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

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Supplementary Material

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

	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

[a]Interplanar angle between the two π–systems (See Supp. Fig. S1). [b]See methods.
[c]Version 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	CHCH	52%	55%
F	Single Proton	CH	15%	10%
C	Bridge	C5HC6H	6%	10%
D	Single Atom	Oδ	5%	0%
U	Bridge	N1HC6H	5%	7%
Y	Bridge	CϵHCζOH	3%	3%
R	Bridge	NηHNηH	2%	0%
R	Bridge	NϵHCδH	2%	0%
E	Single Atom	Oϵ	2%	3%
W	Bridge	CϵHCζH	2%	0%
Y	Bridge	CδHCϵH	2%	3%
Y	Single Proton	CδH	2%	3%
C	Lone Pair	O2	2%	3%
A	Bridge	N9HN3	2%	3%
A	Lone Pair	N3	2%	0%

[a]See Supp. Fig. S2 for atomic numbering.

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.

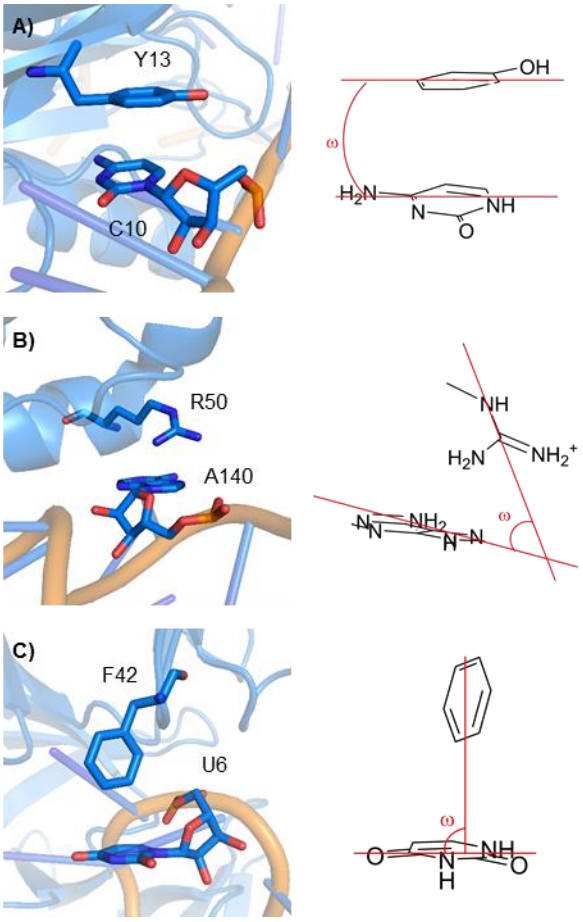
	RNA			DNA[a]		
	Range	Most Common	Mean	Range	Most Common	Mean
A (cyclic)	0-90	5-10 (39%)	28.2 ± 32.8	0-90	5-10 (25%)	25.0±26.4
U/T (cyclic)	0-90	10-15 (25%)	29.5 ± 30.1	0-90	5-10 (31%)	20.6±23.1
G (cyclic)	0-90	20-25 (38%)	19.2 ± 14.4	0-90	10-15 (17%)	25.6±23.1
C (cyclic)	0-90	0-5 (22%)	34.9 ± 29.1	0-90	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

[a]Reference Wilson, *et al.*, 2015.

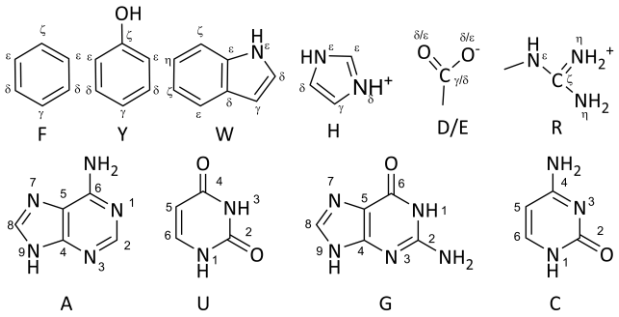
Supplementary Table S4: Comparison of the distance (Å) between nucleobase–amino acid π–systems in RNA or DNA–protein π–interactions found in nature as a function of the nucleobase

	RNA			DNA[a]		
	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

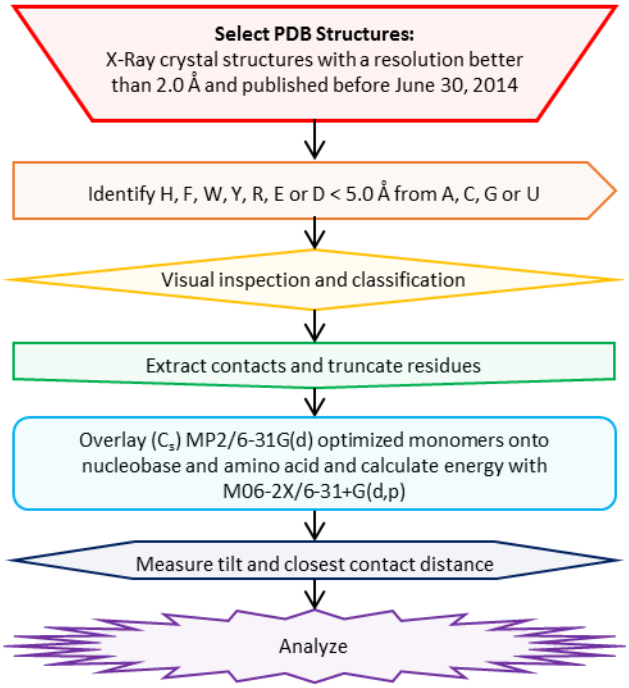
[a]Reference Wilson, *et al.*, 2015.



