

Table S1a: List of 34 plant protein sequences retrieved from NCBI using CSPB as query and parameters as sequence length between 65 to 100 amino acids and E-value <0.0001.

S. No.	Protein ID	Description	Genbank ID	Full/Partial
1	AHG05844.1	cold shock protein 2 [Triticum aestivum]	KJ001173.1	Full
2	AHG05845.1	cold shock protein 3 [Triticum aestivum]	KJ001174.1	Full
3	AHG05843.1	cold shock protein 1 [Triticum aestivum]	KJ001172.1	Full
4	KZV15335.1	cold shock domain containing protein [D. hygrometricum]	KV020106.1	Full
5	EEF25061.1	cold shock domain containing protein, putative [R. communis]	EQ980606.1	Full
6	BAJ94072.1	predicted protein [Hordeum vulgare subsp. vulgare]	AK362868.1	Full
7	XP_017420695.1	PREDICTED: cold shock-like protein CspE [Vigna angularis]	XM_017565206.1	Full
8	KZV14807.1	cold shock domain containing protein [D. hygrometricum]	KV020185.1	Full
9	EEF28187.1	cold shock domain containing protein, putative [R. communis]	EQ974753.1	Full
10	OEL15232.1	hypothetical protein BAE44_0023756 [D. oligosanthos]	KV781798.1	Full
11	KHM99015.1	Glycine-rich protein 2 [Glycine soja]	KN672145.1	Full
12	KNA06212.1	hypothetical protein SOVF_183150 [S. oleracea]	KQ184517.1	Full
13	KDD72850.1	hypothetical protein H632_c2814p0 [Helicosporidium sp. ATCC 50920]	AYPS01002814.1	Full
14	CDM85608.1	unnamed protein product [Triticum aestivum]	HG670306.1	Full
15	KCW55497.1	hypothetical protein EUGRSUZ_I013952 [Eucalyptus grandis]	XM_018862436.1	Glycine domain at C-terminal
16	PPS05738.1	hypothetical protein GOBAR_AA14909 [G. barbadense]	KZ664394.1	Full
17	EAZ41398.1	hypothetical protein OsJ_25919 [O. sativa Japonica Group]	CM000145.1	Full
18	GAU35682.1	hypothetical protein TSUD_162540 [Trifolium subterraneum]	DF973600.1	Full
19	PON34810.1	Cold shock protein [Parasponia andersonii]	JXTB01000642.1	Full
20	XP_010064993.1	PREDICTED: uncharacterized protein LOC104452182 [Eucalyptus grandis]	XM_010066691.2	Full
21	KCW70572.1	hypothetical protein EUGRSUZ_F03759 [E. grandis]	Eucgr.F03759	Partial, Doesn't start with M
22	XP_001422318.1	predicted protein [Ostreococcus lucimarinus CCE9901]	XM_001422281.1	Partial, Doesn't start with M
23	OMO98270.1	Cold-shock protein, DNA-binding protein [C. capsularis]	AWWV01007119.1	Full
24	EEC78743.1	hypothetical protein OsI_18955 [O. sativa Indica Group]	CM000130.1	Full
25	PPD77473.1	hypothetical protein GOBAR_DD25585 [G. barbadense]	KZ648670.1	Full
26	OUS48075.1	cold-shock' DNA-binding domain-domain-containing protein [Ostreococcus tauri]	KZ155776.1	Full
27	XP_022840783.1	Cold-shock protein, DNA-binding [Ostreococcus tauri]	NC_014427.2	Full
28	2MQH_A	Chain A, Solution structure of the Chlamydomonas reinhardtii NAB1 cold shock domain, CSD1	AY157846.2	Partial, glycine & arginine rich domains at C-terminal
29	EAY74459.1	hypothetical protein OsI_02348 [O. sativa Indica Group]	CM000126.1	Full
30	XP_007142927.1	hypothetical protein PHAVU_007G028900g [Phaseolus vulgaris]	NC_023753.1	Full
31	EAZ12267.1	hypothetical protein OsJ_02155 [O. sativa Japonica Group]	CM000138.1	Full
32	EMT00236.1	Cold shock-like protein cspD (A.tauschii_cspD)	KD767246.1	Full
33	EMT17544.1	Cold shock-like protein cspC (A.tauschii_cspC)	KD534513.1	Full
34	EMT17543.1	Cold shock-like protein cspE (A.tauschii_cspE)	KD534513.1	Full

Table S1b: List of selected plant proteins with abbreviated forms used in present study

