Supplementary Material

Evaluating coaxial helical stacking prediction for higher-order junctions

The prediction scenario involved in determining whether a pair of helices in a higher-order junction is stacked or not corresponds to a binary classification system, and therefore the accuracy of prediction can be measured with two parameters, the *sensitivity* and *positive predictive value*:

$$\text{Sensitivity} = \frac{TP}{TP + FN} \times 100\%, \text{ and}$$

$$\text{Positive predicted value} = \frac{TP}{TP + FP} \times 100\%.$$

Here *TP* (*true positives*) is the number of predicted helical stacks that are found to be stacking in the solved structures, *FP* (*false positives*) is the number of predicted helical stacks that are found to be not stacking in the solved structures, and *FN* (*false negatives*) is the number of helical stacks found in the solved junction structures that are not predicted to be stacked.

As Table S7 shows, our results have a sensitivity value of 60%, and positive predictive value of 76%. The higher positive predictive value than sensitivity implies that we make fewer false positive predictions of coaxial stacks than false negatives.

Table S1. List of RNA 3D structures containing 216 junctions

Name	Degree	RNA Type	Coaxial stacks	Family	Nomenclature	Domain	Helix numbers	Proteins/ metabolites
1NKW_31	3WJ	23S rRNA *D. Radiodurans*	H_1H_2	A	$HS_2HS_{14}HS_4$	I	H3-4-23	?
1S72_28	3WJ	23S rRNA *H. Marismortui*	H_1H_2	A	$HS_2HS_{15}HS_4$	I	H3-4-23	L37e, L39e
2AW4_31	3WJ	23S rRNA *E. Coli*	H_1H_2	A	$HS_2HS_{15}HS_4$	I	H3-4-23	L4, L20, L23, L34
2J01_31	3WJ	23S rRNA *T. Thermophilus*	H_1H_2	A	$HS_2HS_{15}HS_4$	I	H3-4-23	L4, L20, L34
1NKW_54	3WJ	23S rRNA *D. Radiodurans*	H_1H_2	A	$2HS_5HS_4$	I	H5-6-7	?
1S72_51	3WJ	23S rRNA *H. Marismortui*	H_1H_2	A	$2HS_5HS_3$	I	H5-6-7	L24, L29, L39e
2AW4_55	3WJ	23S rRNA *E. Coli*	H_1H_2	A	$2HS_5HS_3$	I	H5-6-7	L23, L29, L34
2J01_55	3WJ	23S rRNA *T. Thermophilus*	H_1H_2	A	$2HS_5HS_3$	I	H5-6-7	L29, L34
1NKW_1310	3WJ	23S rRNA *D. Radiodurans*	H_1H_3	A	$HS_4HS_1HS_2$	III	H48-60-?	?
1S72_1403	3WJ	23S rRNA *H. Marismortui*	H_1H_3	A	$HS_4HS_2HS_2$	III	H48-60-?	L19e
2AW4_1297	3WJ	23S rRNA *E. Coli*	H_1H_3	A	$HS_4HS_1HS_2$	III	H48-60-?	-
2J01_1297	3WJ	23S rRNA *T. Thermophilus*	H_1H_3	A	$HS_4HS_1HS_2$	III	H48-60-?	-
1NKW_1318	3WJ	23S rRNA *D. Radiodurans*	H_1H_2	A	$HS_2HS_5HS_1$	III	H49-59.1-?	?
1S72_1411	3WJ	23S rRNA *H. Marismortui*	H_1H_2	A	$HS_2HS_5HS_1$	III	H49-59.1-?	L37e, L39e
2AW4_1305	3WJ	23S rRNA *E. Coli*	H_1H_2	A	$HS_2HS_5HS_1$	III	H49-59.1-?	L34
2J01_1305	3WJ	23S rRNA *T. Thermophilus*	H_1H_2	A	$HS_2HS_5HS_1$	III	H49-59.1-?	L34
1NKW_2072	3WJ	23S rRNA *D. Radiodurans*	H_2H_3	A	$HS_2HS_3HS_5$	V	H75-76-79	?
1S72_2130	3WJ	23S rRNA *H. Marismortui*	H_2H_3	A	$HS_2HS_3HS_5$	V	H75-76-79	L15e
2AW4_2090	3WJ	23S rRNA *E. Coli*	H_2H_3	A	$HS_1HS_3HS_4$	V	H75-76-79	L2, L9, L31
2J01_2090	3WJ	23S rRNA *T. Thermophilus*	H_2H_3	A	$HS_1HS_3HS_4$	V	H75-76-79	L2, L9, L28
1NKW_2788	3WJ	23S rRNA *D. Radiodurans*	H_1H_2	A	$2HS_4HS_3$	VI	H99-100-101	?
1S72_2830	3WJ	23S rRNA *H. Marismortui*	H_1H_2	A	$2HS_4HS_3$	VI	H99-100-101	L22, L3, L31e
2AW4_2811	3WJ	23S rRNA *E. Coli*	H_1H_2	A	$HS_2HS_4HS_5$	VI	H99-100-101	L3, L17, L32
2J01_2813	3WJ	23S rRNA *T. Thermophilus*	H_1H_2	A	$2HS_4HS_3$	VI	H99-100-101	L3, L32
2J00_585	3WJ	16S rRNA *T. Thermophilus*	H_2H_3	A	$HS_1HS_3HS_3$	C	H20-21-22	S8, S12, S15, S17
2AVY_585	3WJ	16S rRNA *E. Coli*	H_2H_3	A	$HS_1HS_3HS_3$	C	H20-21-22	S8, S12, S15
2J00_671	3WJ	16S rRNA *T. Thermophilus*	H_1H_2	A	$2HS_7HS_1$	C	H22-23-23a	S6, S11, S18
2AVY_671	3WJ	16S rRNA *E. Coli*	H_1H_2	A	$HS_4HS_{11}HS_1$	C	H22-23-23a	S11, S18, S21
2J00_825	3WJ	16S rRNA *T. Thermophilus*	H_2H_3	A	$HS_2HS_3HS_5$	C	H25-26-26a	S8
2AVY_825	3WJ	16S rRNA *E. Coli*	H_2H_3	A	$HS_2HS_3HS_5$	C	H25-26-26a	S2, S8
2J00_1059	3WJ	16S rRNA *T. Thermophilus*		A	$HS_7HS_5HS_5$	3' m	H34-35-38	S3, S5, S9, S10, S14
2AVY_1059	3WJ	16S rRNA *E. Coli*		A	$HS_7HS_5HS_9$	3' m	H34-35-38	S3, S9, S10, S14
2A64_61	3WJ	RNase P type B *B. Stearothermophilus*	H_1H_2	A	$2HS_5H$		P5-5.1-7	-
2GDI_13	3WJ	Riboswitch TPP *E. Coli*	H_1H_2	A	$2HS_5HS_2$		P1-2-4	-
2HOJ_13	3WJ	Riboswitch TPP *E. Coli*	H_1H_2	A	$2HS_3HS_2$		P1-2-4	-
2CKY_4	3WJ	Riboswitch TPP *A. Thaliana*	H_1H_2	A	$HS_1HS_5HS_4$		P1-2-4	-
2QBZ_53	3WJ	Riboswitch M-box *B. Subtilis*	H_1H_2	A	$HS_1HS_5HS_4$		P3-4a-5	-
2A64_12	3WJ	RNase P type *B. Stearothermophilus*	H_2H_3	A	$HS_{12}HS_{17}$		P1-2-19	-
1U6B_45	3WJ	GI Intron *Azoarcus*	H_2H_3	B	$HS_{22}HS_{13}$		P3-4-6	-
1NKW_709	3WJ	23S rRNA *D. Radiodurans*	H_2H_3	B	$HS_2HS_3HS_4$	II	H33-34-35	?
1S72_787	3WJ	23S rRNA *H. Marismortui*	H_2H_3	B	$HS_2HS_4HS_4$	II	H33-34-35	L2, L19e
2AW4_696	3WJ	23S rRNA *E. Coli*	H_2H_3	B	$HS_2HS_3HS_4$	II	H33-34-35	L2
2J01_696	3WJ	23S rRNA *T. Thermophilus*	H_2H_3	B	$HS_2HS_3HS_4$	II	H33-34-35	L2
1NKW_1322	3WJ	23S rRNA *D. Radiodurans*		B	$HS_3HS_6HS_2$	III	H50-51-?	?
1S72_1415	3WJ	23S rRNA *H. Marismortui*		B	HS_32HS_2	III	H50-51-?	L23, L39e
2AW4_1309	3WJ	23S rRNA *E. Coli*		B	$HS_3HS_6HS_2$	III	H50-51-?	L23, L34
2J01_1309	3WJ	23S rRNA *T. Thermophilus*		B	$HS_3HS_6HS_2$	III	H50-51-?	L23, L34
1S72_2328	3WJ	23S rRNA *H. Marismortui*		B	$HS_3HS_5HS_4$	V	H83-84-85	L18, L5, L21e
2AW4_2294	3WJ	23S rRNA *E. Coli*		B	$HS_3HS_5HS_4$	V	H83-84-85	L18, L27
2J01_2294	3WJ	23S rRNA *T. Thermophilus*		B	$HS_3HS_5HS_4$	V	H83-84-85	L5, L18, L27
2J00_935	3WJ	16S rRNA *T. Thermophilus*		B	$HS_2HS_5HS_6$	3' m	H28-29-43	S7, S9
2AVY_935	3WJ	16S rRNA *E. Coli*		B	$HS_2HS_5HS_6$	3' m	H28-29-43	S7, S9
2J00_989	3WJ	16S rRNA *T. Thermophilus*	H_2H_3	B	$HS_6HS_2HS_4$	3' m	H32-33-34	S14
2AVY_989	3WJ	16S rRNA *E. Coli*	H_2H_3	B	$HS_6HS_2HS_4$	3' m	H32-33-34	S14

2J00_1002	3WJ	16S rRNA *T. Thermophilus*	H_1H_3	B	$HS_2HS_5HS_4$	3' m	H33-33a-33b	-
2AVY_1002	3WJ	16S rRNA *E. Coli*	H_1H_3	B	$HS_2HS_3HS_2$	3' m	H33-33a-33b	-
2OIU_6	3WJ	L1 ribozyme *Synthetic*	H_1H_2	B	$2HS_2HS_3$		A-B-C	-
3E5C_5	3WJ	Riboswitch (SAM III) *E. Faecalis*	H_2H_3	B	HS_2HS_4H		P1-2-4	SAM
3MXH	3WJ	Riboswitch c-di-GMP *E. Coli*	H_1H_2	B	$HS_6HS_3HS_3$		P1-2-3	c-di-GMP
1NKW_23	3WJ	23S rRNA *D. Radiodurans*	H_1H_2	C	$HS_6HS_9HS_{19}$	I	H2-3-24	?
1S72_20	3WJ	23S rRNA *H. Marismortui*	H_1H_2	C	$HS_7HS_{10}HS_{20}$	I	H2-3-24	L22, L24
2AW4_24	3WJ	23S rRNA *E. Coli*	H_1H_2	C	$HS_5HS_9HS_{18}$	I	H2-3-24	L20, L22, L24
2J01_23	3WJ	23S rRNA *T. Thermophilus*	H_1H_2	C	$HS_6HS_9HS_{19}$	I	H2-3-24	L20, L22, L24, L32
1NKW_307	3WJ	23S rRNA *D. Radiodurans*	H_1H_3	C	$HS_3HS_8HS_3$	I	H18-19-20	?
1S72_301	3WJ	23S rRNA *H. Marismortui*	H_1H_3	C	$HS_6HS_9HS_4$	I	H18-19-20	L4, L24
2AW4_296	3WJ	23S rRNA *E. Coli*	H_1H_3	C	$HS_3HS_8HS_3$	I	H18-19-20	L4, L24
2J01_296	3WJ	23S rRNA *T. Thermophilus*	H_1H_3	C	$HS_3HS_8HS_3$	I	H18-19-20	L24, L4
1NKW_695	3WJ	23S rRNA *D. Radiodurans*	H_1H_2	C	$HS_5HS_3HS_6$	II	H32-33-35a	?
1S72_773	3WJ	23S rRNA *H. Marismortui*	H_1H_2	C	$HS_5HS_3HS_6$	II	H32-33-35.1	L2, L19e
2AW4_682	3WJ	23S rRNA *E. Coli*	H_1H_2	C	$HS_5HS_3HS_6$	II	H32-33-35a	L2, L34
2J01_682	3WJ	23S rRNA *T. Thermophilus*	H_1H_2	C	$HS_5HS_3HS_6$	II	H32-33-35a	L2, L34
1NKW_1065	3WJ	23S rRNA *D. Radiodurans*	H_1H_3	C	$HS_1HS_9HS_3$	II	H42-43-44	?
1S72_1158	3WJ	23S rRNA *H. Marismortui*	H_1H_3	C	$HS_1HS_8HS_2$	II	H42-43-44	-
2AW4_1054	3WJ	23S rRNA *E. Coli*	H_1H_3	C	$HS_1HS_8HS_2$	II	H42-43-44	L2, L33
1S72_1550	3WJ	23S rRNA *H. Marismortui*	H_1H_2	C	$2HS_4HS_{11}$	III	57-58-59	L19e
2J01_1443	3WJ	23S rRNA *T. Thermophilus*	H_1H_2	C	$HS_{12}HS_{13}$	III	57-58-59	-
1NKW_2495	3WJ	23S rRNA *D. Radiodurans*	H_1H_2	C	$HS_2HS_1HS_5$	V	H90-91-92	?
1S72_2551	3WJ	23S rRNA *D. Radiodurans*	H_1H_2	C	$HS_2HS_2HS_5$	V	H90-91-92	L14
2AW4_2516	3WJ	23S rRNA *E. Coli*	H_1H_2	C	$HS_2HS_1HS_5$	V	H90-91-92	-
2J01_2516	3WJ	23S rRNA *T. Thermophilus*	H_1H_2	C	$HS_2HS_1HS_5$	V	H90-91-92	L14
1NKW_11	3WJ	5S rRNA *D. Radiodurans*	H_2H_3	C	$HS_5HS_1HS_3$		H1-2-4	L27
1S72_8	3WJ	5S rRNA *H. Marismortui*	H_2H_3	C	$HS_4HS_3HS_3$		H1-2-4	L18P, L21e
2AW4_9	3WJ	5S rRNA *E. Coli*	H_2H_3	C	$HS_5HS_1HS_3$		H1-2-4	L18, L27, L29, L32
2J01_10	3WJ	5S rRNA *T. Thermophilus*	H_2H_3	C	HS_42HS_1		H1-2-4	L27, L32
1UN6_8	3WJ	5S rRNA *X. Laevis*	H_2H_3	C	HS_42H		H1-2-4	TF IIIA
2J00_45	3WJ	16S rRNA *T. Thermophilus*	H_1H_3	C	$HS_5HS_9HS_2$	5'	H4-5-15	S12, S16
2AVY_45	3WJ	16S rRNA *E. Coli*	H_1H_3	C	$HS_5HS_9HS_2$	5'	H4-5-15	S12, S16
2J00_954	3WJ	16S rRNA *T. Thermophilus*		C	$HS_6HS_{10}HS_3$	3' m	H30-31-32	S10, S13, S14, S19
2AVY_954	3WJ	16S rRNA *E. Coli*		C	$HS_6HS_{10}HS_3$	3' m	H30-31-32	S10, S13, S14, S19
2J00_1072	3WJ	16S rRNA *T. Thermophilus*	H_1H_2	C	$2HS_3HS_3$	3' m	H35-36-37	S2, S5
2AVY_1072	3WJ	16S rRNA *E. Coli*	H_1H_2	C	$2HS_3HS_3$	3' m	H35-36-37	S2, S5
2J00_1115	3WJ	16S rRNA *T. Thermophilus*	H_1H_2	C	$HS_1HS_5HS_8$	3' m	H38-39-40	S9, S10, S14
2AVY_1115	3WJ	16S rRNA *E. Coli*	H_1H_2	C	$HS_1HS_5HS_8$	3' m	H38-39-40	S2, S9
1NYI_14	3WJ	Hammerhead *Synthetic*	H_2H_3	C	$HS_7HS_4HS_2$		I-II-III	-
1E8O_102	3WJ	ALU domain SRP *H. Sapiens*	H_1H_3	C	$2HS_4H$		H1.1-1.2-2	Endothiapepsin
1L9A_127	3WJ	ALU domain SRP *Synthetic*	H_1H_3	C	$2HS_6HS_2$		H6-7-8	-
3KTW_143	3WJ	*SRP19/S-domain SRP RNA S. Solfataricus*	H_1H_3	C	$HS_3HS_4HS_2$		H5-6-8	-
1LNG_144	3WJ	*SRP19/S-domain SRP RNA M. Jannaschii*	H_1H_3	C	$HS_2HS_4HS_1$		H5-6-8	-
2CZJ_6	3WJ	tmRNA *T. Thermophilus*	H_1H_3	C	$HS_{12}HS_6HS_3$		P1-2a-10	SsrA
1U8D_20	3WJ	Riboswitch G *B. Subtilis*	H_1H_3	C	$HS_5HS_{10}HS_2$		P1-2-3	Hypoxanthine
2B57_20	3WJ	Riboswitch G *B. Subtilis*	H_1H_3	C	$HS_5HS_{10}HS_2$		P1-2-3	DAP
2EES_20	3WJ	Riboswitch G *B. Subtilis*	H_1H_3	C	$HS_5HS_{10}HS_2$		P1-2-3	-
1Y26_20	3WJ	Riboswitch A *V. Vulnificus*	H_1H_3	C	$HS_3HS_8HS_2$		P1-2-3	Adenine
3EGZ_4	3WJ	Riboswitch *H. Sapiens*	H_2H_3	C	HS_32HS_7		P1-2-3	Tetracycline
2HO7_5	3WJ	Riboswitch glmS *T. Tengcongensis*	H_1H_2	C	$2HS_2HS_6$		P1-2.1-2.2	-
2NZ4_5	3WJ	Riboswitch glmS *B. Anthracis*	H_1H_2	C	$2HS_2HS_6$		P1-2.1-2.2	-
1Y0Q_195	3WJ	GI Intron *Twort*		C	$HS_2HS_3HS_9$		P9-9.0-9.1	-
1X8W_137	3WJ	GI Intron *Tetrahymena*	H_1H_2	C	$HS_2HS_2HS_4$		P5a-5b-5c	-
2A64_139	3WJ	RNase P type B *B.*	H_1H_3	C	HS_1HS_5H		P7-10.1-11	-