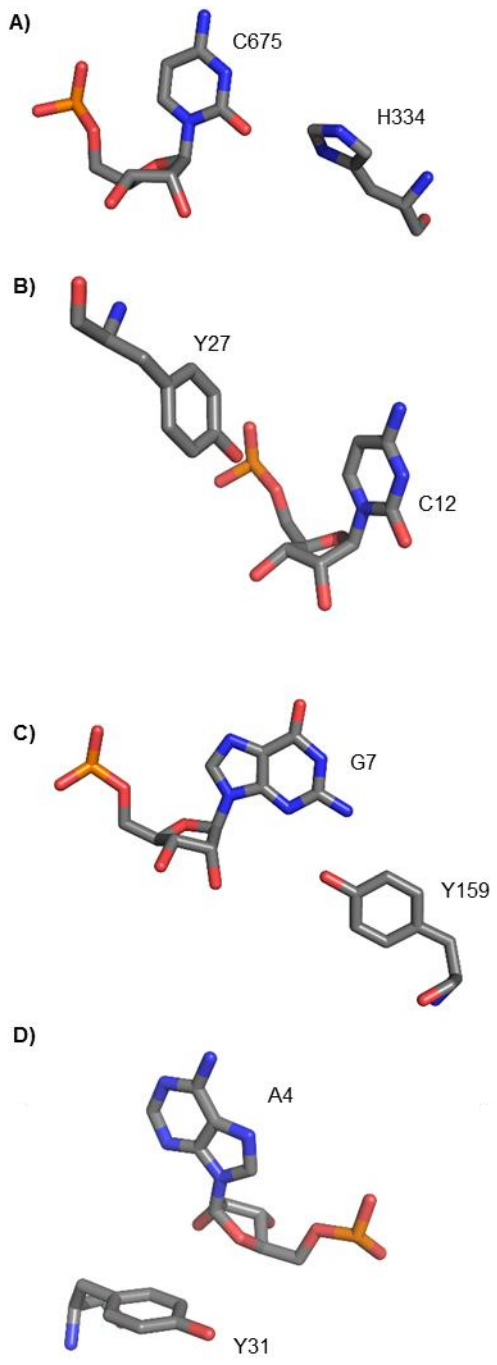
Supplementary Figure S1. Examples of (a) a RNA–protein stacking interaction (PDB ID: 1URN), (b) a RNA–protein inclined interaction (PDB ID: 2PXK), and (c) a RNA–protein stacking interaction (PDB ID: 3RER).



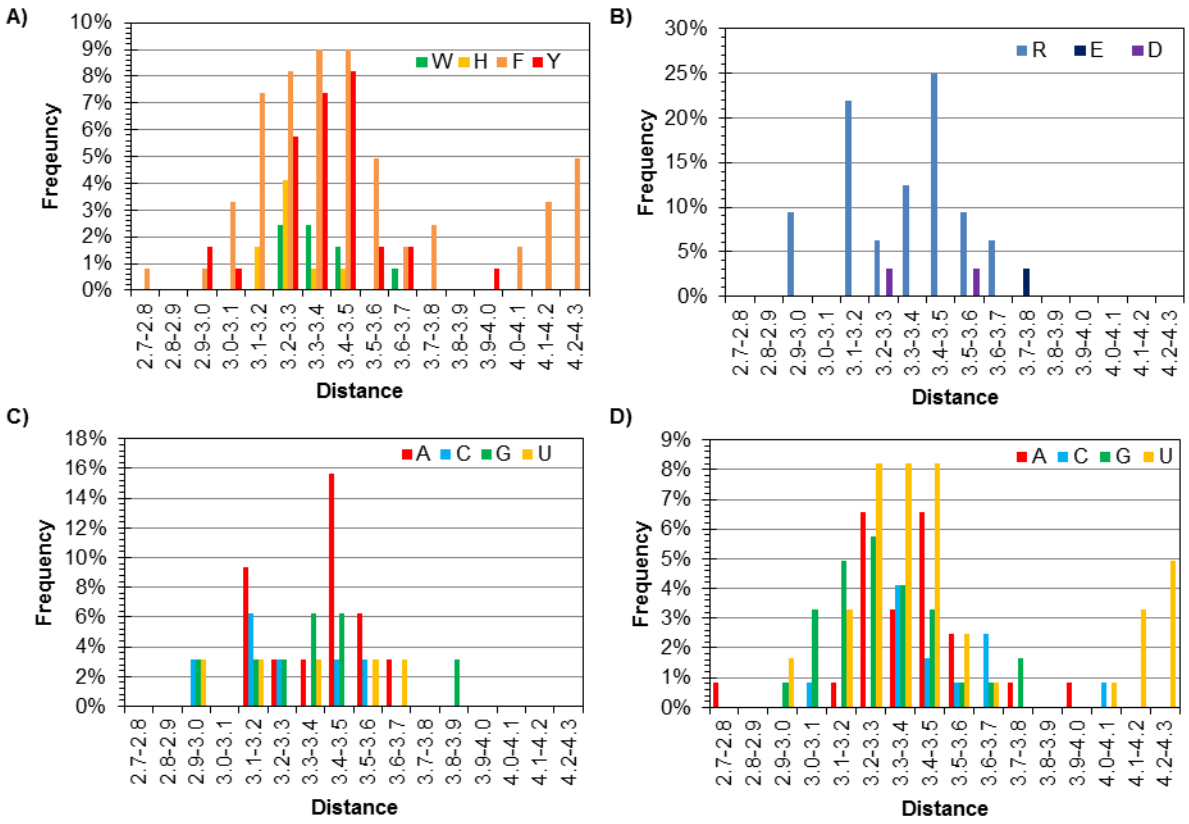
Supplementary Figure S2. Models used in the current study for the nucleobases and amino acids to calculate the interaction energies, as well as the chemical numbering of each residue.



