Supplementary File

Overlapping synthetic peptides as a tool to map protein-protein interactions - FSH as a model system of nonadditive interactions

Tomás A. Santa-Coloma

Laboratory of Cellular and Molecular Biology, Institute for Biomedical Research (BIOMED), School of Medical Sciences, Pontifical Catholic University of Argentina (UCA), and the National Scientific and Technical Research Council (CONICET), Buenos Aires, Argentina.

Table of Contents

Appendix 1- The Gibb equation

The binding equilibrium for a peptide p1 (or any ligand) and a receptor R is,

$$p1 + R \leftrightarrow \ p1::R$$

The free energy of this reaction is

$$\Delta G = \ \Delta G^{\circ}{}_{a} + RT \ln \frac{[p1::R]}{[p1][R]} = \Delta G^{\circ}{}_{a} + RT \ln K_a$$

At equilibrium ΔG = 0; under standard conditions, 25 °C, 1 atm, 1 M (mol/L) concentrations, the free energy for the equilibrium of association is

$$\Delta G^{\circ}{}_{a} = \ -RT \ln K_a$$

On the other hand, the free energy for the dissociation reaction is

$$\Delta G^{\circ}{}_{d} = \ RT \ln K_d$$

where K_a is the equilibrium constant of association and K_d is the equilibrium constant of dissociation ($K_a = 1/ K_d$).

At physiological conditions (pH = 7), the usual nomenclature is

$$\Delta G'^{\circ}{}_{a} = \ -RT \ln K'_a$$

or

$$\Delta G'^{\circ}{}_{d} = \ RT \ln K'_d$$

To simplify terms, we will assume standard conditions and pH and use the equation,

$$\boxed{\Delta G^{\circ} = \ -RT \ln K_a}$$

Appendix 2: ΔG° additivity

According to Gregorio Weber [1, 2], the total free energy of two ligands (in this case the synthetic peptides) corresponding to different anchor sites in the receptor should be,

$$\Delta G°(p1, p2) = \Delta G°(p1) + \Delta G°\left(\frac{p2}{p1}\right)$$

$$\Delta G°(p2, p1) = \Delta G°(p2) + \Delta G°\left(\frac{p1}{p2}\right)$$

Where p2/p1 is the binding of p2 after binding of p1 and vice versa, p1/p2 is the binding of p1 after binding of p2. Since $\Delta G°$ is a state function, a property whose value does not depend on the path taken,

$$\Delta G°(p1) + \Delta G°\left(\frac{p2}{p1}\right) = \Delta G°(p2) + \Delta G°\left(\frac{p1}{p2}\right) =$$

$$\Delta G°(p1) + \Delta G°(p2) + \Delta G°_{interactions}$$

In other words,

$$\Delta G°(p1, p2) = \Delta G°p1 + \Delta G°p2 + \Delta G°_{interactions}$$

Where ΔG°(p1,p2) is the total free energy of the interaction of peptide 1 and peptide 2 with receptor; ΔG°p1 and ΔG°p2 are the free energies corresponding to the binding of each peptide with the corresponding binding site in the receptor, and ΔG°coupling/interactions take into account the interactions between the receptor binding sites in the receptor, including entropic and enthalpic terms, interactions with solvent and other interactions. It will be abbreviated $\Delta G°_{int}$. For a number *i* of peptides/ligands,

$$\Delta G° = (\sum_i \Delta G°_i) + \Delta G°_{\text{int}}$$

For an "ideal" binding with no interactions among the binding sites, without conformational changes, solvent effects, or any other enthalpic or entropic influence, $\Delta G°_{int} = 0$. In the presence of positive cooperativity, $\Delta G°_{int} < 0$; on the other hand, if negative cooperativity is present (antagonism), $\Delta G°_{int} > 0$. Therefore, if the peptides and binding sites behave independently, and no cooperativity or interactions exists, the total free energy is,

$$\Delta G°(p1, p2) = \Delta G°p1 + \Delta G°p2$$

For *i* peptides (or anchor sites),

$$\boxed{\Delta G° = \sum_i \Delta G_i^\circ \quad Model\ 1}$$

Since the free energy of association is $\Delta G_a^\circ = -RT \ln Ka$ then,

$$\Delta G_a^\circ = -RT \ln \prod_i Ka_i$$

Therefore, under ideal conditions, assuming additivity in ΔG_i°, the association constant is the product of affinities of each anchor site [3],

$$Ka\ (total) = \prod_i Ka_i$$

Since $Ka = 1/K_d$,

$$\boxed{Kd\ (total) = \prod_i Kd_i \quad \text{Model 1}}$$

This is an oversimplification, an approximation, valid only if we assume that we do not have cooperativity and no other interactions besides those represented by the term $\sum_i \Delta G_i^\circ$.

Appendix 3: Buried surface areas (BSA) of the hFSH-β subunit.

These BSA values correspond to hFSH-β, indicated in the supplementary Table S2, PISA server interface #4 to #9, PDB entry 4mqw.

Total BSA for FSH-β ≡ BSA (33-53) + BSA (81-95) + BSA (96-99) + BSA (103) + BSA (105).

a) Interface 7: Z-H (receptor chain Z::FSH-β chain H)

BSA (34-37) = 0+26.43+1.59+26.93 = 54.95 $Å^2$ (peptide TRDL)

BSA (49-52) = 0+0+0+0 = 0 $Å^2$ (peptide KTCT)

BSA(33-53) = 54.95 + 0 + 13.41 + 26.73 + 27.77 + 10.68 + 90.14 + 82.89 + 29.27 + 43.25 + 53.96 = 433.05 $Å^2$

BSA (81-95) = 40.02 + 36.62 + 42.46 + 8.35 + 36.87 = 164.32 $Å^2$

BSA (96-99) = 31.60 + 110.92 + 11.99 + 86.25 = 240.76 $Å^2$

BSA (103) = 51.23 $Å^2$

BSA (105) = 0.34 $Å^2$

BSA (89-97) = 40.02+36.62+42.46+8.35+36.87+31.60+110.92 = 306.84 $Å^2$

BSA FSH-β = 433.05 + 164.32 + 240.76+ 51.23 + 0.34 = 889.70 $Å^2$

b) Interface 8: X-B (receptor chain X::FSH-β chain B)

BSA (34-37) = 0+5.2+0.5+22.08 = 27.78

BSA (49-52) = 0+0+0+0 = 0

BSA (33-53) = 27.78 + 0 + 14.39 + 22.97 + 28.08 + 7.96 + 93.09 + 83.50 + 30.73 + 28.28 + 72.23 = 409.01 $Å^2$

BSA (81-95) = 41.98+26.94+43.67+6.5+33.59= 152.68 $Å^2$

BSA (96-99) = 32.48+104.82+10.68+90.05 = 238.03 $Å^2$

BSA (103) = 50.74 $Å^2$

BSA (105) = 0.0 $Å^2$

BSA (89-97) = 41.98+26.94+43.67+6.5+33.59+32.48+104.82 = 289.98 Å^2

BSA FSH-β = 409.01+152.68+238.03+50.74= 850.46 Å^2

c) Interface 9: Y-E (receptor chain Y::FSH-β chain E)

BSA (34-37) = 0+4.53+0.25+25.22 = 30

BSA (49-52) = 0+0+0+0 = 0

BSA (33-53) = 4.53 + 0.25 + 25.22 + 17.23 + 21.55 + 29.57 + 6.86 + 78.76 + 77.05 + 23.83 + 30.15 + 56.16 = 371.16 Å^2.

BSA (81-95) = 42.49 + 25.75 + 43.16 + 6.38 +36.81 = 154.59 Å^2.

BSA (96-99) = 30.29 + 109.30 + 10.03 + 86.24 = 235.86 Å^2.

BSA (103) = 52.21 Å^2.

BSA (105) = 1.20 Å^2.

BSA (89-97) = 42.49+25.75+43.16+6.38+36.81+30.29+109.30 = 294.18 Å^2.

BSA FSH-β = 371.16 + 154.59 +235.86 + 52.21 + 1.20 = 815.02 Å^2.

Averages BSA hFSH-β:

BSA (34-37) = 54.95,27.78,30.00 = 37.58 ± 15.09 Å^2 (n=3).

BSA (49-52) = 0,0,0,0 = 0 ± 0 Å^2 (n=3).

BSA (33-53) = 433.05, 409.01, 371.16 = 404.41 ±31.20 Å^2 (n=3).

BSA (81-95) = 164.32, 152.68, 154.59 = 157.20 ± 6.24 Å^2 (n=3).

BSA (96-99) = 240.76, 238.03, 235.86 = 238.22 ± 2.46 Å^2 (n=3).

BSA (103) = 51.23, 50.74, 52.21 = 51.40 ± 0.75 Å^2 (n=3).

BSA (105) = 0.34, 0, 1.20 = 0.51 ± 0.62 Å^2 (n=3).

BSA (34-47) = 433.05, 409.01, 371.16 = 404.41 ±31.20 Å^2 (n=3); ≡ to (33-53)

BSA (88-106) = 456.65, 441.45, 443.86 = 447.32 ± 8.17 Å^2 (n=3)

BSA (34-47)-(88-106) = 889.70 , 850.46 , 815.02 = 851.73 ± 37.36 Å^2 (n=3).

BSA (89-97) = 297.00 ± 8.78 Å^2 (n=3).

BSA hFSH-β = 851.73 ± 37.36 Å^2 (n=3).

BSA hFSH-α = 1030.6 ± 53.95 Å^2 (n=3).

BSA hFSH (hFSH-α+FSH-β) = 1882.33 ± 91.29 (n=3)

Total BSA hFSH::hFSHR (R-α + R-β interfaces) = 3608.06 ± 166.76 Å^2 (n=3).

For the regression in Figure 9, the hFSH and the hFSH-β values were taken as 1882.33 and 851.73 respectively and values of the peptides as above indicated (also in Table 3).

Appendix 4: Values of C and ω in FSH-β

Considering the FSH-β and the two binding regions A, FSH-β-(33-53) and B, FSH-β-(81-95), with association constants K_{AB} = 1.1 x 10^7 mol^{-1} L, K_A = 1 x 10^4 mol^{-1} L, and K_B= 0.25 x 10^4 mol^{-1} L, respectively, at 25 °C (R=1.9872×10^{-3} kcal K^{-1} mol^{-1}, T = 298.15 K, RT = 0.5925 kcal. mol^{-1}),

$$\omega = \frac{K_{AB}}{K_A.K_B} = \frac{1.1 \times 10^7 M^{-1}}{1x10^4\ M^{-1}\ \ 0.25x10^4\ M^{-1}} = 0.11/0.25 = 0.44$$

$\Delta G^\circ_{int} = -RT \ln \omega$ = - 0.593 ln 0.44 = -0.593 x (- 0.821) = 0.487 kcal/mol

$\Delta G^\circ_A = -RT \ln K_A$ = - 0.593 x ln (1 x 10^4) = -0.593 x 9.210 = -5.462 kcal/mol

$\Delta G^\circ_B = -RT \ln K_B$ = - 0.593 x ln (0.25 x 10^4) = -0.593 x 7.824 = -4.640 kcal/mol

$\Delta G^\circ_{AB} = -RT \ln K_{AB}$ = - 0.593 x ln (0.11 x 10^8) = -0.593 x 16.213= - 9.615 kcal/mol

$$c = \frac{\Delta G^\circ_{AB}}{\Delta G^\circ_A + \Delta G^\circ_B} = \frac{-9.615}{-5.462-4.640} = \frac{-9.615}{-10.102} = 0.952$$

On the other hand, hFSH-β-(33-53)-(81-95) has a observed K_{AB} = 2 x 10^4 mol^{-1} L, far from the predicted value of $K_A.K_B$ = 2.5 x $10^7 mol^{-1}$ L for independent interactions (Model 1). In this case,

$$\boldsymbol{\omega} = 2 \times 10^4 / 1 \times 10^4 * 0.25 \times 10^4 = 8 \times 10^{-4}$$

and

$$\mathbf{c} = -5.87/((-5.46)+(-4{,}64))=-5.87/-10.1= 0.58.$$

Appendix 5: Figure 9A data and R code

Figure 9A data:

Dataset1: values 1-7
Dataset2: values 8-14
Dataset3: values 1-14

	BSA	deltaG	set
1	0	0.00	pre
2	38	-0.28	pre
3	157	-1.14	pre
4	404	-2.93	pre
5	561	-4.07	pre
6	852	-6.18	pre
7	1882	-13.64	pre
8	0	-2.93	obs
9	38	-2.60	obs
10	157	-4.64	obs
11	404	-5.46	obs
12	561	-5.87	obs
13	852	-9.61	obs
14	1882	-13.64	obs

Figure 9A was built using Rstudio and the following user libraries, system libraries, and RStudio code:

User libraries: ggplot2, plyr, reshape2, scales, readxl.
System libraries: base, datasets, graphics, grDevices, methods, stats, and utils.

RStudio code:

```
library(readxl)

Dataset1 <- read_excel("C:/R/DataFSH/Dataset1.xlsx")
View(Dataset1) #BSA and deltaG values 1-7
Dataset2 <- read_excel("C:/R/DataFSH/Dataset2.xlsx")
View(Dataset2) #BSA and deltaG values 8-14
Dataset3 <- read_excel("C:/R/DataFSH/Dataset5.xlsx")
View(Dataset3) #BSA and deltaG values 1-14

lm2 <- lm(deltaG~BSA, data=Dataset2)
anova(lm2)
summary (lm2)

ggplot(Dataset3, aes(BSA, deltaG, shape=set)) +
   geom_point(size=2.5) +
   geom_smooth(method="lm") +
   theme_classic() +
   labs(x = bquote('BSA'~(Å^2)), y = "ΔG°(kcal/mol)") +
   ggtitle("") +
   scale_y_continuous(breaks = seq(-16, 3, 2)) +
   scale_x_continuous(breaks = seq(0, 2250, 250))+
   expand_limits(x = 0, y = 2)
```

Results (corresponding to Figure 9A):

```
> summary (lm2)   # shows the linear regression analysis for lm2 using Dataset2

Call: lm(formula = deltaG ~ BSA, data = Dataset2)

Residuals:
1           2           3           4           5           6           7
0.19689     0.75194     -0.58956     0.03927     0.54981    -1.48009     0.53173

Coefficients:
             Estimate    Std. Error    t value      Pr(>|t|)
(Intercept)  -3.124895   0.441719      -7.074       0.000873 ***
BSA           -0.005870  0.000535      -10.972      0.000109 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
Residual standard error: 0.8636 on 5 degrees of freedom
Multiple R-squared:  0.9601
Adjusted R-squared:  0.9521
F-statistic: 120.4 on 1 and 5 DF,  p-value: 0.0001094
```

The ANOVA results for lm1 are not shown since the line is a perfect line with R=1 and values calculated from the gamma value, FSH affinity, and the BSA values (model 2).

Appendix 6: Hot-Spots and NS in the FSH::FSHR complex.

The results correspond to the output of SPOTON, a software for Hot-Spot detection at protein-protein Interfaces. HS, hot spots; NS, null spots. HS indicated in orange and NS in green.

HS and NS in the FSH::FSHR sequences.

Amino acid residue sequence for chain D (FSH-α).

VQDCPECTLQENPLFSQPGAPILQCMGCCFSRAYPTPLRSKKTMLVQKNVTSESTCCVAKSYNRVTVMGG
FKVENHTACHCSTCYYHKS

Amino acid residue sequence for chain E (FSH-β).

NSCELTNITIAIEKEECRFCISINTTWCAGYCYTRDLVYKDPARPKIQKTCTFKELVYETVRVPGC
AHHADSLYTYPVATQCHCGKCDSDSTDCTVRGLGPSYCSFGE

Amino acid residue sequence for chain Y (FSHR).

CHHRICHCSNRVFLCQESKVTEIPSDLPRNAIELRFVLTKLRVIQKGAFSGFGDLEKIEISQND
VLEVIEADVFSNLPKLHEIRIEKANNLLYINPEAFQNLPNLQYLLISNTGIKHLPDVHKIHSLQ
KVLLDIQDNINIHTIERNSFVGLSFESVILWLNKNGIQEIHNSAFNGTQLDELNLSDNNNLEEL
PNDVFHGASGPVILDISRTRIHSLPSYGLENLKKLRARSTYNLKKLPTLEKLVALMEASLTYPSHCC
AFANWDDLVDVTCSPKPDAFNPCE

HS Table

55	LEU	Y
79	GLN	Y
101	ARG	Y
104	LYS	Y
124	TYR	Y
129	ASN	Y

NS Table:

42	ARG	D
43	SER	D
45	LYS	D
46	THR	D
47	MET	D
48	LEU	D
49	VAL	D
51	LYS	D
65	TYR	D
67	ARG	D
85	SER	D
86	THR	D
87	CYS	D
88	TYR	D
89	TYR	D
91	LYS	D
92	SER	D
40	LYS	E
41	ASP	E
42	PRO	E
43	ALA	E
44	ARG	E
46	LYS	E
87	CYS	E
89	SER	E
90	ASP	E
93	ASP	E

94	CYS	E
95	THR	E
96	VAL	E
97	ARG	E
98	GLY	E
99	LEU	E
103	TYR	E
33	GLN	Y
34	GLU	Y
35	SER	Y
50	GLU	Y
52	ARG	Y
54	VAL	Y
57	LYS	Y
74	LYS	Y
76	GLU	Y
80	ASN	Y
81	ASP	Y
92	SER	Y
98	HIS	Y
99	GLU	Y
103	GLU	Y
105	ALA	Y
106	ASN	Y
123	GLN	Y
126	LEU	Y
130	THR	Y
131	GLY	Y

145	GLN	Y
146	LYS	Y
148	LEU	Y
150	ASP	Y
152	GLN	Y
153	ASP	Y
155	ILE	Y
156	ASN	Y
174	ILE	Y
176	TRP	Y
178	ASN	Y
179	LYS	Y
196	ASP	Y
197	GLU	Y
199	ASN	Y
221	VAL	Y
222	ILE	Y
242	LYS	Y
243	LYS	Y

FIGURES

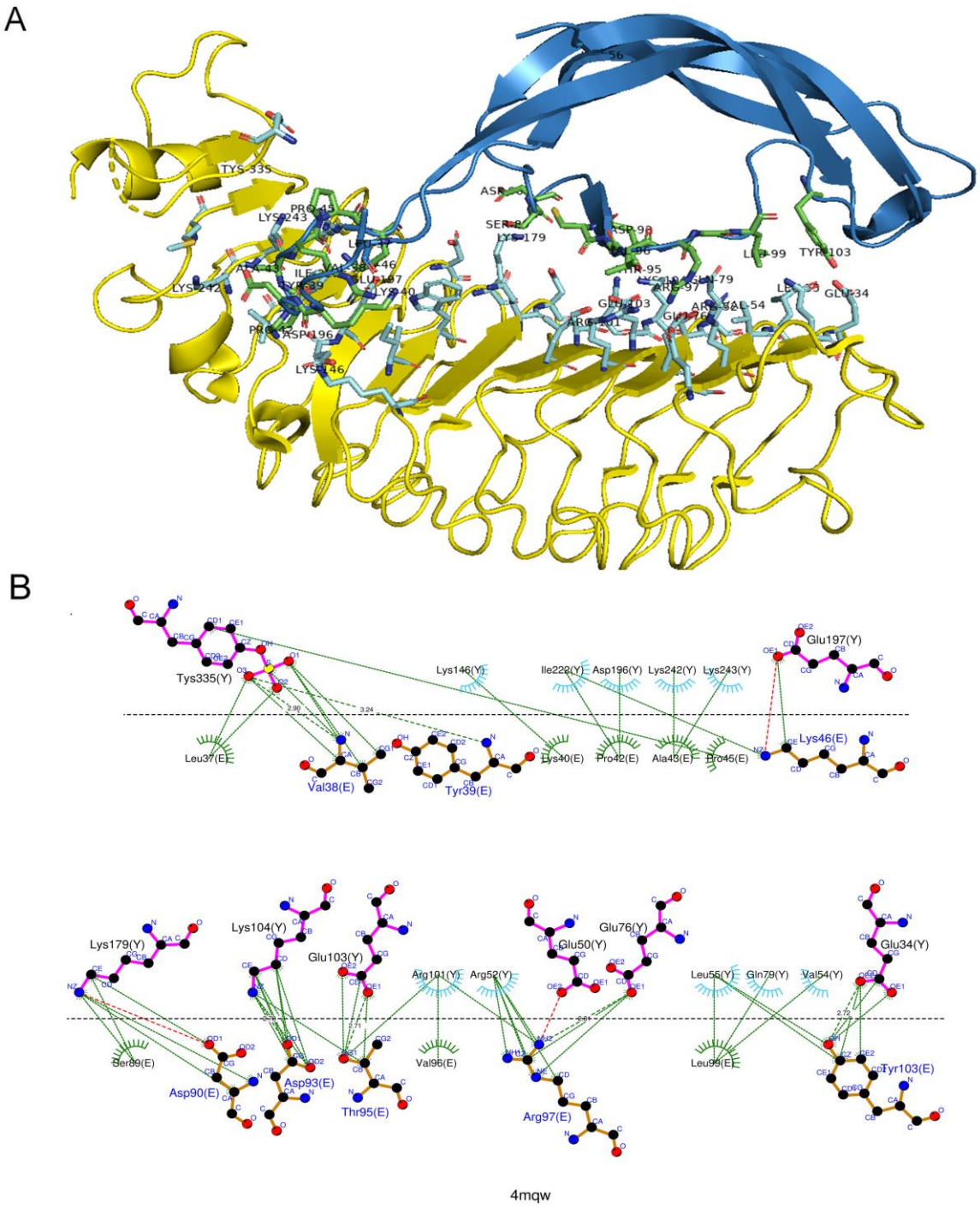


Figure S1: Interaction plots for the FSH-β binding regions in the FSH-β::FSHR complex.

A: interface FSH-β::FSHR. The ball and stick representation were built by using PyMol v2.5 adding the plugin ' interfaceResides.py '. The labeled residues correspond to the interaction residues; green and light blue figures represent hydrophobic residues from chains E and Y respectively. **B**: Interaction plot made by using LigPlot+ v.2.2.5, with program DIMPLOT (www.ebi.ac.uk/thornton-srv/software/LigPlus/).

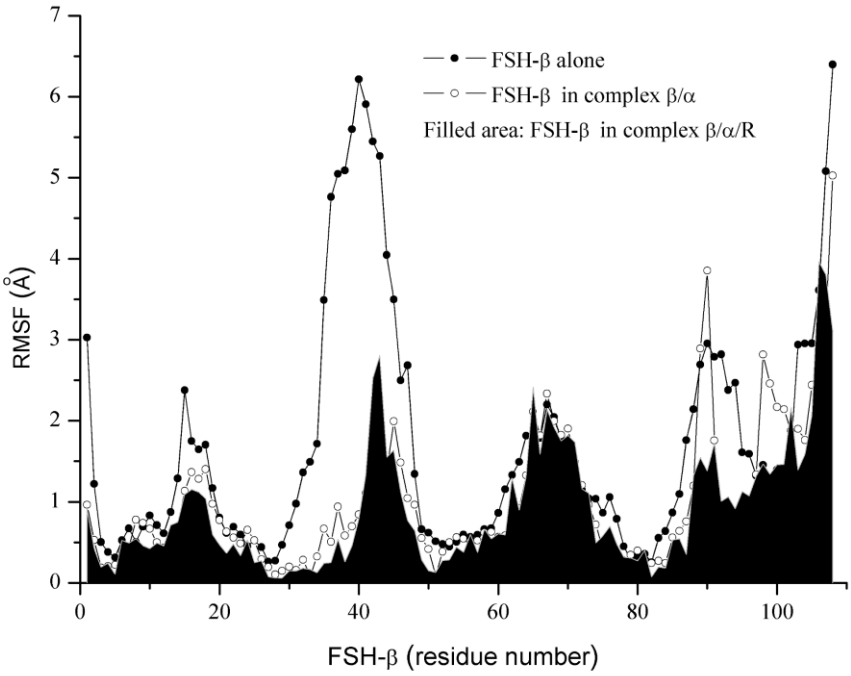
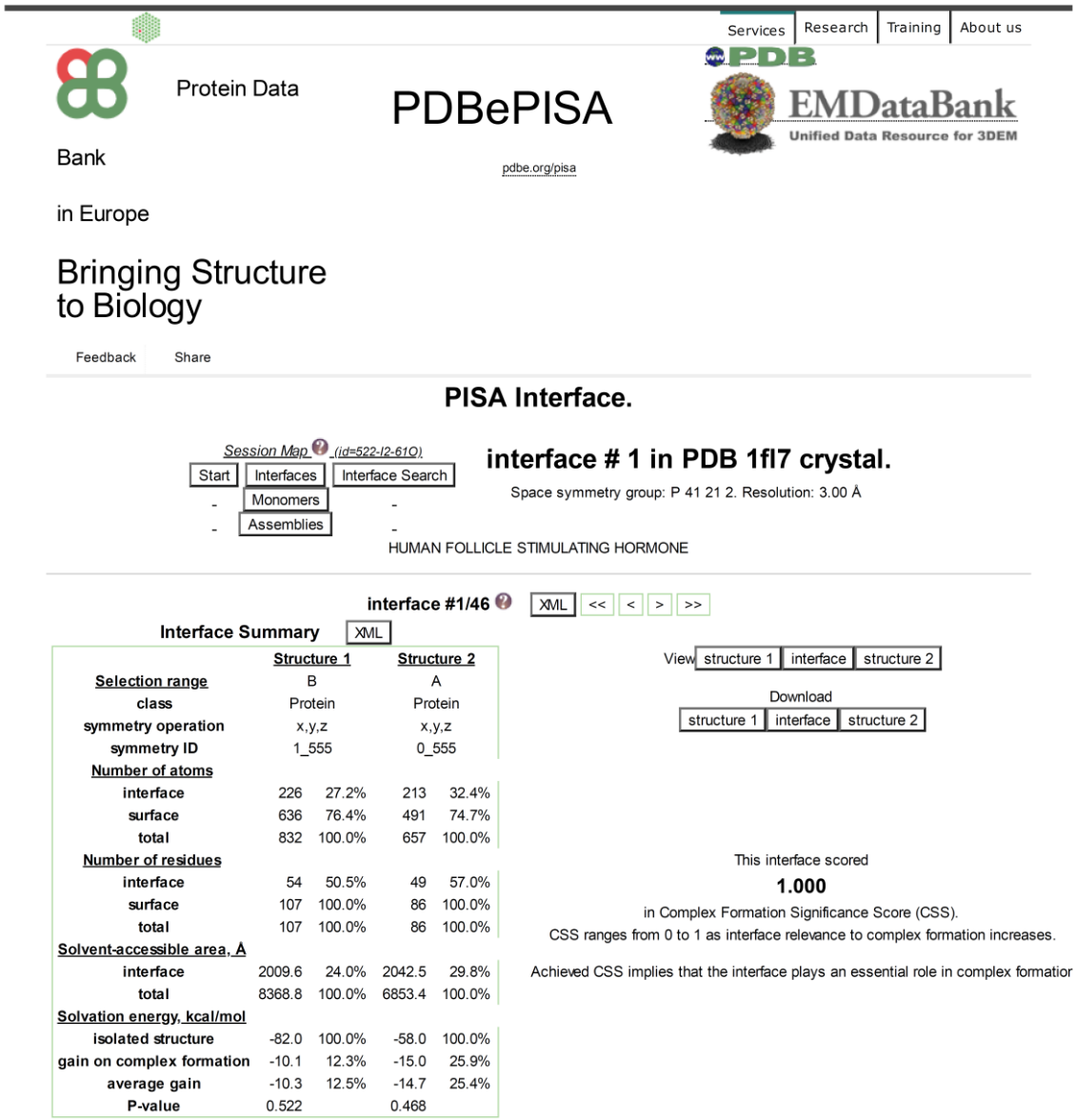


Figure S2: FSH-β chain Flexibility.
Flexibility is indicated as RMSF (Å) according to the data of the crystal structure 4mqw. A: FSH-β (chain E). B: FSH-β in FSH-(α/β) complex (chains E+D). C: FSH-β in FSH-FSHR complex (chains E+D+Y). The values were obtained by using the MD server CABSflex 2.0, a Python package for fast simulations of protein structure flexibility. [4] A progressive reduction of flexibility was obtained from the data corresponding to 50 simulations: FSH-β alone > FSH-β in β/α> FSH-β in the complex α/β/R.

TABLES

Table S1. Interface #1 in PDB 1fl7 crystal



Services | Research | Training | About us

Protein Data Bank in Europe

PDBePISA

pdbe.org/pisa

PDB

EMDataBank

Unified Data Resource for 3DEM

Bringing Structure to Biology

Feedback Share

PISA Interface.

Session Map (id=522-l2-61Q)

Start | Interfaces | Interface Search | Monomers | Assemblies

interface # 1 in PDB 1fl7 crystal.

Space symmetry group: P 41 21 2. Resolution: 3.00 Å

HUMAN FOLLICLE STIMULATING HORMONE

interface #1/46 XML << < > >>

Interface Summary XML

	Structure 1		Structure 2	
Selection range	B		A	
class	Protein		Protein	
symmetry operation	x,y,z		x,y,z	
symmetry ID	1_555		0_555	
Number of atoms				
interface	226	27.2%	213	32.4%
surface	636	76.4%	491	74.7%
total	832	100.0%	657	100.0%
Number of residues				
interface	54	50.5%	49	57.0%
surface	107	100.0%	86	100.0%
total	107	100.0%	86	100.0%
Solvent-accessible area, Å				
interface	2009.6	24.0%	2042.5	29.8%
total	8368.8	100.0%	6853.4	100.0%
Solvation energy, kcal/mol				
isolated structure	-82.0	100.0%	-58.0	100.0%
gain on complex formation	-10.1	12.3%	-15.0	25.9%
average gain	-10.3	12.5%	-14.7	25.4%
P-value	0.522		0.468	

View structure 1 | interface | structure 2

Download structure 1 | interface | structure 2

This interface scored

1.000

in Complex Formation Significance Score (CSS).

CSS ranges from 0 to 1 as interface relevance to complex formation increases.

