Topology of RNA-protein nucleobase-amino acid π - π interactions and comparison to analogous DNA-protein π - π contacts

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	Amino Acid	Nucleobase	Tilt ^a	Our Methodology ^b	3DNA-SNAP ^c
1FXL	Y-A-45	U-B-5	10.82	Yes	Yes
	F-A-84	U-B-9	64.85	Yes	No
	F-A-84	U-B-10	14.40	Yes	Yes
	Y-A-128	U-B-3	5.45	Yes	Yes
	F-A-170	U-B-4	4.73	Yes	Yes
1DFU	Y-P-31	A-N-73	85.16	Yes	No
1H2C	F-A-125	G-R-2	10.47	Yes	Yes
	Y-A-171	A-R-3	74.97	Yes	No
2PXK	R-A-50	A-B-140	47.63	Yes	Yes
3L25	F-B-239	C-F-1	73.40	Yes	No
	F-E-239	C-C-1	74.83	Yes	No
3G9Y	W-A-79	G-C-2	8.77	Yes	Yes
	W-A-79	G-C-3	10.39	Yes	Yes

Supplementary Table S1: Comparison of the contacts found using 3DNA-SNAP and our methodology for representative crystal structures.

^aInterplanar angle between the two π–systems (See Supp. Fig. S1). ^bSee methods. ^cVersion beta-r06-2015oct23 (Lu 2008).

Supplementary Table S2: Most common amino acid or nucleobase edges involved in π - π interactions in nature with an interplanar (tilt) angle greater than 45°.

Residue Edge	Edge Type	Atoms Involved ^a	Frequency in Full Dataset	Frequency in Non-redundant dataset
F	Bridge	СНСН	52%	55%
F	Single Proton	СН	15%	10%
С	Bridge	C5HC6H	6%	10%
D	Single Atom	Οδ	5%	0%
U	Bridge	N1HC6H	5%	7%
Y	Bridge	ϹͼΗϹζΟΗ	3%	3%
R	Bridge	ΝηΗΝηΗ	2%	0%
R	Bridge	ΝєΗϹδΗ	2%	0%
E	Single Atom	Oe	2%	3%
W	Bridge	СєНСζН	2%	0%
Y	Bridge	CδHC∈H	2%	3%
Y	Single Proton	CδH	2%	3%
С	Lone Pair	02	2%	3%
А	Bridge	N9HN3	2%	3%
А	Lone Pair	N3	2%	0%

^aSee Supp. Fig. S2 for atomic numbering.

		RNA			DNA ^a			
	Range	Most Common	Mean	Range	Most Common	Mean		
A (cyclic)	0-90	5-10 (39%)	28.2 ± 32.8	0-90	5-10 (25%)	25.0±26.4		
U/T (cyclic)	0-90	10-15 (25%)	29.5 ± 30.1	0-90	5-10 (31%)	20.6±23.1		
G (cyclic)	0-90	20-25 (38%)	19.2 ± 14.4	0-90	10-15 (17%)	25.6±23.1		
C (cyclic)	0-90	0-5 (22%)	34.9 ± 29.1	0-90	5-10 (26%)	26.8±24.4		
A (acyclic)	0-85	0-5 (19%) 5-10 (19%)	19.7 ± 16.7	0-90	5-10 (22%)	35.3±28.8		
U/T (acyclic)	5-25	20-25 (50%)	18.6 ± 4.4	0-90	5-10 (17%)	34.7±32.0		
G (acyclic)	5-65	5-10 (45%)	18.6 ± 16.8	0-90	5-10 (15%)	50.4±30.6		
C (acyclic)	0-80	75-80 (21%)	36.5 ± 26.7	0-90	20-25 (16%)	42.7±27.2		

Supplementary Table S3: Comparison of the relative orientation (tilt angle or ω , degrees) of different nucleobase–amino acid π –systems in RNA or DNA–protein π –interactions found in nature as a function of the nucleobase.

^{*a*}Reference Wilson, *et al.*, 2015.

		RNA		DNAª				
	Range	Most Common	Mean	Range	Most Common	Mean		
A (cyclic)	2.7-4.0	3.4-3.5 (32%)	3.369 ± 0.173	2.9-4.3	3.4-3.5 (23%)	3.493±0.315		
U/T (cyclic)	2.8-4.3	3.4-3.5 (22%)	3.483 ± 0.314	2.6-4.0	3.4-3.5 (28%)	3.459±0.213		
G (cyclic)	2.9-3.8	3.1-3.2 (20%)	3.217 ± 0.193	3.1-4.3	3.3-3.4 (20%)	3.492±0.209		
C (cyclic)	3.0-4.1	3.3-3.4 (22%) 3.4-3.5 (22%)	3.436 ± 0.200	2.9-4.3	3.4-3.5 (17%)	3.479±0.215		
A (acyclic)	2.7-3.8	3.4-3.5 (26%)	3.305 ± 0.209	2.9-4.5	3.3-3.4 (19%)	3.489±0.302		
U/T (acyclic)	2.9-3.7	3.5-3.6 (30%)	3.373 ± 0.202	2.8-4.3	3.4-3.5 (21%) 3.5-3.6 (21%)	3.493±0.275		
G (acyclic)	2.9-3.9	3.3-3.4 (27%)	3.304 ± 0.228	2.9-4.8	3.1-3.2 (19%)	3.421±0.382		
C (acyclic)	2.9-3.6	3.1-3.2 (36%)	3.245 ± 0.199	2.8-4.7	3.3-3.4 (12%)	3.651±0.494		

Supplementary Table S4: Comparison of the distance (Å) between nucleobase–amino acid π –systems in RNA or DNA–protein π –interactions found in nature as a function of the nucleobase

^{*a*}Reference Wilson, *et al.*, 2015.