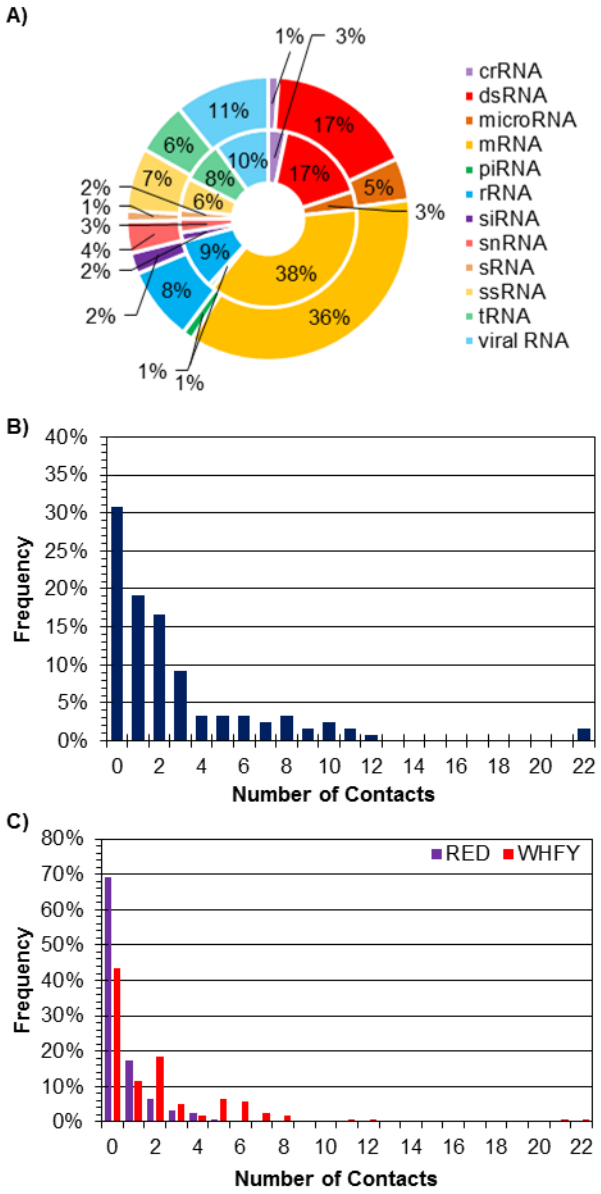
Supplementary Figure S3. Approach used in the current study to identify and classify RNA–protein nucleobase–amino acid π–π interactions. For full description of our approach see the Methods section in the main manuscript.



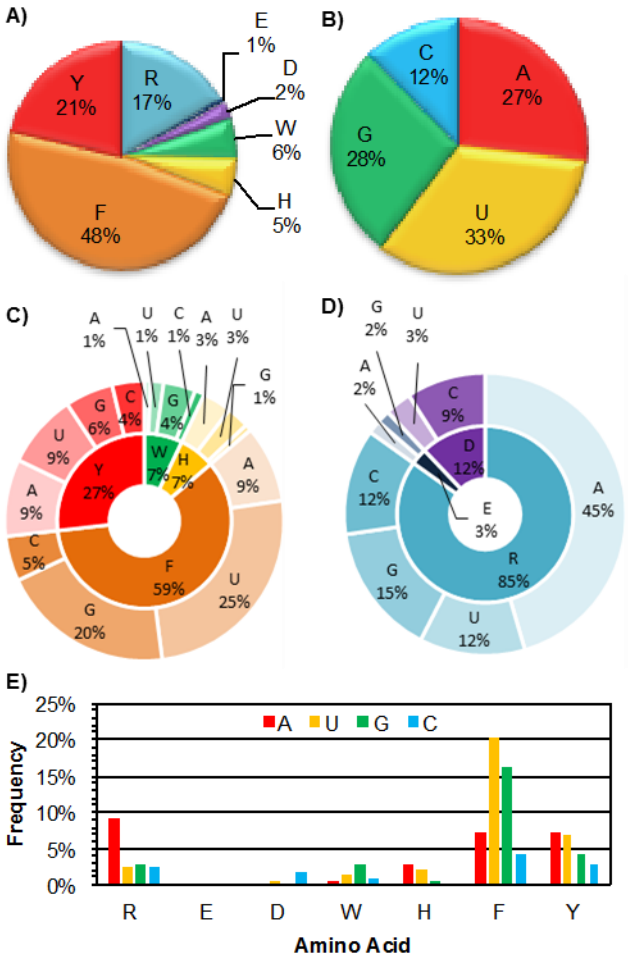
Supplementary Figure S4. Previously identified RNA–protein nucleobase–amino acid π–π contacts through the use of automated search routines (Baker and Grant 2007) that instead represent A) a non-interacting pair (PDB ID: 1ASZ), B) a phosphate interaction (PDB ID: 1E8O), C) a nucleobase–amino acid hydrogen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



