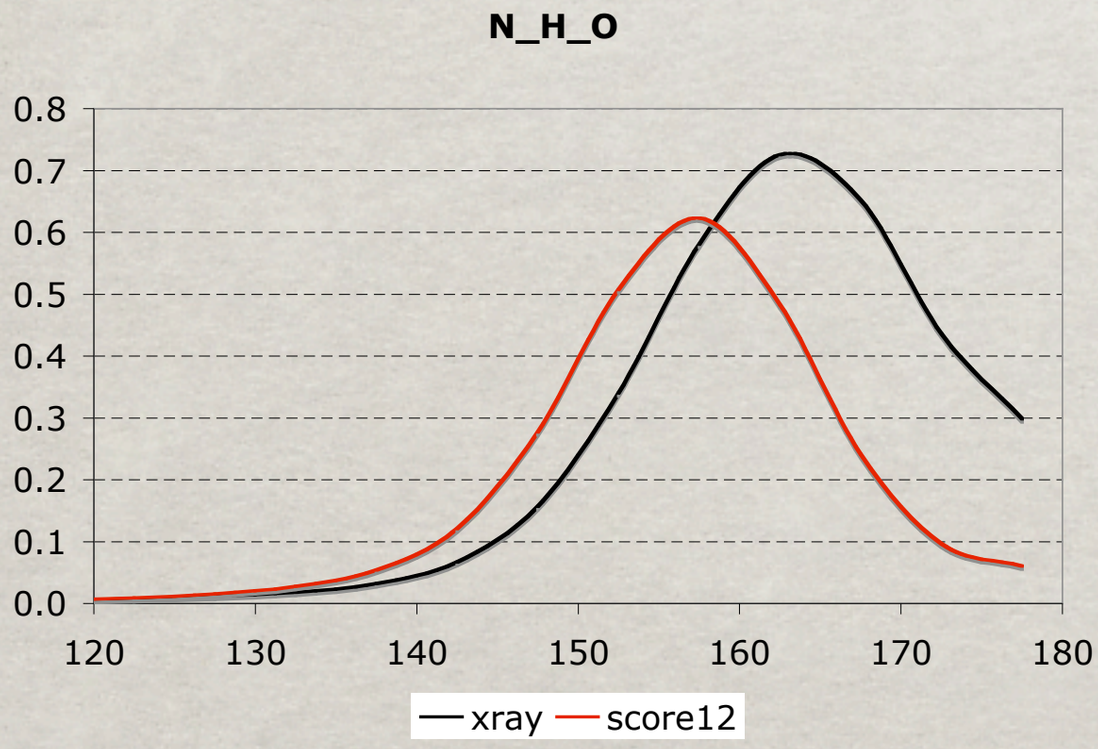
3.5
4.0
4.5
5.0
5.5
DISTANCE
xray
score12


N_H_O
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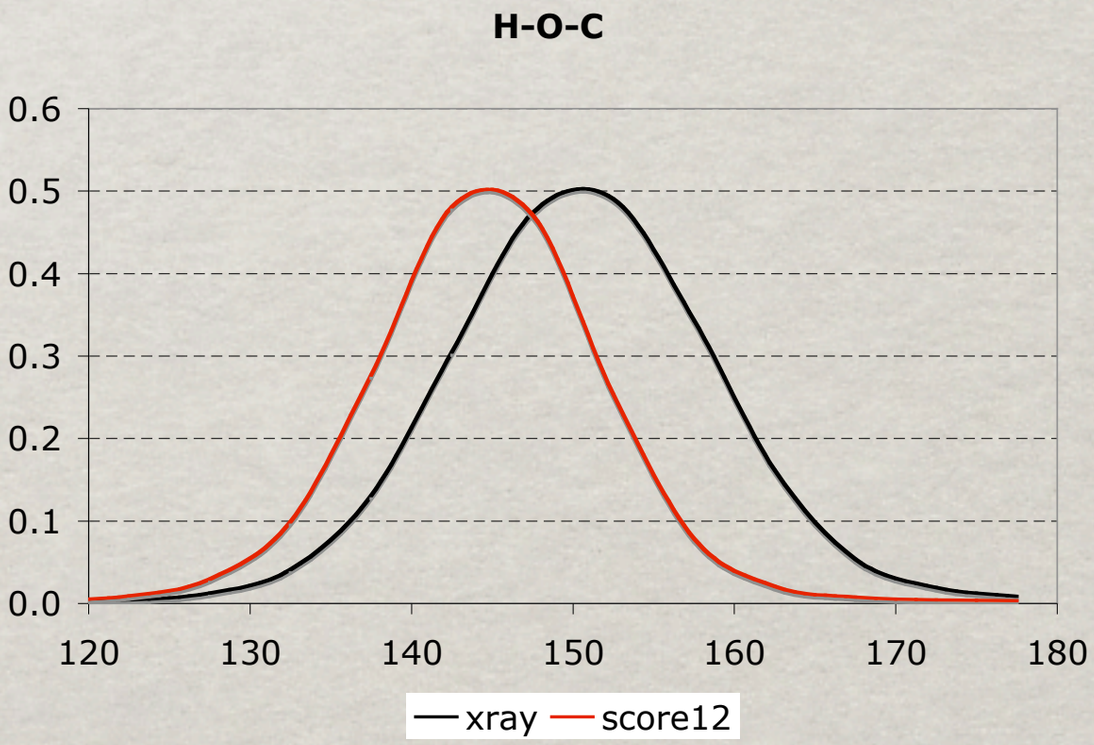
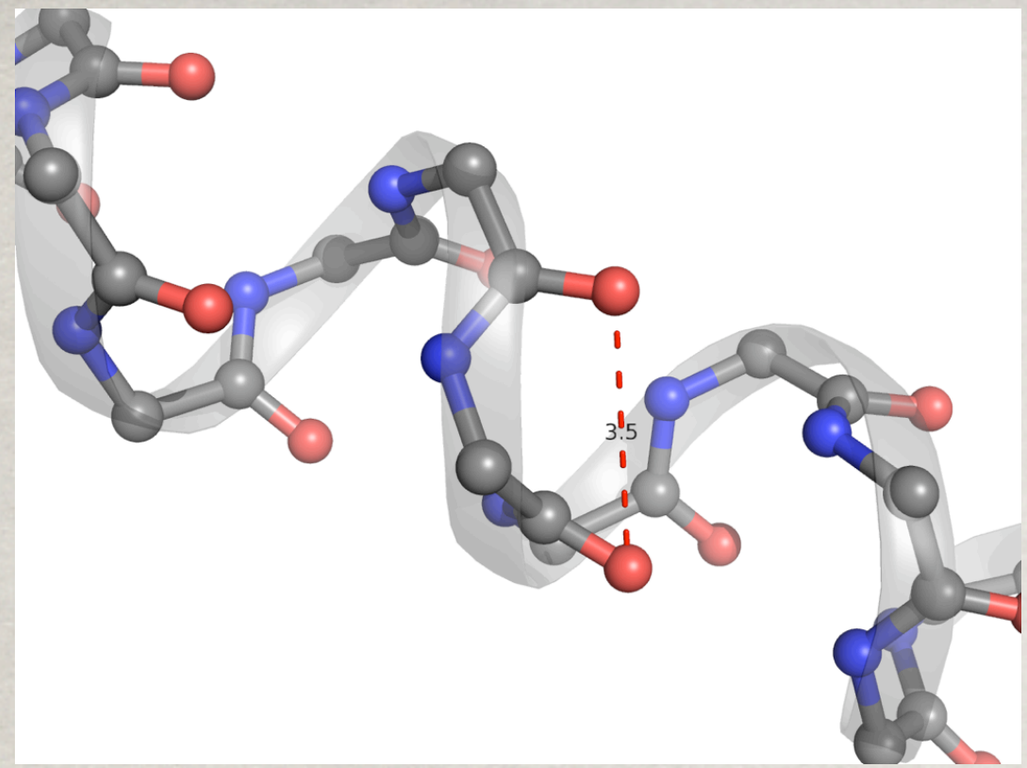
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
120
130
140
150
160
170
180
xray
score12


H-O-C
0.0
0.1
0.2
0.3
0.4
0.5
0.6
120
130
140
150
160
170
180
xray
score12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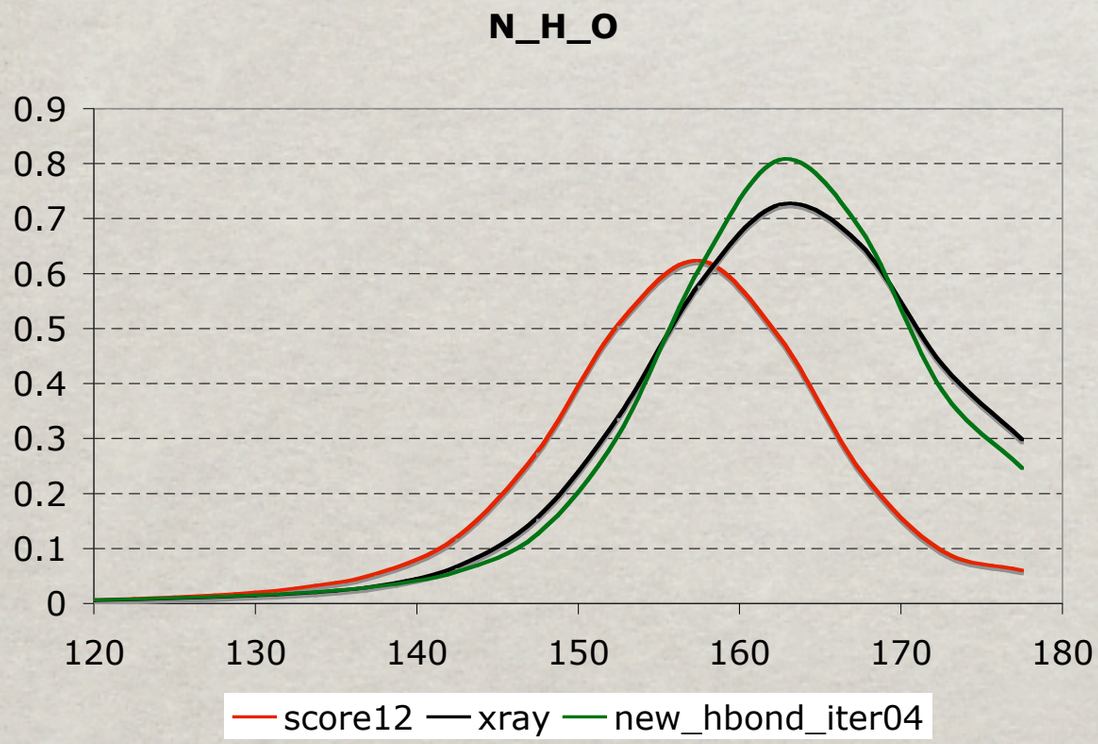
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0.6
0.5
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0.1
0
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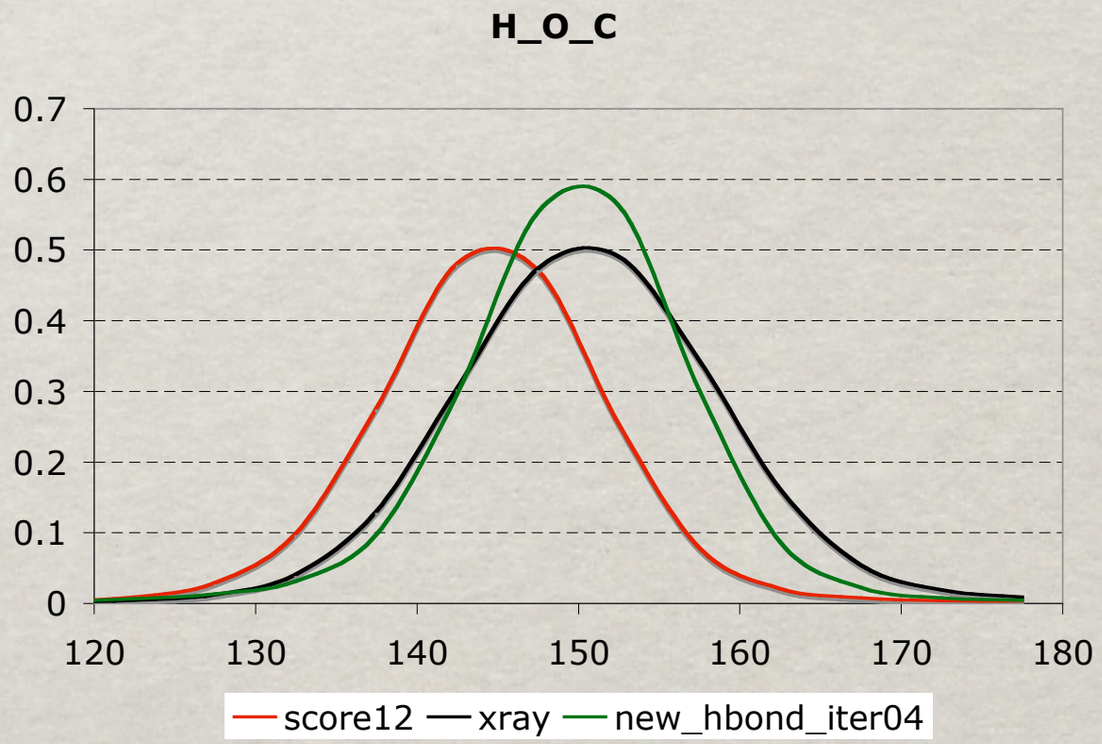
150
160
170
180
score12
xray
new_hbond_iter04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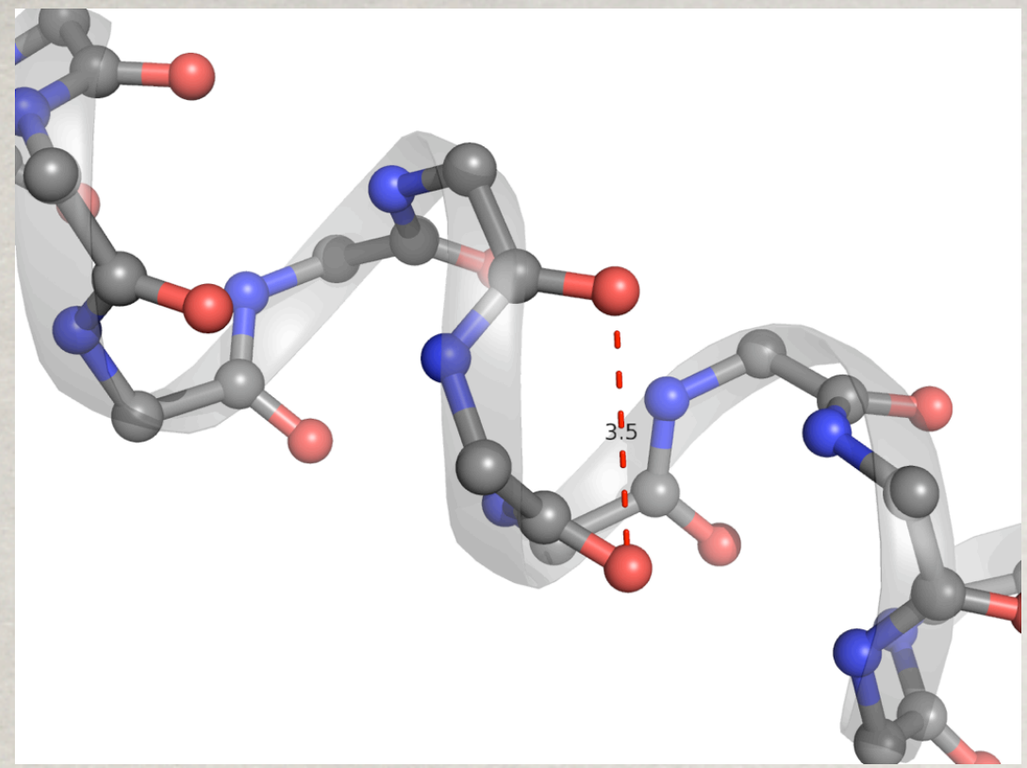
score12
xray
new_hbond_iter04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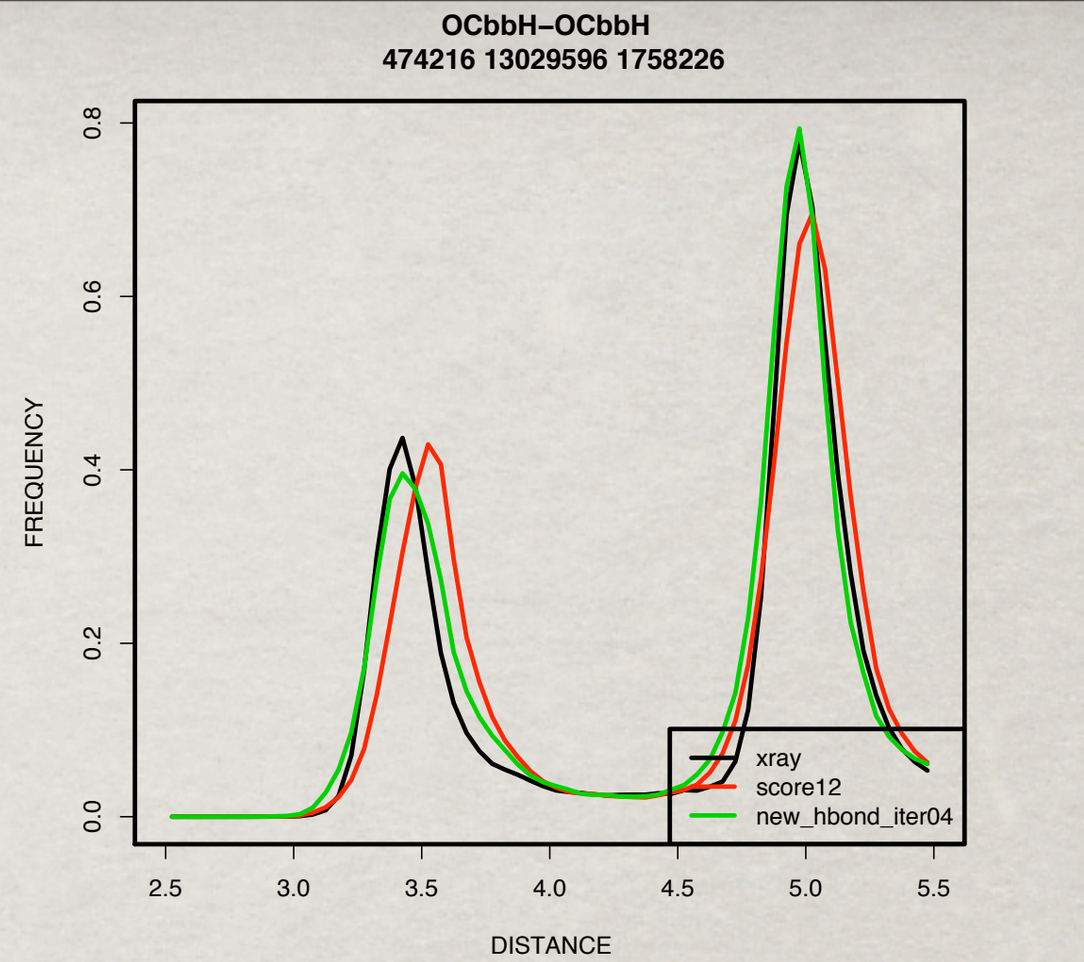
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5.5
DISTANCE
xray
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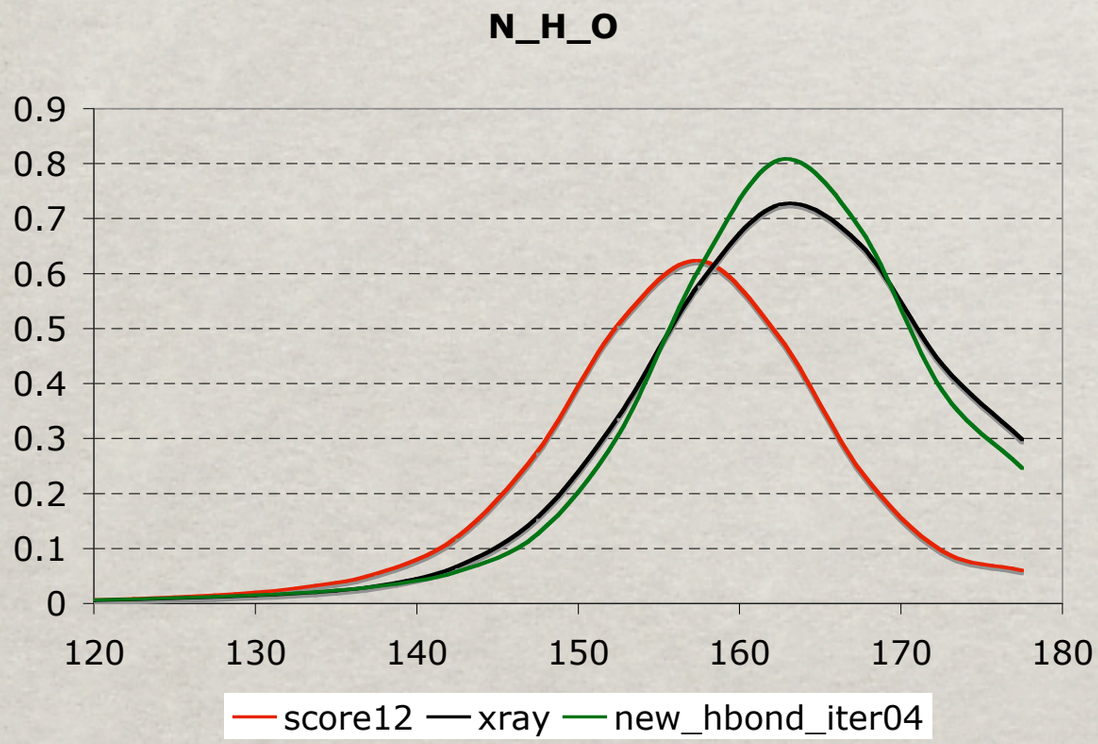
new_hbond_iter04


N_H_O
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0.7
0.6
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150
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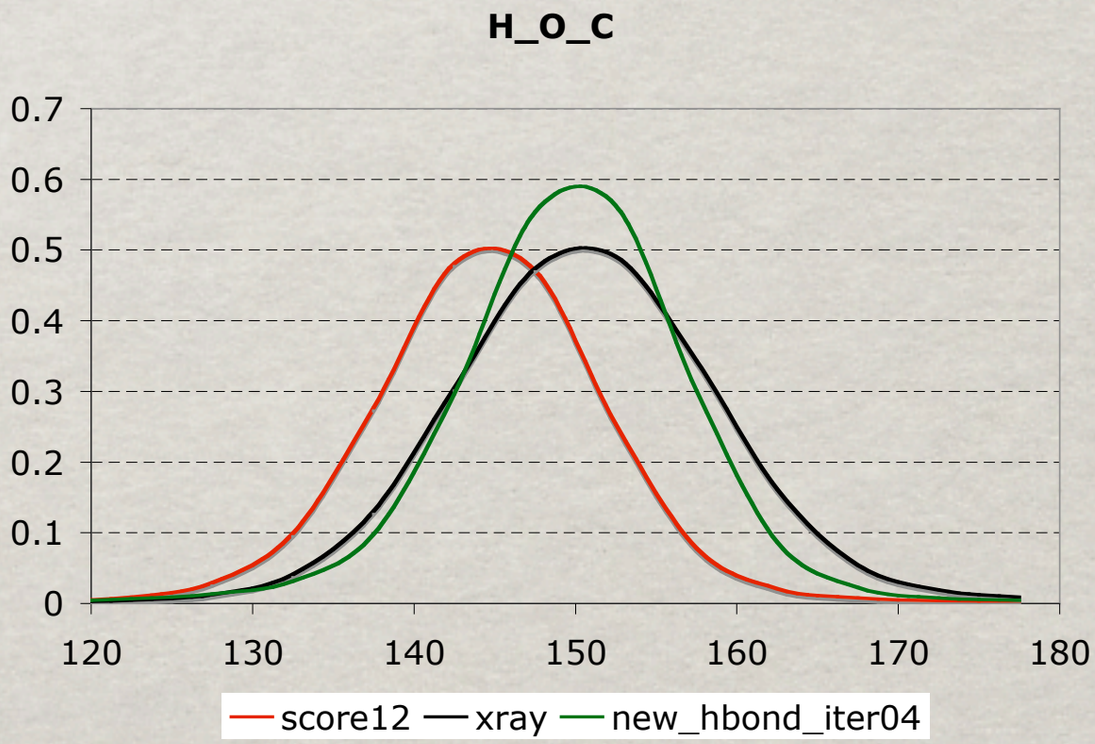
170
180
score12
xray
new_hbond_iter04


H_O_C
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
120
130
140
150
160
170
180
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xray
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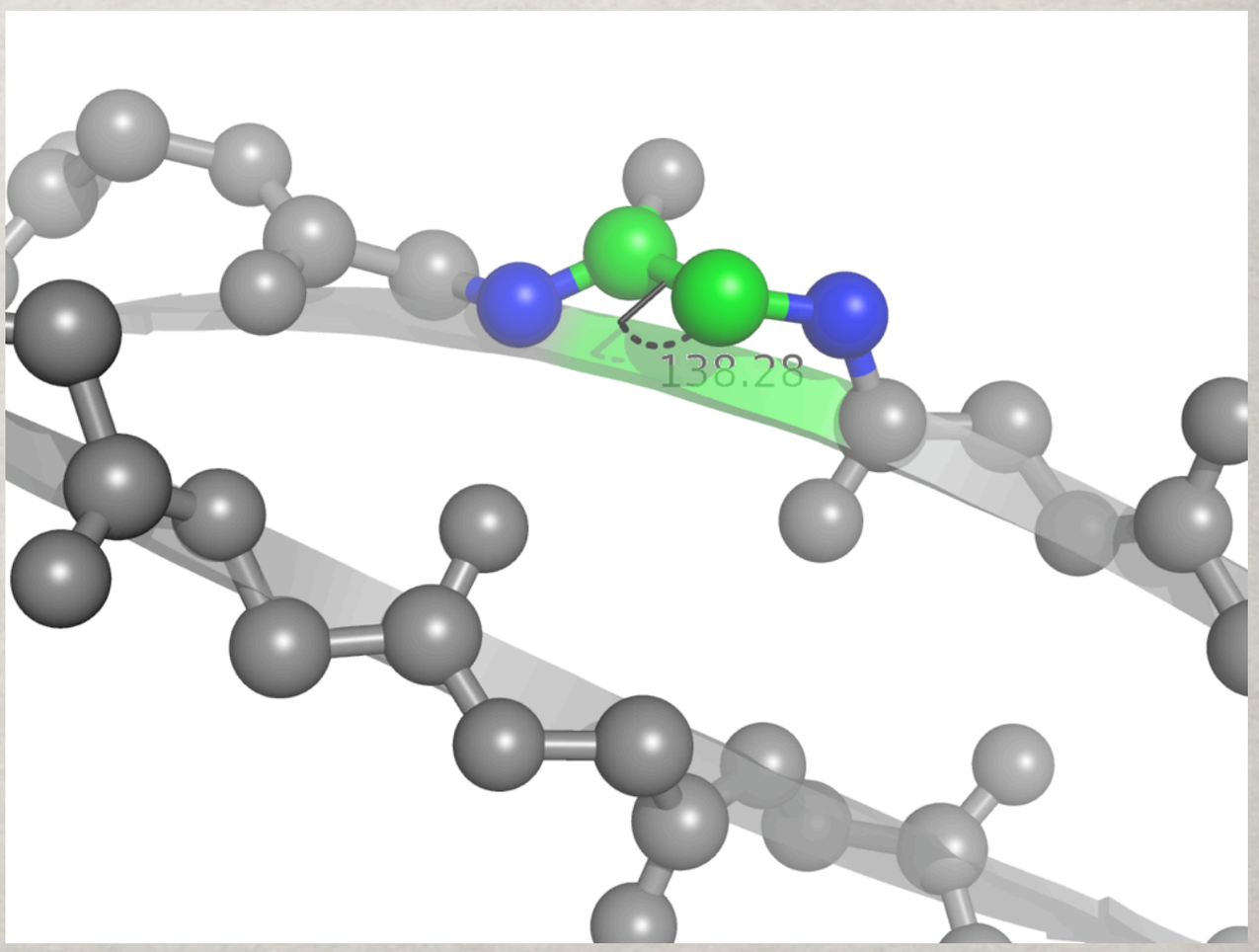
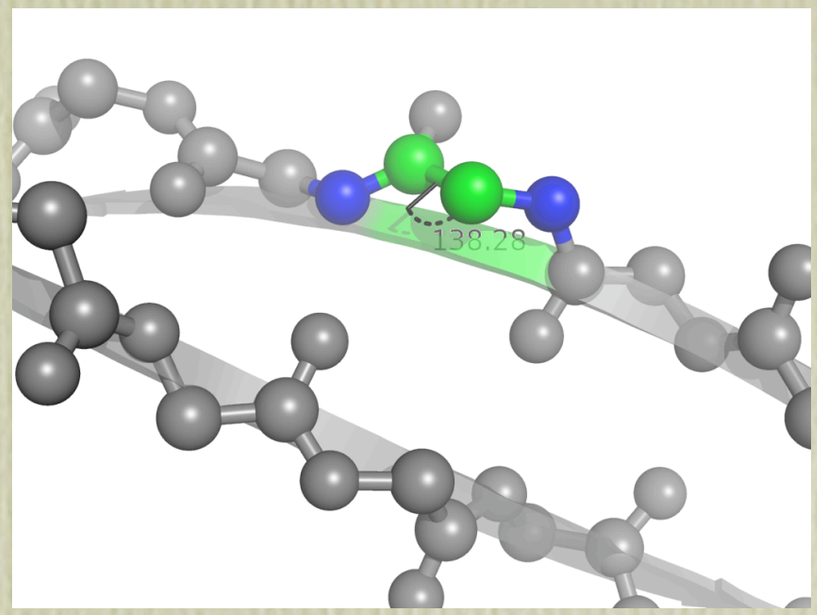
- Angular dependence of short-range backbone hydrogen bond (Helix)
- Ramachandran potential
- Non-polar hydrogen bond