Supplementary Figure S1. Examples of (a) a RNA–protein stacking interaction (PDB ID: 1URN), (b) a RNA– protein inclined interaction (PDB ID: 2PXK), and (c) a RNA–protein stacking interaction (PDB ID: 3RER).



Supplementary Figure S2. Models used in the current study for the nucleobases and amino acids to calculate the interaction energies, as well as the chemical numbering of each residue.



Supplementary Figure S3. Approach used in the current study to identify and classify RNA–protein nucleobase–amino acid π – π interactions. For full description of our approach see the Methods section in the main manuscript.



Supplementary Figure S4. Previously identified RNA–protein nucleobase–amino acid π – π contacts through the use of automated search routines (Baker and Grant 2007) that instead represent A) a non-interacting pair (PDB ID: 1ASZ), B) a phosphate interaction (PDB ID: 1E8O), C) a nucleobase–amino acid hydrogen bonding (PDB ID: 1U63), and D) a ribose interactions (PDB ID: 1DFU).



Supplementary Figure S5. Frequency of the closest heavy atom distance for π - π contacts in the non-redundant dataset as a function of the protein (a and b) or RNA (c and d) component for the cyclic (a and c) and acyclic (b and d) amino acids.



Supplementary Figure S6. A) Distribution in the RNA types searched (inner circle) and the RNA types that form at least one protein π - π contact (outer circle) in the full dataset. B) Overall number of RNA-protein π - π contacts found in each crystal structure searched in the full dataset. C) Number of RNA-protein π - π contacts found in each crystal structure searched as a function of the amino acid (cyclic versus acyclic) classification in the full dataset.



Supplementary Figure S7. Distribution in the composition of the RNA–protein π – π contacts in the full dataset as a function of A) amino acid, B) nucleobase, C) the aromatic (cyclic) amino acids, D) the acyclic amino acids, and E) both (cyclic and acyclic) amino acid classes.



Supplementary Figure S8. Frequency of the tilt angle (degrees) between the ring planes for all π - π interactions in the full dataset as a function of the protein (A and B) or RNA (C and D) component for the cyclic (A and C) and acyclic (B and D) amino acids.



Supplementary Figure S9. Frequency of the closest heavy atom distance for π - π contacts in the full dataset as a function of the protein (A and B) or RNA (C and D) component for the cyclic (A and C) and acyclic (B and D) amino acids.



Supplementary Figure S10. Frequency of the binding energy (kJ mol⁻¹) for nucleobase–amino acid π – π interactions in the full dataset as a function of the protein (A and B) or RNA (C and D) component for the neutral (A and C) and charged (B and D) π –containing amino acids.



Supplementary Figure S11. Number of DNA-protein π - π contacts found in each crystal structure searched regardless of the amino acid type.

Supp. Table S5. Full details of the crystal structures searched, the nucleobase–amino acid pairs identified and the classification of each π –interaction. An * represents structures or interactions removed from the dataset to obtain the non-redundant dataset.

PDB ID	A	mino Aci	d	N	9					
	Res ID	Chain	Res #	Res ID	Chain	Res #				
1A34 No contacts										
1B2M	Е	А	58	G	С	105				
1B2M	Y	А	45	G	С	105				
*1B2M	Y	А	45	G	D	105				
*1C9S	Е	L	36	А	W	105				
*1C9S	F	Т	32	А	W	142				
*1C9S	F	Ν	32	А	W	112				
*1C9S	F	0	32	А	W	117				
*1C9S	F	М	32	А	W	107				
*1C9S	F	L	32	А	W	102				
*1C9S	F	V	32	А	W	152				
*1C9S	F	U	32	А	W	147				
*1C9S	F	S	32	А	W	137				
*1C9S	F	R	32	А	W	132				
*1C9S	F	Q	32	А	W	127				
*1C9S	F	Ν	32	G	W	111				
*1C9S	F	Т	32	G	W	141				
*1C9S	F	М	32	G	w	106				
*1C9S	F	R	32	G	W	131				
*1C9S	F	0	32	G	w	116				
*1C9S	F	L	32	G	W	101				
*1C9S	F	V	32	G	w	151				
*1C9S	F	U	32	G	W	146				
*1C9S	F	S	32	G	W	136				
*1C9S	F	Q	32	G	W	126				
*1C9S	F	Р	32	G	W	121				
*1DUL	R	А	50	А	В	140				
*1FXL	F	А	170	U	В	4				
*1FXL	F	А	84	U	В	10				
*1FXL	F	А	84	U	В	9				
*1FXL	Y	А	45	U	В	5				
*1FXL	Y	А	128	U	В	3				
1GTF	F	0	32	G	W	118				
1GTF	F	Ν	32	G	W	113				
1GTF	F	М	32	G	W	108				
1GTF	F	L	32	G	W	103				
1GTF	F	V	32	G	W	153				
1GTF	F	U	32	G	W	148				
1GTF	F	Т	32	G	W	143				
1GTF	F	S	32	G	W	138				
1GTF	F	R	32	G	W	133				