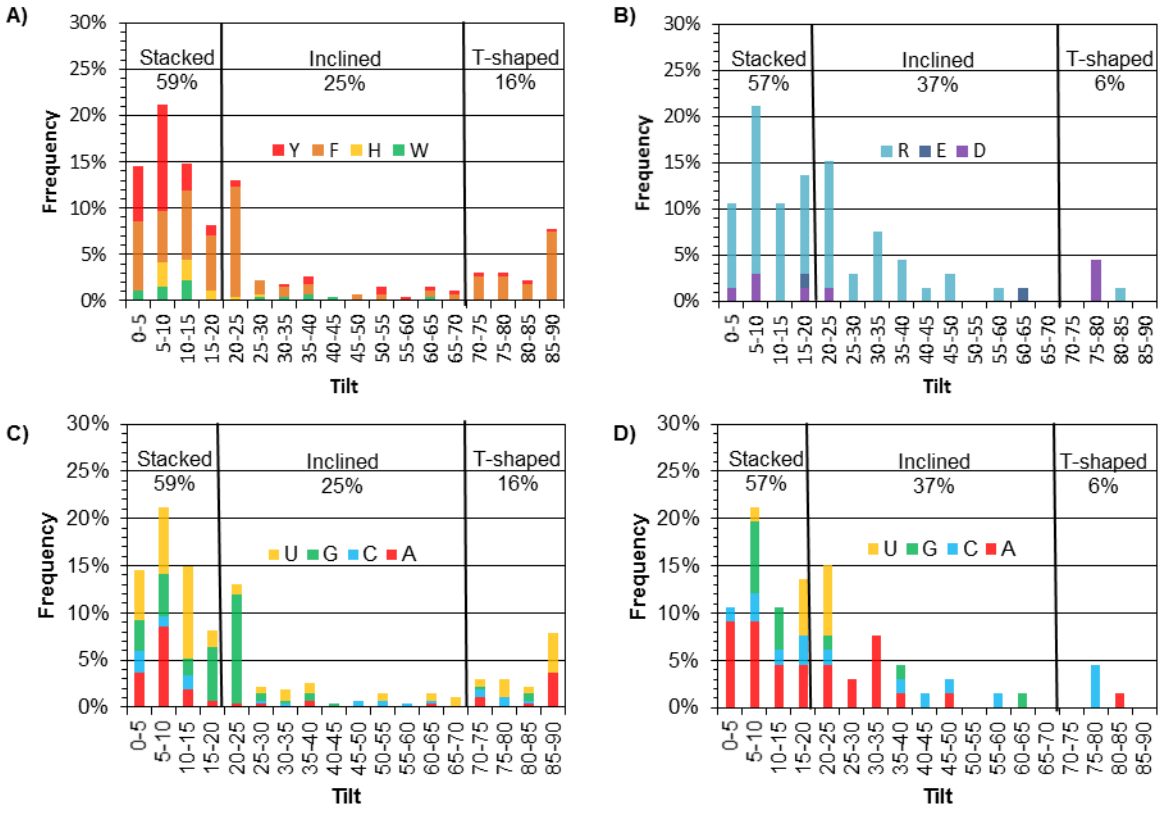
Supplementary Figure S5. Frequency of the closest heavy atom distance for π–π contacts in the non-redundant dataset as a function of the protein (a and b) or RNA (c and d) component for the cyclic (a and c) and acyclic (b and d) amino acids.