Achieved CSS implies that the interface plays an essential role in complex formatior

Hydrogen bonds XML

##	Structure 1	Dist. [Å]	Structure 2
1	B:VAL 38[N]	3.35	A:GLN 27[OE1]
2	B:ASP 36[N]	2.92	A:CYS 28[O]
3	B:THR 34[N]	2.77	A:GLY 30[O]
4	B:THR 34[OG1]	3.78	A:GLY 30[O]
5	B:CYS 32[N]	3.31	A:CYS 32[O]
6	B:GLY 30[N]	3.04	A:SER 34[O]
7	B:THR 50[OG1]	2.71	A:SER 34[OG]
8	B:CYS 51[N]	3.32	A:SER 34[OG]
9	B:CYS 28[N]	3.70	A:ALA 36[O]
10	B:LEU 99[N]	3.85	A:TYR 37[OH]
11	B:GLY 100[N]	3.26	A:TYR 37[OH]
12	B:ASP 93[N]	2.74	A:VAL 53[O]
13	B:THR 95[N]	2.89	A:SER 55[O]
14	B:THR 95[OG1]	3.78	A:SER 55[O]
15	B:GLY 98[N]	2.96	A:GLU 56[OE2]
16	B:LYS 40[NZ]	2.56	A:GLU 77[OE1]
17	B:THR 34[O]	2.83	A:GLY 30[N]
18	B:CYS 32[O]	3.09	A:CYS 32[N]
19	B:GLY 30[O]	2.88	A:SER 34[N]
20	B:CYS 51[O]	3.37	A:SER 34[OG]
21	B:CYS 28[O]	3.13	A:ALA 36[N]
22	B:MET 109[O]	3.18	A:ARG 42[NH1]
23	B:MET 109[O]	3.08	A:ARG 42[NH2]
24	B:GLU 15[OE2]	2.72	A:LYS 45[NZ]
25	B:SER 89[O]	2.68	A:LYS 51[NZ]
26	B:SER 89[OG]	3.88	A:LYS 51[NZ]
27	B:THR 92[O]	3.61	A:LYS 51[NZ]
28	B:SER 91[O]	3.51	A:ASN 52[N]
29	B:SER 91[O]	3.18	A:VAL 53[N]
30	B:ASP 93[OD2]	3.89	A:THR 54[OG1]
31	B:ASP 93[O]	3.17	A:SER 55[N]
32	B:THR 95[O]	3.03	A:SER 57[N]
33	B:THR 95[O]	3.07	A:SER 57[OG]
34	B:THR 34[OG1]	2.79	A:CYS 60[N]
35	B:ASP 36[OD2]	2.93	A:ALA 62[N]
36	B:VAL 38[O]	2.87	A:GLU 77[N]
37	B:ASP 36[OD1]	2.85	A:TYR 88[OH]

Salt bridges XML

##	Structure 1	Dist. [Å]	Structure 2
1	B:LYS 40[NZ]	2.56	A:GLU 77[OE1]
2	B:LYS 40[NZ]	2.68	A:GLU 77[OE2]
3	B:GLU 108[OE1]	3.40	A:LYS 45[NZ]
4	B:GLU 15[OE2]	2.72	A:LYS 45[NZ]
5	B:ASP 36[OD2]	3.78	A:HIS 79[NE2]

No disulfide bonds found
No covalent bonds found

Interfacing residues (not a contact table) XML Display level: Residues

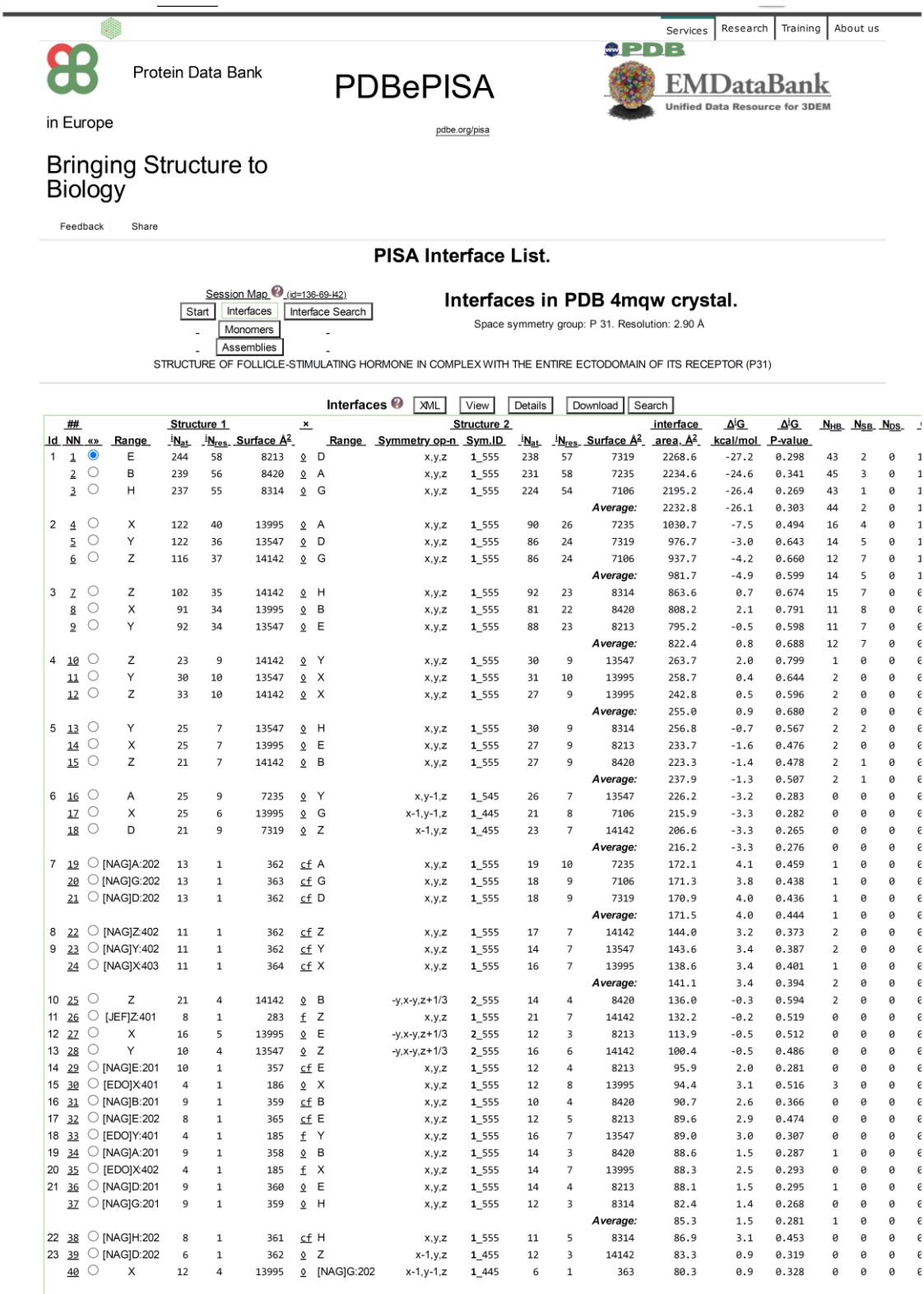
Inaccessible residues HSDC Residues making **H**ydrogen/**D**isulphide bond, **S**alt bridge or **C**ovalent link
Solvent-accessible residues Interfacing residues
ASA Accessible Surface Area, Å² **BSA** Buried Surface Area, Å² **ΔᴵG** Solvation energy effect, kcal/mol |||| Buried area percentage, one bar per 10%

##	Structure 1	HSDC	ASA	BSA	ΔᴵG	##	Structure 2	HSDC	ASA	BSA	ΔᴵG
1	B:CYS 3		38.56	0.00	0.00	1	A:GLN 5		186.16	0.00	0.00
2	B:GLU 4		130.37	0.00	0.00	2	A:ASP 6		146.79	0.00	0.00
3	B:LEU 5		73.11	0.00	0.00	3	A:CYS 7		83.00	41.75 |||||	1.29
4	B:THR 6		58.45	0.00	0.00	4	A:PRO 8		76.23	10.71 ||	0.17
5	B:ASN 7		113.67	0.00	0.00	5	A:GLU 9		148.72	0.00	0.00
6	B:ILE 8		48.10	12.55 |||	0.20	6	A:CYS 10		13.77	0.00	0.00
7	B:THR 9		54.17	0.00	0.00	7	A:THR 11		57.25	0.00	0.00
8	B:ILE 10		25.45	20.60 ||||||||	0.33	8	A:LEU 12		48.03	0.00	0.00
9	B:ALA 11		25.35	5.03 ||	-0.06	9	A:GLN 13		93.88	0.00	0.00
10	B:ILE 12		3.92	0.00	0.00	10	A:GLU 14		107.22	0.00	0.00
11	B:GLU 13		58.21	33.41 |||||	-0.11	11	A:ASN 15		14.45	3.54 |||	-0.05
12	B:LYS 14		17.63	0.00	0.00	12	A:PRO 16		99.82	0.00	0.00
13	B:GLU 15	HS	103.95	38.92 ||||	-0.01	13	A:PHE 17		177.98	0.00	0.00
14	B:GLU 16		88.03	0.00	0.00	14	A:PHE 18		70.39	27.80 ||||	0.44
15	B:CYS 17		11.87	0.00	0.00	15	A:SER 19		27.40	0.00	0.00
16	B:ARG 18		179.19	0.00	0.00	16	A:GLN 20		74.31	0.00	0.00
17	B:PHE 19		58.94	0.00	0.00	17	A:PRO 21		130.14	0.00	0.00
18	B:CYS 20		35.68	0.00	0.00	18	A:GLY 22		88.29	0.00	0.00

19	B:ILE	21		33.46	0.00	0.00	19	A:ALA	23		65.06	0.00	0.00
20	B:SER	22		88.49	0.00	0.00	20	A:PRO	24		65.36	0.00	0.00
21	B:ILE	23		24.69	0.00	0.00	21	A:ILE	25		6.19	5.52 |||||||||	0.09
22	B:ASN	24		106.45	0.00	0.00	22	A:LEU	26		58.49	0.61 |	-0.01
23	B:THR	25		7.90	0.00	0.00	23	A:GLN	27	H	58.60	47.95 ||||||||	-0.47
24	B:ALA	26		23.88	0.00	0.00	24	A:CYS	28	H	13.02	13.02 |||||||||	-0.13
25	B:TRP	27		52.70	52.70 ||||||||||	0.77	25	A:MET	29		80.60	44.86 ||||||	0.96
26	B:CYS	28	H	24.69	23.33 |||||||||	-0.17	26	A:GLY	30	H	37.74	35.56 |||||||||	-0.17
27	B:ALA	29		47.75	31.06 |||||||	0.50	27	A:CYS	31		34.41	28.06 ||||||||	0.72
28	B:GLY	30	H	47.27	34.22 ||||||||	-0.24	28	A:CYS	32	H	35.77	32.17 ||||||||	-0.11
29	B:TYR	31		194.21	84.14 |||||	1.12	29	A:PHE	33		161.73	64.02 ||||	0.90
30	B:CYS	32	H	43.32	37.55 ||||||||	-0.11	30	A:SER	34	H	61.20	58.67 |||||||||	0.03
31	B:TYR	33		177.11	75.21 |||||	0.48	31	A:ARG	35		126.78	64.71 ||||||	-0.43
32	B:THR	34	H	69.70	65.94 ||||||||	-0.38	32	A:ALA	36	H	68.73	67.50 |||||||||	0.28
33	B:ARG	35		163.42	28.34 ||	0.45	33	A:TYR	37	H	63.67	62.37 |||||||||	0.49
34	B:ASP	36	HS	120.19	98.82 ||||||||	-0.22	34	A:PRO	38		108.93	97.33 ||||||||	1.43
35	B:LEU	37		72.95	19.48 |||	0.28	35	A:THR	39		17.59	6.72 ||||	-0.07
36	B:VAL	38	H	154.01	150.22 |||||||||	1.72	36	A:PRO	40		76.81	69.12 ||||||||	1.11
37	B:TYR	39		177.47	80.89 |||||	1.11	37	A:LEU	41		130.80	83.68 |||||||	1.26
38	B:LYS	40	HS	137.35	73.25 ||||||	0.29	38	A:ARG	42	H	211.38	137.30 ||||||	-0.14
39	B:ASP	41		78.52	9.98 ||	-0.11	39	A:SER	43		42.25	17.86 |||||	0.28
40	B:PRO	42		126.53	0.00	0.00	40	A:LYS	44		82.79	8.94 ||	-0.04
41	B:ALA	43		72.57	0.00	0.00	41	A:LYS	45	HS	145.57	55.46 ||||	-0.96
42	B:ARG	44		204.84	50.00 |||	-0.19	42	A:THR	46		116.80	0.00	0.00
43	B:PRO	45		89.48	19.89 |||	0.12	43	A:MET	47		44.03	20.75 |||||	0.35
44	B:LYS	46		95.07	10.62 ||	-0.08	44	A:LEU	48		169.26	0.00	0.00
45	B:ILE	47		106.25	27.94 |||	0.15	45	A:VAL	49		110.41	0.00	0.00
46	B:GLN	48		57.58	31.44 |||||	0.38	46	A:GLN	50		126.95	0.00	0.00
47	B:LYS	49		107.77	3.67 |	-0.04	47	A:LYS	51	H	117.71	73.46 ||||||	-0.25
48	B:THR	50	H	55.42	47.20 |||||||	-0.05	48	A:ASN	52	H	111.10	39.83 ||||	0.12
49	B:CYS	51	H	32.55	32.55 |||||||||	-0.02	49	A:VAL	53	H	96.58	96.24 |||||||||	1.14
50	B:THR	52		18.18	15.35 ||||||||	0.09	50	A:THR	54	H	34.63	31.62 |||||||||	0.33
51	B:PHE	53		35.35	7.31 |||	0.12	51	A:SER	55	H	74.87	74.87 |||||||||	0.01
52	B:LYS	54		104.29	0.00	0.00	52	A:GLU	56	H	70.86	56.52 |||||||	0.13
53	B:GLU	55		96.97	0.00	0.00	53	A:SER	57	H	68.83	49.92 |||||||	-0.12
54	B:LEU	56		56.03	7.60 ||	0.12	54	A:THR	58		39.26	9.02 |||	-0.06
55	B:VAL	57		80.61	0.00	0.00	55	A:CYS	59		42.79	38.31 ||||||||	0.62
56	B:TYR	58		138.57	27.49 ||	-0.16	56	A:CYS	60	H	25.99	25.63 ||||||||	-0.15
57	B:GLU	59		71.26	0.00	0.00	57	A:VAL	61		19.75	8.04 |||||	0.13
58	B:THR	60		80.76	0.00	0.00	58	A:ALA	62	H	20.53	3.79 ||	0.01
59	B:VAL	61		41.80	0.00	0.00	59	A:LYS	63		124.56	0.00	0.00
60	B:ARG	62		149.46	0.00	0.00	60	A:SER	64		47.67	0.00	0.00
61	B:VAL	63		8.37	0.00	0.00	61	A:TYR	65		106.90	0.00	0.00
62	B:PRO	64		62.25	0.00	0.00	62	A:ASN	66		91.32	0.00	0.00
63	B:GLY	65		18.84	0.00	0.00	63	A:ARG	67		118.63	0.00	0.00
64	B:CYS	66		52.87	0.00	0.00	64	A:VAL	68		53.16	0.00	0.00
65	B:ALA	67		88.20	0.00	0.00	65	A:THR	69		84.35	0.00	0.00
66	B:HIS	68		160.87	0.00	0.00	66	A:VAL	70		25.74	0.00	0.00
67	B:HIS	69		79.72	0.00	0.00	67	A:MET	71		158.85	0.00	0.00
68	B:ALA	70		89.10	0.00	0.00	68	A:GLY	72		52.96	0.00	0.00
69	B:ASP	71		52.00	0.00	0.00	69	A:GLY	73		61.15	0.00	0.00
70	B:SER	72		51.78	0.00	0.00	70	A:PHE	74		101.92	25.28 |||	0.40
71	B:LEU	73		134.25	0.00	0.00	71	A:LYS	75		115.00	8.09 |	-0.09
72	B:TYR	74		100.92	21.21 |||	-0.24	72	A:VAL	76		21.42	20.92 ||||||||	0.33
73	B:THR	75		77.39	0.00	0.00	73	A:GLU	77	HS	62.72	48.61 |||||||	-0.23
74	B:TYR	76		16.89	2.68 ||	0.04	74	A:ASN	78		27.92	0.00	0.00
75	B:PRO	77		49.69	40.74 ||||||||	0.61	75	A:HIS	79	S	23.16	21.20 |||||||||	1.14
76	B:VAL	78		14.01	0.00	0.00	76	A:THR	80		71.26	0.00	0.00
77	B:ALA	79		8.02	0.00	0.00	77	A:ALA	81		31.07	0.00	0.00
78	B:THR	80		69.78	0.00	0.00	78	A:CYS	82		24.98	0.00	0.00
79	B:GLN	81		99.29	0.00	0.00	79	A:HIS	83		68.66	0.00	0.00
80	B:CYS	82		22.23	0.00	0.00	80	A:CYS	84		54.38	0.00	0.00
81	B:HIS	83		59.06	0.00	0.00	81	A:SER	85		31.74	1.44 |	0.02
82	B:CYS	84		38.90	0.00	0.00	82	A:THR	86		95.96	36.49 ||||	0.58
83	B:GLY	85		13.80	0.00	0.00	83	A:CYS	87		44.98	15.72 ||||	0.46

84	B:LYS	86		127.23	0.00		0.00	84	A:TYR	88	H	137.22	28.22	||| -0.06
85	B:CYS	87		33.33	6.53	||	0.10	85	A:TYR	89		190.87	108.19	|||||| 1.59
86	B:ASP	88		72.43	0.00		0.00	86	A:HIS	90		137.18	115.08	|||||||| 1.75
87	B:SER	89	H	88.61	21.52	|||	-0.25							
88	B:ASP	90		136.24	3.11	|	0.05							
89	B:SER	91	H	80.36	44.98	||||||	-0.16							
90	B:THR	92	H	44.27	43.04	||||||||	0.53							
91	B:ASP	93	H	120.07	77.87	|||||||	0.27							
92	B:CYS	94		65.19	16.84	|||	0.27							
93	B:THR	95	H	73.08	40.28	||||||	-0.37							
94	B:VAL	96		157.53	83.13	||||||	0.81							
95	B:ARG	97		212.15	17.07	|	0.08							
96	B:GLY	98	H	45.83	25.76	||||||	0.14							
97	B:LEU	99	H	140.39	64.68	|||||	0.95							
98	B:GLY	100	H	39.61	29.56	||||||||	0.15							
99	B:PRO	101		83.27	62.13	||||||||	0.83							
100	B:SER	102		68.06	0.00		0.00							
101	B:TYR	103		105.97	45.37	|||||	-0.06							
102	B:CYS	104		23.53	0.00		0.00							
103	B:SER	105		24.56	17.02	||||||	0.13							
104	B:PHE	106		118.65	0.00		0.00							
105	B:GLY	107		29.87	0.98	|	-0.01							
106	B:GLU	108	S	100.08	54.14	||||||	-0.29							
107	B:MET	109	H	218.69	34.29	||	0.19							

Table S2. Interfaces in PDB 4mqw crystal.



Services | Research | Training | About us

Protein Data Bank in Europe

PDBePISA

pdbe.org/pisa

PDB EMDataBank Unified Data Resource for 3DEM

Bringing Structure to Biology

Feedback Share

PISA Interface List.

Session Map (id=136-69-l42)

Start | Interfaces | Interface Search | Monomers | Assemblies

Interfaces in PDB 4mqw crystal.

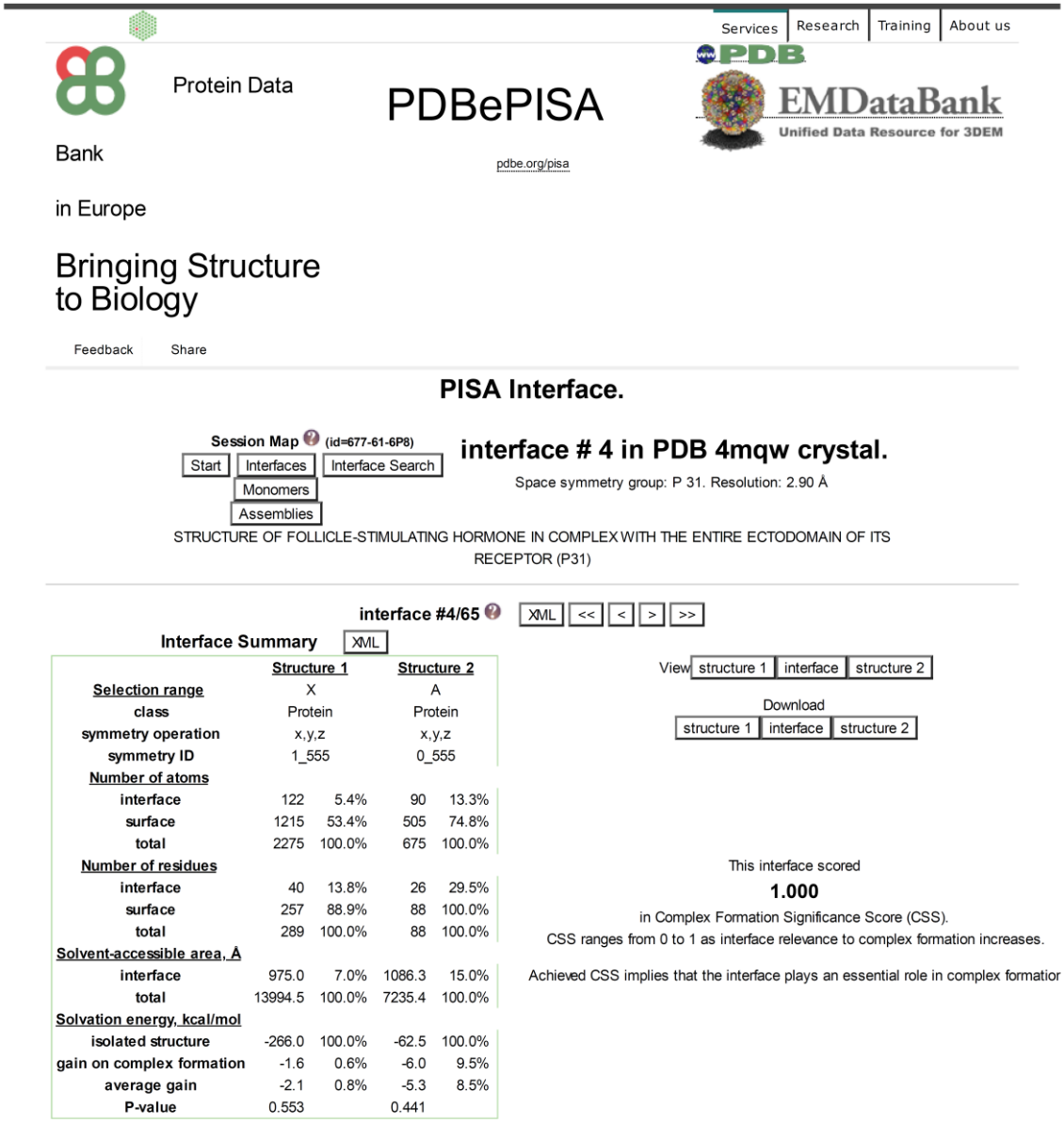
Space symmetry group: P 31. Resolution: 2.90 Å

STRUCTURE OF FOLLICLE-STIMULATING HORMONE IN COMPLEX WITH THE ENTIRE ECTODOMAIN OF ITS RECEPTOR (P31)

Interfaces | XML | View | Details | Download | Search

	##			Structure 1			×		Structure 2					interface	Δ^iG	Δ^iG	N_{HB}	N_{SB}	N_{DS}	
Id	NN	«»	Range	$^iN_{at}$	$^iN_{res}$	Surface Å^2		Range	Symmetry op-n	Sym.ID	$^iN_{at}$	$^iN_{res}$	Surface Å^2	area, Å^2	kcal/mol	P-value				
1	1	◉	E	244	58	8213	◊	D	x,y,z	1_555	238	57	7319	2268.6	-27.2	0.298	43	2	0	1
	2	○	B	239	56	8420	◊	A	x,y,z	1_555	231	58	7235	2234.6	-24.6	0.341	45	3	0	1
	3	○	H	237	55	8314	◊	G	x,y,z	1_555	224	54	7106	2195.2	-26.4	0.269	43	1	0	1
													Average:	2232.8	-26.1	0.303	44	2	0	1
2	4	○	X	122	40	13995	◊	A	x,y,z	1_555	90	26	7235	1030.7	-7.5	0.494	16	4	0	1
	5	○	Y	122	36	13547	◊	D	x,y,z	1_555	86	24	7319	976.7	-3.0	0.643	14	5	0	1
	6	○	Z	116	37	14142	◊	G	x,y,z	1_555	86	24	7106	937.7	-4.2	0.660	12	7	0	1
													Average:	981.7	-4.9	0.599	14	5	0	1
3	7	○	Z	102	35	14142	◊	H	x,y,z	1_555	92	23	8314	863.6	0.7	0.674	15	7	0	0
	8	○	X	91	34	13995	◊	B	x,y,z	1_555	81	22	8420	808.2	2.1	0.791	11	8	0	0
	9	○	Y	92	34	13547	◊	E	x,y,z	1_555	88	23	8213	795.2	-0.5	0.598	11	7	0	0
													Average:	822.4	0.8	0.688	12	7	0	0
4	10	○	Z	23	9	14142	◊	Y	x,y,z	1_555	30	9	13547	263.7	2.0	0.799	1	0	0	0
	11	○	Y	30	10	13547	◊	X	x,y,z	1_555	31	10	13995	258.7	0.4	0.644	2	0	0	0
	12	○	Z	33	10	14142	◊	X	x,y,z	1_555	27	9	13995	242.8	0.5	0.596	2	0	0	0
													Average:	255.0	0.9	0.680	2	0	0	0
5	13	○	Y	25	7	13547	◊	H	x,y,z	1_555	30	9	8314	256.8	-0.7	0.567	2	2	0	0
	14	○	X	25	7	13995	◊	E	x,y,z	1_555	27	9	8213	233.7	-1.6	0.476	2	0	0	0
	15	○	Z	21	7	14142	◊	B	x,y,z	1_555	27	9	8420	223.3	-1.4	0.478	2	1	0	0
													Average:	237.9	-1.3	0.507	2	1	0	0
6	16	○	A	25	9	7235	◊	Y	x,y-1,z	1_545	26	7	13547	226.2	-3.2	0.283	0	0	0	0
	17	○	X	25	6	13995	◊	G	x-1,y-1,z	1_445	21	8	7106	215.9	-3.3	0.282	0	0	0	0
	18	○	D	21	9	7319	◊	Z	x-1,y,z	1_455	23	7	14142	206.6	-3.3	0.265	0	0	0	0
													Average:	216.2	-3.3	0.276	0	0	0	0
7	19	○	[NAG]A:202	13	1	362	cf	A	x,y,z	1_555	19	10	7235	172.1	4.1	0.459	1	0	0	0
	20	○	[NAG]G:202	13	1	363	cf	G	x,y,z	1_555	18	9	7106	171.3	3.8	0.438	1	0	0	0
	21	○	[NAG]D:202	13	1	362	cf	D	x,y,z	1_555	18	9	7319	170.9	4.0	0.436	1	0	0	0
													Average:	171.5	4.0	0.444	1	0	0	0
8	22	○	[NAG]Z:402	11	1	362	cf	Z	x,y,z	1_555	17	7	14142	144.0	3.2	0.373	2	0	0	0
9	23	○	[NAG]Y:402	11	1	362	cf	Y	x,y,z	1_555	14	7	13547	143.6	3.4	0.387	2	0	0	0
	24	○	[NAG]X:403	11	1	364	cf	X	x,y,z	1_555	16	7	13995	138.6	3.4	0.401	1	0	0	0
													Average:	141.1	3.4	0.394	2	0	0	0
10	25	○	Z	21	4	14142	◊	B	-y,x-y,z+1/3	2_555	14	4	8420	136.0	-0.3	0.594	2	0	0	0
11	26	○	[JEF]Z:401	8	1	283	f	Z	x,y,z	1_555	21	7	14142	132.2	-0.2	0.519	0	0	0	0
12	27	○	X	16	5	13995	◊	E	-y,x-y,z+1/3	2_555	12	3	8213	113.9	-0.5	0.512	0	0	0	0
13	28	○	Y	10	4	13547	◊	Z	-y,x-y,z+1/3	2_555	16	6	14142	100.4	-0.5	0.486	0	0	0	0
14	29	○	[NAG]E:201	10	1	357	cf	E	x,y,z	1_555	12	4	8213	95.9	2.0	0.281	0	0	0	0
15	30	○	[EDO]X:401	4	1	186	◊	X	x,y,z	1_555	12	8	13995	94.4	3.1	0.516	3	0	0	0
16	31	○	[NAG]B:201	9	1	359	cf	B	x,y,z	1_555	10	4	8420	90.7	2.6	0.366	0	0	0	0
17	32	○	[NAG]E:202	8	1	365	cf	E	x,y,z	1_555	12	5	8213	89.6	2.9	0.474	0	0	0	0
18	33	○	[EDO]Y:401	4	1	185	f	Y	x,y,z	1_555	16	7	13547	89.0	3.0	0.307	0	0	0	0
19	34	○	[NAG]A:201	9	1	358	◊	B	x,y,z	1_555	14	3	8420	88.6	1.5	0.287	1	0	0	0
20	35	○	[EDO]X:402	4	1	185	f	X	x,y,z	1_555	14	7	13995	88.3	2.5	0.293	0	0	0	0
21	36	○	[NAG]D:201	9	1	360	◊	E	x,y,z	1_555	14	4	8213	88.1	1.5	0.295	1	0	0	0
	37	○	[NAG]G:201	9	1	359	◊	H	x,y,z	1_555	12	3	8314	82.4	1.4	0.268	0	0	0	0
													Average:	85.3	1.5	0.281	1	0	0	0
22	38	○	[NAG]H:202	8	1	361	cf	H	x,y,z	1_555	11	5	8314	86.9	3.1	0.453	0	0	0	0
23	39	○	[NAG]D:202	6	1	362	◊	Z	x-1,y,z	1_455	12	3	14142	83.3	0.9	0.319	0	0	0	0
	40	○	X	12	4	13995	◊	[NAG]G:202	x-1,y-1,z	1_445	6	1	363	80.3	0.9	0.328	0	0	0	0

	41	○ [NAG]A:202	6	1	362	o	Y	x,y-1,z	1_545	12	4	13547	79.4	0.8	0.323	0	0	0	0
												Average:	81.0	0.9	0.323	0	0	0	0
24	42	○ [NAG]B:202	9	1	360	cf	B	x,y,z	1_555	8	4	8420	80.3	1.8	0.318	0	0	0	0
25	43	○ X	11	5	13995	o	H	-y,x-y,z+1/3	2_555	8	2	8314	80.3	-1.8	0.235	0	0	0	0
26	44	○ [NAG]D:201	8	1	360	cf	D	x,y,z	1_555	8	4	7319	78.0	2.3	0.328	2	0	0	0
27	45	○ [NAG]G:201	9	1	359	cf	G	x,y,z	1_555	9	4	7106	77.8	2.2	0.273	2	0	0	0
	46	○ [NAG]A:201	8	1	358	cf	A	x,y,z	1_555	7	4	7235	71.9	2.5	0.324	2	0	0	0
												Average:	74.8	2.4	0.298	2	0	0	0
28	47	○ [NAG]H:201	9	1	361	cf	H	x,y,z	1_555	10	5	8314	77.2	2.4	0.328	0	0	0	0
29	48	○ [EDO]B:203	4	1	187	o	B	x,y,z	1_555	13	6	8420	69.4	1.9	0.845	0	0	0	0
30	49	○ Z	8	2	14142	f	[EDO]B:203	-y,x-y,z+1/3	2_555	4	1	187	49.2	1.5	0.791	0	0	0	0
31	50	○ [NAG]G:201	6	1	359	o	Y	x,y,z	1_555	7	2	13547	47.6	1.2	0.267	2	0	0	0
	51	○ [NAG]D:201	4	1	360	o	X	x,y,z	1_555	4	2	13995	39.1	1.1	0.350	2	0	0	0
												Average:	43.4	1.2	0.308	2	0	0	0
32	52	○ [EDO]B:204	4	1	185	f	B	x,y,z	1_555	3	2	8420	44.7	1.3	0.938	1	0	0	0
33	53	○ [NAG]A:201	5	1	358	o	Z	x,y,z	1_555	7	2	14142	41.3	0.8	0.263	2	0	0	0
34	54	○ [NAG]A:202	8	1	362	o	D	x,y-1,z	1_545	3	2	7319	38.3	2.1	0.273	0	0	0	0
	55	○ [NAG]D:202	4	1	362	o	G	x-1,y,z	1_455	2	1	7106	16.7	0.9	0.416	0	0	0	0
	56	○ A	2	2	7235	o	[NAG]G:202	x-1,y-1,z	1_445	4	1	363	12.6	0.7	0.378	0	0	0	0
												Average:	22.5	1.3	0.356	0	0	0	0
35	57	○ X	9	4	13995	o	B	-y,x-y,z+1/3	2_555	3	2	8420	37.8	0.3	0.599	0	0	0	0
36	58	○ D	4	2	7319	o	G	x-1,y,z	1_455	2	1	7106	27.4	0.9	0.705	0	0	0	0
	59	○ A	4	2	7235	o	D	x,y-1,z	1_545	1	1	7319	26.9	0.7	0.668	0	0	0	0
	60	○ A	2	1	7235	o	G	x-1,y-1,z	1_445	3	2	7106	25.6	0.7	0.639	0	0	0	0
												Average:	26.6	0.8	0.671	0	0	0	0
37	61	○ [NAG]B:202	1	1	360	f	[NAG]B:201	x,y,z	1_555	2	1	359	24.1	1.1	0.415	0	0	0	0
38	62	○ [NAG]E:202	2	1	365	f	[NAG]E:201	x,y,z	1_555	1	1	357	11.9	0.8	0.439	0	0	0	0
39	63	○ Y	3	1	13547	o	H	-y,x-y,z+1/3	2_555	4	1	8314	8.7	-0.1	0.540	0	0	0	0
40	64	○ [EDO]X:401	1	1	186	f	A	x,y,z	1_555	2	1	7235	4.7	0.1	0.835	0	0	0	0
41	65	○ X	1	1	13995	o	Y	-y,x-y,z+1/3	2_555	1	1	13547	2.2	-0.0	0.548	0	0	0	0



Services | Research | Training | About us

Protein Data Bank in Europe

PDBePISA

pdbe.org/pisa

PDB

EMDataBank
Unified Data Resource for 3DEM

Bringing Structure to Biology

Feedback Share

PISA Interface.