PDB ID	A	mino Aci	d	Nucleotide			
	Res ID	Chain	Res #	Res ID	Chain	Res #	
1GTF	F	0	32	U	W	119	
1GTF	F	Ν	32	U	W	114	
1GTF	F	М	32	U	W	109	
1GTF	F	L	32	U	W	104	
1GTF	F	V	32	U	W	154	
1GTF	F	U	32	U	W	149	
1GTF	F	Т	32	U	W	144	
1GTF	F	S	32	U	W	139	
1GTF	F	R	32	U	W	134	
1GTF	F	Q	32	U	W	129	
1GTF	F	Р	32	U	W	124	
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1H2C	Y	А	171	А	R	3	
*1HQ1	R	А	50	А	В	140	
1J1U	F	А	261	G	В	535	
1JBS			No co	ntacts			
1JID	R	А	14	G	В	148	
1JID	R	А	101	G	В	147	
1K8W	R	А	141	G	В	412	
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*1R9F	W	А	39	G	С	19	
1SDS			No co	ntacts			
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*1URN	Y	В	13	С	Q	10	
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*1UTF	F	J	32	G	9	103	
*1UTF	F	I	32	G	8	103	
*1UTF	F	В	32	G	1	103	
*1UTF	F	С	32	G	2	103	
*1UTF	F	А	32	G	0	103	
*1UTF	F	К	32	G	Z	103	
*1UTF	F	Н	32	G	7	103	
*1UTF	F	D	32	G	3	103	
*1UTF	F	Е	32	G	4	103	
*1UTF	F	F	32	G	5	103	
*1UTV	F	I	32	G	8	103	
*1UTV	F	Н	32	G	7	103	

	А	mino Aci	d	N	lucleotid	е		A	mino Aci	d	
10010	Res ID	Chain	Res #	Res ID	Chain	Res #	10010	Res ID	Chain	Res #	Res I
*1UTV	F	E	32	G	4	103	 *2PXF	R	Α	50	Α
*1UTV	F	F	32	G	5	103	*2PXK	R	А	50	А
*1UTV	F	D	32	G	3	103	*2PXV	R	А	50	А
*1UTV	F	С	32	G	2	103	2Q66	н	А	314	А
*1UTV	F	В	32	G	1	103	2Q66	F	А	140	А
*1UTV	F	А	32	G	0	103	2R8S	D	Н	109	U
*1UTV	F	К	32	G	Z	103	2R8S	Y	Н	106	U
*1UTV	F	J	32	G	9	103	2R8S	Y	L	49	U
*1UTV	F	G	32	G	6	103	2V00	F	А	35	U
*1UVJ			No co	ntacts			*2V00	F	В	35	U
*1UVL	R	С	291	С	D	7	*2V00	F	В	55	U
*1UVL	D	А	399	С	В	7	2V00	F	А	55	U
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*1UVL	D	С	399	С	D	7	*2V00	Y	В	23	U
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*1UVL	F	А	156	U	В	4	2X1F	Y	А	21	G
*1UVL	F	С	156	U	D	4	*2XLK			No co	ntacts
1UVM	F	С	156	U	F	5	2XNR	F	А	333	С
*1UVM	F	В	156	U	Е	5	2XNR	F	А	368	U
*1UVM	F	А	156	U	D	5	*2XS2	R	А	115	U
*1WMQ			No co	ntacts			*2XS2	F	А	43	U
*1WPU			No co	ntacts			*2XS2	F	А	84	U
*1ZH5	F	В	35	U	С	9	*2XS5	R	А	115	U
*1ZH5	F	В	28	U	D	1	*2XS5	R	В	115	U
*1ZH5	F	А	28	U	С	1	*2XS5	F	А	84	U
*1ZH5	F	А	35	U	D	9	*2XS5	F	А	43	U
*1ZH5	Y	В	23	U	С	8	*2XS5	F	В	43	U
*1ZH5	Y	А	23	U	D	8	*2XS5	F	В	84	U
2ANR			No co	ntacts			*2XS5	Y	В	88	С
2ASB			No co	ntacts			*2XS5	Y	А	88	С
2B3J	R	А	70	G	F	37	2XS7	R	А	115	U
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*2B3J	R	В	70	G	Е	37	2XS7	F	А	43	U
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*2B3J	F	D	145	G	Н	36	2ZKO			No co	ntacts
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2JLV			No co	ntacts			3BOY			No co	ntacts
2NUG			No co	ntacts			*3BSN			No co	ntacts
2PO1	Н	А	66	А	С	395	*3BSO			No co	ntacts
*2PXB	R	А	50	А	В	140	3D2S	F	D	202	С
*2PXD	R	А	50	А	В	140	3D2S	F	В	202	С
*2PXE	R	А	50	А	В	140	3D2S	F	Α	202	G