S. No.	Protein ID	Name of protein	Genbank ID	Abbreviated form
1	EMT17544.1	Cold shock-like protein cspC (<i>A. tauschii</i> _cspC)	KD534513.1	<i>A. tauschii</i> _cspC
2	EMT00236.1	Cold shock-like protein cspD (<i>A. tauschii</i> _cspD)	KD767246.1	<i>A. tauschii</i> _cspD
3	EMT17543.1	Cold shock-like protein cspE (<i>A. tauschii</i> _cspDE)	KD534513.1	<i>A. tauschii</i> _cspE
4	KZV14807.1	Cold shock domain containing protein [<i>D. hygrometricum</i>]	KV020185.1	<i>D. hygrometricum</i> _csd1
5	KZV15335.1	Cold shock domain containing protein [<i>D. hygrometricum</i>]	KV020106.1	<i>D. hygrometricum</i> _csd2
6	BAJ94072.1	Predicted protein [<i>Hordeum vulgare</i> subsp. <i>vulgare</i>]	AK362868.1	<i>H. vulgare</i> _csd
7	EEF25061.1	Cold shock domain containing protein, putative [<i>R. communis</i>]	EQ980606.1	<i>R. communis</i> _csd1
8	EEF28187.1	Cold shock domain containing protein, putative [<i>R. communis</i>]	EQ974753.1	<i>R. communis</i> _csd2
9	AHG05843.1	Cold shock protein 1 [<i>Triticum aestivum</i>]	KJ001172.1	<i>T. aestivum</i> _csp1
10	AHG05844.1	Cold shock protein 2 [<i>Triticum aestivum</i>]	KJ001173.1	<i>T. aestivum</i> _csp2
11	AHG05845.1	Cold shock protein 3 [<i>Triticum aestivum</i>]	KJ001174.1	<i>T. aestivum</i> _csp3
12	CDM85608.1	Unnamed protein product [<i>Triticum aestivum</i>]	HG670306.1	<i>T. aestivum</i> _UP

Table S2: Sequence identity matrix of CSPB with 12 plant CSPs selected on the basis of sequence identity ($\geq 40\%$)

S. No.	Name of protein	CSPB	<i>A.tauschii_cspC</i>	<i>A.tauschii_cspD</i>	<i>A.tauschii_cspE</i>	<i>D.hygrometricum_csd1</i>	<i>D.hygrometricum_csd2</i>	<i>H.vulgare_csd</i>	<i>R.communis_csd1</i>	<i>R.communis_csd2</i>	<i>T.aestivum_csp1</i>	<i>T.aestivum_csp2</i>	<i>T.aestivum_csp3</i>	<i>T.aestivum_UP</i>
1	CSPB	ID												
2	<i>A.tauschii_cspC</i>	0.50	ID											
3	<i>A.tauschii_cspD</i>	0.42	0.37	ID										
4	<i>A.tauschii_cspE</i>	0.57	0.67	0.36	ID									
5	<i>D.hygrometricum_csd1</i>	0.51	0.46	0.35	0.51	ID								
6	<i>D.hygrometricum_csd2</i>	0.54	0.46	0.33	0.51	0.74	ID							
7	<i>H.vulgare_csd</i>	0.45	0.80	0.34	0.64	0.44	0.46	ID						
8	<i>R.communis_csd1</i>	0.53	0.49	0.40	0.59	0.63	0.54	0.47	ID					
9	<i>R.communis_csd2</i>	0.53	0.46	0.40	0.55	0.59	0.57	0.42	0.73	ID				
10	<i>T.aestivum_csp1</i>	0.57	0.67	0.36	1.00	0.51	0.51	0.64	0.59	0.55	ID			
11	<i>T.aestivum_csp2</i>	0.59	0.63	0.35	0.86	0.51	0.53	0.59	0.55	0.54	0.86	ID		
12	<i>T.aestivum_csp3</i>	0.50	0.99	0.37	0.67	0.46	0.46	0.79	0.49	0.46	0.67	0.63	ID	
13	<i>T.aestivum_UP</i>	0.49	0.41	0.33	0.49	0.63	0.61	0.40	0.53	0.51	0.49	0.49	0.41	ID

Table S3: Prediction of sub-cellular localization of CSPs on the basis of sequence composition