1NBS_132	3WJ	*Stearothermophilus* RNase P type B *B. Subtilis*	H_1H_3	C	HS_1HS_5H		P7-8-9-10	-
1U9S _78	4WJ	RNase P type A *T. thermophilus*	H_1H_4, H_2H_3	H	$2HS_1HS_2H$		P7-8-9-10	-
2A2E _70	4WJ	RNase P type A *T. Maritima*	H_1H_4, H_2H_3	H	HS_13HS_1		P7-8-9-10	-
1NBS _89	4WJ	RNase P type B *B. Subtilis*	H_1H_4, H_2H_3	H	$2HS_1HS_2H$		P7-8-9-10	-
2A64 _90	4WJ	RNase P type B *B. Stearothermophilus*	H_1H_4, H_2H_3	H	$2HS_1HS_2H$		P7-8-9-10	-
1M5O _13	4WJ	Hairpin Ribozyme *S. Tobacco ringspot virus*	H_1H_4, H_2H_3	H	4H		A-B-C-D	-
1S72 _1827	4WJ	23S rRNA *H. Marismortui*	H_1H_4, H_2H_3	H	$HS_3HS_3HS_3HS_4$	IV	H64-65-66-67	L2, L37e
2AW4 _1771	4WJ	23S rRNA *E. Coli*	H_1H_4, H_2H_3	H	$HS_3HS_3HS_2HS_3$	IV	H64-65-66-67	L2
2J01 _1771	4WJ	23S rRNA *T. Thermophilus*	H_1H_4, H_2H_3	H	$HS_3HS_3HS_2HS_3$	IV	H64-65-66-67	L2
1KH6 _4	4WJ	IRES *Hepatitis C Virus*	H_1H_4, H_2H_3	cH	HS_22HS_1H		III-IIIa-IIIb-IIIc	-
2AVY _141	4WJ	16S rRNA *E. Coli*	H_1H_4, H_2H_3	cH	$HS_3HS_7HS_4HS_1$	5'	H7-8-9-10	S20
2J00 _141	4WJ	16S rRNA *T. Thermophilus*	H_1H_4, H_2H_3	cH	$HS_1HS_4HS_3HS_1$	5'	H7-8-9-10	S20
1NKW _2621	4WJ	23S rRNA *D. Radiodurans*	H_1H_4, H_2H_3	cH	$HS_2HS_1HS_4HS_2$	VI	H94-95-96-97	?
1S72 _2678	4WJ	23S rRNA *H. Marismortui*	H_1H_4, H_2H_3	cH	$HS_22HS_2HS_1$	VI	H94-95-96-97	L3, L13, L14
2AW4 _2642	4WJ	23S rRNA *E. Coli*	H_1H_4, H_2H_3	cH	$HS_2HS_1HS_3HS_1$	VI	H94-95-96-97	L3, L13, L14
2J01 _2642	4WJ	23S rRNA *T. Thermophilus*	H_1H_4, H_2H_3	cH	$HS_2HS_1HS_3HS_1$	VI	H94-95-96-97	L3, L13, L14
3F2Q_7	4WJ	Riboswitch (FMN) *F. Nucleatum*	H_1H_4, H_2H_3	cH	$HS_6HS_3HS_1HS_7$		P1-P2-X-P6	FNM
3F2Q_31	4WJ	Riboswitch (FMN) *F. Nucleatum*	H_1H_4, H_2H_3	cH	$2HS_2HS_3HS_2$		X-P3-P4-P5	FNM
1NKW _1457	4WJ	23S rRNA *D. Radiodurans*	H_1H_2, H_3H_4	cH	$HS_1HS_3HS_6HS_4$	III	H56-57-58-59	?
2AW4 _1443	4WJ	23S rRNA *E. Coli*	H_1H_2, H_3H_4	cH	$3HS_3HS_4$	III	H56-57-58-59	-
3F4E_7	4WJ	Riboswitch FNM *F. Nucleatum*	H_1H_4	cH	$HS_6HS_3HS_1HS_7$		P1-2-6-?	FNM
3F4E_31	4WJ	Riboswitch FNM *F. Nucleatum*	H_1H_4	cH	$2HS_3HS_4HS_2$		P3-4-5-?	FNM
3IVK_53	4WJ	RNA-polymerase Ribozyme M. Musculus	H_1H_2	cH	$2HS_22H$		P4-5-6-7	-
2AVY _568	4WJ	16S rRNA *E. Coli*	H_1H_4, H_2H_3	cL	$HS_7HS_4HS_{10}HS_1$	C	H19-20-24-25	S8, S12
2J00 _568	4WJ	16S rRNA *T. Thermophilus*	H_1H_4, H_2H_3	cL	$HS_7HS_4HS_{10}HS_1$	C	H19-20-24-25	S8, S12
1NKW _1282	4WJ	23S rRNA *D. Radiodurans*	H_1H_4, H_2H_3	cL	HS_52HS_2H	III	H47A-47-48-61	?
1S72 _1373	4WJ	23S rRNA *H. Marismortui*	H_1H_4, H_2H_3	cL	HS_72HS_3H	III	H47A-47-48-61	L19e, L31e
2AW4 _1269	4WJ	23S rRNA *E. Coli*	H_1H_4, H_2H_3	cL	HS_52HS_2H	III	H47A-47-48-61	L17, L22
2J01 _1269	4WJ	23S rRNA *T. Thermophilus*	H_1H_4, H_2H_3	cL	HS_52HS_2H	III	H49A-49-50-51	L17, L22
1EFW _6	4WJ	Asp-tRNA *T. Thermophilus*	H_1H_4, H_2H_3	cL	$HS_2HS_1HS_5H$		H1-2-3-4	-
1EHZ _6	4WJ	Phe-tRNA *Yeast*	H_1H_4, H_2H_3	cL	$HS_2HS_1HS_5H$		H1-2-3-4	-
1N78 _506	4WJ	Glu-tRNA *T. Thermophilus*	H_1H_4, H_2H_3	cL	$HS_2HS_1HS_4H$		H1-2-3-4	-
1QRS _6	4WJ	Gln-tRNA *E. Coli*	H_1H_4, H_2H_3	cL	$HS_2HS_1HS_5H$		H1-2-3-4	-
1U0B _6	4WJ	Cys-tRNA *E. Coli*	H_1H_4,	cL	$HS_2HS_1HS_4H$		H1-2-3-4	-

2GIS _7	4WJ	Riboswitch (SAM I) *Synthetic*	H_2H_3 H_1H_4, H_2H_3	cL	$HS_6HS_1HS_8HS_3$		P1-2A-3-4	-
2AVY _114	4WJ	16S rRNA *E. Coli*	H_1H_4	cK	HS_62HS_2	5'	H7-11-12-13A	S16, S17
2J00 _114	4WJ	16S rRNA *T. Thermophilus*	H_1H_4	cK	HS_62HS_2	5'	H7-11-12-13A	S16, S17
1NKW _2263	4WJ	23S rRNA *D. Radiodurans*	H_3H_4	cK	$HS_4HS_4HS_1HS_1$	V	H82-83-86-87	?
1S72 _2318	4WJ	23S rRNA *H. Marismortui*	H_3H_4	cK	$HS_3HS_3HS_1HS_1$	V	H82-83-86-87	L18, L21e, L44e
2AW4 _2284	4WJ	23S rRNA *E. Coli*	H_3H_4	cK	$HS_3HS_3HS_1HS_1$	V	H82-83-86-87	L18, L33, L35
2J01 _2284	4WJ	23S rRNA *T. Thermophilus*	H_3H_4	cK	$HS_3HS_3HS_1HS_1$	V	H83A-83-86-87	L27, L33, L35
1NKW _1360	4WJ	23S rRNA *D. Radiodurans*	H_3H_4	cK	$HS_1HS_3HS_4HS_2$	III	H51-52-53-54	?
1S72 _1452	4WJ	23S rRNA *H. Marismortui*	H_3H_4	cK	$HS_1HS_3HS_2HS_1$	III	H51-52-53-54	L23
2AW4 _1346	4WJ	23S rRNA *E. Coli*	H_3H_4	cK	$HS_2HS_3HS_2HS_1$	III	H49A-49-50-51	L23
2J01 _1347	4WJ	23S rRNA *T. Thermophilus*	H_3H_4	cK	$HS_1HS_3HS_2H$	III	H51-52-53-54	L23
2AVY _18	4WJ	16S rRNA *E. Coli*	H_1H_2	cK	$HS_7HS_{10}HS_1HS_3$	C	H2-3-19-27	S5, S12
2J00 _18	4WJ	16S rRNA *T. Thermophilus*	H_1H_2	cK	$HS_7HS_{10}HS_1HS_3$	C	H2-3-19-28	S4, S5, S8, S12
1U9S _118	4WJ	RNase P type A *T. thermophilus*	H_3H_4	π	$HS_{12}HS_7HS_1HS_4$		P11-12-13-14	-
2A2E _110	4WJ	RNase P type A *T. Maritima*	H_3H_4	π	$HS_{10}HS_7HS_2HS_4$		P11-12-13-14	-
1NKW _1682	4WJ	23S rRNA *D. Radiodurans*		cW	$HS_{15}2HS_{12}HS_5$	IV	H61-62-63-64	?
1S72 _1743	4WJ	23S rRNA *H. Marismortui*		cW	$HS_{15}2HS_{12}HS_5$	IV	H61-62-63-64	L3, L14, L19e
2AW4 _1665	4WJ	23S rRNA *E. Coli*		cW	$HS_{15}2HS_{12}HS_5$	IV	H61-62-63-64	L3, L14, L19
2J01 _1665	4WJ	23S rRNA *T. Thermophilus*		cW	$HS_{15}2HS_{12}HS_5$	IV	H61-62-63-64	L3, L14, L19
1S72 _42	4WJ	23S rRNA *H. Marismortui*		ψ	$HS_6HS_4HS_5HS_1$	I	H4-5-8-10	L37e, L39e
1NKW _1824	4WJ	23S rRNA *D. Radiodurans*		ψ	$HS_1HS_2HS_{22}HS_{10}$	IV	H64-65-66-67	?
1S72 _1888	4WJ	23S rRNA *H. Marismortui*		ψ	$HS_12HS_{20}HS_{10}$	IV	H67-68-69-71	-
2AW4 _1832	4WJ	23S rRNA *E. Coli*		ψ	$HS_12HS_{20}HS_{10}$	IV	H64-65-66-67	L2
2J01 _1832	4WJ	23S rRNA *T. Thermophilus*		ψ	$HS_12HS_{20}HS_{10}$	IV	H64-65-66-67	L2
1NKW _244	4WJ	23S rRNA *D. Radiodurans*		ψ	$HS_5HS_6HS_6HS_2$	I	H14-16-21-22	?
2AW4 _267	4WJ	23S rRNA *E. Coli*		ψ	$HS_2HS_8HS_6HS_2$	I	H14-16-21-22	L31
1NKW_608	4WJ	23S rRNA *D. Radiodurans*		X	$HS_{10}HS_9HS_3HS_{11}$	I	H27-28-29-31	?
2AW4 _600	4WJ	23S rRNA *E. Coli*		X	$HS_2HS_3HS_2HS_5$	I	H27-28-29-31	L15, L35
2J01 _600	4WJ	23S rRNA *T. Thermophilus*		X	$HS_2HS_3HS_2HS_2$	I	H27-28-29-31	L4, L15, L35
2IHX _166	4WJ	*Sarcoma Virus*		cX	$HS_3HS_42HS_3$		A-B-C-O3	NC
2AVY _942	4WJ	16S rRNA *E. Coli*		cX	$HS_2HS_5HS_{11}HS_{10}$	3'M	H29-30-41-42	S7, S9, S13
2J00 _940	4WJ	16S rRNA *T. Thermophilus*		cX	$HS_4HS_5HS_{11}HS_{12}$	3'M	H29-30-41-42	S7, S9, S13, THX
1U6B_8	5WJ	GI intron *Azoarcus*	H_1H_2, H_3H_4		$HS_3HS_32HS_{13}HS_2$		P2-3-8-7.1-10	-
1Y0Q_43	5WJ	GI intron *Twort*	H_2H_3, H_4H_5		$HS_42HS_{10}HS_3HS_5$		P3-4-6-7.1-7.2	-
1S72_238	5WJ	23S rRNA *H. Marismortui*	H_1H_2, H_3H_5		$HS_4HS_5HS_6HS_6HS_2$	I	H14-15-16-21-22	L15e, L4
2J01_267	5WJ	23S rRNA *T. Thermophilus*	H_1H_2, H_3H_5		$HS_4HS_5HS_5HS_6HS_2$	I	H14-15-16-21-22	L9, L28
2BTE_6	5WJ	Leuyl-tRNA *T. Thermophilus*	H_1H_5, H_2H_3		HS_23HS_2H		H1-2-3-4-5	-
2NR0_6	5WJ	Leucyl-tRNA *E. Coli*	H_1H_5, H_2H_3		$HS_2HS_4HS_1HS_2H$		H1-2-3-4-5	-
2J01_45	5WJ	23S rRNA *T. Thermophilus*	H_2H_5, H_3H_4		$HS_6HS_42HS_1HS_1$	I	H4A-5-8-9-10	L34
2AW4_46	5WJ	23S rRNA *E. Coli*	H_2H_5, H_3H_4		$HS_6HS_42HS_1HS_1$	I	H4A-5-8-9-10	L34
1NKW_45	5WJ	23S rRNA *D. Radiodurans*	H_2H_5, H_3H_4		$HS_6HS_42HS_1HS_1$	I	H4A-5-8-9-10	?
3BWP_23	5WJ	GII intron *O. Iheyensis*	H_2H_3		$HS_3HS_2HS_2HS_3HS_3$		IA-IB-IC-ID1-I(ii)	-
2J00_35	5WJ	16S rRNA *T. Thermophilus*	H_3H_4		$HS_2HS_2HS_4HS_6HS_2$	5'	H3-4-16-17-18	S4, S12
2AVY_35	5WJ	16S rRNA *E. Coli*	H_3H_4		$HS_2HS_2HS_5HS_7HS_2$	5'	H3-4-16-17-18	S4, S12, S16
1NKW_592	5WJ	23S rRNA *D. Radiodurans*	H_4H_5		$HS_4HS_2HS_22HS_5$	II	H26-27-32-	?