Nucleotide

В

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В

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Х

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Res ID Chain

	A	mino Aci	d	Ν	lucleotid	e		A	mino Aci	d	
	Res ID	Chain	Res #	Res ID	Chain	Res #	10010	Res ID	Chain	Res #	Res I
3DD2	R	Н	233	А	В	7	*3PEW			No co	ntacts
3DD2	R	Н	165	А	В	15	3PEY			No co	ntacts
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3H5Y			No co	ontacts			3PF5	F	В	17	U
*3I5X	F	А	576	U	В	1	3PF5	W	В	8	U
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*3162	F	А	576	U	В	1	*3Q0Q	R	А	814	А
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*3K62	R	А	288	А	В	7	*3Q0Q	н	Α	852	А
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*3K62	Н	А	454	U	В	3	*3Q0Q	Y	А	924	А
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*3K62	Y	А	416	G	В	4	*3Q0Q	Y	А	1003	U
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*3K62	Y	А	245	U	В	8	3Q0R	R	А	814	А
*3K64	R	А	288	А	В	7	3Q0R	R	А	888	А
*3K64	н	А	326	А	В	7	3Q0R	R	Α	888	G
*3K64	н	А	454	U	В	3	3Q0R	Н	Α	852	А
*3K64	Y	А	501	G	В	2	3Q0R	Y	А	778	А
*3K64	Y	A	416	G	В	4	3Q0R	Y	A	924	A
*3K64	Y	A	245	U	В	9	3Q0R	Y	A	1003	G
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*3L25	F	В	239	С	F	1	*3Q0S	R	A	814	A
3LQX	R	A	50	A	В	140	*3Q0S	R	A	742	С
*3NMR	D	A	187	U	В	4	*3Q0S	R	A	814	U
*3NMR	F	A	111	G	В	3	*3Q0S	Н	A	852	A
*3NMR	F	A	111	U	В	4	*3Q0S	н	A	1039	U
*3NMR	F -	A	152	U	В	5	*3Q0S	Y	A	924	A
3NNA	F -	A	111	G	В	3	*3Q0S	Y	A	778	C
3NNA	+	A	152	U	В	5	*3Q0S	Y	A	1003	G
3NNA	F	A	111	U	В	4	*3Q0S	Y	A	//8	0
3080	W	A	501	0	C	/	*3Q0S	Y	A	1003	U
3080	W	A	501	U	C	8	SQGC	н	A	454	G
BOIN	ĸ	A	129	A	C	8	SQGC	н	A	326	U
30IN	К	A	136	U	Ĺ	/	3QGC	H	A	454	U
			NO CO				3QGC	Y	A	245	A
30AR			INO CO	intacts			 JUGC	Ŷ	A	416	G

Nucleotide Res ID Chain Res #

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		A	mino Aci	d	Nucleotide		
	10010	Res ID	Chain	Res #	Res ID	Chain	Res #
ł	3QGC	Y	Α	501	G	В	2
	3QGC	Y	А	501	U	В	1
	3QGC	Y	А	288	U	В	8
	3R2C	R	А	102	С	R	3
	*3R2C	R	В	102	С	S	3
	3R2C	R	А	102	G	R	1
	*3R2C	R	В	102	G	S	1
	3R2C	R	J	16	U	R	8
	3R2C	F	А	104	U	R	4
	3R2C	F	А	122	U	R	8
	*3R2C	F	В	104	U	S	4
	*3R2C	F	В	122	U	S	8
	3R2C	w	В	72	G	S	9
	*3RER	F	В	42	А	К	8
	*3RER	F	Е	42	U	К	5
	*3RER	F	D	42	U	К	4
	*3RER	F	Е	42	U	К	6
	*3RER	F	А	42	U	К	7
	3SQW			No co	ntacts		
	3T5N	R	А	300	А	С	3
	3T5N	R	А	300	U	С	4
	3T5N	Y	А	308	А	С	3
	*3U4M			No co	ntacts		
	3UMY	R	А	129	А	В	2169
	3WBM			No co	ntacts		
	4AL5	R	А	115	С	В	9
	4AL5	R	А	111	С	В	6
	4AL5	F	А	158	А	В	5
	4AL5	F	А	155	G	В	20
	4ALP	F	А	77	U	Е	1
	4ALP	F	D	77	U	Е	2
	4ARC	R	А	416	С	В	75
	4ARC	R	А	719	U	В	16
	4ARC	Y	А	330	С	В	75
	4C8Y	Н	А	37	А	С	29
	4D25	F	А	348	А	D	3
	*4ED5	F	В	151	U	С	4
	4ED5	F	В	65	U	С	10
	4ED5	F	А	151	U	D	4
	*4ED5	Y	В	26	U	С	5
	*4ED5	Ŷ	B	109	- U	c	3
	4ED5	Ŷ	Ā	109	Ŭ	D	3
	4FD5	Ŷ	A	26	U U	D	5
	*4F02	R	D	94	Δ	F	6
	4F02	R	D	179	Δ	F	2
	-102	1/	0	1/3	~	L	5