Session Map (id=677-61-6P8)

Start | Interfaces | Interface Search | Monomers | Assemblies

interface # 4 in PDB 4mqw crystal.

Space symmetry group: P 31. Resolution: 2.90 Å

STRUCTURE OF FOLLICLE-STIMULATING HORMONE IN COMPLEX WITH THE ENTIRE ECTODOMAIN OF ITS RECEPTOR (P31)

interface #4/65 XML << < > >>

Interface Summary XML

	Structure 1		Structure 2	
Selection range	X		A	
class	Protein		Protein	
symmetry operation	x,y,z		x,y,z	
symmetry ID	1_555		0_555	
Number of atoms				
interface	122	5.4%	90	13.3%
surface	1215	53.4%	505	74.8%
total	2275	100.0%	675	100.0%
Number of residues				
interface	40	13.8%	26	29.5%
surface	257	88.9%	88	100.0%
total	289	100.0%	88	100.0%
Solvent-accessible area, Å				
interface	975.0	7.0%	1086.3	15.0%
total	13994.5	100.0%	7235.4	100.0%
Solvation energy, kcal/mol				
isolated structure	-266.0	100.0%	-62.5	100.0%
gain on complex formation	-1.6	0.6%	-6.0	9.5%
average gain	-2.1	0.8%	-5.3	8.5%
P-value	0.553		0.441	

View structure 1 | interface | structure 2

Download structure 1 | interface | structure 2

This interface scored

1.000

in Complex Formation Significance Score (CSS).

CSS ranges from 0 to 1 as interface relevance to complex formation increases.

Achieved CSS implies that the interface plays an essential role in complex formatior

Hydrogen bonds [XML]

##	Structure 1	Dist. [Å]	Structure 2
1	X:ASN 106[ND2]	3.39	A:LYS 45[O]
2	X:ASN 106[N]	3.29	A:THR 46[O]
3	X:ASN 129[ND2]	3.02	A:VAL 49[O]
4	X:LYS 74[NZ]	3.03	A:SER 85[OG]
5	X:LYS 74[NZ]	3.63	A:THR 86[OG1]
6	X:TYS 335[O2]	2.99	A:ASN 15[ND2]
7	X:TYS 335[O2]	3.54	A:GLN 27[NE2]
8	X:TYS 335[O3]	3.19	A:GLN 27[NE2]
9	X:ASP 81[OD2]	2.81	A:ARG 42[NH1]
10	X:ASP 81[OD2]	2.84	A:ARG 42[NH2]
11	X:GLN 79[OE1]	2.72	A:SER 43[OG]
12	X:ASN 129[OD1]	3.01	A:LEU 48[N]
13	X:ASN 129[OD1]	2.81	A:VAL 49[N]
14	X:ASP 153[OD1]	3.17	A:LYS 51[NZ]
15	X:GLN 145[OE1]	3.87	A:TYR 65[OH]
16	X:GLU 99[OE1]	3.32	A:TYR 88[OH]

Salt bridges [XML]

##	Structure 1	Dist. [Å]	Structure 2
1	X:ASP 81[OD2]	2.81	A:ARG 42[NH1]
2	X:ASP 81[OD2]	2.84	A:ARG 42[NH2]
3	X:ASP 153[OD1]	3.17	A:LYS 51[NZ]
4	X:ASP 153[OD2]	3.32	A:LYS 51[NZ]

No disulfide bonds found

No covalent bonds found

Interfacing residues (not a contact table) [XML] Display level: Residues

Inaccessible residues — HSDC — Residues making **H**ydrogen/**D**isulphide bond, **S**alt bridge or **C**ovalent link

Solvent-accessible residues — Interfacing residues

ASA Accessible Surface Area, Å² **BSA** Buried Surface Area, Å² **ΔⁱG** Solvation energy effect, kcal/mol |||| Buried area percentage, one bar per 10%

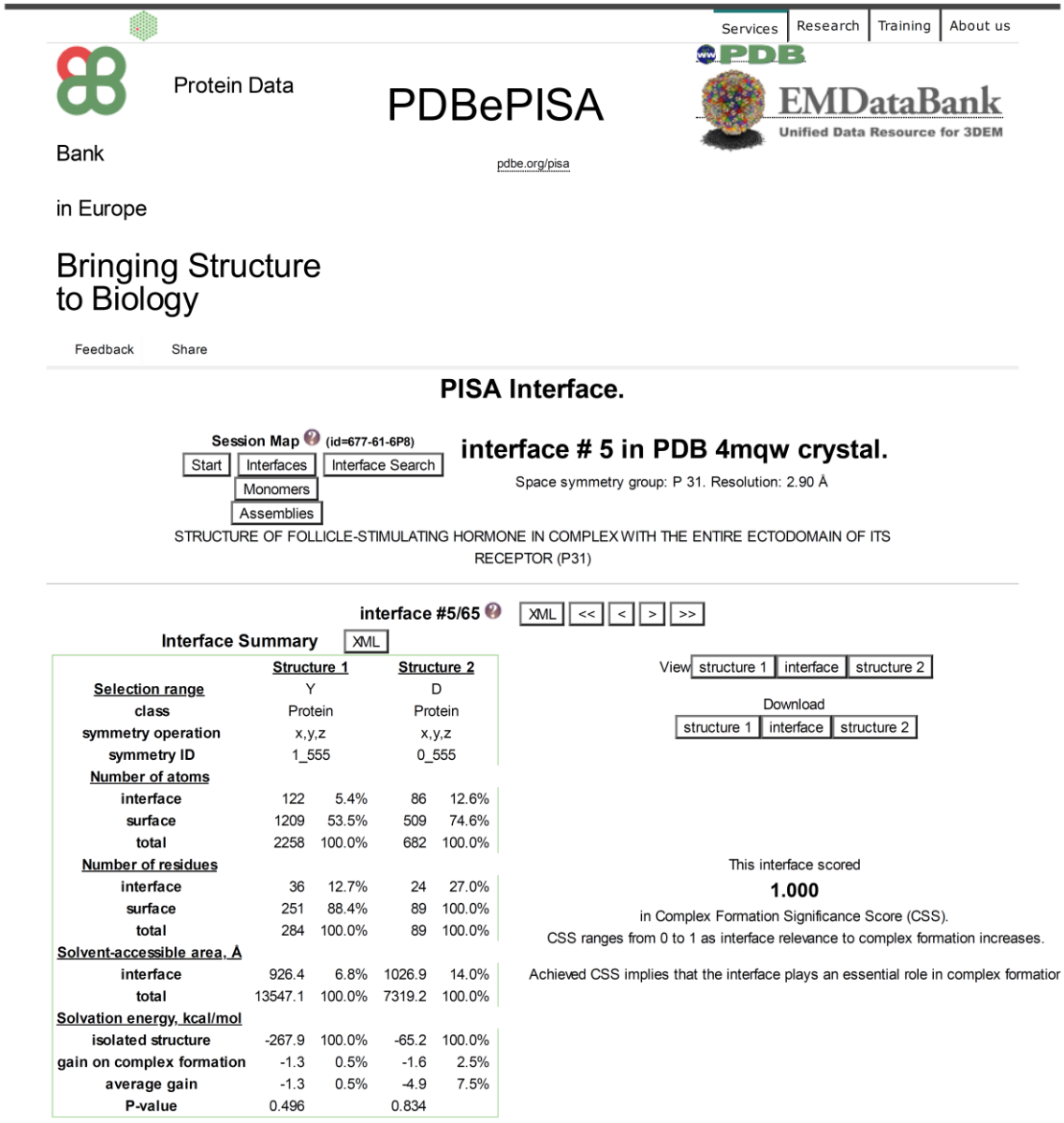
##	Structure 1	HSDC	ASA	BSA	ΔⁱG	##	Structure 2	HSDC	ASA	BSA	ΔⁱG
1	X:CYS 18		117.41	0.00	0.00	1	A:GLN 5		239.47	0.00	0.00
2	X:HIS 19		165.43	0.00	0.00	2	A:ASP 6		132.62	0.00	0.00
3	X:HIS 20		16.04	0.00	0.00	3	A:CYS 7		85.51	0.00	0.00
4	X:ARG 21		141.01	0.00	0.00	4	A:PRO 8		99.49	0.00	0.00
5	X:ILE 22		38.64	0.00	0.00	5	A:GLU 9		134.32	0.00	0.00
6	X:CYS 23		1.96	0.00	0.00	6	A:CYS 10		7.68	0.00	0.00
7	X:HIS 24		102.08	0.00	0.00	7	A:THR 11		66.48	0.00	0.00
8	X:CYS 25		19.34	0.00	0.00	8	A:LEU 12		51.74	0.00	0.00
9	X:SER 26		67.76	0.00	0.00	9	A:GLN 13		89.90	0.00	0.00
10	X:ASN 27		131.63	0.00	0.00	10	A:GLU 14		113.33	0.00	0.00
11	X:ARG 28		95.77	0.00	0.00	11	A:ASN 15	H	21.63	15.87 |||||||	-0.18
12	X:VAL 29		31.93	0.00	0.00	12	A:PRO 16		122.46	0.00	0.00
13	X:PHE 30		4.22	0.00	0.00	13	A:LEU 17		133.37	54.84 |||||	0.88
14	X:LEU 31		34.30	0.00	0.00	14	A:PHE 18		53.15	23.61 |||||	0.38
15	X:CYS 32		0.00	0.00	0.00	15	A:SER 19		13.60	0.00	0.00
16	X:GLN 33		53.36	0.00	0.00	16	A:GLN 20		118.64	0.00	0.00
17	X:GLU 34		76.97	0.00	0.00	17	A:PRO 21		128.12	0.00	0.00
18	X:SER 35		65.12	4.11 |	-0.05	18	A:GLY 22		87.95	0.00	0.00
19	X:LYS 36		114.91	0.00	0.00	19	A:ALA 23		57.30	0.00	0.00
20	X:VAL 37		0.00	0.00	0.00	20	A:PRO 24		53.39	0.00	0.00
21	X:THR 38		78.40	0.00	0.00	21	A:ILE 25		7.53	0.00	0.00
22	X:GLU 39		108.01	0.00	0.00	22	A:LEU 26		61.96	0.00	0.00
23	X:ILE 40		18.44	0.00	0.00	23	A:GLN 27	H	62.27	18.55 |||	-0.20
24	X:PRO 41		7.37	0.00	0.00	24	A:CYS 28		12.63	0.00	0.00
25	X:SER 42		102.92	0.00	0.00	25	A:MET 29		74.55	0.00	0.00
26	X:ASP 43		66.04	0.00	0.00	26	A:GLY 30		36.65	0.00	0.00
27	X:LEU 44		6.23	0.00	0.00	27	A:CYS 31		33.45	0.00	0.00
28	X:PRO 45		50.57	0.00	0.00	28	A:CYS 32		31.91	0.00	0.00
29	X:ARG 46		117.44	0.00	0.00	29	A:PHE 33		153.33	0.00	0.00
30	X:ASN 47		71.77	0.00	0.00	30	A:SER 34		66.84	0.00	0.00
31	X:ALA 48		0.00	0.00	0.00	31	A:ARG 35		123.74	0.00	0.00
32	X:ILE 49		40.68	0.84 |	0.01	32	A:ALA 36		71.72	0.00	0.00
33	X:GLU 50		27.95	0.00	0.00	33	A:TYR 37		65.05	0.00	0.00
34	X:LEU 51		0.17	0.00	0.00	34	A:PRO 38		110.22	0.00	0.00
35	X:ARG 52		83.22	0.00	0.00	35	A:THR 39		9.54	0.00	0.00
36	X:PHE 53		0.78	0.00	0.00	36	A:PRO 40		68.88	0.00	0.00
37	X:VAL 54		16.75	0.00	0.00	37	A:LEU 41		137.97	0.00	0.00
38	X:LEU 55		77.49	42.42 ||||||	0.64	38	A:ARG 42	HS	165.44	91.62 ||||||	-0.46
39	X:THR 56		0.98	0.49 |||||	-0.01	39	A:SER 43	H	41.95	22.95 ||||||	0.04
40	X:LYS 57		76.97	13.09 ||	0.08	40	A:LYS 44		53.57	0.00	0.00

41	X:LEU	58		0.33	0.00	0.00	41	A:LYS	45	H	161.80	24.42 ||	-0.18
42	X:ARG	59		151.06	0.00	0.00	42	A:THR	46	H	106.13	106.13 |||||||||	0.51
43	X:VAL	60		52.85	0.00	0.00	43	A:MET	47		40.41	29.39 |||||||	0.68
44	X:ILE	61		0.67	0.00	0.00	44	A:LEU	48	H	183.03	119.63 ||||||	1.71
45	X:GLN	62		68.32	0.00	0.00	45	A:VAL	49	H	102.57	65.98 ||||||	0.90
46	X:LYS	63		128.72	0.00	0.00	46	A:GLN	50		105.04	0.00	0.00
47	X:GLY	64		32.05	0.00	0.00	47	A:LYS	51	HS	116.64	46.44 ||||	-0.52
48	X:ALA	65		22.92	0.00	0.00	48	A:ASN	52		99.46	0.00	0.00
49	X:PHE	66		0.78	0.00	0.00	49	A:VAL	53		105.04	0.00	0.00
50	X:SER	67		27.75	0.00	0.00	50	A:THR	54		36.23	0.00	0.00
51	X:GLY	68		42.87	0.00	0.00	51	A:SER	55		81.02	0.00	0.00
52	X:PHE	69		2.82	0.00	0.00	52	A:GLU	56		75.90	0.00	0.00
53	X:GLY	70		32.66	0.00	0.00	53	A:SER	57		42.97	0.00	0.00
54	X:ASP	71		45.91	0.00	0.00	54	A:THR	58		37.27	0.00	0.00
55	X:LEU	72		0.00	0.00	0.00	55	A:CYS	59		43.46	0.00	0.00
56	X:GLU	73		58.33	21.09 ||||	-0.24	56	A:CYS	60		28.85	0.00	0.00
57	X:LYS	74	H	63.94	35.94 ||||||	-0.32	57	A:VAL	61		53.32	0.00	0.00
58	X:ILE	75		1.22	0.00	0.00	58	A:ALA	62		27.43	0.00	0.00
59	X:GLU	76		25.86	0.00	0.00	59	A:LYS	63		128.57	20.47 ||	0.08
60	X:ILE	77		0.17	0.00	0.00	60	A:SER	64		49.94	0.00	0.00
61	X:SER	78		3.15	0.00	0.00	61	A:TYR	65	H	83.31	14.51 ||	-0.11
62	X:GLN	79	H	82.45	42.40 ||||||	-0.00	62	A:ASN	66		92.14	0.00	0.00
63	X:ASN	80		0.78	0.46 ||||||	0.00	63	A:ARG	67		170.73	15.28 |	-0.23
64	X:ASP	81	HS	58.65	42.15 ||||||||	-0.11	64	A:VAL	68		50.10	0.00	0.00
65	X:VAL	82		43.99	0.00	0.00	65	A:THR	69		89.82	0.00	0.00
66	X:LEU	83		0.17	0.00	0.00	66	A:VAL	70		28.57	0.00	0.00
67	X:GLU	84		61.99	0.00	0.00	67	A:MET	71		144.53	56.11 ||||	1.28
68	X:VAL	85		43.16	0.00	0.00	68	A:GLY	72		87.45	0.00	0.00
69	X:ILE	86		0.00	0.00	0.00	69	A:GLY	73		54.07	0.00	0.00
70	X:GLU	87		61.82	0.00	0.00	70	A:PHE	74		89.86	16.25 ||	0.26
71	X:ALA	88		11.18	0.00	0.00	71	A:LYS	75		179.90	0.00	0.00
72	X:ASP	89		56.55	0.00	0.00	72	A:VAL	76		21.74	0.98 |	0.02
73	X:VAL	90		0.00	0.00	0.00	73	A:GLU	77		70.41	0.00	0.00
74	X:PHE	91		0.00	0.00	0.00	74	A:ASN	78		40.82	0.00	0.00
75	X:SER	92		9.18	0.00	0.00	75	A:HIS	79		27.75	0.00	0.00
76	X:ASN	93		105.91	0.00	0.00	76	A:THR	80		72.14	0.00	0.00
77	X:LEU	94		1.92	0.00	0.00	77	A:ALA	81		36.08	0.00	0.00
78	X:PRO	95		78.79	0.00	0.00	78	A:CYS	82		31.31	0.00	0.00
79	X:LYS	96		106.98	0.00	0.00	79	A:HIS	83		64.63	5.82 |	-0.22
80	X:LEU	97		0.00	0.00	0.00	80	A:CYS	84		53.38	0.00	0.00
81	X:HIS	98		35.96	6.74 ||	0.11	81	A:SER	85	H	37.33	20.49 ||||||	-0.23
82	X:GLU	99	H	21.31	20.94 ||||||||	-0.33	82	A:THR	86	H	86.71	56.50 ||||||	0.30
83	X:ILE	100		0.00	0.00	0.00	83	A:CYS	87		10.78	4.05 ||||	-0.05
84	X:ARG	101		51.99	14.70 |||	-0.11	84	A:TYR	88	H	154.81	117.22 |||||||	0.42
85	X:ILE	102		0.00	0.00	0.00	85	A:TYR	89		201.54	49.79 |||	0.54
86	X:GLU	103		24.62	0.00	0.00	86	A:HIS	90		95.16	0.00	0.00
87	X:LYS	104		75.54	35.26 |||||	0.49	87	A:LYS	91		167.35	76.09 |||||	0.36
88	X:ALA	105		0.00	0.00	0.00	88	A:SER	92		168.49	13.31 |	-0.02
89	X:ASN	106	H	98.48	64.23 |||||||	0.36							
90	X:ASN	107		65.03	0.00	0.00							
91	X:LEU	108		0.00	0.00	0.00							
92	X:LEU	109		87.05	0.17 |	0.00							
93	X:TYR	110		111.98	0.00	0.00							
94	X:ILE	111		22.81	0.00	0.00							
95	X:ASN	112		36.77	0.00	0.00							
96	X:PRO	113		69.35	0.00	0.00							
97	X:GLU	114		65.94	0.00	0.00							
98	X:ALA	115		0.00	0.00	0.00							
99	X:PHE	116		0.61	0.00	0.00							
100	X:GLN	117		31.41	0.00	0.00							
101	X:ASN	118		89.74	0.00	0.00							
102	X:LEU	119		0.00	0.00	0.00							
103	X:PRO	120		32.62	0.00	0.00							
104	X:ASN	121		52.49	0.00	0.00							
105	X:LEU	122		0.00	0.00	0.00							

106	X:GLN 123		78.52	17.37	|||	-0.09
107	X:TYR 124		56.32	53.99	||||||||||	0.42
108	X:LEU 125		0.00	0.00		0.00
109	X:LEU 126		18.40	12.56	|||||||	0.20
110	X:ILE 127		0.00	0.00		0.00
111	X:SER 128		19.44	2.01	||	0.03
112	X:ASN 129	H	79.38	74.09	|||||||||	-0.91
113	X:THR 130		6.42	6.42	||||||||||	-0.02
114	X:GLY 131		5.69	5.69	||||||||||	0.09
115	X:ILE 132		1.84	0.00		0.00
116	X:LYS 133		103.06	0.00		0.00
117	X:HIS 134		116.06	0.00		0.00
118	X:LEU 135		28.08	0.00		0.00
119	X:PRO 136		6.39	0.00		0.00
120	X:ASP 137		40.32	0.00		0.00
121	X:VAL 138		1.04	0.00		0.00
122	X:HIS 139		76.69	0.00		0.00
123	X:LYS 140		68.01	0.00		0.00
124	X:ILE 141		0.00	0.00		0.00
125	X:HIS 142		74.76	0.00		0.00
126	X:SER 143		0.00	0.00		0.00
127	X:LEU 144		113.01	0.00		0.00
128	X:GLN 145	H	56.52	26.35	|||||	-0.41
129	X:LYS 146		124.02	0.00		0.00
130	X:VAL 147		3.24	0.00		0.00
131	X:LEU 148		35.97	30.63	|||||||||	0.49
132	X:LEU 149		0.17	0.00		0.00
133	X:ASP 150		8.71	8.71	||||||||||	0.08
134	X:ILE 151		0.00	0.00		0.00
135	X:GLN 152		41.14	21.68	||||||	-0.22
136	X:ASP 153	HS	53.59	38.85	|||||||	-0.31
137	X:ASN 154		0.00	0.00		0.00
138	X:ILE 155		125.97	48.10	||||	0.77
139	X:ASN 156		39.39	7.42	||	-0.08
140	X:ILE 157		0.33	0.00		0.00
141	X:HIS 158		75.11	0.00		0.00
142	X:THR 159		36.76	0.00		0.00
143	X:ILE 160		0.00	0.00		0.00
144	X:GLU 161		85.53	0.00		0.00
145	X:ARG 162		165.10	0.00		0.00
146	X:ASN 163		46.44	0.00		0.00
147	X:SER 164		25.88	0.00		0.00
148	X:PHE 165		4.42	0.00		0.00
149	X:VAL 166		50.44	0.00		0.00
150	X:GLY 167		15.24	0.00		0.00
151	X:LEU 168		0.52	0.00		0.00
152	X:SER 169		23.80	0.00		0.00
153	X:PHE 170		136.08	0.00		0.00
154	X:GLU 171		66.06	0.00		0.00
155	X:SER 172		7.94	0.00		0.00
156	X:VAL 173		5.67	0.00		0.00
157	X:ILE 174		47.63	15.56	||||	0.25
158	X:LEU 175		0.00	0.00		0.00
159	X:TRP 176		70.77	42.86	|||||||	0.69
160	X:LEU 177		0.00	0.00		0.00
161	X:ASN 178		12.65	6.55	||||||	-0.07
162	X:LYS 179		86.60	12.89	||	-0.48
163	X:ASN 180		8.95	0.00		0.00
164	X:GLY 181		8.20	0.00		0.00
165	X:ILE 182		0.00	0.00		0.00
166	X:GLN 183		79.83	0.00		0.00
167	X:GLU 184		100.82	0.00		0.00
168	X:ILE 185		6.46	0.00		0.00
169	X:HIS 186		77.74	0.00		0.00
170	X:ASN 187		70.65	0.00		0.00

171	X:SER 188	17.73	0.00	0.00
172	X:ALA 189	0.00	0.00	0.00
173	X:PHE 190	0.00	0.00	0.00
174	X:ASN 191	49.38	0.00	0.00
175	X:GLY 192	43.55	0.00	0.00
176	X:THR 193	13.94	0.00	0.00
177	X:GLN 194	82.42	0.00	0.00
178	X:LEU 195	3.13	0.00	0.00
179	X:ASP 196	44.38	0.00	0.00
180	X:GLU 197	33.79	0.00	0.00
181	X:LEU 198	0.74	0.00	0.00
182	X:ASN 199	24.88	6.40 |||	-0.07
183	X:LEU 200	0.17	0.00	0.00
184	X:SER 201	3.44	0.00	0.00
185	X:ASP 202	37.50	0.00	0.00
186	X:ASN 203	0.84	0.00	0.00
187	X:ASN 204	83.66	0.00	0.00
188	X:ASN 205	60.70	0.00	0.00
189	X:LEU 206	0.17	0.00	0.00
190	X:GLU 207	70.33	0.00	0.00
191	X:GLU 208	105.96	0.00	0.00
192	X:LEU 209	11.35	0.00	0.00
193	X:PRO 210	23.77	0.00	0.00
194	X:ASN 211	84.55	0.00	0.00
195	X:ASP 212	62.70	0.00	0.00
196	X:VAL 213	0.33	0.00	0.00
197	X:PHE 214	4.64	0.00	0.00
198	X:HIS 215	94.02	0.00	0.00
199	X:GLY 216	41.75	0.00	0.00
200	X:ALA 217	18.58	0.00	0.00
201	X:SER 218	62.10	0.00	0.00
202	X:GLY 219	3.38	0.00	0.00
203	X:PRO 220	0.17	0.00	0.00
204	X:VAL 221	53.88	0.00	0.00
205	X:ILE 222	39.84	0.00	0.00
206	X:LEU 223	0.00	0.00	0.00
207	X:ASP 224	22.05	0.00	0.00
208	X:ILE 225	0.00	0.00	0.00
209	X:SER 226	1.74	0.00	0.00
210	X:ARG 227	98.61	0.00	0.00
211	X:THR 228	6.83	0.00	0.00
212	X:ARG 229	100.35	0.00	0.00
213	X:ILE 230	0.00	0.00	0.00
214	X:HIS 231	91.24	0.00	0.00
215	X:SER 232	51.34	0.00	0.00
216	X:LEU 233	15.30	0.00	0.00
217	X:PRO 234	1.90	0.00	0.00
218	X:SER 235	75.23	0.00	0.00
219	X:TYR 236	79.03	0.00	0.00
220	X:GLY 237	2.01	0.00	0.00
221	X:LEU 238	4.89	0.00	0.00
222	X:GLU 239	85.37	0.00	0.00
223	X:ASN 240	66.91	0.00	0.00
224	X:LEU 241	0.00	0.00	0.00
225	X:LYS 242	88.31	0.00	0.00
226	X:LYS 243	48.45	0.00	0.00
227	X:LEU 244	0.27	0.00	0.00
228	X:ARG 245	75.08	0.00	0.00
229	X:ALA 246	2.16	0.00	0.00
230	X:ARG 247	100.10	0.00	0.00
231	X:SER 248	44.82	0.00	0.00
232	X:THR 249	1.27	0.00	0.00
233	X:TYR 250	132.42	0.00	0.00
234	X:ASN 251	47.21	0.00	0.00
235	X:LEU 252	9.22	0.00	0.00

236	X:LYS 253		133.11	0.00	0.00
237	X:LYS 254		150.57	0.00	0.00
238	X:LEU 255		32.64	0.00	0.00
239	X:PRO 256		23.71	0.00	0.00
240	X:THR 257		78.49	0.00	0.00
241	X:LEU 258		51.85	0.00	0.00
242	X:GLU 259		124.91	0.00	0.00
243	X:LYS 260		85.06	0.00	0.00
244	X:LEU 261		0.00	0.00	0.00
245	X:VAL 262		100.48	0.00	0.00
246	X:ALA 263		33.58	0.00	0.00
247	X:LEU 264		8.22	0.00	0.00
248	X:MET 265		76.48	0.00	0.00
249	X:GLU 266		45.27	0.00	0.00
250	X:ALA 267		1.29	0.00	0.00
251	X:SER 268		20.32	0.00	0.00
252	X:LEU 269		3.39	0.00	0.00
253	X:THR 270		27.67	0.00	0.00
254	X:TYR 271		53.44	0.00	0.00
255	X:PRO 272		26.30	0.00	0.00
256	X:SER 273		54.37	0.00	0.00
257	X:HIS 274		22.75	0.00	0.00
258	X:CYS 275		8.43	0.00	0.00
259	X:CYS 276		37.49	0.00	0.00
260	X:ALA 277		76.03	0.00	0.00
261	X:PHE 278		9.70	0.00	0.00
262	X:ALA 279		56.30	0.00	0.00
263	X:ASN 280		121.34	0.00	0.00
264	X:TRP 281		54.95	0.00	0.00
265	X:ARG 282		132.03	0.00	0.00
266	X:ILE 291		165.39	0.00	0.00
267	X:CYS 292		58.06	0.00	0.00
268	X:ASN 293		111.81	24.26 |||	0.05
269	X:LYS 294		142.04	22.00 ||	0.34
270	X:ASP 334		154.37	0.00	0.00
271	X:TYS 335	H	285.76	112.36 ||||	0.26
272	X:ASP 336		98.65	0.00	0.00
273	X:LEU 337		89.94	14.73 ||	0.24
274	X:CYS 338		133.42	18.49 ||	-0.19
275	X:VAL 342		205.83	0.00	0.00
276	X:ASP 343		58.65	0.00	0.00
277	X:VAL 344		23.35	0.00	0.00
278	X:THR 345		92.80	0.00	0.00
279	X:CYS 346		15.28	0.00	0.00
280	X:SER 347		31.08	0.00	0.00
281	X:PRO 348		36.93	0.00	0.00
282	X:LYS 349		153.42	0.00	0.00
283	X:PRO 350		47.86	0.00	0.00
284	X:ASP 351		120.71	0.00	0.00
285	X:ALA 352		100.21	0.00	0.00
286	X:PHE 353		129.97	0.00	0.00
287	X:ASN 354		53.47	0.00	0.00
288	X:PRO 355		108.21	0.00	0.00
289	X:CYS 356		109.92	0.00	0.00