							36-46	
1S72_640	5WJ	23S rRNA *H. Marismortui*	H_4H_5		$HS_4HS_2HS_2HS_4HS_{10}$	II	H26-27-32-36-46	L4, L5, L32e
2AW4_583	5WJ	23S rRNA *E. Coli*	H_4H_5		$HS_4HS_2HS_2HS_2HS_8$	II	H26-27-32-36-46	L4, L15, L20, L21
2J01_583	5WJ	23S rRNA *T. Thermophilus*	H_4H_5		$HS_4HS_2HS_2HS_2HS_8$	II	H26-27-32-36-46	L4, L15, L20
1S72_657	5WJ	23S rRNA *H. Marismortui*	H_4H_5		$HS_2HS_3HS_5HS_1HS_3$	II	H27-28-29-30-31	L15, L18e
2AVY_57	5WJ	16S rRNA *E. Coli*	H_4H_5		$HS_2HS_6HS_1HS_1HS_3$	5'	H5-6-7-13-14	S16, S20
2J00_56	5WJ	16S rRNA *T. Thermophilus*	H_4H_5		$HS_3HS_6HS_1HS_1HS_4$	5'	H5-6-7-13-14	S16, S20
1NKW_2036	5WJ	23S rRNA *D. Radiodurans*	H_2H_3		$HS_9HS_8HS_{11}HS_7HS_8$	V	H73-74-89-90-93	?
1S72_2097	5WJ	23S rRNA *H. Marismortui*	H_2H_3		$HS_6HS_8HS_9HS_4HS_4$	V	H73-74-89-90-93	-
2AW4_2056	5WJ	23S rRNA *E. Coli*	H_2H_3		$HS_6HS_8HS_9HS_4HS_4$	V	H73-74-89-90-93	L3, L4, L32
2J01_2053	5WJ	23S rRNA *T. Thermophilus*	H_2H_3		$HS_9HS_8HS_{11}HS_7HS_8$	V	H73-34-89-90-93	L3, L4, L16, L32
3DIL_8	5WJ	Riboswitch *T. Maritima*	H_1H_2		$HS_4HS_32HS_1HS_4$		P1-2-2A-3-4-5	Lysine
3EOH_23	5WJ	GII intron O. Iheyensis	H_2H_3		HS3HS2HS2HS3HS3		IA-B-C-D1-D2	-
2A64_20	6WJ	RNase P type B *B. Stearothermophilus*	H_1H_2, H_5H_6		$HS_1HS_{13}HS_3HS_32HS_8$		P2-3-5-15-15.1-15.2	-
1NKW_2056	6WJ	23S rRNA *D. Radiodurans*	H_1H_2		$HS_2HS_22HS_2HS_{10}HS_{13}$	V	H74-75-80-81-82-88	?
2J01_2073	6WJ	23S rRNA *T. Thermophilus*	H_1H_2		$HS_2HS_22HS_2HS_{10}HS_{13}$	V	H74-75-80-81-82-88	L2, L15, L27, L28, L33, L35
1S72_2114	6WJ	23S rRNA *H. Marismortui*	H_1H_2		$HS_2HS_3HS_2HS_2HS_{10}HS_{10}$	V	H74-75-80-81-82-88	L2, L15, L21e, L44e
2AW4_2073	6WJ	23S rRNA *E. Coli*	H_1H_2		$HS_2HS_22HS_2HS_{10}HS_{13}$	V	H74-75-80-81-82-88	L2, L27, L33, L35, L15
1S72_38	6WJ	23S rRNA *H. Marismortui*	H_2H_3		$HS_2HS_4HS_{11}HS_3HS_3HS_9$	I	H4-4A-11-12-13-14	L37e, L15e
2J01_43	6WJ	23S rRNA *T. Thermophilus*	H_2H_3		$2HS_4HS_{11}HS_3HS_3HS_9$	I	H4-4A-11-12-13-14	L34
2AW4_44	6WJ	23S rRNA *E. Coli*	H_2H_3		$2HS_4HS_{11}HS_3HS_3HS_9$	I	H4-4A-11-12-13-14	L34
1NKW_43	6WJ	23S rRNA *D. Radiodurans*	H_2H_3		$2HS_4HS_{11}HS_3HS_3HS_9$	I	H4-4A-11-12-13-14	?
1NKW_829	7WJ	23S rRNA *D. Radiodurans*	H_2H_3, H_6H_7		$HS_42HS_2HS_4HS_3HS_3HS_7$	II	H36-37-38-39-40-41-45	?
2AW4_816	7WJ	23S rRNA *E. Coli*	H_2H_3, H_6H_7		$HS_4HS_2HS_5HS_4HS_32HS_4$	II	H36-37-38-39-40-41-45	L15, L20, L21, L30, L35
2J01_816	7WJ	23S rRNA *T. Thermophilus*	H_2H_3, H_6H_7		$HS_42HS_2HS_5HS_32HS_4$	II	H36-37-38-39-40-41-45	L15, L20, L21, L29, L34
1S72_909	7WJ	23S rRNA *H. Marismortui*	H_2H_3, H_6H_7		$HS_4HS_2HS_5HS_4HS_32HS_4$	II	H36-37-38-39-40-41-45	L15, L30, L32e
2J01_6	9WJ	23S rRNA *T. Thermophilus*	H_4H_5		$HS_7HS_7HS_{18}HS_7HS_11HS_2HS_4HS_{19}HS_5$	I	H1-2-25-26-47-72-73-94-99	L3, L13, L20, L21, L22, L32
1NKW_7	10WJ	23S rRNA *D. Radiodurans*	H_4H_5, H_9H_{10}		$HS_8HS_9HS_{18}HS_7HS_11HS_2HS_4HS_2HS_4HS_4$	I	H1-2-25-26-47-72-73-94-98-99	?
2AW4_7	10WJ	23S rRNA *E. Coli*	H_4H_5, H_9H_{10}		$HS_6HS_7HS_{18}HS_7HS_11HS_2HS_4HS_2HS_5HS_5$	I	H1-2-25-26-47-72-73-94-98-99	L3, L4, L13, L20, L21, L22, L32

List of RNA 3D structures containing 110 three-way junctions, 65 four-way junctions, 25 five-way junctions, 9 six-way junctions, 4 seven-way junctions, 1 nine-way junction, and 2 ten-way junctions. The name column lists the PDB code, and the number of the first residue of helix H_1 in a junction. The nomenclature is based on Lilley et. al., (1) and the helices are numbered according to the scheme in Leffers et al. (2). The last column describes proteins interacting to each junction.

Table S2. List of feature parameters for three-way junctions.

PDB	Coaxial	Family	|L1|	|L2|	|L3|	Min(|L2|,|L3|)	Min(|L1|,|L3|)	Min(|L1|,|L2|)	|L1'|	|L2'|	|L3'|	ΔG(H1,H2)	ΔG(H2,H3)	ΔG(H3,H1)	A(L1)	A(L2)	A(L3)
1NKW_23	H1H2	C	6	9	19	9	6	6	6	9	19	5.7	6.1	7	0	4	3
1S72_20	H1H2	C	6	10	20	10	6	6	6	10	20	5.7	6.3	7	0	3	3
2AW4_24	H1H2	C	5	9	18	9	5	5	5	9	18	6	6.1	6.9	0	4	5
2J01_23	H1H2	C	6	9	19	9	6	6	6	9	19	5.7	6.1	7	0	4	3
1NKW_31	H1H2	A	2	14	4	4	2	2	2	4	14	6.9	6.6	6.3	0	0	3
1S72_28	H1H2	A	2	15	4	4	2	2	2	4	15	6.9	6.7	6.3	0	2	2
2AW4_31	H1H2	A	2	15	4	4	2	2	2	4	15	6.9	6.7	6.3	0	2	3
2J01_31	H1H2	A	2	15	4	4	2	2	2	4	15	6.9	6.7	6.3	0	0	3
1NKW_54	H1H2	A	0	5	4	4	0	0	0	4	5	-2.2	6	6.3	0	4	0
1S72_51	H1H2	A	0	5	3	3	0	0	0	3	5	-2.2	6	6.6	0	2	0
2AW4_55	H1H2	A	0	5	3	3	0	0	0	3	5	-2.2	6	6.6	0	2	0
2J01_55	H1H2	A	0	5	3	3	0	0	0	3	5	-2.2	6	6.6	0	2	0
1NKW_307	H1H3	C	3	8	3	3	3	3	3	3	8	6.6	6	6.6	2	0	0
1S72_301	H1H3	C	6	9	4	4	4	6	4	6	9	5.7	6.1	6.3	2	0	0
2AW4_296	H1H3	C	3	8	3	3	3	3	3	3	8	6.6	6	6.6	2	0	0
2J01_296	H1H3	C	3	8	3	3	3	3	3	3	8	6.6	6	6.6	2	0	0
1NKW_695	H1H2	C	5	3	6	3	5	3	3	5	6	6	6.6	5.7	0	0	2
1S72_773	H1H2	C	5	3	6	3	5	3	3	5	6	6	6.6	5.7	0	0	0
2AW4_682	H1H2	C	5	3	6	3	5	3	3	5	6	6	6.6	5.7	0	0	2
2J01_682	H1H2	C	5	3	6	3	5	3	3	5	6	6	6.6	5.7	0	0	2
1NKW_709	H2H3	B	2	3	4	3	2	2	2	3	4	6.9	6.6	6.3	0	2	0
1S72_787	H2H3	B	2	4	4	4	2	2	2	4	4	6.9	6.3	6.3	0	0	0
2AW4_696	H2H3	B	2	3	4	3	2	2	2	3	4	6.9	6.6	6.3	0	2	0
2J01_696	H2H3	B	2	3	4	3	2	2	2	3	4	6.9	6.6	6.3	0	2	0
1NKW_1065	H1H3	C	1	9	3	3	1	1	1	3	9	0.5	6.1	6.6	0	3	0
1S72_1158	H1H3	C	1	8	2	2	1	1	1	2	8	0.5	6	6.9	0	3	0
2AW4_1054	H1H3	C	1	8	2	2	1	1	1	2	8	0.5	6	6.9	0	3	0
1NKW_1310	H1H3	A	4	1	2	1	2	1	1	2	4	6.3	0.7	6.9	2	0	2
1S72_1403	H1H3	A	4	2	2	2	2	2	2	2	4	6.3	6.9	6.9	2	0	2
2AW4_1297	H1H3	A	4	1	2	1	2	1	1	2	4	6.3	0.6	6.9	2	0	2

2J01_1297	H1H3	A	4	1	2	1	2	1	1	2	4	6.3	0.7	6.9	2	0	0
1NKW_1318	H1H2	A	2	5	1	1	1	2	1	2	5	6.9	6	0.6	2	3	0
1S72_1411	H1H2	A	2	5	1	1	1	2	1	2	5	6.9	6	1	2	2	0
2AW4_1305	H1H2	A	2	5	1	1	1	2	1	2	5	6.9	6	0.6	2	3	0
2J01_1305	H1H2	A	2	5	1	1	1	2	1	2	5	6.9	6	0.6	2	3	0
1NKW_1322	none	B	3	6	2	2	2	3	2	3	6	6.6	5.7	6.9	0	3	0
1S72_1415	none	B	3	6	2	2	2	3	2	3	6	6.6	5.7	6.9	0	0	0
2AW4_1309	none	B	3	6	2	2	2	3	2	3	6	6.6	5.7	6.9	0	0	0
2J01_1309	none	B	3	6	2	2	2	3	2	3	6	6.6	5.7	6.9	0	0	0
1S72_1550	H1H2	C	0	4	11	4	0	0	0	4	11	-1.4	6.3	6.4	0	2	3
2J01_1443	H1H2	C	1	0	13	0	1	0	0	1	13	7.2	-3.4	6.6	0	0	2
1NKW_2072	H2H3	A	2	3	5	3	2	2	2	3	5	6.9	6.6	6	0	2	0
1S72_2130	H2H3	A	2	3	5	3	2	2	2	3	5	6.9	6.6	6	0	0	0
2AW4_2090	H2H3	A	1	3	4	3	1	1	1	3	4	0.9	6.6	6.3	0	2	0
2J01_2090	H2H3	A	1	3	4	3	1	1	1	3	4	0.9	6.6	6.3	0	2	0
1S72_2328	none	B	3	5	4	4	3	3	3	4	5	6.6	6	6.3	0	2	4
2AW4_2294	none	B	3	5	4	4	3	3	3	4	5	6.6	6	6.3	2	0	2
2J01_2294	none	B	3	5	4	4	3	3	3	4	5	6.6	6	6.3	0	0	2
1NKW_2495	H1H2	C	2	1	5	1	2	1	1	2	5	6.9	1.3	6	0	0	3
1S72_2551	H1H2	C	2	2	6	2	2	2	2	2	6	6.9	6.9	5.7	0	0	3
2AW4_2516	H1H2	C	2	1	5	1	2	1	1	2	5	6.9	1.4	6	0	0	3
2J01_2516	H1H2	C	2	1	5	1	2	1	1	2	5	6.9	1.3	6	0	0	3
1NKW_2788	H1H2	A	0	4	3	3	0	0	0	3	4	-2.4	6.3	6.6	0	2	0
1S72_2830	H1H2	A	0	4	3	3	0	0	0	3	4	-3.3	6.3	6.6	0	0	0
2AW4_2811	H1H2	A	2	4	5	4	2	2	2	4	5	6.9	6.3	6	2	0	2
2J01_2813	H1H2	A	0	4	3	3	0	0	0	3	4	-3.3	6.3	6.6	0	0	0
1NKW_11	H2H3	C	5	1	3	1	3	1	1	3	5	6	0.7	6.6	0	0	0
1S72_8	H2H3	C	4	3	3	3	3	3	3	3	4	6.3	6.6	6.6	0	0	0
2AW4_9	H2H3	C	5	1	3	1	3	1	1	3	5	6	0.7	6.6	0	0	2
2J01_10	H2H3	C	4	0	1	0	1	0	0	1	4	6.3	-1.4	1	0	0	0
1UN6_8	H2H3	C	4	0	0	0	0	0	0	0	4	6.3	-1.5	-1.4	0	0	0
2J00_45	H1H3	C	5	9	2	2	2	5	2	5	9	6	6.1	6.9	2	2	0

2AVY_45	H1H3	C	5	9	2	2	2	5	2	5	9	6	6.1	6.9	2	2	0
2J00_585	H2H3	A	1	3	3	3	1	1	1	3	3	0.6	6.6	6.6	0	0	0
2AVY_585	H2H3	A	1	3	3	3	1	1	1	3	3	0.6	6.6	6.6	0	0	0
2J00_671	H1H2	A	4	11	1	1	1	4	1	4	11	6.3	6.4	0.7	2	2	0
2AVY_671	H1H2	A	4	11	1	1	1	4	1	4	11	6.3	6.4	0.5	2	2	0
2J00_825	H2H3	A	2	3	5	3	2	2	2	3	5	6.9	6.6	6	0	2	2
2AVY_825	H2H3	A	2	3	5	3	2	2	2	3	5	6.9	6.6	6	0	0	2
2J00_935	none	B	2	5	6	5	2	2	2	5	6	6.9	6	5.7	2	0	2
2AVY_935	none	B	2	5	6	5	2	2	2	5	6	6.9	6	5.7	2	0	2
2J00_954	none	C	6	10	3	3	3	6	3	6	10	5.7	6.3	6.6	2	2	0
2AVY_954	none	C	6	10	3	3	3	6	3	6	10	5.7	6.3	6.6	2	2	0
2J00_989	H2H3	B	6	2	4	2	4	2	2	4	6	5.7	6.9	6.3	0	0	0
2AVY_989	H2H3	B	6	2	4	2	4	2	2	4	6	5.7	6.9	6.3	0	0	0
2J00_1000	H1H3	B	5	5	6	5	5	5	5	5	6	6	6	5.7	2	0	0
2AVY_1002	H1H3	B	2	3	2	2	2	2	2	2	3	6.9	6.6	6.9	2	0	2
2J00_1059	none	A	7	5	9	5	7	5	5	7	9	5.9	6	6.1	0	2	0
2AVY_1059	none	A	7	5	9	5	7	5	5	7	9	5.9	6	6.1	0	2	0
2J00_1072	H1H2	C	0	3	3	3	0	0	0	3	3	-1	6.6	6.6	0	0	0
2AVY_1072	H1H2	C	0	3	3	3	0	0	0	3	3	-1	6.6	6.6	0	0	0
2J00_1115	H1H2	C	1	5	8	5	1	1	1	5	8	0.7	6	6	0	0	2
2AVY_1115	H1H2	C	1	5	8	5	1	1	1	5	8	1.3	6	6	0	0	2
1NYI_14	H2H3	C	7	4	2	2	2	4	2	4	7	5.9	6.3	6.9	0	3	0
1E8O_102	H1H3	C	0	4	0	0	0	0	0	0	4	-1.4	6.3	-2.1	0	0	0
1L9A_127	H1H3	C	0	6	1	1	0	0	0	1	6	-1.5	5.7	1.1	0	0	0
1LNG_144	H1H3	C	2	4	1	1	1	2	1	2	4	6.9	6.3	0.5	0	0	0
2CZJ_4	H1H3	C	14	3	2	2	2	3	2	3	14	6.6	6.6	6.9	3	0	0
1U8D_20	H1H2	C	5	10	2	2	2	5	2	5	10	6	6.3	6.9	2	2	0
2B57_20	H1H3	C	5	10	2	2	2	5	2	5	10	6	6.3	6.9	2	2	0
2EES_20	H1H3	C	5	10	2	2	2	5	2	5	10	6	6.3	6.9	2	2	0
1Y26_20	H1H3	C	3	8	2	2	2	3	2	3	8	6.6	6	6.9	2	0	0
2HO7_5	H1H2	C	0	2	6	2	0	0	0	2	6	-1.5	6.9	5.7	0	0	0
2NZ4_5	H1H2	C	0	2	6	2	0	0	0	2	6	-2.4	6.9	5.7	0	0	0

2GDI_13	H1H2	A	0	5	2	2	0	0	0	2	5	-2.4	6	6.9	0	0	0
2HOJ_13	H1H2	A	0	3	2	2	0	0	0	2	3	-2.4	6.6	6.9	0	2	0
2CKY_4	H1H2	A	1	5	4	4	1	1	1	4	5	1.3	6	6.3	0	2	0
2QBZ_53	H1H2	A	1	5	4	4	1	1	1	4	5	0.9	6	6.3	0	2	2
2OIU_6	H1H2	B	0	2	3	2	0	0	0	2	3	-2.4	6.9	6.6	0	0	0
1U6B_45	H2H3	B	4	0	13	0	4	0	0	4	13	6.3	-0.6	6.6	3	0	0
1Y0Q_195	none	C	2	3	9	3	2	2	2	3	9	6.9	6.6	6.1	0	2	2
1X8W_137	H1H2	C	2	2	4	2	2	2	2	2	4	6.9	6.9	6.3	2	0	0
2A64_12	H2H3	A	1	0	17	0	1	0	0	1	17	0.7	-1.4	6.8	0	0	2
2A64_61	H1H2	C	0	5	0	0	0	0	0	0	5	-2.1	6	-2.1	0	0	0
2A64_139	H1H3	C	1	5	0	0	0	1	0	1	5	0.7	6	-3.3	0	3	0
1NBS_132	H1H3	C	1	5	0	0	0	1	0	1	5	1.5	6	-3.3	0	3	0
3E5C_5	H2H3	B	2	4	0	0	0	2	0	2	4	6.9	6.3	-3.3	0	2	0
3EGZ_4	H2H3	C	3	0	7	0	3	0	0	3	7	6.6	-2.1	5.9	0	0	3
3KTW_143	H1H3	C	3	4	2	2	2	3	2	3	4	6.6	6.3	6.9	0	0	0
3MXH_13	H1H2	B	6	3	3	3	3	3	3	3	6	5.7	6.6	6.6	0	3	0

Feature parameters are described in the Materials and Methods section.