S. No.	Name of protein	Parameters considered for prediction of sequence localization					Cytoplasmic	Mitochondrial	Chloroplast	Most likely location
		Amino acid composition	Di-peptide composition	Partitioned amino acid composition	Physioco-chemical composition	Neighboring sequence composition				
1	CSPB	Cytoplasmic	Chloroplast	Cytoplasmic	Cytoplasmic	Cytoplasmic	1.778*	0.581	1.061	Cytoplasmic
2	<i>A.tauschii_cspC</i>	Cytoplasmic	Cytoplasmic	Mitochondrial	Cytoplasmic	Cytoplasmic	2.592*	0.809	0.525	Cytoplasmic
3	<i>A.tauschii_cspD</i>	Mitochondrial	Mitochondrial	Cytoplasmic	Mitochondrial	Mitochondrial	1.222*	1.267*	0.903	Mitochondrial
4	<i>A.tauschii_cspE</i>	Cytoplasmic	Cytoplasmic	Cytoplasmic	Chloroplast	Cytoplasmic	2.029*	1.007	1.042	Cytoplasmic
5	<i>D.hygrometricum_csd1</i>	Cytoplasmic	Mitochondrial	Cytoplasmic	Nuclear	Cytoplasmic	2.338*	1.087	0.44	Cytoplasmic
6	<i>D.hygrometricum_csd2</i>	Cytoplasmic	Cytoplasmic	Cytoplasmic	Cytoplasmic	Cytoplasmic	2.509*	0.924	0.459	Cytoplasmic
7	<i>H.vulgare_csd</i>	Cytoplasmic	Cytoplasmic	Cytoplasmic	Mitochondrial	Cytoplasmic	2.153*	0.984	0.817	Cytoplasmic
8	<i>R.communis_csd1</i>	Cytoplasmic	Mitochondrial	Cytoplasmic	Chloroplast	Cytoplasmic	1.799*	0.893	0.865	Cytoplasmic
9	<i>R.communis_csd2</i>	Cytoplasmic	Mitochondrial	Cytoplasmic	Chloroplast	Cytoplasmic	1.688*	1.148*	0.693	Cytoplasmic
10	<i>T.aestivum_csp1</i>	Cytoplasmic	Cytoplasmic	Cytoplasmic	Chloroplast	Cytoplasmic	2.029*	1.007	1.042	Cytoplasmic
11	<i>T.aestivum_csp2</i>	Cytoplasmic	Mitochondrial	Cytoplasmic	Mitochondrial	Cytoplasmic	1.758*	1.141*	0.762	Cytoplasmic
12	<i>T.aestivum_csp3</i>	Cytoplasmic	Cytoplasmic	Mitochondrial	Chloroplast	Cytoplasmic	2.662*	0.858	0.561	Cytoplasmic
13	<i>T.aestivum_UP</i>	Cytoplasmic	Mitochondrial	Cytoplasmic	Mitochondrial	Mitochondrial	1.745*	1.674*	0.674	Cytoplasmic

* indicates probable location of a protein scored on basis of amino acid sequence composition, di-peptide composition, partitioned amino acid composition, physico-chemical properties of amino acid sequence and neighboring sequence composition. Most likely location of a sequence is determined from combined results obtained from all parameters.

Table S4 : Description of major templates used for homology modelling of CSPs

S. No.	Name of protein	Template (PDB ID)	% Sequence identity ID1/ID2	Template description (gene name, Species, function)	C-score	Tm score	RMSD value (Å)
1	CSPB	1csqA	100/100	CspB, <i>Bacillus subtilis</i> , Transcription regulation	1.22	0.88±0.07	1.0±1.0
2	<i>A.tauschii_cspC</i>	3i2zA	81/69	CspE, <i>Salmonella typhimurium</i> , Gene regulation	0.10	0.73±0.11	3.3±2.3
3	<i>A.tauschii_cspD</i>	1mjcA	49/37	CspA, <i>E. coli</i> , Transcriptional activation	-0.66	0.63±0.14	5.0±3.3
4	<i>A.tauschii_cspE</i>	3i2zA	80/80	CspE, <i>Salmonella typhimurium</i> , Gene regulation	1.25	0.89±0.07	1.0±1.0
5	<i>D.hygrometricum_csd1</i>	3i2zA	58/61	CspE, <i>Salmonella typhimurium</i> , Gene regulation	1.19	0.88±0.07	1.1±1.1
6	<i>D.hygrometricum_csd2</i>	3i2zA	54/56	CspE, <i>Salmonella typhimurium</i> , Gene regulation	1.19	0.88±0.07	1.1±1.1
7	<i>H.vulgare_csd</i>	3i2zA	76/65	CspE, <i>Salmonella typhimurium</i> , Gene regulation	-0.43	0.66±0.13	4.5±3.0
8	<i>R.communis_csd1</i>	1mjcA	61/61	CspA, <i>E. coli</i> , Transcriptional activation	1.08	0.86±0.07	1.3±1.3
9	<i>R.communis_csd2</i>	1mjcA	57/57	CspA, <i>E. coli</i> , Transcriptional activation	1.07	0.86±0.07	1.3±1.3
10	<i>T.aestivum_csp1</i>	3i2zA	80/80	CspE, <i>Salmonella typhimurium</i> , Gene regulation	1.25	0.89±0.07	1.0±1.0
11	<i>T.aestivum_csp2</i>	3i2zA	75/75	CspE, <i>Salmonella typhimurium</i> , Gene regulation	1.27	0.89±0.07	1.0±1.0
12	<i>T.aestivum_csp3</i>	3i2zA	81/69	CspE, <i>Salmonella typhimurium</i> , Gene regulation	-0.08	0.70±0.12	3.7±2.5
13	<i>T.aestivum_UP</i>	3i2zA	49/49	CspE, <i>Salmonella typhimurium</i> , Gene regulation	1.08	0.86±0.07	1.3±1.3

ID1: Percentage sequence identity of the templates in the threading aligned region with the query sequence.