Res IDChainRes #Res IDChainRes #4F02RA94AB34F02FA102AB4*4F02FD142AE34F02FD102AE34F02YA56AB8*4F02YD56AE8*4F02YD14AE64F02YD14AE64F02YA429GC24F03YA429GC24F04FA339CX3*4078FA337UX24H08FA337UX3*4H78YD25AK1*4H78YA25AI1*4H78YC25AI1*4H78YA20CB1*4H79FA20AD1*4H79YA20AD1*4H78YA25AD1*4H79YA20CB1*4H79YA20CB1*4H79YA20GB1*4H7	PDB ID	Aı	mino Aci	d	Nucleotide			
4F02 R A 94 A B 6 4F02 F A 102 A B 4 *4F02 F D 142 A E 4 *4F02 F D 102 A E 3 4F02 Y A 56 A B 8 *4F02 Y D 56 A E 8 *4F02 Y D 14 A E 6 4F02 Y A 429 G C 2 4GV3 Y A 429 G C 2 4GV6 Y A 429 G C 2 4HOR F A 337 U X 2 4HOS F A 337 U X 2 4HOS F A 337 U X 3 *4HT8 Y B 25 A I 1 *4HT8		Res ID	Chain	Res #	Res ID	Chain	Res #	
4F02FA102AB34F02FD142AB4*4F02FD102AE34F02YA56AB8*4F02YD56AE8*4F02YD14AE64F02YA14AB6*4GV3YA429GC24GV6YA429GC24HORFA337UX24HOSFA339UX3*4HORFA339UX3*4HRYD25AK1*4HT8YA25AI1*4HT8YF25AI1*4HT8YA25AD74HT9FA20CB1*4HT9YA20CB14HT9YA20GG4014HT9YA20GG4014HT9YA20GB4114HT9YA20GG4014HT9YA20GB4114HT9YA20GB4114HT9	4F02	R	А	94	А	В	6	
4F02FA142AB4*4F02FD102AE34F02YA56AB8*4F02YD56AE8*4F02YD14AE6*4F02YA429GC24GV3YA429GC24GV6YA339CX3*4H0RFA337UX24H0SFA337UX3*4H78YD25AK1*4H78YB25AI1*4H78YF25AI1*4H78YB25AD74H79FA25AD74H79FA25AD74H79FA25AD14H79YA25AD14H79YA25AD14H79YA25AD14H79YA25AD14H79YA25AD14H79YA25AD14H79YB25AD14H79Y <t< td=""><td>4F02</td><td>F</td><td>А</td><td>102</td><td>А</td><td>В</td><td>3</td></t<>	4F02	F	А	102	А	В	3	
*4F02FD142AE4*4F02FD102AE34F02YD56AE8*4F02YD14AE64F02YA429GC24GV3YA429GC24GV6YA339CX3*4H0RFA337UX24H0SFA337UX24H0SFA339UX3*4H78YD25AK1*4H78YB25AI1*4H78YF25AI1*4H79FA25AD74H79FA25AD74H79FA25AD14H79YA25AD14H79YA25AD14H79YA25AD14H79YA25AD14H79YA25AD14H79YA26AD14H79YA26AD14H79YA26AD14H79Y <t< td=""><td>4F02</td><td>F</td><td>А</td><td>142</td><td>А</td><td>В</td><td>4</td></t<>	4F02	F	А	142	А	В	4	
*4F02 F D 102 A E 3 4F02 Y A 56 A B 8 *4F02 Y D 14 A E 6 *4F02 Y A 14 A B 6 *4F02 Y A 429 G C 2 4GV3 Y A 429 G C 2 *4HOR F A 339 C X 3 *4HOR F A 337 U X 3 *4HOR F A 337 U X 3 *4HOR F A 337 U X 3 *4HOR F A 339 U X 3 *4HOR F A 25 A K 1 *4HT8 Y B 25 A I 1 *4HT8 Y A 25 A D 1 *4HT9 Y A 25 A D 1 *4HT9 Y A 20 C B 1 *4HT9 Y <td>*4F02</td> <td>F</td> <td>D</td> <td>142</td> <td>А</td> <td>Е</td> <td>4</td>	*4F02	F	D	142	А	Е	4	
4F02 Y A 56 A B 8 *4F02 Y D 14 A E 6 *4F02 Y A 14 A B 6 *4F02 Y A 14 A B 6 *4F02 Y A 429 G C 2 4GV6 Y A 429 G C 2 *4HOR F A 339 C X 3 *4HOS F A 337 U X 2 4HOS F A 337 U X 3 *4HT8 Y D 25 A K 1 *4HT8 Y B 25 A K 7 *4HT8 Y F 25 A I 1 *4HT8 Y E 25 A I 7 *4HT8 Y A 25 A D 7 *4HT9 F A 42 U E 5 4HT9 Y A 20 C B 1 *4HT9 Y	*4F02	F	D	102	А	Е	3	
*4F02 Y D 56 A E 8 *4F02 Y D 14 A E 6 *4F02 Y A 14 A B 6 *4GV3 Y A 429 G C 2 *4HOR F A 339 C X 3 *4HOR F A 337 U X 2 4HOS F A 337 U X 3 *4HOR F A 337 U X 3 *4HOS F A 337 U X 3 *4HT8 Y D 25 A K 1 *4HT8 Y E 25 A I 1 *4HT9 F A 42 U E 5 4HT9 Y A 25 A D 1 4HT9 Y A 20 C B 11 4HT9	4F02	Y	А	56	А	В	8	
*4F02 Y D 14 A E 6 4F02 Y A 14 A B 6 *4GV3 Y A 429 G C 2 4GV6 Y A 429 G C 2 *4HOR F A 339 C X 3 *4HOR F A 337 U X 2 4HOS F A 337 U X 3 *4HOS F A 337 U X 3 *4HTS Y D 25 A K 1 *4HT8 Y B 25 A I 1 *4HT8 Y E 25 A D 1 *4HT9 Y B 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y B 20 C B 119 *4JJN	*4F02	Y	D	56	А	Е	8	
4F02 Y A 14 A B 6 *4GV3 Y A 429 G C 2 4GV6 Y A 429 G C 2 *4HOR F A 339 C X 3 *4HOR F A 337 U X 2 4HOS F A 337 U X 3 *4HOS F A 337 U X 3 *4HOS F A 337 U X 3 *4HT8 Y D 25 A K 1 *4HT8 Y B 25 A I 1 *4HT8 Y F 25 A D 7 4HT9 F A 42 U E 5 4HT9 Y A 25 A D 1 4HT9 Y B 25 A D 1 4HT9	*4F02	Y	D	14	А	Е	6	