Table S3. List of feature parameters for four-way junctions.

PDB	Coaxial	Family	|L1|	|L2|	|L3|	|L4|	Min(|L2|,|L4|)	Min(|L1|,|L3|)	|L1'|	|L2'|	|L3'|	|L4'|	ΔG(H1,H2)	ΔG(H2,H3)	ΔG(H3,H4)	ΔG(H4,H1)	A(L1)	A(L2)	A(L3)	A(L4)
1U9S_78	H1H4, H2H3	H	0	1	2	0	0	0	0	0	1	2	-3.4	0.7	6.9	-3.3	0	0	0	0
2A2E_70	H1H4, H2H3	H	1	0	0	1	0	0	0	0	1	1	1.3	-3.3	-2.4	1.3	0	0	0	0
1NBS_89	H1H4, H2H3	H	0	1	2	0	0	0	0	0	1	2	-3.4	0.8	6.9	-3.3	0	0	0	0
2A64_90	H1H4, H2H3	H	0	1	2	0	0	0	0	0	1	2	-3.4	0.8	6.9	-3.3	0	0	0	0
1M5O_13	H1H4, H2H3	H	0	0	0	0	0	0	0	0	0	0	-0.9	-1.3	-2.1	-2.1	0	0	0	0
1S72_1827	H1H4, H2H3	H	3	3	3	4	3	3	3	3	3	4	6.6	6.6	6.6	6.3	0	0	2	2
2AW4_1771	H1H4, H2H3	H	3	3	2	3	3	2	2	3	3	3	6.6	6.6	6.9	6.6	0	0	0	2
2J01_1771	H1H4, H2H3	H	3	3	2	3	3	2	2	3	3	3	6.6	6.6	6.9	6.6	0	0	0	2
1KH6_4	H1H4, H2H3	cH	2	0	1	0	0	1	0	0	1	2	6.9	-2.4	-2.1	-3.3	2	0	0	0
2AVY_141	H1H4, H2H3	cH	3	7	4	1	1	3	1	3	4	7	6.6	5.9	6.3	0.8	0	2	3	0
2J00_141	H1H4, H2H3	cH	1	4	3	1	1	1	1	1	3	4	0.6	6.3	6.6	0.7	0	0	3	0
1NKW_2621	H1H4, H2H3	cH	2	1	4	2	1	2	1	2	2	4	6.9	0.5	6.3	6.9	0	0	2	0
1S72_2678	H1H4, H2H3	cH	2	0	2	1	0	2	0	1	2	2	6.9	-3.3	6.9	0.6	2	0	0	0
2AW4_2642	H1H4, H2H3	cH	2	1	3	1	1	2	1	1	2	3	6.9	0.5	6.6	0.7	0	0	2	0
2J01_2642	H1H4, H2H3	cH	2	1	3	1	1	2	1	1	2	3	6.9	0.5	6.6	0.7	0	0	2	0
1NKW_1457	H1H2, H3H4	cH	1	3	6	4	3	1	1	3	4	6	1.5	6.6	5.7	6.3	0	0	0	2
2AW4_1443	H1H2, H3H4	cH	0	0	3	4	0	0	0	0	3	4	-1.5	-0.6	6.6	6.3	0	0	0	2
3F2Q_7	H1H4, H2H3	cH	6	3	1	7	3	1	1	3	6	7	5.7	6.6	0.5	5.9	0	0	0	0
3F2Q_31	H1H4, H2H3	cH	0	2	3	2	2	0	0	2	2	3	-3.3	6.9	6.6	6.9	0	0	0	0
2AVY_568	H1H4, H2H3	cL	7	4	10	1	1	7	1	4	7	10	5.9	6.3	6.3	0.6	3	3	3	0
2J00_568	H1H4, H2H3	cL	7	4	10	1	1	7	1	4	7	10	5.9	6.3	6.3	0.6	3	3	3	0
1NKW_1282	H1H4, H2H3	cL	5	0	2	0	0	2	0	0	2	5	6	-2.4	6.9	-3.3	2	0	0	0
1S72_1373	H1H4, H2H3	cL	7	0	3	0	0	3	0	0	3	7	5.9	-2.4	6.6	-3.3	0	0	0	0
2AW4_1269	H1H4, H2H3	cL	5	0	2	0	0	2	0	0	2	5	6	-2.4	6.9	-2.1	2	0	0	0
2J01_1269	H1H4, H2H3	cL	5	0	2	0	0	2	0	0	2	5	6	-2.4	6.9	-3.3	2	0	0	0
1EFW_6	H1H4, H2H3	cL	2	1	5	0	0	2	0	1	2	5	6.9	0.5	6	-1.5	0	0	0	0
1EHZ_6	H1H4, H2H3	cL	2	1	5	0	0	2	0	1	2	5	6.9	0.7	6	-2.4	0	0	0	0
1N78_506	H1H4, H2H3	cL	2	1	4	0	0	2	0	1	2	4	6.9	0.6	6.3	-2.1	0	0	3	0
1QRS_6	H1H4, H2H3	cL	2	1	5	0	0	2	0	1	2	5	6.9	0.6	6	-2.2	0	0	0	0
1U0B_6	H1H4, H2H3	cL	2	1	4	0	0	2	0	1	2	4	6.9	1.1	6.3	-0.9	0	0	0	0
2GIS_7	H1H4, H2H3	cL	6	1	8	3	1	6	1	3	6	8	5.7	0.6	6	6.6	2	0	2	3
2AVY_114	H1H4	cK	6	0	2	0	0	2	0	0	2	6	5.7	-1.4	6.9	-3.3	2	0	0	0
2J00_114	H1H4	cK	6	0	2	0	0	2	0	0	2	6	5.7	-1.5	6.9	-3.3	2	0	0	0
1NKW_2263	H3H4	cK	4	4	1	1	1	1	1	1	4	4	6.3	6.3	0.5	0.5	3	0	0	0
1S72_2318	H3H4	cK	3	3	1	1	1	1	1	1	3	3	6.6	6.6	1	0.9	0	0	0	0
2AW4_2284	H3H4	cK	3	3	1	1	1	1	1	1	3	3	6.6	6.6	0.5	0.5	2	0	0	0

2J01_2284	H3H4	cK	3	3	1	1	1	1	1	1	3	3	6.6	6.6	0.5	0.5	3	0	0	0
1S72_1452	H3H4	cK	1	3	2	1	1	1	1	1	2	3	0.6	6.6	6.9	1.1	0	2	0	0
1NKW_1360	H3H4	cK	1	3	4	2	2	1	1	2	3	4	0.8	6.6	6.3	6.9	0	0	0	0
2AW4_1346	H3H4	cK	2	3	2	1	1	2	1	2	2	3	6.9	6.6	6.9	1.1	0	2	0	0
2J01_1347	H3H4	cK	1	3	2	0	0	1	0	1	2	3	0.5	6.6	6.9	-2.2	0	0	0	0
2AVY_18	H1H2	cK	7	10	1	3	3	1	1	3	7	10	5.9	6.3	0.6	6.6	0	2	0	3
2J00_18	H1H2	cK	7	10	1	3	3	1	1	3	7	10	5.9	6.3	0.6	6.6	0	0	0	3
1U9S_118	H1H4, H2H3	cH	6	3	1	7	3	1	1	3	6	7	5.7	6.6	0.5	5.9	0	0	0	0
2A2E_110	H1H4, H2H3	cH	0	3	4	2	2	0	0	2	3	4	-3.3	6.6	6.3	6.9	0	2	0	0
1NKW_1682	H1H2, H3H4	cH	0	2	0	0	0	0	0	0	0	2	-2.2	6.9	-3.3	-2.2	0	0	0	0
1S72_1743	H3H4	π	12	7	1	4	4	1	1	4	7	12	6.5	5.9	0.6	6.3	2	3	0	0
2AW4_1665	H3H4	π	10	7	2	4	4	2	2	4	7	10	6.3	5.9	6.9	6.3	2	2	0	0
2J01_1665		cW	15	0	12	5	0	12	0	5	12	15	6.7	-2.4	6.5	6	2	0	2	0
1S72_42		cW	15	0	12	5	0	12	0	5	12	15	6.7	0.3	6.5	6	2	0	0	0
1NKW_1824		cW	15	0	12	5	0	12	0	5	12	15	6.7	-1.4	6.5	6	4	0	2	0
1S72_1888		cW	15	0	12	5	0	12	0	5	12	15	6.7	-1.4	6.5	6	2	0	2	0
2AW4_1832		ψ	6	4	5	1	1	5	1	4	5	6	5.7	6.3	6	0.9	2	2	2	0
2J01_1832		ψ	1	2	22	10	2	1	1	2	10	22	0.6	6.9	7.1	6.3	0	0	3	3
1NKW_244		ψ	1	0	20	10	0	1	0	1	10	20	0.9	-2.4	7	6.3	0	0	2	2
2AW4_267		ψ	1	0	20	10	0	1	0	1	10	20	0.9	-2.4	7	6.3	0	0	3	2
1NKW_608		ψ	1	0	20	10	0	1	0	1	10	20	1.4	-2.4	7	6.3	0	0	3	3
2AW4_600		ψ	5	6	6	2	2	5	2	5	6	6	6	5.7	5.7	6.9	3	2	2	2
2J01_600		ψ	2	8	6	2	2	2	2	2	6	8	6.9	6	5.7	6.9	0	0	2	2
2IHX_166		X	10	9	3	11	9	3	3	9	10	11	6.3	6.1	6.6	6.4	2	0	0	0
2AVY_942		X	2	3	2	5	3	2	2	2	3	5	6.9	6.6	6.9	6	2	2	0	2
2J00_940		X	2	3	2	2	2	2	2	2	2	3	6.9	6.6	6.9	6.9	0	0	0	0
3F4E_7		cX	3	4	0	3	3	0	0	3	3	4	6.6	6.3	-1.5	6.6	0	0	0	0
3F4E_31		cX	2	5	11	10	5	2	2	5	10	11	6.9	6	6.4	6.3	0	2	0	2
3IVK_53		cX	4	5	11	12	5	4	4	5	11	12	6.3	6	6.4	6.5	0	2	0	2

Feature parameters are described in the Materials and Methods section.

Table S4. List of feature parameters for five to ten-way junctions.

PDB	Degree	Class	|Li-1|	|Li|	|Li+1|	Min(|Li-1|, |Li+1|)	ΔG(Hi-1,Hi)	ΔG(Hi,Hi+1)	ΔG(Hi+1,Hi+2)	A(Li-1)	A(Li)	A(Li+1)
1U6B_8	5WJ	Coaxial	2	3	3	2	6.9	6.6	6.6	0	0	0
1U6B_8	5WJ	Non-coaxial	3	3	0	0	6.6	6.6	-3.3	0	0	0
1U6B_8	5WJ	Coaxial	3	0	13	3	6.6	-3.3	6.6	0	0	2
1U6B_8	5WJ	Non-coaxial	0	13	2	0	-3.3	6.6	6.9	0	2	0
1U6B_8	5WJ	Non-coaxial	13	2	3	3	6.6	6.9	6.6	2	0	0
1Y0Q_43	5WJ	Non-coaxial	5	4	0	0	6	6.3	-0.6	3	2	0
1Y0Q_43	5WJ	Coaxial	4	0	10	4	6.3	-0.6	6.3	2	0	2
1Y0Q_43	5WJ	Non-coaxial	0	10	3	0	-0.6	6.3	6.6	0	2	0
1Y0Q_43	5WJ	Coaxial	10	3	5	5	6.3	6.6	6	2	0	3
1Y0Q_43	5WJ	Non-coaxial	3	5	4	3	6.6	6	6.3	0	3	2
2BTE_6	5WJ	Non-coaxial	0	2	0	0	-3.3	6.9	-1.4	0	0	0
2BTE_6	5WJ	Coaxial	2	0	0	0	6.9	-1.4	-1.4	0	0	0
2BTE_6	5WJ	Non-coaxial	0	0	2	0	-1.4	-1.4	6.9	0	0	0
2BTE_6	5WJ	Non-coaxial	0	2	0	0	-1.4	6.9	-3.3	0	0	0
2BTE_6	5WJ	Coaxial	2	0	2	2	6.9	-3.3	6.9	0	0	0
2NR0_6	5WJ	Non-coaxial	0	2	4	0	-2.4	6.9	6.3	0	0	0
2NR0_6	5WJ	Coaxial	2	4	1	1	6.9	6.3	1	0	0	0
2NR0_6	5WJ	Non-coaxial	4	1	2	2	6.3	1	6.9	0	0	0
2NR0_6	5WJ	Non-coaxial	1	2	0	0	1	6.9	-2.4	0	0	0
2NR0_6	5WJ	Coaxial	2	0	2	2	6.9	-2.4	6.9	0	0	0
2AVY_57	5WJ	Non-coaxial	3	2	6	3	6.6	6.9	5.7	0	2	0
2AVY_57	5WJ	Non-coaxial	2	6	1	1	6.9	5.7	0.7	2	0	0
2AVY_57	5WJ	Non-coaxial	6	1	1	1	5.7	0.7	0.5	0	0	0
2AVY_57	5WJ	Coaxial	1	1	3	1	0.7	0.5	6.6	0	0	0
2AVY_57	5WJ	Non-coaxial	1	3	2	1	0.5	6.6	6.9	0	0	2
2J00_56	5WJ	Non-coaxial	4	3	6	4	6.3	6.6	5.7	0	2	0
2J00_56	5WJ	Non-coaxial	3	6	1	1	6.6	5.7	0.7	2	0	0
2J00_56	5WJ	Non-coaxial	6	1	1	1	5.7	0.7	0.5	0	0	0
2J00_56	5WJ	Coaxial	1	1	4	1	0.7	0.5	6.3	0	0	0
2J00_56	5WJ	Non-coaxial	1	4	3	1	0.5	6.3	6.6	0	0	2
3BWP_23	5WJ	Non-coaxial	3	3	2	2	6.6	6.6	6.9	2	0	0
3BWP_23	5WJ	Coaxial	3	2	2	2	6.6	6.9	6.9	0	0	0
3BWP_23	5WJ	Non-coaxial	2	2	3	2	6.9	6.9	6.6	0	0	3
3BWP_23	5WJ	Non-coaxial	2	3	3	2	6.9	6.6	6.6	0	3	2
3BWP_23	5WJ	Non-coaxial	3	3	3	3	6.6	6.6	6.6	3	2	0
2J00_35	5WJ	Non-coaxial	2	2	2	2	6.9	6.9	6.9	0	0	0
2J00_35	5WJ	Non-coaxial	2	2	4	2	6.9	6.9	6.3	0	0	2
2J00_35	5WJ	Coaxial	2	4	6	2	6.9	6.3	5.7	0	2	2
2J00_35	5WJ	Non-coaxial	4	6	2	2	6.3	5.7	6.9	2	2	0
2J00_35	5WJ	Non-coaxial	6	2	2	2	5.7	6.9	6.9	2	0	0
2AVY_35	5WJ	Non-coaxial	2	2	2	2	6.9	6.9	6.9	2	0	0
2AVY_35	5WJ	Non-coaxial	2	2	5	2	6.9	6.9	6	0	0	0
2AVY_35	5WJ	Coaxial	2	5	7	2	6.9	6	5.9	0	0	2
2AVY_35	5WJ	Non-coaxial	5	7	2	2	6	5.9	6.9	0	2	2
2AVY_35	5WJ	Non-coaxial	7	2	2	2	5.9	6.9	6.9	2	2	0
1NKW_592	5WJ	Non-coaxial	5	4	2	2	6	6.3	6.9	0	0	0