Ramachandran potential



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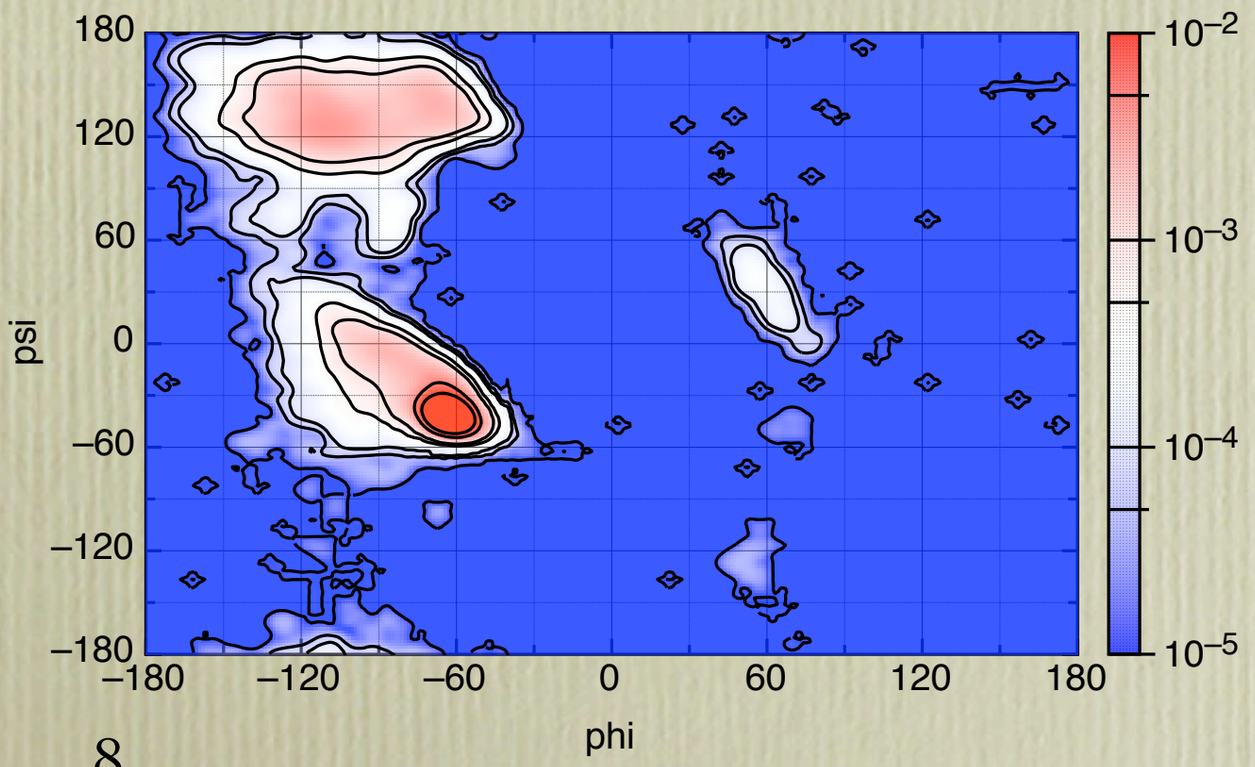

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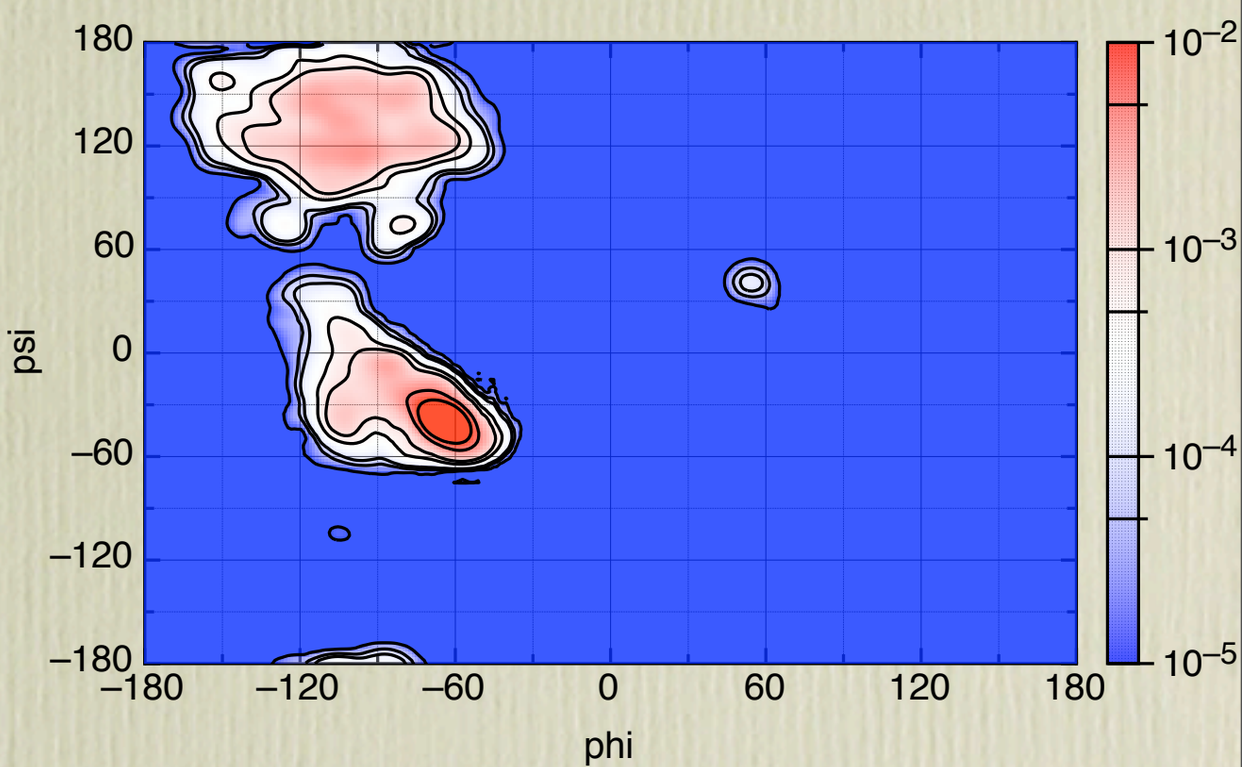
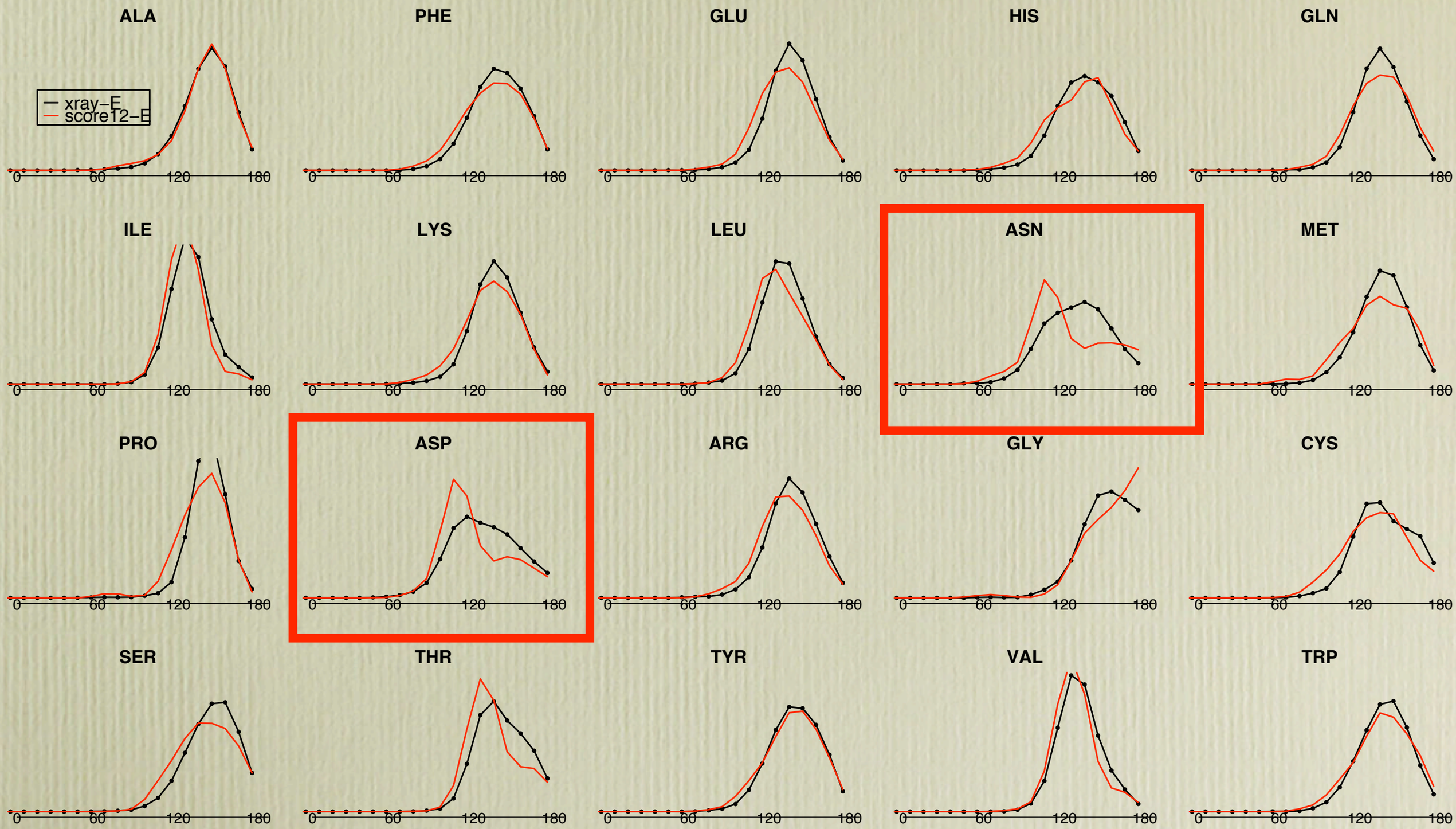


psi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GLN
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LEU
ASN
MET
PRO
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ARG
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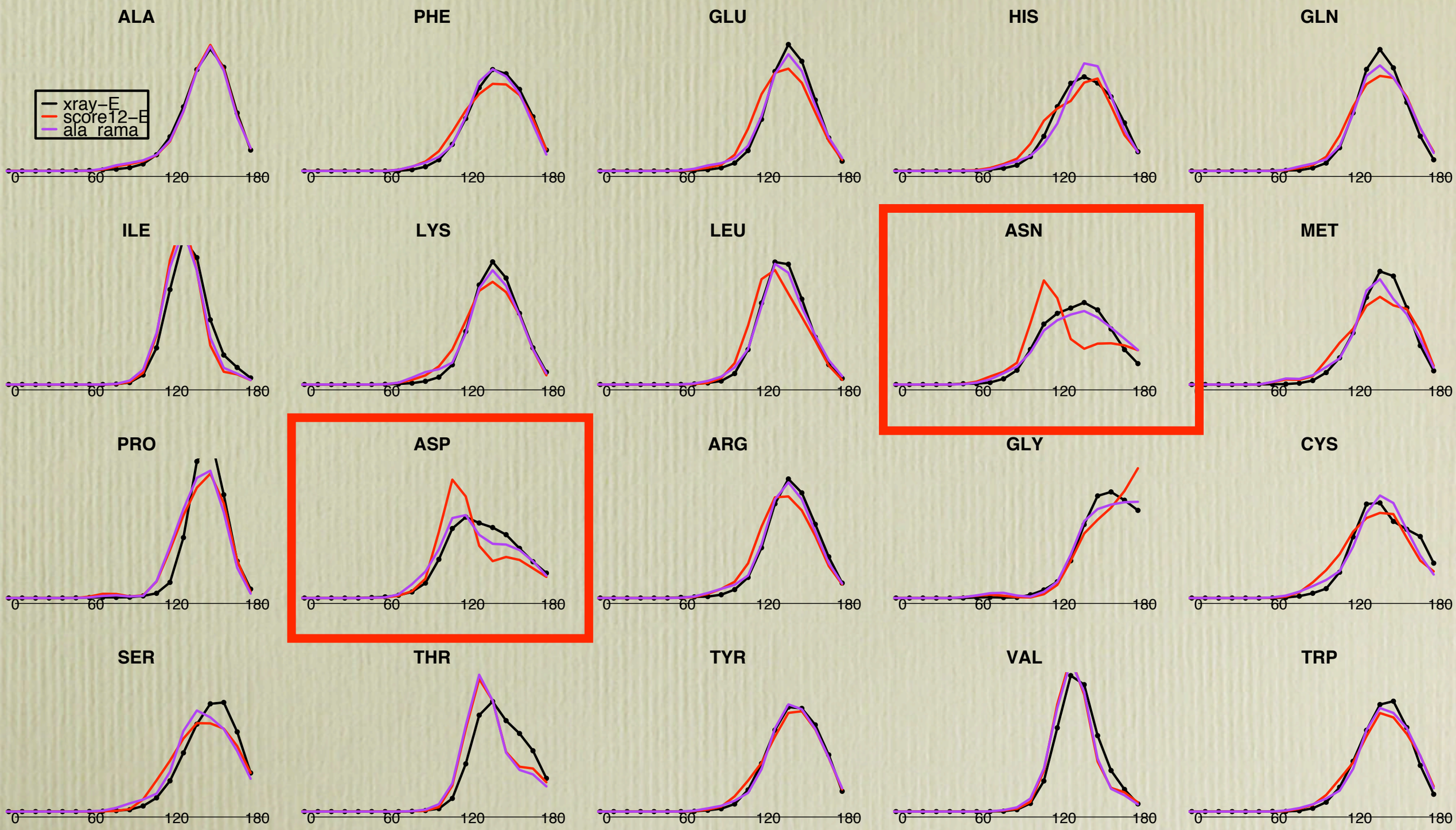
SER
THR
TYR
VAL
TRP
xray-E
score12-E
0
60
120
180

psi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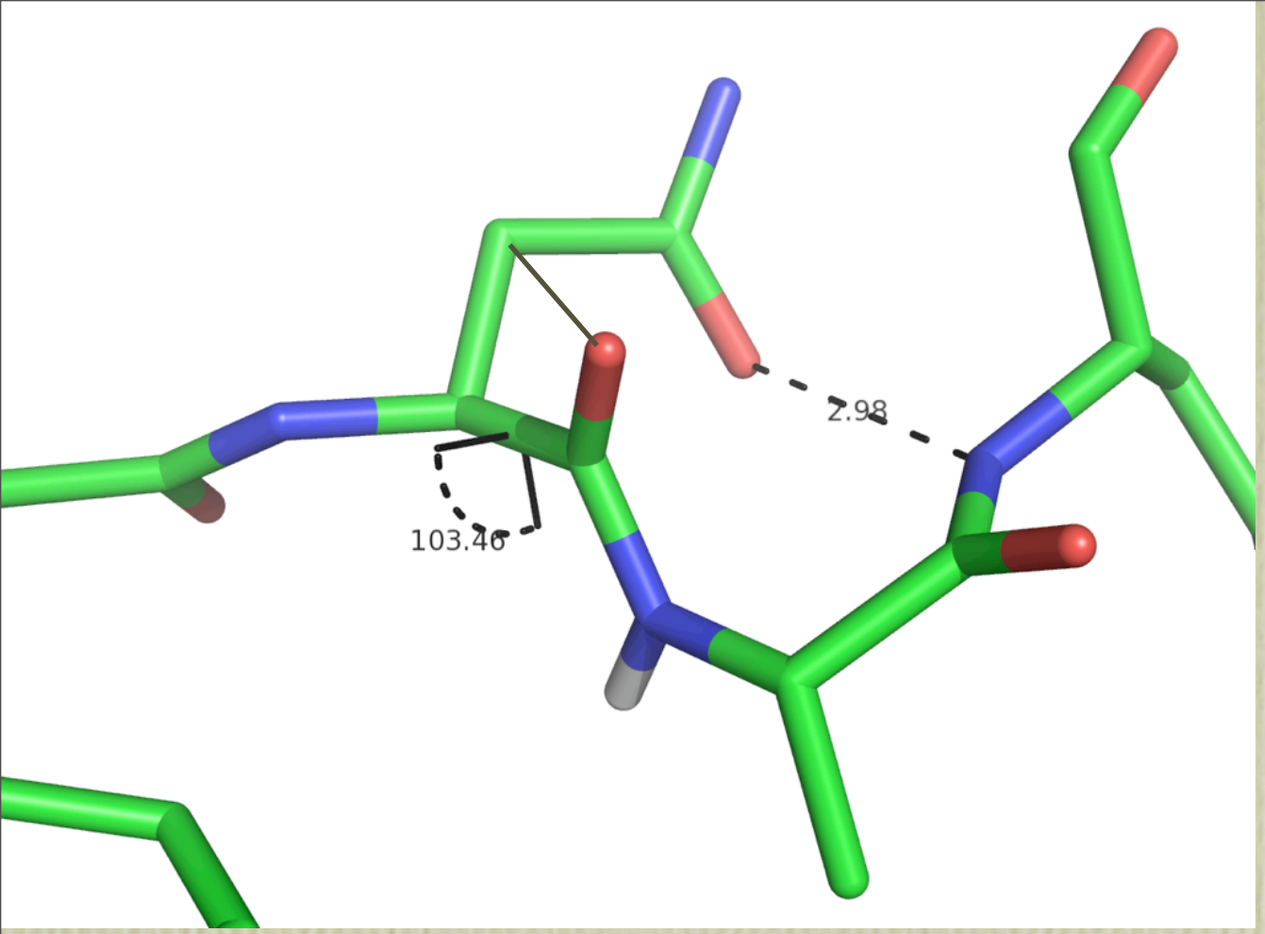
0
60
120
180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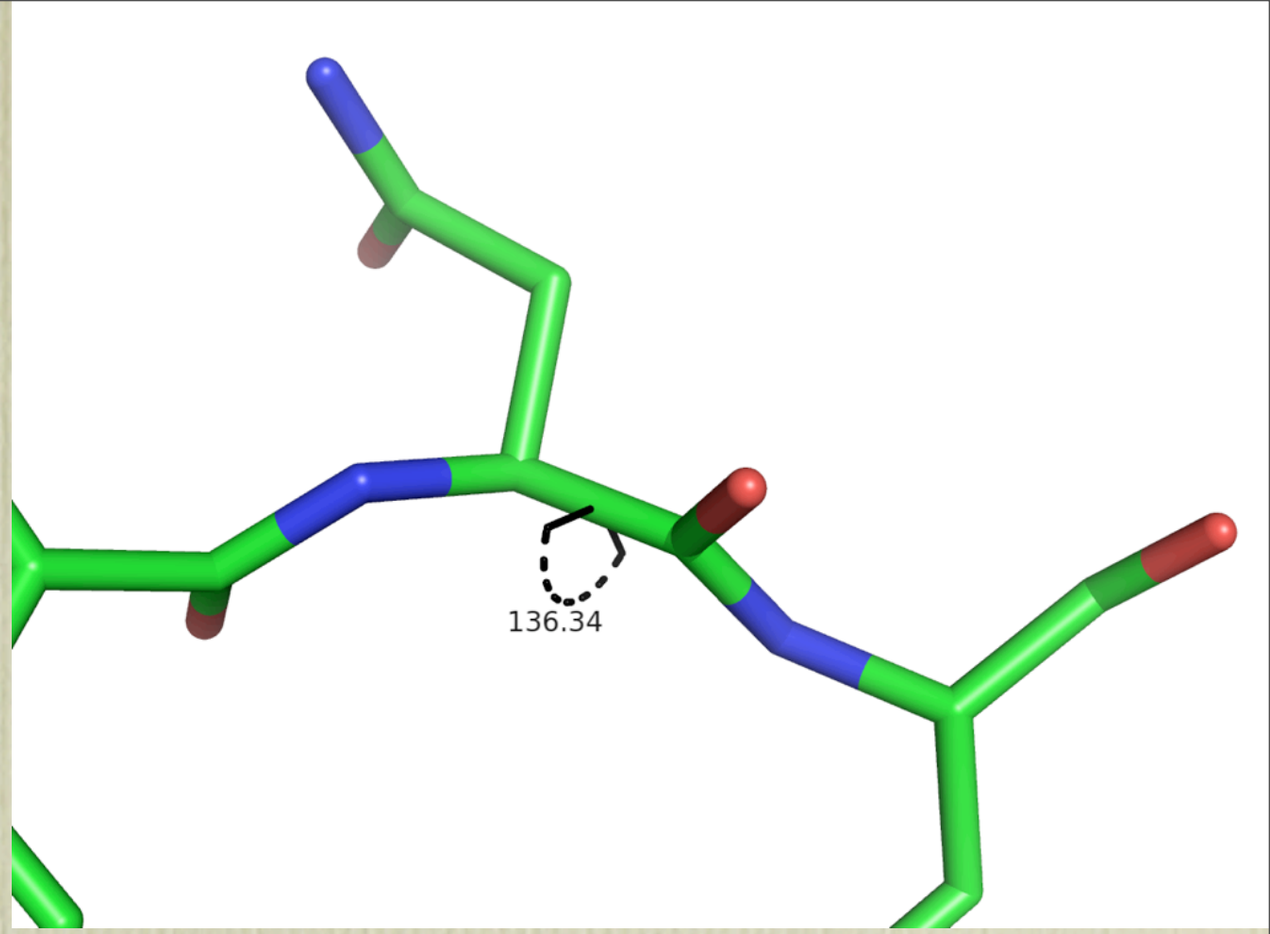
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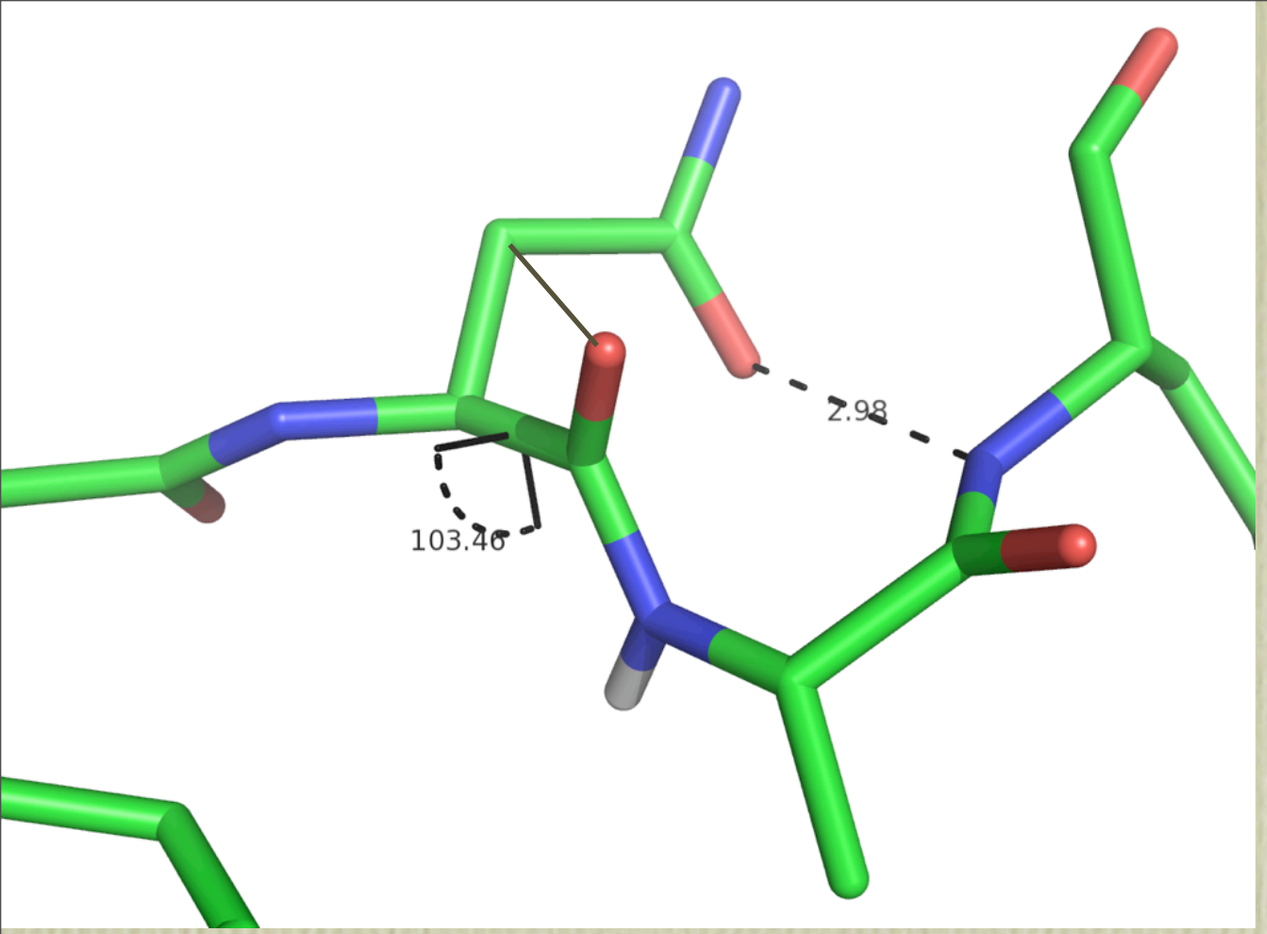
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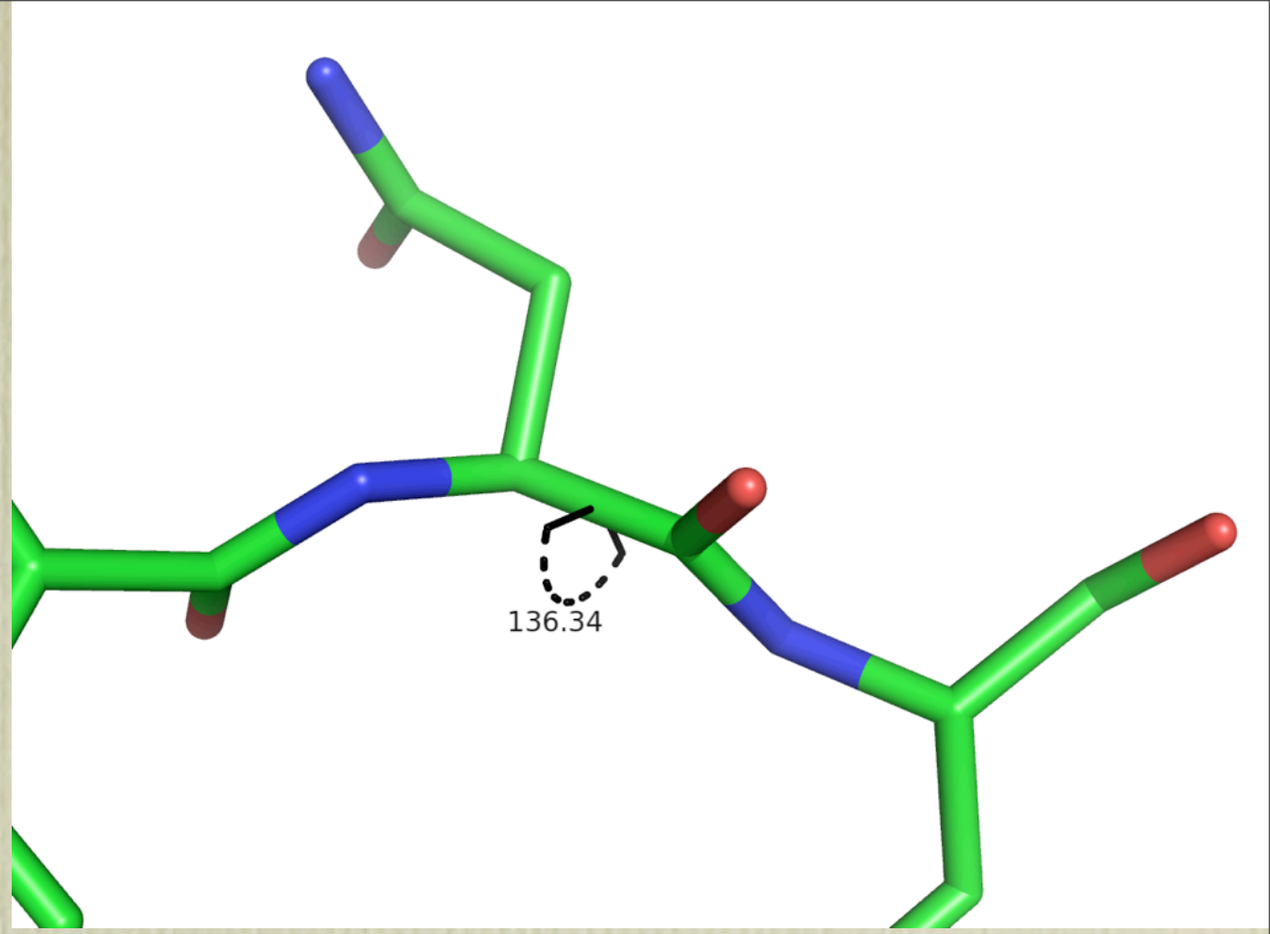
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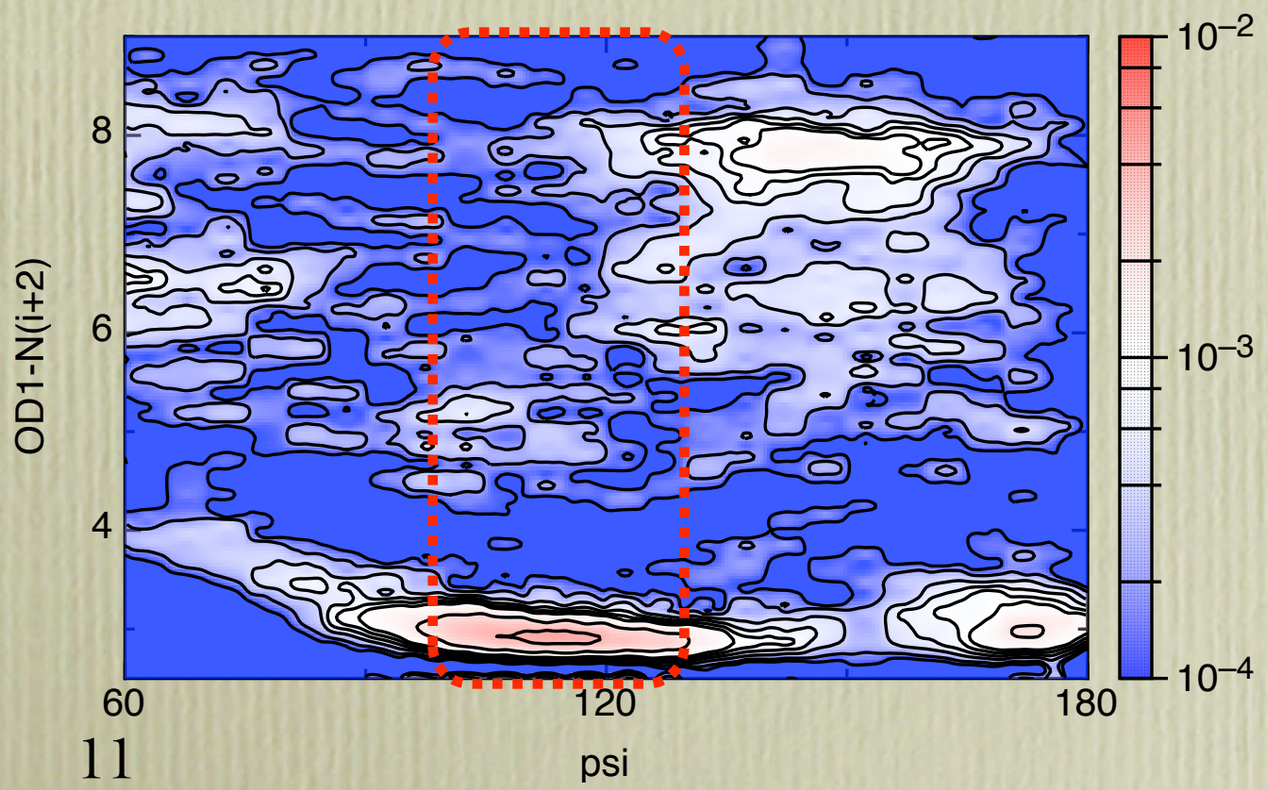
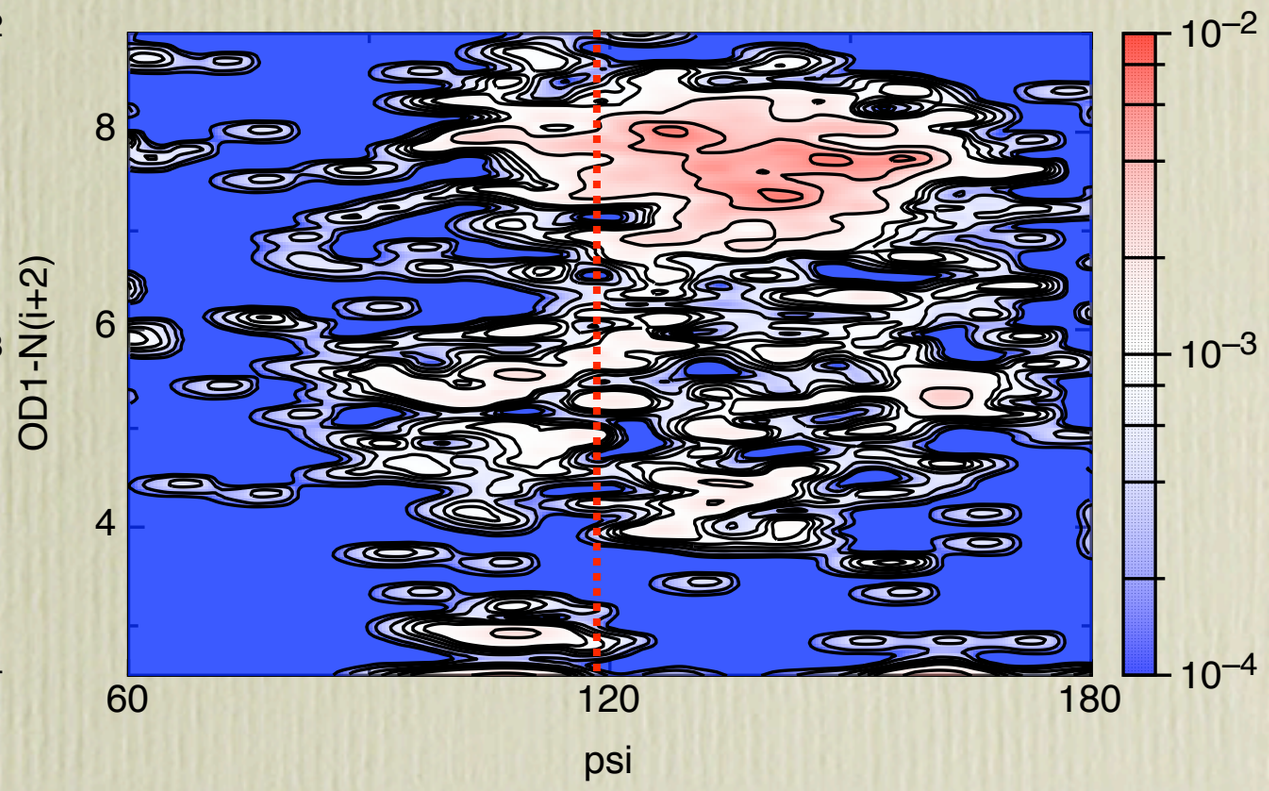
xray-L