	Structure 1		Structure 2	
Selection range	Y		D	
class	Protein		Protein	
symmetry operation	x,y,z		x,y,z	
symmetry ID	1_555		0_555	
Number of atoms				
interface	122	5.4%	86	12.6%
surface	1209	53.5%	509	74.6%
total	2258	100.0%	682	100.0%
Number of residues				
interface	36	12.7%	24	27.0%
surface	251	88.4%	89	100.0%
total	284	100.0%	89	100.0%
Solvent-accessible area, Å				
interface	926.4	6.8%	1026.9	14.0%
total	13547.1	100.0%	7319.2	100.0%
Solvation energy, kcal/mol				
isolated structure	-267.9	100.0%	-65.2	100.0%
gain on complex formation	-1.3	0.5%	-1.6	2.5%
average gain	-1.3	0.5%	-4.9	7.5%
P-value	0.496		0.834	

Hydrogen bonds XML

##	Structure 1	Dist. [Å]	Structure 2
1	Y:ASN 106[N]	3.41	D:THR 46[O]
2	Y:ASN 129[ND2]	2.82	D:VAL 49[O]
3	Y:LYS 74[NZ]	3.23	D:SER 85[OG]
4	Y:TYS 335[O1]	2.72	D:ASN 15[ND2]
5	Y:TYS 335[O1]	3.14	D:GLN 27[NE2]
6	Y:ASP 81[OD2]	3.10	D:ARG 42[NH1]
7	Y:GLN 79[OE1]	2.66	D:SER 43[OG]
8	Y:ASN 129[OD1]	3.09	D:LEU 48[N]
9	Y:ASN 129[OD1]	2.76	D:VAL 49[N]
10	Y:ASP 153[OD1]	2.93	D:LYS 51[NZ]
11	Y:GLN 145[OE1]	3.61	D:ARG 67[NH2]
12	Y:GLU 99[OE2]	3.48	D:THR 86[OG1]
13	Y:GLU 99[OE1]	3.47	D:TYR 88[OH]
14	Y:ASP 150[OD2]	2.75	D:LYS 91[NZ]

Salt bridges XML

##	Structure 1	Dist. [Å]	Structure 2
1	Y:ASP 81[OD2]	3.10	D:ARG 42[NH1]
2	Y:ASP 153[OD1]	2.93	D:LYS 51[NZ]
3	Y:ASP 153[OD2]	3.21	D:LYS 51[NZ]
4	Y:ASP 150[OD1]	3.62	D:LYS 91[NZ]
5	Y:ASP 150[OD2]	2.75	D:LYS 91[NZ]

No disulfide bonds found

No covalent bonds found

Interfacing residues (not a contact table) XML Display level: Residues

Inaccessible residues HSDC Residues making **H**ydrogen/**D**isulphide bond, **S**alt bridge or **C**ovalent link

Solvent-accessible residues Interfacing residues

ASA Accessible Surface Area, Å² **BSA** Buried Surface Area, Å² **Δ^iG** Solvation energy effect, kcal/mol |||| Buried area percentage, one bar per 10%

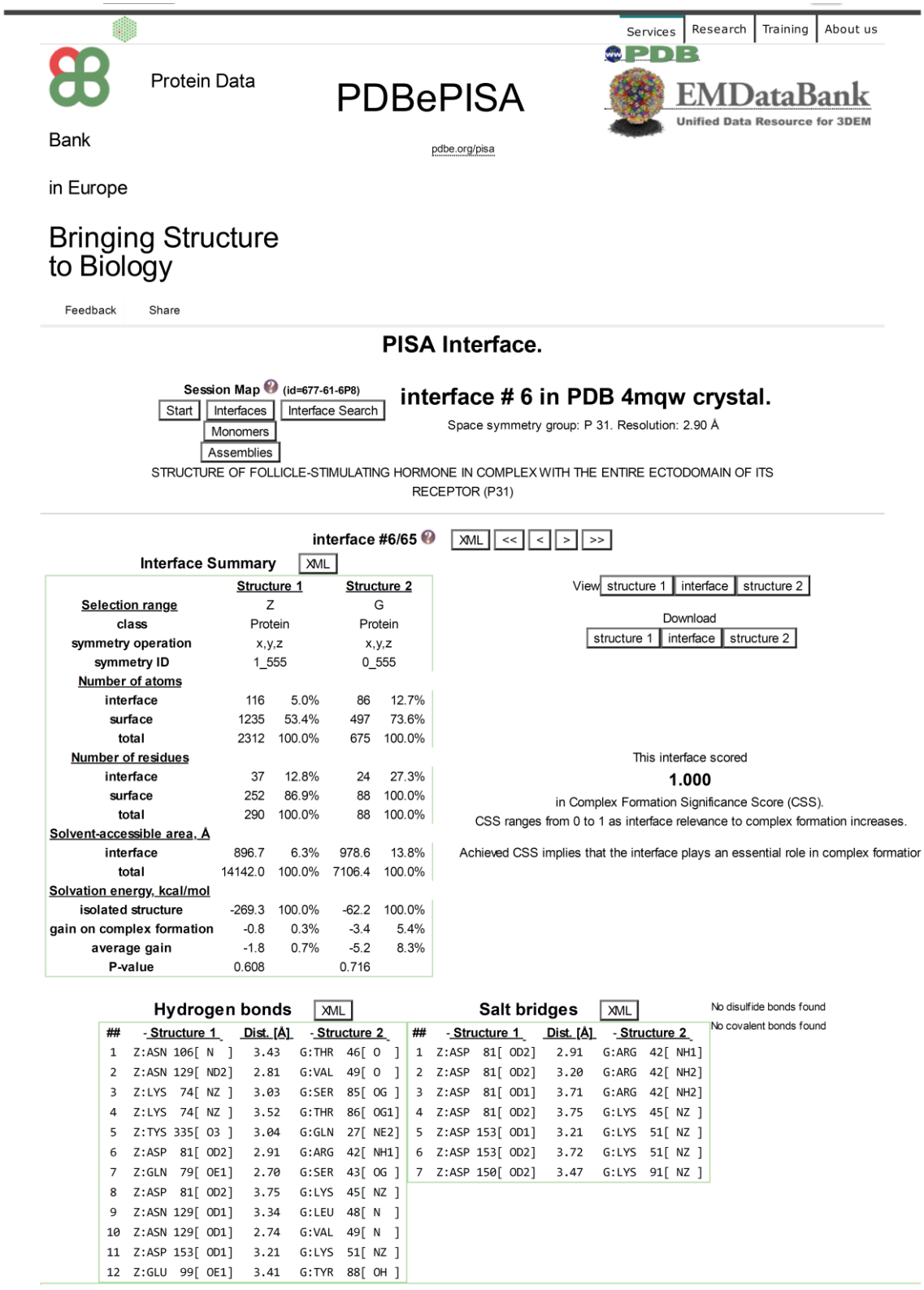
##	Structure 1	HSDC	ASA	BSA	Δ^iG	##	Structure 2	HSDC	ASA	BSA	Δ^iG
1	Y:CYS 18		116.02	0.00	0.00	1	D:VAL 4		205.59	0.00	0.00
2	Y:HIS 19		161.36	0.00	0.00	2	D:GLN 5		177.24	0.00	0.00
3	Y:HIS 20		15.73	0.00	0.00	3	D:ASP 6		129.63	0.00	0.00
4	Y:ARG 21		156.33	0.00	0.00	4	D:CYS 7		92.21	0.00	0.00
5	Y:ILE 22		35.96	0.00	0.00	5	D:PRO 8		97.84	0.00	0.00
6	Y:CYS 23		2.42	0.00	0.00	6	D:GLU 9		137.54	0.00	0.00
7	Y:HIS 24		97.25	0.00	0.00	7	D:CYS 10		15.01	0.00	0.00
8	Y:CYS 25		21.51	0.00	0.00	8	D:THR 11		67.99	0.00	0.00
9	Y:SER 26		79.07	0.00	0.00	9	D:LEU 12		53.36	0.00	0.00
10	Y:ASN 27		139.31	0.00	0.00	10	D:GLN 13		92.91	0.00	0.00
11	Y:ARG 28		99.27	0.00	0.00	11	D:GLU 14		117.47	0.00	0.00
12	Y:VAL 29		33.72	0.00	0.00	12	D:ASN 15	H	19.84	11.84 ||||||	-0.15
13	Y:PHE 30		3.90	0.00	0.00	13	D:PRO 16		124.10	0.00	0.00
14	Y:LEU 31		36.93	0.00	0.00	14	D:LEU 17		109.94	44.50 |||||	0.71
15	Y:CYS 32		0.16	0.00	0.00	15	D:PHE 18		49.69	18.83 ||||	0.30
16	Y:GLN 33		57.37	0.00	0.00	16	D:SER 19		19.73	0.00	0.00
17	Y:GLU 34		83.98	0.00	0.00	17	D:GLN 20		107.80	0.00	0.00
18	Y:SER 35		69.97	5.31 |	-0.06	18	D:PRO 21		126.81	0.00	0.00
19	Y:LYS 36		123.23	0.00	0.00	19	D:GLY 22		83.76	0.00	0.00
20	Y:VAL 37		0.84	0.00	0.00	20	D:ALA 23		54.99	0.00	0.00
21	Y:THR 38		84.84	0.00	0.00	21	D:PRO 24		54.51	0.00	0.00
22	Y:GLU 39		123.18	0.00	0.00	22	D:ILE 25		6.19	0.00	0.00
23	Y:ILE 40		20.95	0.00	0.00	23	D:LEU 26		60.16	0.00	0.00
24	Y:PRO 41		6.58	0.00	0.00	24	D:GLN 27	H	67.81	19.35 |||	-0.22
25	Y:SER 42		104.31	0.00	0.00	25	D:CYS 28		13.84	0.00	0.00
26	Y:ASP 43		72.40	0.00	0.00	26	D:MET 29		70.89	0.00	0.00
27	Y:LEU 44		3.08	0.00	0.00	27	D:GLY 30		38.18	0.00	0.00
28	Y:PRO 45		48.31	0.00	0.00	28	D:CYS 31		34.59	0.00	0.00
29	Y:ARG 46		122.20	0.00	0.00	29	D:CYS 32		33.16	0.00	0.00
30	Y:ASN 47		72.74	0.00	0.00	30	D:PHE 33		154.98	0.00	0.00
31	Y:ALA 48		0.00	0.00	0.00	31	D:SER 34		63.15	0.00	0.00
32	Y:ILE 49		37.50	0.00	0.00	32	D:ARG 35		128.14	0.00	0.00
33	Y:GLU 50		27.88	0.00	0.00	33	D:ALA 36		72.89	0.00	0.00
34	Y:LEU 51		0.00	0.00	0.00	34	D:TYR 37		66.19	0.00	0.00
35	Y:ARG 52		75.47	0.00	0.00	35	D:PRO 38		109.37	0.00	0.00
36	Y:PHE 53		0.62	0.00	0.00	36	D:THR 39		8.79	0.00	0.00
37	Y:VAL 54		18.75	0.00	0.00	37	D:PRO 40		67.54	0.00	0.00
38	Y:LEU 55		81.34	49.35 ||||||	0.74	38	D:LEU 41		144.60	0.00	0.00
39	Y:THR 56		0.12	0.00	0.00	39	D:ARG 42	HS	165.31	93.85 ||||||	-0.64
40	Y:LYS 57		74.45	16.75 |||	0.04	40	D:SER 43	H	41.44	23.53 ||||||	0.05
41	Y:LEU 58		1.33	0.00	0.00	41	D:LYS 44		50.13	0.00	0.00
42	Y:ARG 59		137.80	0.00	0.00	42	D:LYS 45		156.16	32.51 |||	-0.41

43	Y:VAL	60		51.82	0.00		0.00	43	D:THR	46	H	105.14	105.14	||||||||	0.53
44	Y:ILE	61		0.67	0.00		0.00	44	D:MET	47		45.98	32.45	||||||	0.78
45	Y:GLN	62		62.91	0.00		0.00	45	D:LEU	48	H	189.33	118.41	||||||	1.59
46	Y:LYS	63		141.36	0.00		0.00	46	D:VAL	49	H	102.89	67.22	||||||	0.93
47	Y:GLY	64		26.22	0.00		0.00	47	D:GLN	50		100.02	0.00		0.00
48	Y:ALA	65		19.89	0.00		0.00	48	D:LYS	51	HS	115.35	43.61	||||	-0.53
49	Y:PHE	66		0.00	0.00		0.00	49	D:ASN	52		98.11	0.00		0.00
50	Y:SER	67		29.69	0.00		0.00	50	D:VAL	53		101.43	0.00		0.00
51	Y:GLY	68		38.46	0.00		0.00	51	D:THR	54		37.52	0.00		0.00
52	Y:PHE	69		4.69	0.00		0.00	52	D:SER	55		80.36	0.00		0.00
53	Y:GLY	70		36.03	0.00		0.00	53	D:GLU	56		71.71	0.00		0.00
54	Y:ASP	71		48.21	0.00		0.00	54	D:SER	57		41.51	0.00		0.00
55	Y:LEU	72		0.00	0.00		0.00	55	D:THR	58		40.21	0.00		0.00
56	Y:GLU	73		59.55	0.00		0.00	56	D:CYS	59		45.30	0.00		0.00
57	Y:LYS	74	H	61.52	31.50	|||||	-0.15	57	D:CYS	60		27.37	0.00		0.00
58	Y:ILE	75		1.63	0.00		0.00	58	D:VAL	61		53.74	0.00		0.00
59	Y:GLU	76		23.90	0.00		0.00	59	D:ALA	62		28.86	0.00		0.00
60	Y:ILE	77		0.43	0.00		0.00	60	D:LYS	63		135.71	0.00		0.00
61	Y:SER	78		2.42	0.00		0.00	61	D:SER	64		47.51	0.00		0.00
62	Y:GLN	79	H	75.74	38.88	|||||	-0.09	62	D:TYR	65		78.06	6.99	|	-0.08
63	Y:ASN	80		0.79	0.00		0.00	63	D:ASN	66		83.64	0.00		0.00
64	Y:ASP	81	HS	63.67	50.18	|||||||	-0.19	64	D:ARG	67	H	183.45	34.38	||	-0.77
65	Y:VAL	82		42.97	0.00		0.00	65	D:VAL	68		51.11	0.00		0.00
66	Y:LEU	83		0.50	0.00		0.00	66	D:THR	69		80.85	0.00		0.00
67	Y:GLU	84		67.24	0.00		0.00	67	D:VAL	70		24.78	0.00		0.00
68	Y:VAL	85		40.18	0.00		0.00	68	D:MET	71		109.33	0.00		0.00
69	Y:ILE	86		0.61	0.00		0.00	69	D:GLY	72		78.00	0.00		0.00
70	Y:GLU	87		66.68	0.00		0.00	70	D:GLY	73		62.66	0.00		0.00
71	Y:ALA	88		11.20	0.00		0.00	71	D:PHE	74		102.98	13.12	||	0.21
72	Y:ASP	89		55.28	0.00		0.00	72	D:LYS	75		179.84	0.00		0.00
73	Y:VAL	90		0.00	0.00		0.00	73	D:VAL	76		21.03	0.00		0.00
74	Y:PHE	91		0.00	0.00		0.00	74	D:GLU	77		78.70	0.00		0.00
75	Y:SER	92		4.65	0.00		0.00	75	D:ASN	78		38.23	0.00		0.00
76	Y:ASN	93		102.22	0.00		0.00	76	D:HIS	79		25.00	0.00		0.00
77	Y:LEU	94		0.58	0.00		0.00	77	D:THR	80		74.29	0.00		0.00
78	Y:PRO	95		73.93	0.00		0.00	78	D:ALA	81		32.78	0.00		0.00
79	Y:LYS	96		106.57	0.00		0.00	79	D:CYS	82		27.08	0.00		0.00
80	Y:LEU	97		0.00	0.00		0.00	80	D:HIS	83		65.34	5.25	|	-0.19
81	Y:HIS	98		38.02	5.61	||	0.07	81	D:CYS	84		52.58	0.00		0.00
82	Y:GLU	99	H	28.62	26.59	||||||||	-0.37	82	D:SER	85	H	35.24	20.44	|||||	-0.23
83	Y:ILE	100		0.00	0.00		0.00	83	D:THR	86	H	88.33	58.23	||||||	0.31
84	Y:ARG	101		60.29	14.92	|||	-0.10	84	D:CYS	87		9.94	3.93	||||	-0.04
85	Y:ILE	102		0.17	0.00		0.00	85	D:TYR	88	H	157.92	119.78	||||||	0.34
86	Y:GLU	103		25.89	0.00		0.00	86	D:TYR	89		196.16	50.75	|||	0.48
87	Y:LYS	104		80.75	37.03	|||||	0.49	87	D:HIS	90		97.11	0.16	|	0.00
88	Y:ALA	105		0.00	0.00		0.00	88	D:LYS	91	HS	158.24	73.21	|||||	-1.25
89	Y:ASN	106	H	95.27	63.12	||||||	0.39	89	D:SER	92		166.95	29.46	||	-0.07
90	Y:ASN	107		69.38	0.00		0.00								
91	Y:LEU	108		0.00	0.00		0.00								
92	Y:LEU	109		81.15	0.17	|	0.00								
93	Y:TYR	110		111.49	0.00		0.00								
94	Y:ILE	111		25.85	0.00		0.00								
95	Y:ASN	112		33.82	0.00		0.00								
96	Y:PRO	113		66.53	0.00		0.00								
97	Y:GLU	114		66.13	0.00		0.00								
98	Y:ALA	115		0.00	0.00		0.00								
99	Y:PHE	116		1.09	0.00		0.00								
100	Y:GLN	117		34.61	0.00		0.00								
101	Y:ASN	118		76.63	0.00		0.00								
102	Y:LEU	119		0.00	0.00		0.00								
103	Y:PRO	120		36.78	0.00		0.00								
104	Y:ASN	121		51.50	0.00		0.00								
105	Y:LEU	122		0.00	0.00		0.00								
106	Y:GLN	123		71.85	14.49	|||	-0.05								
107	Y:TYR	124		52.14	48.95	||||||||	0.42								

108	Y:LEU 125		0.00	0.00		0.00
109	Y:LEU 126		17.73	9.70	|||||	0.16
110	Y:ILE 127		0.00	0.00		0.00
111	Y:SER 128		19.41	0.00		0.00
112	Y:ASN 129	H	83.24	76.63	|||||||||	-0.86
113	Y:THR 130		6.62	6.62	|||||||||	0.03
114	Y:GLY 131		5.36	5.36	|||||||||	0.09
115	Y:ILE 132		4.01	0.00		0.00
116	Y:LYS 133		96.36	0.00		0.00
117	Y:HIS 134		116.35	0.00		0.00
118	Y:LEU 135		27.23	0.00		0.00
119	Y:PRO 136		8.21	0.00		0.00
120	Y:ASP 137		40.39	0.00		0.00
121	Y:VAL 138		3.08	0.00		0.00
122	Y:HIS 139		78.98	0.00		0.00
123	Y:LYS 140		71.91	0.00		0.00
124	Y:ILE 141		0.00	0.00		0.00
125	Y:HIS 142		66.97	0.00		0.00
126	Y:SER 143		0.00	0.00		0.00
127	Y:LEU 144		114.14	4.79	|	-0.05
128	Y:GLN 145	H	65.96	31.26	|||||	-0.45
129	Y:LYS 146		122.05	0.00		0.00
130	Y:VAL 147		2.87	0.00		0.00
131	Y:LEU 148		37.75	32.48	||||||||	0.52
132	Y:LEU 149		0.50	0.00		0.00
133	Y:ASP 150	HS	9.20	9.20	|||||||||	0.07
134	Y:ILE 151		0.00	0.00		0.00
135	Y:GLN 152		42.10	24.19	||||||	-0.20
136	Y:ASP 153	HS	57.13	43.37	||||||||	-0.32
137	Y:ASN 154		0.00	0.00		0.00
138	Y:ILE 155		127.03	49.94	||||	0.80
139	Y:ASN 156		35.49	6.27	||	-0.07
140	Y:ILE 157		0.00	0.00		0.00
141	Y:HIS 158		73.84	0.00		0.00
142	Y:THR 159		35.88	0.00		0.00
143	Y:ILE 160		0.00	0.00		0.00
144	Y:GLU 161		87.10	0.00		0.00
145	Y:ARG 162		157.60	0.00		0.00
146	Y:ASN 163		49.31	0.00		0.00
147	Y:SER 164		20.64	0.00		0.00
148	Y:PHE 165		4.64	0.00		0.00
149	Y:VAL 166		50.10	0.00		0.00
150	Y:GLY 167		13.03	0.00		0.00
151	Y:LEU 168		1.08	0.00		0.00
152	Y:SER 169		22.12	0.00		0.00
153	Y:PHE 170		139.67	0.00		0.00
154	Y:GLU 171		66.22	7.59	||	-0.11
155	Y:SER 172		9.89	0.00		0.00
156	Y:VAL 173		4.52	0.00		0.00
157	Y:ILE 174		47.68	13.89	|||	0.22
158	Y:LEU 175		0.00	0.00		0.00
159	Y:TRP 176		69.84	43.33	|||||||	0.69
160	Y:LEU 177		0.00	0.00		0.00
161	Y:ASN 178		12.50	9.75	|||||||	-0.11
162	Y:LYS 179		88.68	15.32	||	-0.29
163	Y:ASN 180		9.57	0.00		0.00
164	Y:GLY 181		15.18	0.00		0.00
165	Y:ILE 182		0.00	0.00		0.00
166	Y:GLN 183		69.64	0.00		0.00
167	Y:GLU 184		85.97	0.00		0.00
168	Y:ILE 185		6.16	0.00		0.00
169	Y:HIS 186		71.48	0.00		0.00
170	Y:ASN 187		72.36	0.00		0.00
171	Y:SER 188		23.07	0.00		0.00
172	Y:ALA 189		0.00	0.00		0.00

173	Y:PHE 190	0.00	0.00	0.00
174	Y:ASN 191	40.79	0.00	0.00
175	Y:GLY 192	43.58	0.00	0.00
176	Y:THR 193	10.22	0.00	0.00
177	Y:GLN 194	89.98	0.00	0.00
178	Y:LEU 195	3.35	0.00	0.00
179	Y:ASP 196	44.83	0.00	0.00
180	Y:GLU 197	38.40	0.00	0.00
181	Y:LEU 198	0.31	0.00	0.00
182	Y:ASN 199	25.92	10.77 |||||	-0.12
183	Y:LEU 200	0.00	0.00	0.00
184	Y:SER 201	2.46	0.00	0.00
185	Y:ASP 202	31.09	0.00	0.00
186	Y:ASN 203	0.34	0.00	0.00
187	Y:ASN 204	83.39	0.00	0.00
188	Y:ASN 205	84.41	0.00	0.00
189	Y:LEU 206	0.00	0.00	0.00
190	Y:GLU 207	70.26	0.00	0.00
191	Y:GLU 208	117.57	0.00	0.00
192	Y:LEU 209	16.19	0.00	0.00
193	Y:PRO 210	39.50	0.00	0.00
194	Y:ASN 211	82.90	0.00	0.00
195	Y:ASP 212	55.27	0.00	0.00
196	Y:VAL 213	0.00	0.00	0.00
197	Y:PHE 214	4.09	0.00	0.00
198	Y:HIS 215	88.48	0.00	0.00
199	Y:GLY 216	45.36	0.00	0.00
200	Y:ALA 217	14.23	0.00	0.00
201	Y:SER 218	61.69	0.00	0.00
202	Y:GLY 219	2.90	0.00	0.00
203	Y:PRO 220	0.00	0.00	0.00
204	Y:VAL 221	48.86	0.00	0.00
205	Y:ILE 222	35.14	0.00	0.00
206	Y:LEU 223	0.00	0.00	0.00
207	Y:ASP 224	21.97	0.00	0.00
208	Y:ILE 225	0.00	0.00	0.00
209	Y:SER 226	0.41	0.00	0.00
210	Y:ARG 227	96.32	0.00	0.00
211	Y:THR 228	5.61	0.00	0.00
212	Y:ARG 229	112.51	0.00	0.00
213	Y:ILE 230	0.33	0.00	0.00
214	Y:HIS 231	90.17	0.00	0.00
215	Y:SER 232	38.40	0.00	0.00
216	Y:LEU 233	7.37	0.00	0.00
217	Y:PRO 234	2.42	0.00	0.00
218	Y:SER 235	66.02	0.00	0.00
219	Y:TYR 236	83.82	0.00	0.00
220	Y:GLY 237	1.00	0.00	0.00
221	Y:LEU 238	4.88	0.00	0.00
222	Y:GLU 239	87.35	0.00	0.00
223	Y:ASN 240	66.57	0.00	0.00
224	Y:LEU 241	0.00	0.00	0.00
225	Y:LYS 242	76.85	0.00	0.00
226	Y:LYS 243	60.31	0.00	0.00
227	Y:LEU 244	0.76	0.00	0.00
228	Y:ARG 245	68.70	0.00	0.00
229	Y:ALA 246	1.67	0.00	0.00
230	Y:ARG 247	94.38	0.00	0.00
231	Y:SER 248	47.42	0.00	0.00
232	Y:THR 249	1.31	0.00	0.00
233	Y:TYR 250	129.53	0.00	0.00
234	Y:ASN 251	38.49	0.00	0.00
235	Y:LEU 252	3.62	0.00	0.00
236	Y:LYS 253	131.16	0.00	0.00
237	Y:LYS 254	128.33	0.00	0.00

238	Y:LEU 255		18.87	0.00		0.00
239	Y:PRO 256		16.26	0.00		0.00
240	Y:THR 257		82.05	0.00		0.00
241	Y:LEU 258		53.81	0.00		0.00
242	Y:GLU 259		125.02	0.00		0.00
243	Y:LYS 260		84.05	0.00		0.00
244	Y:LEU 261		0.62	0.00		0.00
245	Y:VAL 262		109.03	0.00		0.00
246	Y:ALA 263		27.80	0.00		0.00
247	Y:LEU 264		8.88	0.00		0.00
248	Y:MET 265		103.47	0.00		0.00
249	Y:GLU 266		51.50	0.00		0.00
250	Y:ALA 267		1.21	0.00		0.00
251	Y:SER 268		18.06	0.00		0.00
252	Y:LEU 269		3.15	0.00		0.00
253	Y:THR 270		25.58	0.00		0.00
254	Y:TYR 271		68.22	0.00		0.00
255	Y:PRO 272		43.96	0.00		0.00
256	Y:SER 273		49.02	0.00		0.00
257	Y:HIS 274		22.67	0.00		0.00
258	Y:CYS 275		5.12	0.00		0.00
259	Y:CYS 276		20.11	0.00		0.00
260	Y:ALA 277		68.64	0.00		0.00
261	Y:PHE 278		5.23	0.00		0.00
262	Y:ALA 279		76.36	0.00		0.00
263	Y:ASN 280		79.69	0.00		0.00
264	Y:TRP 281		91.13	0.00		0.00
265	Y:ASP 334		191.42	1.06	|	0.01
266	Y:TYS 335	H	273.27	105.50	||||	-0.09
267	Y:ASP 336		143.78	3.68	|	0.06
268	Y:LEU 337		151.48	12.88	|	0.21
269	Y:VAL 342		202.97	0.00		0.00
270	Y:ASP 343		90.42	0.00		0.00
271	Y:VAL 344		24.43	0.00		0.00
272	Y:THR 345		82.06	0.00		0.00
273	Y:CYS 346		10.46	0.00		0.00
274	Y:SER 347		27.66	0.00		0.00
275	Y:PRO 348		41.67	0.00		0.00
276	Y:LYS 349		126.58	0.00		0.00
277	Y:PRO 350		42.97	0.00		0.00
278	Y:ASP 351		125.29	0.00		0.00
279	Y:ALA 352		82.91	0.00		0.00
280	Y:PHE 353		199.77	0.00		0.00
281	Y:ASN 354		53.01	0.00		0.00
282	Y:PRO 355		122.71	0.00		0.00
283	Y:CYS 356		52.99	0.00		0.00
284	Y:GLU 357		146.32	0.00		0.00



Services | Research | Training | About us

Protein Data Bank in Europe

PDBePISA

pdbe.org/pisa

PDB EMDataBank Unified Data Resource for 3DEM

Bringing Structure to Biology

Feedback Share

PISA Interface.

Session Map (id=677-61-6P8)

Start | Interfaces | Interface Search | Monomers | Assemblies

interface # 6 in PDB 4mqw crystal.

Space symmetry group: P 31. Resolution: 2.90 Å

STRUCTURE OF FOLLICLE-STIMULATING HORMONE IN COMPLEX WITH THE ENTIRE ECTODOMAIN OF ITS RECEPTOR (P31)

interface #6/65 XML << < > >>

Interface Summary XML

	Structure 1		Structure 2	
Selection range	Z		G	
class	Protein		Protein	
symmetry operation	x,y,z		x,y,z	
symmetry ID	1_555		0_555	
Number of atoms				
interface	116	5.0%	86	12.7%
surface	1235	53.4%	497	73.6%
total	2312	100.0%	675	100.0%
Number of residues				
interface	37	12.8%	24	27.3%
surface	252	86.9%	88	100.0%
total	290	100.0%	88	100.0%
Solvent-accessible area, Å				
interface	896.7	6.3%	978.6	13.8%
total	14142.0	100.0%	7106.4	100.0%
Solvation energy, kcal/mol				
isolated structure	-269.3	100.0%	-62.2	100.0%
gain on complex formation	-0.8	0.3%	-3.4	5.4%
average gain	-1.8	0.7%	-5.2	8.3%
P-value	0.608		0.716	

View structure 1 | interface | structure 2

Download structure 1 | interface | structure 2

This interface scored

1.000

in Complex Formation Significance Score (CSS).