1NKW_592	5WJ	Non-coaxial	4	2	2	2	6.3	6.9	6.9	0	0	0
1NKW_592	5WJ	Non-coaxial	2	2	0	0	6.9	6.9	-3.4	0	0	0
1NKW_592	5WJ	Coaxial	2	0	5	2	6.9	-3.4	6	0	0	0
1NKW_592	5WJ	Non-coaxial	0	5	4	0	-3.4	6	6.3	0	0	0
1S72_640	5WJ	Non-coaxial	10	4	2	2	6.3	6.3	6.9	4	0	0
1S72_640	5WJ	Non-coaxial	4	2	2	2	6.3	6.9	6.9	0	0	0
1S72_640	5WJ	Non-coaxial	2	2	4	2	6.9	6.9	6.3	0	0	0
1S72_640	5WJ	Coaxial	2	4	10	2	6.9	6.3	6.3	0	0	4
1S72_640	5WJ	Non-coaxial	4	10	4	4	6.3	6.3	6.3	0	4	0
2AW4_583	5WJ	Non-coaxial	8	4	2	2	6	6.3	6.9	2	0	0
2AW4_583	5WJ	Non-coaxial	4	2	2	2	6.3	6.9	6.9	0	0	0
2AW4_583	5WJ	Non-coaxial	2	2	2	2	6.9	6.9	6.9	0	0	0
2AW4_583	5WJ	Coaxial	2	2	8	2	6.9	6.9	6	0	0	2
2AW4_583	5WJ	Non-coaxial	2	8	4	2	6.9	6	6.3	0	2	0
2J01_583	5WJ	Non-coaxial	8	4	2	2	6	6.3	6.9	2	0	0
2J01_583	5WJ	Non-coaxial	4	2	2	2	6.3	6.9	6.9	0	0	0
2J01_583	5WJ	Non-coaxial	2	2	2	2	6.9	6.9	6.9	0	0	0
2J01_583	5WJ	Coaxial	2	2	8	2	6.9	6.9	6	0	0	2
2J01_583	5WJ	Non-coaxial	2	8	4	2	6.9	6	6.3	0	2	0
1S72_657	5WJ	Non-coaxial	3	2	3	3	6.6	6.9	6.6	0	2	0
1S72_657	5WJ	Non-coaxial	2	3	5	2	6.9	6.6	6	2	0	0
1S72_657	5WJ	Non-coaxial	3	5	1	1	6.6	6	0.6	0	0	0
1S72_657	5WJ	Coaxial	5	1	3	3	6	0.6	6.6	0	0	0
1S72_657	5WJ	Non-coaxial	1	3	2	1	0.6	6.6	6.9	0	0	2
1NKW_2036	5WJ	Non-coaxial	8	9	8	8	6	6.1	6	0	4	2
1NKW_2036	5WJ	Coaxial	9	8	11	9	6.1	6	6.4	4	2	0
1NKW_2036	5WJ	Non-coaxial	8	11	7	7	6	6.4	5.9	2	0	0
1NKW_2036	5WJ	Non-coaxial	11	7	8	8	6.4	5.9	6	0	0	0
1NKW_2036	5WJ	Non-coaxial	7	8	9	7	5.9	6	6.1	0	0	4
1S72_2097	5WJ	Non-coaxial	4	6	8	4	6.3	5.7	6	0	2	2
1S72_2097	5WJ	Coaxial	6	8	9	6	5.7	6	6.1	2	2	0
1S72_2097	5WJ	Non-coaxial	8	9	4	4	6	6.1	6.3	2	0	0
1S72_2097	5WJ	Non-coaxial	9	4	4	4	6.1	6.3	6.3	0	0	0
1S72_2097	5WJ	Non-coaxial	4	4	6	4	6.3	6.3	5.7	0	0	2
2AW4_2056	5WJ	Non-coaxial	4	6	8	4	6.3	5.7	6	0	3	2
2AW4_2056	5WJ	Coaxial	6	8	9	6	5.7	6	6.1	3	2	0
2AW4_2056	5WJ	Non-coaxial	8	9	4	4	6	6.1	6.3	2	0	0
2AW4_2056	5WJ	Non-coaxial	9	4	4	4	6.1	6.3	6.3	0	0	0
2AW4_2056	5WJ	Non-coaxial	4	4	6	4	6.3	6.3	5.7	0	0	3
2J01_2053	5WJ	Non-coaxial	8	9	8	8	6	6.1	6	0	4	2
2J01_2053	5WJ	Coaxial	9	8	11	9	6.1	6	6.4	4	2	0
2J01_2053	5WJ	Non-coaxial	8	11	7	7	6	6.4	5.9	2	0	0
2J01_2053	5WJ	Non-coaxial	11	7	8	8	6.4	5.9	6	0	0	0
2J01_2053	5WJ	Non-coaxial	7	8	9	7	5.9	6	6.1	0	0	4
3DIL_8	5WJ	Coaxial	4	4	3	3	6.3	6.3	6.6	0	0	0
3DIL_8	5WJ	Non-coaxial	4	3	0	0	6.3	6.6	-1	0	0	0
3DIL_8	5WJ	Non-coaxial	3	0	1	1	6.6	-1	1.3	0	0	0
3DIL_8	5WJ	Coaxial	0	1	4	0	-1	1.3	6.3	0	0	0

3DIL_8	5WJ	Non-coaxial	1	4	4	1	1.3	6.3	6.3	0	0	0
3EOH_23	5WJ	Non-coaxial	3	3	2	2	6.6	6.6	6.9	2	0	0
3EOH_23	5WJ	Coaxial	3	2	2	2	6.6	6.9	6.9	0	0	0
3EOH_23	5WJ	Non-coaxial	2	2	3	2	6.9	6.9	6.6	0	0	3
3EOH_23	5WJ	Non-coaxial	2	3	3	2	6.9	6.6	6.6	0	3	2
3EOH_23	5WJ	Non-coaxial	3	3	3	3	6.6	6.6	6.6	3	2	0
2A64_20	6WJ	Coaxial	8	1	13	8	6	0.6	6.6	0	0	3
2A64_20	6WJ	Non-coaxial	1	13	3	1	0.6	6.6	6.6	0	3	3
2A64_20	6WJ	Non-coaxial	13	3	3	3	6.6	6.6	6.6	3	3	0
2A64_20	6WJ	Non-coaxial	3	3	0	0	6.6	6.6	-2.4	3	0	0
2A64_20	6WJ	Coaxial	3	0	8	3	6.6	-2.4	6	0	0	0
2A64_20	6WJ	Non-coaxial	0	8	1	0	-2.4	6	0.6	0	0	0
1NKW_2056	6WJ	Coaxial	13	2	2	2	6.6	6.9	6.9	3	0	0
1NKW_2056	6WJ	Non-coaxial	2	2	0	0	6.9	6.9	-2.4	0	0	0
1NKW_2056	6WJ	Non-coaxial	2	0	2	2	6.9	-2.4	6.9	0	0	0
1NKW_2056	6WJ	Non-coaxial	0	2	10	0	-2.4	6.9	6.3	0	0	2
1NKW_2056	6WJ	Non-coaxial	2	10	13	2	6.9	6.3	6.6	0	2	3
1NKW_2056	6WJ	Non-coaxial	10	13	2	2	6.3	6.6	6.9	2	3	0
2J01_2073	6WJ	Coaxial	13	2	2	2	6.6	6.9	6.9	3	0	0
2J01_2073	6WJ	Non-coaxial	2	2	0	0	6.9	6.9	-2.4	0	0	0
2J01_2073	6WJ	Non-coaxial	2	0	2	2	6.9	-2.4	6.9	0	0	0
2J01_2073	6WJ	Non-coaxial	0	2	10	0	-2.4	6.9	6.3	0	0	2
2J01_2073	6WJ	Non-coaxial	2	10	13	2	6.9	6.3	6.6	0	2	3
2J01_2073	6WJ	Non-coaxial	10	13	2	2	6.3	6.6	6.9	2	3	0
1S72_2114	6WJ	Coaxial	10	2	3	3	6.3	6.9	6.6	3	0	0
1S72_2114	6WJ	Non-coaxial	2	3	2	2	6.9	6.6	6.9	0	0	0
1S72_2114	6WJ	Non-coaxial	3	2	2	2	6.6	6.9	6.9	0	0	0
1S72_2114	6WJ	Non-coaxial	2	2	10	2	6.9	6.9	6.3	0	0	2
1S72_2114	6WJ	Non-coaxial	2	10	10	2	6.9	6.3	6.3	0	2	3
1S72_2114	6WJ	Non-coaxial	10	10	2	2	6.3	6.3	6.9	2	3	0
2AW4_2073	6WJ	Coaxial	13	2	2	2	6.6	6.9	6.9	3	0	0
2AW4_2073	6WJ	Non-coaxial	2	2	0	0	6.9	6.9	-2.1	0	0	0
2AW4_2073	6WJ	Non-coaxial	2	0	2	2	6.9	-2.1	6.9	0	0	0
2AW4_2073	6WJ	Non-coaxial	0	2	10	0	-2.1	6.9	6.3	0	0	0
2AW4_2073	6WJ	Non-coaxial	2	10	13	2	6.9	6.3	6.6	0	0	3
2AW4_2073	6WJ	Non-coaxial	10	13	2	2	6.3	6.6	6.9	0	3	0
1S72_38	6WJ	Non-coaxial	9	2	4	4	6.1	6.9	6.3	3	0	2
1S72_38	6WJ	Coaxial	2	4	11	2	6.9	6.3	6.4	0	2	3
1S72_38	6WJ	Non-coaxial	4	11	3	3	6.3	6.4	6.6	2	3	0
1S72_38	6WJ	Non-coaxial	11	3	3	3	6.4	6.6	6.6	3	0	0
1S72_38	6WJ	Non-coaxial	3	3	9	3	6.6	6.6	6.1	0	0	3
1S72_38	6WJ	Non-coaxial	3	9	2	2	6.6	6.1	6.9	0	3	0
2J01_43	6WJ	Non-coaxial	6	0	4	4	5.7	-3.4	6.3	2	0	2
2J01_43	6WJ	Coaxial	0	4	11	0	-3.4	6.3	6.4	0	2	3
2J01_43	6WJ	Non-coaxial	4	11	3	3	6.3	6.4	6.6	2	3	0
2J01_43	6WJ	Non-coaxial	11	3	3	3	6.4	6.6	6.6	3	0	0
2J01_43	6WJ	Non-coaxial	3	3	6	3	6.6	6.6	5.7	0	0	2
2J01_43	6WJ	Non-coaxial	3	6	0	0	6.6	5.7	-3.4	0	2	0

2AW4_44	6WJ	Non-coaxial	6	0	4	4	5.7	-3.3	6.3	3	0	2
2AW4_44	6WJ	Coaxial	0	4	11	0	-3.3	6.3	6.4	0	2	4
2AW4_44	6WJ	Non-coaxial	4	11	3	3	6.3	6.4	6.6	2	4	0
2AW4_44	6WJ	Non-coaxial	11	3	3	3	6.4	6.6	6.6	4	0	0
2AW4_44	6WJ	Non-coaxial	3	3	6	3	6.6	6.6	5.7	0	0	3
2AW4_44	6WJ	Non-coaxial	3	6	0	0	6.6	5.7	-3.3	0	3	0
1NKW_43	6WJ	Non-coaxial	6	0	4	4	5.7	-3.4	6.3	3	0	2
1NKW_43	6WJ	Coaxial	0	4	11	0	-3.4	6.3	6.4	0	2	3
1NKW_43	6WJ	Non-coaxial	4	11	3	3	6.3	6.4	6.6	2	3	0
1NKW_43	6WJ	Non-coaxial	11	3	3	3	6.4	6.6	6.6	3	0	0
1NKW_43	6WJ	Non-coaxial	3	3	6	3	6.6	6.6	5.7	0	0	3
1NKW_43	6WJ	Non-coaxial	3	6	0	0	6.6	5.7	-3.4	0	3	0
1NKW_829	7WJ	Non-coaxial	7	4	0	0	5.9	6.3	-0.6	0	3	0
1NKW_829	7WJ	Coaxial	4	0	2	2	6.3	-0.6	6.9	3	0	0
1NKW_829	7WJ	Non-coaxial	0	2	4	0	-0.6	6.9	6.3	0	0	0
1NKW_829	7WJ	Non-coaxial	2	4	3	2	6.9	6.3	6.6	0	0	0
1NKW_829	7WJ	Non-coaxial	4	3	3	3	6.3	6.6	6.6	0	0	0
1NKW_829	7WJ	Coaxial	3	3	7	3	6.6	6.6	5.9	0	0	0
1NKW_829	7WJ	Non-coaxial	3	7	4	3	6.6	5.9	6.3	0	0	3
2AW4_816	7WJ	Non-coaxial	4	4	2	2	6.3	6.3	6.9	0	3	0
2AW4_816	7WJ	Coaxial	4	2	5	4	6.3	6.9	6	3	0	0
2AW4_816	7WJ	Non-coaxial	2	5	4	2	6.9	6	6.3	0	0	2
2AW4_816	7WJ	Non-coaxial	5	4	3	3	6	6.3	6.6	0	2	0
2AW4_816	7WJ	Non-coaxial	4	3	0	0	6.3	6.6	-3.4	2	0	0
2AW4_816	7WJ	Coaxial	3	0	4	3	6.6	-3.4	6.3	0	0	0
2AW4_816	7WJ	Non-coaxial	0	4	4	0	-3.4	6.3	6.3	0	0	3
2J01_816	7WJ	Non-coaxial	4	4	0	0	6.3	6.3	-0.6	0	3	0
2J01_816	7WJ	Coaxial	4	0	2	2	6.3	-0.6	6.9	3	0	0
2J01_816	7WJ	Non-coaxial	0	2	5	0	-0.6	6.9	6	0	0	0
2J01_816	7WJ	Non-coaxial	2	5	3	2	6.9	6	6.6	0	0	0
2J01_816	7WJ	Non-coaxial	5	3	0	0	6	6.6	-3.3	0	0	0
2J01_816	7WJ	Coaxial	3	0	4	3	6.6	-3.3	6.3	0	0	0
2J01_816	7WJ	Non-coaxial	0	4	4	0	-3.3	6.3	6.3	0	0	3
1S72_909	7WJ	Non-coaxial	4	4	2	2	6.3	6.3	6.9	0	3	0
1S72_909	7WJ	Coaxial	4	2	5	4	6.3	6.9	6	3	0	0
1S72_909	7WJ	Non-coaxial	2	5	4	2	6.9	6	6.3	0	0	0
1S72_909	7WJ	Non-coaxial	5	4	3	3	6	6.3	6.6	0	0	0
1S72_909	7WJ	Non-coaxial	4	3	0	0	6.3	6.6	-3.3	0	0	0
1S72_909	7WJ	Coaxial	3	0	4	3	6.6	-3.3	6.3	0	0	0
1S72_909	7WJ	Non-coaxial	0	4	4	0	-3.3	6.3	6.3	0	0	3
2J01_6	9WJ	Non-coaxial	5	7	7	5	6	5.9	5.9	0	2	2
2J01_6	9WJ	Non-coaxial	7	7	18	7	5.9	5.9	6.9	2	2	2
2J01_6	9WJ	Non-coaxial	7	18	7	7	5.9	6.9	5.9	2	2	0
2J01_6	9WJ	Coaxial	18	7	11	11	6.9	5.9	6.4	2	0	3
2J01_6	9WJ	Non-coaxial	7	11	2	2	5.9	6.4	6.9	0	3	0
2J01_6	9WJ	Non-coaxial	11	2	4	4	6.4	6.9	6.3	3	0	0
2J01_6	9WJ	Non-coaxial	2	4	19	2	6.9	6.3	7	0	0	2
2J01_6	9WJ	Non-coaxial	4	19	5	4	6.3	7	6	0	2	0

2J01_6	9WJ	Non-coaxial	19	5	7	7	7	6	5.9	2	0	2
1NKW_7	10WJ	Non-coaxial	4	8	9	4	6.3	6	6.1	0	2	2
1NKW_7	10WJ	Non-coaxial	8	9	18	8	6	6.1	6.9	2	2	2
1NKW_7	10WJ	Non-coaxial	9	18	7	7	6.1	6.9	5.9	2	2	0
1NKW_7	10WJ	Coaxial	18	7	11	11	6.9	5.9	6.4	2	0	3
1NKW_7	10WJ	Non-coaxial	7	11	2	2	5.9	6.4	6.9	0	3	0
1NKW_7	10WJ	Non-coaxial	11	2	4	4	6.4	6.9	6.3	3	0	0
1NKW_7	10WJ	Non-coaxial	2	4	2	2	6.9	6.3	6.9	0	0	0
1NKW_7	10WJ	Non-coaxial	4	2	4	4	6.3	6.9	6.3	0	0	2
1NKW_7	10WJ	Coaxial	2	4	4	2	6.9	6.3	6.3	0	2	0
1NKW_7	10WJ	Non-coaxial	4	4	8	4	6.3	6.3	6	2	0	2
2AW4_7	10WJ	Non-coaxial	5	6	7	5	6	5.7	5.9	0	2	2
2AW4_7	10WJ	Non-coaxial	6	7	18	6	5.7	5.9	6.9	2	2	2
2AW4_7	10WJ	Non-coaxial	7	18	7	7	5.9	6.9	5.9	2	2	2
2AW4_7	10WJ	Coaxial	18	7	11	11	6.9	5.9	6.4	2	2	3
2AW4_7	10WJ	Non-coaxial	7	11	2	2	5.9	6.4	6.9	2	3	0
2AW4_7	10WJ	Non-coaxial	11	2	4	4	6.4	6.9	6.3	3	0	0
2AW4_7	10WJ	Non-coaxial	2	4	2	2	6.9	6.3	6.9	0	0	0
2AW4_7	10WJ	Non-coaxial	4	2	5	4	6.3	6.9	6	0	0	2
2AW4_7	10WJ	Coaxial	2	5	5	2	6.9	6	6	0	2	0
2AW4_7	10WJ	Non-coaxial	5	5	6	5	6	6	5.7	2	0	2

Feature parameters are described in the Materials and Methods section.