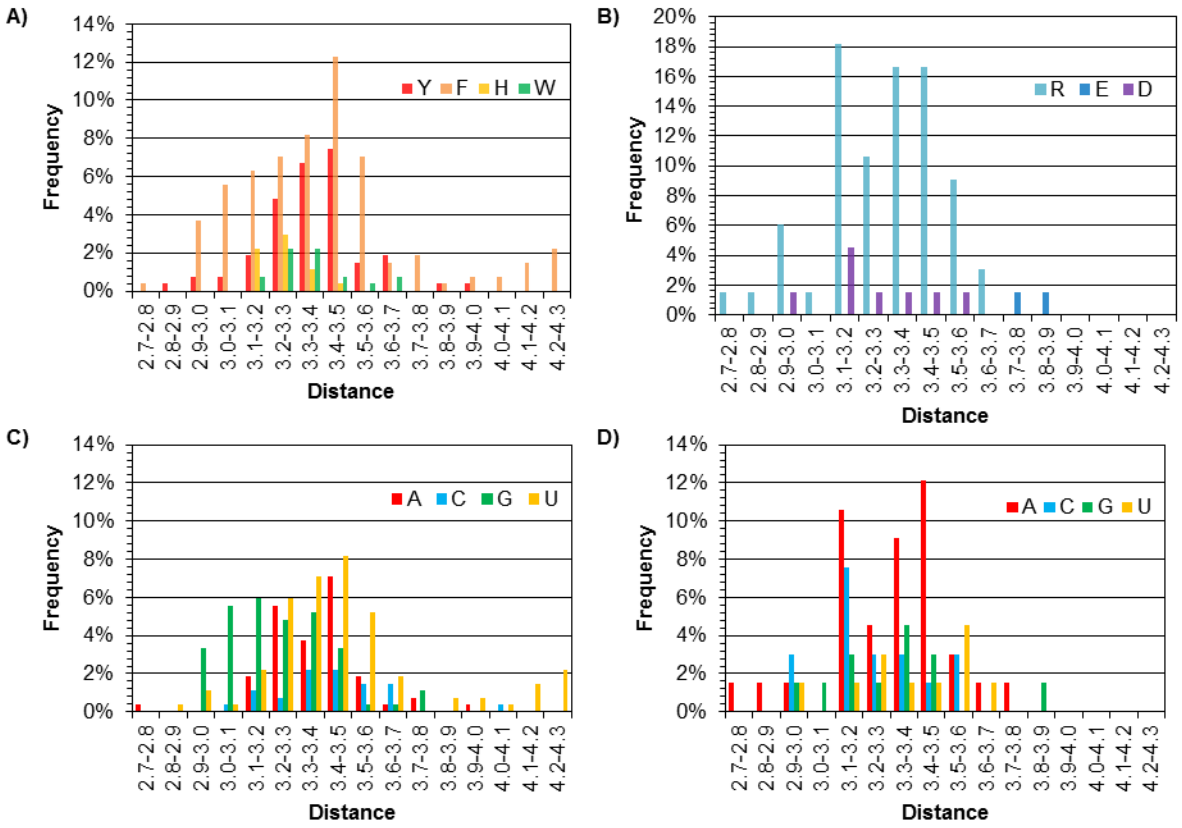
Supplementary Figure S6. A) Distribution in the RNA types searched (inner circle) and the RNA types that form at least one protein π–π contact (outer circle) in the full dataset. B) Overall number of RNA–protein π–π contacts found in each crystal structure searched in the full dataset. C) Number of RNA–protein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



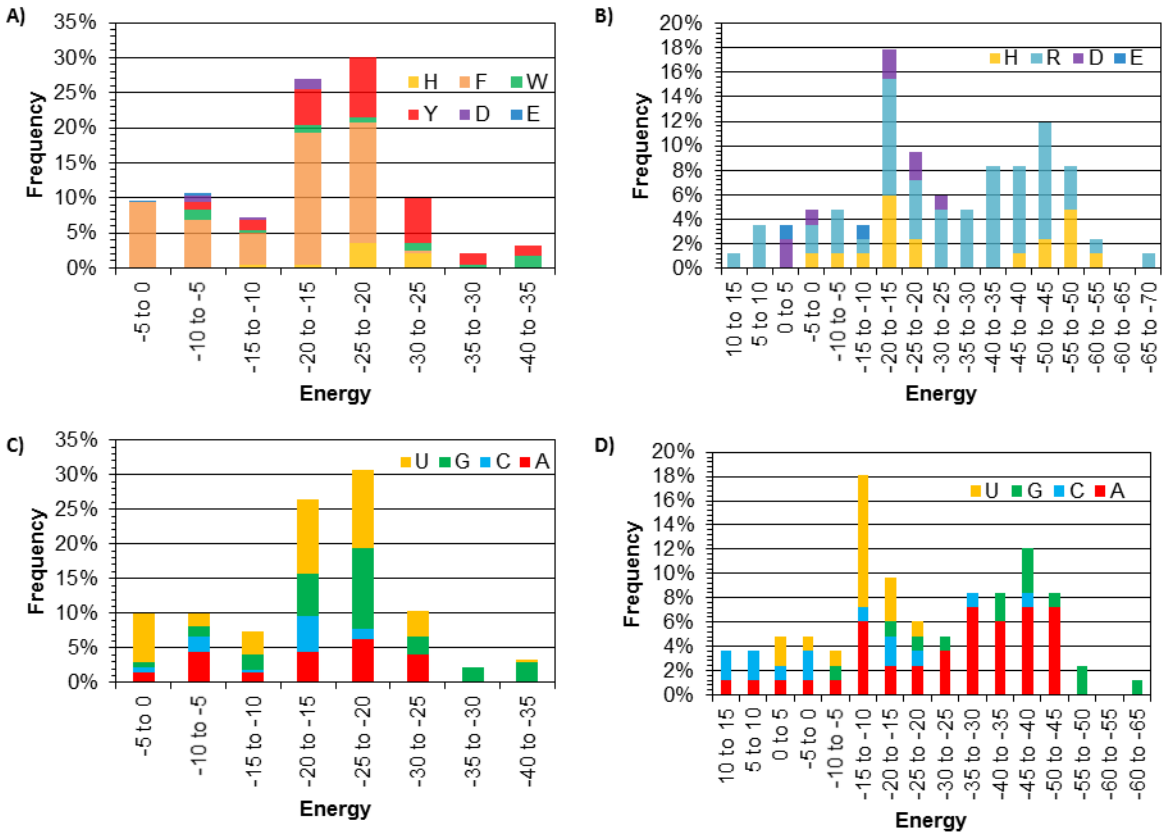
Supplementary Figure S7. Distribution in the composition of the RNA–protein π–π contacts in the full dataset as a function of A) amino acid, B) nucleobase, C) the aromatic (cyclic) amino acids, D) the acyclic amino acids, and E) both (cyclic and acyclic) amino acid classes.