OD1-N(i+2)
8
6
4
60
120
180
psi
10^{-2}
10^{-3}
10^{-4}

xray-E


OD1-N(i+2)
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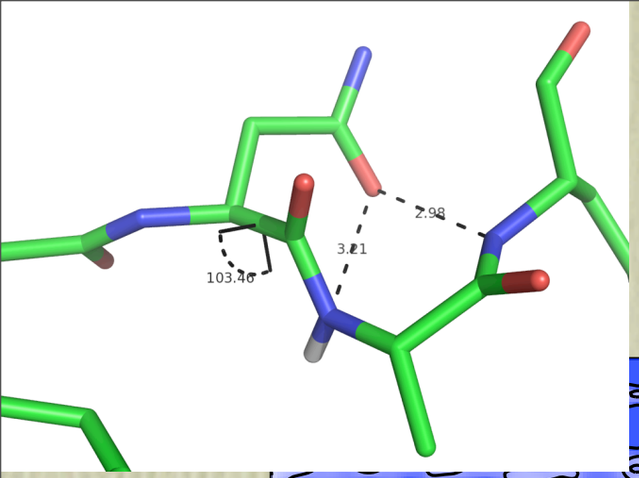
6
4
60
120
180
psi
10^{-2}
10^{-3}
10^{-4}



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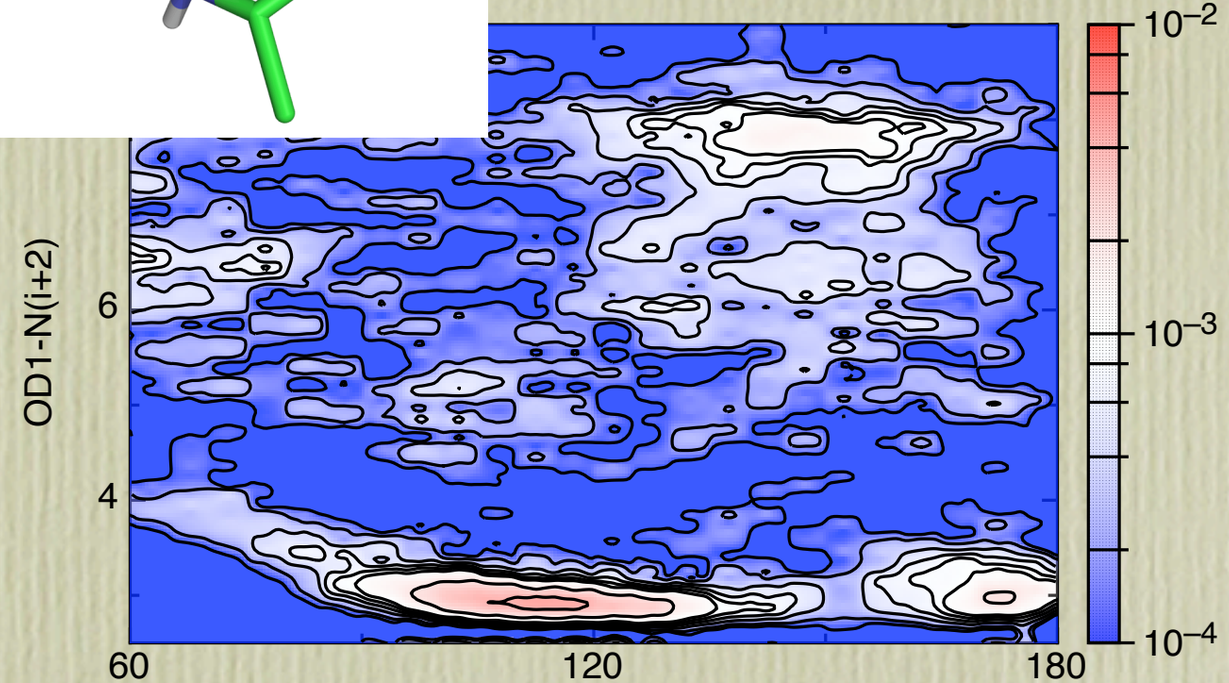

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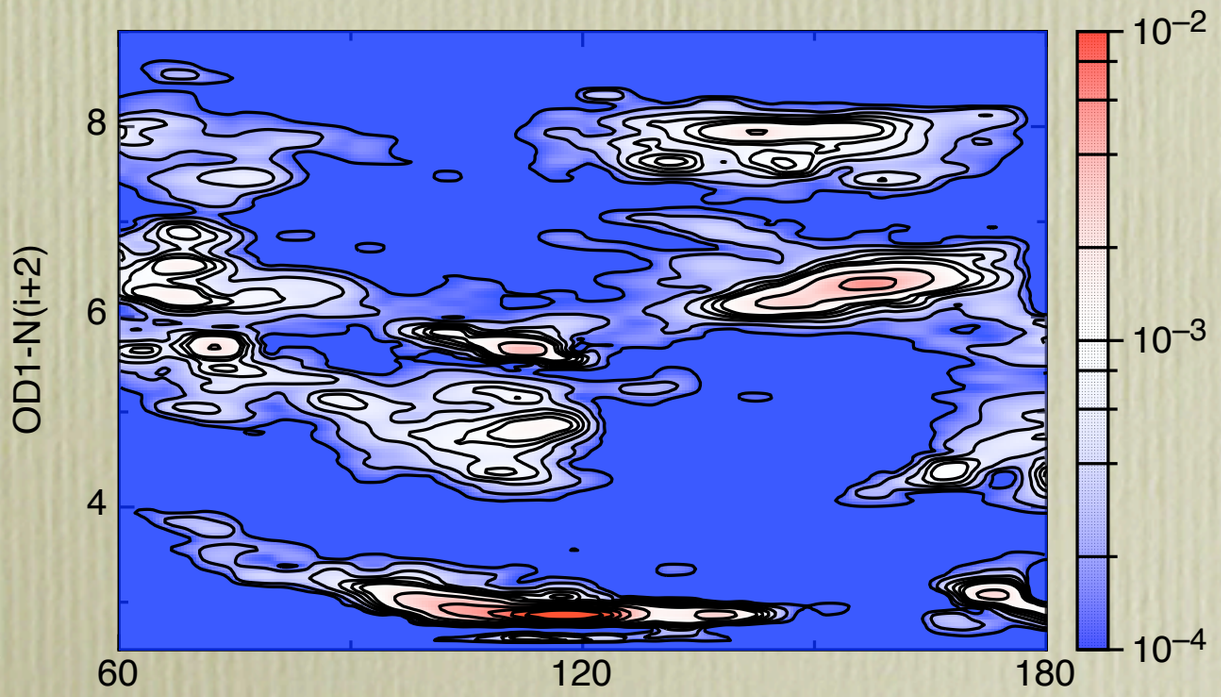

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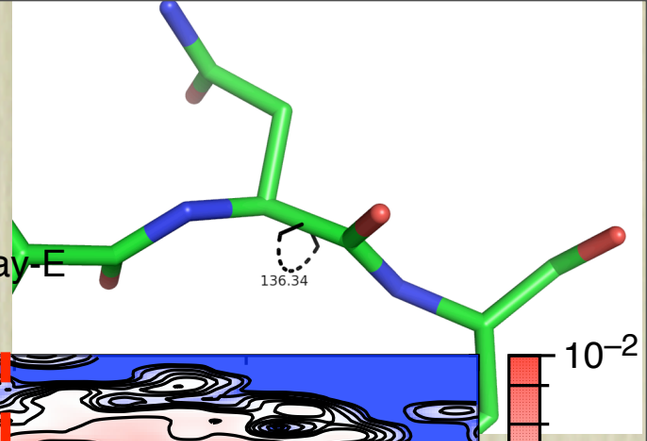

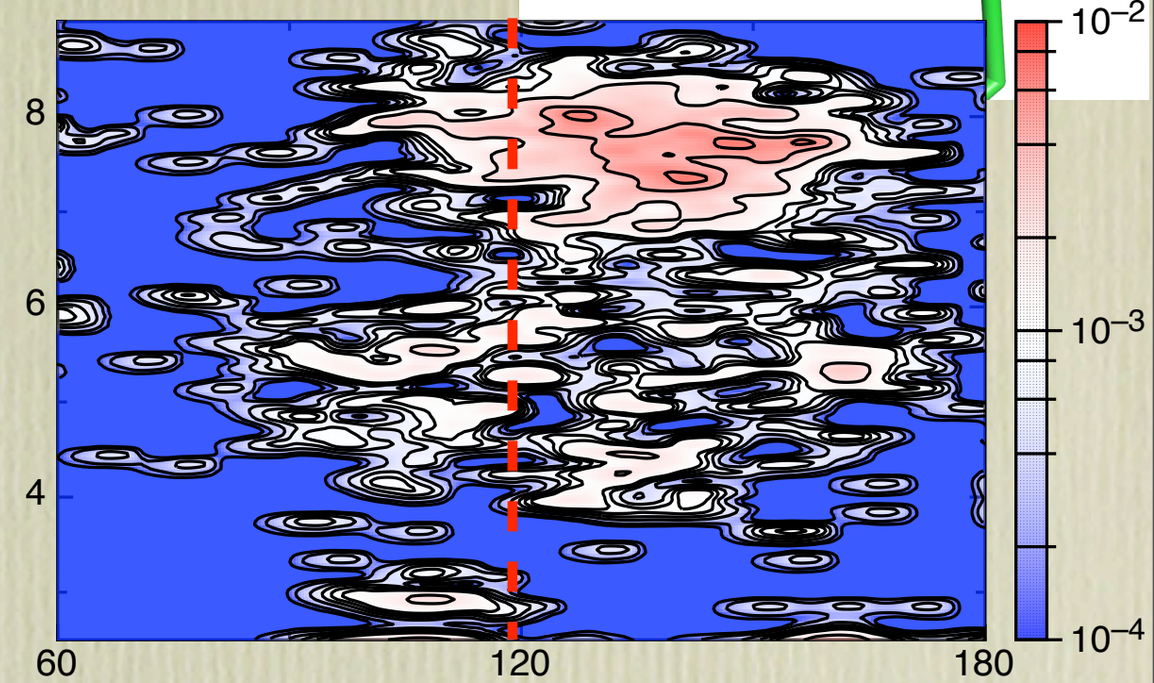

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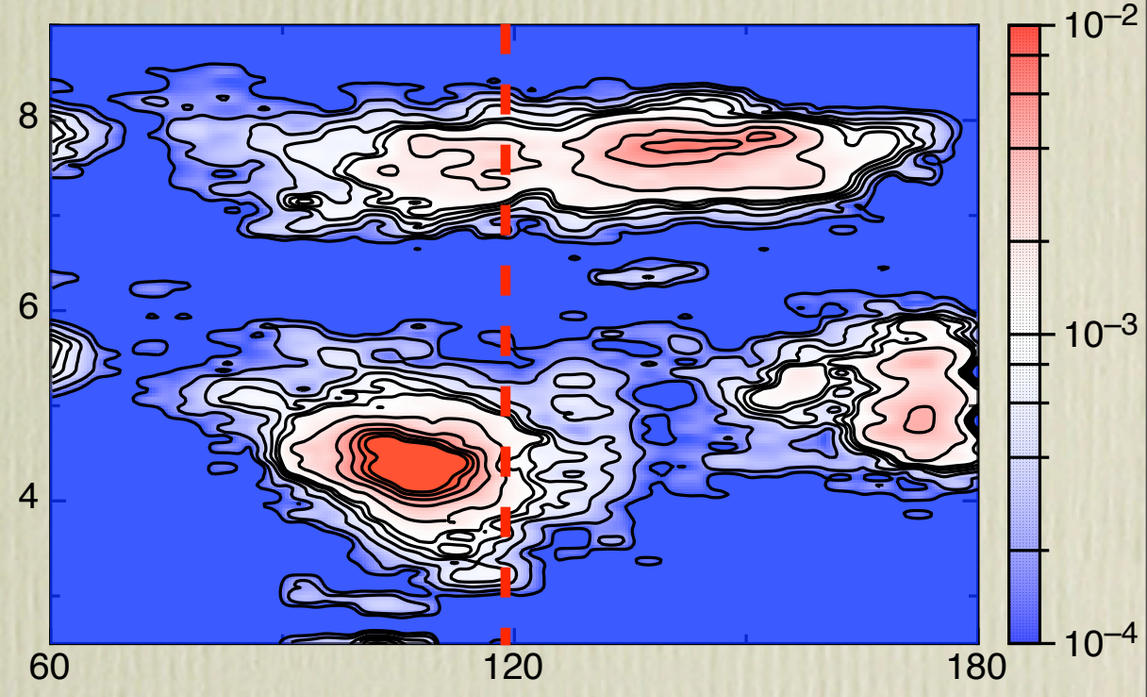

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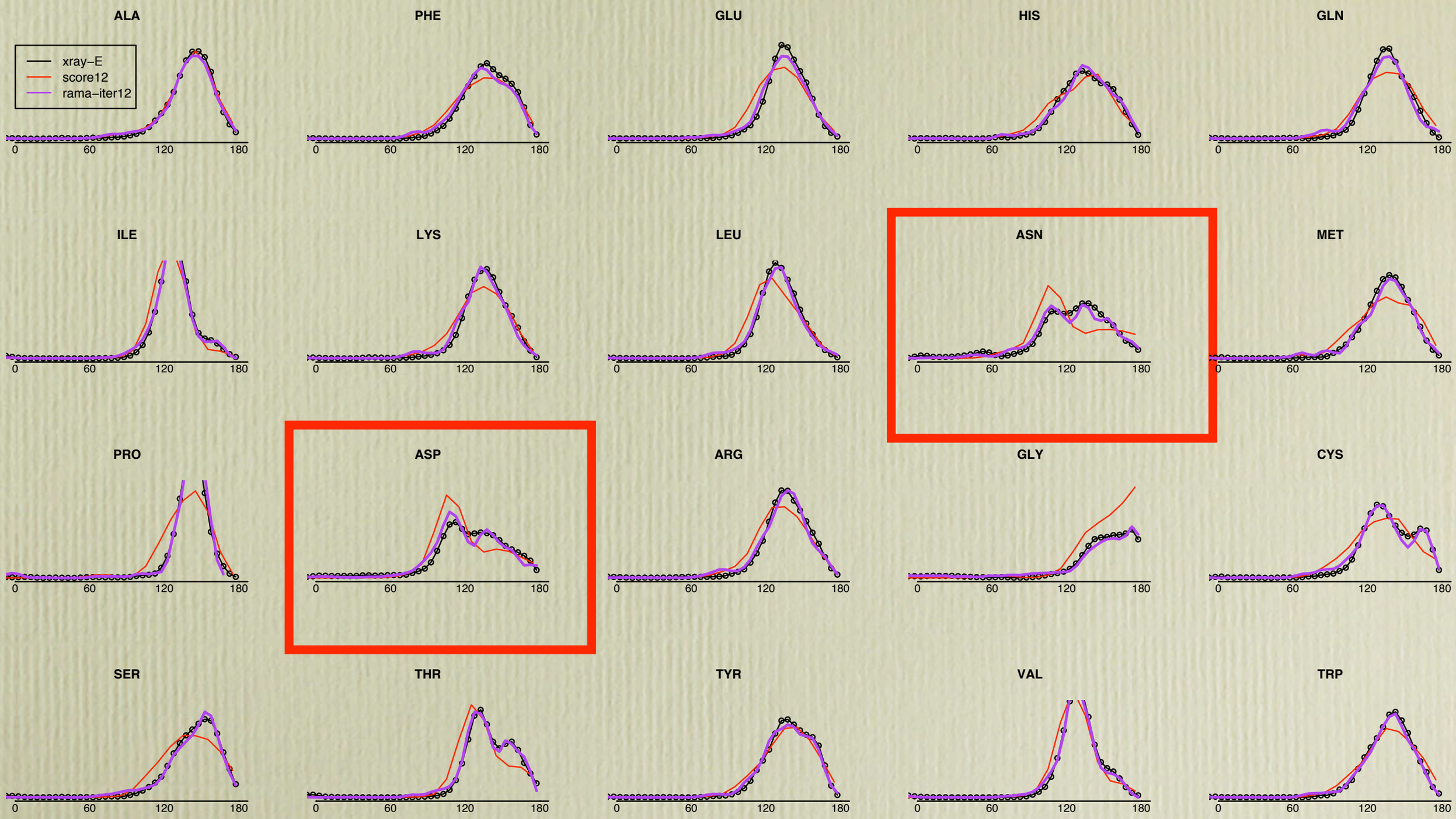
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rama–iter12
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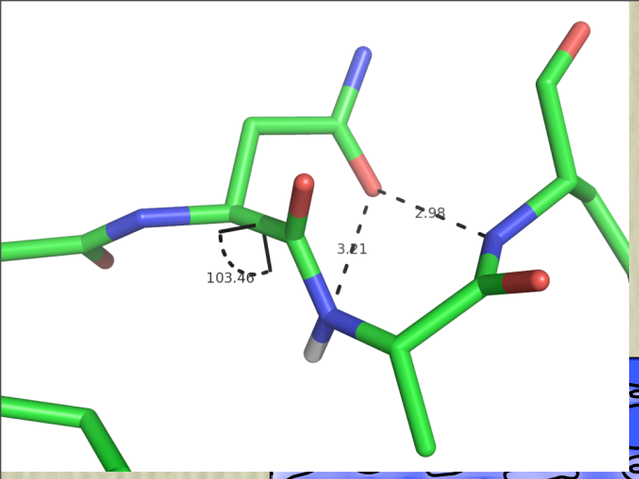
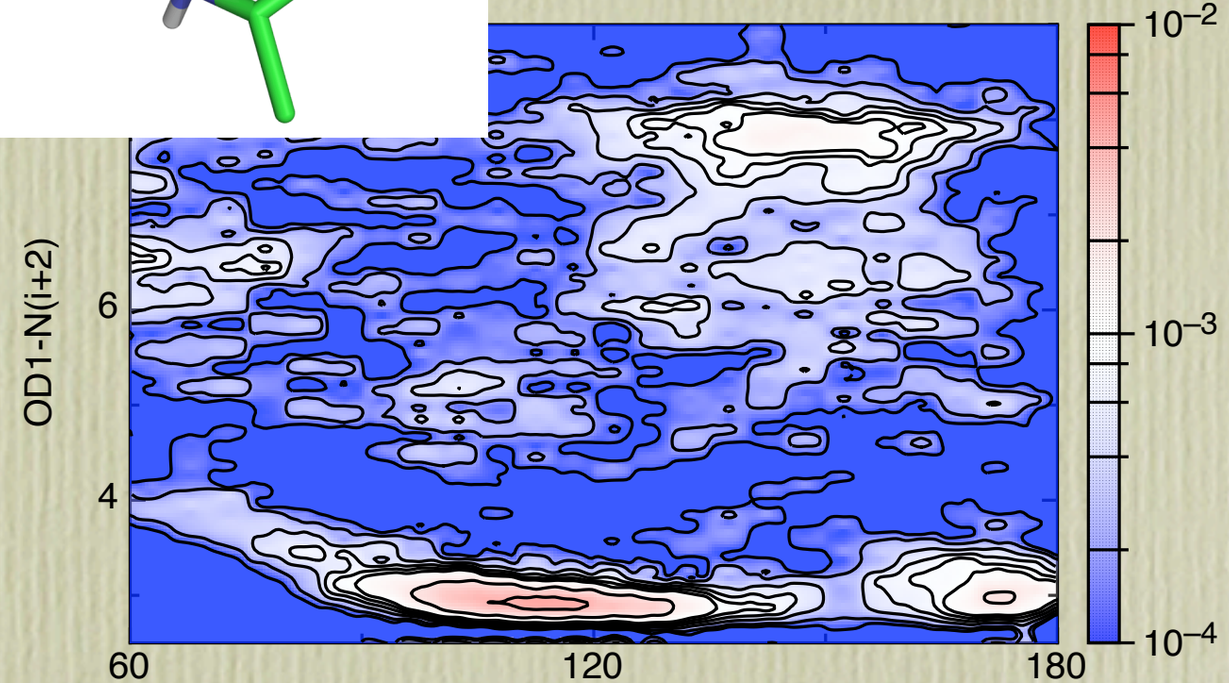
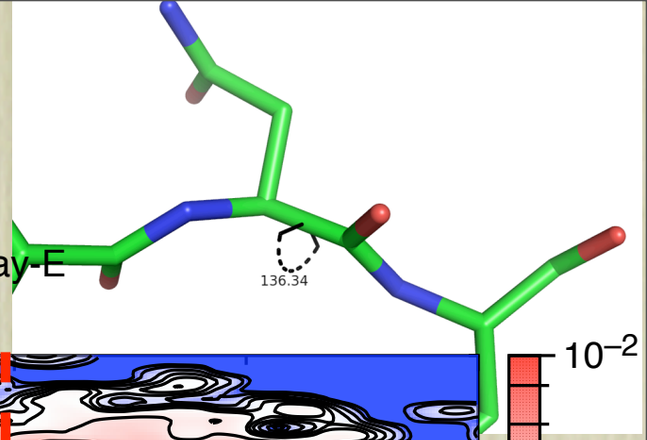
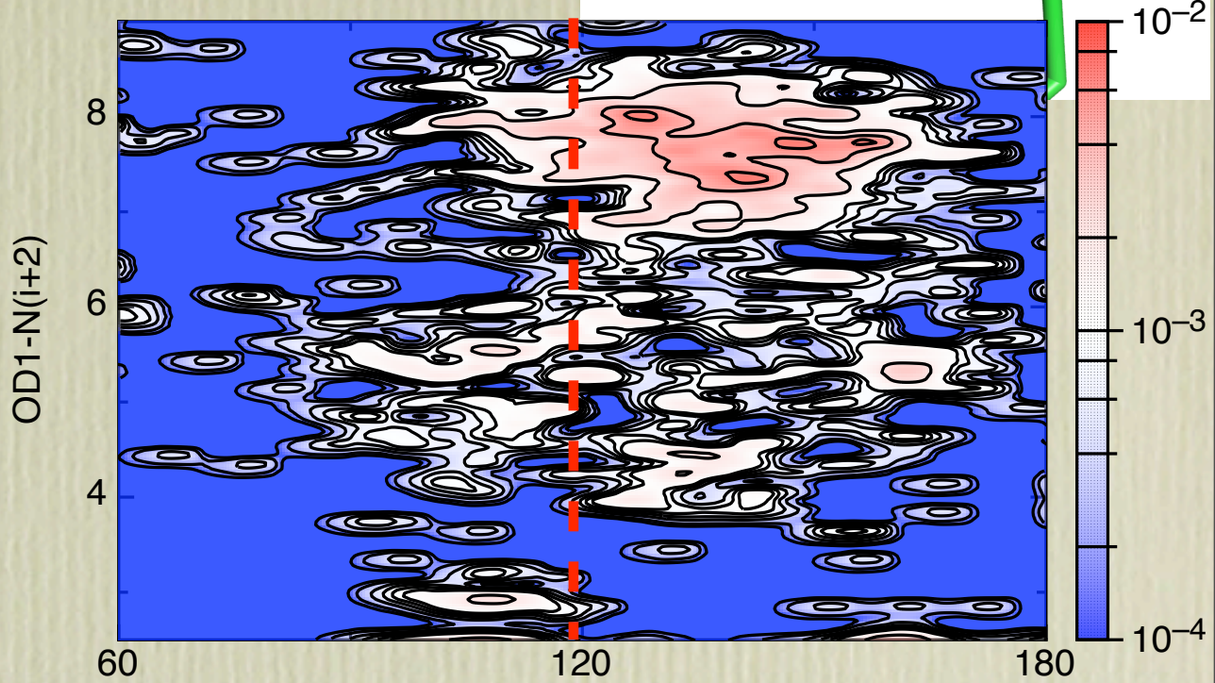


xray-L



xray-E





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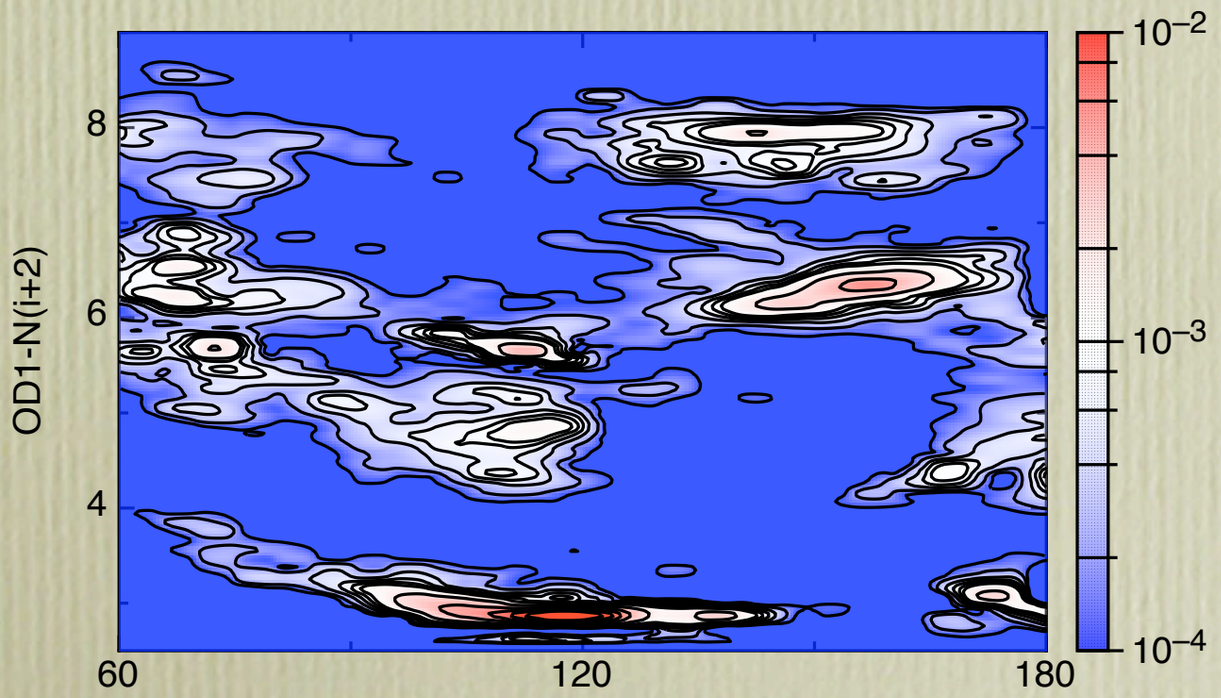