ID2: Percentage sequence identity of the whole template chains with query sequence.

Table S5: Number of residues in favoured, allowed and outlier region before and after MD simulations.

S. No.	Name of protein	Before simulation			After simulation		
		No. of residues in favoured region	No. of residues in allowed region	No. of residues in outlier region	No. of residues in favoured region	No. of residues in allowed region	No. of residues in outlier region
1	<i>A.tauschii_cspC</i>	68 (87.2%)	8 (10.3%)	2 (2.6%)	72 (93.5%)	5 (6.5%)	0
2	<i>A.tauschii_cspD</i>	66 (75.9%)	18 (20.7%)	3 (3.4%)	80 (92.0%)	7 (8.0%)	0
3	<i>A.tauschii_cspE</i>	56 (83.6%)	8 (11.9%)	3 (4.5%)	65 (97.0%)	2 (3.0%)	0
4	<i>D.hygrometricum_csd1</i>	58 (86.6%)	7 (10.4%)	2 (3.0%)	67 (100.0%)	0	0
5	<i>D.hygrometricum_csd2</i>	58 (86.6%)	8 (11.9%)	1 (1.5%)	63 (94.0%)	4 (6.0%)	0
6	<i>H.vulgare_csd</i>	62 (74.7%)	13 (15.7%)	8 (9.6%)	71 (85.5%)	11 (13.3%)	1 (1.2%)
7	<i>R.communis_csd1</i>	55 (84.6%)	6 (9.2%)	4 (6.2%)	58 (89.2%)	7 (10.8%)	0
8	<i>R.communis_csd2</i>	60 (92.3%)	3 (4.6%)	2 (3.1%)	62 (95.4%)	3 (4.6%)	0
9	<i>T.aestivum_csp1</i>	56 (83.6%)	8 (11.9%)	3 (4.5%)	62 (92.5%)	5 (7.5%)	0
10	<i>T.aestivum_csp2</i>	61 (91.0%)	4 (6.0%)	2 (3.0%)	61 (91.0%)	6 (9.0%)	0
11	<i>T.aestivum_csp3</i>	69 (88.5%)	5 (6.4%)	4 (5.1%)	69 (89.6%)	8 (10.4%)	0
12	<i>T.aestivum_UP</i>	61 (89.7%)	4 (5.9%)	3 (4.4%)	67 (98.5%)	1 (1.5%)	0