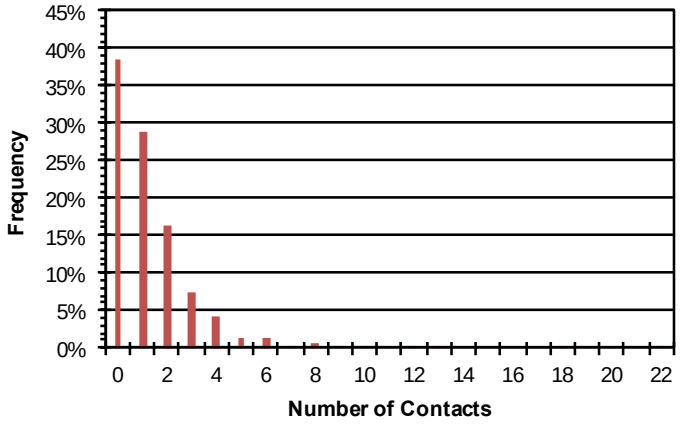
Supplementary Figure S8. Frequency of the tilt angle (degrees) between the ring planes for all π–π interactions in the full dataset as a function of the protein (A and B) or RNA (C and D) component for the cyclic (A and C) and acyclic (B and D) amino acids.



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	Amino Acid			Nucleotide		
	Res ID	Chain	Res #	Res ID	Chain	Res #
1A34	No contacts					
1B2M	E	A	58	G	C	105
1B2M	Y	A	45	G	C	105
*1B2M	Y	A	45	G	D	105
*1C9S	E	L	36	A	W	105
*1C9S	F	T	32	A	W	142
*1C9S	F	N	32	A	W	112
*1C9S	F	O	32	A	W	117
*1C9S	F	M	32	A	W	107
*1C9S	F	L	32	A	W	102
*1C9S	F	V	32	A	W	152
*1C9S	F	U	32	A	W	147
*1C9S	F	S	32	A	W	137
*1C9S	F	R	32	A	W	132
*1C9S	F	Q	32	A	W	127
*1C9S	F	N	32	G	W	111
*1C9S	F	T	32	G	W	141
*1C9S	F	M	32	G	W	106
*1C9S	F	R	32	G	W	131
*1C9S	F	O	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	P	32	G	W	121
*1DUL	R	A	50	A	B	140
*1FXL	F	A	170	U	B	4
*1FXL	F	A	84	U	B	10
*1FXL	F	A	84	U	B	9
*1FXL	Y	A	45	U	B	5
*1FXL	Y	A	128	U	B	3
1GTF	F	O	32	G	W	118
1GTF	F	N	32	G	W	113
1GTF	F	M	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	T	32	G	W	143
1GTF	F	S	32	G	W	138
1GTF	F	R	32	G	W	133
1GTF	F	O	32	U	W	119
1GTF	F	N	32	U	W	114
1GTF	F	M	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	T	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	P	32	U	W	124
1H2C	F	A	125	G	R	2
1H2C	Y	A	171	A	R	3
*1HQ1	R	A	50	A	B	140
1J1U	F	A	261	G	B	535
1JBS	No contacts					
1JID	R	A	14	G	B	148
1JID	R	A	101	G	B	147
1K8W	R	A	141	G	B	412
*1R9F	W	A	42	C	B	1
*1R9F	W	A	39	G	C	19
1SDS	No contacts					
1URN	D	A	92	C	P	12
*1URN	D	C	92	C	R	12
*1URN	D	B	92	C	Q	12
1URN	F	A	56	A	P	11
*1URN	F	B	56	A	Q	11
*1URN	F	C	56	A	R	11
1URN	Y	A	13	C	P	10
*1URN	Y	C	13	C	R	10
*1URN	Y	B	13	C	Q	10
*1UTF	F	E	32	A	4	104
*1UTF	F	G	32	G	6	103
*1UTF	F	J	32	G	9	103
*1UTF	F	I	32	G	8	103
*1UTF	F	B	32	G	1	103
*1UTF	F	C	32	G	2	103
*1UTF	F	A	32	G	0	103
*1UTF	F	K	32	G	Z	103
*1UTF	F	H	32	G	7	103
*1UTF	F	D	32	G	3	103
*1UTF	F	E	32	G	4	103
*1UTF	F	F	32	G	5	103
*1UTV	F	I	32	G	8	103
*1UTV	F	H	32	G	7	103

PDB ID	Amino Acid			Nucleotide		
	Res ID	Chain	Res #	Res ID	Chain	Res #
*1UTV	F	E	32	G	4	103
*1UTV	F	F	32	G	5	103
*1UTV	F	D	32	G	3	103
*1UTV	F	C	32	G	2	103
*1UTV	F	B	32	G	1	103
*1UTV	F	A	32	G	0	103
*1UTV	F	K	32	G	Z	103
*1UTV	F	J	32	G	9	103
*1UTV	F	G	32	G	6	103
*1UVJ	No contacts					
*1UVL	R	C	291	C	D	7
*1UVL	D	A	399	C	B	7
*1UVL	D	E	399	C	F	7
*1UVL	D	C	399	C	D	7
*1UVL	F	E	156	U	F	4
*1UVL	F	A	156	U	B	4
*1UVL	F	C	156	U	D	4
1UVM	F	C	156	U	F	5
*1UVM	F	B	156	U	E	5
*1UVM	F	A	156	U	D	5
*1WMQ	No contacts					
*1WPU	No contacts					
*1ZH5	F	B	35	U	C	9
*1ZH5	F	B	28	U	D	1
*1ZH5	F	A	28	U	C	1
*1ZH5	F	A	35	U	D	9
*1ZH5	Y	B	23	U	C	8
*1ZH5	Y	A	23	U	D	8
2ANR	No contacts					
2ASB	No contacts					
2B3J	R	A	70	G	F	37
*2B3J	R	C	70	G	H	37
*2B3J	R	B	70	G	E	37
2B3J	F	D	144	C	H	35
*2B3J	F	A	144	C	E	35
*2B3J	F	D	145	G	H	36
*2B3J	F	C	145	G	G	36
2B3J	F	A	145	G	E	36
2F8K	No contacts					
2JLV	No contacts					
2NUG	No contacts					
2PO1	H	A	66	A	C	395
*2PXB	R	A	50	A	B	140
*2PXD	R	A	50	A	B	140
*2PXE	R	A	50	A	B	140