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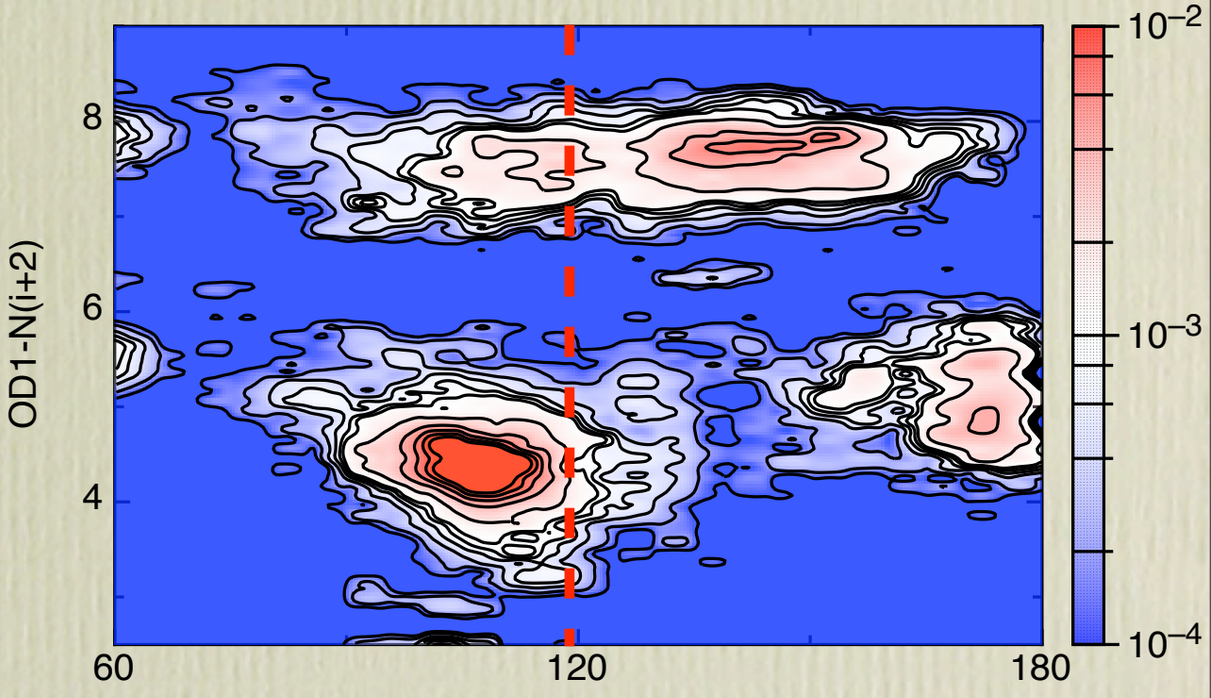
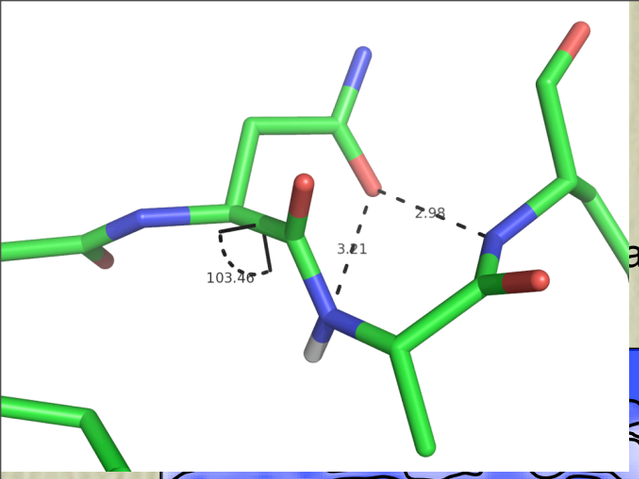
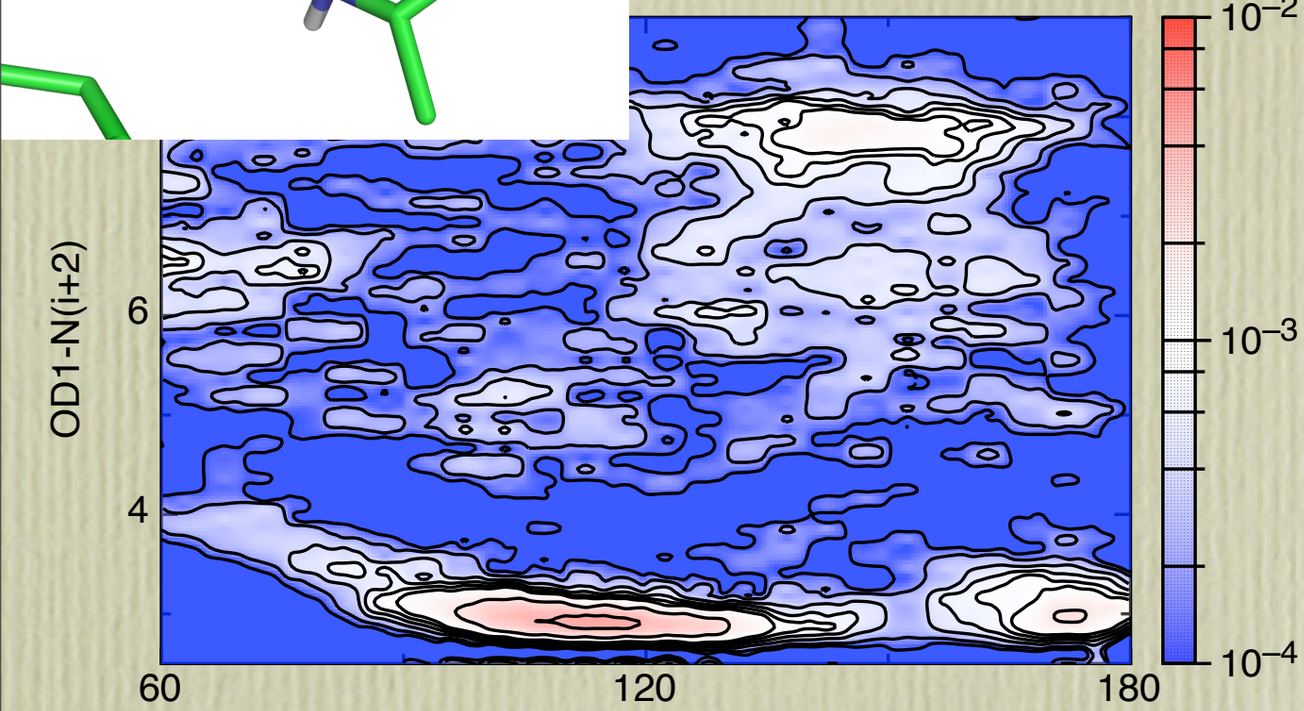
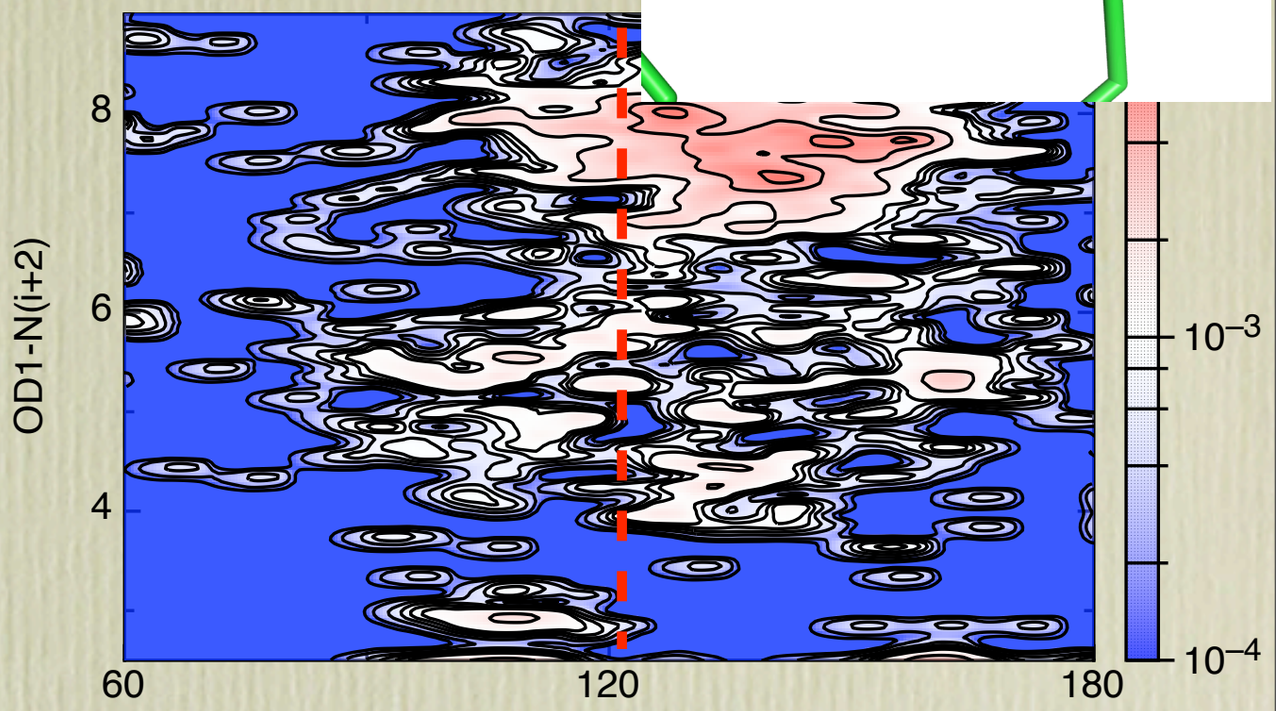




ay-L

xray-



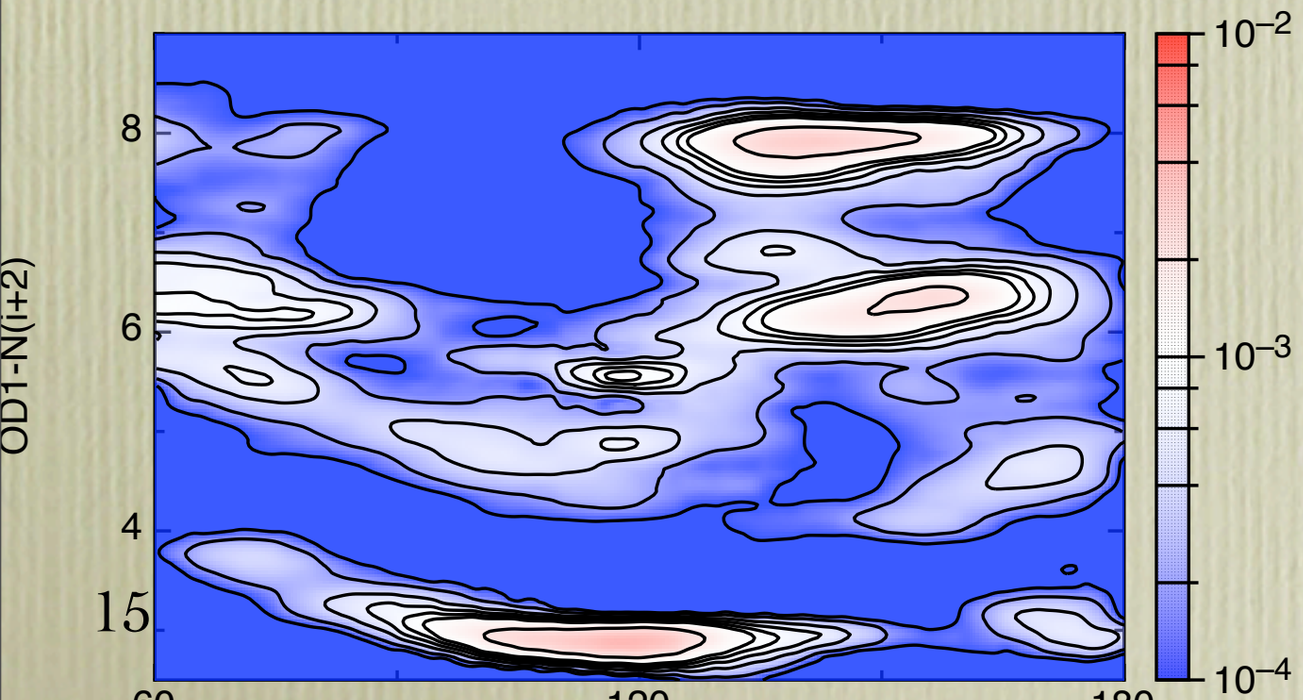


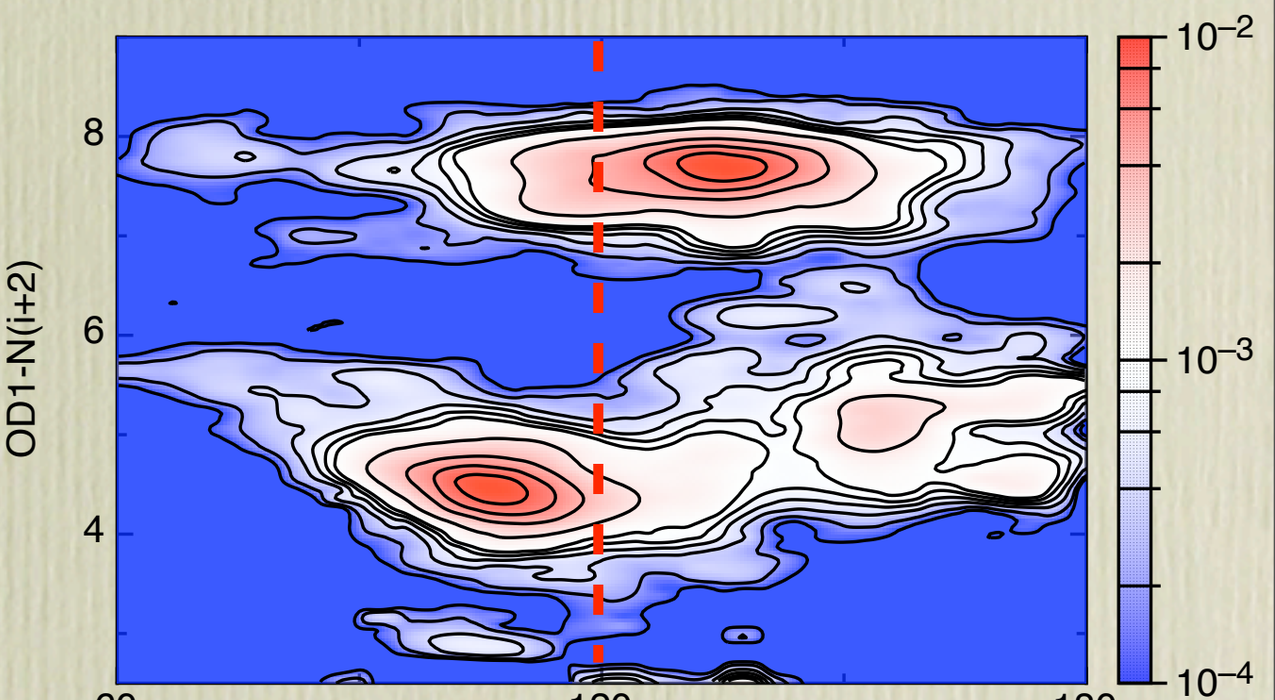
psi

rama-iter12-L

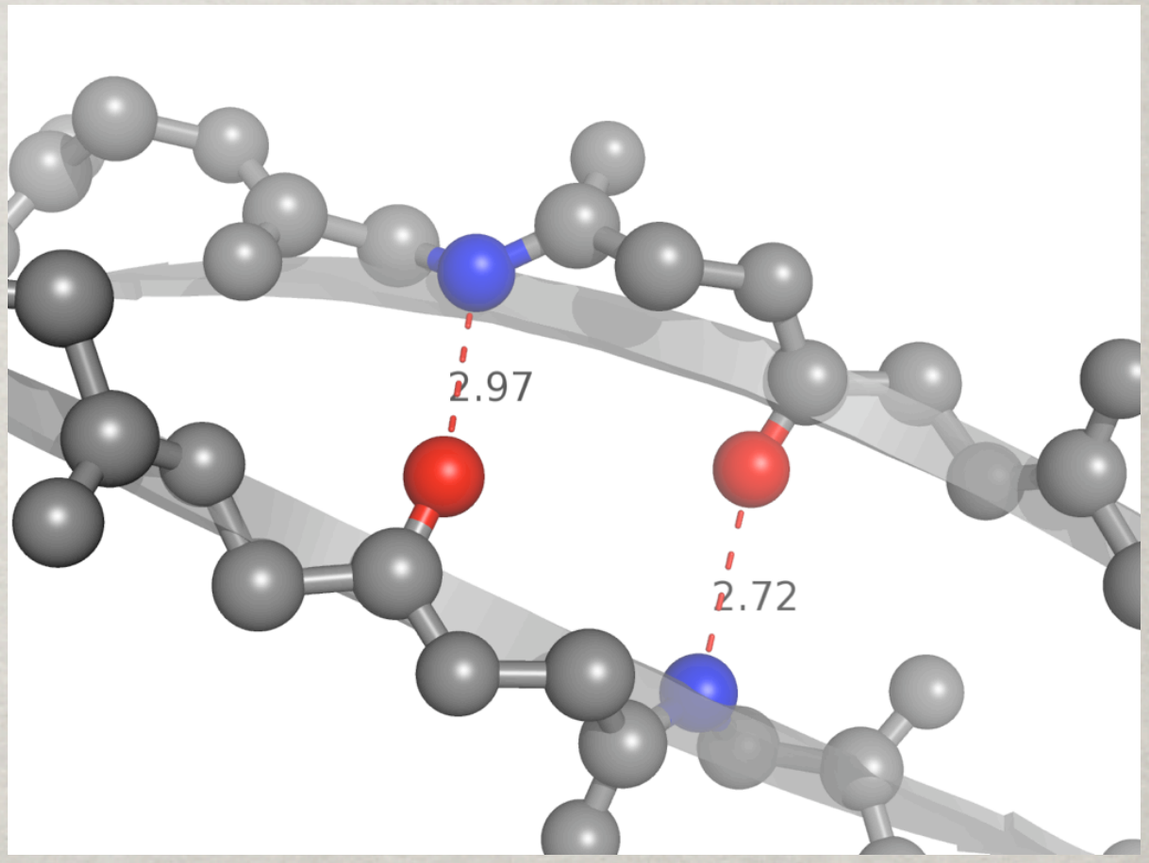
psi

rama-iter12-E





- Angular dependence of short-range backbone hydrogen bond (Helix)
- Ramachandran potential
- Non-polar hydrogen bond



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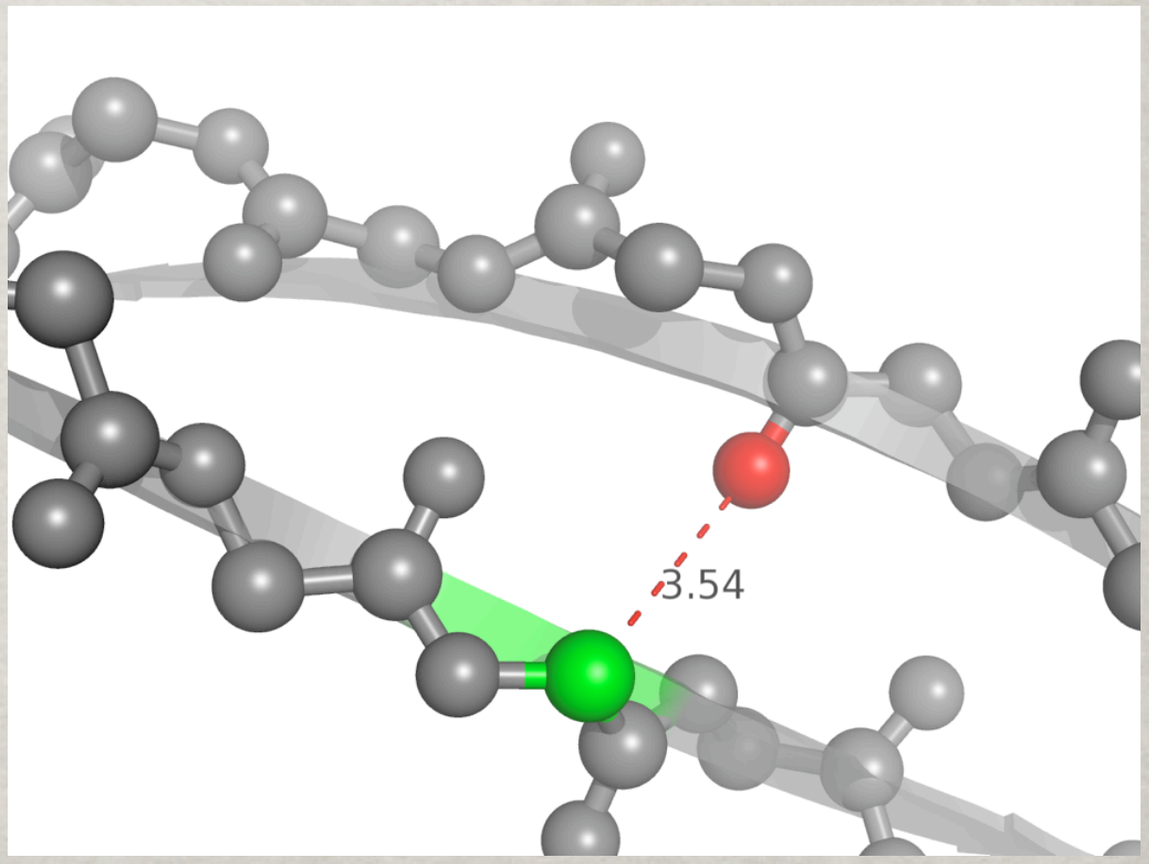
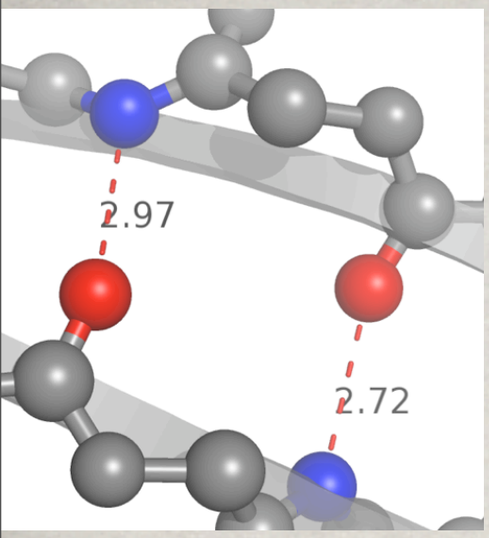
- Non-polar hydrogen bond

