

Supplementary Table S1.

List of across-bulged motifs found in the representative set of PDB structures.

Classes of base-phosphate interactions (BPh) are given according to the classification from (Zirbel et al. 2009).

PDB entry	Chain	A-minors		Adenine(s) thread is	Unique motif	Across-bulged motif's nucleotides	Base triple / non-canonical base pair	Adenine(s) thread	Adenine(s) thread (sequence)	Thread with bulged bases	Thread with bulged bases (sequence)	Bulged base (s)	Bulged bases involved in	Molecule	Organism
		Adenines	Base pairs												
4yaz	R	A78 A79	(C7, G77) (G8, C76)	3' - thread	I	U3-G8, C76-A82	A6, A80 cWH	A78-A80	--AAa	C5-A6	-C---a	C5		Cyclic di-GMP-I riboswitch	geobacter
6tdt	C	A30	(G11, U28)	3' - thread	II	A7-C12 G27-A32	U10, A29 cWW	A29-A30	a-A--	C9-U10	-C---u	C9	RNA-protein int.	Cas13b sgRNA	prevotella buccae
4v9f	9	A56 A57	(U28, A54) (C29, G53)	3' - thread	III	G20-C29 G53-C60	U55, C27, G58 cWW, cSW	U55-G58	u-AAg	G22-C27	gUUGcc	U23, U24		5S rRNA	haloarcularia marismortui
5dm6	Y	A59 A60	(A31, U57) (C32, G56)	3' - thread	III	U24-C32 G56-A63	G58, C30, A61 cWW, cSW	G58-A61	g-AAa	G26-C30	gAa-cc	A27	7BPh with G56	5S rRNA	deinococcus radiodurans
5fdv	1B	A57 A58	(A29, U55) (C30, G54)	3' - thread	III	G54-G61 U22-C30	G56, C28, A59 cWW, cSW	G56-A59	g-AAa	G24-C28	gAa-cc	A25	A-minor with (C3, G118)	5S rRNA	thermus thermophilus
5j7l	DB	A57 A58	(A29, U55) (C30, G54)	3' - thread	III	G54-G61 U22-C30	G56, C28, A59 cWW, cSW	G56-A59	g-AAa	G24-C28	gUc-cc	U25	U-minor with (C3, G117)	5S rRNA	escherichia coli
5t5h	D	A54 A55	(A27, U52) (C28, G51)	3' - thread	III	C20-C28 G51-G58	U53, C26, G56 cWW, cSW	U53-G56	u-AAg	A22-C26	aGu-gc	G23	G-minor with (G1, C118)	5S rRNA	trypanosoma cruzi
5tbw	AS	A55 A56	(A27, U53) (C28, G52)	3' - thread	III	A20-C28 G52-U59	U54, C26, G57 cWW, cSW	U54-G57	u-AAg	A22-C26	AAa-gc	A22, A23	A22: RNA-protein int.; A23: A-minor with (G1, C120)	5S rRNA	saccharomyces cerevisiae
6er1	Ax	A57 A58	(A29, U55) (C30, G54)	3' - thread	III	A22-C30 G54-U61	U56, C28, A59 cWW, cSW	U56-A59	u-AAa	G24-C28	gAa-cc	A25	A-minor with (C4, G117)	5S rRNA	spinacea oleracea
6hma	B	A55 A56	(A27, U53) (C28, G52)	3' - thread	III	A20-C28 G52-U59	U54, C26, G57 cWW, cSW	U54-G57	u-AAg	G22-C26	gUc-ac	U23		5S rRNA	staphylococcus aureus
6qzp	L7	A54 A55	(G27, C52) (C28, G51)	3' - thread	III	U20-C28 G51-A58	U53, C26, G56 cWW, cSW	U53-G56	u-AAg	A22-C26	AAC-gc	A22, A23, C24	A-minor with (G1, C118); C-minor with (U2, A117)	5S rRNA	homo sapiens