*4GV3 Y A 429 G C 2 4GV6 Y A 429 G C 2 *4HOR F A 339 C X 3 *4HOR F A 337 U X 2 4HOS F A 337 U X 3 *4HOS F A 337 U X 3 *4HOS F A 337 U X 3 *4HT8 Y D 25 A K 1 *4HT8 Y B 25 A I 1 *4HT8 Y F 25 A I 7 4HT9 F A 42 U E 5 4HT9 Y A 25 A D 1 4HT9 Y A 20 C B 1 4HT9 Y A 20 C B 11 4HT9	4F02	Y	А	14	А	В	6	
44VOR Y A 429 G C 2 *4HOR F A 337 C X 2 4HOS F A 337 U X 2 4HOS F A 337 U X 2 4HOS F A 337 U X 3 *4HT8 Y D 25 A K 1 *4HT8 Y B 25 A I 1 *4HT8 Y A 25 A I 4 *4HT8 Y E 25 A I 7 4HT9 F A 42 U E 4 4HT9 Y A 25 A D 1 4HT9 Y A 20 C B 1 4HT9 Y A 20 G 419	*4GV3	Y	А	429	G	С	2	
*4HOR F A 339 C X 3 *4HOR F A 337 U X 2 4HOS F A 337 U X 3 *4HOS F A 339 U X 3 *4HT8 Y D 25 A K 4 *4HT8 Y B 25 A K 7 *4HT8 Y A 25 A I 1 *4HT8 Y A 25 A I 4 *4HT8 Y E 25 A I 7 4HT9 F B 42 U E 5 4HT9 Y A 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y B 25 A D 1 4J1X	4GV6	Y	А	429	G	С	2	
*4HOR F A 337 C X 2 4HOS F A 337 U X 2 4HOS F A 337 U X 3 *4HT8 Y D 25 A K 1 *4HT8 Y B 25 A K 7 *4HT8 Y B 25 A I 1 *4HT8 Y A 25 A I 1 *4HT8 Y F 25 A I 4 *4HT9 F B 42 U E 5 4HT9 F A 42 U E 4 4HT9 Y A 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y B 25 A D 1 4J17L	*4HOR	F	А	339	С	Х	3	
4HOS F A 337 U X 2 4HOS F A 339 U X 3 *4HT8 Y D 25 A K 1 *4HT8 Y B 25 A K 4 *4HT8 Y B 25 A I 1 *4HT8 Y A 25 A I 4 *4HT8 Y A 25 A I 4 *4HT8 Y E 25 A I 4 *4HT9 F B 42 U E 5 4HT9 F A 25 A D 1 4HT9 Y A 25 A D 1 4HT9 Y A 20 C B 1 4HT9 Y A 20 G 419 *4JNX W D 17 G G 419 *4JNX W	*4HOR	F	А	337	С	Х	2	
4HOS F A 339 U X 3 *4HT8 Y D 25 A K 1 *4HT8 Y B 25 A K 7 *4HT8 Y B 25 A K 7 *4HT8 Y A 25 A I 1 *4HT8 Y A 25 A I 4 *4HT8 Y F 25 A I 4 *4HT9 F A 42 U E 5 4HT9 F A 42 U E 4 4HT9 Y A 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y B 20 C B 1 *4J39 W A 20 G 419 *4J7L No contacts<	4HOS	F	А	337	U	Х	2	
*4HT8 Y D 25 A K 1 *4HT8 Y B 25 A K 7 *4HT8 Y B 25 A I 1 *4HT8 Y A 25 A I 1 *4HT8 Y F 25 A I 4 *4HT8 Y E 25 A I 4 *4HT9 F B 42 U E 5 4HT9 F A 42 U E 4 4HT9 Y A 25 A D 1 4HT9 Y A 20 C B 1 4HT9 Y A 20 G 419 *4J30 W <	4HOS	F	А	339	U	Х	3	
*4HT8 Y C 25 A K 4 *4HT8 Y B 25 A I 1 *4HT8 Y A 25 A I 1 *4HT8 Y F 25 A I 4 *4HT8 Y E 25 A I 7 4HT9 F B 42 U E 4 4HT9 F A 42 U E 4 4HT9 F A 42 U E 4 4HT9 Y A 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y B 20 C B 1 4HT9 Y A 20 C B 1 *4J30 W A 17 G B 419 *4JNX <t< td=""><td>*4HT8</td><td>Y</td><td>D</td><td>25</td><td>А</td><td>Κ</td><td>1</td></t<>	*4HT8	Y	D	25	А	Κ	1	
*4HT8 Y B 25 A K 7 *4HT8 Y F 25 A I 4 *4HT8 Y F 25 A I 7 4HT8 Y E 25 A I 7 4HT9 F B 42 U E 5 4HT9 F A 42 U E 4 4HT9 F A 42 U E 4 4HT9 Y C 25 A D 7 4HT9 Y B 25 A D 1 4IH9 Y B 25 A D 1 4IH9 Y B 20 C B 1 *4J39 W A 20 C B 419 *4J7L No contacts No contacts 4419 419 419 419 419 419 419 419 419 410 411 411 4	*4HT8	Y	С	25	А	К	4	
*4HT8 Y A 25 A I 1 *4HT8 Y F 25 A I 7 4HT8 Y E 25 A I 7 4HT9 F B 42 U E 5 4HT9 F A 42 U E 4 4HT9 Y C 25 A D 7 4HT9 Y A 25 A D 1 4HT9 Y B 25 A D 1 4I19 Y B 25 A D 1 4I19 Y B 25 A D 1 4I19 Y A 20 C B 1 *4J32 W A 20 C B 419 *4J7X W A 17 G B 401 *4JNX W D 20 G B 401 4JNX	*4HT8	Y	В	25	А	К	7	
*4HT8 Y F 25 A I 4 *4HT8 Y E 25 A I 7 4HT9 F B 42 U E 4 4HT9 F A 42 U E 4 4HT9 F A 42 U E 4 4HT9 Y C 25 A D 4 4HT9 Y A 25 A D 1 4HT9 Y B 25 A D 1 4IH9 Y B 20 C B 1 *4J39 W A 20 C B 19 *4J7L No contacts No contacts 419 419 *4JNX W D 17 G G 419 *4JNX W A 20 G B 401 *4JNX W A 20 G B 401 4JZU No c	*4HT8	Y	А	25	А	I	1	