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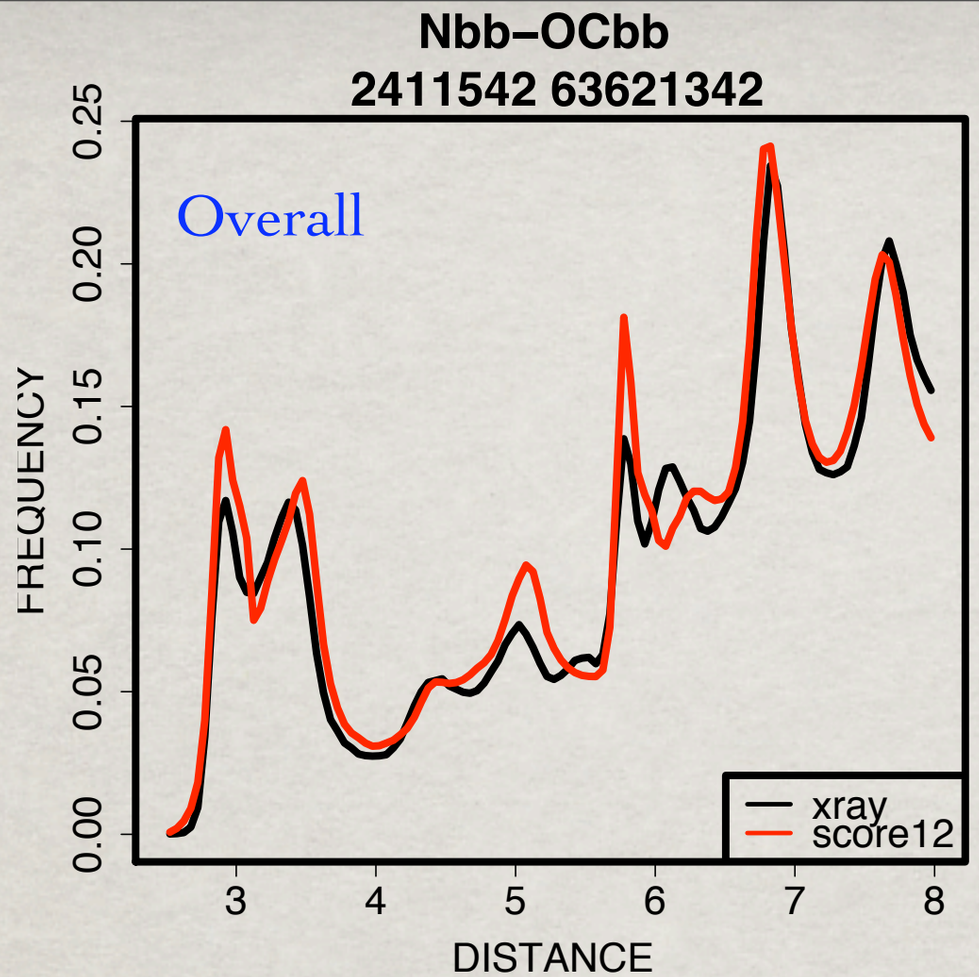
Nbb–OCbb
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Overall
FREQUENCY
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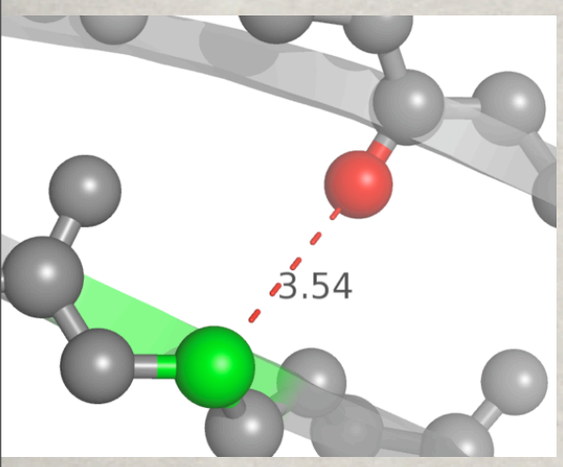
xray
score12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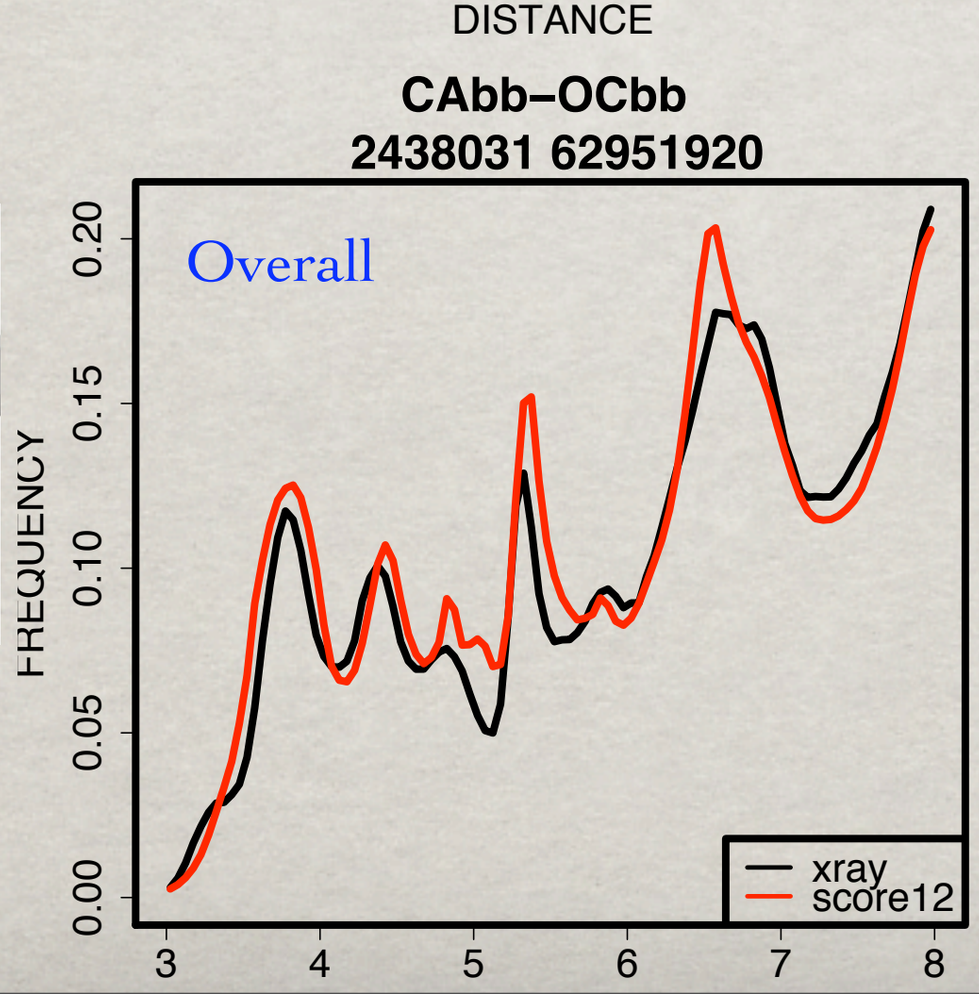
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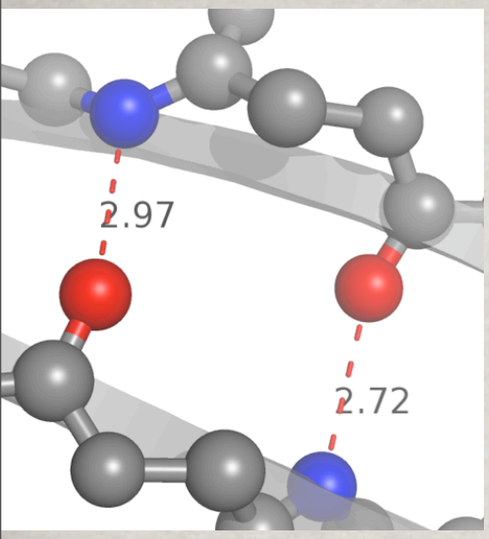
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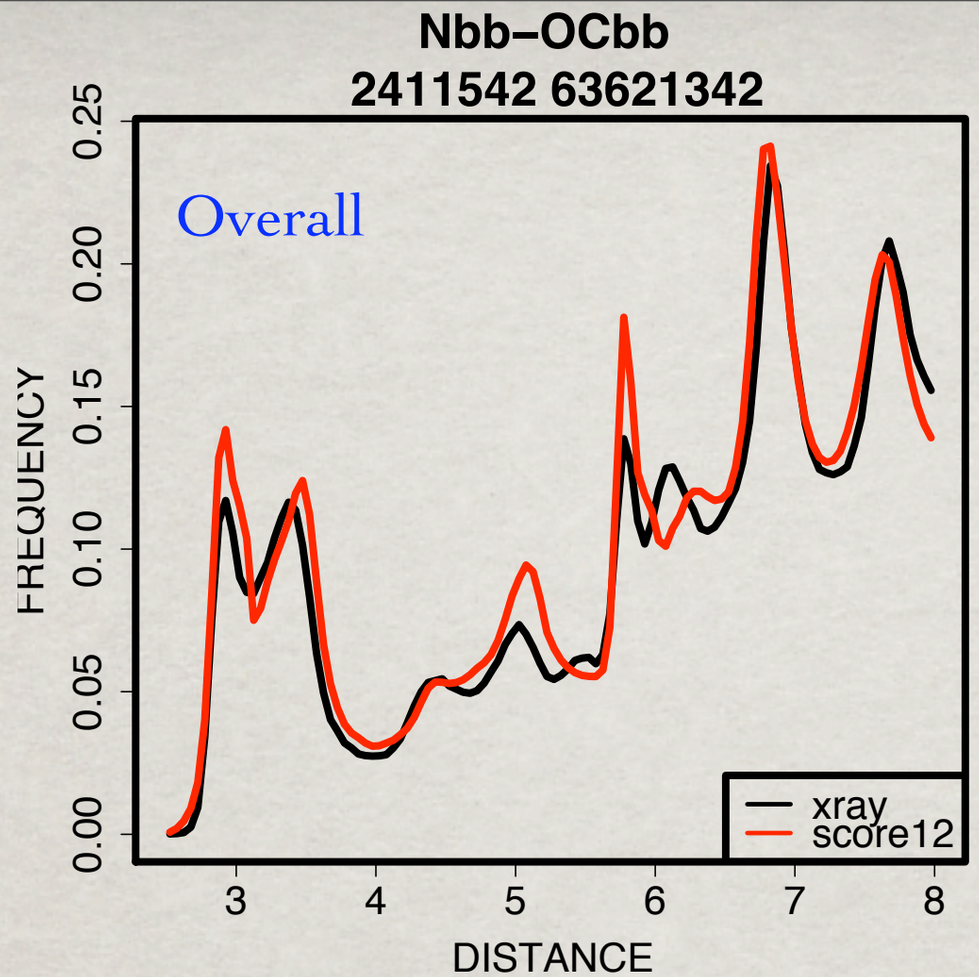
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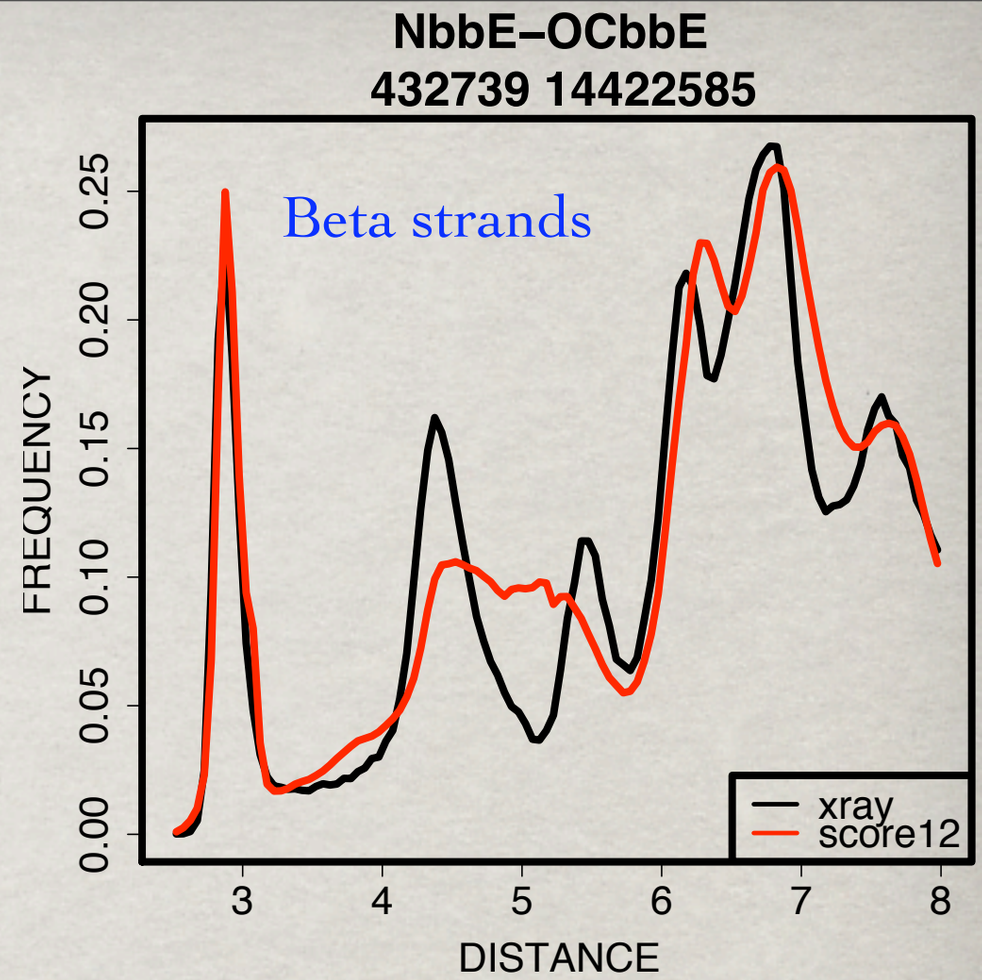
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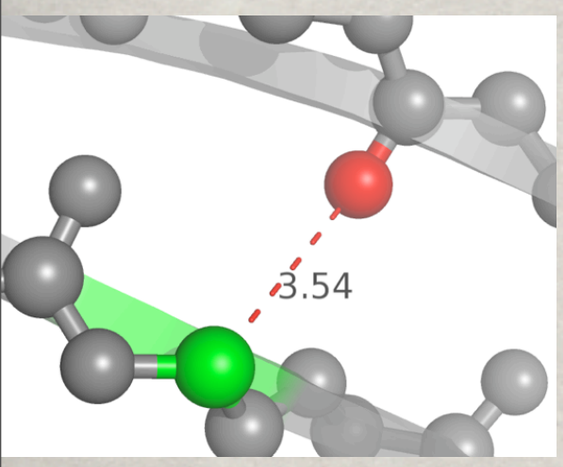
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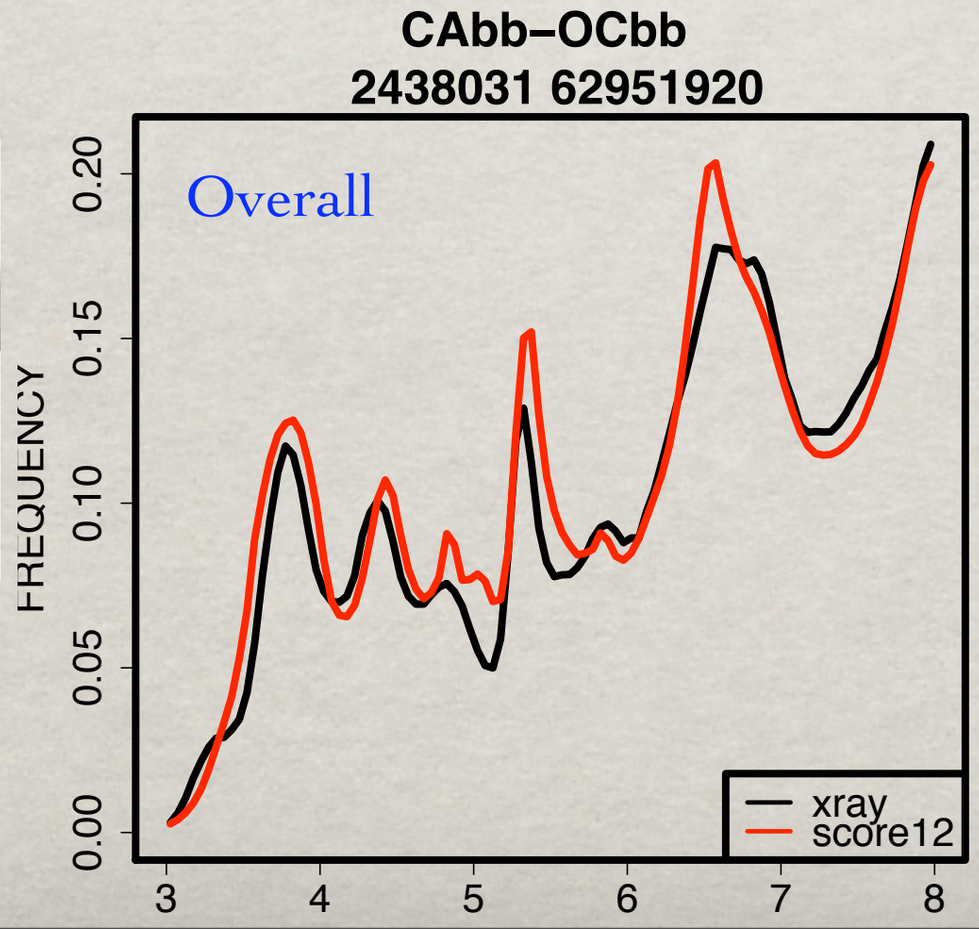
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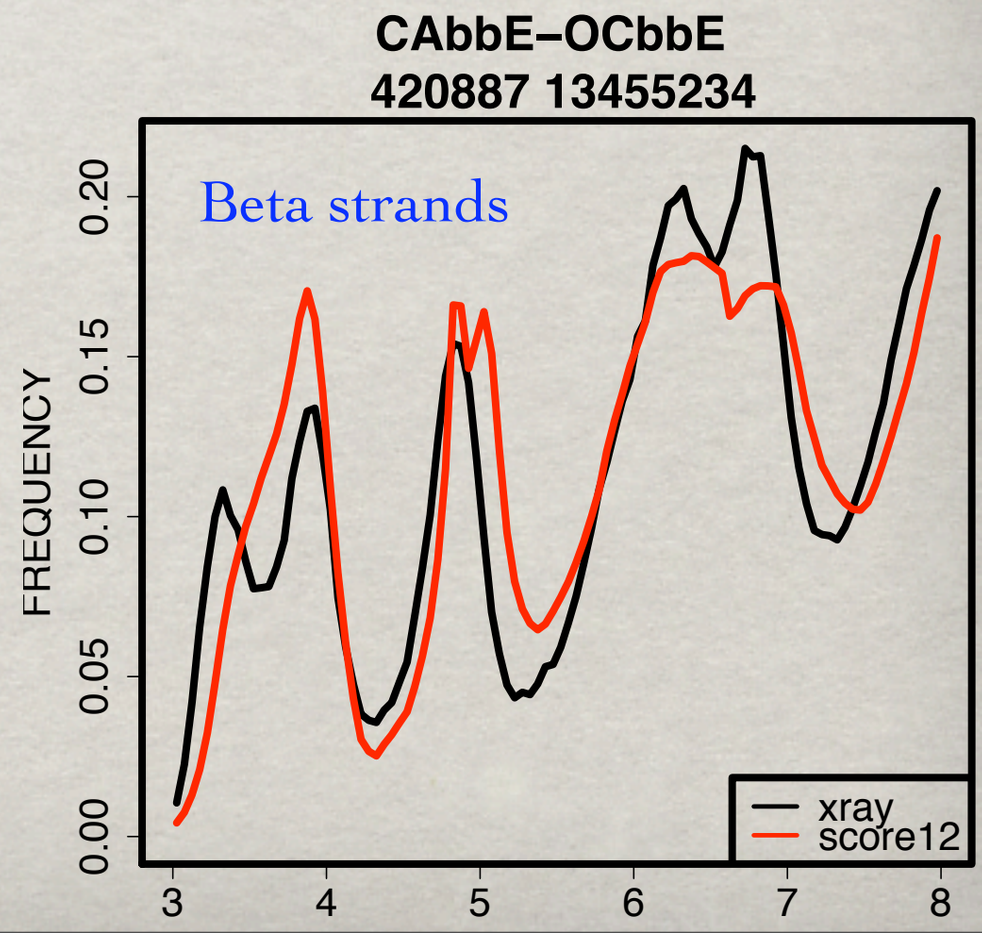
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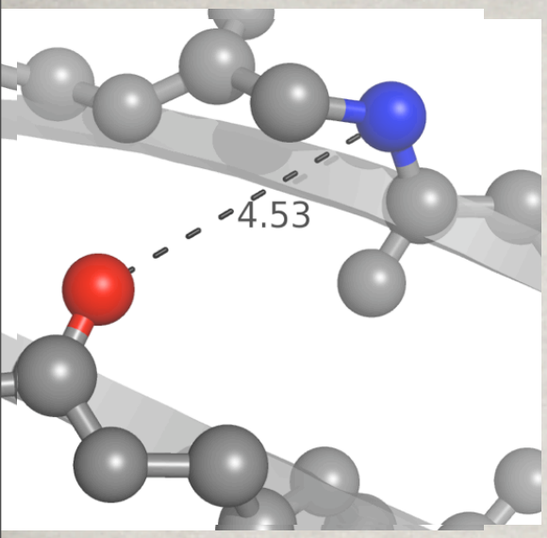
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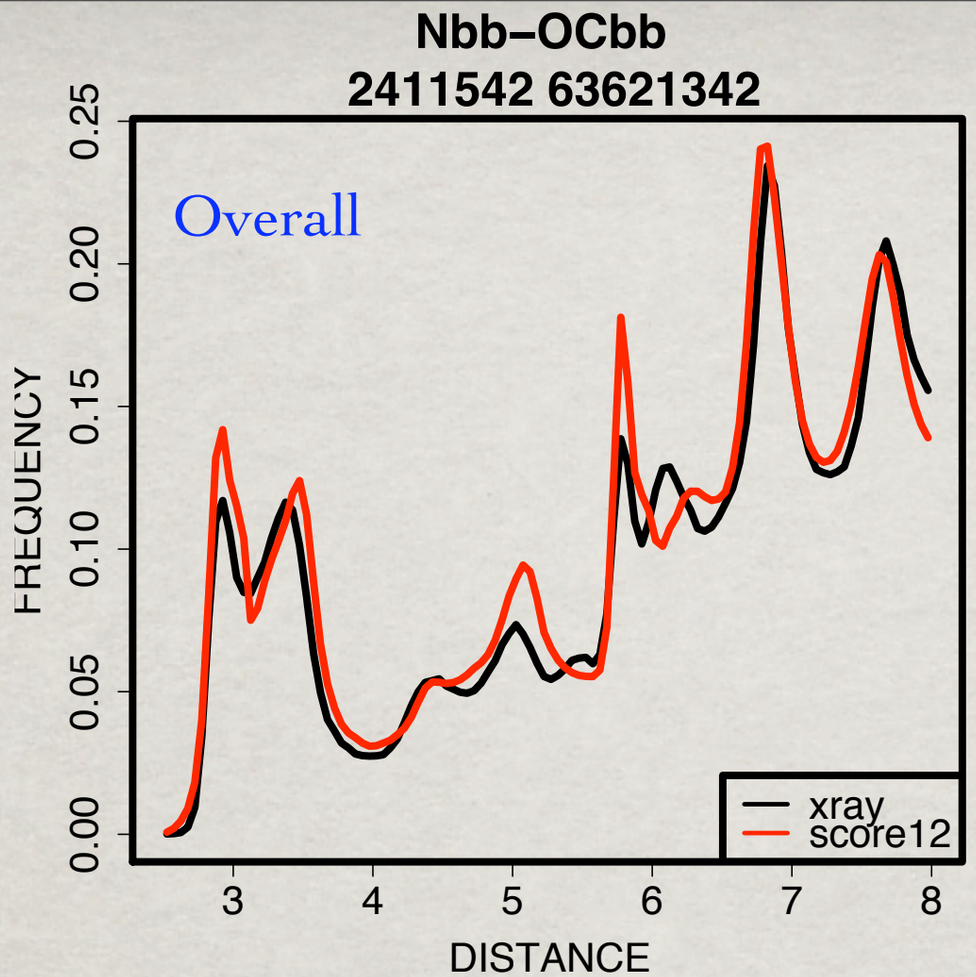
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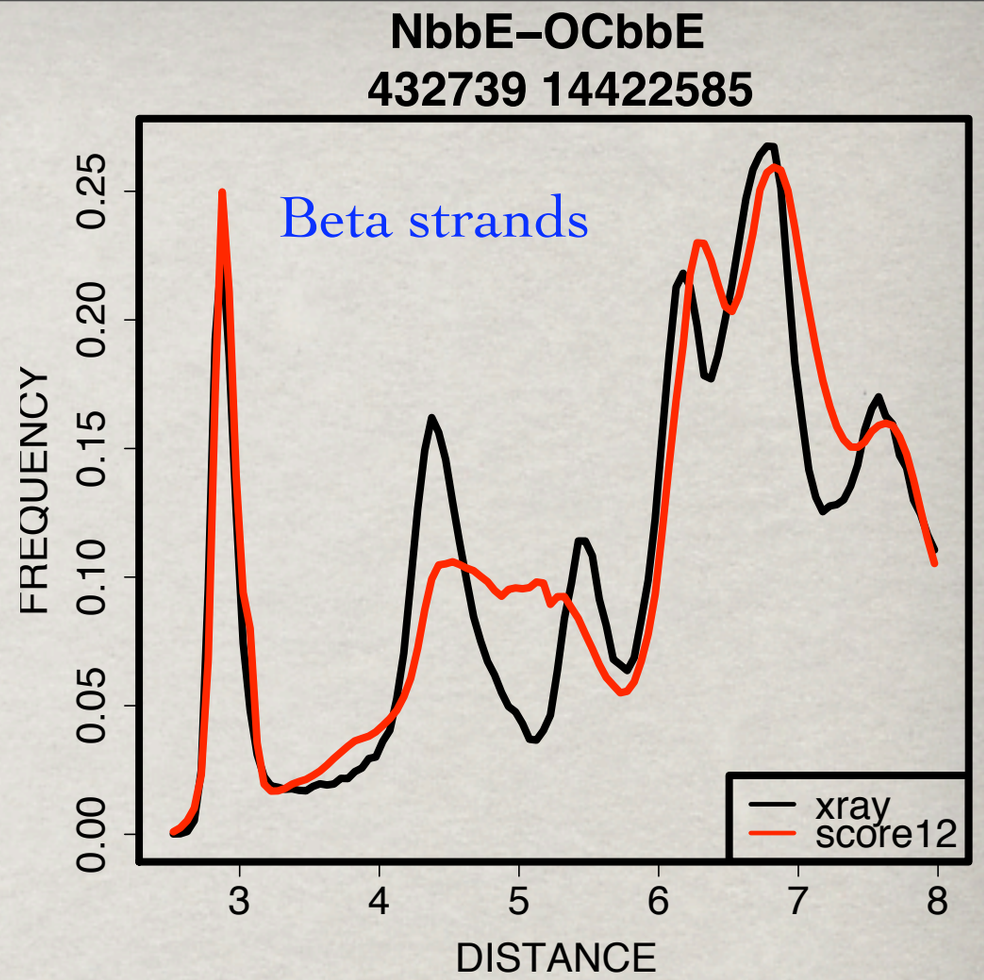
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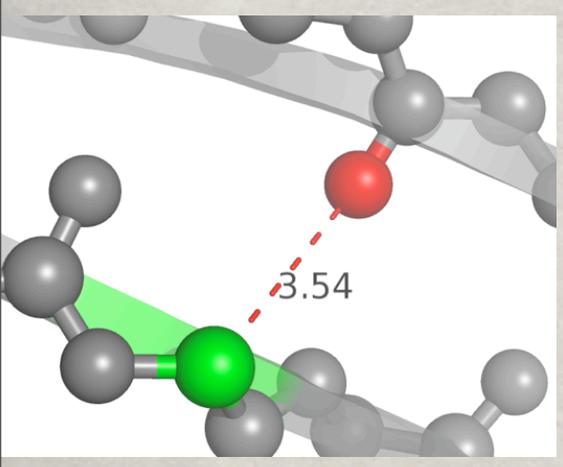
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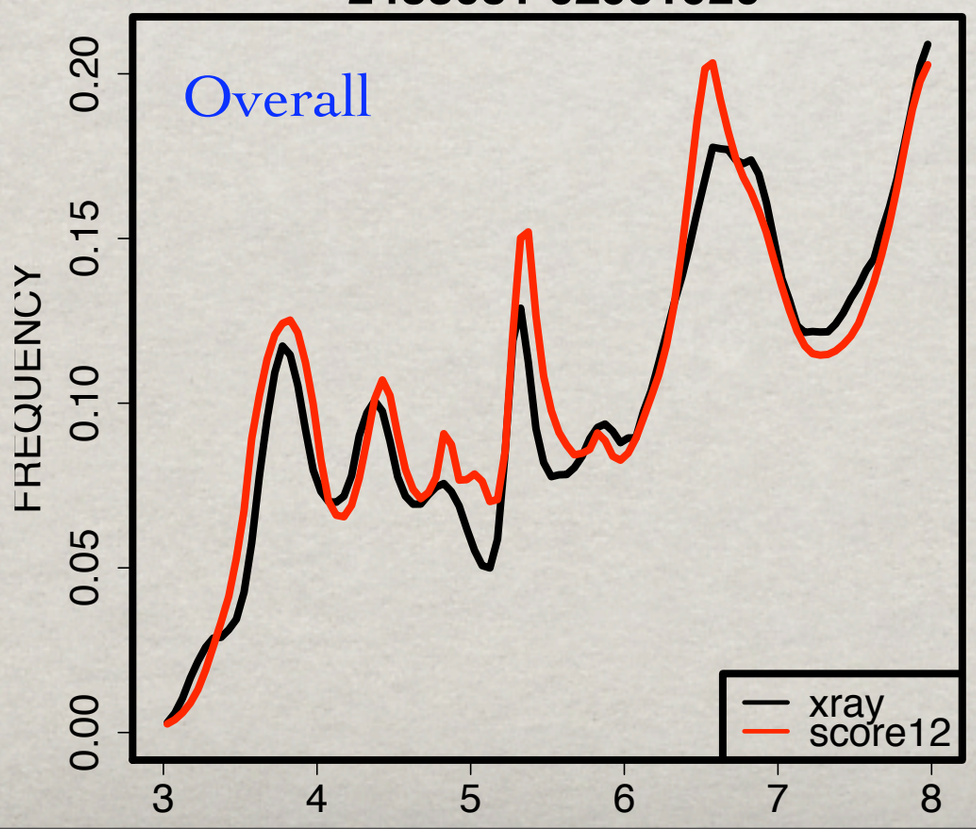
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Overall
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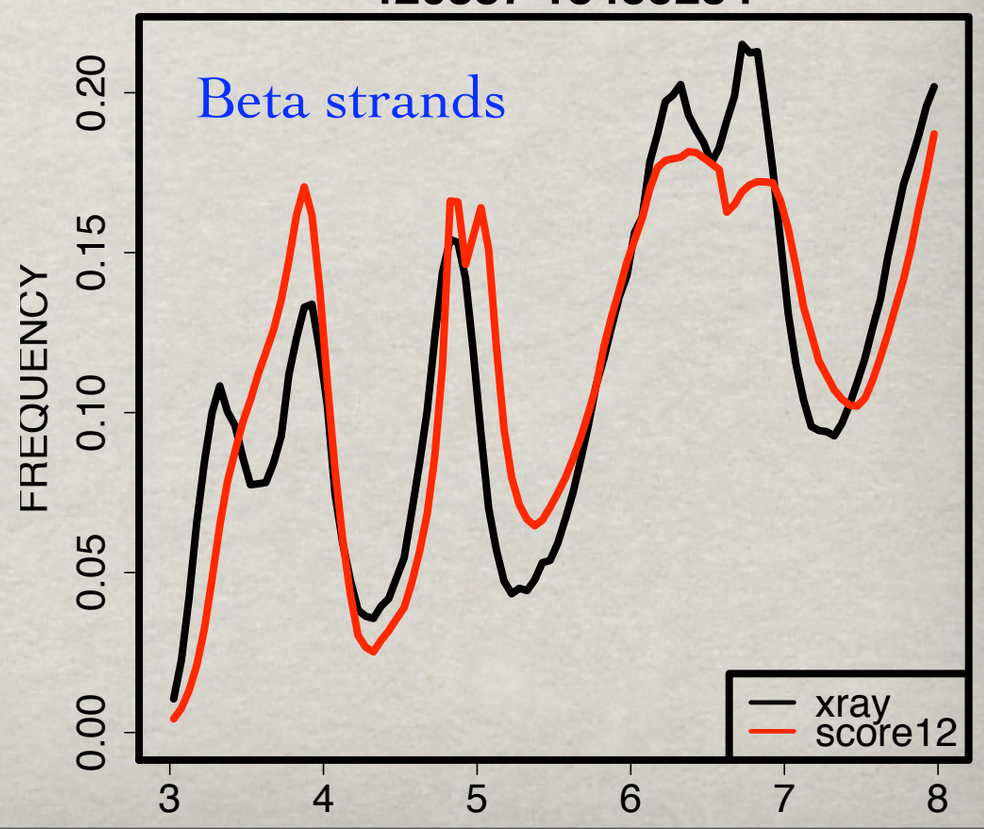
xray
score12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Beta strands
FREQUENCY
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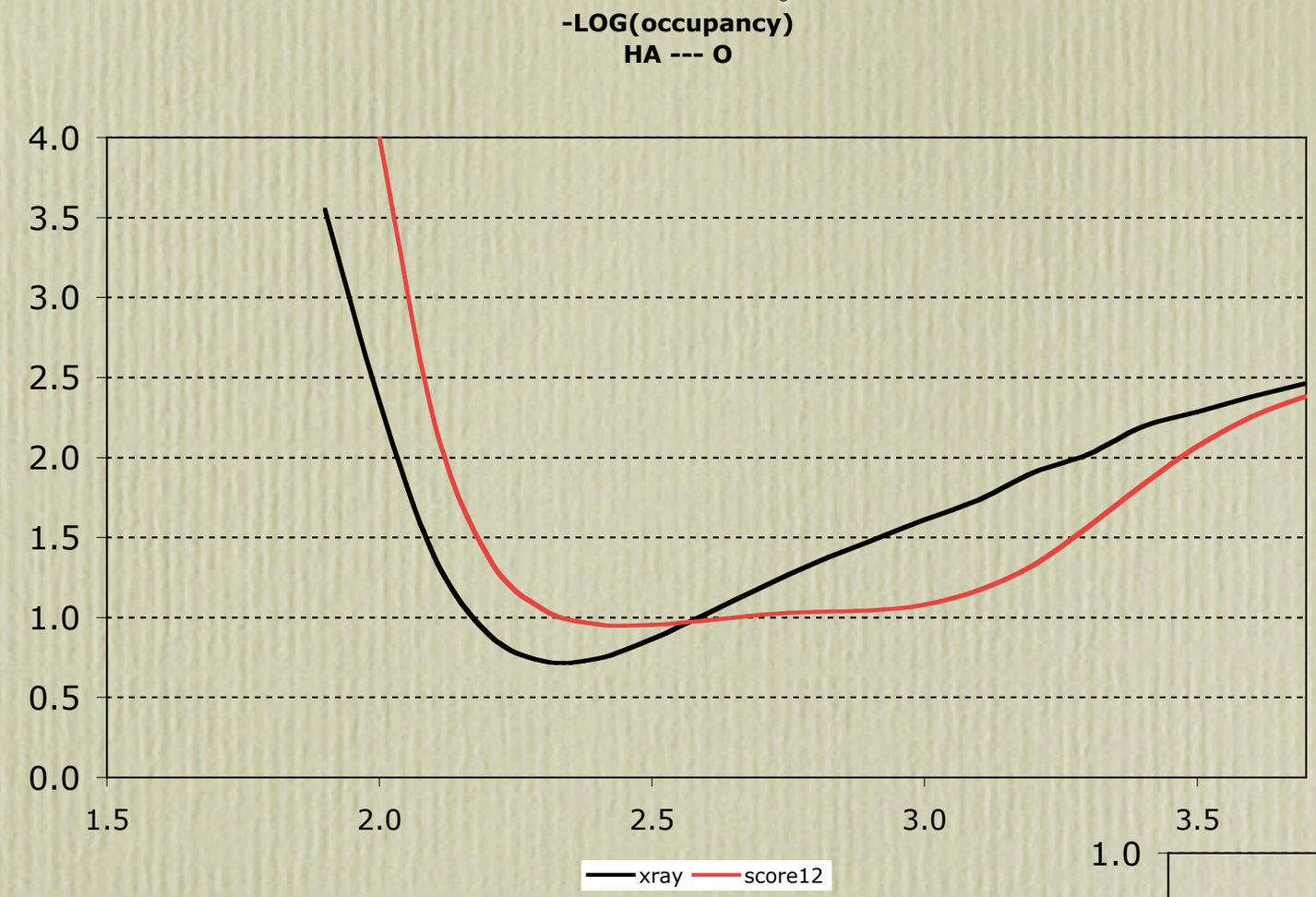
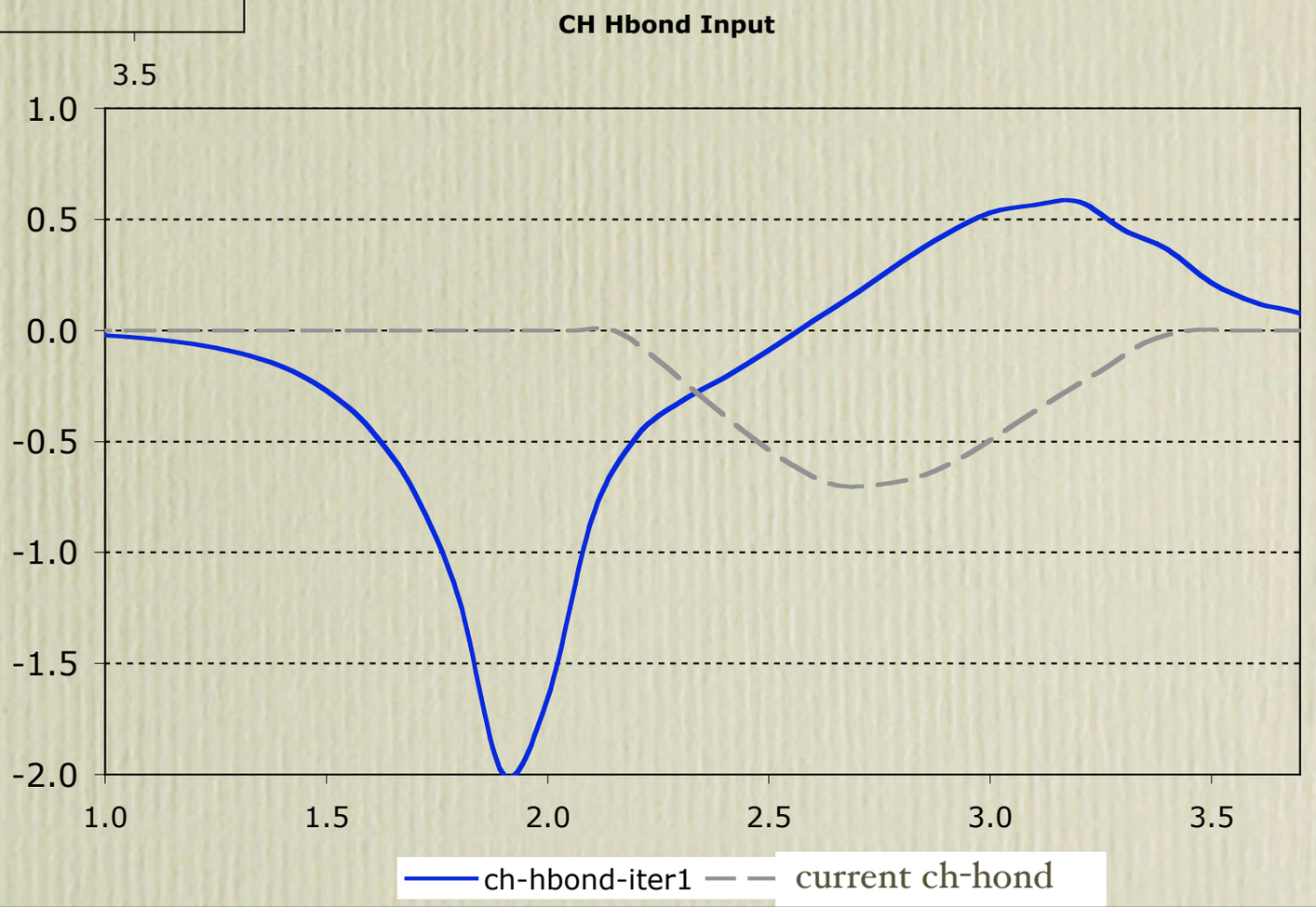
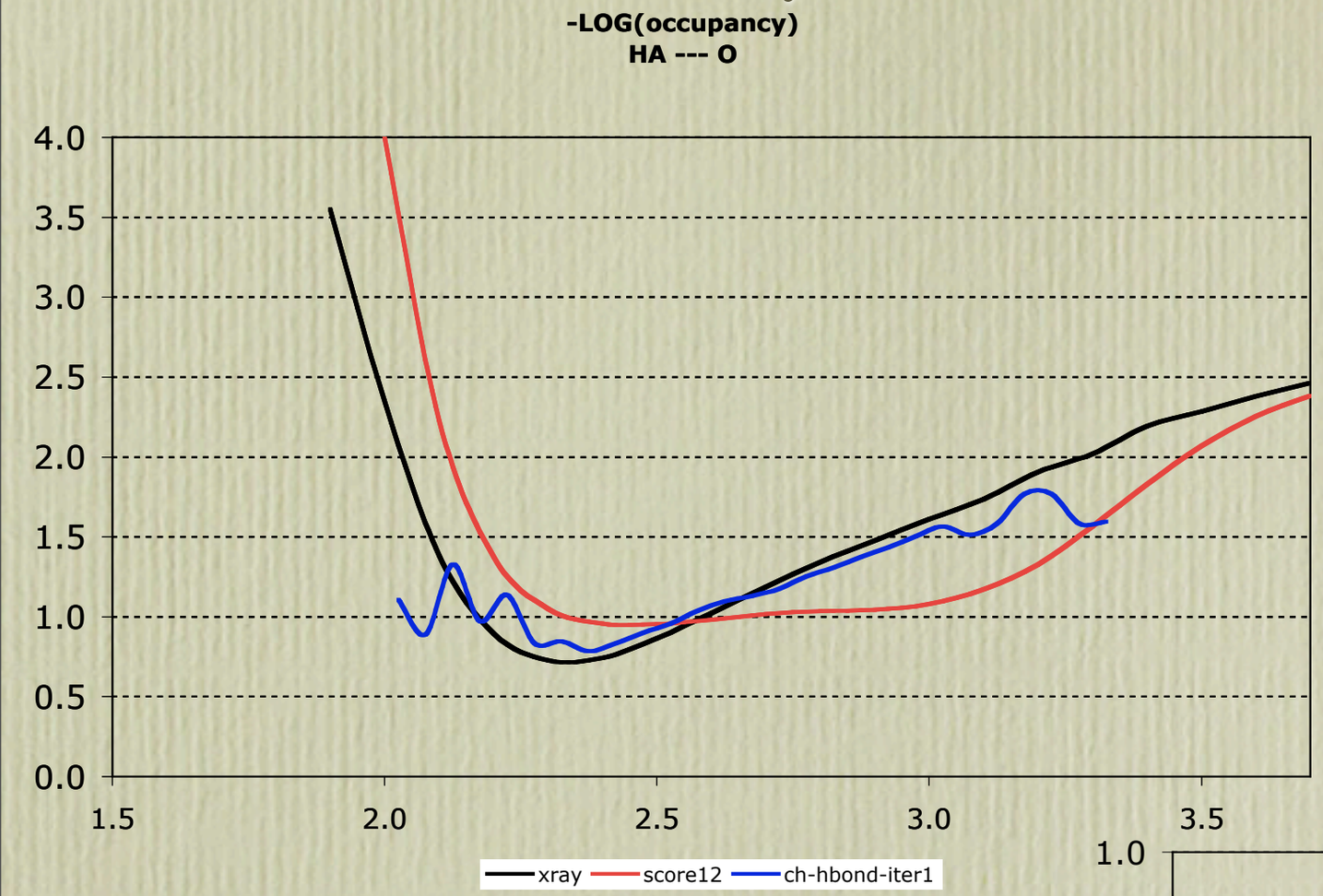
DISTANCE
xray
score12