PDB ID	Amino Acid			Nucleotide		
	Res ID	Chain	Res #	Res ID	Chain	Res #
*2PXF	R	A	50	A	B	140
*2PXK	R	A	50	A	B	140
*2PXV	R	A	50	A	B	140
2Q66	H	A	314	A	X	3
2Q66	F	A	140	A	X	3
2R8S	D	H	109	U	R	130
2R8S	Y	H	106	U	R	130
2R8S	Y	L	49	U	R	130
2VOO	F	A	35	U	C	-1
*2VOO	F	B	35	U	D	-1
*2VOO	F	B	55	U	D	-1
2VOO	F	A	55	U	C	-1
2VOO	Y	A	23	U	C	-2
*2VOO	Y	B	23	U	D	-2
2X1F	H	A	109	G	B	1
2X1F	Y	A	21	G	B	1
*2XLK	No contacts					
2XNR	F	A	333	C	C	2
2XNR	F	A	368	U	C	3
*2XS2	R	A	115	U	B	5
*2XS2	F	A	43	U	B	4
*2XS2	F	A	84	U	B	5
*2XS5	R	A	115	U	C	4
*2XS5	R	B	115	U	D	4
*2XS5	F	A	84	U	C	4
*2XS5	F	A	43	U	C	3
*2XS5	F	B	43	U	D	3
*2XS5	F	B	84	U	D	4
*2XS5	Y	B	88	C	C	5
*2XS5	Y	A	88	C	D	5
2XS7	R	A	115	U	B	5
2XS7	F	A	84	U	B	5
2XS7	F	A	43	U	B	4
2Y8W	No contacts					
*2Y8Y	No contacts					
2ZKO	No contacts					
2ZUE	Y	A	85	A	B	920
2ZUE	Y	A	587	C	B	935
3B0U	No contacts					
3BOY	No contacts					
*3BSN	No contacts					
*3BSO	No contacts					
3D2S	F	D	202	C	H	3
3D2S	F	B	202	C	F	3
3D2S	F	A	202	G	E	5

PDB ID	Amino Acid			Nucleotide		
	Res ID	Chain	Res #	Res ID	Chain	Res #
3DD2	R	H	233	A	B	7
3DD2	R	H	165	A	B	15
3EQT	F	A	601	C	D	8
*3EQT	F	B	601	C	C	8
3G9Y	W	A	79	G	C	2
3G9Y	W	A	79	G	C	3
*3GPQ	R	B	144	A	F	1
3GPQ	R	A	144	A	E	1
*3H5X	No contacts					
3H5Y	No contacts					
*3I5X	F	A	576	U	B	1
*3I5X	F	A	224	U	B	10
*3I62	F	A	576	U	B	1
3IEV	W	A	280	A	D	1534
3IEV	Y	A	276	C	D	1538
3IEV	Y	A	276	U	D	1537
*3K62	R	A	288	A	B	7
*3K62	H	A	326	A	B	7
*3K62	H	A	454	U	B	3
*3K62	Y	A	245	C	B	9
*3K62	Y	A	416	G	B	4
*3K62	Y	A	501	G	B	2
*3K62	Y	A	245	U	B	8
*3K64	R	A	288	A	B	7
*3K64	H	A	326	A	B	7
*3K64	H	A	454	U	B	3
*3K64	Y	A	501	G	B	2
*3K64	Y	A	416	G	B	4
*3K64	Y	A	245	U	B	9
3L25	F	E	239	C	C	1
*3L25	F	B	239	C	F	1
3LQX	R	A	50	A	B	140
*3NMR	D	A	187	U	B	4
*3NMR	F	A	111	G	B	3
*3NMR	F	A	111	U	B	4
*3NMR	F	A	152	U	B	5
3NNA	F	A	111	G	B	3
3NNA	F	A	152	U	B	5
3NNA	F	A	111	U	B	4
3O8C	W	A	501	U	C	7
3O8C	W	A	501	U	C	8
3OIN	R	A	129	A	C	8
3OIN	R	A	136	C	C	7
*3OVA	No contacts					
3OVB	No contacts					