CSS ranges from 0 to 1 as interface relevance to complex formation increases.

Achieved CSS implies that the interface plays an essential role in complex formatior

Hydrogen bonds XML

##	Structure 1	Dist. [Å]	Structure 2
1	Z:ASN 106[N]	3.43	G:THR 46[O]
2	Z:ASN 129[ND2]	2.81	G:VAL 49[O]
3	Z:LYS 74[NZ]	3.03	G:SER 85[OG]
4	Z:LYS 74[NZ]	3.52	G:THR 86[OG1]
5	Z:TYS 335[O3]	3.04	G:GLN 27[NE2]
6	Z:ASP 81[OD2]	2.91	G:ARG 42[NH1]
7	Z:GLN 79[OE1]	2.70	G:SER 43[OG]
8	Z:ASP 81[OD2]	3.75	G:LYS 45[NZ]
9	Z:ASN 129[OD1]	3.34	G:LEU 48[N]
10	Z:ASN 129[OD1]	2.74	G:VAL 49[N]
11	Z:ASP 153[OD1]	3.21	G:LYS 51[NZ]
12	Z:GLU 99[OE1]	3.41	G:TYR 88[OH]

Salt bridges XML

##	Structure 1	Dist. [Å]	Structure 2
1	Z:ASP 81[OD2]	2.91	G:ARG 42[NH1]
2	Z:ASP 81[OD2]	3.20	G:ARG 42[NH2]
3	Z:ASP 81[OD1]	3.71	G:ARG 42[NH2]
4	Z:ASP 81[OD2]	3.75	G:LYS 45[NZ]
5	Z:ASP 153[OD1]	3.21	G:LYS 51[NZ]
6	Z:ASP 153[OD2]	3.72	G:LYS 51[NZ]
7	Z:ASP 150[OD2]	3.47	G:LYS 91[NZ]

No disulfide bonds found

No covalent bonds found

Interfacing residues (not a contact table) XML Display level: Residues

Inaccessible residues HSDC Residues making **H**ydrogen/**D**isulphide bond, **S**alt bridge or **C**ovalent link

Solvent-accessible residues Interfacing residues

ASA Accessible Surface Area, Å² **BSA** Buried Surface Area, Å² **ΔᴵG** Solvation energy effect, kcal/mol |||| Buried area percentage, one bar per 10%

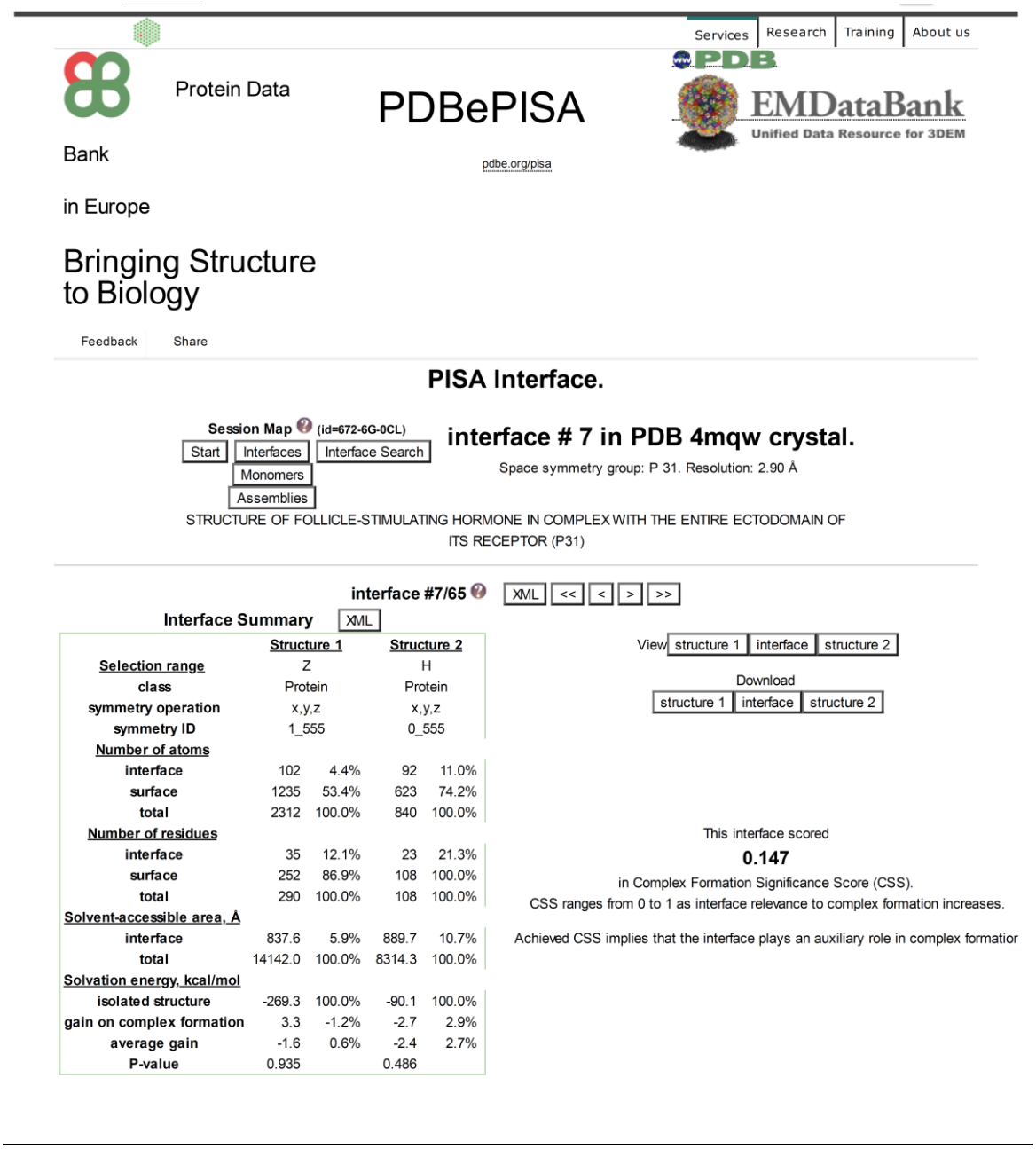
##	Structure 1	HSDC	ASA	BSA	ΔᴵG	##	Structure 2	HSDC	ASA	BSA	ΔᴵG
1	Z:CYS 18		128.01	0.00	0.00	1	G:GLN 5		236.95	0.00	0.00
2	Z:HIS 19		167.66	0.00	0.00	2	G:ASP 6		129.00	0.00	0.00
3	Z:HIS 20		14.05	0.00	0.00	3	G:CYS 7		89.39	0.00	0.00
4	Z:ARG 21		143.54	0.00	0.00	4	G:PRO 8		85.61	0.00	0.00
5	Z:ILE 22		42.09	0.00	0.00	5	G:GLU 9		145.16	0.00	0.00
6	Z:CYS 23		2.27	0.00	0.00	6	G:CYS 10		13.49	0.00	0.00
7	Z:HIS 24		97.00	0.00	0.00	7	G:THR 11		65.57	0.00	0.00
8	Z:CYS 25		23.23	0.00	0.00	8	G:LEU 12		58.93	0.00	0.00
9	Z:SER 26		70.63	0.00	0.00	9	G:GLN 13		96.13	0.00	0.00
10	Z:ASN 27		141.13	0.00	0.00	10	G:GLU 14		110.69	0.00	0.00
11	Z:ARG 28		101.49	0.00	0.00	11	G:ASN 15		26.02	17.36 |||||||	-0.22
12	Z:VAL 29		25.25	0.00	0.00	12	G:PRO 16		124.80	0.00	0.00
13	Z:PHE 30		5.92	0.00	0.00	13	G:LEU 17		105.71	27.44 |||	0.44
14	Z:LEU 31		38.60	0.00	0.00	14	G:PHE 18		44.31	18.35 |||||	0.29
15	Z:CYS 32		0.00	0.00	0.00	15	G:SER 19		17.04	0.00	0.00
16	Z:GLN 33		53.76	0.00	0.00	16	G:GLN 20		101.15	0.00	0.00
17	Z:GLU 34		80.61	0.00	0.00	17	G:PRO 21		127.03	0.00	0.00
18	Z:SER 35		64.58	4.53		-0.05	18	G:GLY 22		84.34	0.00	0.00
19	Z:LYS 36		113.02	0.00	0.00	19	G:ALA 23		60.12	0.00	0.00
20	Z:VAL 37		1.51	0.00	0.00	20	G:PRO 24		50.40	0.00	0.00
21	Z:THR 38		81.53	0.00	0.00	21	G:ILE 25		8.20	0.00	0.00
22	Z:GLU 39		122.49	0.00	0.00	22	G:LEU 26		60.29	0.00	0.00
23	Z:ILE 40		31.49	0.00	0.00	23	G:GLN 27	H	59.00	14.80 |||	-0.16
24	Z:PRO 41		6.44	0.00	0.00	24	G:CYS 28		11.51	0.00	0.00
25	Z:SER 42		104.54	0.00	0.00	25	G:MET 29		68.31	0.00	0.00
26	Z:ASP 43		69.41	0.00	0.00	26	G:GLY 30		37.95	0.00	0.00
27	Z:LEU 44		3.48	0.00	0.00	27	G:CYS 31		37.57	0.00	0.00
28	Z:PRO 45		45.83	0.00	0.00	28	G:CYS 32		32.29	0.00	0.00
29	Z:ARG 46		124.53	0.00	0.00	29	G:PHE 33		149.11	0.00	0.00
30	Z:ASN 47		75.08	0.00	0.00	30	G:SER 34		66.75	0.00	0.00
31	Z:ALA 48		0.00	0.00	0.00	31	G:ARG 35		127.72	0.00	0.00
32	Z:ILE 49		42.18	0.00	0.00	32	G:ALA 36		70.40	0.00	0.00
33	Z:GLU 50		26.48	0.00	0.00	33	G:TYR 37		66.92	0.00	0.00
34	Z:LEU 51		0.00	0.00	0.00	34	G:PRO 38		106.50	0.00	0.00
35	Z:ARG 52		82.33	0.00	0.00	35	G:THR 39		9.23	0.00	0.00
36	Z:PHE 53		0.16	0.00	0.00	36	G:PRO 40		67.88	0.00	0.00
37	Z:VAL 54		18.75	0.00	0.00	37	G:LEU 41		149.06	0.00	0.00
38	Z:LEU 55		76.01	43.37 ||||||	0.69	38	G:ARG 42	HS	154.18	86.98 ||||||	-0.57
39	Z:THR 56		0.12	0.00	0.00	39	G:SER 43	H	40.52	24.16 ||||||	0.09
40	Z:LYS 57		63.73	11.27 ||	-0.13	40	G:LYS 44		51.54	0.00	0.00
41	Z:LEU 58		0.00	0.00	0.00	41	G:LYS 45	HS	156.56	30.03 ||	-0.43
42	Z:ARG 59		137.62	0.00	0.00	42	G:THR 46	H	100.81	100.81 |||||||||	0.44
43	Z:VAL 60		63.55	0.00	0.00	43	G:MET 47		41.42	29.42 |||||||	0.76
44	Z:ILE 61		0.00	0.00	0.00	44	G:LEU 48	H	181.53	118.64 ||||||	1.71
45	Z:GLN 62		134.49	0.00	0.00	45	G:VAL 49	H	103.67	67.08 |||||||	0.93
46	Z:LYS 63		130.31	0.00	0.00	46	G:GLN 50		106.58	0.00	0.00
47	Z:GLY 64		21.52	0.00	0.00	47	G:LYS 51	HS	118.57	45.18 ||||	-0.29
48	Z:ALA 65		23.40	0.00	0.00	48	G:ASN 52		101.89	0.00	0.00
49	Z:PHE 66		0.32	0.00	0.00	49	G:VAL 53		102.06	0.00	0.00
50	Z:SER 67		27.30	0.00	0.00	50	G:THR 54		36.22	0.00	0.00
51	Z:GLY 68		37.80	0.00	0.00	51	G:SER 55		80.42	0.00	0.00
52	Z:PHE 69		2.66	0.00	0.00	52	G:GLU 56		75.05	0.00	0.00
53	Z:GLY 70		33.66	0.00	0.00	53	G:SER 57		42.46	0.00	0.00
54	Z:ASP 71		43.04	0.00	0.00	54	G:THR 58		34.48	0.00	0.00
55	Z:LEU 72		0.83	0.00	0.00	55	G:CYS 59		43.81	0.00	0.00
56	Z:GLU 73		60.31	2.33		-0.04	56	G:CYS 60		29.94	0.00	0.00
57	Z:LYS 74	H	66.35	36.00 ||||||	-0.30	57	G:VAL 61		49.58	0.00	0.00
58	Z:ILE 75		1.94	0.00	0.00	58	G:ALA 62		26.89	0.00	0.00

59	Z:GLU	76		21.77	0.00		0.00	59	G:LYS	63		133.54	2.36 |	-0.03
60	Z:ILE	77		0.00	0.00		0.00	60	G:SER	64		50.40	0.00	0.00
61	Z:SER	78		4.23	0.00		0.00	61	G:TYR	65		83.24	12.15 ||	-0.06
62	Z:GLN	79	H	78.72	42.00 ||||||		-0.05	62	G:ASN	66		92.75	0.00	0.00
63	Z:ASN	80		0.91	0.91 ||||||||||		-0.00	63	G:ARG	67		163.67	9.03 |	-0.10
64	Z:ASP	81	HS	71.73	54.79 |||||||		-0.11	64	G:VAL	68		53.38	0.00	0.00
65	Z:VAL	82		52.34	0.00		0.00	65	G:THR	69		86.46	0.00	0.00
66	Z:LEU	83		0.00	0.00		0.00	66	G:VAL	70		23.43	0.00	0.00
67	Z:GLU	84		71.87	0.00		0.00	67	G:MET	71		106.56	0.00	0.00
68	Z:VAL	85		42.50	0.00		0.00	68	G:GLY	72		77.60	0.00	0.00
69	Z:ILE	86		0.24	0.00		0.00	69	G:GLY	73		63.99	0.00	0.00
70	Z:GLU	87		66.16	0.00		0.00	70	G:PHE	74		103.47	16.88 ||	0.27
71	Z:ALA	88		11.05	0.00		0.00	71	G:LYS	75		179.78	0.00	0.00
72	Z:ASP	89		57.17	0.00		0.00	72	G:VAL	76		16.39	0.00	0.00
73	Z:VAL	90		0.00	0.00		0.00	73	G:GLU	77		73.57	0.00	0.00
74	Z:PHE	91		0.00	0.00		0.00	74	G:ASN	78		33.49	0.00	0.00
75	Z:SER	92		11.95	0.00		0.00	75	G:HIS	79		25.90	0.00	0.00
76	Z:ASN	93		98.56	0.00		0.00	76	G:THR	80		65.70	0.00	0.00
77	Z:LEU	94		1.69	0.00		0.00	77	G:ALA	81		32.45	0.00	0.00
78	Z:PRO	95		76.07	0.00		0.00	78	G:CYS	82		31.78	0.00	0.00
79	Z:LYS	96		108.83	0.00		0.00	79	G:HIS	83		62.47	6.11 |	-0.23
80	Z:LEU	97		0.00	0.00		0.00	80	G:CYS	84		55.25	0.00	0.00
81	Z:HIS	98		37.64	7.33 ||		0.09	81	G:SER	85	H	36.17	19.93 |||||	-0.23
82	Z:GLU	99	H	24.46	22.88 ||||||||		-0.32	82	G:THR	86	H	87.89	57.72 ||||||	0.33
83	Z:ILE	100		0.00	0.00		0.00	83	G:CYS	87		11.08	4.42 |||	-0.05
84	Z:ARG	101		62.92	14.09 |||		-0.10	84	G:TYR	88	H	154.17	115.06 |||||||	0.38
85	Z:ILE	102		0.00	0.00		0.00	85	G:TYR	89		203.60	52.58 |||	0.52
86	Z:GLU	103		26.39	0.00		0.00	86	G:HIS	90		92.23	0.00	0.00
87	Z:LYS	104		75.96	32.80 |||||		0.48	87	G:LYS	91	S	162.30	72.29 |||||	-0.36
88	Z:ALA	105		0.00	0.00		0.00	88	G:SER	92		164.97	29.86 ||	-0.05
89	Z:ASN	106	H	96.44	63.90 |||||||		0.36							
90	Z:ASN	107		63.48	0.00		0.00							
91	Z:LEU	108		0.00	0.00		0.00							
92	Z:LEU	109		80.26	0.00		0.00							
93	Z:TYR	110		119.49	0.00		0.00							
94	Z:ILE	111		27.72	0.00		0.00							
95	Z:ASN	112		32.75	0.00		0.00							
96	Z:PRO	113		62.64	0.00		0.00							
97	Z:GLU	114		67.46	0.00		0.00							
98	Z:ALA	115		0.00	0.00		0.00							
99	Z:PHE	116		0.93	0.00		0.00							
100	Z:GLN	117		34.54	0.00		0.00							
101	Z:ASN	118		79.48	0.00		0.00							
102	Z:LEU	119		0.00	0.00		0.00							
103	Z:PRO	120		42.31	0.00		0.00							
104	Z:ASN	121		45.81	0.00		0.00							
105	Z:LEU	122		0.00	0.00		0.00							
106	Z:GLN	123		76.16	15.15 ||		-0.03							
107	Z:TYR	124		53.33	51.24 |||||||||		0.43							
108	Z:LEU	125		0.00	0.00		0.00							
109	Z:LEU	126		17.91	11.89 |||||||		0.19							
110	Z:ILE	127		0.00	0.00		0.00							
111	Z:SER	128		19.42	1.17 |		0.02							
112	Z:ASN	129	H	82.74	76.91 |||||||||		-0.86							
113	Z:THR	130		5.78	5.78 ||||||||||		-0.00							
114	Z:GLY	131		5.52	5.19 |||||||||		0.08							
115	Z:ILE	132		3.01	0.00		0.00							
116	Z:LYS	133		97.78	0.00		0.00							
117	Z:HIS	134		111.54	0.00		0.00							
118	Z:LEU	135		24.85	0.00		0.00							
119	Z:PRO	136		9.57	0.00		0.00							
120	Z:ASP	137		43.61	0.00		0.00							
121	Z:VAL	138		3.38	0.00		0.00							
122	Z:HIS	139		75.77	0.00		0.00							
123	Z:LYS	140		59.03	0.00		0.00							

124	Z:ILE 141		0.00	0.00		0.00
125	Z:HIS 142		67.35	0.00		0.00
126	Z:SER 143		0.00	0.00		0.00
127	Z:LEU 144		115.27	0.00		0.00
128	Z:GLN 145		54.94	19.44	||||	-0.33
129	Z:LYS 146		122.41	0.00		0.00
130	Z:VAL 147		2.31	0.00		0.00
131	Z:LEU 148		39.71	33.14	||||||||	0.53
132	Z:LEU 149		0.00	0.00		0.00
133	Z:ASP 150	S	11.20	11.08	|||||||||	-0.13
134	Z:ILE 151		0.00	0.00		0.00
135	Z:GLN 152		39.37	23.76	||||||	-0.25
136	Z:ASP 153	HS	54.76	39.90	|||||||	-0.22
137	Z:ASN 154		0.00	0.00		0.00
138	Z:ILE 155		122.94	45.38	||||	0.73
139	Z:ASN 156		37.16	7.15	||	-0.08
140	Z:ILE 157		0.00	0.00		0.00
141	Z:HIS 158		83.18	0.00		0.00
142	Z:THR 159		27.36	0.00		0.00
143	Z:ILE 160		0.00	0.00		0.00
144	Z:GLU 161		84.53	0.00		0.00
145	Z:ARG 162		157.58	0.00		0.00
146	Z:ASN 163		49.29	0.00		0.00
147	Z:SER 164		17.81	0.00		0.00
148	Z:PHE 165		2.36	0.00		0.00
149	Z:VAL 166		47.62	0.00		0.00
150	Z:GLY 167		17.16	0.00		0.00
151	Z:LEU 168		1.73	0.00		0.00
152	Z:SER 169		19.04	0.00		0.00
153	Z:PHE 170		134.84	0.00		0.00
154	Z:GLU 171		66.02	0.00		0.00
155	Z:SER 172		10.42	0.00		0.00
156	Z:VAL 173		3.67	0.00		0.00
157	Z:ILE 174		48.19	15.22	||||	0.24
158	Z:LEU 175		0.00	0.00		0.00
159	Z:TRP 176		71.19	44.26	||||||	0.71
160	Z:LEU 177		0.00	0.00		0.00
161	Z:ASN 178		11.04	7.86	|||||||	-0.09
162	Z:LYS 179		94.56	19.14	|||	-0.32
163	Z:ASN 180		11.65	0.00		0.00
164	Z:GLY 181		9.53	0.00		0.00
165	Z:ILE 182		0.00	0.00		0.00
166	Z:GLN 183		74.45	0.00		0.00
167	Z:GLU 184		75.36	0.00		0.00
168	Z:ILE 185		4.66	0.00		0.00
169	Z:HIS 186		71.72	0.00		0.00
170	Z:ASN 187		70.36	0.00		0.00
171	Z:SER 188		17.69	0.00		0.00
172	Z:ALA 189		0.00	0.00		0.00
173	Z:PHE 190		0.31	0.00		0.00
174	Z:ASN 191		40.07	0.00		0.00
175	Z:GLY 192		41.50	0.00		0.00
176	Z:THR 193		12.77	0.00		0.00
177	Z:GLN 194		77.86	0.00		0.00
178	Z:LEU 195		1.08	0.00		0.00
179	Z:ASP 196		48.79	0.00		0.00
180	Z:GLU 197		33.11	0.74	|	-0.01
181	Z:LEU 198		0.47	0.00		0.00
182	Z:ASN 199		24.09	8.15	||||	-0.09
183	Z:LEU 200		0.17	0.00		0.00
184	Z:SER 201		4.79	0.00		0.00
185	Z:ASP 202		39.40	0.00		0.00
186	Z:ASN 203		0.67	0.00		0.00
187	Z:ASN 204		74.95	0.00		0.00
188	Z:ASN 205		83.63	0.00		0.00

189	Z:LEU 206	0.00	0.00	0.00
190	Z:GLU 207	66.12	0.00	0.00
191	Z:GLU 208	98.42	0.00	0.00
192	Z:LEU 209	14.65	0.00	0.00
193	Z:PRO 210	41.36	0.00	0.00
194	Z:ASN 211	80.33	0.00	0.00
195	Z:ASP 212	58.59	0.00	0.00
196	Z:VAL 213	0.00	0.00	0.00
197	Z:PHE 214	3.83	0.00	0.00
198	Z:HIS 215	87.93	0.00	0.00
199	Z:GLY 216	42.03	0.00	0.00
200	Z:ALA 217	22.99	0.00	0.00
201	Z:SER 218	70.89	0.00	0.00
202	Z:GLY 219	1.64	0.00	0.00
203	Z:PRO 220	0.00	0.00	0.00
204	Z:VAL 221	47.20	0.00	0.00
205	Z:ILE 222	37.84	0.00	0.00
206	Z:LEU 223	0.00	0.00	0.00
207	Z:ASP 224	21.19	0.00	0.00
208	Z:ILE 225	0.00	0.00	0.00
209	Z:SER 226	0.90	0.00	0.00
210	Z:ARG 227	100.60	0.00	0.00
211	Z:THR 228	5.26	0.00	0.00
212	Z:ARG 229	122.40	0.00	0.00
213	Z:ILE 230	0.00	0.00	0.00
214	Z:HIS 231	91.70	0.00	0.00
215	Z:SER 232	55.82	0.00	0.00
216	Z:LEU 233	11.92	0.00	0.00
217	Z:PRO 234	6.70	0.00	0.00
218	Z:SER 235	54.54	0.00	0.00
219	Z:TYR 236	81.31	0.00	0.00
220	Z:GLY 237	5.46	0.00	0.00
221	Z:LEU 238	0.63	0.00	0.00
222	Z:GLU 239	85.67	0.00	0.00
223	Z:ASN 240	62.02	0.00	0.00
224	Z:LEU 241	0.00	0.00	0.00
225	Z:LYS 242	89.66	0.00	0.00
226	Z:LYS 243	55.10	0.00	0.00
227	Z:LEU 244	0.37	0.00	0.00
228	Z:ARG 245	67.43	0.00	0.00
229	Z:ALA 246	2.20	0.00	0.00
230	Z:ARG 247	95.62	0.00	0.00
231	Z:SER 248	44.55	0.00	0.00
232	Z:THR 249	1.67	0.00	0.00
233	Z:TYR 250	124.63	0.00	0.00
234	Z:ASN 251	46.69	0.00	0.00
235	Z:LEU 252	4.38	0.00	0.00
236	Z:LYS 253	131.30	0.00	0.00
237	Z:LYS 254	156.95	0.00	0.00
238	Z:LEU 255	33.55	0.00	0.00
239	Z:PRO 256	17.86	0.00	0.00
240	Z:THR 257	60.77	0.00	0.00
241	Z:LEU 258	1.87	0.00	0.00
242	Z:GLU 259	111.59	0.00	0.00
243	Z:LYS 260	65.88	0.00	0.00
244	Z:LEU 261	0.50	0.00	0.00
245	Z:VAL 262	82.75	0.00	0.00
246	Z:ALA 263	30.04	0.00	0.00
247	Z:LEU 264	0.00	0.00	0.00
248	Z:MET 265	74.67	0.00	0.00
249	Z:GLU 266	55.64	0.00	0.00
250	Z:ALA 267	0.90	0.00	0.00
251	Z:SER 268	25.31	0.00	0.00
252	Z:LEU 269	4.19	0.00	0.00
253	Z:THR 270	27.20	0.00	0.00

254	Z:TYR 271		56.36	0.00		0.00
255	Z:PRO 272		41.84	0.00		0.00
256	Z:SER 273		50.32	0.00		0.00
257	Z:HIS 274		18.27	0.00		0.00
258	Z:CYS 275		0.80	0.00		0.00
259	Z:CYS 276		28.31	0.00		0.00
260	Z:ALA 277		57.24	0.00		0.00
261	Z:PHE 278		8.81	0.00		0.00
262	Z:ALA 279		45.06	0.00		0.00
263	Z:ASN 280		104.34	0.00		0.00
264	Z:TRP 281		98.97	0.00		0.00
265	Z:ARG 282		157.61	0.00		0.00
266	Z:ARG 283		127.10	0.00		0.00
267	Z:PRO 290		196.59	0.00		0.00
268	Z:ILE 291		155.21	0.00		0.00
269	Z:CYS 292		137.93	0.00		0.00
270	Z:ASP 334		197.05	0.00		0.00
271	Z:TYS 335	H	283.01	89.90	||||	-0.65
272	Z:ASP 336		86.30	10.21	||	0.16
273	Z:LEU 337		114.45	17.42	||	0.28
274	Z:CYS 338		52.15	0.00		0.00
275	Z:ASN 339		123.36	0.45	|	0.01
276	Z:VAL 342		184.80	0.00		0.00
277	Z:ASP 343		63.88	0.00		0.00
278	Z:VAL 344		17.80	0.00		0.00
279	Z:THR 345		91.76	0.00		0.00
280	Z:CYS 346		11.75	0.00		0.00
281	Z:SER 347		36.26	0.00		0.00
282	Z:PRO 348		41.49	0.00		0.00
283	Z:LYS 349		100.18	0.00		0.00
284	Z:PRO 350		42.69	0.00		0.00
285	Z:ASP 351		109.76	0.00		0.00
286	Z:ALA 352		89.22	0.00		0.00
287	Z:PHE 353		187.75	0.00		0.00
288	Z:ASN 354		53.59	0.00		0.00
289	Z:PRO 355		149.42	0.00		0.00
290	Z:CYS 356		73.40	0.00		0.00



Services | Research | Training | About us

Protein Data Bank in Europe

PDBePISA

pdbe.org/pisa

PDB

EMDataBank
Unified Data Resource for 3DEM

Bringing Structure to Biology

Feedback Share

PISA Interface.

Session Map (id=672-6G-0CL)

Start | Interfaces | Interface Search | Monomers | Assemblies

interface # 7 in PDB 4mqw crystal.

Space symmetry group: P 31. Resolution: 2.90 Å

STRUCTURE OF FOLLICLE-STIMULATING HORMONE IN COMPLEX WITH THE ENTIRE ECTODOMAIN OF ITS RECEPTOR (P31)

interface #7/65 XML << < > >>

Interface Summary XML

	Structure 1		Structure 2	
Selection range	Z		H	
class	Protein		Protein	
symmetry operation	x,y,z		x,y,z	
symmetry ID	1_555		0_555	
Number of atoms				
interface	102	4.4%	92	11.0%
surface	1235	53.4%	623	74.2%
total	2312	100.0%	840	100.0%
Number of residues				
interface	35	12.1%	23	21.3%
surface	252	86.9%	108	100.0%
total	290	100.0%	108	100.0%
Solvent-accessible area, Å				
interface	837.6	5.9%	889.7	10.7%
total	14142.0	100.0%	8314.3	100.0%
Solvation energy, kcal/mol				
isolated structure	-269.3	100.0%	-90.1	100.0%
gain on complex formation	3.3	-1.2%	-2.7	2.9%
average gain	-1.6	0.6%	-2.4	2.7%
P-value	0.935		0.486	

View structure 1 | interface | structure 2

Download structure 1 | interface | structure 2

This interface scored

0.147

in Complex Formation Significance Score (CSS).

CSS ranges from 0 to 1 as interface relevance to complex formation increases.