*4HT8 Y E 25 A I 7 4HT9 F B 42 U E 4 4HT9 F A 42 U E 4 4HT9 F A 42 U E 4 4HT9 Y C 25 A D 7 4HT9 Y A 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y A 20 C B 1 *4J39 W A 20 C B 1 *4J7L No contacts * No contacts * *4JNX W D 17 G G 419 *4JNX W A 20 G B 401 *4JNX W A 20 G B 401 *4JNX W A 20 G B 20 *4KNQ A	*4HT8	Y	F	25	А	I	4	
4HT9 F B 42 U E 5 4HT9 F A 42 U E 4 4HT9 Y C 25 A D 7 4HT9 Y A 25 A D 4 4HT9 Y B 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y B 25 A D 1 4HT9 Y B 20 C B 1 4H19 Y B 20 C B 1 4H19 Y A 20 C B 1 *4J39 W A 20 C B 19 *4J7L No contacts No contacts 419 419 *4JNX W A 20 G B 401 *4JNX W A 20 G B 401 4JZU No contac	*4HT8	Y	Е	25	А	I	7	
4HT9 F A 42 U E 4 4HT9 Y C 25 A D 7 4HT9 Y A 25 A D 4 4HT9 Y B 25 A D 1 4H19 Y B 20 C B 1 *4J32 W A 20 G 419 419 *4JNX W A 17 G B 419 *4JNX W A 20 G B 401 4LT No contacts No contacts No 1 1 4KRE	4HT9	F	В	42	U	Е	5	
4HT9 Y C 25 A D 7 4HT9 Y A 25 A D 1 4HT9 Y B 25 A D 1 4II9 Y B 25 A D 1 4II9 Y B 25 A D 1 4II9 Y B 20 C B 1 *4J39 W A 20 C B 1 *4J7L No contacts No contacts 1 1 *4J7M W D 17 G G 419 *4JNX W A 17 G B 419 *4JNX W A 20 G B 401 *4JNX W A 20 G B 401 *4JNX W A 20 G B 401 4KRE R A 708 A R 20 4KRE F </td <td>4HT9</td> <td>F</td> <td>А</td> <td>42</td> <td>U</td> <td>Е</td> <td>4</td>	4HT9	F	А	42	U	Е	4	
4HT9 Y A 25 A D 4 4HT9 Y B 25 A D 1 4II9 No contacts No contacts B 1 *4J39 W A 20 C B 1 *4J7L No contacts No contacts 1 *4J7M No contacts 1 19 *4JNX W D 17 G G 419 *4JNX W A 20 G 401 19 *4JNX W A 17 G B 419 *4JNX W A 20 G 401 *4JNX W A 20 G 401 *4JNX W D 20 G B 401 4KRE R A 708 A R 9 4KRE F A 292 A R 1 4KRE F A 20 G B 201	4HT9	Y	С	25	А	D	7	
4HT9 Y B 25 A D 1 4II9 No contacts No contacts B 1 *4J39 W A 20 C B 1 *4J39 W A 20 C B 1 *4J39 W A 20 C B 1 *4J7L No contacts No contacts No 1 4J7M W D 17 G G 419 *4JNX W A 17 G B 419 *4JNX W A 20 G B 401 *4JNX W A 20 G B 401 *4JNX W D 20 G B 401 *4JNX W D 20 G B 401 *4JNX W D 20 G B 401 4KRE R A 708 A R 20 4KRE F	4HT9	Y	А	25	А	D	4	
4II9 No contacts *4J39 W A 20 C B 1 *4J39 W A 20 C B 1 *4J39 W A 20 C B 1 *4J7L No contacts No contacts 1 1 *4J7M No contacts No contacts 1 *4JNX W D 17 G G 419 *4JNX W A 20 G B 419 *4JNX W A 20 G B 401 *4JNX W A 20 G B 401 *4JNX W A 20 G B 401 4KNQ No contacts No contacts 1	4HT9	Y	В	25	А	D	1	
*4J39 W A 20 C B 1 *4J7L No contacts No contacts No contacts No contacts 4J7M No contacts No contacts No contacts No contacts *4JGN W D 17 G G 419 *4JNX W A 17 G B 419 *4JNX W A 20 G G 401 *4JNX W A 20 G B 401 *4JNX W A 20 G B 401 *4JNX W D 20 G B 401 *4JNX W D 20 G B 401 4JZU No contacts No contacts No 1	4119			No co	ntacts			
*4J7L No contacts 4J7M No contacts *4JGN No contacts *4JNX W D 17 G G 419 *4JNX W D 17 G B 419 *4JNX W A 17 G B 419 *4JNX W A 20 G G 401 *4JNX W A 20 G B 401 *4JNX W D 20 G B 401 *4JNX W D 20 G B 401 *4JNX W D 20 G B 401 4JZU No contacts No contacts V No contacts V 4KRE F A 292 A R 20 4KRE F A 527 A R 1 4KTG W A 17 C E 219 4KTG W A 20 <t< td=""><td>*4J39</td><td>W</td><td>А</td><td>20</td><td>С</td><td>В</td><td>1</td></t<>	*4J39	W	А	20	С	В	1	
4J7M No contacts *4JGN No contacts *4JNX W D 17 G G 419 *4JNX W A 17 G B 419 *4JNX W A 17 G G 419 *4JNX W A 20 G G 401 *4JNX W A 20 G B 401 *4JNX W D 20 G B 401 *4JNX W D 20 G B 401 4JZU No contacts No contacts V A 708 A R 9 4KRE F A 292 A R 20 A R 10 4KRE Y A 527 A R 11 4 20 G B 201 201 201 201 201 201 201 201 201 201 201 201 201 201 201	*4J7L			No co	ntacts			