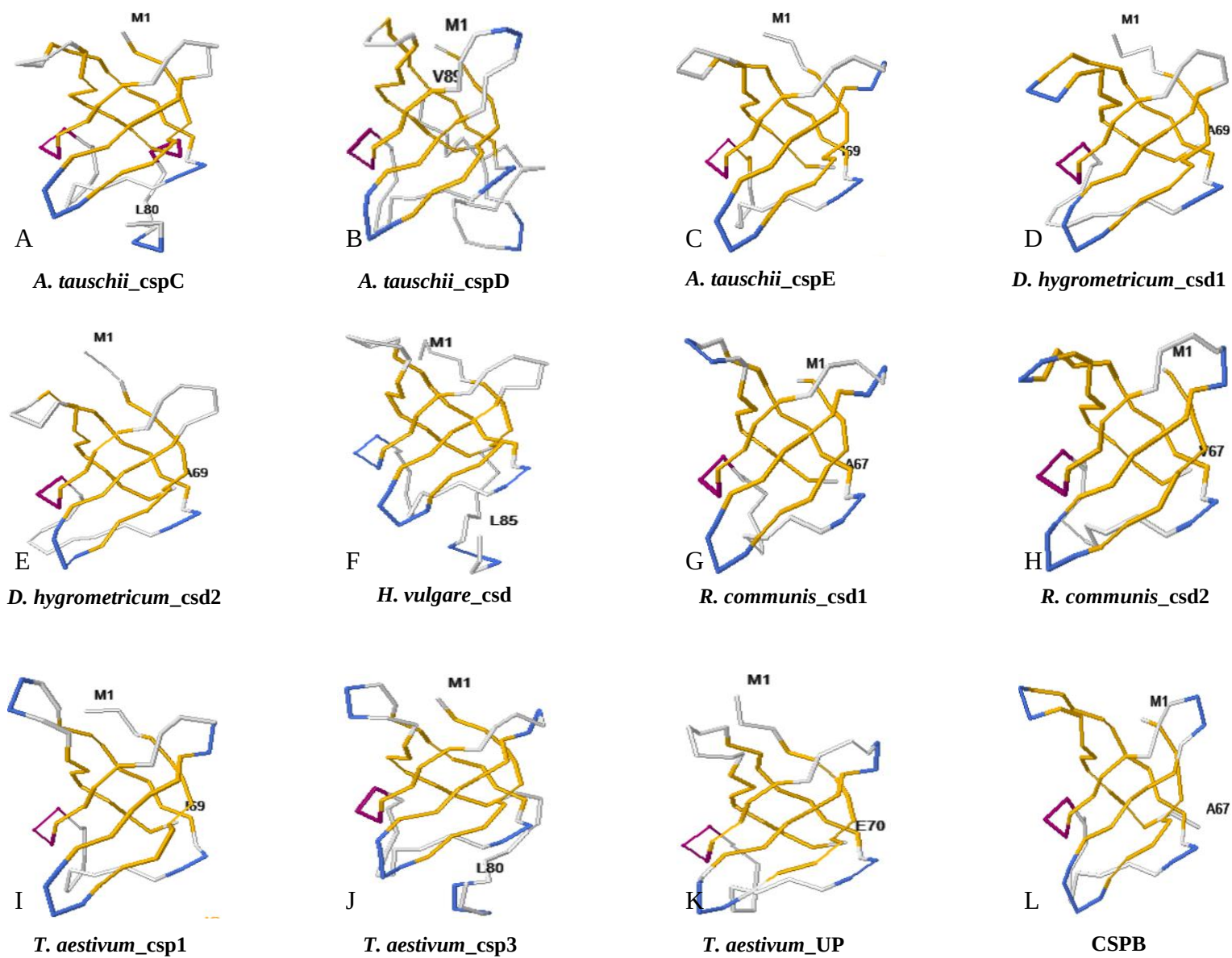


Figure S1: 3D structure models of CSPB and plant CSPs predicted by I-TASSER server. Labels on the models represent first and last amino acid residue denoted by single letter code and identity (M1 indicates methionine at first position). Backbones of 3D models are shown in color scheme. Beta-strands are shown in yellow color.