Achieved CSS implies that the interface plays an auxiliary role in complex formatior

Hydrogen bonds [XML]

##	Structure 1	Dist. [Å]	Structure 2
1	Z:LYS 146[NZ]	3.52	H:LYS 40[O]
2	Z:LYS 243[NZ]	2.91	H:ALA 43[O]
3	Z:LYS 179[NZ]	3.20	H:SER 89[O]
4	Z:LYS 104[NZ]	2.93	H:ASP 93[OD1]
5	Z:ARG 101[NH1]	3.77	H:THR 95[OG1]
6	Z:TYS 335[O3]	3.12	H:VAL 38[N]
7	Z:TYS 335[O1]	3.45	H:VAL 38[N]
8	Z:TYS 335[O1]	3.08	H:TYR 39[N]
9	Z:GLU 197[OE1]	2.75	H:LYS 46[NZ]
10	Z:GLU 103[OE2]	2.94	H:THR 95[OG1]
11	Z:GLU 76[OE1]	3.59	H:ARG 97[NE]
12	Z:GLU 50[OE2]	3.24	H:ARG 97[NH2]
13	Z:GLU 76[OE1]	3.63	H:ARG 97[NH2]
14	Z:GLU 34[OE1]	2.73	H:TYR 103[OH]
15	Z:GLU 34[OE2]	2.69	H:TYR 103[OH]

Salt bridges [XML]

##	Structure 1	Dist. [Å]	Structure 2
1	Z:LYS 179[NZ]	3.93	H:ASP 90[OD2]
2	Z:LYS 104[NZ]	2.93	H:ASP 93[OD1]
3	Z:LYS 104[NZ]	3.03	H:ASP 93[OD2]
4	Z:GLU 197[OE1]	2.75	H:LYS 46[NZ]
5	Z:GLU 76[OE1]	3.59	H:ARG 97[NE]
6	Z:GLU 50[OE2]	3.24	H:ARG 97[NH2]
7	Z:GLU 76[OE1]	3.63	H:ARG 97[NH2]

No disulfide bonds found
No covalent bonds found

Interfacing residues (not a contact table) [XML] Display level: Residues

Inaccessible residues HSDC Residues making **H**ydrogen/**D**isulphide bond, **S**alt bridge or **C**ovalent link
Solvent-accessible residues Interfacing residues
ASA Accessible Surface Area, Å² **BSA** Buried Surface Area, Å² **Δ^{i}G** Solvation energy effect, kcal/mol |||| Buried area percentage, one bar per 10%

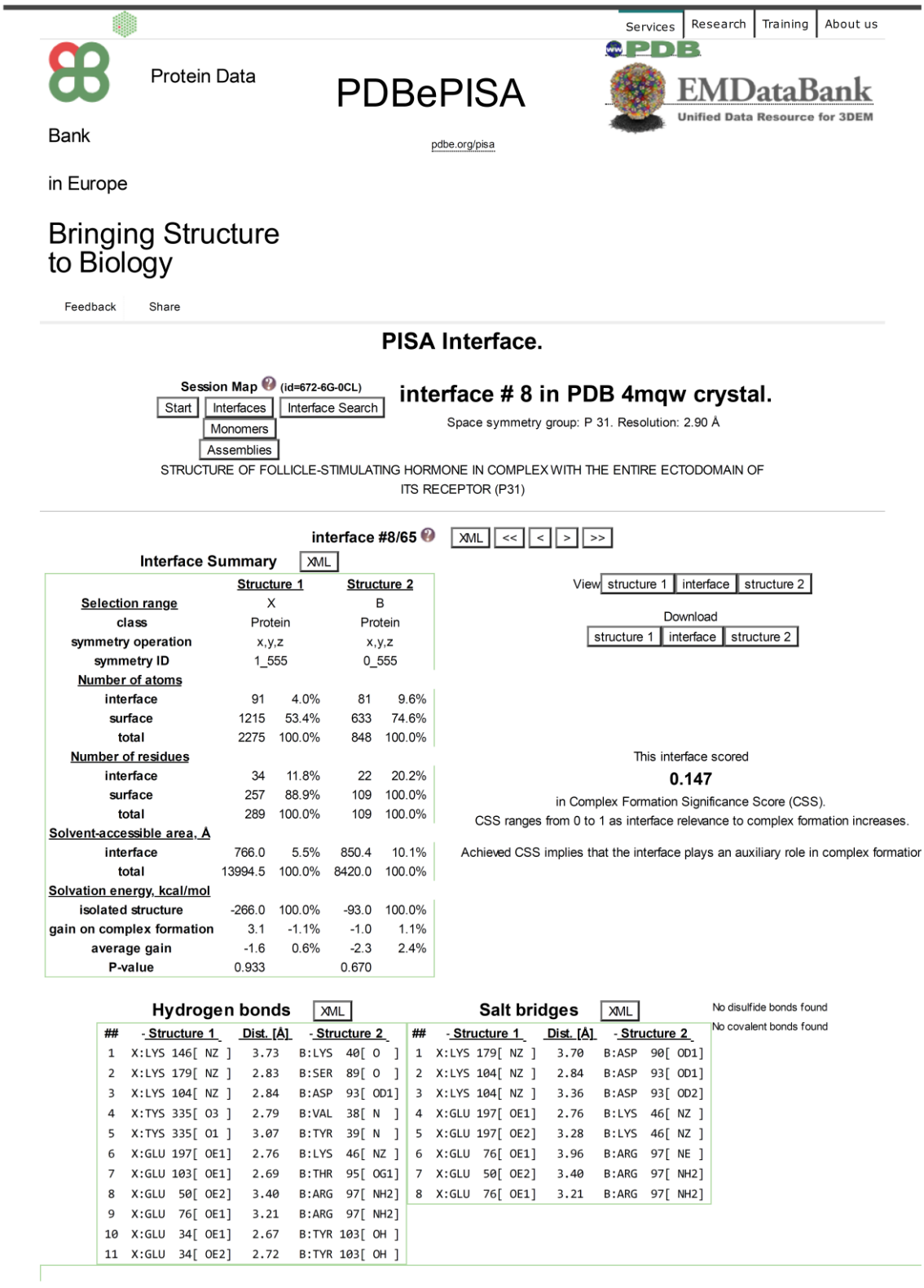
##	Structure 1	HSDC	ASA	BSA	Δ^{i}G	##	Structure 2	HSDC	ASA	BSA	Δ^{i}G
1	Z:CYS 18		128.01	0.00	0.00	1	H:ASN 1		149.26	0.00	0.00
2	Z:HIS 19		167.66	0.00	0.00	2	H:SER 2		75.46	0.00	0.00
3	Z:HIS 20		14.05	0.00	0.00	3	H:CYS 3		18.00	0.00	0.00
4	Z:ARG 21		143.54	0.00	0.00	4	H:GLU 4		112.15	0.00	0.00
5	Z:ILE 22		42.09	0.00	0.00	5	H:LEU 5		74.17	0.00	0.00
6	Z:CYS 23		2.27	0.00	0.00	6	H:THR 6		50.76	0.00	0.00
7	Z:HIS 24		97.00	0.00	0.00	7	H:ASN 7		126.98	0.00	0.00
8	Z:CYS 25		23.23	0.00	0.00	8	H:ILE 8		46.09	0.00	0.00
9	Z:SER 26		70.63	0.00	0.00	9	H:THR 9		61.58	0.00	0.00
10	Z:ASN 27		141.13	0.00	0.00	10	H:ILE 10		24.22	0.00	0.00
11	Z:ARG 28		101.49	0.00	0.00	11	H:ALA 11		21.78	0.00	0.00
12	Z:VAL 29		25.25	0.00	0.00	12	H:ILE 12		3.59	0.00	0.00
13	Z:PHE 30		5.92	0.00	0.00	13	H:GLU 13		73.95	0.00	0.00
14	Z:LEU 31		38.60	0.00	0.00	14	H:LYS 14		8.06	0.00	0.00
15	Z:CYS 32		0.00	0.00	0.00	15	H:GLU 15		132.58	0.00	0.00
16	Z:GLN 33		53.76	14.47 |||	-0.18	16	H:GLU 16		92.35	0.00	0.00
17	Z:GLU 34	H	80.61	24.27 ||||	-0.29	17	H:CYS 17		15.14	0.00	0.00
18	Z:SER 35		64.58	0.00	0.00	18	H:ARG 18		177.65	0.00	0.00
19	Z:LYS 36		113.02	0.00	0.00	19	H:PHE 19		65.31	0.00	0.00
20	Z:VAL 37		1.51	0.00	0.00	20	H:CYS 20		34.45	0.00	0.00
21	Z:THR 38		81.53	0.00	0.00	21	H:ILE 21		35.72	0.00	0.00
22	Z:GLU 39		122.49	0.00	0.00	22	H:SER 22		79.81	0.00	0.00
23	Z:ILE 40		31.49	0.00	0.00	23	H:ILE 23		38.74	0.00	0.00
24	Z:PRO 41		6.44	0.00	0.00	24	H:ASN 24		119.93	0.00	0.00
25	Z:SER 42		104.54	0.00	0.00	25	H:THR 25		7.91	0.00	0.00
26	Z:ASP 43		69.41	0.00	0.00	26	H:THR 26		43.16	0.00	0.00
27	Z:LEU 44		3.48	0.00	0.00	27	H:TRP 27		50.46	0.00	0.00
28	Z:PRO 45		45.83	0.00	0.00	28	H:CYS 28		27.09	0.00	0.00
29	Z:ARG 46		124.53	0.00	0.00	29	H:ALA 29		50.24	0.00	0.00
30	Z:ASN 47		75.08	0.00	0.00	30	H:GLY 30		40.82	0.00	0.00
31	Z:ALA 48		0.00	0.00	0.00	31	H:TYR 31		173.39	0.00	0.00
32	Z:ILE 49		42.18	0.00	0.00	32	H:CYS 32		31.36	0.00	0.00
33	Z:GLU 50	HS	26.48	5.44 |||	-0.06	33	H:TYR 33		136.66	0.00	0.00
34	Z:LEU 51		0.00	0.00	0.00	34	H:THR 34		70.08	0.00	0.00
35	Z:ARG 52		82.33	40.14 |||||	-0.73	35	H:ARG 35		169.87	26.43 ||	-0.34
36	Z:PHE 53		0.16	0.00	0.00	36	H:ASP 36		119.22	1.59 |	-0.02
37	Z:VAL 54		18.75	9.21 |||||	0.15	37	H:LEU 37		50.31	26.93 ||||||	0.43
38	Z:LEU 55		76.01	32.64 |||||	0.52	38	H:VAL 38	H	150.20	13.41 |	0.12
39	Z:THR 56		0.12	0.00	0.00	39	H:TYR 39	H	166.26	26.73 ||	0.33
40	Z:LYS 57		63.73	0.00	0.00	40	H:LYS 40	H	120.38	27.77 |||	0.09

41	Z:LEU	58		0.00	0.00		0.00	41	H:ASP	41		46.93	10.68 |||	-0.10
42	Z:ARG	59		137.62	0.00		0.00	42	H:PRO	42		126.34	90.14 |||||||	0.95
43	Z:VAL	60		63.55	0.00		0.00	43	H:ALA	43	H	94.54	82.89 ||||||||	0.82
44	Z:ILE	61		0.00	0.00		0.00	44	H:ARG	44		64.22	29.27 |||||	-0.29
45	Z:GLN	62		134.49	0.00		0.00	45	H:PRO	45		95.65	43.25 |||||	0.69
46	Z:LYS	63		130.31	0.00		0.00	46	H:LYS	46	HS	124.33	53.96 |||||	-0.35
47	Z:GLY	64		21.52	0.00		0.00	47	H:ILE	47		117.62	0.00	0.00
48	Z:ALA	65		23.40	0.00		0.00	48	H:GLN	48		129.80	0.00	0.00
49	Z:PHE	66		0.32	0.00		0.00	49	H:LYS	49		110.58	0.00	0.00
50	Z:SER	67		27.30	0.00		0.00	50	H:THR	50		58.91	0.00	0.00
51	Z:GLY	68		37.80	0.00		0.00	51	H:CYS	51		26.72	0.00	0.00
52	Z:PHE	69		2.66	0.00		0.00	52	H:THR	52		17.90	0.00	0.00
53	Z:GLY	70		33.66	0.00		0.00	53	H:PHE	53		36.69	0.00	0.00
54	Z:ASP	71		43.04	0.00		0.00	54	H:LYS	54		99.19	0.00	0.00
55	Z:LEU	72		0.83	0.00		0.00	55	H:GLU	55		87.20	0.00	0.00
56	Z:GLU	73		60.31	0.00		0.00	56	H:LEU	56		55.44	0.00	0.00
57	Z:LYS	74		66.35	0.84 |		0.01	57	H:VAL	57		70.53	0.00	0.00
58	Z:ILE	75		1.94	0.00		0.00	58	H:TYR	58		142.32	0.00	0.00
59	Z:GLU	76	HS	21.77	17.66 ||||||||		-0.25	59	H:GLU	59		77.38	0.00	0.00
60	Z:ILE	77		0.00	0.00		0.00	60	H:THR	60		78.61	0.00	0.00
61	Z:SER	78		4.23	3.61 ||||||||		0.01	61	H:VAL	61		32.79	0.00	0.00
62	Z:GLN	79		78.72	36.72 |||||		-0.53	62	H:ARG	62		166.39	0.00	0.00
63	Z:ASN	80		0.91	0.00		0.00	63	H:VAL	63		3.84	0.00	0.00
64	Z:ASP	81		71.73	0.00		0.00	64	H:PRO	64		67.37	0.00	0.00
65	Z:VAL	82		52.34	0.00		0.00	65	H:GLY	65		27.87	0.00	0.00
66	Z:LEU	83		0.00	0.00		0.00	66	H:CYS	66		47.88	0.00	0.00
67	Z:GLU	84		71.87	0.00		0.00	67	H:ALA	67		100.84	0.00	0.00
68	Z:VAL	85		42.50	0.00		0.00	68	H:HIS	68		175.34	0.00	0.00
69	Z:ILE	86		0.24	0.00		0.00	69	H:HIS	69		89.54	0.00	0.00
70	Z:GLU	87		66.16	0.00		0.00	70	H:ALA	70		88.06	0.00	0.00
71	Z:ALA	88		11.05	0.00		0.00	71	H:ASP	71		78.79	0.00	0.00
72	Z:ASP	89		57.17	0.00		0.00	72	H:SER	72		48.28	0.00	0.00
73	Z:VAL	90		0.00	0.00		0.00	73	H:LEU	73		117.20	0.00	0.00
74	Z:PHE	91		0.00	0.00		0.00	74	H:TYR	74		104.77	0.00	0.00
75	Z:SER	92		11.95	0.00		0.00	75	H:THR	75		63.86	0.00	0.00
76	Z:ASN	93		98.56	0.00		0.00	76	H:TYR	76		11.15	0.00	0.00
77	Z:LEU	94		1.69	0.00		0.00	77	H:PRO	77		46.24	0.00	0.00
78	Z:PRO	95		76.07	0.00		0.00	78	H:VAL	78		13.06	0.00	0.00
79	Z:LYS	96		108.83	0.00		0.00	79	H:ALA	79		4.66	0.00	0.00
80	Z:LEU	97		0.00	0.00		0.00	80	H:THR	80		68.39	0.00	0.00
81	Z:HIS	98		37.64	0.00		0.00	81	H:GLN	81		78.53	0.00	0.00
82	Z:GLU	99		24.46	0.77 |		-0.00	82	H:CYS	82		21.67	0.00	0.00
83	Z:ILE	100		0.00	0.00		0.00	83	H:HIS	83		55.31	0.00	0.00
84	Z:ARG	101	H	62.92	48.83 |||||||		-0.86	84	H:CYS	84		30.69	0.00	0.00
85	Z:ILE	102		0.00	0.00		0.00	85	H:GLY	85		7.50	0.00	0.00
86	Z:GLU	103	H	26.39	25.18 ||||||||		-0.31	86	H:LYS	86		149.55	0.00	0.00
87	Z:LYS	104	HS	75.96	43.16 |||||		-0.32	87	H:CYS	87		38.06	0.00	0.00
88	Z:ALA	105		0.00	0.00		0.00	88	H:ASP	88		73.57	0.00	0.00
89	Z:ASN	106		96.44	0.00		0.00	89	H:SER	89	H	88.38	40.02 |||||	0.03
90	Z:ASN	107		63.48	0.00		0.00	90	H:ASP	90	S	140.52	36.62 |||	-0.18
91	Z:LEU	108		0.00	0.00		0.00	91	H:SER	91		77.03	0.00	0.00
92	Z:LEU	109		80.26	0.00		0.00	92	H:THR	92		43.28	0.00	0.00
93	Z:TYR	110		119.49	0.00		0.00	93	H:ASP	93	HS	121.94	42.46 ||||	-0.40
94	Z:ILE	111		27.72	0.00		0.00	94	H:CYS	94		64.33	8.35 ||	-0.10
95	Z:ASN	112		32.75	0.00		0.00	95	H:THR	95	H	84.75	36.87 |||||	-0.03
96	Z:PRO	113		62.64	0.00		0.00	96	H:VAL	96		123.24	31.60 |||	0.50
97	Z:GLU	114		67.46	0.00		0.00	97	H:ARG	97	HS	200.20	110.92 ||||||	-0.98
98	Z:ALA	115		0.00	0.00		0.00	98	H:GLY	98		59.92	11.99 |||	0.11
99	Z:PHE	116		0.93	0.00		0.00	99	H:LEU	99		140.75	86.25 |||||||	1.37
100	Z:GLN	117		34.54	0.00		0.00	100	H:GLY	100		43.73	0.00	0.00
101	Z:ASN	118		79.48	0.00		0.00	101	H:PRO	101		75.93	0.00	0.00
102	Z:LEU	119		0.00	0.00		0.00	102	H:SER	102		51.67	0.00	0.00
103	Z:PRO	120		42.31	0.00		0.00	103	H:TYR	103	H	99.55	51.23 |||||	-0.01
104	Z:ASN	121		45.81	0.00		0.00	104	H:CYS	104		14.50	0.00	0.00
105	Z:LEU	122		0.00	0.00		0.00	105	H:SER	105		66.45	0.34 |	0.01

106	Z:GLN 123		76.16	0.00	0.00	106	H:PHE 106	77.61	0.00	0.00
107	Z:TYR 124		53.33	0.00	0.00	107	H:GLY 107	42.58	0.00	0.00
108	Z:LEU 125		0.00	0.00	0.00	108	H:GLU 108	180.71	0.00	0.00
109	Z:LEU 126		17.91	4.02 |||	0.06					
110	Z:ILE 127		0.00	0.00	0.00					
111	Z:SER 128		19.42	3.06 ||	-0.03					
112	Z:ASN 129		82.74	2.18 |	-0.02					
113	Z:THR 130		5.78	0.00	0.00					
114	Z:GLY 131		5.52	0.00	0.00					
115	Z:ILE 132		3.01	0.00	0.00					
116	Z:LYS 133		97.78	0.00	0.00					
117	Z:HIS 134		111.54	0.00	0.00					
118	Z:LEU 135		24.85	0.00	0.00					
119	Z:PRO 136		9.57	0.00	0.00					
120	Z:ASP 137		43.61	0.00	0.00					
121	Z:VAL 138		3.38	0.00	0.00					
122	Z:HIS 139		75.77	0.00	0.00					
123	Z:LYS 140		59.03	0.00	0.00					
124	Z:ILE 141		0.00	0.00	0.00					
125	Z:HIS 142		67.35	0.00	0.00					
126	Z:SER 143		0.00	0.00	0.00					
127	Z:LEU 144		115.27	0.00	0.00					
128	Z:GLN 145		54.94	0.00	0.00					
129	Z:LYS 146	H	122.41	38.77 ||||	-0.57					
130	Z:VAL 147		2.31	0.00	0.00					
131	Z:LEU 148		39.71	0.00	0.00					
132	Z:LEU 149		0.00	0.00	0.00					
133	Z:ASP 150		11.20	0.00	0.00					
134	Z:ILE 151		0.00	0.00	0.00					
135	Z:GLN 152		39.37	11.29 |||	-0.19					
136	Z:ASP 153		54.76	8.23 ||	-0.04					
137	Z:ASN 154		0.00	0.00	0.00					
138	Z:ILE 155		122.94	0.00	0.00					
139	Z:ASN 156		37.16	0.00	0.00					
140	Z:ILE 157		0.00	0.00	0.00					
141	Z:HIS 158		83.18	0.00	0.00					
142	Z:THR 159		27.36	0.00	0.00					
143	Z:ILE 160		0.00	0.00	0.00					
144	Z:GLU 161		84.53	0.00	0.00					
145	Z:ARG 162		157.58	0.00	0.00					
146	Z:ASN 163		49.29	0.00	0.00					
147	Z:SER 164		17.81	0.00	0.00					
148	Z:PHE 165		2.36	0.00	0.00					
149	Z:VAL 166		47.62	0.00	0.00					
150	Z:GLY 167		17.16	0.00	0.00					
151	Z:LEU 168		1.73	0.00	0.00					
152	Z:SER 169		19.04	0.00	0.00					
153	Z:PHE 170		134.84	0.00	0.00					
154	Z:GLU 171		66.02	0.00	0.00					
155	Z:SER 172		10.42	0.00	0.00					
156	Z:VAL 173		3.67	0.00	0.00					
157	Z:ILE 174		48.19	25.44 |||||	0.41					
158	Z:LEU 175		0.00	0.00	0.00					
159	Z:TRP 176		71.19	7.67 ||	0.12					
160	Z:LEU 177		0.00	0.00	0.00					
161	Z:ASN 178		11.04	0.15 |	-0.00					
162	Z:LYS 179	HS	94.56	64.36 ||||||	-0.11					
163	Z:ASN 180		11.65	0.00	0.00					
164	Z:GLY 181		9.53	0.00	0.00					
165	Z:ILE 182		0.00	0.00	0.00					
166	Z:GLN 183		74.45	0.00	0.00					
167	Z:GLU 184		75.36	0.00	0.00					
168	Z:ILE 185		4.66	0.00	0.00					
169	Z:HIS 186		71.72	0.00	0.00					
170	Z:ASN 187		70.36	0.00	0.00					

171	Z:SER 188		17.69	0.00		0.00
172	Z:ALA 189		0.00	0.00		0.00
173	Z:PHE 190		0.31	0.00		0.00
174	Z:ASN 191		40.07	0.00		0.00
175	Z:GLY 192		41.50	0.00		0.00
176	Z:THR 193		12.77	0.00		0.00
177	Z:GLN 194		77.86	0.00		0.00
178	Z:LEU 195		1.08	0.00		0.00
179	Z:ASP 196		48.79	35.40	||||||||	-0.03
180	Z:GLU 197	HS	33.11	19.00	||||||	-0.25
181	Z:LEU 198		0.47	0.00		0.00
182	Z:ASN 199		24.09	0.00		0.00
183	Z:LEU 200		0.17	0.00		0.00
184	Z:SER 201		4.79	0.00		0.00
185	Z:ASP 202		39.40	9.51	|||	-0.03
186	Z:ASN 203		0.67	0.00		0.00
187	Z:ASN 204		74.95	0.00		0.00
188	Z:ASN 205		83.63	0.00		0.00
189	Z:LEU 206		0.00	0.00		0.00
190	Z:GLU 207		66.12	0.00		0.00
191	Z:GLU 208		98.42	0.00		0.00
192	Z:LEU 209		14.65	0.00		0.00
193	Z:PRO 210		41.36	0.00		0.00
194	Z:ASN 211		80.33	0.00		0.00
195	Z:ASP 212		58.59	0.00		0.00
196	Z:VAL 213		0.00	0.00		0.00
197	Z:PHE 214		3.83	0.00		0.00
198	Z:HIS 215		87.93	0.00		0.00
199	Z:GLY 216		42.03	0.00		0.00
200	Z:ALA 217		22.99	0.00		0.00
201	Z:SER 218		70.89	0.00		0.00
202	Z:GLY 219		1.64	0.00		0.00
203	Z:PRO 220		0.00	0.00		0.00
204	Z:VAL 221		47.20	26.45	|||||	0.42
205	Z:ILE 222		37.84	31.13	||||||||	0.50
206	Z:LEU 223		0.00	0.00		0.00
207	Z:ASP 224		21.19	0.00		0.00
208	Z:ILE 225		0.00	0.00		0.00
209	Z:SER 226		0.90	0.00		0.00
210	Z:ARG 227		100.60	0.00		0.00
211	Z:THR 228		5.26	0.00		0.00
212	Z:ARG 229		122.40	0.00		0.00
213	Z:ILE 230		0.00	0.00		0.00
214	Z:HIS 231		91.70	0.00		0.00
215	Z:SER 232		55.82	0.00		0.00
216	Z:LEU 233		11.92	0.00		0.00
217	Z:PRO 234		6.70	0.00		0.00
218	Z:SER 235		54.54	0.00		0.00
219	Z:TYR 236		81.31	0.00		0.00
220	Z:GLY 237		5.46	0.00		0.00
221	Z:LEU 238		0.63	0.00		0.00
222	Z:GLU 239		85.67	0.00		0.00
223	Z:ASN 240		62.02	0.00		0.00
224	Z:LEU 241		0.00	0.00		0.00
225	Z:LYS 242		89.66	23.25	|||	-0.40
226	Z:LYS 243	H	55.10	32.31	|||||	-0.62
227	Z:LEU 244		0.37	0.00		0.00
228	Z:ARG 245		67.43	0.00		0.00
229	Z:ALA 246		2.20	0.00		0.00
230	Z:ARG 247		95.62	0.00		0.00
231	Z:SER 248		44.55	0.00		0.00
232	Z:THR 249		1.67	0.00		0.00
233	Z:TYR 250		124.63	0.00		0.00
234	Z:ASN 251		46.69	0.00		0.00
235	Z:LEU 252		4.38	0.00		0.00

236	Z:LYS 253		131.30	0.00	0.00
237	Z:LYS 254		156.95	0.00	0.00
238	Z:LEU 255		33.55	0.00	0.00
239	Z:PRO 256		17.86	0.00	0.00
240	Z:THR 257		60.77	0.00	0.00
241	Z:LEU 258		1.87	0.00	0.00
242	Z:GLU 259		111.59	0.00	0.00
243	Z:LYS 260		65.88	0.00	0.00
244	Z:LEU 261		0.50	0.00	0.00
245	Z:VAL 262		82.75	0.00	0.00
246	Z:ALA 263		30.04	0.00	0.00
247	Z:LEU 264		0.00	0.00	0.00
248	Z:MET 265		74.67	6.00 |	0.10
249	Z:GLU 266		55.64	0.00	0.00
250	Z:ALA 267		0.90	0.00	0.00
251	Z:SER 268		25.31	0.00	0.00
252	Z:LEU 269		4.19	0.00	0.00
253	Z:THR 270		27.20	0.00	0.00
254	Z:TYR 271		56.36	0.00	0.00
255	Z:PRO 272		41.84	0.00	0.00
256	Z:SER 273		50.32	0.00	0.00
257	Z:HIS 274		18.27	0.00	0.00
258	Z:CYS 275		0.80	0.00	0.00
259	Z:CYS 276		28.31	0.00	0.00
260	Z:ALA 277		57.24	0.00	0.00
261	Z:PHE 278		8.81	0.00	0.00
262	Z:ALA 279		45.06	0.00	0.00
263	Z:ASN 280		104.34	0.00	0.00
264	Z:TRP 281		98.97	0.00	0.00
265	Z:ARG 282		157.61	0.00	0.00
266	Z:ARG 283		127.10	0.00	0.00
267	Z:PRO 290		196.59	0.00	0.00
268	Z:ILE 291		155.21	0.00	0.00
269	Z:CYS 292		137.93	0.00	0.00
270	Z:ASP 334		197.05	30.30 ||	-0.18
271	Z:TYS 335	H	283.01	152.96 ||||||	0.34
272	Z:ASP 336		86.30	0.00	0.00
273	Z:LEU 337		114.45	3.16 |	0.05
274	Z:CYS 338		52.15	0.00	0.00
275	Z:ASN 339		123.36	0.00	0.00
276	Z:VAL 342		184.80	0.00	0.00
277	Z:ASP 343		63.88	0.00	0.00
278	Z:VAL 344		17.80	0.00	0.00
279	Z:THR 345		91.76	0.00	0.00
280	Z:CYS 346		11.75	0.00	0.00
281	Z:SER 347		36.26	0.00	0.00
282	Z:PRO 348		41.49	0.00	0.00
283	Z:LYS 349		100.18	0.00	0.00
284	Z:PRO 350		42.69	0.00	0.00
285	Z:ASP 351		109.76	0.00	0.00
286	Z:ALA 352		89.22	0.00	0.00
287	Z:PHE 353		187.75	0.00	0.00
288	Z:ASN 354		53.59	0.00	0.00
289	Z:PRO 355		149.42	0.00	0.00
290	Z:CYS 356		73.40	0.00	0.00



Services | Research | Training | About us

Protein Data Bank in Europe

PDBePISA

pdbe.org/pisa

PDB EMDataBank Unified Data Resource for 3DEM

Bringing Structure to Biology

Feedback Share

PISA Interface.

Session Map (id=672-6G-0CL)

Start | Interfaces | Interface Search | Monomers | Assemblies

interface # 8 in PDB 4mqw crystal.

Space symmetry group: P 31. Resolution: 2.90 Å

STRUCTURE OF FOLLICLE-STIMULATING HORMONE IN COMPLEX WITH THE ENTIRE ECTODOMAIN OF ITS RECEPTOR (P31)

interface #8/65 XML << < > >>

Interface Summary XML

	Structure 1		Structure 2	
Selection range	X		B	
class	Protein		Protein	
symmetry operation	x,y,z		x,y,z	
symmetry ID	1_555		0_555	
Number of atoms				
interface	91	4.0%	81	9.6%
surface	1215	53.4%	633	74.6%
total	2275	100.0%	848	100.0%
Number of residues				
interface	34	11.8%	22	20.2%
surface	257	88.9%	109	100.0%
total	289	100.0%	109	100.0%
Solvent-accessible area, Å				
interface	766.0	5.5%	850.4	10.1%
total	13994.5	100.0%	8420.0	100.0%
Solvation energy, kcal/mol				
isolated structure	-266.0	100.0%	-93.0	100.0%
gain on complex formation	3.1	-1.1%	-1.0	1.1%
average gain	-1.6	0.6%	-2.3	2.4%
P-value	0.933		0.670	

View structure 1 | interface | structure 2

Download structure 1 | interface | structure 2

This interface scored

0.147

in Complex Formation Significance Score (CSS).

CSS ranges from 0 to 1 as interface relevance to complex formation increases.