*4JGN No contacts *4JNX W D 17 G G 419 *4JNX W A 17 G B 419 *4JNX W A 17 G B 419 *4JNX W A 20 G G 401 *4JNX W D 20 G B 401 4JZU No contacts No contacts 1 20 4 R 9 4KRE R A 708 A R 20 4KRE F A 292 A R 1 4KRE Y A 527 A R 1 4KTG W A 17 C E 219 4LGT No contacts <td>4J7M</td> <td></td> <td></td> <td>No co</td> <td>ntacts</td> <td></td> <td></td>	4J7M			No co	ntacts			
*4JNX W D 17 G G 419 *4JNX W A 17 G B 419 *4JNX W A 20 G G 401 *4JNX W A 20 G B 401 *4JNX W D 20 G B 401 4JZU No contacts No contacts V A 708 A R 9 4KRE F A 292 A R 20 A R 20 4KRE F A 292 A R 20 A R 20 4KRE F A 292 A R 20 A 1 1 4KRE Y A 527 A R 1	*4JGN			No co	ntacts			
*4JNX W A 17 G B 419 *4JNX W A 20 G G 401 *4JNX W D 20 G B 401 *4JNX W D 20 G B 401 *4JNX W D 20 G B 401 4JZU No contacts No contacts F A 708 A R 9 4KRE F A 292 A R 20 4 R 20 4KRE F A 292 A R 20 11 <t< td=""><td>*4JNX</td><td>W</td><td>D</td><td>17</td><td>G</td><td>G</td><td>419</td></t<>	*4JNX	W	D	17	G	G	419	
*4JNX W A 20 G G 401 *4JNX W D 20 G B 401 4JXU D 20 G B 401 4JZU No contacts No contacts S *4KNQ No contacts No contacts S 4KRE R A 708 A R 9 4KRE F A 292 A R 20 4KRE Y A 527 A R 1 4KTG W A 17 C E 219 4KTG W A 20 G B 201 4LGT No contacts No contacts No contacts S 4MDX F B 10 U C 2	*4JNX	W	А	17	G	В	419	
*4JNX W D 20 G B 401 4JZU No contacts No contacts No contacts No contacts *4KNQ No contacts No contacts No contacts No contacts 4KRE R A 708 A R 9 4KRE F A 292 A R 20 4KRE Y A 527 A R 1 4KTG W A 17 C E 219 4KTG W A 20 G B 201 4LGT No contacts No contacts No contacts No contacts 4MDX F B 10 U C 2	*4JNX	W	А	20	G	G	401	
4JZU No contacts *4KNQ No contacts 4KRE R A 708 A R 9 4KRE R A 708 A R 9 4KRE F A 292 A R 20 4KRE Y A 527 A R 1 4KTG W A 17 C E 219 4KTG W A 20 G B 201 4LGT No contacts No contacts No contacts No contacts 4MDX F B 10 U C 2	*4JNX	W	D	20	G	В	401	
*4KNQ No contacts 4KRE R A 708 A R 9 4KRE F A 292 A R 20 4KRE F A 527 A R 1 4KRG W A 17 C E 219 4KTG W A 20 G B 201 4LGT No contacts No contacts No contacts 4M40 10 U C 2	4JZU			No co	ntacts			
4KRE R A 708 A R 9 4KRE F A 292 A R 20 4KRE Y A 527 A R 1 4KRG W A 17 C E 219 4KTG W A 20 G B 201 4LGT No contacts 4M40 No contacts 4MDX F B 10 U C 2	*4KNQ			No co	ntacts			
4KRE F A 292 A R 20 4KRE Y A 527 A R 1 4KTG W A 17 C E 219 4KTG W A 20 G B 201 4KTG W A 20 G B 201 4LGT No contacts 4M40 No contacts 4MDX F B 10 U C 2	4KRE	R	А	708	А	R	9	
4KRE Y A 527 A R 1 4KTG W A 17 C E 219 4KTG W A 20 G B 201 4LGT No contacts No contacts 1 1 4M40 No contacts 1 1 1 4MDX F B 10 U C 2	4KRE	F	А	292	А	R	20	
4KTG W A 17 C E 219 4KTG W A 20 G B 201 4LGT No contacts 4M40 No contacts 4MDX F B 10 U C 2	4KRE	Y	А	527	А	R	1	
4KTG W A 20 G B 201 4LGT No contacts No contacts 4M40 No contacts 4MDX F B 10 U C 2	4KTG	W	А	17	С	Е	219	
4LGTNo contacts4M4ONo contacts4MDXFB10UC2	4KTG	W	А	20	G	В	201	
4M4ONo contacts4MDXFB10UC2	4LGT			No co	ntacts			
4MDX F B 10 U C 2	4M40			No co	ntacts			
	4MDX	F	В	10	U	С	2	

PDB ID	Amino Acid			Nucleotide		
	Res ID	Chain	Res	Res ID	Chain	Res
4N0T	R	А	38	G	В	50
4N0T	F	А	154	А	В	53
4N0T	F	А	154	С	В	58
4N0T	F	А	257	С	В	43
4N0T	F	А	292	G	В	55
4N0T	F	А	154	U	В	54
4N0T	W	А	120	А	В	49
4N0T	Y	А	162	G	В	50
4NGD	F	А	950	U	В	12
*4NKU	Y	В	212	U	Н	59
4NKU	Y	А	212	U	D	59
*1GTF	F	Q	32	G	W	128
1GTF	F	Р	32	G	W	123
40HY	W	А	233	G	В	1
1DFU	Y	Р	31	А	Ν	73
1DI2	No contacts					