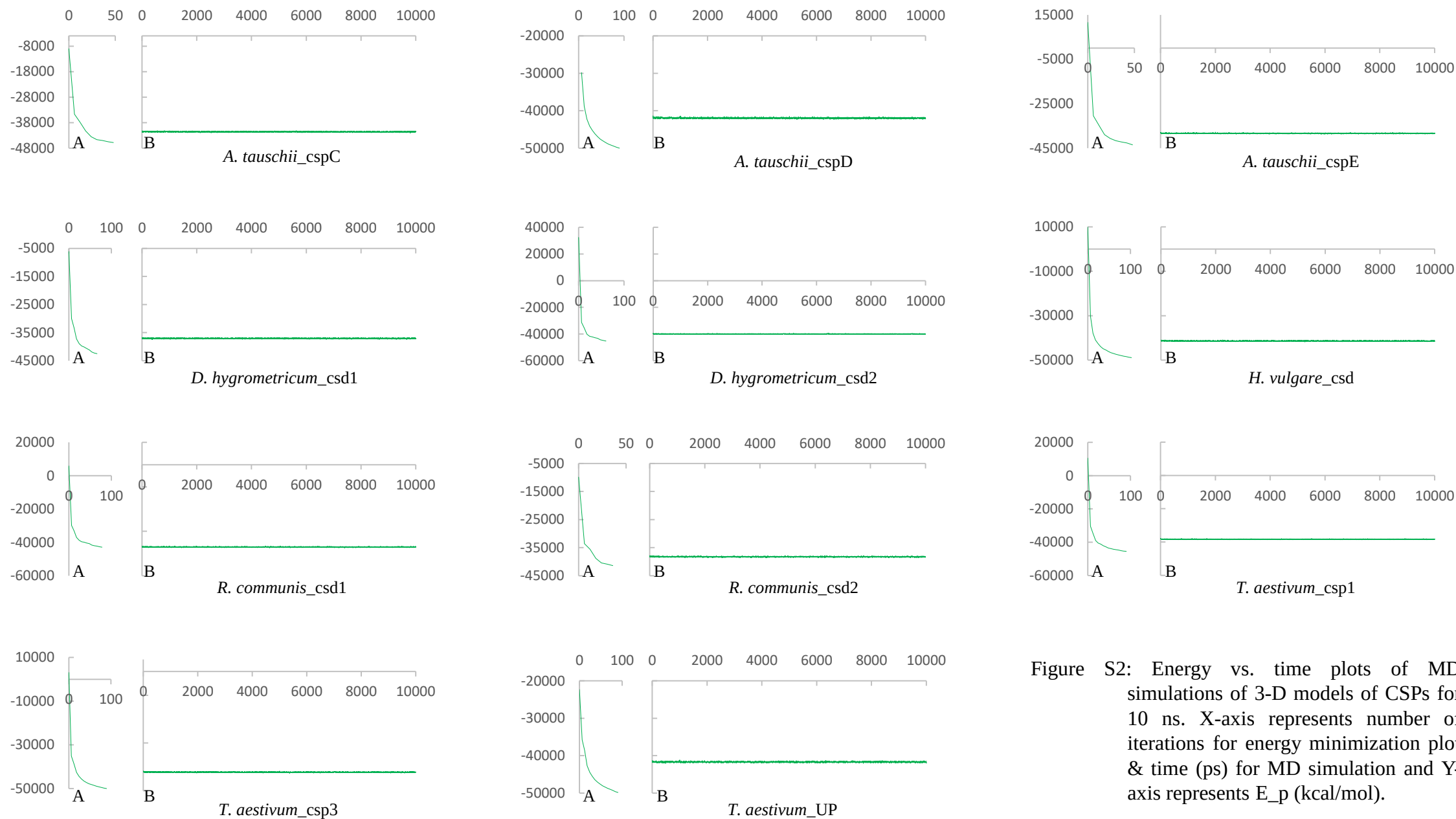


Figure S2: Energy vs. time plots of MD simulations of 3-D models of CSPs for 10 ns. X-axis represents number of iterations for energy minimization plot & time (ps) for MD simulation and Y-axis represents E_p (kcal/mol).

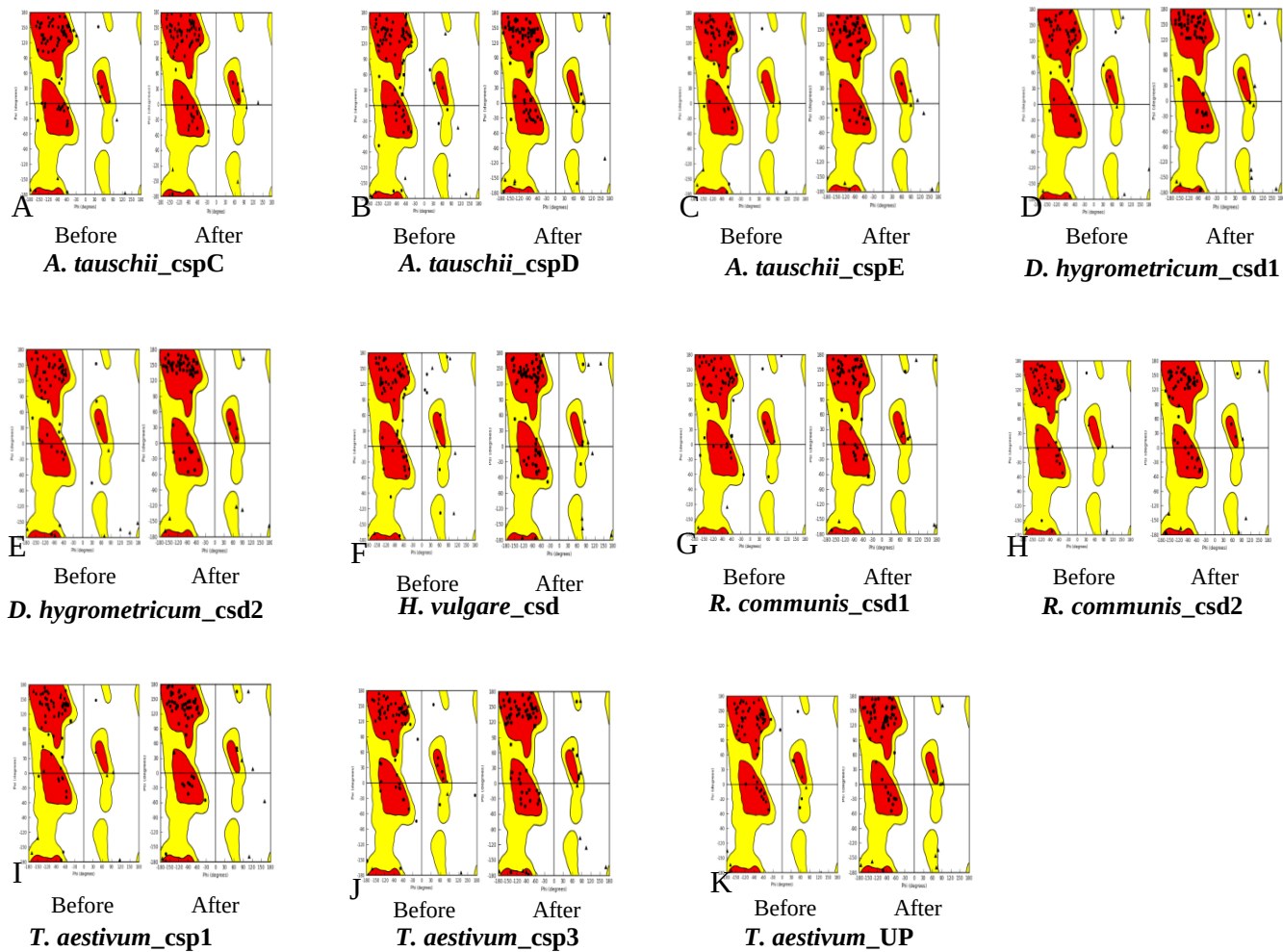
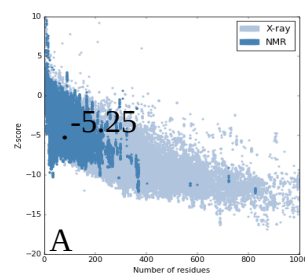
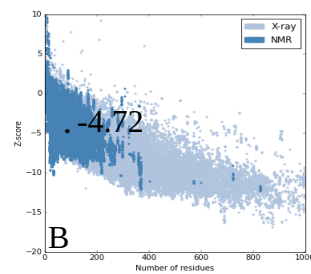