Achieved CSS implies that the interface plays an auxiliary role in complex formatior

Hydrogen bonds XML

##	Structure 1	Dist. [Å]	Structure 2
1	X:LYS 146[NZ]	3.73	B:LYS 40[O]
2	X:LYS 179[NZ]	2.83	B:SER 89[O]
3	X:LYS 104[NZ]	2.84	B:ASP 93[OD1]
4	X:TYS 335[O3]	2.79	B:VAL 38[N]
5	X:TYS 335[O1]	3.07	B:TYR 39[N]
6	X:GLU 197[OE1]	2.76	B:LYS 46[NZ]
7	X:GLU 103[OE1]	2.69	B:THR 95[OG1]
8	X:GLU 50[OE2]	3.40	B:ARG 97[NH2]
9	X:GLU 76[OE1]	3.21	B:ARG 97[NH2]
10	X:GLU 34[OE1]	2.67	B:TYR 103[OH]
11	X:GLU 34[OE2]	2.72	B:TYR 103[OH]

Salt bridges XML

##	Structure 1	Dist. [Å]	Structure 2
1	X:LYS 179[NZ]	3.70	B:ASP 90[OD1]
2	X:LYS 104[NZ]	2.84	B:ASP 93[OD1]
3	X:LYS 104[NZ]	3.36	B:ASP 93[OD2]
4	X:GLU 197[OE1]	2.76	B:LYS 46[NZ]
5	X:GLU 197[OE2]	3.28	B:LYS 46[NZ]
6	X:GLU 76[OE1]	3.96	B:ARG 97[NE]
7	X:GLU 50[OE2]	3.40	B:ARG 97[NH2]
8	X:GLU 76[OE1]	3.21	B:ARG 97[NH2]

No disulfide bonds found

No covalent bonds found

Interfacing residues (not a contact table) XML Display level: Residues

Inaccessible residues HSDC Residues making **H**ydrogen/**D**isulphide bond, **S**alt bridge or **C**ovalent link

Solvent-accessible residues Interfacing residues

ASA Accessible Surface Area, Å² **BSA** Buried Surface Area, Å² **$\Delta^i G$** Solvation energy effect, kcal/mol |||| Buried area percentage, one bar per 10%

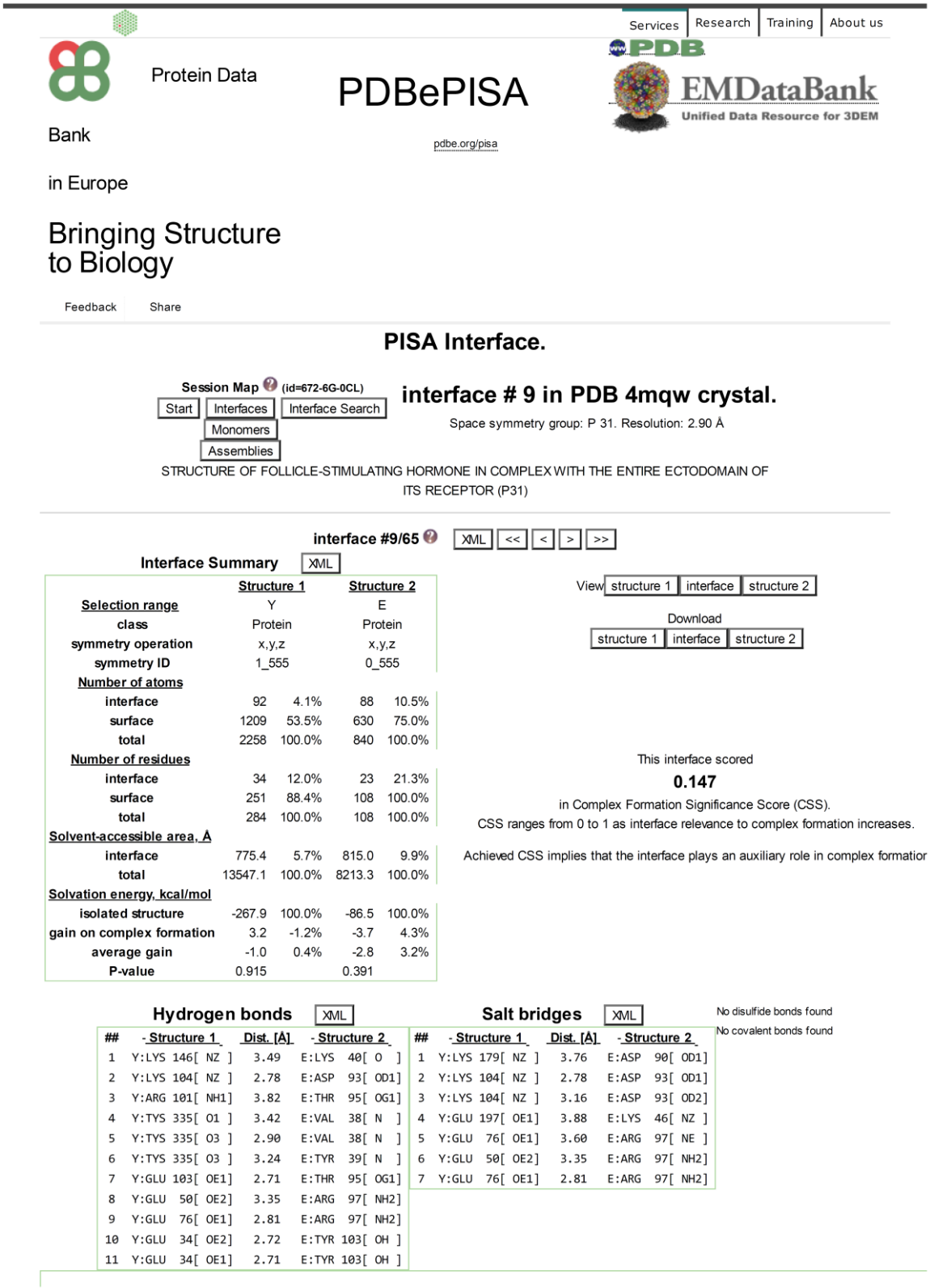
##	Structure 1	HSDC	ASA	BSA	$\Delta^i G$	##	Structure 2	HSDC	ASA	BSA	$\Delta^i G$
1	X:CYS 18		117.41	0.00	0.00	1	B:ASN 1		147.44	0.00	0.00
2	X:HIS 19		165.43	0.00	0.00	2	B:SER 2		57.28	0.00	0.00
3	X:HIS 20		16.04	0.00	0.00	3	B:CYS 3		18.80	0.00	0.00
4	X:ARG 21		141.01	0.00	0.00	4	B:GLU 4		106.86	0.00	0.00
5	X:ILE 22		38.64	0.00	0.00	5	B:LEU 5		83.92	0.00	0.00
6	X:CYS 23		1.96	0.00	0.00	6	B:THR 6		44.78	0.00	0.00
7	X:HIS 24		102.08	0.00	0.00	7	B:ASN 7		130.56	0.00	0.00
8	X:CYS 25		19.34	0.00	0.00	8	B:ILE 8		41.50	0.00	0.00
9	X:SER 26		67.76	0.00	0.00	9	B:THR 9		30.40	0.00	0.00
10	X:ASN 27		131.63	0.00	0.00	10	B:ILE 10		25.66	0.00	0.00
11	X:ARG 28		95.77	0.00	0.00	11	B:ALA 11		26.64	0.00	0.00
12	X:VAL 29		31.93	0.00	0.00	12	B:ILE 12		5.94	0.00	0.00
13	X:PHE 30		4.22	0.00	0.00	13	B:GLU 13		70.22	0.00	0.00
14	X:LEU 31		34.30	0.00	0.00	14	B:LYS 14		11.18	0.00	0.00
15	X:CYS 32		0.00	0.00	0.00	15	B:GLU 15		129.36	0.00	0.00
16	X:GLN 33		53.36	16.00 |||	-0.18	16	B:GLU 16		88.78	0.00	0.00
17	X:GLU 34	H	76.97	22.69 |||	-0.22	17	B:CYS 17		14.57	0.00	0.00
18	X:SER 35		65.12	0.00	0.00	18	B:ARG 18		176.03	0.00	0.00
19	X:LYS 36		114.91	0.00	0.00	19	B:PHE 19		65.01	0.00	0.00
20	X:VAL 37		0.00	0.00	0.00	20	B:CYS 20		31.94	0.00	0.00
21	X:THR 38		78.40	0.00	0.00	21	B:ILE 21		36.84	0.00	0.00
22	X:GLU 39		108.01	0.00	0.00	22	B:SER 22		74.86	0.00	0.00
23	X:ILE 40		18.44	0.00	0.00	23	B:ILE 23		30.12	0.00	0.00
24	X:PRO 41		7.37	0.00	0.00	24	B:ASN 24		125.73	0.00	0.00
25	X:SER 42		102.92	0.00	0.00	25	B:THR 25		10.08	0.00	0.00
26	X:ASP 43		66.04	0.00	0.00	26	B:THR 26		44.06	0.00	0.00
27	X:LEU 44		6.23	0.00	0.00	27	B:TRP 27		52.54	0.00	0.00
28	X:PRO 45		50.57	0.00	0.00	28	B:CYS 28		26.15	0.00	0.00
29	X:ARG 46		117.44	0.00	0.00	29	B:ALA 29		48.01	0.00	0.00
30	X:ASN 47		71.77	0.00	0.00	30	B:GLY 30		42.52	0.00	0.00
31	X:ALA 48		0.00	0.00	0.00	31	B:TYR 31		174.47	0.00	0.00
32	X:ILE 49		40.68	0.00	0.00	32	B:CYS 32		35.81	0.00	0.00
33	X:GLU 50	HS	27.95	5.16 ||	-0.06	33	B:TYR 33		140.39	0.00	0.00
34	X:LEU 51		0.17	0.00	0.00	34	B:THR 34		72.32	0.00	0.00
35	X:ARG 52		83.22	41.50 |||||	-0.86	35	B:ARG 35		167.76	5.20 |	0.08
36	X:PHE 53		0.78	0.00	0.00	36	B:ASP 36		123.51	0.50 |	-0.01
37	X:VAL 54		16.75	6.02 ||||	0.10	37	B:LEU 37		45.36	22.08 |||||	0.35
38	X:LEU 55		77.49	35.07 |||||	0.56	38	B:VAL 38	H	153.08	14.39 |	0.15
39	X:THR 56		0.98	0.00	0.00	39	B:TYR 39	H	172.35	22.97 ||	0.25
40	X:LYS 57		76.97	0.00	0.00	40	B:LYS 40	H	122.03	28.08 |||	0.11
41	X:LEU 58		0.33	0.00	0.00	41	B:ASP 41		47.27	7.96 ||	-0.17
42	X:ARG 59		151.06	0.00	0.00	42	B:PRO 42		127.95	93.09 ||||||||	0.95
43	X:VAL 60		52.85	0.00	0.00	43	B:ALA 43		95.82	83.50 ||||||||	0.86
44	X:ILE 61		0.67	0.00	0.00	44	B:ARG 44		68.83	30.73 |||||	-0.91
45	X:GLN 62		68.32	0.00	0.00	45	B:PRO 45		93.35	28.28 ||||	0.45
46	X:LYS 63		128.72	0.00	0.00	46	B:LYS 46	HS	132.93	72.23 ||||||	-1.34
47	X:GLY 64		32.05	0.00	0.00	47	B:ILE 47		115.77	0.00	0.00
48	X:ALA 65		22.92	0.00	0.00	48	B:GLN 48		131.39	0.00	0.00
49	X:PHE 66		0.78	0.00	0.00	49	B:LYS 49		118.88	0.00	0.00
50	X:SER 67		27.75	0.00	0.00	50	B:THR 50		57.20	0.00	0.00
51	X:GLY 68		42.87	0.00	0.00	51	B:CYS 51		27.30	0.00	0.00
52	X:PHE 69		2.82	0.00	0.00	52	B:THR 52		16.12	0.00	0.00
53	X:GLY 70		32.66	0.00	0.00	53	B:PHE 53		38.44	0.00	0.00
54	X:ASP 71		45.91	0.00	0.00	54	B:LYS 54		96.17	0.00	0.00
55	X:LEU 72		0.00	0.00	0.00	55	B:GLU 55		93.16	0.00	0.00
56	X:GLU 73		58.33	0.00	0.00	56	B:LEU 56		54.25	0.00	0.00
57	X:LYS 74		63.94	0.00	0.00	57	B:VAL 57		76.39	0.00	0.00
58	X:ILE 75		1.22	0.00	0.00	58	B:TYR 58		141.24	0.00	0.00

59	X:GLU	76	HS	25.86	20.70	||||||||	-0.27	59	B:GLU	59		80.17	0.00	0.00
60	X:ILE	77		0.17	0.00		0.00	60	B:THR	60		81.87	0.00	0.00
61	X:SER	78		3.15	1.36	|||||	-0.00	61	B:VAL	61		36.14	0.00	0.00
62	X:GLN	79		82.45	40.05	|||||	-0.57	62	B:ARG	62		140.67	0.00	0.00
63	X:ASN	80		0.78	0.00		0.00	63	B:VAL	63		3.18	0.00	0.00
64	X:ASP	81		58.65	0.00		0.00	64	B:PRO	64		62.18	0.00	0.00
65	X:VAL	82		43.99	0.00		0.00	65	B:GLY	65		21.47	0.00	0.00
66	X:LEU	83		0.17	0.00		0.00	66	B:CYS	66		75.65	0.00	0.00
67	X:GLU	84		61.99	0.00		0.00	67	B:ALA	67		59.55	0.00	0.00
68	X:VAL	85		43.16	0.00		0.00	68	B:HIS	68		188.80	0.00	0.00
69	X:ILE	86		0.00	0.00		0.00	69	B:HIS	69		84.22	0.00	0.00
70	X:GLU	87		61.82	0.00		0.00	70	B:ALA	70		85.28	0.00	0.00
71	X:ALA	88		11.18	0.00		0.00	71	B:ASP	71		71.22	0.00	0.00
72	X:ASP	89		56.55	0.00		0.00	72	B:SER	72		42.84	0.00	0.00
73	X:VAL	90		0.00	0.00		0.00	73	B:LEU	73		100.89	0.00	0.00
74	X:PHE	91		0.00	0.00		0.00	74	B:TYR	74		101.80	0.00	0.00
75	X:SER	92		9.18	0.00		0.00	75	B:THR	75		66.61	0.00	0.00
76	X:ASN	93		105.91	0.00		0.00	76	B:TYR	76		16.56	0.00	0.00
77	X:LEU	94		1.92	0.00		0.00	77	B:PRO	77		42.81	0.00	0.00
78	X:PRO	95		78.79	0.00		0.00	78	B:VAL	78		13.06	0.00	0.00
79	X:LYS	96		106.98	0.00		0.00	79	B:ALA	79		4.54	0.00	0.00
80	X:LEU	97		0.00	0.00		0.00	80	B:THR	80		68.21	0.00	0.00
81	X:HIS	98		35.96	0.00		0.00	81	B:GLN	81		80.34	0.00	0.00
82	X:GLU	99		21.31	0.12	|	-0.00	82	B:CYS	82		21.05	0.00	0.00
83	X:ILE	100		0.00	0.00		0.00	83	B:HIS	83		57.35	0.00	0.00
84	X:ARG	101		51.99	37.29	|||||||	-0.61	84	B:CYS	84		33.07	0.00	0.00
85	X:ILE	102		0.00	0.00		0.00	85	B:GLY	85		7.92	0.00	0.00
86	X:GLU	103	H	24.62	22.37	||||||||	-0.25	86	B:LYS	86		147.43	0.00	0.00
87	X:LYS	104	HS	75.54	40.28	|||||	-0.25	87	B:CYS	87		36.31	0.00	0.00
88	X:ALA	105		0.00	0.00		0.00	88	B:ASP	88		66.60	0.00	0.00
89	X:ASN	106		98.48	0.00		0.00	89	B:SER	89	H	91.60	41.98	||||| -0.03
90	X:ASN	107		65.03	0.00		0.00	90	B:ASP	90	S	138.02	26.94	|| -0.10
91	X:LEU	108		0.00	0.00		0.00	91	B:SER	91		75.73	0.00	0.00
92	X:LEU	109		87.05	0.00		0.00	92	B:THR	92		44.74	0.00	0.00
93	X:TYR	110		111.98	0.00		0.00	93	B:ASP	93	HS	117.58	43.67	|||| -0.48
94	X:ILE	111		22.81	0.00		0.00	94	B:CYS	94		65.13	6.50	| -0.07
95	X:ASN	112		36.77	0.00		0.00	95	B:THR	95	H	85.24	33.59	|||| -0.03
96	X:PRO	113		69.35	0.00		0.00	96	B:VAL	96		122.87	32.48	||| 0.52
97	X:GLU	114		65.94	0.00		0.00	97	B:ARG	97	HS	196.83	104.82	|||||| -1.06
98	X:ALA	115		0.00	0.00		0.00	98	B:GLY	98		59.80	10.68	|| 0.13
99	X:PHE	116		0.61	0.00		0.00	99	B:LEU	99		147.68	90.05	||||||| 1.42
100	X:GLN	117		31.41	0.00		0.00	100	B:GLY	100		41.30	0.00	0.00
101	X:ASN	118		89.74	0.00		0.00	101	B:PRO	101		84.43	0.00	0.00
102	X:LEU	119		0.00	0.00		0.00	102	B:SER	102		51.35	0.00	0.00
103	X:PRO	120		32.62	0.00		0.00	103	B:TYR	103	H	108.70	50.74	||||| -0.08
104	X:ASN	121		52.49	0.00		0.00	104	B:CYS	104		17.93	0.00	0.00
105	X:LEU	122		0.00	0.00		0.00	105	B:SER	105		62.80	0.00	0.00
106	X:GLN	123		78.52	0.00		0.00	106	B:PHE	106		77.72	0.00	0.00
107	X:TYR	124		56.32	0.00		0.00	107	B:GLY	107		32.50	0.00	0.00
108	X:LEU	125		0.00	0.00		0.00	108	B:GLU	108		173.16	0.00	0.00
109	X:LEU	126		18.40	4.01	|||	0.06	109	B:MET	109		189.77	0.00	0.00
110	X:ILE	127		0.00	0.00		0.00							
111	X:SER	128		19.44	0.86	|	-0.01							
112	X:ASN	129		79.38	4.41	|	-0.04							
113	X:THR	130		6.42	0.00		0.00							
114	X:GLY	131		5.69	0.00		0.00							
115	X:ILE	132		1.84	0.00		0.00							
116	X:LYS	133		103.06	0.00		0.00							
117	X:HIS	134		116.06	0.00		0.00							
118	X:LEU	135		28.08	0.00		0.00							
119	X:PRO	136		6.39	0.00		0.00							
120	X:ASP	137		40.32	0.00		0.00							
121	X:VAL	138		1.04	0.00		0.00							
122	X:HIS	139		76.69	0.00		0.00							
123	X:LYS	140		68.01	0.00		0.00							

124	X:ILE 141		0.00	0.00		0.00
125	X:HIS 142		74.76	0.00		0.00
126	X:SER 143		0.00	0.00		0.00
127	X:LEU 144		113.01	0.00		0.00
128	X:GLN 145		56.52	0.00		0.00
129	X:LYS 146	H	124.02	43.27	||||	-0.20
130	X:VAL 147		3.24	0.00		0.00
131	X:LEU 148		35.97	0.00		0.00
132	X:LEU 149		0.17	0.00		0.00
133	X:ASP 150		8.71	0.00		0.00
134	X:ILE 151		0.00	0.00		0.00
135	X:GLN 152		41.14	12.27	|||	-0.21
136	X:ASP 153		53.59	6.17	||	-0.07
137	X:ASN 154		0.00	0.00		0.00
138	X:ILE 155		125.97	0.00		0.00
139	X:ASN 156		39.39	0.00		0.00
140	X:ILE 157		0.33	0.00		0.00
141	X:HIS 158		75.11	0.00		0.00
142	X:THR 159		36.76	0.00		0.00
143	X:ILE 160		0.00	0.00		0.00
144	X:GLU 161		85.53	0.00		0.00
145	X:ARG 162		165.10	0.00		0.00
146	X:ASN 163		46.44	0.00		0.00
147	X:SER 164		25.88	0.00		0.00
148	X:PHE 165		4.42	0.00		0.00
149	X:VAL 166		50.44	0.00		0.00
150	X:GLY 167		15.24	0.00		0.00
151	X:LEU 168		0.52	0.00		0.00
152	X:SER 169		23.80	0.00		0.00
153	X:PHE 170		136.08	0.00		0.00
154	X:GLU 171		66.06	0.00		0.00
155	X:SER 172		7.94	0.00		0.00
156	X:VAL 173		5.67	0.00		0.00
157	X:ILE 174		47.63	30.93	||||||	0.49
158	X:LEU 175		0.00	0.00		0.00
159	X:TRP 176		70.77	10.33	||	0.17
160	X:LEU 177		0.00	0.00		0.00
161	X:ASN 178		12.65	1.16	|	-0.01
162	X:LYS 179	HS	86.60	58.57	||||||	-0.54
163	X:ASN 180		8.95	0.00		0.00
164	X:GLY 181		8.20	0.00		0.00
165	X:ILE 182		0.00	0.00		0.00
166	X:GLN 183		79.83	0.00		0.00
167	X:GLU 184		100.82	0.00		0.00
168	X:ILE 185		6.46	0.00		0.00
169	X:HIS 186		77.74	0.00		0.00
170	X:ASN 187		70.65	0.00		0.00
171	X:SER 188		17.73	0.00		0.00
172	X:ALA 189		0.00	0.00		0.00
173	X:PHE 190		0.00	0.00		0.00
174	X:ASN 191		49.38	0.00		0.00
175	X:GLY 192		43.55	0.00		0.00
176	X:THR 193		13.94	0.00		0.00
177	X:GLN 194		82.42	0.00		0.00
178	X:LEU 195		3.13	0.00		0.00
179	X:ASP 196		44.38	34.64	|||||||	-0.04
180	X:GLU 197	HS	33.79	16.71	|||||	-0.18
181	X:LEU 198		0.74	0.00		0.00
182	X:ASN 199		24.88	0.00		0.00
183	X:LEU 200		0.17	0.00		0.00
184	X:SER 201		3.44	0.00		0.00
185	X:ASP 202		37.50	4.19	||	0.01
186	X:ASN 203		0.84	0.00		0.00
187	X:ASN 204		83.66	0.00		0.00
188	X:ASN 205		60.70	0.00		0.00

189	X:LEU 206	0.17	0.00		0.00
190	X:GLU 207	70.33	0.00		0.00
191	X:GLU 208	105.96	0.00		0.00
192	X:LEU 209	11.35	0.00		0.00
193	X:PRO 210	23.77	0.00		0.00
194	X:ASN 211	84.55	0.00		0.00
195	X:ASP 212	62.70	0.00		0.00
196	X:VAL 213	0.33	0.00		0.00
197	X:PHE 214	4.64	0.00		0.00
198	X:HIS 215	94.02	0.00		0.00
199	X:GLY 216	41.75	0.00		0.00
200	X:ALA 217	18.58	0.00		0.00
201	X:SER 218	62.10	0.00		0.00
202	X:GLY 219	3.38	0.00		0.00
203	X:PRO 220	0.17	0.00		0.00
204	X:VAL 221	53.88	29.80	||||||	0.48
205	X:ILE 222	39.84	29.62	||||||||	0.47
206	X:LEU 223	0.00	0.00		0.00
207	X:ASP 224	22.05	0.00		0.00
208	X:ILE 225	0.00	0.00		0.00
209	X:SER 226	1.74	0.00		0.00
210	X:ARG 227	98.61	0.00		0.00
211	X:THR 228	6.83	0.00		0.00
212	X:ARG 229	100.35	0.00		0.00
213	X:ILE 230	0.00	0.00		0.00
214	X:HIS 231	91.24	0.00		0.00
215	X:SER 232	51.34	0.00		0.00
216	X:LEU 233	15.30	0.00		0.00
217	X:PRO 234	1.90	0.00		0.00
218	X:SER 235	75.23	0.00		0.00
219	X:TYR 236	79.03	0.00		0.00
220	X:GLY 237	2.01	0.00		0.00
221	X:LEU 238	4.89	0.00		0.00
222	X:GLU 239	85.37	0.00		0.00
223	X:ASN 240	66.91	0.00		0.00
224	X:LEU 241	0.00	0.00		0.00
225	X:LYS 242	88.31	18.53	|||	-0.48
226	X:LYS 243	48.45	24.36	||||||	-0.02
227	X:LEU 244	0.27	0.00		0.00
228	X:ARG 245	75.08	0.00		0.00
229	X:ALA 246	2.16	0.00		0.00
230	X:ARG 247	100.10	0.00		0.00
231	X:SER 248	44.82	0.00		0.00
232	X:THR 249	1.27	0.00		0.00
233	X:TYR 250	132.42	0.00		0.00
234	X:ASN 251	47.21	0.00		0.00
235	X:LEU 252	9.22	0.00		0.00
236	X:LYS 253	133.11	0.00		0.00
237	X:LYS 254	150.57	0.00		0.00
238	X:LEU 255	32.64	0.00		0.00
239	X:PRO 256	23.71	0.00		0.00
240	X:THR 257	78.49	0.00		0.00
241	X:LEU 258	51.85	0.00		0.00
242	X:GLU 259	124.91	0.00		0.00
243	X:LYS 260	85.06	0.00		0.00
244	X:LEU 261	0.00	0.00		0.00
245	X:VAL 262	100.48	0.00		0.00
246	X:ALA 263	33.58	0.00		0.00
247	X:LEU 264	8.22	0.00		0.00
248	X:MET 265	76.48	6.19	|	0.10
249	X:GLU 266	45.27	0.00		0.00
250	X:ALA 267	1.29	0.00		0.00
251	X:SER 268	20.32	0.00		0.00
252	X:LEU 269	3.39	0.00		0.00
253	X:THR 270	27.67	0.00		0.00

254	X:TYR 271		53.44	0.00	0.00
255	X:PRO 272		26.30	0.00	0.00
256	X:SER 273		54.37	0.00	0.00
257	X:HIS 274		22.75	0.00	0.00
258	X:CYS 275		8.43	0.00	0.00
259	X:CYS 276		37.49	0.00	0.00
260	X:ALA 277		76.03	0.00	0.00
261	X:PHE 278		9.70	0.00	0.00
262	X:ALA 279		56.30	0.00	0.00
263	X:ASN 280		121.34	0.00	0.00
264	X:TRP 281		54.95	0.00	0.00
265	X:ARG 282		132.03	0.00	0.00
266	X:ILE 291		165.39	0.00	0.00
267	X:CYS 292		58.06	0.00	0.00
268	X:ASN 293		111.81	0.00	0.00
269	X:LYS 294		142.04	0.00	0.00
270	X:ASP 334		154.37	6.84 |	-0.04
271	X:TYS 335	H	285.76	129.02 |||||	-0.33
272	X:ASP 336		98.65	0.00	0.00
273	X:LEU 337		89.94	0.00	0.00
274	X:CYS 338		133.42	5.52 |	-0.06
275	X:VAL 342		205.83	0.00	0.00
276	X:ASP 343		58.65	0.00	0.00
277	X:VAL 344		23.35	0.00	0.00
278	X:THR 345		92.80	0.00	0.00
279	X:CYS 346		15.28	0.00	0.00
280	X:SER 347		31.08	0.00	0.00
281	X:PRO 348		36.93	0.00	0.00
282	X:LYS 349		153.42	0.00	0.00
283	X:PRO 350		47.86	0.00	0.00
284	X:ASP 351		120.71	0.00	0.00
285	X:ALA 352		100.21	0.00	0.00
286	X:PHE 353		129.97	0.00	0.00
287	X:ASN 354		53.47	0.00	0.00
288	X:PRO 355		108.21	0.00	0.00
289	X:CYS 356		109.92	0.00	0.00



Services | Research | Training | About us

Protein Data Bank in Europe

PDBePISA

pdbe.org/pisa

PDB EMDataBank Unified Data Resource for 3DEM

Bringing Structure to Biology

Feedback Share

PISA Interface.

Session Map (id=672-6G-0CL)

Start | Interfaces | Interface Search | Monomers | Assemblies

interface # 9 in PDB 4mqw crystal.

Space symmetry group: P 31. Resolution: 2.90 Å

STRUCTURE OF FOLLICLE-STIMULATING HORMONE IN COMPLEX WITH THE ENTIRE ECTODOMAIN OF ITS RECEPTOR (P31)

interface #9/65 XML << < > >>

Interface Summary XML

	Structure 1		Structure 2	
Selection range	Y		E	
class	Protein		Protein	
symmetry operation	x,y,z		x,y,z	
symmetry ID	1_555		0_555	
Number of atoms				
interface	92	4.1%	88	10.5%
surface	1209	53.5%	630	75.0%
total	2258	100.0%	840	100.0%
Number of residues				
interface	34	12.0%	23	21.3%
surface	251	88.4%	108	100.0%
total	284	100.0%	108	100.0%
Solvent-accessible area, Å				
interface	775.4	5.7%	815.0	9.9%
total	13547.1	100.0%	8213.3	100.0%
Solvation energy, kcal/mol				
isolated structure	-267.9	100.0%	-86.5	100.0%
gain on complex formation	3.2	-1.2%	-3.7	4.3%
average gain	-1.0	0.4%	-2.8	3.2%
P-value	0.915		0.391	

View structure 1 | interface | structure 2

Download structure 1 | interface | structure 2

This interface scored

0.147

in Complex Formation Significance Score (CSS).

CSS ranges from 0 to 1 as interface relevance to complex formation increases.