PDB ID	Amino Acid			Nucleotide		
	Res ID	Chain	Res #	Res ID	Chain	Res #
*3PEW	No contacts					
3PEY	No contacts					
*3PF4	H	B	29	U	R	1
*3PF4	F	B	27	C	R	2
*3PF4	F	B	17	U	R	3
*3PF4	W	B	8	U	R	4
3PF5	H	B	29	U	R	1
3PF5	F	A	17	U	S	1
3PF5	F	B	27	U	R	2
3PF5	F	B	17	U	R	3
3PF5	W	B	8	U	R	4
*3Q0Q	R	A	742	A	B	8
*3Q0Q	R	A	814	A	B	6
*3Q0Q	R	A	888	A	B	5
*3Q0Q	R	A	888	A	B	4
*3Q0Q	H	A	852	A	B	6
*3Q0Q	H	A	852	A	B	5
*3Q0Q	Y	A	778	A	B	8
*3Q0Q	Y	A	924	A	B	4
*3Q0Q	Y	A	1003	G	B	2
*3Q0Q	Y	A	1003	U	B	1
3Q0R	R	A	742	A	B	8
3Q0R	R	A	814	A	B	6
3Q0R	R	A	888	A	B	4
3Q0R	R	A	888	G	B	5
3Q0R	H	A	852	A	B	6
3Q0R	Y	A	778	A	B	8
3Q0R	Y	A	924	A	B	4
3Q0R	Y	A	1003	G	B	2
3Q0R	Y	A	924	U	B	3
*3Q0S	R	A	814	A	B	6
*3Q0S	R	A	742	C	B	8
*3Q0S	R	A	814	U	B	7
*3Q0S	H	A	852	A	B	6
*3Q0S	H	A	1039	U	B	1
*3Q0S	Y	A	924	A	B	4
*3Q0S	Y	A	778	C	B	8
*3Q0S	Y	A	1003	G	B	2
*3Q0S	Y	A	778	U	B	7
*3Q0S	Y	A	1003	U	B	1
3QGC	H	A	454	G	B	2
3QGC	H	A	326	U	B	7
3QGC	H	A	454	U	B	3
3QGC	Y	A	245	A	B	9
3QGC	Y	A	416	G	B	4

PDB ID	Amino Acid			Nucleotide		
	Res ID	Chain	Res #	Res ID	Chain	Res #
3QGC	Y	A	501	G	B	2
3QGC	Y	A	501	U	B	1
3QGC	Y	A	288	U	B	8
3R2C	R	A	102	C	R	3
*3R2C	R	B	102	C	S	3
3R2C	R	A	102	G	R	1
*3R2C	R	B	102	G	S	1
3R2C	R	J	16	U	R	8
3R2C	F	A	104	U	R	4
3R2C	F	A	122	U	R	8
*3R2C	F	B	104	U	S	4
*3R2C	F	B	122	U	S	8
3R2C	W	B	72	G	S	9
*3RER	F	B	42	A	K	8
*3RER	F	E	42	U	K	5
*3RER	F	D	42	U	K	4
*3RER	F	E	42	U	K	6
*3RER	F	A	42	U	K	7
3SQW	No contacts					
3T5N	R	A	300	A	C	3
3T5N	R	A	300	U	C	4
3T5N	Y	A	308	A	C	3
*3U4M	No contacts					
3UMY	R	A	129	A	B	2169
3WBM	No contacts					
4AL5	R	A	115	C	B	9
4AL5	R	A	111	C	B	6
4AL5	F	A	158	A	B	5
4AL5	F	A	155	G	B	20
4ALP	F	A	77	U	E	1
4ALP	F	D	77	U	E	2
4ARC	R	A	416	C	B	75
4ARC	R	A	719	U	B	16
4ARC	Y	A	330	C	B	75
4C8Y	H	A	37	A	C	29
4D25	F	A	348	A	D	3
*4ED5	F	B	151	U	C	4
4ED5	F	B	65	U	C	10
4ED5	F	A	151	U	D	4
*4ED5	Y	B	26	U	C	5
*4ED5	Y	B	109	U	C	3
4ED5	Y	A	109	U	D	3
4ED5	Y	A	26	U	D	5
*4F02	R	D	94	A	E	6
4F02	R	D	179	A	E	3

PDB ID	Amino Acid			Nucleotide		
	Res ID	Chain	Res #	Res ID	Chain	Res #
4F02	R	A	94	A	B	6
4F02	F	A	102	A	B	3
4F02	F	A	142	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	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	C	X	2
4HOS	F	A	337	U	X	2
4HOS	F	A	339	U	X	3
*4HT8	Y	D	25	A	K	1
*4HT8	Y	C	25	A	K	4
*4HT8	Y	B	25	A	K	7
*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	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
4II9	No contacts					
*4J39	W	A	20	C	B	1
*4J7L	No contacts					
4J7M	No contacts					
*4JGN	No contacts					
*4JNX	W	D	17	G	G	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					
*4KNQ	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					
4M4O	No contacts					
4MDX	F	B	10	U	C	2

PDB ID	Amino Acid			Nucleotide		
	Res ID	Chain	Res	Res ID	Chain	Res
4N0T	R	A	38	G	B	50
4N0T	F	A	154	A	B	53
4N0T	F	A	154	C	B	58
4N0T	F	A	257	C	B	43
4N0T	F	A	292	G	B	55
4N0T	F	A	154	U	B	54
4N0T	W	A	120	A	B	49
4N0T	Y	A	162	G	B	50
4NGD	F	A	950	U	B	12
*4NKU	Y	B	212	U	H	59
4NKU	Y	A	212	U	D	59
*1GTF	F	Q	32	G	W	128
1GTF	F	P	32	G	W	123
4OHY	W	A	233	G	B	1
1DFU	Y	P	31	A	N	73
1DI2	No contacts					