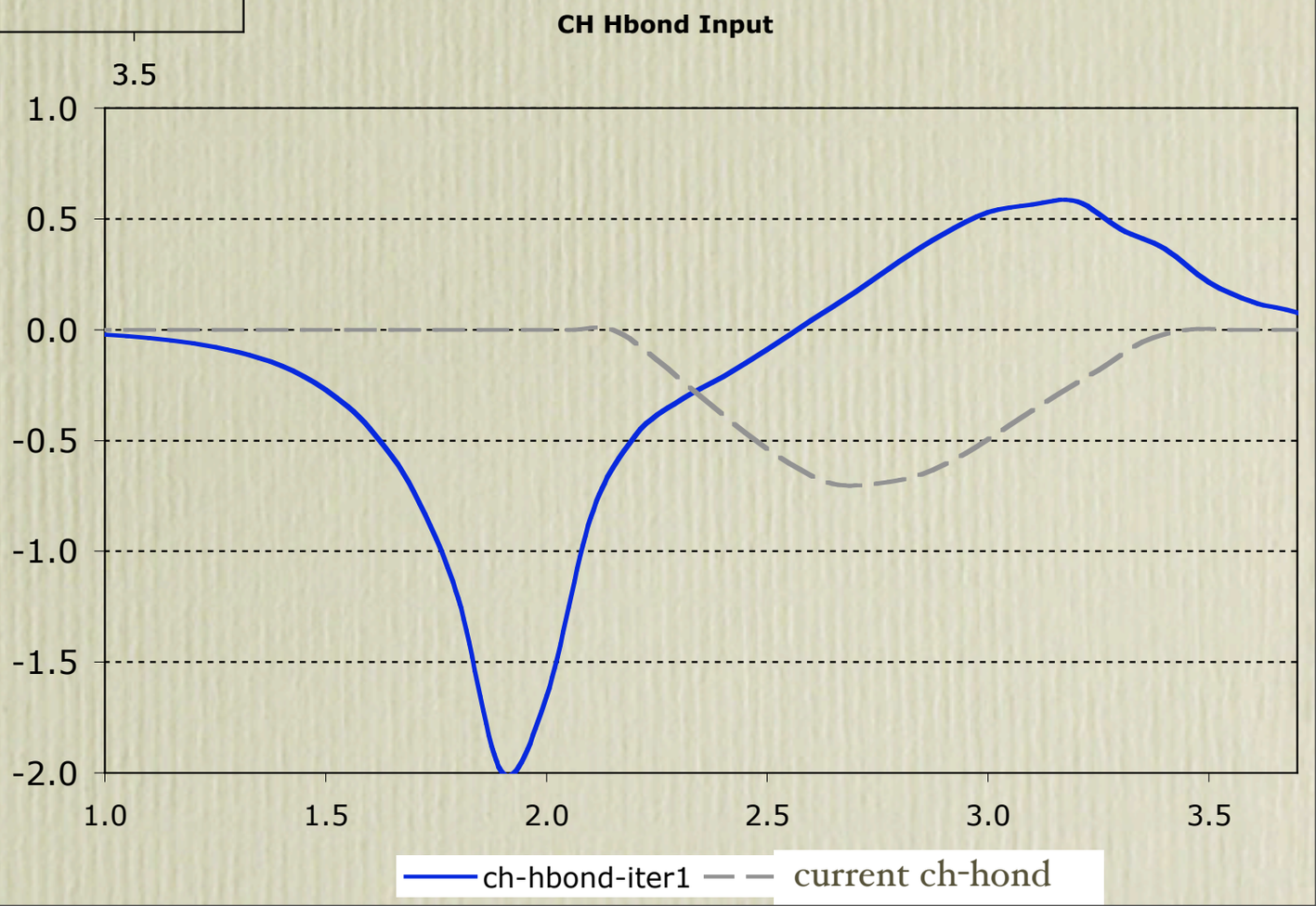
Iteratively correct CH HBond potential



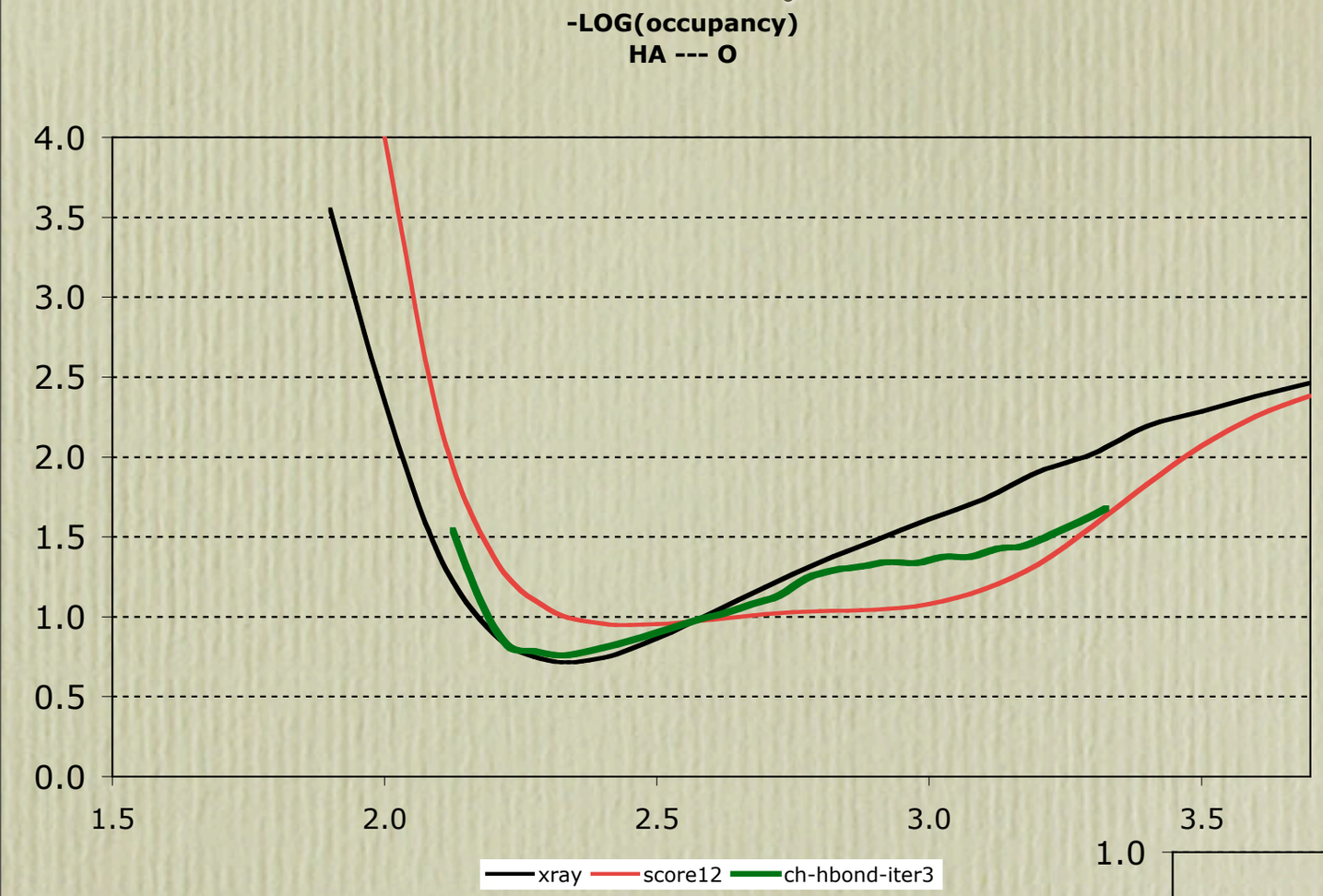


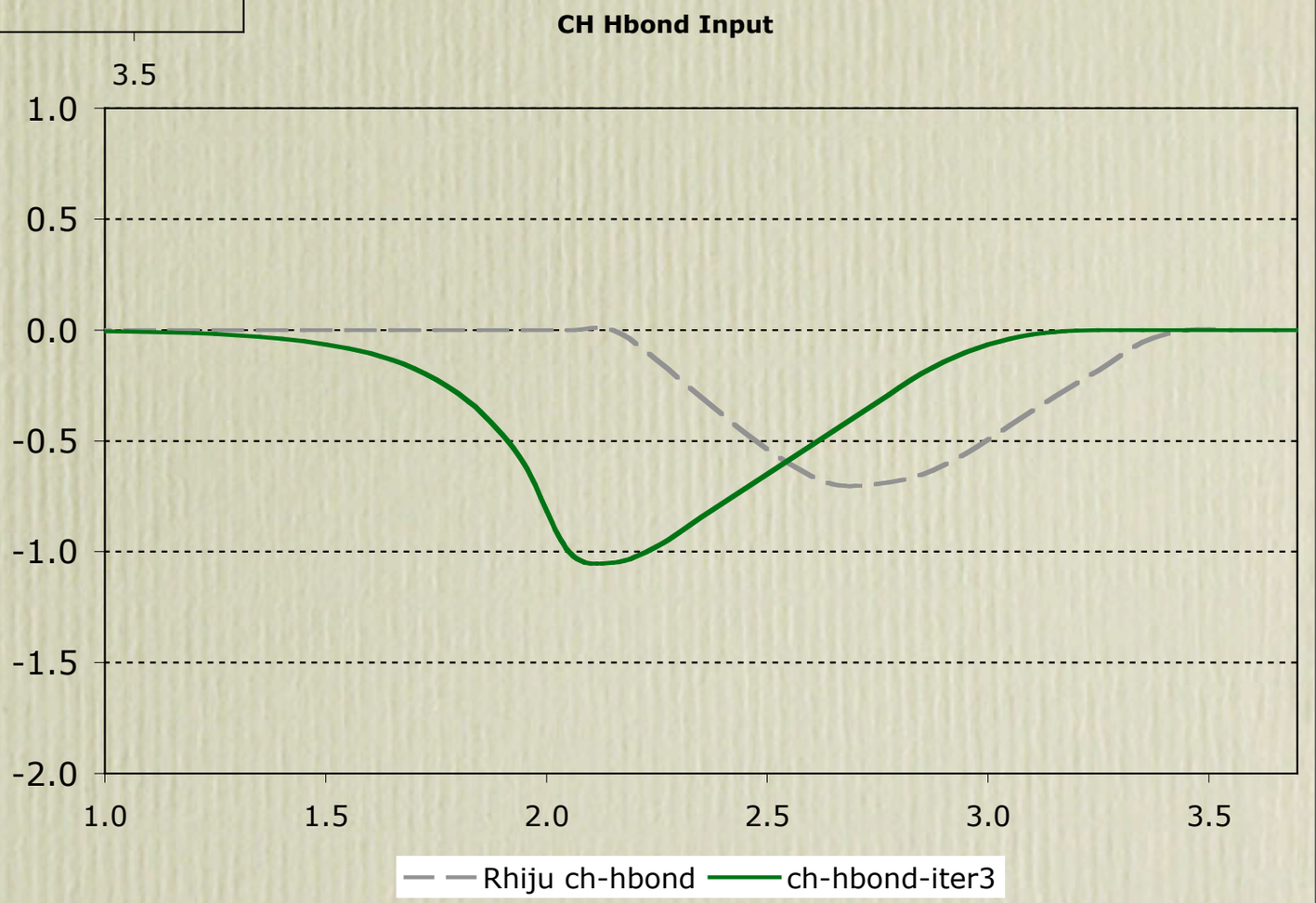
Iteratively correct CH HBond potential

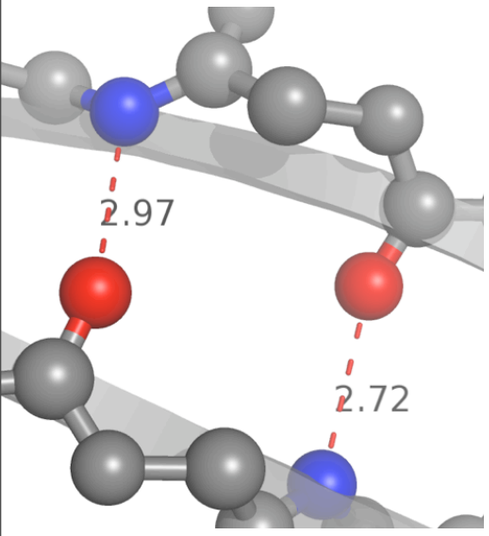




Iteratively correct CH HBond potential



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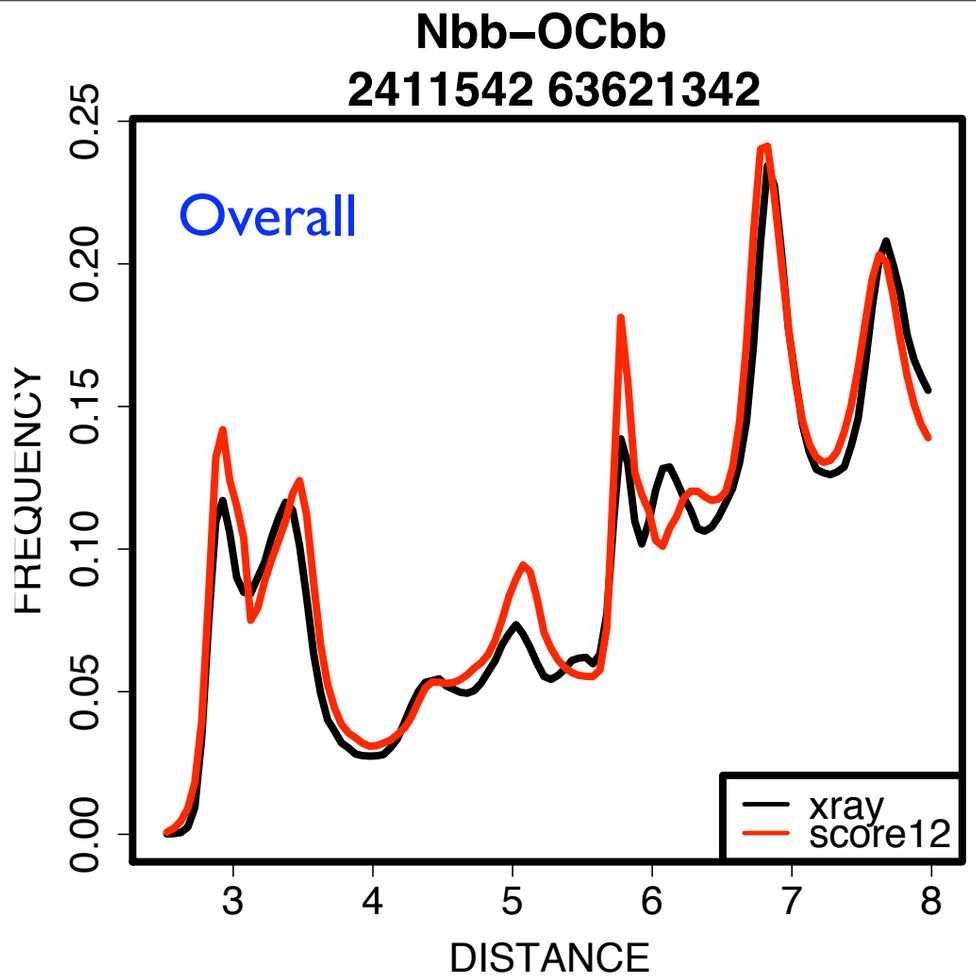
Nbb–OCbb
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Overall
FREQUENCY
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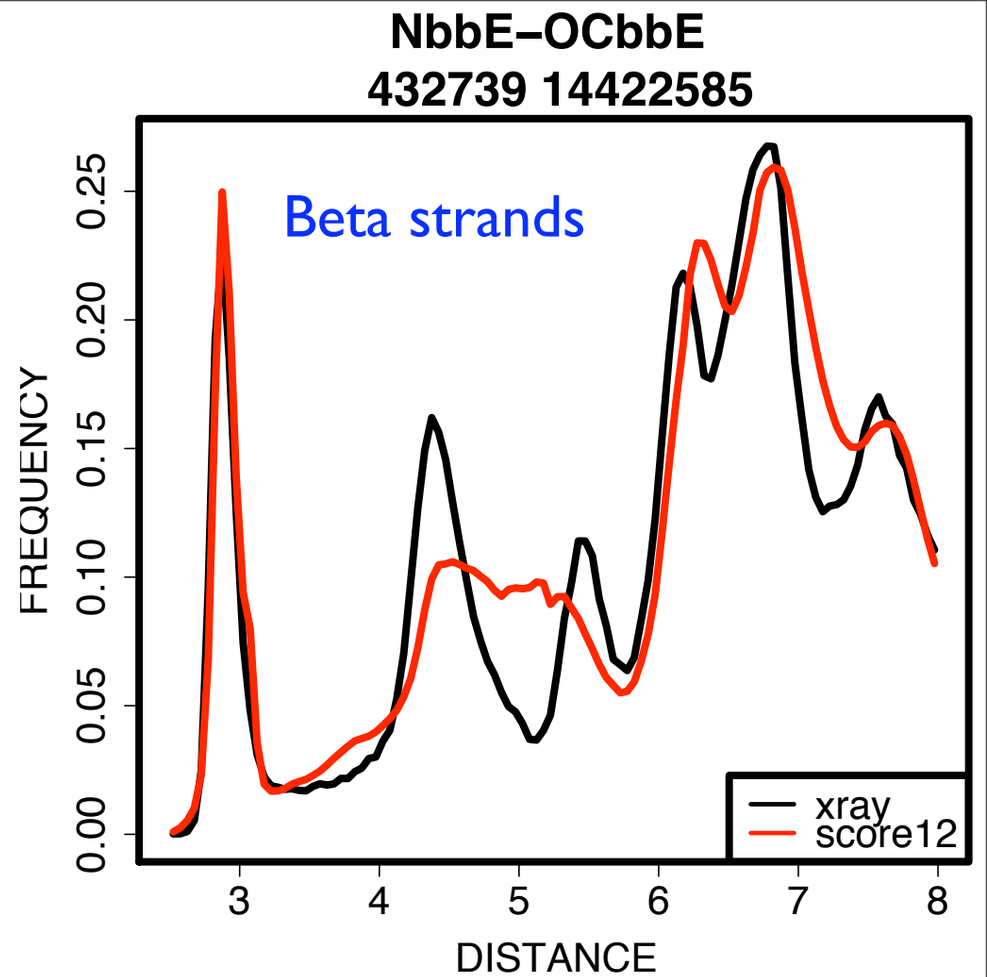
DISTANCE
xray
score12