Table S5. List of correct and incorrect prediction instances computed for each three-way junction.

Name	Coaxial Stacking prediction. No assumption of the junction family		Coaxial Stacking prediction. Junction family is assumed to be known		Junction family prediction. No assumption of the coaxial stacking		Junction family prediction. Coaxial stacking is assumed to be known	
	CORRECT	INCORRECT	CORRECT	INCORRECT	CORRECT	INCORRECT	CORRECT	INCORRECT
1NKW_23	75	0	75	0	75	0	75	0
1S72_20	75	0	75	0	75	0	75	0
2AW4_24	75	0	75	0	75	0	75	0
2J01_23	75	0	75	0	75	0	75	0
1NKW_31	75	0	75	0	75	0	75	0
1S72_28	75	0	75	0	75	0	75	0
2AW4_31	75	0	75	0	75	0	75	0
2J01_31	75	0	75	0	75	0	75	0
1NKW_54	75	0	75	0	75	0	75	0
1S72_51	75	0	75	0	75	0	75	0
2AW4_55	75	0	75	0	75	0	75	0
2J01_55	75	0	75	0	75	0	75	0
1NKW_307	73	2	75	0	75	0	75	0
1S72_301	0	75	0	75	75	0	75	0
2AW4_296	73	2	75	0	75	0	75	0
2J01_296	73	2	75	0	75	0	75	0
1NKW_695	75	0	75	0	75	0	75	0
1S72_773	75	0	75	0	75	0	75	0
2AW4_682	75	0	75	0	75	0	75	0
2J01_682	75	0	75	0	75	0	75	0
1NKW_709	75	0	75	0	75	0	74	1
1S72_787	6	69	69	6	67	8	75	0
2AW4_696	75	0	75	0	75	0	74	1
2J01_696	75	0	75	0	75	0	74	1
1NKW_1065	17	58	51	24	75	0	74	1
1S72_1158	72	3	73	2	75	0	74	1
2AW4_1054	72	3	73	2	75	0	74	1
1NKW_1310	75	0	75	0	75	0	74	1
1S72_1403	75	0	75	0	2	73	13	62
2AW4_1297	75	0	75	0	75	0	74	1
2J01_1297	74	1	75	0	75	0	74	1
1NKW_1318	75	0	75	0	75	0	75	0
1S72_1411	75	0	75	0	75	0	75	0
2AW4_1305	75	0	75	0	75	0	75	0
2J01_1305	75	0	75	0	75	0	75	0
1NKW_1322	75	0	75	0	74	1	75	0
1S72_1415	75	0	75	0	74	1	75	0
2AW4_1309	75	0	75	0	74	1	75	0

2J01_1309	75	0	75	0	74	1	75	0
1S72_1550	75	0	75	0	62	13	57	18
2J01_1443	1	74	2	73	31	44	71	4
1NKW_2072	75	0	75	0	75	0	75	0
1S72_2130	75	0	75	0	75	0	75	0
2AW4_2090	75	0	75	0	75	0	74	1
2J01_2090	75	0	75	0	75	0	74	1
1S72_2328	70	5	73	2	75	0	75	0
2AW4_2294	75	0	75	0	75	0	75	0
2J01_2294	75	0	74	1	75	0	75	0
1NKW_2495	73	2	75	0	75	0	73	2
1S72_2551	75	0	75	0	73	2	75	0
2AW4_2516	73	2	75	0	75	0	73	2
2J01_2516	73	2	75	0	75	0	73	2
1NKW_2788	75	0	75	0	75	0	75	0
1S72_2830	75	0	75	0	75	0	75	0
2AW4_2811	0	75	16	59	61	14	75	0
2J01_2813	75	0	75	0	75	0	75	0
1NKW_11	75	0	75	0	69	6	68	7
1S72_8	35	40	24	51	7	68	0	75
2AW4_9	73	2	72	3	69	6	68	7
2J01_10	65	10	67	8	75	0	75	0
1UN6_8	66	9	67	8	75	0	75	0
2J00_45	75	0	75	0	75	0	75	0
2AVY_45	75	0	75	0	75	0	75	0
2J00_585	75	0	75	0	67	8	66	9
2AVY_585	75	0	75	0	67	8	66	9
2J00_671	71	4	74	1	71	4	69	6
2AVY_671	71	4	73	2	71	4	69	6
2J00_825	74	1	74	1	75	0	75	0
2AVY_825	73	2	75	0	75	0	75	0
2J00_935	68	7	70	5	64	11	66	9
2AVY_935	68	7	70	5	64	11	66	9
2J00_954	66	9	69	6	75	0	75	0
2AVY_954	66	9	69	6	75	0	75	0
2J00_989	70	5	73	2	68	7	68	7
2AVY_989	70	5	73	2	68	7	68	7
2J00_1000	0	75	0	75	0	75	0	75
2AVY_1002	75	0	73	2	0	75	0	75
2J00_1059	70	5	69	6	68	7	71	4
2AVY_1059	70	5	69	6	68	7	71	4
2J00_1072	75	0	75	0	68	7	69	6
2AVY_1072	75	0	75	0	68	7	69	6

2J00_1115	74	1	75	0	72	3	74	1
2AVY_1115	74	1	75	0	72	3	74	1
1NYI_14	0	75	0	75	23	52	12	63
1E8O_102	2	73	2	73	75	0	75	0
1L9A_127	0	75	3	72	75	0	75	0
1LNG_144	0	75	0	75	0	75	5	70
2CZJ_4	75	0	75	0	75	0	75	0
1U8D_20	0	75	0	75	75	0	75	0
2B57_20	66	9	60	15	75	0	75	0
2EES_20	65	10	64	11	75	0	75	0
1Y26_20	75	0	75	0	75	0	75	0
2HO7_5	75	0	75	0	75	0	75	0
2NZ4_5	75	0	75	0	74	1	75	0
2GDI_13	75	0	75	0	75	0	75	0
2HOJ_13	75	0	75	0	68	7	66	9
2CKY_4	75	0	75	0	75	0	75	0
2QBZ_53	75	0	75	0	75	0	75	0
2OIU_6	75	0	75	0	0	75	0	75
1U6B_45	68	7	73	2	0	75	0	75
1Y0Q_195	0	75	0	75	0	75	0	75
1X8W_137	0	75	4	71	0	75	1	74
2A64_12	4	71	4	71	0	75	0	75
2A64_61	3	72	1	74	75	0	74	1
2A64_139	70	5	68	7	75	0	75	0
1NBS_132	70	5	68	7	75	0	75	0
3E5C_5	0	75	1	74	0	75	0	75
3EGZ_4	15	60	5	70	75	0	75	0
3KTW_143	10	65	45	30	0	75	31	44
3MXH_13	0	75	0	75	0	75	0	75

To evaluate the random forests classifier, the 10-fold cross-validation procedure is performed 75 times. Each time a junction element is randomly assigned to a partition unit, where is evaluated using the remaining nine units for training. The number of times a junction is correctly or incorrectly predicted is reported here.

Table S6. List of correct and incorrect prediction instances computed for each four-way junction.

Name	Coaxial Stacking prediction. No assumption of the junction family		Coaxial Stacking prediction. Junction family is assumed to be known		Junction family prediction. No assumption of the coaxial stacking		Junction family prediction. Coaxial stacking is assumed to be known	
	CORRECT	INCORRECT	CORRECT	INCORRECT	CORRECT	INCORRECT	CORRECT	INCORRECT
1U9S_78	75	0	75	0	75	0	74	1
2A2E_70	75	0	75	0	26	49	10	65
1NBS_89	75	0	75	0	75	0	74	1
2A64_90	75	0	75	0	75	0	74	1
1M5O_13	70	5	72	3	58	17	67	8
1S72_1827	75	0	74	1	59	16	43	32
2AW4_1771	70	5	74	1	72	3	72	3
2J01_1771	70	5	74	1	72	3	72	3
1KH6_4	75	0	75	0	0	75	0	75
2AVY_141	75	0	75	0	47	28	45	30
2J00_141	1	74	75	0	1	74	75	0
1NKW_2621	75	0	75	0	75	0	75	0
1S72_2678	75	0	75	0	4	71	1	74
2AW4_2642	75	0	75	0	75	0	74	1
2J01_2642	75	0	75	0	75	0	74	1
1NKW_1457	0	75	0	75	28	47	62	13
2AW4_1443	0	75	0	75	50	25	47	28
3F2Q_7	68	7	66	9	71	4	72	3
3F2Q_31	63	12	75	0	73	2	75	0
2AVY_568	67	8	70	5	71	4	73	2
2J00_568	67	8	70	5	71	4	73	2
1NKW_1282	74	1	75	0	75	0	75	0
1S72_1373	34	41	75	0	75	0	75	0
2AW4_1269	74	1	75	0	75	0	75	0
2J01_1269	74	1	75	0	75	0	75	0
1EFW_6	75	0	75	0	75	0	75	0
1EHZ_6	75	0	75	0	75	0	75	0
1N78_506	75	0	75	0	71	4	74	1
1QRS_6	75	0	75	0	75	0	75	0
1U0B_6	75	0	75	0	75	0	75	0
2GIS_7	8	67	68	7	0	75	0	75
2AVY_114	70	5	74	1	72	3	66	9
2J00_114	70	5	74	1	72	3	66	9
1NKW_2263	74	1	75	0	75	0	75	0
1S72_2318	75	0	75	0	75	0	75	0
2AW4_2284	75	0	75	0	75	0	75	0
2J01_2284	75	0	75	0	75	0	75	0
1S72_1452	75	0	75	0	75	0	75	0

1NKW_1360	0	75	38	37	0	75	74	1
2AW4_1346	51	24	74	1	28	47	75	0
2J01_1347	11	64	74	1	73	2	75	0
2AVY_18	73	2	72	3	72	3	70	5
2J00_18	73	2	72	3	72	3	70	5
1U9S_118	42	33	58	17	7	68	34	41
2A2E_110	2	73	6	69	27	48	71	4
1NKW_1682	75	0	75	0	75	0	75	0
1S72_1743	75	0	75	0	75	0	75	0
2AW4_1665	75	0	75	0	75	0	75	0
2J01_1665	75	0	75	0	75	0	75	0
1S72_42	0	75	1	74	0	75	0	75
1NKW_1824	75	0	75	0	75	0	75	0
1S72_1888	75	0	75	0	75	0	75	0
2AW4_1832	75	0	75	0	75	0	75	0
2J01_1832	75	0	75	0	75	0	75	0
1NKW_244	70	5	75	0	71	4	75	0
2AW4_267	60	15	75	0	63	12	69	6
1NKW_608	74	1	75	0	0	75	0	75
2AW4_600	1	74	69	6	0	75	18	57
2J01_600	0	75	11	64	0	75	0	75
2IHX_166	0	75	0	75	0	75	0	75
2AVY_942	75	0	75	0	68	7	66	9
2J00_940	75	0	75	0	69	6	67	8
3F4E_7	68	7	66	9	71	4	72	3
3F4E_31	4	71	75	0	67	8	75	0
3IVK_53	0	75	0	75	0	75	0	75

To evaluate the random forests classifier, the 10-fold cross-validation procedure is performed 75 times. Each time a junction element is randomly assigned to a partition unit, where is evaluated using the remaining nine units for training. The number of times a junction is correctly or incorrectly predicted is reported here.

Table S7. List of prediction values computed for each pair of helices in a higher-order junction.

Name	Degree	Helix pair	TP	FP	TN	FN
1U6B_8	5WJ	H1H2	0	0	0	75
1U6B_8	5WJ	H2H3	0	0	75	0
1U6B_8	5WJ	H3H4	75	0	0	0
1U6B_8	5WJ	H4H5	0	0	75	0
1U6B_8	5WJ	H5H1	0	0	75	0
1Y0Q_43	5WJ	H1H2	0	0	75	0
1Y0Q_43	5WJ	H2H3	75	0	0	0
1Y0Q_43	5WJ	H3H4	0	0	75	0
1Y0Q_43	5WJ	H4H5	0	0	0	75
1Y0Q_43	5WJ	H5H1	0	0	75	0
2BTE_6	5WJ	H1H2	0	0	75	0
2BTE_6	5WJ	H2H3	75	0	0	0
2BTE_6	5WJ	H3H4	0	68	7	0
2BTE_6	5WJ	H4H5	0	0	75	0
2BTE_6	5WJ	H5H1	0	0	0	75
2NR0_6	5WJ	H1H2	0	0	75	0
2NR0_6	5WJ	H2H3	0	0	0	75
2NR0_6	5WJ	H3H4	0	0	75	0
2NR0_6	5WJ	H4H5	0	0	75	0
2NR0_6	5WJ	H5H1	0	0	0	75
2AVY_57	5WJ	H1H2	0	0	75	0
2AVY_57	5WJ	H2H3	0	0	75	0
2AVY_57	5WJ	H3H4	0	5	70	0
2AVY_57	5WJ	H4H5	0	0	0	75
2AVY_57	5WJ	H5H1	0	0	75	0
2J00_56	5WJ	H1H2	0	0	75	0
2J00_56	5WJ	H2H3	0	0	75	0
2J00_56	5WJ	H3H4	0	5	70	0
2J00_56	5WJ	H4H5	0	0	0	75
2J00_56	5WJ	H5H1	0	2	73	0
3BWP_23	5WJ	H1H2	0	0	75	0
3BWP_23	5WJ	H2H3	0	0	0	75
3BWP_23	5WJ	H3H4	0	0	75	0
3BWP_23	5WJ	H4H5	0	2	73	0
3BWP_23	5WJ	H5H1	0	0	75	0
2J00_35	5WJ	H1H2	0	0	75	0
2J00_35	5WJ	H2H3	0	0	75	0
2J00_35	5WJ	H3H4	0	0	0	75
2J00_35	5WJ	H4H5	0	0	75	0
2J00_35	5WJ	H5H1	0	0	75	0
2AVY_35	5WJ	H1H2	0	0	75	0
2AVY_35	5WJ	H2H3	0	0	75	0
2AVY_35	5WJ	H3H4	0	0	0	75
2AVY_35	5WJ	H4H5	0	0	75	0
2AVY_35	5WJ	H5H1	0	0	75	0
1NKW_592	5WJ	H1H2	0	0	75	0
1NKW_592	5WJ	H2H3	0	1	74	0
1NKW_592	5WJ	H3H4	0	0	75	0
1NKW_592	5WJ	H4H5	75	0	0	0
1NKW_592	5WJ	H5H1	0	0	75	0
1S72_640	5WJ	H1H2	0	0	75	0
1S72_640	5WJ	H2H3	0	1	74	0
1S72_640	5WJ	H3H4	0	0	75	0
1S72_640	5WJ	H4H5	0	0	0	75
1S72_640	5WJ	H5H1	0	0	75	0
2AW4_583	5WJ	H1H2	0	0	75	0
2AW4_583	5WJ	H2H3	0	1	74	0
2AW4_583	5WJ	H3H4	0	0	75	0
2AW4_583	5WJ	H4H5	65	0	0	10
2AW4_583	5WJ	H5H1	0	0	75	0
2J01_583	5WJ	H1H2	0	0	75	0
2J01_583	5WJ	H2H3	0	1	74	0
2J01_583	5WJ	H3H4	0	0	75	0