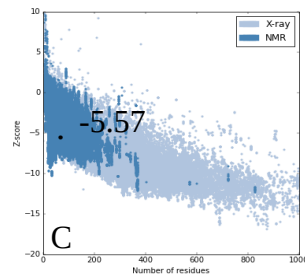
Figure S3: Ramachandran plots of 3D structure models of CSPs before and after MD simulations for 10 ns



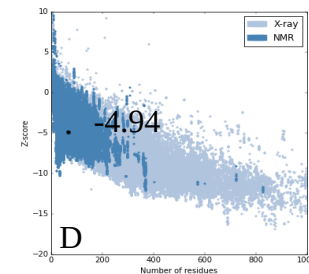
A. tauschii_cspC



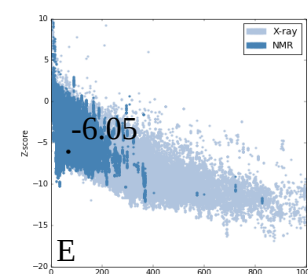
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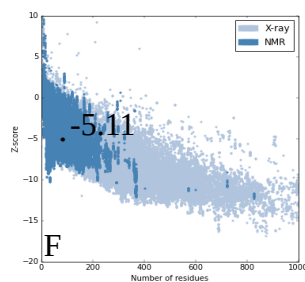
A. tauschii_cspE



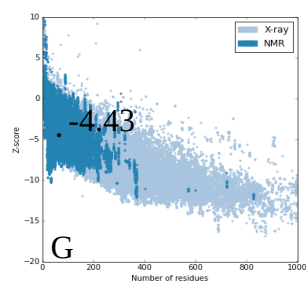
D. hygrometricum_csd1



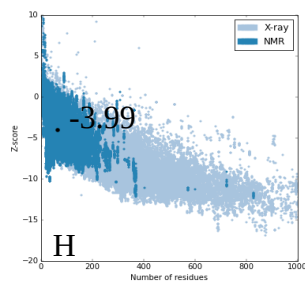
D. hygrometricum_csd2



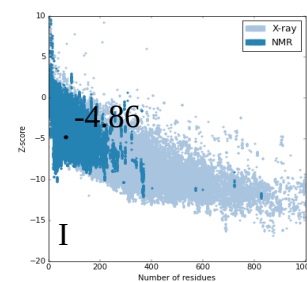
H. vulgare_csd



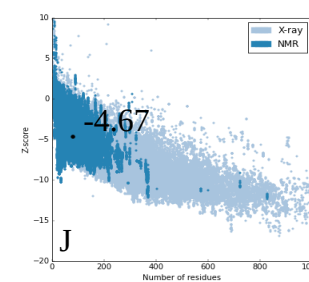
R. communis_csd1



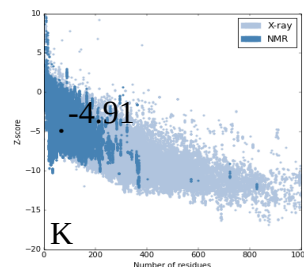
R. communis_csd2



T. aestivum_csp1



T. aestivum_csp3



T. aestivum_UP

Figure S4: Z-plots of refined 3D models using ProSA web server to assess overall model quality. Black dot on the plot corresponds to z-score of 3D model. Light blue area on the plot shows z-scores for protein structures solved by X-ray crystallography and dark blue area on plot shows z-scores for protein structures solved by NMR. Value on each plot shows z-score value of refined 3D model.