Achieved CSS implies that the interface plays an auxiliary role in complex formatior

Hydrogen bonds XML

##	Structure 1	Dist. [Å]	Structure 2
1	Y:LYS 146[NZ]	3.49	E:LYS 40[O]
2	Y:LYS 104[NZ]	2.78	E:ASP 93[OD1]
3	Y:ARG 101[NH1]	3.82	E:THR 95[OG1]
4	Y:TYS 335[O1]	3.42	E:VAL 38[N]
5	Y:TYS 335[O3]	2.90	E:VAL 38[N]
6	Y:TYS 335[O3]	3.24	E:TYR 39[N]
7	Y:GLU 103[OE1]	2.71	E:THR 95[OG1]
8	Y:GLU 50[OE2]	3.35	E:ARG 97[NH2]
9	Y:GLU 76[OE1]	2.81	E:ARG 97[NH2]
10	Y:GLU 34[OE2]	2.72	E:TYR 103[OH]
11	Y:GLU 34[OE1]	2.71	E:TYR 103[OH]

Salt bridges XML

##	Structure 1	Dist. [Å]	Structure 2
1	Y:LYS 179[NZ]	3.76	E:ASP 90[OD1]
2	Y:LYS 104[NZ]	2.78	E:ASP 93[OD1]
3	Y:LYS 104[NZ]	3.16	E:ASP 93[OD2]
4	Y:GLU 197[OE1]	3.88	E:LYS 46[NZ]
5	Y:GLU 76[OE1]	3.60	E:ARG 97[NE]
6	Y:GLU 50[OE2]	3.35	E:ARG 97[NH2]
7	Y:GLU 76[OE1]	2.81	E:ARG 97[NH2]

No disulfide bonds found

No covalent bonds found

Interfacing residues (not a contact table) XML Display level: Residues

Inaccessible residues HSDC Residues making **H**ydrogen/**D**isulphide bond, **S**alt bridge or **C**ovalent link

Solvent-accessible residues Interfacing residues

ASA Accessible Surface Area, Å² **BSA** Buried Surface Area, Å² **$\Delta^i G$** Solvation energy effect, kcal/mol |||| Buried area percentage, one bar per 10%

##	Structure 1	HSDC	ASA	BSA	$\Delta^i G$	##	Structure 2	HSDC	ASA	BSA	$\Delta^i G$
1	Y:CYS 18		116.02	0.00	0.00	1	E:ASN 1		151.77	0.00	0.00
2	Y:HIS 19		161.36	0.00	0.00	2	E:SER 2		61.70	0.00	0.00
3	Y:HIS 20		15.73	0.00	0.00	3	E:CYS 3		15.73	0.00	0.00
4	Y:ARG 21		156.33	0.00	0.00	4	E:GLU 4		111.81	0.00	0.00
5	Y:ILE 22		35.96	0.00	0.00	5	E:LEU 5		82.85	0.00	0.00
6	Y:CYS 23		2.42	0.00	0.00	6	E:THR 6		48.90	0.00	0.00
7	Y:HIS 24		97.25	0.00	0.00	7	E:ASN 7		129.12	0.00	0.00
8	Y:CYS 25		21.51	0.00	0.00	8	E:ILE 8		37.03	0.00	0.00
9	Y:SER 26		79.07	0.00	0.00	9	E:THR 9		60.65	0.00	0.00
10	Y:ASN 27		139.31	0.00	0.00	10	E:ILE 10		26.06	0.00	0.00
11	Y:ARG 28		99.27	0.00	0.00	11	E:ALA 11		21.77	0.00	0.00
12	Y:VAL 29		33.72	0.00	0.00	12	E:ILE 12		6.66	0.00	0.00
13	Y:PHE 30		3.90	0.00	0.00	13	E:GLU 13		71.80	0.00	0.00
14	Y:LEU 31		36.93	0.00	0.00	14	E:LYS 14		5.94	0.00	0.00
15	Y:CYS 32		0.16	0.00	0.00	15	E:GLU 15		134.78	0.00	0.00
16	Y:GLN 33		57.37	18.58 ||||	-0.22	16	E:GLU 16		79.46	0.00	0.00
17	Y:GLU 34	H	83.98	23.56 |||	-0.27	17	E:CYS 17		16.53	0.00	0.00
18	Y:SER 35		69.97	0.00	0.00	18	E:ARG 18		174.21	0.00	0.00
19	Y:LYS 36		123.23	0.00	0.00	19	E:PHE 19		67.17	0.00	0.00
20	Y:VAL 37		0.84	0.00	0.00	20	E:CYS 20		32.01	0.00	0.00
21	Y:THR 38		84.84	0.00	0.00	21	E:ILE 21		33.86	0.00	0.00
22	Y:GLU 39		123.18	0.00	0.00	22	E:SER 22		83.86	0.00	0.00
23	Y:ILE 40		20.95	0.00	0.00	23	E:ILE 23		30.77	0.00	0.00
24	Y:PRO 41		6.58	0.00	0.00	24	E:ASN 24		119.72	0.00	0.00
25	Y:SER 42		104.31	0.00	0.00	25	E:THR 25		9.89	0.00	0.00
26	Y:ASP 43		72.40	0.00	0.00	26	E:THR 26		47.52	0.00	0.00
27	Y:LEU 44		3.08	0.00	0.00	27	E:TRP 27		52.15	0.00	0.00
28	Y:PRO 45		48.31	0.00	0.00	28	E:CYS 28		26.94	0.00	0.00
29	Y:ARG 46		122.20	0.00	0.00	29	E:ALA 29		46.57	0.00	0.00
30	Y:ASN 47		72.74	0.00	0.00	30	E:GLY 30		42.96	0.00	0.00
31	Y:ALA 48		0.00	0.00	0.00	31	E:TYR 31		176.73	0.00	0.00
32	Y:ILE 49		37.50	0.00	0.00	32	E:CYS 32		32.15	0.00	0.00
33	Y:GLU 50	HS	27.88	7.37 |||	-0.08	33	E:TYR 33		137.15	0.00	0.00
34	Y:LEU 51		0.00	0.00	0.00	34	E:THR 34		71.75	0.00	0.00
35	Y:ARG 52		75.47	35.68 |||||	-0.74	35	E:ARG 35		168.96	4.53 |	0.07
36	Y:PHE 53		0.62	0.00	0.00	36	E:ASP 36		122.04	0.25 |	-0.00
37	Y:VAL 54		18.75	7.02 ||||	0.11	37	E:LEU 37		50.64	25.22 |||||	0.40
38	Y:LEU 55		81.34	31.99 ||||	0.51	38	E:VAL 38	H	154.26	17.23 ||	0.17
39	Y:THR 56		0.12	0.00	0.00	39	E:TYR 39	H	167.72	21.55 ||	0.26
40	Y:LYS 57		74.45	0.00	0.00	40	E:LYS 40	H	121.47	29.57 |||	0.17
41	Y:LEU 58		1.33	0.00	0.00	41	E:ASP 41		50.15	6.86 ||	-0.09
42	Y:ARG 59		137.80	0.00	0.00	42	E:PRO 42		117.84	78.76 |||||||	0.93
43	Y:VAL 60		51.82	0.00	0.00	43	E:ALA 43		93.31	77.05 ||||||||	0.82
44	Y:ILE 61		0.67	0.00	0.00	44	E:ARG 44		56.87	23.83 |||||	-0.06
45	Y:GLN 62		62.91	0.00	0.00	45	E:PRO 45		96.24	30.15 ||||	0.48
46	Y:LYS 63		141.36	0.00	0.00	46	E:LYS 46	S	124.31	56.16 |||||	0.27
47	Y:GLY 64		26.22	0.00	0.00	47	E:ILE 47		119.76	0.00	0.00
48	Y:ALA 65		19.89	0.00	0.00	48	E:GLN 48		131.28	0.00	0.00
49	Y:PHE 66		0.00	0.00	0.00	49	E:LYS 49		114.58	0.00	0.00
50	Y:SER 67		29.69	0.00	0.00	50	E:THR 50		56.13	0.00	0.00
51	Y:GLY 68		38.46	0.00	0.00	51	E:CYS 51		29.21	0.00	0.00
52	Y:PHE 69		4.69	0.00	0.00	52	E:THR 52		17.26	0.00	0.00
53	Y:GLY 70		36.03	0.00	0.00	53	E:PHE 53		39.28	0.00	0.00
54	Y:ASP 71		48.21	0.00	0.00	54	E:LYS 54		101.66	0.00	0.00
55	Y:LEU 72		0.00	0.00	0.00	55	E:GLU 55		82.18	0.00	0.00
56	Y:GLU 73		59.55	0.00	0.00	56	E:LEU 56		52.69	0.00	0.00
57	Y:LYS 74		61.52	0.51 |	0.01	57	E:VAL 57		75.24	0.00	0.00
58	Y:ILE 75		1.63	0.00	0.00	58	E:TYR 58		143.25	0.00	0.00

59	Y:GLU	76	HS	23.90	18.03	||||||||	-0.25	59	E:GLU	59		82.28	0.00	0.00
60	Y:ILE	77		0.43	0.00		0.00	60	E:THR	60		85.68	0.00	0.00
61	Y:SER	78		2.42	2.18	||||||||	-0.02	61	E:VAL	61		36.80	0.00	0.00
62	Y:GLN	79		75.74	36.86	|||||	-0.54	62	E:ARG	62		167.14	0.00	0.00
63	Y:ASN	80		0.79	0.00		0.00	63	E:VAL	63		2.67	0.00	0.00
64	Y:ASP	81		63.67	0.00		0.00	64	E:PRO	64		67.76	0.00	0.00
65	Y:VAL	82		42.97	0.00		0.00	65	E:GLY	65		23.31	0.00	0.00
66	Y:LEU	83		0.50	0.00		0.00	66	E:CYS	66		65.04	0.00	0.00
67	Y:GLU	84		67.24	0.00		0.00	67	E:ALA	67		77.16	0.00	0.00
68	Y:VAL	85		40.18	0.00		0.00	68	E:HIS	68		186.32	0.00	0.00
69	Y:ILE	86		0.61	0.00		0.00	69	E:HIS	69		91.84	0.00	0.00
70	Y:GLU	87		66.68	0.00		0.00	70	E:ALA	70		87.86	0.00	0.00
71	Y:ALA	88		11.20	0.00		0.00	71	E:ASP	71		84.95	0.00	0.00
72	Y:ASP	89		55.28	0.00		0.00	72	E:SER	72		43.49	0.00	0.00
73	Y:VAL	90		0.00	0.00		0.00	73	E:LEU	73		114.44	0.00	0.00
74	Y:PHE	91		0.00	0.00		0.00	74	E:TYR	74		101.42	0.00	0.00
75	Y:SER	92		4.65	0.00		0.00	75	E:THR	75		64.66	0.00	0.00
76	Y:ASN	93		102.22	0.00		0.00	76	E:TYR	76		14.80	0.00	0.00
77	Y:LEU	94		0.58	0.00		0.00	77	E:PRO	77		42.65	0.00	0.00
78	Y:PRO	95		73.93	0.00		0.00	78	E:VAL	78		12.06	0.00	0.00
79	Y:LYS	96		106.57	0.00		0.00	79	E:ALA	79		4.53	0.00	0.00
80	Y:LEU	97		0.00	0.00		0.00	80	E:THR	80		62.83	0.00	0.00
81	Y:HIS	98		38.02	0.00		0.00	81	E:GLN	81		75.72	0.00	0.00
82	Y:GLU	99		28.62	0.00		0.00	82	E:CYS	82		22.91	0.00	0.00
83	Y:ILE	100		0.00	0.00		0.00	83	E:HIS	83		61.34	0.00	0.00
84	Y:ARG	101	H	60.29	45.37	||||||||	-0.81	84	E:CYS	84		31.24	0.00	0.00
85	Y:ILE	102		0.17	0.00		0.00	85	E:GLY	85		6.66	0.00	0.00
86	Y:GLU	103	H	25.89	23.48	|||||||||	-0.29	86	E:LYS	86		128.81	0.00	0.00
87	Y:LYS	104	HS	80.75	43.73	||||||	-0.31	87	E:CYS	87		38.49	0.00	0.00
88	Y:ALA	105		0.00	0.00		0.00	88	E:ASP	88		42.81	0.00	0.00
89	Y:ASN	106		95.27	0.00		0.00	89	E:SER	89		88.28	42.49 |||||	0.11
90	Y:ASN	107		69.38	0.00		0.00	90	E:ASP	90	S	136.81	25.75 ||	-0.01
91	Y:LEU	108		0.00	0.00		0.00	91	E:SER	91		77.36	0.00	0.00
92	Y:LEU	109		81.15	0.00		0.00	92	E:THR	92		43.72	0.00	0.00
93	Y:TYR	110		111.49	0.00		0.00	93	E:ASP	93	HS	119.38	43.16 ||||	-0.49
94	Y:ILE	111		25.85	0.00		0.00	94	E:CYS	94		68.73	6.38 |	-0.07
95	Y:ASN	112		33.82	0.00		0.00	95	E:THR	95	H	82.20	36.81 |||||	0.01
96	Y:PRO	113		66.53	0.00		0.00	96	E:VAL	96		123.76	30.29 |||	0.48
97	Y:GLU	114		66.13	0.00		0.00	97	E:ARG	97	HS	199.51	109.30 ||||||	-1.19
98	Y:ALA	115		0.00	0.00		0.00	98	E:GLY	98		59.76	10.03 ||	0.14
99	Y:PHE	116		1.09	0.00		0.00	99	E:LEU	99		143.22	86.24 |||||||	1.31
100	Y:GLN	117		34.61	0.00		0.00	100	E:GLY	100		42.19	0.00	0.00
101	Y:ASN	118		76.63	0.00		0.00	101	E:PRO	101		77.40	0.00	0.00
102	Y:LEU	119		0.00	0.00		0.00	102	E:SER	102		50.65	0.00	0.00
103	Y:PRO	120		36.78	0.00		0.00	103	E:TYR	103	H	90.30	52.21 ||||||	-0.03
104	Y:ASN	121		51.50	0.00		0.00	104	E:CYS	104		8.55	0.00	0.00
105	Y:LEU	122		0.00	0.00		0.00	105	E:SER	105		64.24	1.20 |	0.01
106	Y:GLN	123		71.85	0.00		0.00	106	E:PHE	106		61.46	0.00	0.00
107	Y:TYR	124		52.14	0.00		0.00	107	E:GLY	107		48.76	0.00	0.00
108	Y:LEU	125		0.00	0.00		0.00	108	E:GLU	108		165.02	0.00	0.00
109	Y:LEU	126		17.73	3.35 ||		0.05							
110	Y:ILE	127		0.00	0.00		0.00							
111	Y:SER	128		19.41	0.86 |		-0.01							
112	Y:ASN	129		83.24	3.37 |		-0.03							
113	Y:THR	130		6.62	0.00		0.00							
114	Y:GLY	131		5.36	0.00		0.00							
115	Y:ILE	132		4.01	0.00		0.00							
116	Y:LYS	133		96.36	0.00		0.00							
117	Y:HIS	134		116.35	0.00		0.00							
118	Y:LEU	135		27.23	0.00		0.00							
119	Y:PRO	136		8.21	0.00		0.00							
120	Y:ASP	137		40.39	0.00		0.00							
121	Y:VAL	138		3.08	0.00		0.00							
122	Y:HIS	139		78.98	0.00		0.00							
123	Y:LYS	140		71.91	0.00		0.00							

124	Y:ILE 141		0.00	0.00		0.00
125	Y:HIS 142		66.97	0.00		0.00
126	Y:SER 143		0.00	0.00		0.00
127	Y:LEU 144		114.14	0.00		0.00
128	Y:GLN 145		65.96	0.00		0.00
129	Y:LYS 146	H	122.05	36.11	|||	-0.93
130	Y:VAL 147		2.87	0.00		0.00
131	Y:LEU 148		37.75	0.00		0.00
132	Y:LEU 149		0.50	0.00		0.00
133	Y:ASP 150		9.20	0.00		0.00
134	Y:ILE 151		0.00	0.00		0.00
135	Y:GLN 152		42.10	13.25	||||	-0.22
136	Y:ASP 153		57.13	8.51	||	-0.08
137	Y:ASN 154		0.00	0.00		0.00
138	Y:ILE 155		127.03	0.00		0.00
139	Y:ASN 156		35.49	0.00		0.00
140	Y:ILE 157		0.00	0.00		0.00
141	Y:HIS 158		73.84	0.00		0.00
142	Y:THR 159		35.88	0.00		0.00
143	Y:ILE 160		0.00	0.00		0.00
144	Y:GLU 161		87.10	0.00		0.00
145	Y:ARG 162		157.60	0.00		0.00
146	Y:ASN 163		49.31	0.00		0.00
147	Y:SER 164		20.64	0.00		0.00
148	Y:PHE 165		4.64	0.00		0.00
149	Y:VAL 166		50.10	0.00		0.00
150	Y:GLY 167		13.03	0.00		0.00
151	Y:LEU 168		1.08	0.00		0.00
152	Y:SER 169		22.12	0.00		0.00
153	Y:PHE 170		139.67	0.00		0.00
154	Y:GLU 171		66.22	0.00		0.00
155	Y:SER 172		9.89	0.00		0.00
156	Y:VAL 173		4.52	0.00		0.00
157	Y:ILE 174		47.68	22.41	|||||	0.36
158	Y:LEU 175		0.00	0.00		0.00
159	Y:TRP 176		69.84	7.36	||	0.12
160	Y:LEU 177		0.00	0.00		0.00
161	Y:ASN 178		12.50	0.58			-0.01
162	Y:LYS 179	S	88.68	60.05	|||||||	-0.42
163	Y:ASN 180		9.57	0.00		0.00
164	Y:GLY 181		15.18	0.00		0.00
165	Y:ILE 182		0.00	0.00		0.00
166	Y:GLN 183		69.64	0.00		0.00
167	Y:GLU 184		85.97	0.00		0.00
168	Y:ILE 185		6.16	0.00		0.00
169	Y:HIS 186		71.48	0.00		0.00
170	Y:ASN 187		72.36	0.00		0.00
171	Y:SER 188		23.07	0.00		0.00
172	Y:ALA 189		0.00	0.00		0.00
173	Y:PHE 190		0.00	0.00		0.00
174	Y:ASN 191		40.79	0.00		0.00
175	Y:GLY 192		43.58	0.00		0.00
176	Y:THR 193		10.22	0.00		0.00
177	Y:GLN 194		89.98	0.00		0.00
178	Y:LEU 195		3.35	0.00		0.00
179	Y:ASP 196		44.83	28.86	|||||||	0.03
180	Y:GLU 197	S	38.40	17.60	|||||	-0.16
181	Y:LEU 198		0.31	0.00		0.00
182	Y:ASN 199		25.92	0.00		0.00
183	Y:LEU 200		0.00	0.00		0.00
184	Y:SER 201		2.46	0.00		0.00
185	Y:ASP 202		31.09	3.91	||	-0.05
186	Y:ASN 203		0.34	0.00		0.00
187	Y:ASN 204		83.39	0.00		0.00
188	Y:ASN 205		84.41	0.00		0.00

189	Y:LEU 206	0.00	0.00		0.00
190	Y:GLU 207	70.26	0.00		0.00
191	Y:GLU 208	117.57	0.00		0.00
192	Y:LEU 209	16.19	0.00		0.00
193	Y:PRO 210	39.50	0.00		0.00
194	Y:ASN 211	82.90	0.00		0.00
195	Y:ASP 212	55.27	0.00		0.00
196	Y:VAL 213	0.00	0.00		0.00
197	Y:PHE 214	4.09	0.00		0.00
198	Y:HIS 215	88.48	0.00		0.00
199	Y:GLY 216	45.36	0.00		0.00
200	Y:ALA 217	14.23	0.00		0.00
201	Y:SER 218	61.69	0.00		0.00
202	Y:GLY 219	2.90	0.00		0.00
203	Y:PRO 220	0.00	0.00		0.00
204	Y:VAL 221	48.86	30.12	|||||||	0.48
205	Y:ILE 222	35.14	33.30	|||||||||	0.53
206	Y:LEU 223	0.00	0.00		0.00
207	Y:ASP 224	21.97	0.00		0.00
208	Y:ILE 225	0.00	0.00		0.00
209	Y:SER 226	0.41	0.00		0.00
210	Y:ARG 227	96.32	0.00		0.00
211	Y:THR 228	5.61	0.00		0.00
212	Y:ARG 229	112.51	0.00		0.00
213	Y:ILE 230	0.33	0.00		0.00
214	Y:HIS 231	90.17	0.00		0.00
215	Y:SER 232	38.40	0.00		0.00
216	Y:LEU 233	7.37	0.00		0.00
217	Y:PRO 234	2.42	0.00		0.00
218	Y:SER 235	66.02	0.00		0.00
219	Y:TYR 236	83.82	0.00		0.00
220	Y:GLY 237	1.00	0.00		0.00
221	Y:LEU 238	4.88	0.00		0.00
222	Y:GLU 239	87.35	0.00		0.00
223	Y:ASN 240	66.57	0.00		0.00
224	Y:LEU 241	0.00	0.00		0.00
225	Y:LYS 242	76.85	20.78	|||	-0.25
226	Y:LYS 243	60.31	31.94	|||||	0.18
227	Y:LEU 244	0.76	0.00		0.00
228	Y:ARG 245	68.70	1.60	|	-0.06
229	Y:ALA 246	1.67	0.00		0.00
230	Y:ARG 247	94.38	0.00		0.00
231	Y:SER 248	47.42	0.00		0.00
232	Y:THR 249	1.31	0.00		0.00
233	Y:TYR 250	129.53	0.00		0.00
234	Y:ASN 251	38.49	0.00		0.00
235	Y:LEU 252	3.62	0.00		0.00
236	Y:LYS 253	131.16	0.00		0.00
237	Y:LYS 254	128.33	0.00		0.00
238	Y:LEU 255	18.87	0.00		0.00
239	Y:PRO 256	16.26	0.00		0.00
240	Y:THR 257	82.05	0.00		0.00
241	Y:LEU 258	53.81	0.00		0.00
242	Y:GLU 259	125.02	0.00		0.00
243	Y:LYS 260	84.05	0.00		0.00
244	Y:LEU 261	0.62	0.00		0.00
245	Y:VAL 262	109.03	0.00		0.00
246	Y:ALA 263	27.80	0.00		0.00
247	Y:LEU 264	8.88	0.00		0.00
248	Y:MET 265	103.47	1.91	|	0.08
249	Y:GLU 266	51.50	0.00		0.00
250	Y:ALA 267	1.21	0.00		0.00
251	Y:SER 268	18.06	0.00		0.00
252	Y:LEU 269	3.15	0.00		0.00
253	Y:THR 270	25.58	0.00		0.00

254	Y:TYR 271		68.22	0.00		0.00
255	Y:PRO 272		43.96	0.00		0.00
256	Y:SER 273		49.02	0.00		0.00
257	Y:HIS 274		22.67	0.00		0.00
258	Y:CYS 275		5.12	0.00		0.00
259	Y:CYS 276		20.11	0.00		0.00
260	Y:ALA 277		68.64	0.00		0.00
261	Y:PHE 278		5.23	0.00		0.00
262	Y:ALA 279		76.36	0.00		0.00
263	Y:ASN 280		79.69	0.00		0.00
264	Y:TRP 281		91.13	0.00		0.00
265	Y:ASP 334		191.42	6.92	|	-0.08
266	Y:TYS 335	H	273.27	148.20	||||||	0.15
267	Y:ASP 336		143.78	0.00		0.00
268	Y:LEU 337		151.48	0.00		0.00
269	Y:VAL 342		202.97	0.00		0.00
270	Y:ASP 343		90.42	0.00		0.00
271	Y:VAL 344		24.43	0.00		0.00
272	Y:THR 345		82.06	0.00		0.00
273	Y:CYS 346		10.46	0.00		0.00
274	Y:SER 347		27.66	0.00		0.00
275	Y:PRO 348		41.67	0.00		0.00
276	Y:LYS 349		126.58	0.00		0.00
277	Y:PRO 350		42.97	0.00		0.00
278	Y:ASP 351		125.29	0.00		0.00
279	Y:ALA 352		82.91	0.00		0.00
280	Y:PHE 353		199.77	0.00		0.00
281	Y:ASN 354		53.01	0.00		0.00
282	Y:PRO 355		122.71	0.00		0.00
283	Y:CYS 356		52.99	0.00		0.00
284	Y:GLU 357		146.32	0.00		0.00

<< < > >>

PDBe PISA v1.52 [20/10/2014]

PDBe
Protein Data Bank in Europe

is a member of

PDB

EMDataBank
Unified Data Resource for 3DEM

Table S3: Predicted $\Delta G°_i$values for each FSH-β residue in the FSH-β::FSHR interaction. Only the additive terms $\Delta G°_i$are shown. The values were calculated by using the equation [12]. $\Delta G°_i = \Delta G° - \Delta G°_{na}$. $\Delta G°_i$values were plotted in Figure 9B.

Residue	BSA#7 Chain H	BSA#8 Chain B	BSA#9 Chain E	Media	SD	ΔGi	ΔGi SD
ASN 1	0	0	0	0	0	0	0
SER 2	0	0	0	0	0	0	0
CYS 3	0	0	0	0	0	0	0
GLU 4	0	0	0	0	0	0	0
LEU 5	0	0	0	0	0	0	0
THR 6	0	0	0	0	0	0	0
ASN 7	0	0	0	0	0	0	0
ILE 8	0	0	0	0	0	0	0
THR 9	0	0	0	0	0	0	0
ILE 10	0	0	0	0	0	0	0
ALA 11	0	0	0	0	0	0	0
ILE 12	0	0	0	0	0	0	0
GLU 13	0	0	0	0	0	0	0
LYS 14	0	0	0	0	0	0	0
GLU 15	0	0	0	0	0	0	0
GLU 16	0	0	0	0	0	0	0
CYS 17	0	0	0	0	0	0	0
ARG 18	0	0	0	0	0	0	0
PHE 19	0	0	0	0	0	0	0
CYS 20	0	0	0	0	0	0	0
ILE 21	0	0	0	0	0	0	0
SER 22	0	0	0	0	0	0	0
ILE 23	0	0	0	0	0	0	0
ASN 24	0	0	0	0	0	0	0
THR 25	0	0	0	0	0	0	0
THR 26	0	0	0	0	0	0	0
TRP 27	0	0	0	0	0	0	0
CYS 28	0	0	0	0	0	0	0
ALA 29	0	0	0	0	0	0	0
GLY 30	0	0	0	0	0	0	0
TYR 31	0	0	0	0	0	0	0
CYS 32	0	0	0	0	0	0	0
TYR 33	0	0	0	0	0	0	0
THR 34	0	0	0	0	0	0	0
ARG 35	26.4274	5.19531	4.52626	12.04966	12.45598	-0.07073	-0.07311
ASP 36	1.59406	0.495477	0.245811	0.778449	0.717286	-0.00457	-0.00421
LEU 37	26.9296	22.0761	25.218	24.74123	2.461625	-0.14522	-0.01445
VAL 38	13.4099	14.3852	17.2322	15.0091	1.98606	-0.0881	-0.01166

TYR 39	26.7336	22.966	21.5544	23.75133	2.677422	-0.13941	-0.01572
LYS 40	27.7733	28.0754	29.5747	28.47447	0.964729	-0.16714	-0.00566
ASP 41	10.6805	7.96472	6.86229	8.502503	1.965093	-0.04991	-0.01153
PRO 42	90.1435	93.0863	78.7632	87.331	7.564418	-0.51261	-0.0444
ALA 43	82.893	83.499	77.0466	81.1462	3.563264	-0.4763	-0.02092
ARG 44	29.2696	30.7315	23.8312	27.9441	3.636103	-0.16402	-0.02134
PRO 45	43.247	28.2789	30.1546	33.8935	8.154479	-0.19894	-0.04786
LYS 46	53.9647	72.2339	56.1649	60.78783	9.973442	-0.35681	-0.05854
ILE 47	0	0	0	0	0	0	0
GLN 48	0	0	0	0	0	0	0
LYS 49	0	0	0	0	0	0	0
THR 50	0	0	0	0	0	0	0
CYS 51	0	0	0	0	0	0	0
THR 52	0	0	0	0	0	0	0
PHE 53	0	0	0	0	0	0	0
LYS 54	0	0	0	0	0	0	0
GLU 55	0	0	0	0	0	0	0
LEU 56	0	0	0	0	0	0	0
VAL 57	0	0	0	0	0	0	0
TYR 58	0	0	0	0	0	0	0
GLU 59	0	0	0	0	0	0	0
THR 60	0	0	0	0	0	0	0
VAL 61	0	0	0	0	0	0	0
ARG 62	0	0	0	0	0	0	0
VAL 63	0	0	0	0	0	0	0
PRO 64	0	0	0	0	0	0	0
GLY 65	0	0	0	0	0	0	0
CYS 66	0	0	0	0	0	0	0
ALA 67	0	0	0	0	0	0	0
HIS 68	0	0	0	0	0	0	0
HIS 69	0	0	0	0	0	0	0
ALA 70	0	0	0	0	0	0	0
ASP 71	0	0	0	0	0	0	0
SER 72	0	0	0	0	0	0	0
LEU 73	0	0	0	0	0	0	0
TYR 74	0	0	0	0	0	0	0
THR 75	0	0	0	0	0	0	0
TYR 76	0	0	0	0	0	0	0
PRO 77	0	0	0	0	0	0	0
VAL 78	0	0	0	0	0	0	0
ALA 79	0	0	0	0	0	0	0
THR 80	0	0	0	0	0	0	0
GLN 81	0	0	0	0	0	0	0
CYS 82	0	0	0	0	0	0	0
HIS 83	0	0	0	0	0	0	0

CYS 84	0	0	0	0	0	0	0
GLY 85	0	0	0	0	0	0	0
LYS 86	0	0	0	0	0	0	0
CYS 87	0	0	0	0	0	0	0
ASP 88	0	0	0	0	0	0	0
SER 89	40.0227	41.9822	42.4924	41.4991	1.3038	-0.24359	-0.00765
ASP 90	36.6246	26.9406	25.7465	29.77057	5.965719	-0.17474	-0.03502
SER 91	0	0	0	0	0	0	0
THR 92	0	0	0	0	0	0	0
ASP 93	42.4564	43.6669	43.1599	43.0944	0.607902	-0.25295	-0.00357
CYS 94	8.34642	6.50421	6.38069	7.077107	1.100991	-0.04154	-0.00646
THR 95	36.8722	33.5917	36.8131	35.759	1.877169	-0.20989	-0.01102
VAL 96	31.5954	32.4799	30.2882	31.4545	1.102623	-0.18463	-0.00647
ARG 97	110.918	104.817	109.302	108.3457	3.16093	-0.63596	-0.01855
GLY 98	11.9929	10.6833	10.0336	10.90327	0.998	-0.064	-0.00586
LEU 99	86.2462	90.0467	86.244	87.5123	2.194855	-0.51367	-0.01288
GLY 100	0	0	0	0	0	0	0
PRO 101	0	0	0	0	0	0	0
SER 102	0	0	0	0	0	0	0
TYR 103	51.2272	50.739	52.2106	51.39227	0.749558	-0.30166	-0.0044
CYS 104	0	0	0	0	0	0	0
SER 105	0.33585	0	1.20342	0.51309	0.620979	-0.00301	-0.00364
PHE 106	0	0	0	0	0	0	0
GLY 107	0	0	0	0	0	0	0
GLU 108	0	0	0	0	0	0	0
MET 109	0	0	0	0	0	0	0

Total $\Delta G°_i$ of -2.37 ± -0.18 kcal mol^{-1} for region FSH-β-(34-47) and -2.63 ± -0.05 kcal mol^{-1} for region FSH-β-(88-106). To calculate $\Delta G°$, $\Delta G°_{na}$ = - 3.13 kcal mol^{-1} should be added. The contribution to $\Delta G°$ of each binding regions is similar, with a little higher contribution of region FSH-β-(88-106).

References

1. Weber, G., Energetics of ligand binding to proteins. *Adv. Protein Chem.* **1975**, 29, 1-83.
2. Weber, G., Ligand binding and internal equilibria in proteins. *Biochemistry* **1972**, 11, 864-78.
3. Santa-Coloma, T. A.; Crabb, J. W.; Reichert, L. E., Jr., A synthetic peptide encompassing two discontinuous regions of hFSH-beta subunit mimics the receptor binding surface of the hormone. *Mol. Cell. Endocrinol.* **1991**, 78, 197-204.
4. Kurcinski, M.; Oleniecki, T.; Ciemny, M. P.; Kuriata, A.; Kolinski, A.; Kmiecik, S., CABS-flex standalone: a simulation environment for fast modeling of protein flexibility. *Bioinformatics* **2018**, 35, 694-695.