NbbE–OCbbE
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Beta strands
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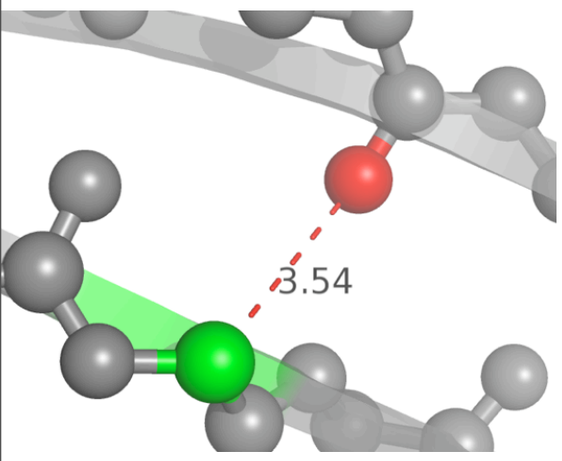
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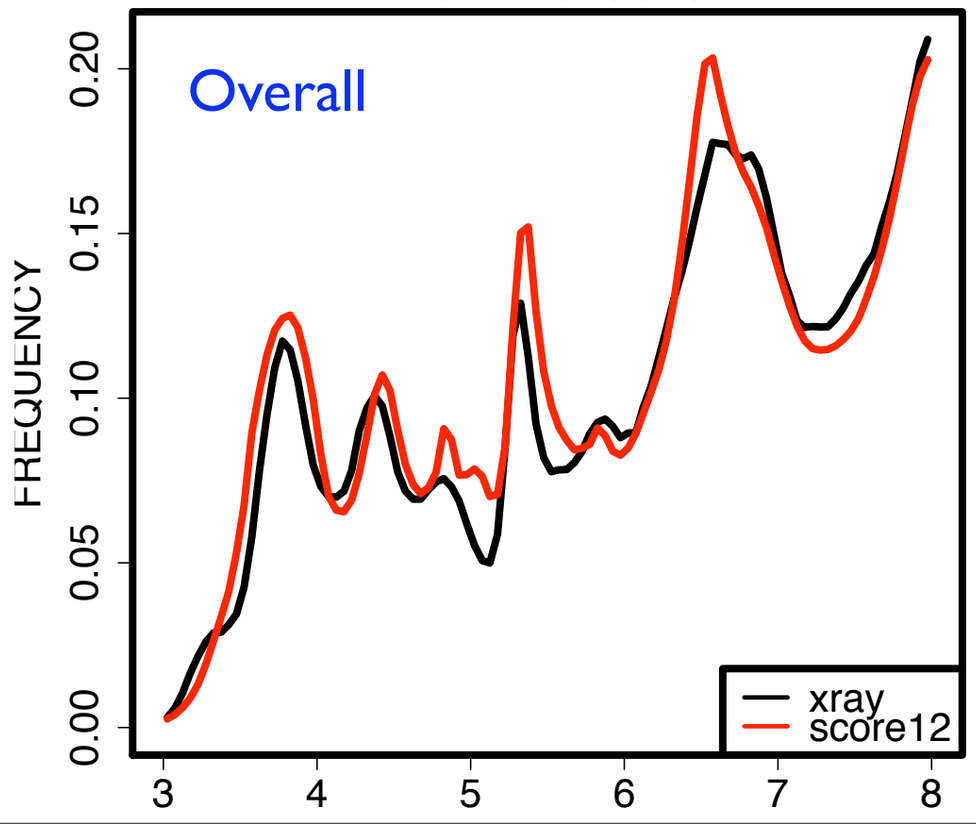
CAbb–OCbb
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Overall
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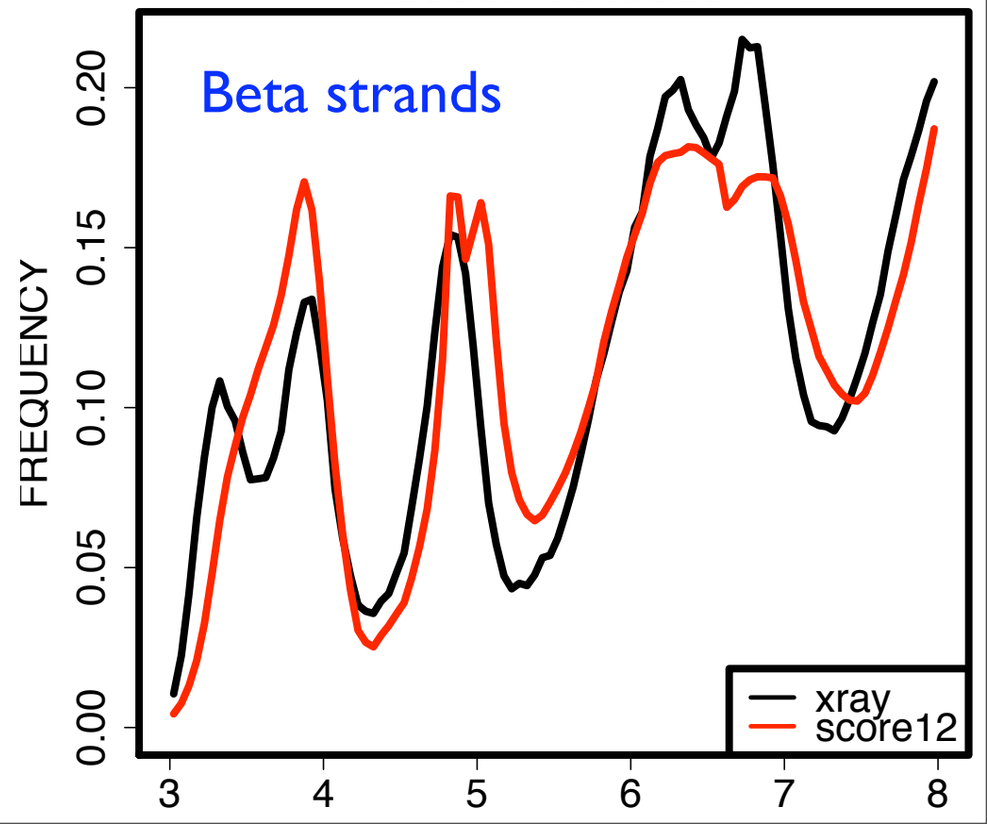
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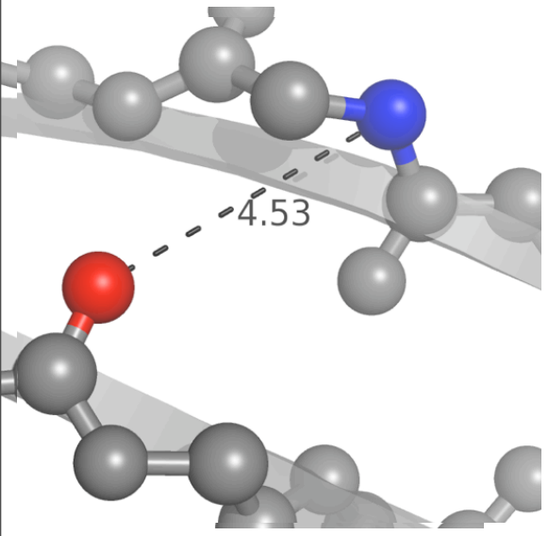
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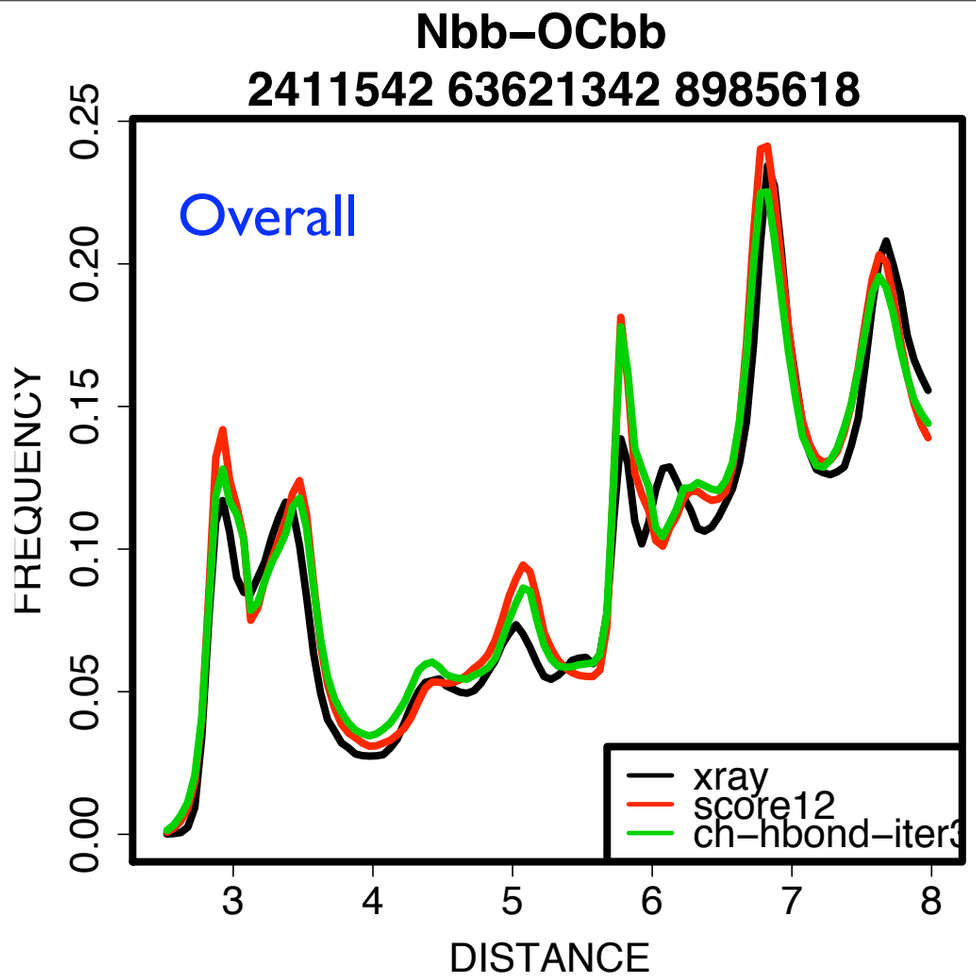
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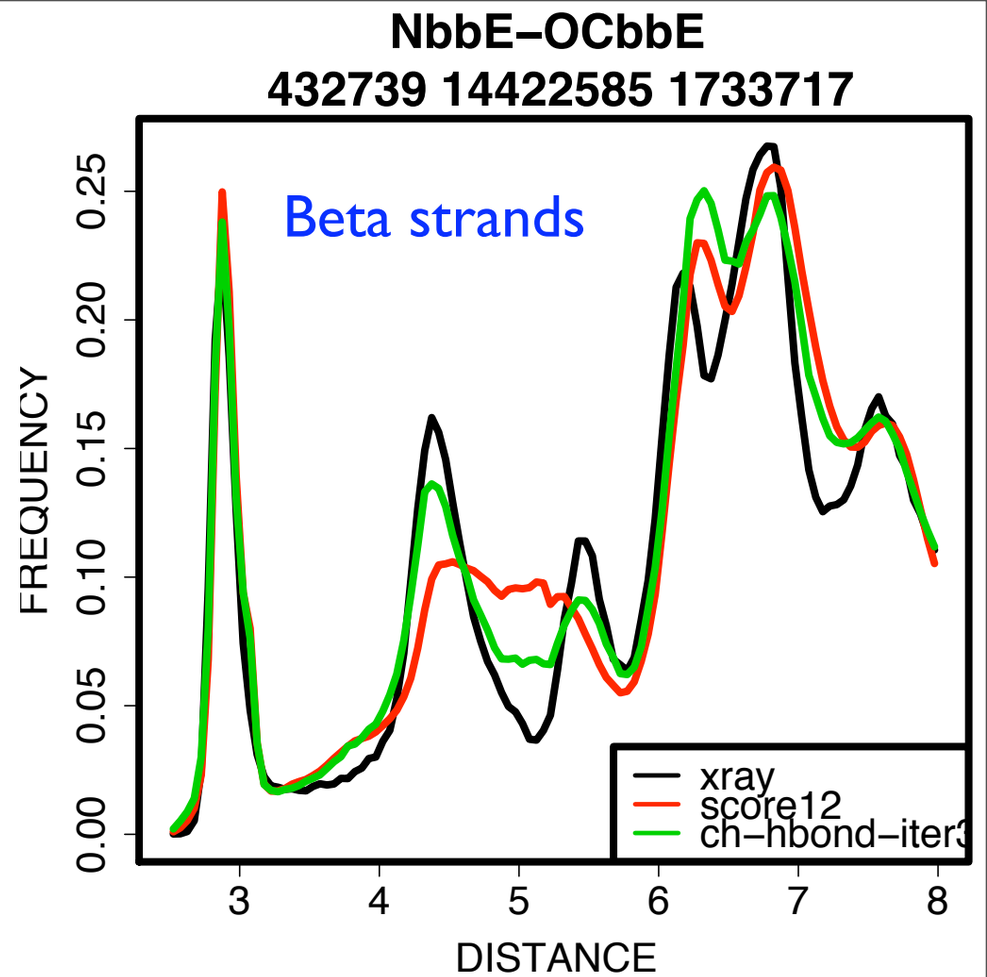
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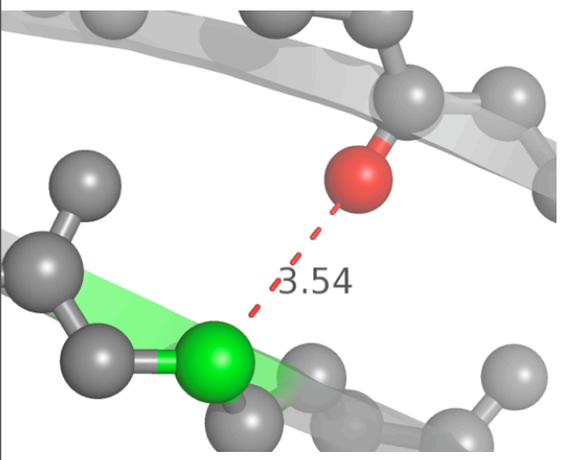
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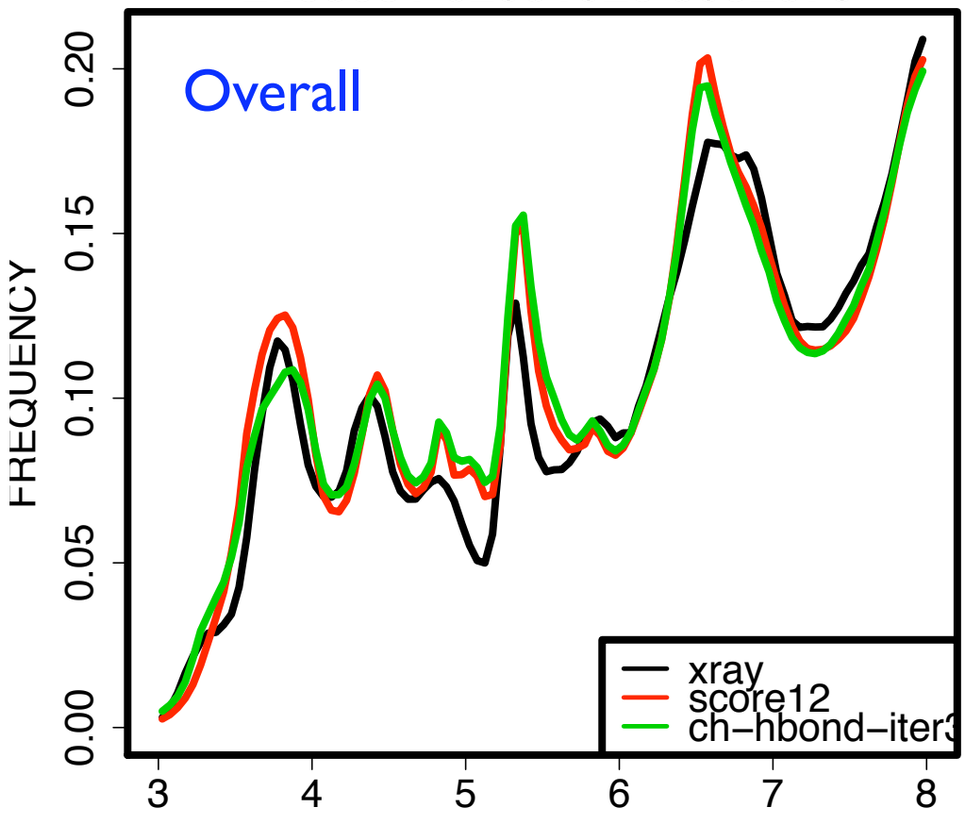
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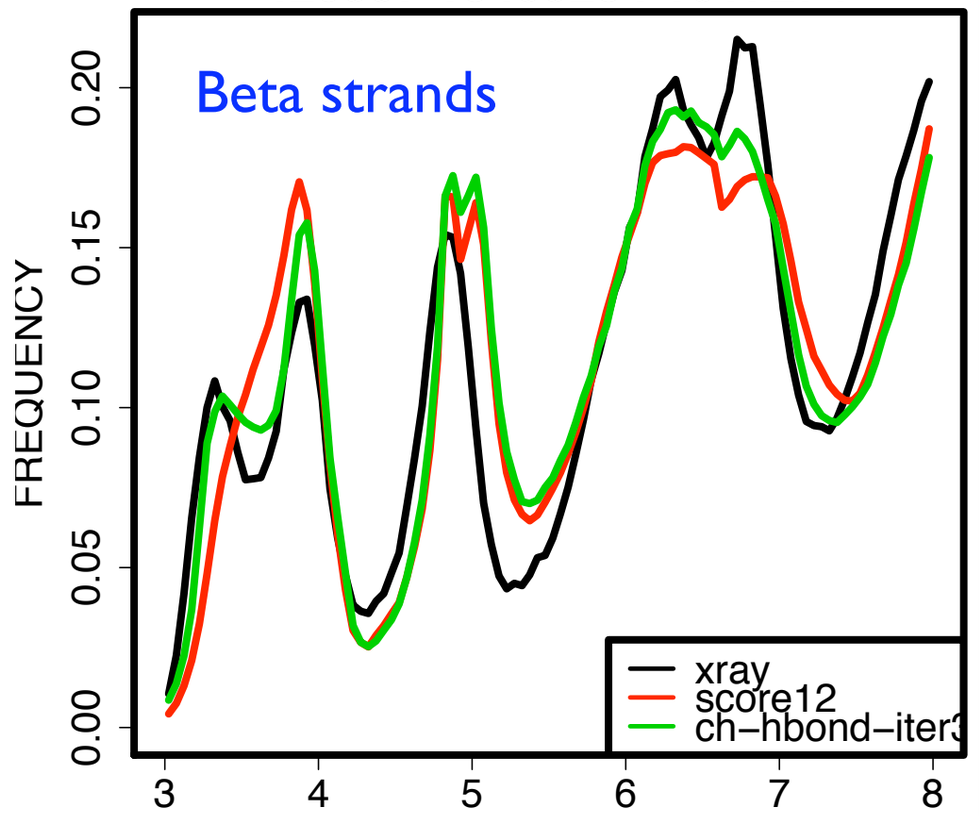
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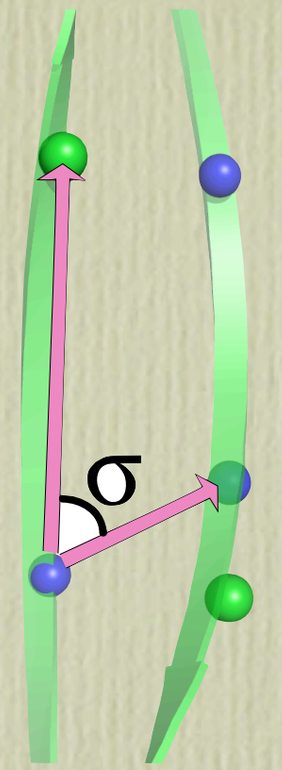
sspair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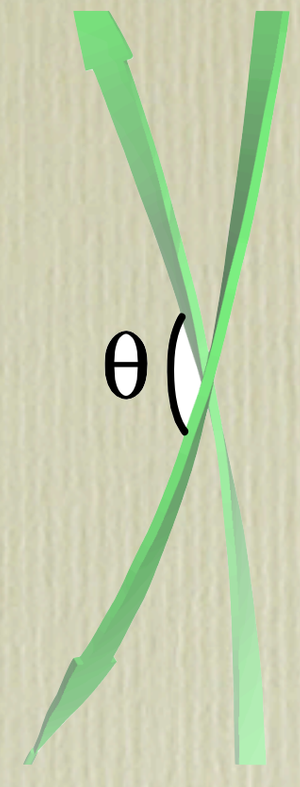
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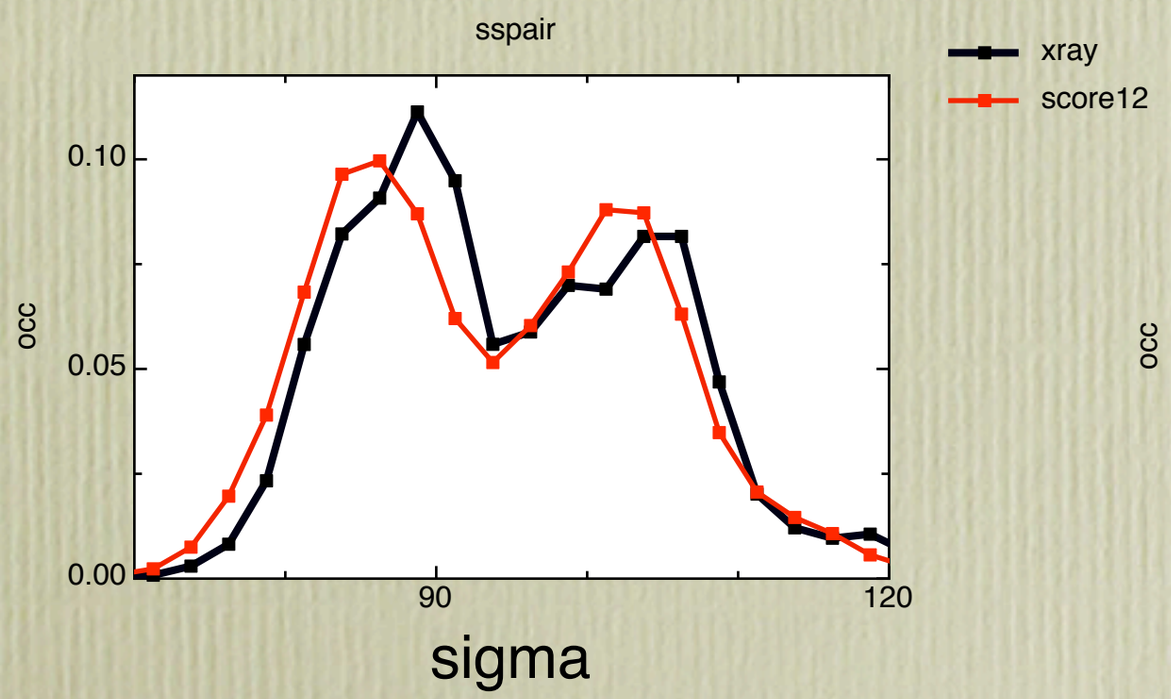
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0.00
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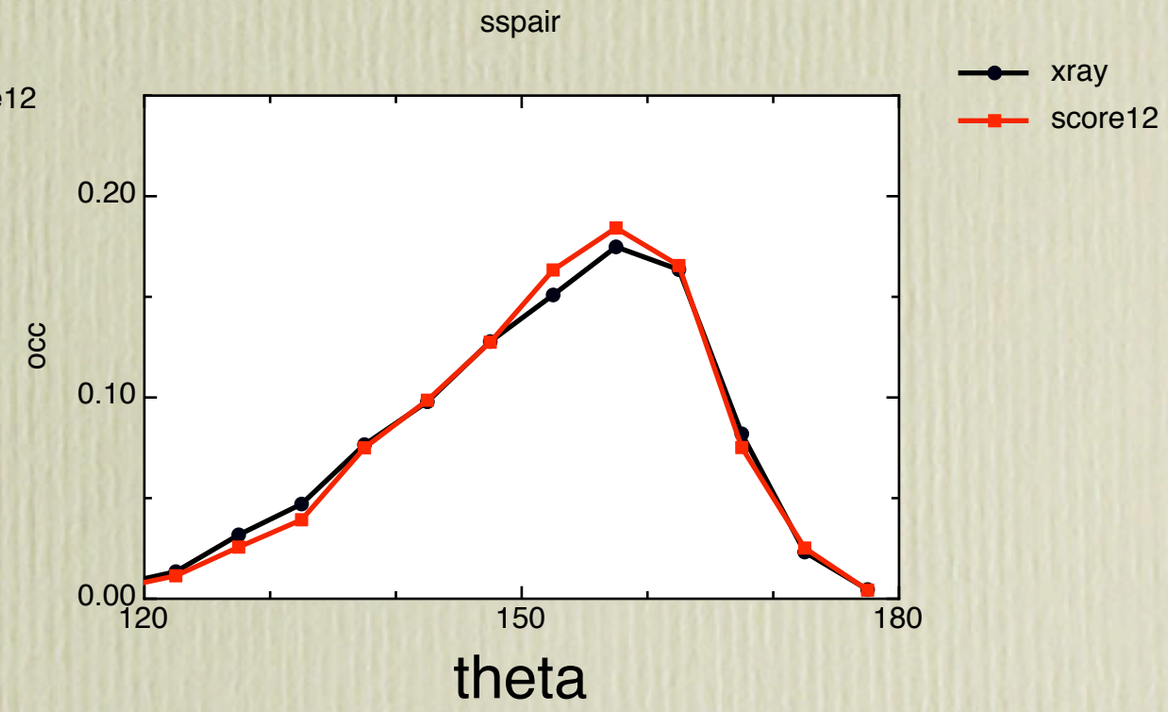
120
sigma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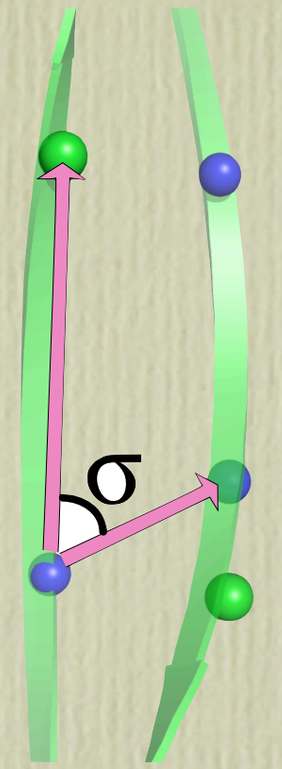
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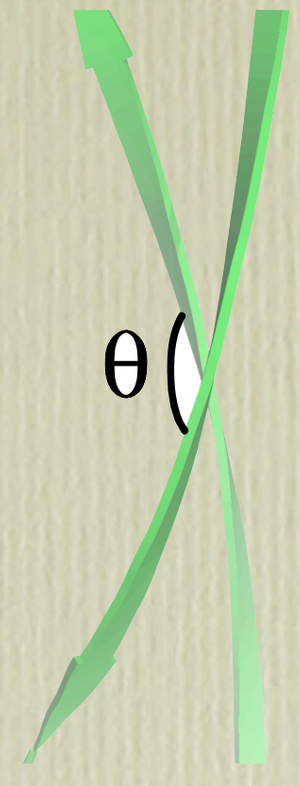
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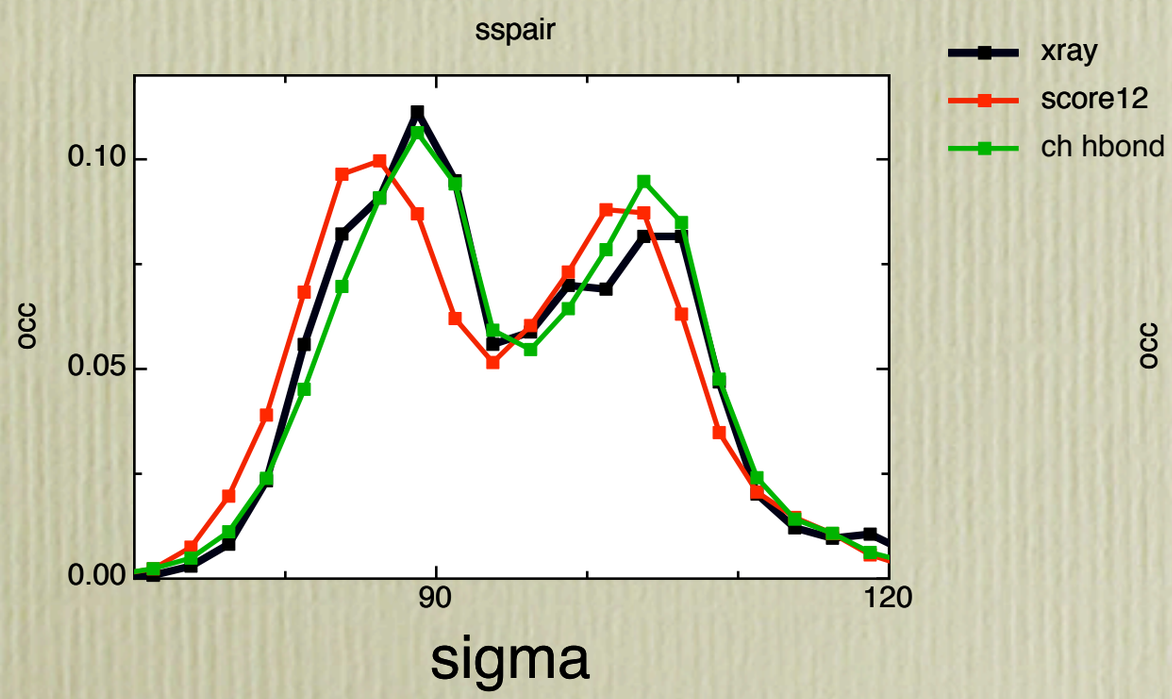
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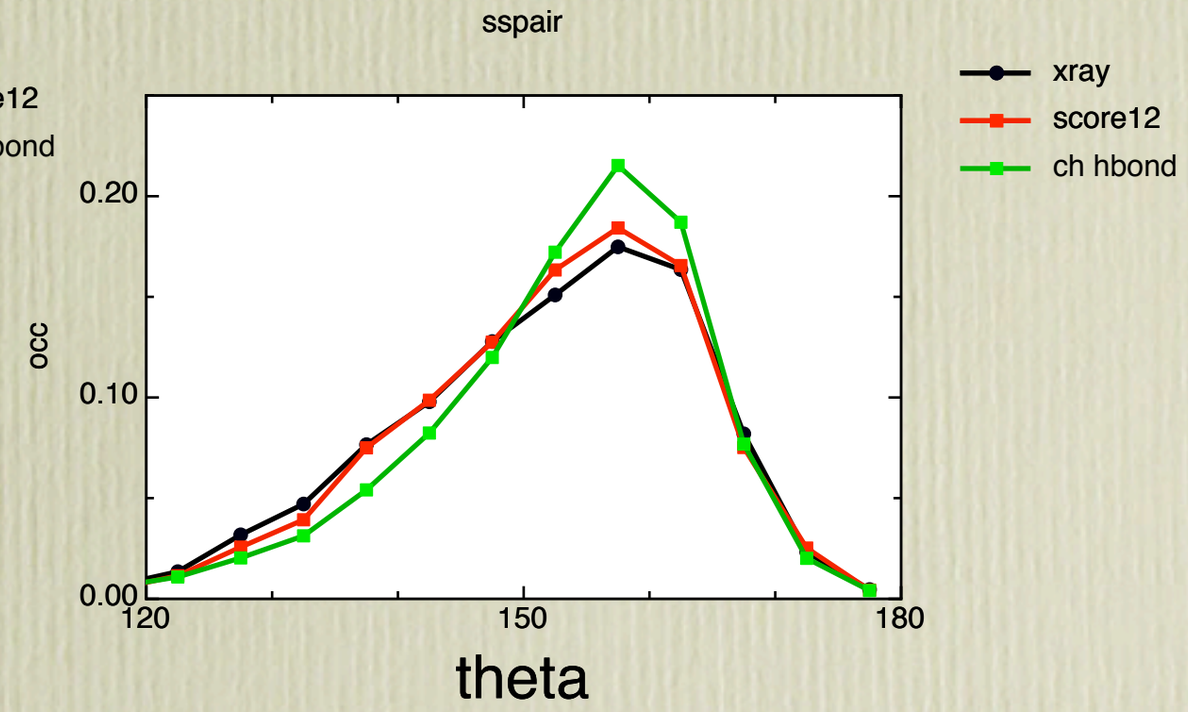
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theta