2J01_583	5WJ	H4H5	62	0	0	13
2J01_583	5WJ	H5H1	0	0	75	0
1S72_657	5WJ	H1H2	0	0	75	0
1S72_657	5WJ	H2H3	0	1	74	0
1S72_657	5WJ	H3H4	0	0	75	0
1S72_657	5WJ	H4H5	75	0	0	0
1S72_657	5WJ	H5H1	0	0	75	0
1NKW_2036	5WJ	H1H2	0	0	75	0
1NKW_2036	5WJ	H2H3	68	0	0	7
1NKW_2036	5WJ	H3H4	0	0	75	0
1NKW_2036	5WJ	H4H5	0	0	75	0
1NKW_2036	5WJ	H5H1	0	0	75	0
1S72_2097	5WJ	H1H2	0	0	75	0
1S72_2097	5WJ	H2H3	0	0	0	75
1S72_2097	5WJ	H3H4	0	0	75	0
1S72_2097	5WJ	H4H5	0	0	75	0
1S72_2097	5WJ	H5H1	0	0	75	0
2AW4_2056	5WJ	H1H2	0	0	75	0
2AW4_2056	5WJ	H2H3	72	0	0	3
2AW4_2056	5WJ	H3H4	0	0	75	0
2AW4_2056	5WJ	H4H5	0	0	75	0
2AW4_2056	5WJ	H5H1	0	0	75	0
2J01_2053	5WJ	H1H2	0	0	75	0
2J01_2053	5WJ	H2H3	68	0	0	7
2J01_2053	5WJ	H3H4	0	0	75	0
2J01_2053	5WJ	H4H5	0	0	75	0
2J01_2053	5WJ	H5H1	0	0	75	0
3DIL_8	5WJ	H1H2	0	0	0	75
3DIL_8	5WJ	H2H3	0	0	75	0
3DIL_8	5WJ	H3H4	0	75	0	0
3DIL_8	5WJ	H4H5	0	0	0	75
3DIL_8	5WJ	H5H1	0	0	75	0
3EOH_23	5WJ	H1H2	0	0	75	0
3EOH_23	5WJ	H2H3	0	0	0	75
3EOH_23	5WJ	H3H4	0	0	75	0
3EOH_23	5WJ	H4H5	0	3	72	0
3EOH_23	5WJ	H5H1	0	0	75	0
2A64_20	6WJ	H1H2	71	0	0	4
2A64_20	6WJ	H2H3	0	0	75	0
2A64_20	6WJ	H3H4	0	0	75	0
2A64_20	6WJ	H4H5	0	0	75	0
2A64_20	6WJ	H5H6	75	0	0	0
2A64_20	6WJ	H6H1	0	0	75	0
1NKW_2056	6WJ	H1H2	74	0	0	1
1NKW_2056	6WJ	H2H3	0	0	75	0
1NKW_2056	6WJ	H3H4	0	50	25	0
1NKW_2056	6WJ	H4H5	0	0	75	0
1NKW_2056	6WJ	H5H6	0	0	75	0
1NKW_2056	6WJ	H6H1	0	0	75	0
2J01_2073	6WJ	H1H2	74	0	0	1
2J01_2073	6WJ	H2H3	0	0	75	0
2J01_2073	6WJ	H3H4	0	43	32	0
2J01_2073	6WJ	H4H5	0	0	75	0
2J01_2073	6WJ	H5H6	0	0	75	0
2J01_2073	6WJ	H6H1	0	0	75	0
1S72_2114	6WJ	H1H2	0	0	0	75
1S72_2114	6WJ	H2H3	0	0	75	0
1S72_2114	6WJ	H3H4	0	60	15	0
1S72_2114	6WJ	H4H5	0	44	31	0
1S72_2114	6WJ	H5H6	0	0	75	0
1S72_2114	6WJ	H6H1	0	0	75	0
2AW4_2073	6WJ	H1H2	74	0	0	1
2AW4_2073	6WJ	H2H3	0	0	75	0
2AW4_2073	6WJ	H3H4	0	10	65	0
2AW4_2073	6WJ	H4H5	0	0	75	0
2AW4_2073	6WJ	H5H6	0	0	75	0

2AW4_2073	6WJ	H6H1	0	0	75	0
1S72_38	6WJ	H1H2	0	71	4	0
1S72_38	6WJ	H2H3	47	0	0	28
1S72_38	6WJ	H3H4	0	0	75	0
1S72_38	6WJ	H4H5	0	0	75	0
1S72_38	6WJ	H5H6	0	0	75	0
1S72_38	6WJ	H6H1	0	0	75	0
2J01_43	6WJ	H1H2	0	0	75	0
2J01_43	6WJ	H2H3	66	0	0	9
2J01_43	6WJ	H3H4	0	0	75	0
2J01_43	6WJ	H4H5	0	0	75	0
2J01_43	6WJ	H5H6	0	0	75	0
2J01_43	6WJ	H6H1	0	0	75	0
2AW4_44	6WJ	H1H2	0	10	65	0
2AW4_44	6WJ	H2H3	72	0	0	3
2AW4_44	6WJ	H3H4	0	0	75	0
2AW4_44	6WJ	H4H5	0	0	75	0
2AW4_44	6WJ	H5H6	0	0	75	0
2AW4_44	6WJ	H6H1	0	0	75	0
1NKW_43	6WJ	H1H2	0	1	74	0
1NKW_43	6WJ	H2H3	66	0	0	9
1NKW_43	6WJ	H3H4	0	0	75	0
1NKW_43	6WJ	H4H5	0	0	75	0
1NKW_43	6WJ	H5H6	0	0	75	0
1NKW_43	6WJ	H6H1	0	0	75	0
1NKW_829	7WJ	H1H2	0	0	75	0
1NKW_829	7WJ	H2H3	75	0	0	0
1NKW_829	7WJ	H3H4	0	0	75	0
1NKW_829	7WJ	H4H5	0	26	49	0
1NKW_829	7WJ	H5H6	0	75	0	0
1NKW_829	7WJ	H6H7	0	0	0	75
1NKW_829	7WJ	H7H1	0	71	4	0
2AW4_816	7WJ	H1H2	0	0	75	0
2AW4_816	7WJ	H2H3	71	0	0	4
2AW4_816	7WJ	H3H4	0	0	75	0
2AW4_816	7WJ	H4H5	0	0	75	0
2AW4_816	7WJ	H5H6	0	0	75	0
2AW4_816	7WJ	H6H7	75	0	0	0
2AW4_816	7WJ	H7H1	0	0	75	0
2J01_816	7WJ	H1H2	0	0	75	0
2J01_816	7WJ	H2H3	75	0	0	0
2J01_816	7WJ	H3H4	0	0	75	0
2J01_816	7WJ	H4H5	0	0	75	0
2J01_816	7WJ	H5H6	0	0	75	0
2J01_816	7WJ	H6H7	75	0	0	0
2J01_816	7WJ	H7H1	0	0	75	0
1S72_909	7WJ	H1H2	0	0	75	0
1S72_909	7WJ	H2H3	71	0	0	4
1S72_909	7WJ	H3H4	0	0	75	0
1S72_909	7WJ	H4H5	0	0	75	0
1S72_909	7WJ	H5H6	0	0	75	0
1S72_909	7WJ	H6H7	75	0	0	0
1S72_909	7WJ	H7H1	0	0	75	0
2J01_6	9WJ	H1H2	0	0	75	0
2J01_6	9WJ	H2H3	0	0	75	0
2J01_6	9WJ	H3H4	0	0	75	0
2J01_6	9WJ	H4H5	75	0	0	0
2J01_6	9WJ	H5H6	0	0	75	0
2J01_6	9WJ	H6H7	0	0	75	0
2J01_6	9WJ	H7H8	0	0	75	0
2J01_6	9WJ	H8H9	0	0	75	0
2J01_6	9WJ	H9H1	0	69	6	0
1NKW_7	10WJ	H1H2	0	0	75	0
1NKW_7	10WJ	H2H3	0	0	75	0
1NKW_7	10WJ	H3H4	0	0	75	0
1NKW_7	10WJ	H4H5	75	0	0	0

1NKW_7	10WJ	H5H6	0	0	75	0
1NKW_7	10WJ	H6H7	0	0	75	0
1NKW_7	10WJ	H7H8	0	0	75	0
1NKW_7	10WJ	H8H9	0	0	75	0
1NKW_7	10WJ	H9H10	75	0	0	0
1NKW_7	10WJ	H10H1	0	0	75	0
2AW4_7	10WJ	H1H2	0	0	75	0
2AW4_7	10WJ	H2H3	0	0	75	0
2AW4_7	10WJ	H3H4	0	0	75	0
2AW4_7	10WJ	H4H5	75	0	0	0
2AW4_7	10WJ	H5H6	0	0	75	0
2AW4_7	10WJ	H6H7	0	0	75	0
2AW4_7	10WJ	H7H8	0	0	75	0
2AW4_7	10WJ	H8H9	0	1	74	0
2AW4_7	10WJ	H9H10	0	0	0	75
2AW4_7	10WJ	H10H1	0	0	75	0
Total			**2146**	**696**	**11529**	**1454**
Positive predictive value = 76				**Sensitivity = 60**		

To evaluate the random forests classifier, the 10-fold cross-validation procedure is performed 75 times. Each time, a pair of consecutive helices HiHi+1 is randomly assigned to a partition unit, where is evaluated using the remaining nine units for training. In addition, the training data is augmented using information for every pair of consecutive helices from 3 and 4-way junctions. The values for true positive (TP), false positive (FP), true negative (TN), and false negative (FN) are reported here.

Table S8. List of correct and incorrect prediction instances computed for each three and four-way junction in a two step procedure.

Name	3WJ Coaxial Stacking prediction		3WJ Junction family prediction		Name	4WJ Coaxial Stacking prediction		4WJ Junction family prediction	
	CORRECT	INCORRECT	CORRECT	INCORRECT		CORRECT	INCORRECT	CORRECT	INCORRECT
1NKW_23	75	0	75	0	1U9S_78	75	0	75	0
1S72_20	75	0	75	0	2A2E_70	75	0	14	61
2AW4_24	75	0	75	0	1NBS_89	75	0	75	0
2J01_23	75	0	75	0	2A64_90	75	0	75	0
1NKW_31	75	0	75	0	1M5O_13	71	4	62	13
1S72_28	75	0	75	0	1S72_1827	75	0	41	34
2AW4_31	75	0	75	0	2AW4_1771	71	4	73	2
2J01_31	75	0	75	0	2J01_1771	71	4	73	2
1NKW_54	75	0	75	0	1KH6_4	75	0	0	75
1S72_51	75	0	75	0	2AVY_141	66	9	48	27
2AW4_55	75	0	75	0	2J00_141	3	72	1	74
2J01_55	75	0	75	0	1NKW_2621	75	0	73	2
1NKW_307	75	0	74	1	1S72_2678	75	0	0	75
1S72_301	0	75	75	0	2AW4_2642	75	0	73	2
2AW4_296	75	0	74	1	2J01_2642	75	0	73	2
2J01_296	75	0	74	1	1NKW_1457	0	75	73	2
1NKW_695	75	0	75	0	2AW4_1443	0	75	50	25
1S72_773	75	0	75	0	3F2Q_7	70	5	74	1
2AW4_682	75	0	75	0	3F2Q_31	74	1	73	2
2J01_682	75	0	75	0	2AVY_568	70	5	73	2
1NKW_709	75	0	75	0	2J00_568	70	5	73	2
1S72_787	62	13	16	59	1NKW_1282	75	0	75	0
2AW4_696	75	0	75	0	1S72_1373	75	0	31	44
2J01_696	75	0	75	0	2AW4_1269	75	0	75	0
1NKW_1065	57	18	73	2	2J01_1269	75	0	75	0
1S72_1158	75	0	75	0	1EFW_6	75	0	75	0
2AW4_1054	75	0	75	0	1EHZ_6	75	0	75	0
1NKW_1310	73	2	73	2	1N78_506	75	0	70	5
1S72_1403	75	0	18	57	1QRS_6	75	0	75	0
2AW4_1297	73	2	73	2	1U0B_6	75	0	74	1
2J01_1297	73	2	73	2	2GIS_7	0	75	0	75
1NKW_1318	75	0	74	1	2AVY_114	72	3	67	8
1S72_1411	75	0	74	1	2J00_114	72	3	67	8
2AW4_1305	75	0	74	1	1NKW_2263	75	0	75	0
2J01_1305	75	0	74	1	1S72_2318	75	0	75	0
1NKW_1322	75	0	75	0	2AW4_2284	75	0	75	0
1S72_1415	75	0	75	0	2J01_2284	75	0	75	0

2AW4_1309	75	0	75	0
2J01_1309	75	0	75	0
1S72_1550	75	0	52	23
2J01_1443	1	74	18	57
1NKW_2072	75	0	75	0
1S72_2130	75	0	74	1
2AW4_2090	75	0	75	0
2J01_2090	75	0	75	0
1S72_2328	75	0	74	1
2AW4_2294	74	1	75	0
2J01_2294	75	0	75	0
1NKW_2495	75	0	74	1
1S72_2551	75	0	75	0
2AW4_2516	75	0	74	1
2J01_2516	75	0	74	1
1NKW_2788	75	0	75	0
1S72_2830	75	0	75	0
2AW4_2811	16	59	50	25
2J01_2813	75	0	75	0
1NKW_11	75	0	71	4
1S72_8	38	37	33	42
2AW4_9	75	0	70	5
2J01_10	61	14	75	0
1UN6_8	61	14	75	0
2J00_45	75	0	75	0
2AVY_45	75	0	75	0
2J00_585	74	1	68	7
2AVY_585	74	1	68	7
2J00_671	67	8	71	4
2AVY_671	67	8	71	4
2J00_825	75	0	75	0
2AVY_825	75	0	74	1
2J00_935	72	3	70	5
2AVY_935	72	3	70	5
2J00_954	69	6	75	0
2AVY_954	69	6	75	0
2J00_989	72	3	69	6
2AVY_989	72	3	69	6
2J00_1000	3	72	31	44
2AVY_1002	75	0	0	75
2J00_1059	67	8	68	7
2AVY_1059	67	8	68	7
2J00_1072	75	0	69	6
1S72_1452	75	0	72	3
1NKW_1360	0	75	0	75
2AW4_1346	36	39	35	40
2J01_1347	66	9	9	66
2AVY_18	68	7	71	4
2J00_18	68	7	71	4
1U9S_118	62	13	33	42
2A2E_110	2	73	4	71
1NKW_1682	74	1	75	0
1S72_1743	74	1	75	0
2AW4_1665	74	1	75	0
2J01_1665	74	1	75	0
1S72_42	0	75	0	75
1NKW_1824	75	0	75	0
1S72_1888	75	0	75	0
2AW4_1832	75	0	75	0
2J01_1832	75	0	75	0
1NKW_244	67	8	63	12
2AW4_267	57	18	57	18
1NKW_608	72	3	0	75
2AW4_600	0	75	0	75
2J01_600	0	75	0	75
2IHX_166	0	75	0	75
2AVY_942	75	0	70	5
2J00_940	75	0	70	5
3F4E_7	70	5	74	1
3F4E_31	59	16	7	68
3IVK_53	0	75	0	75

2AVY_1072	75	0	69	6
2J00_1115	75	0	71	4
2AVY_1115	75	0	71	4
1NYI_14	0	75	74	1
1E8O_102	3	72	75	0
1L9A_127	0	75	75	0
1LNG_144	0	75	0	75
2CZJ_4	75	0	75	0
1U8D_20	0	75	75	0
2B57_20	62	13	75	0
2EES_20	62	13	75	0
1Y26_20	75	0	75	0
2HO7_5	75	0	75	0
2NZ4_5	75	0	75	0
2GDI_13	74	1	75	0
2HOJ_13	74	1	64	11
2CKY_4	75	0	75	0
2QBZ_53	75	0	75	0
2OIU_6	75	0	0	75
1U6B_45	58	17	0	75
1Y0Q_195	0	75	1	74
1X8W_137	0	75	0	75
2A64_12	2	73	0	75
2A64_61	0	75	75	0
2A64_139	67	8	75	0
1NBS_132	67	8	75	0
3E5C_5	0	75	0	75
3EGZ_4	2	73	75	0
3KTW_143	0	75	2	73
3MXH_13	0	75	1	74

To evaluate the random forests classifier, the 10-fold cross-validation procedure is performed 75 times. Each time a junction element is randomly assigned to a partition unit, where is evaluated using the remaining nine units for training. The random forest classifier is first implemented to determine the coaxial stacking (family type), and implemented a second time to predict the junction family type (coaxial stacking) using the results from the first prediction as a feature parameter. The number of times a junction is correctly or incorrectly predicted is reported here.

Table S9. List of training and test dataset used to compare our method with the work of Tyagi and Mathews.