4y4o	1a	A1146	(C1128, G1144)	3' - thread	IV	A1123-C1129 G1143-U1150	C1145, G1127, U1148 cWW, cSW	C1145-U1148	c-Acu	U1125-G1127	uU---g	U1126	cross-strand stack with U1281; RNA-protein int.; 5BPh with A1280	16S rRNA	thermus thermophilus
6er1	BA	A1095	(C1078, G1093)	3' - thread	IV	A1073-C1079 G1092-U1099	A1094, G1077, C1097 cWW, cSW	A1094-C1097	a-Acc	U1075-G1077	uU---g	U1076	cross-strand stack with C1230; RNA-protein int.; 5BPh with A1229	16S rRNA	spinacea oleracea
4y4o	1a	A373 A374	(C370, G391) (G371, C390)	5' - thread	V	C370-G377 C386-G391	C372, A389, U375 tWH, cWW	C372-U375	c-AAu	G388-A389	-G---a	G388	G-minor with (C58, G354); 4BPh with G369	16S rRNA	thermus thermophilus
5j7l	AA	A373 A374	(C370, G391) (A371, U390)	5' - thread	V	C370-G377 C386-G391	C372, A389, U375 tWH, cWW	C372-U375	c-AAu	G388-A389	-G---a	G388	G-minor with (C58, G354); 4BPh with G369	16S rRNA	escherichia coli
5ngm	Aa	A381 A382	(C378, G399) (G379, C398)	5' - thread	V	C378-G385 C394-G399	C380, A397, U383 tWH, cWW	C380-U383	c-AAu	G396-A397	-G---a	G396	cross-strand stack with C59; 4BPh with C377	16S rRNA	staphylococcus aureus
6er1	BA	A345 A346	(C342, G363) (G343, C362)	5' - thread	V	C342-G349 C358-G363	C344, A361, U347 tWH, cWW	C344-U347	c-AAu	G360-A361	-G---a	G360	G-minor with (C60, G326); 4BPh with C341	16S rRNA	spinacea oleracea
4v88	A6	A445 A446	(C442, G462) (C443, G461)	5' - thread	V	C442-C449 G457-G462	C444, A460, U447 tWH, cWW	C444-U447	c-AAu	G459-A460	-G---a	G459	G-minor with (C54, G426); 4BPh with A441	18S rRNA	saccharomyces cerevisiae
6az1	1	A488 A489	(C485, G510) (C486, G509)	5' - thread	V	C485-U492 A505-G510	C487, A508, U490 tWH, cWW	C487-U490	c-AAu	G507-A508	-G---a	G507	G-minor with (C54, G469); 4BPh with G484	18S rRNA	leishmania donovani
6qzp	S2	A493	(C490, G510)	5' - thread	V	C490-C497 G505-G510	C492, A508, U495 tWH, cWW	C492-U495	c-Acu	G507-A508	-G---a	G507	G-minor with (C53, G474); 4BPh with A489	18S rRNA	homo sapiens
4y4o	2A	A1321 A1322	(C1318, G1334) (G1319, C1333)	5' - thread	VI	C1318-G1324 C1330-G1334	C1320, A1331, U1323 tWH, cWW	C1320-U1323	c-AAu	A1331-G1332	aG----	G1332	cross-strand stack with A1609	23S rRNA	thermus thermophilus
5dm6	X	A1321 A1322	(G1318, C1334) (G1319, C1333)	5' - thread	VI	G1318-G1324 C1330-G1334	G1320, C1331, G1323 tHH, cWW	G1320-G1323	g-AAg	C1331-G1332	cG----	G1332	cross-strand stack with A1609	23S rRNA	deinococcus radiodurans
5j7l	DA	A1321 A1322	(U1318, G1334) (C1319, G1333)	5' - thread	VI	U1318-G1324 C1330-G1334	C1320, G1331, C1323 tWH, cWW	C1320-C1323	c-AAc	G1331-G1332	gG----	G1332	cross-strand stack with A1609	23S rRNA	escherichia coli