Acknowledgement

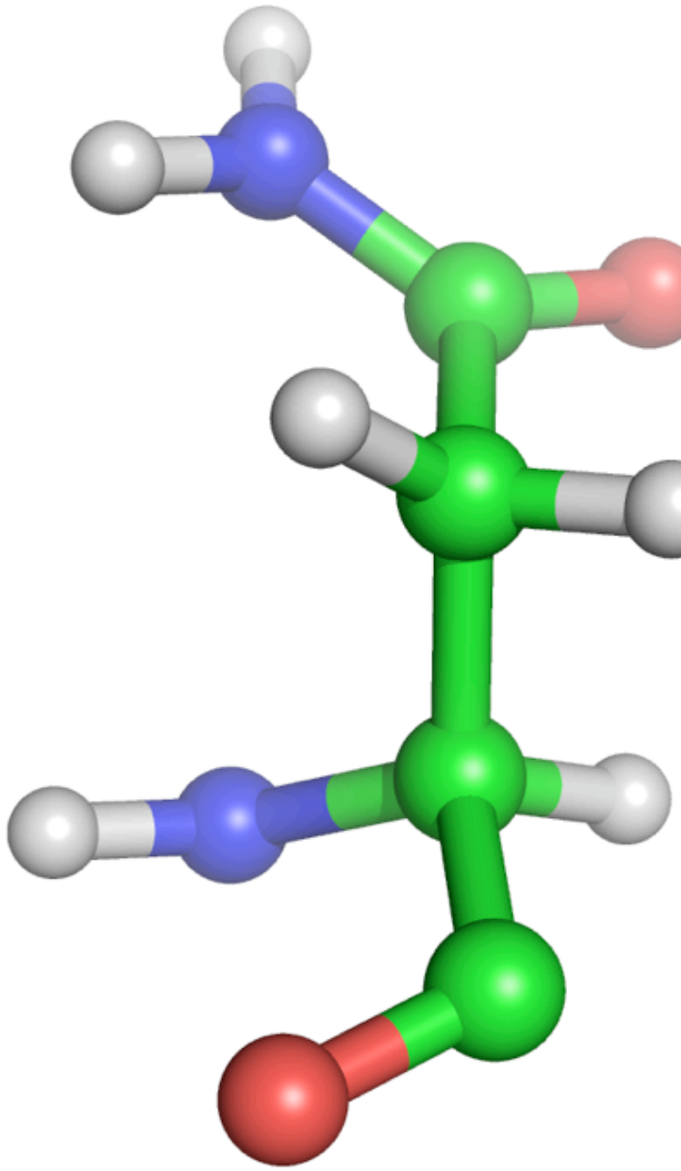
mini/coding: Andrew LF, Mike, Oliver, James,
Rob, Will, Ingemar, David Kim, Patrick

datasets: Mike, Sarel, Nobu

Discussions: Rhiju Das, Roland Dunbrack

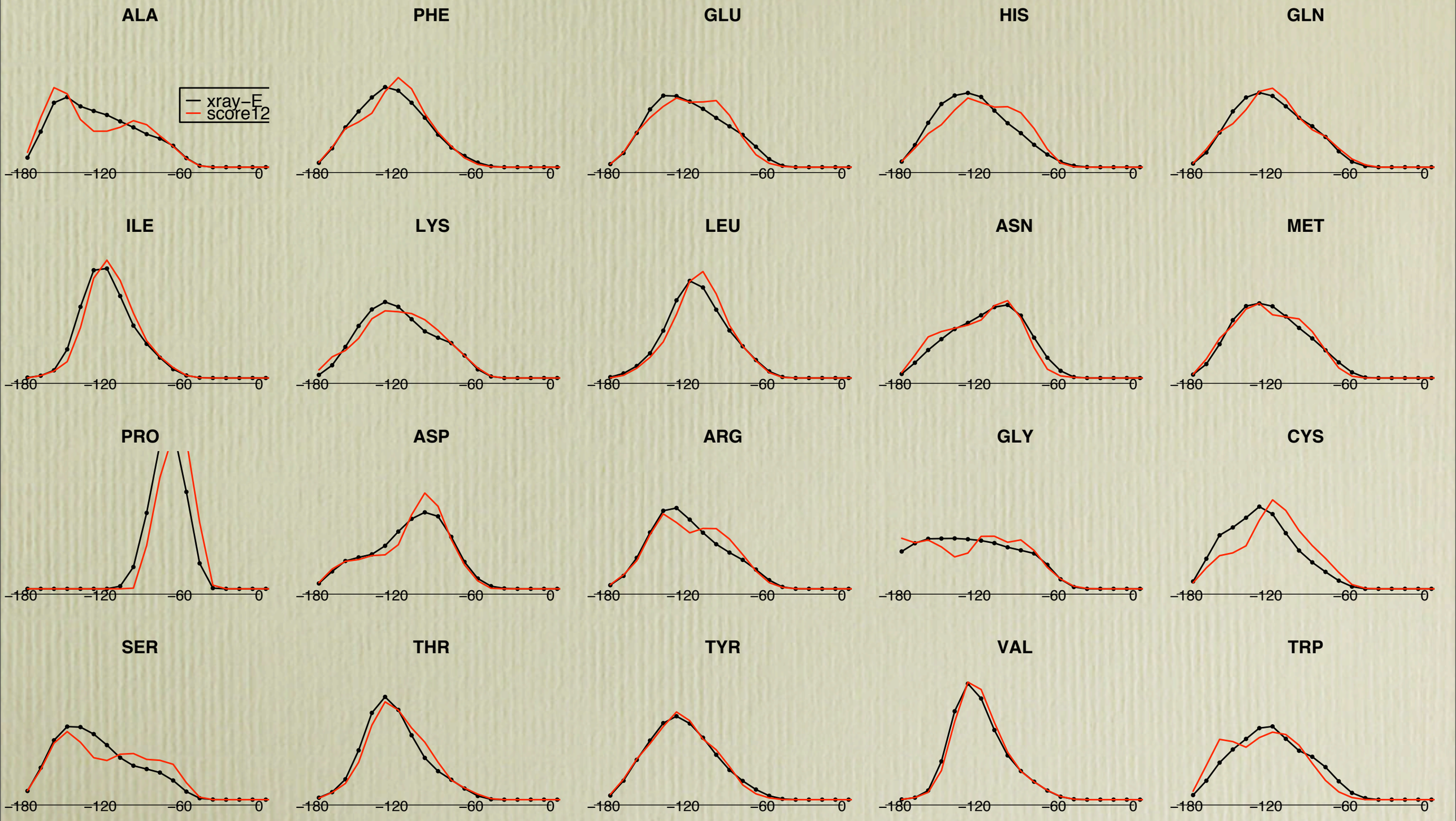
David Baker

Full-atom Idealized Coordinates



RES	ATOM	ATOM	ATOM	ATOM	PDB	ICOO	diff
ASP	**OD2**	**CG**	**CB**	**OD1**	**180.0**	**171.4**	**8.6**
GLU	**OE2**	**CD**	**CG**	**OE1**	**180.0**	**173.9**	**6.1**
ASN	1HB	CB	CA	CG	121.0	132.8	11.8
CYS	**CB**	**CA**	**N**		**69.4**	**77.2**	**7.8**
ASN	2HB	CB	CA		70.5	86.7	16.2
GLN	2HG	CG	CB		71.1	85.4	14.3
GLN	1HG	CG	CB		71.1	57.2	13.9
ARG	HE	NE	CD		62.0	50.4	11.6
ASN	1HB	CB	CA		70.5	59.2	11.3
ASP	2HB	CB	CA		70.5	79.9	9.4
LEU	1HB	CB	CA		71.5	80.6	9.1
TRP	HD1	CD1	CG		55.1	63.1	8.0
HIS	HD2	CD2	NE2		53.6	59.9	6.3
GLU	2HG	CG	CB		71.1	76.4	5.3
HIS	HE1	CE1	ND1		54.2	59.4	5.2

phi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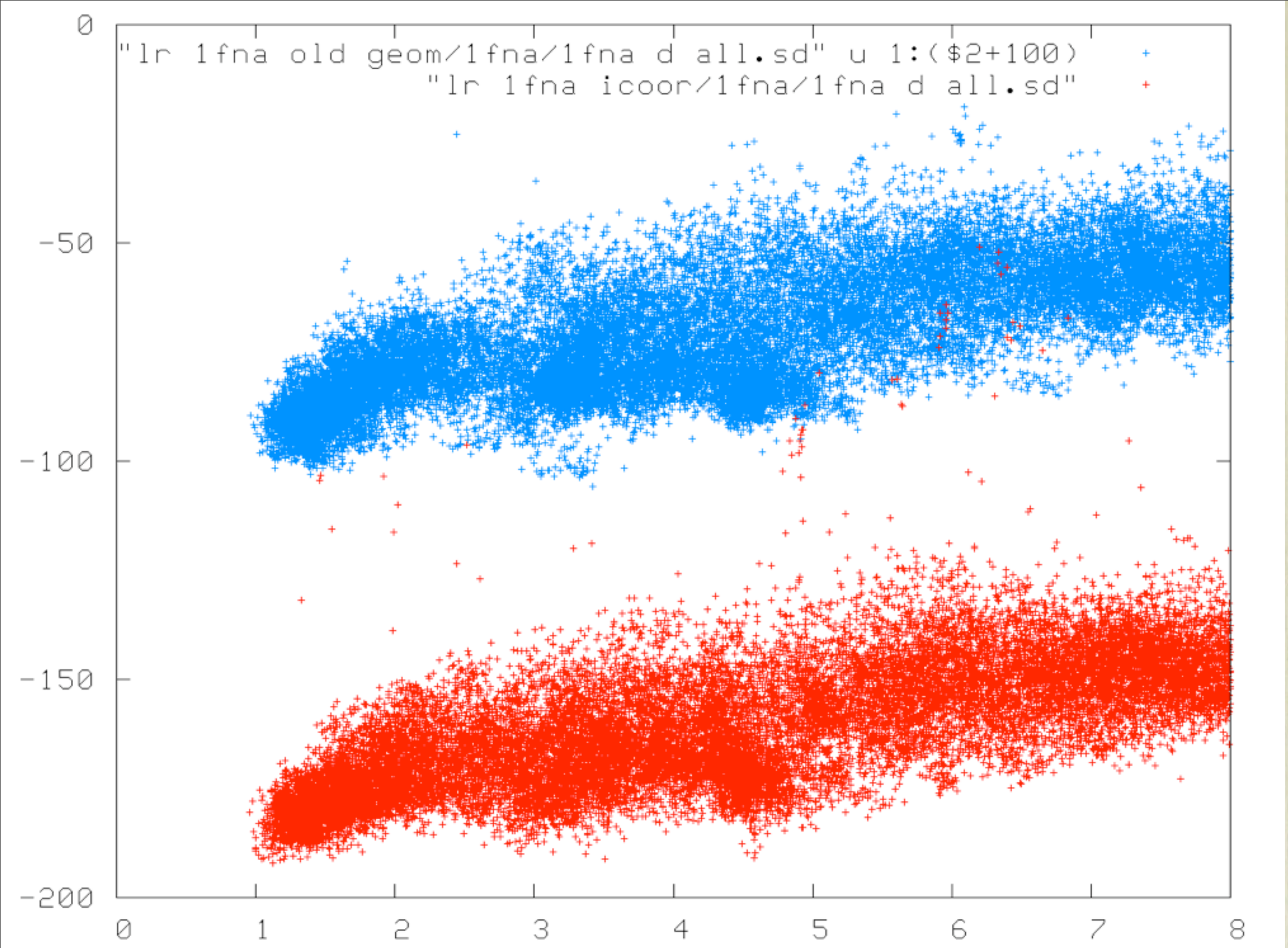
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2
3
4
5
6
7
8

PROTEINS: Structure, Function, and Genetics 34:82–95 (1999)

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2. Weak hydrogen bond between HA and O
3. Backbone Φ-Ψ

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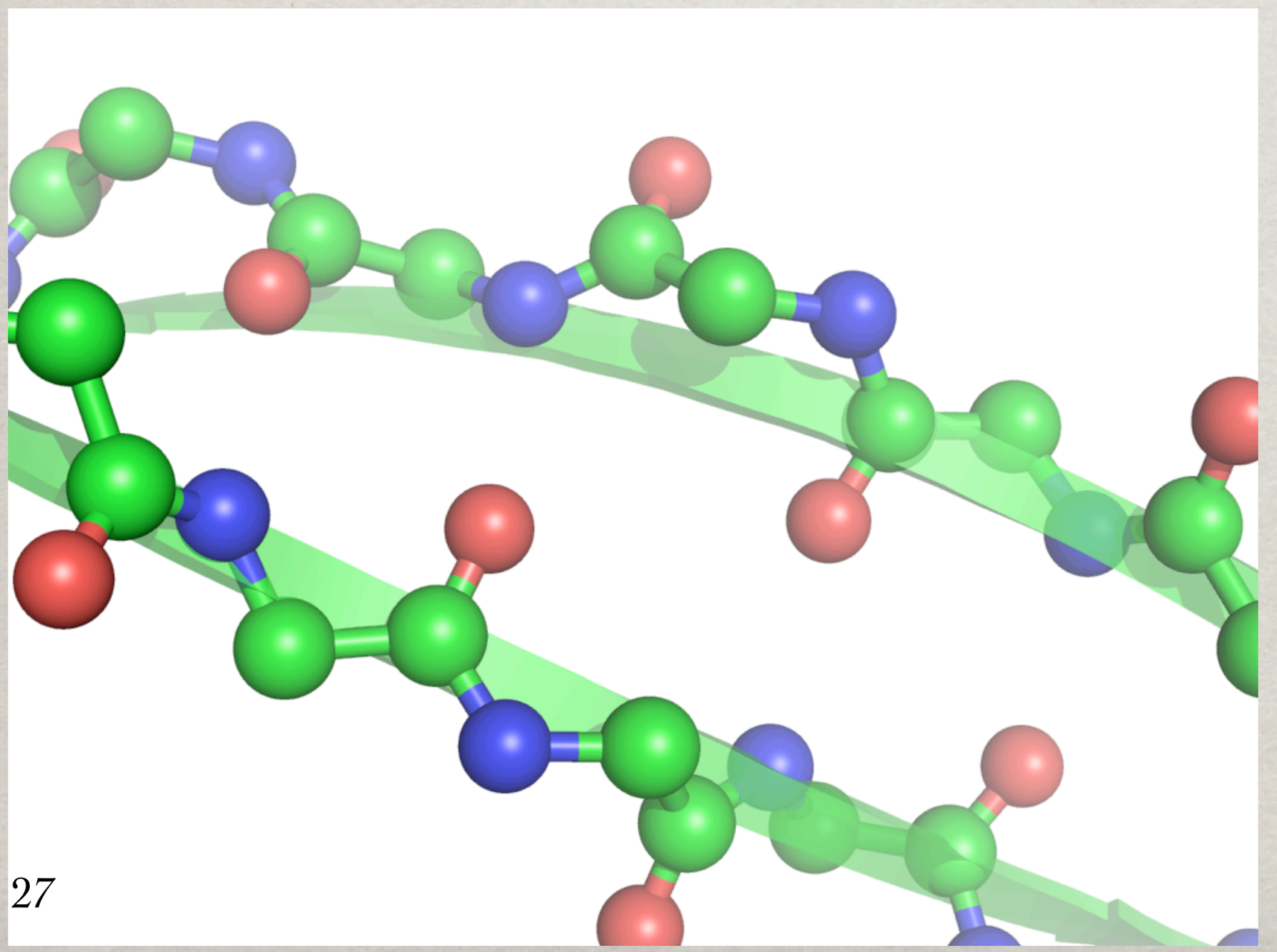

27

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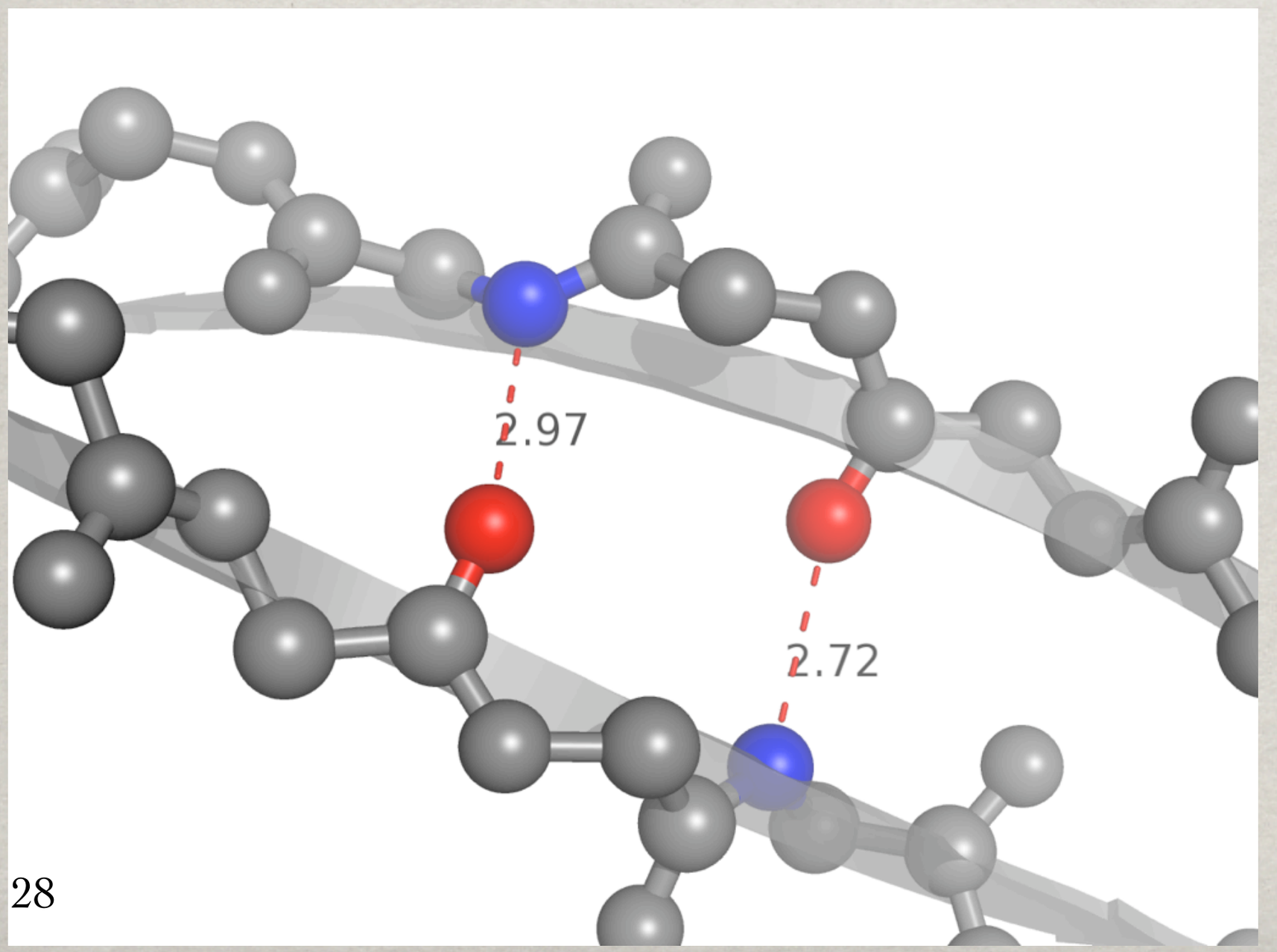

28

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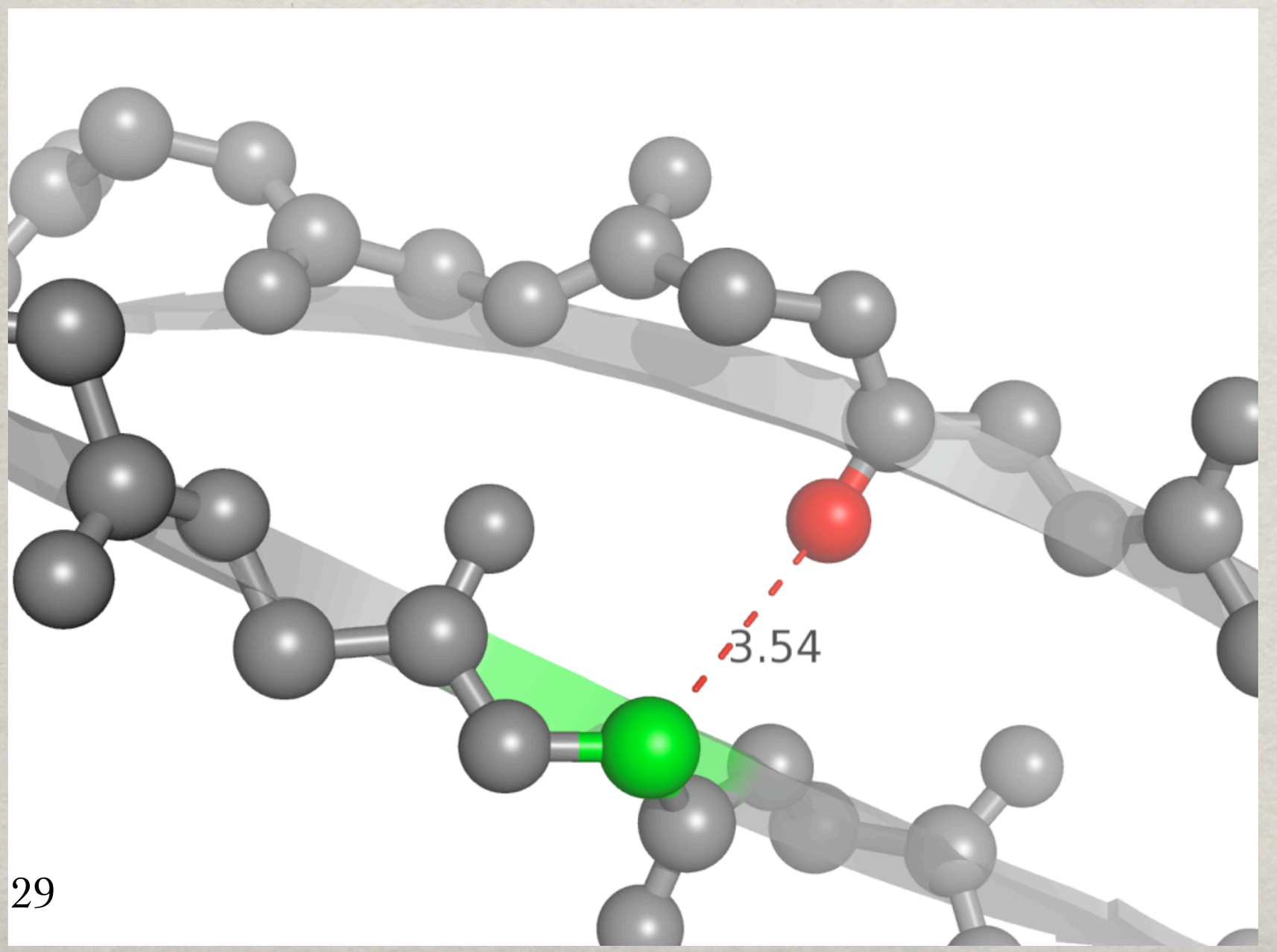

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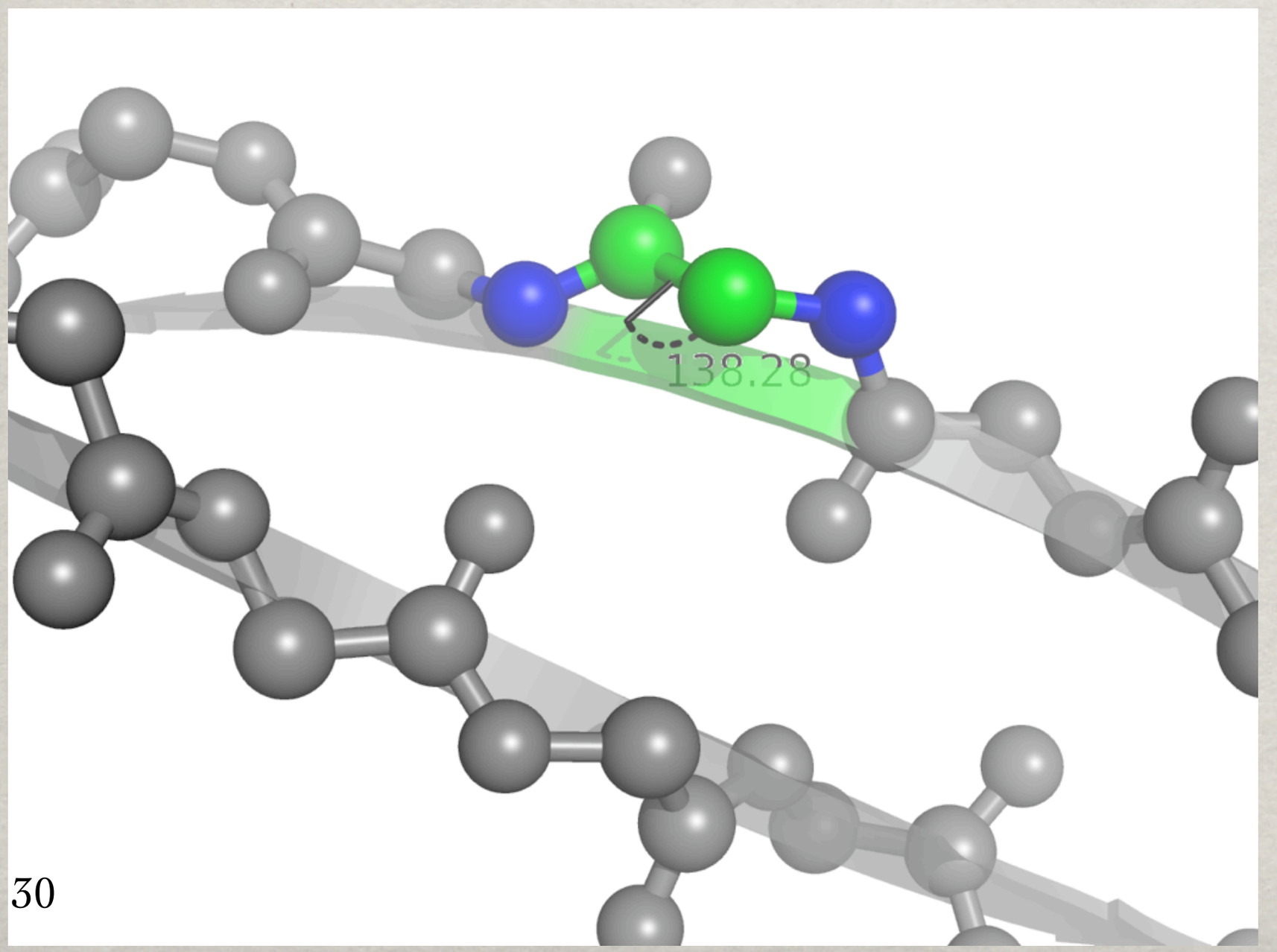

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