Training dataset for predicting coaxial stacking on 3-way junctions								
2AW4_24	2J01_696	2J01_2294	2AVY_825	1Y26_20	2A64_61	2J00_989	1S72_8	1NBS_132
2J01_23	2AW4_1297	2AW4_2516	2AVY_935	2HO7_5	2A64_139	2J00_1000	1NKW_23	1NYI_14
2AW4_31	2J01_1297	2J01_2516	2AVY_954	2NZ4_5	3E5C_5	2J00_1059	1NKW_307	1X8W_137
2J01_31	2AW4_1305	2AW4_2811	2AVY_989	2GDI_13	3EGZ_4	2J00_1115	1NKW_695	
2AW4_55	2J01_1305	2J01_2813	2AVY_1002	2HOJ_13	3KTW_143	1S72_20	1NKW_709	
2J01_55	2AW4_1309	2AW4_9	2AVY_1059	2CKY_4	3MXH_13	1S72_301	1NKW_1065	
2AW4_296	2J01_1309	2J01_10	2AVY_1072	2QBZ_53	2J00_45	1S72_787	1NKW_1322	
2J01_296	2J01_1443	1UN6_8	2AVY_1115	2OIU_6	2J00_585	1S72_1158	1NKW_2495	
2AW4_682	2AW4_2090	2AVY_45	2CZJ_4	1U6B_45	2J00_825	1S72_1415	1NKW_2788	
2J01_682	2J01_2090	2AVY_585	2B57_20	1Y0Q_195	2J00_935	1S72_2328	1NKW_11	
2AW4_696	2AW4_2294	2AVY_671	2EES_20	2A64_12	2J00_954	1S72_2551	1U8D_20	

Test dataset and results for predicting coaxial stacking on 3-way junctions								
Name	Our method	Tyagi & Mathews	Name	Our method	Tyagi & Mathews	Name	Our method	Tyagi & Mathews
1E8O_102	Incorrect	Correct	1S72_2130	Correct	Incorrect	1NKW_1310	Correct	Incorrect
1LNG_144	Incorrect	Correct	1S72_2830	Correct	Incorrect	1NKW_1318	Correct	Incorrect
1S72_51	Correct	Correct	1S72_773	Correct	Incorrect	1NKW_2072	Correct	Incorrect
1S72_1550	Correct	Correct	2J00_1072	Correct	Correct	2AW4_1054	Correct	Incorrect
1S72_28	Correct	Incorrect	2J00_671	Correct	Incorrect	1L9A_127	Incorrect	Correct
1S72_1403	Correct	Incorrect	1NKW_31	Correct	Incorrect	1J2B_906	Incorrect	Incorrect
1S72_1411	Correct	Incorrect	1NKW_54	Correct	Incorrect			

Training dataset for predicting coaxial stacking on 4-way junctions								
2A2E_70	2J01_2642	2J01_1269	2AW4_2284	2AW4_1665	2J01_600	2J00_141	1S72_1743	1M5O_13
2A64_90	2AW4_1443	1EFW_6	2J01_2284	2J01_1665	2IHX_166	2J00_568	1NKW_2621	
2AW4_1771	3F2Q_7	1QRS_6	2AW4_1346	2AW4_1832	2AVY_942	2J00_18	1NKW_1457	
2J01_1771	3F2Q_31	1U0B_6	2J01_1347	2J01_1832	3F4E_7	2J00_940	1NKW_1360	
2AVY_141	2AVY_568	2GIS_7	2AVY_18	2AW4_267	3F4E_31	1S72_1827	1NKW_244	
2AW4_2642	2AW4_1269	2AVY_114	2A2E_110	2AW4_600	3IVK_53	1S72_2678	1NKW_608	

Test dataset and results for predicting coaxial stacking on 4-way junctions								
Name	Our method	Tyagi & Mathews	Name	Our method	Tyagi & Mathews	Name	Our method	Tyagi & Mathews
1N78_506	Correct	Correct	1S72_42	Incorrect	Incorrect	1C0A_606	Correct	Correct
1EHZ_6	Correct	Correct	1S72_1888	Correct	Incorrect	1EIY_6	Correct	Correct
1NBS_89	Correct	Incorrect	2J00_114	Correct	Incorrect	1H4S_6	Correct	Correct
1U9S_78	Correct	Correct	1NKW_1282	Correct	Correct	2FMT_6	Correct	Correct
1U9S_118	Incorrect	Correct	1NKW_2263	Correct	Correct	1J1U_506	Correct	Correct
1KH6_4	Correct	Correct	1NKW_1682	Correct	Incorrect	1QTQ_906	Correct	Correct
1S72_1373	Correct	Correct	1NKW_1824	Correct	Incorrect	1FIR_6	Correct	Incorrect
1S72_2318	Correct	Correct	1B23_6	Correct	Correct	trna05_6	Correct	Correct
1S72_1452	Correct	Incorrect	1QU2_6	Correct	Correct	1YFG_6	Correct	Correct

Prediction of coaxial stacking for both three and four-way junctions are performed.

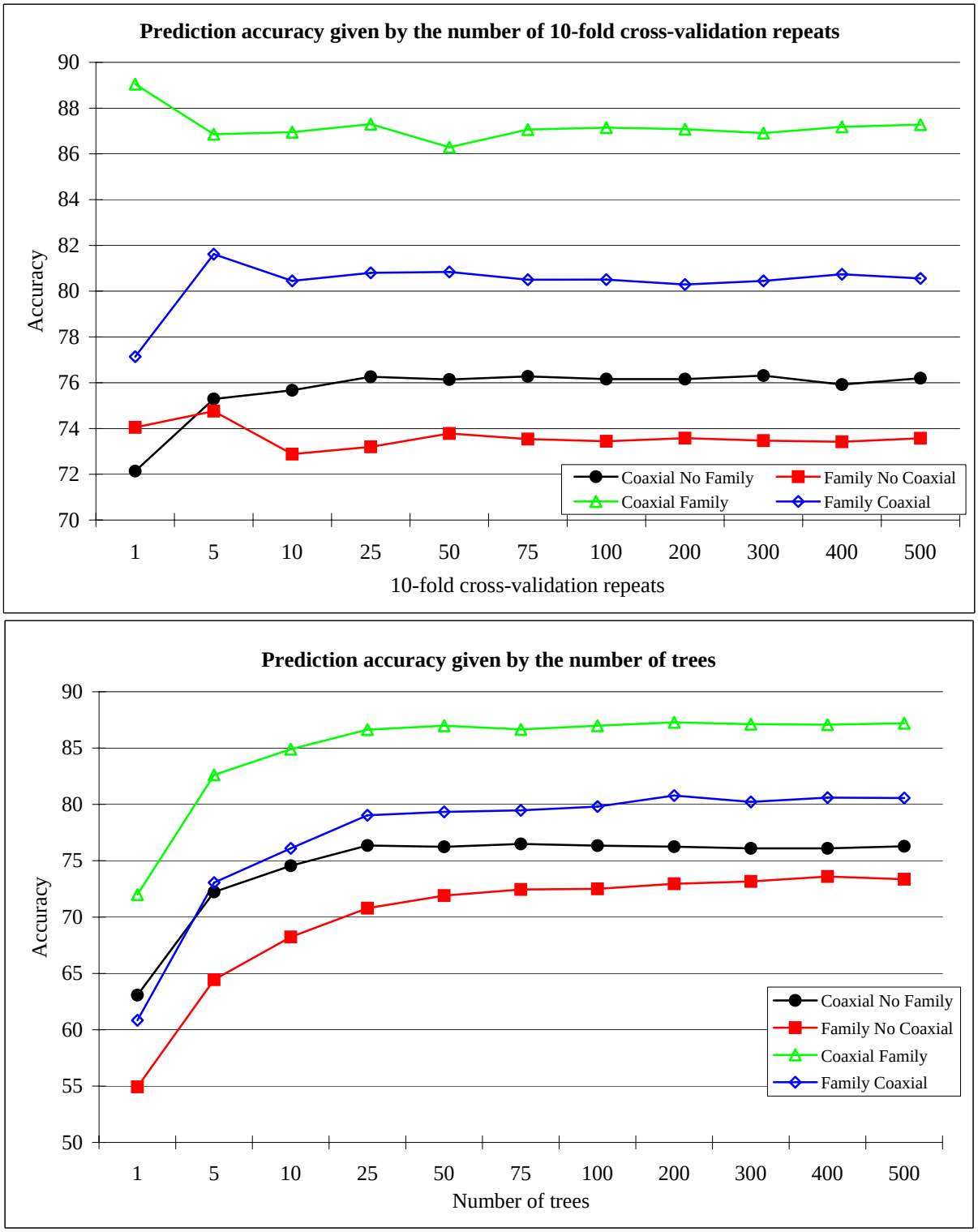
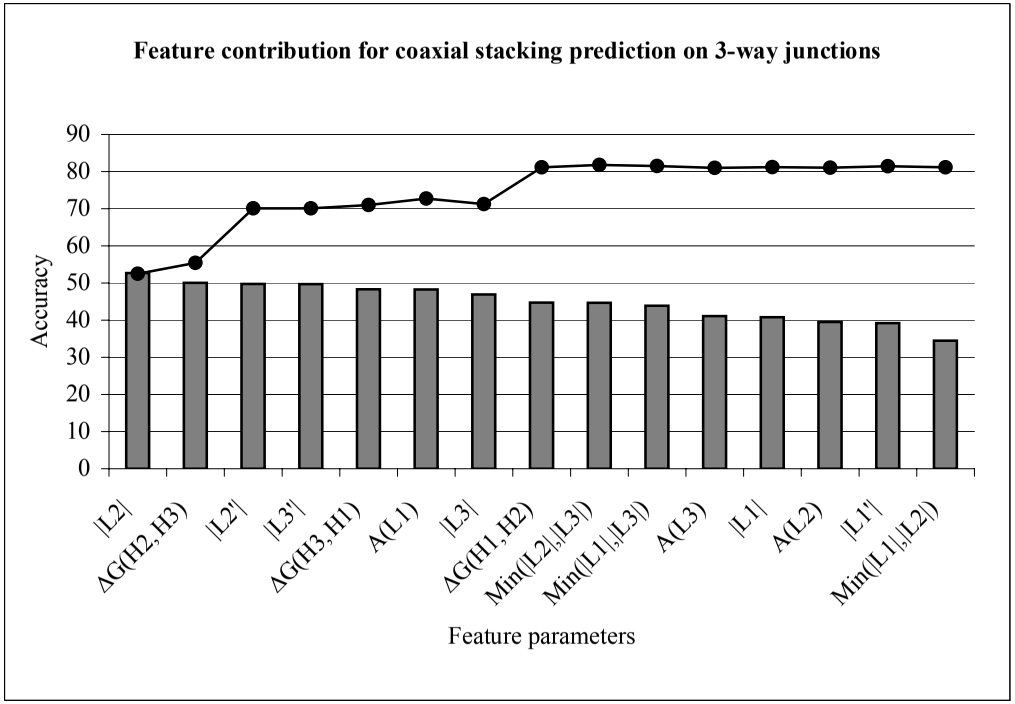
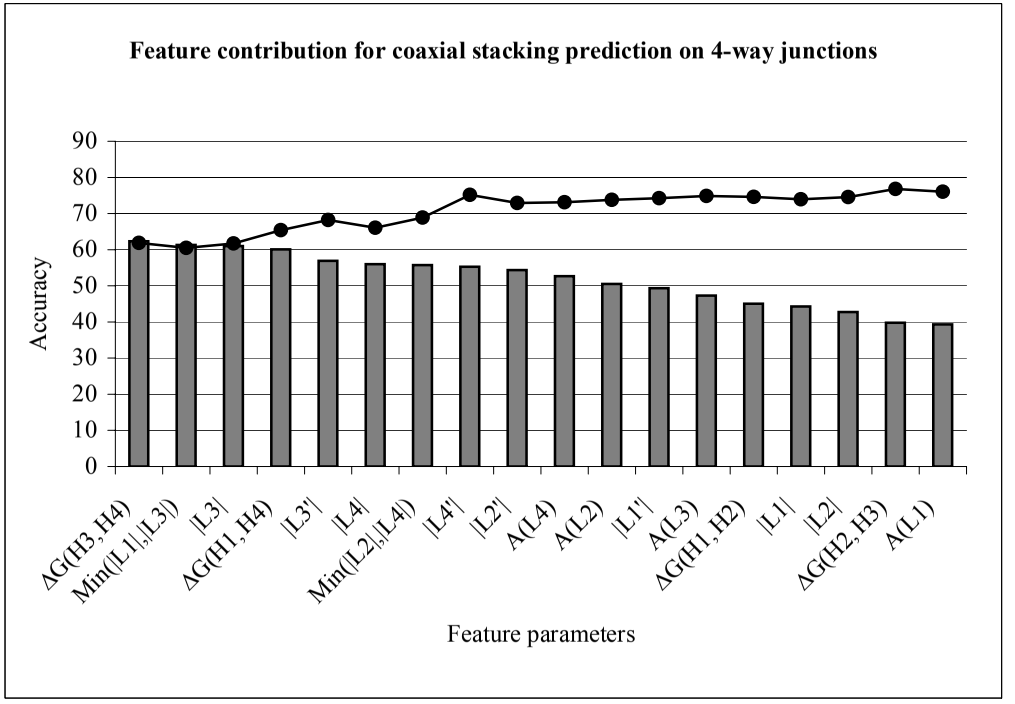
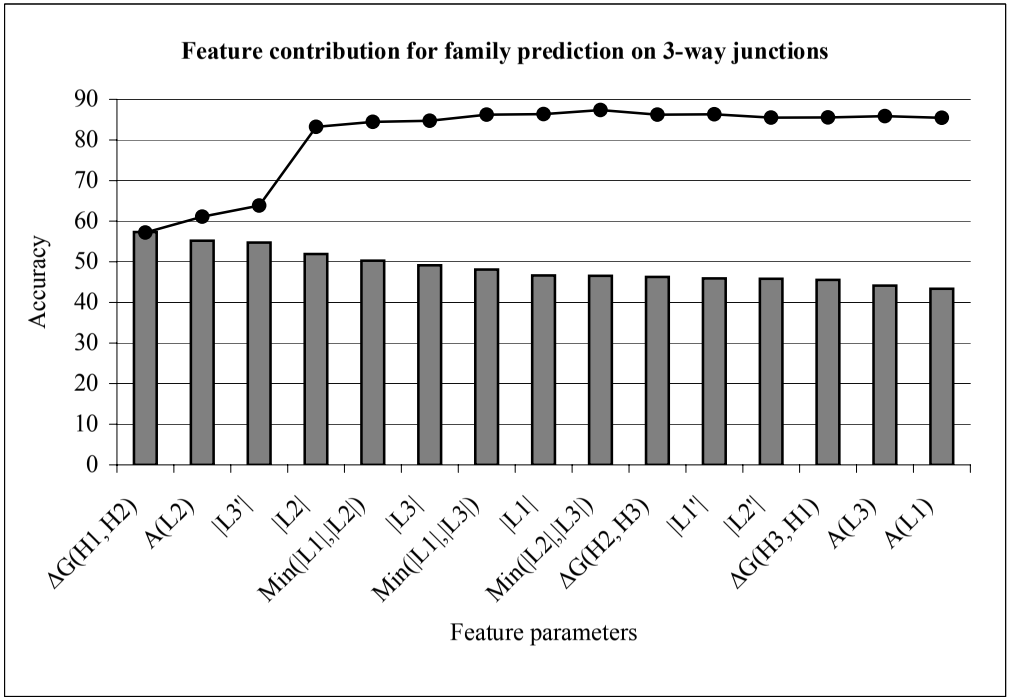


Figure S1. Prediction accuracy of 4-way junctions given by different parameter values for 10-fold cross-validation repeats (top), as well as the number of tree elements per random forest (bottom). The parameters are analyzed for both coaxial stacking prediction with (green) and without (black) knowledge of family information, and junction family prediction with (blue) and without (red) coaxial stacking knowledge as described in the Results section.







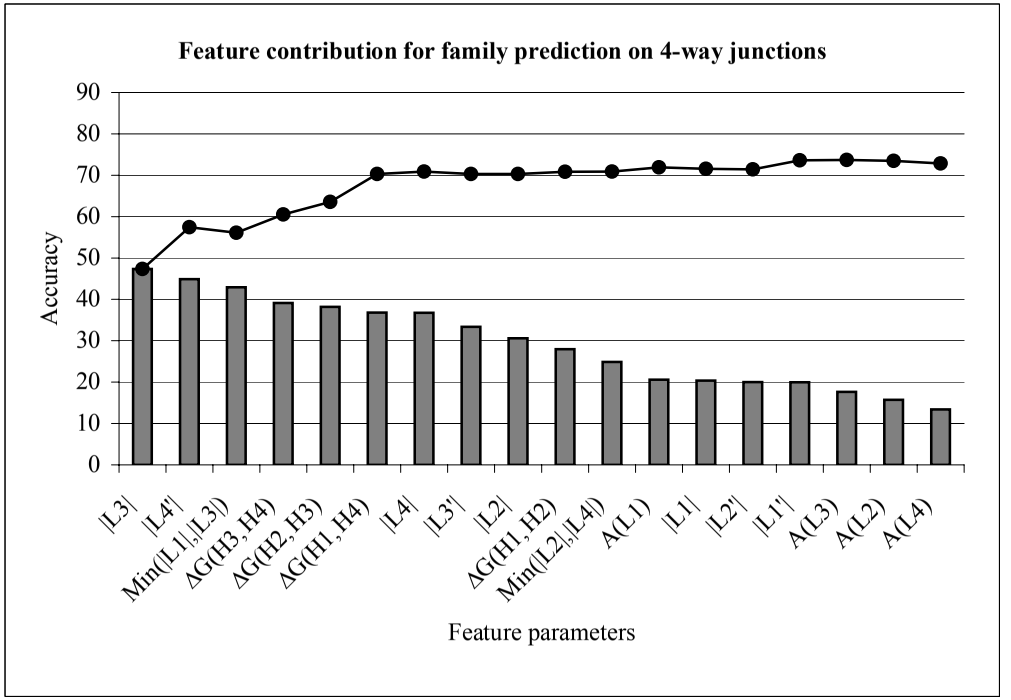


Figure S2. Analysis on the feature parameter contribution for coaxial stacking prediction (top) as well as junction family topology (bottom) for three (left) and four-way junctions (right). Prediction performance for each feature is given individually using bars. The cumulative graph is presented using a polygonal graph.

References

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2. Leffers, H., Kjems, J., Ostergaard, L., Larsen, N. and Garrett, R.A. (1987) Evolutionary relationships amongst archaebacteria. A comparative study of 23 S ribosomal RNAs of a sulphur-dependent extreme thermophile, an extreme halophile and a thermophilic methanogen. *J Mol Biol*, **195**, 43-61.