6er1	AA	A1342 A1343	(C1339, G1355) (G1340, C1354)	5' - thread	VI	C1339-G1345 C1351-G1355	C1341, C1352, G1344 tWH, cWW	C1341-G1344	c-AAg	C1352-A1353	cA----	A1353	cross-strand stack with A1645	23S rRNA	spinacea oleracea
6hma	A	A1358 A1359	(A1355, U1371) (G1356, C1370)	5' - thread	VI	A1355-G1361 C1367-U1371	G1357, C1368, G1360 tHH, cWW	G1357-G1360	g-AAg	C1368-G1369	cG----	G1369	cross-strand stack with A1653	23S rRNA	staphylococcus aureus
6qzp	L5	A2417 A2418	(G2414, C2430) (U2415, A2429)	5' - thread	VI	G2414-A2420 U2426-C2430	G2416, G2427, C2419 tWH, cWW	G2416-C2419	g-AAc	G2427-A2428	gA----	A2428	RNA-protein int.; cross-strand stack with A2789	28S rRNA	homo sapiens
4v9f	Ø	A961	(G958, C1008)	5' - thread	VII	A957-A965 U1003-U1009	C959, A1005, C963 tWH, cWW	C959-C963	cgAcc	A1005-A1007	aAA---	A1006, A1007	A-minors with (U2297, A2311), (C2298, G2310)	23S rRNA	haloarcularia marismortui
4y4o	2A	A866	(G864, C912)	5' - thread	VII	A863-A870 U907-U913	C865, A909, U868 tWH, cWW	C865-U868	c-Acu	A909-A911	aAA---	A910, A911	A-minors with (C2263, G2277), (C2264, G2276)	23S rRNA	thermus thermophilus
5dm6	X	A866	(G864, C912)	5' - thread	VII	A863-A870 U907-U913	C865, A909, U868 tWH, cWW	C865-U868	c-Acu	A909-A911	aAA---	A910, A911	A-minors with (C2263, G2277), (C2264, G2276)	23S rRNA	deinococcus radiodurans
6er1	AA	A876	(G874, C921)	5' - thread	VII	A873-U880 G916-U922	C875, A918, U878 tWH, cWW	C875-U878	c-Acu	A918-A920	aAA---	A919, A920	A-minors with (C2280, G2294), (C2281, G2293)	23S rRNA	spinacea oleracea
6hma	A	A911	(G909, C957)	5' - thread	VII	A908-U915 A952-U958	C910, A954, U913 tWH, cWW	C910-U913	c-Acu	A954-A956	aAA---	A955, A956	A-minors with (C2290, G2304), (C2291, G2303)	23S rRNA	staphylococcus aureus
5tbw	1	A1002 A1003	(A998, U1050) (G999, C1049)	5' - thread	VII	A998-A1006 U1044-U1050	C1000, A1046, U1004 tWH, cWW	C1000-U1004	cgAAu	A1046-A1048	aAA---	A1047, A1048	A-minors with (G2632, C2646), (U2633, G2645)	25S rRNA	saccharomyces cerevisiae
6qzp	L5	A1742 A1743	(A1738, U1790) (G1739, C1789)	5' - thread	VII	A1738-A1746 U1784-U1790	C1740, A1786, U1744 tWH, cWW	C1740-U1744	cgAAu	A1786-A1788	aAA---	A1787, A1788	A-minors with (G4209, C4223), (U4210, G4222)	28S rRNA	homo sapiens
6az3	1	A1053 A1054	(A1049, U1101) (G1050, C1100)	5' - thread	VII	A1049-A1057 U1095-U1101	C1051, A1097, U1055 tWH, cWW	C1051-U1055	caAAu	A1097-A1099	aAA---	A1098, A1099	A-minors with (G1060, C1074), (U1061, G1073) of chain 2	rRNA alpha	leishmania donovani
6eri	AA	U2699 C2700	(A2696, U2746) (C2697, G2745)	5' - thread	VIII	A2696-G2703 C2741-U2746	C2698, A2743, U2701 tWH, cWW	C2698-U2701	c-UCu	A2743-A2744	aA---	A2744	cross-strand stack with A1700	23S rRNA	spinacea oleracea