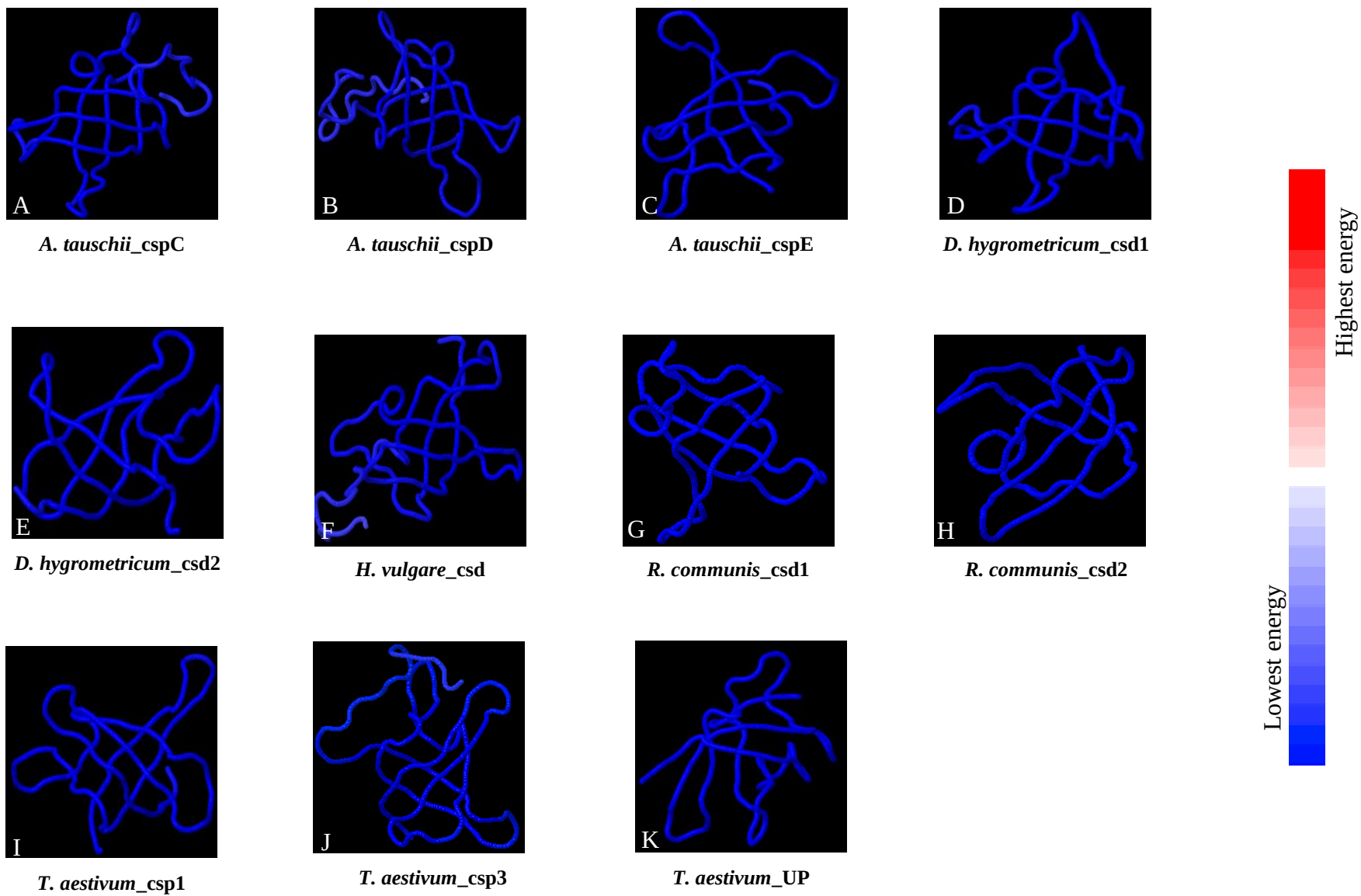


Figure S5: Energy levels of refined 3D models shown in color scheme. Change in color from blue to red shows increase in energy.

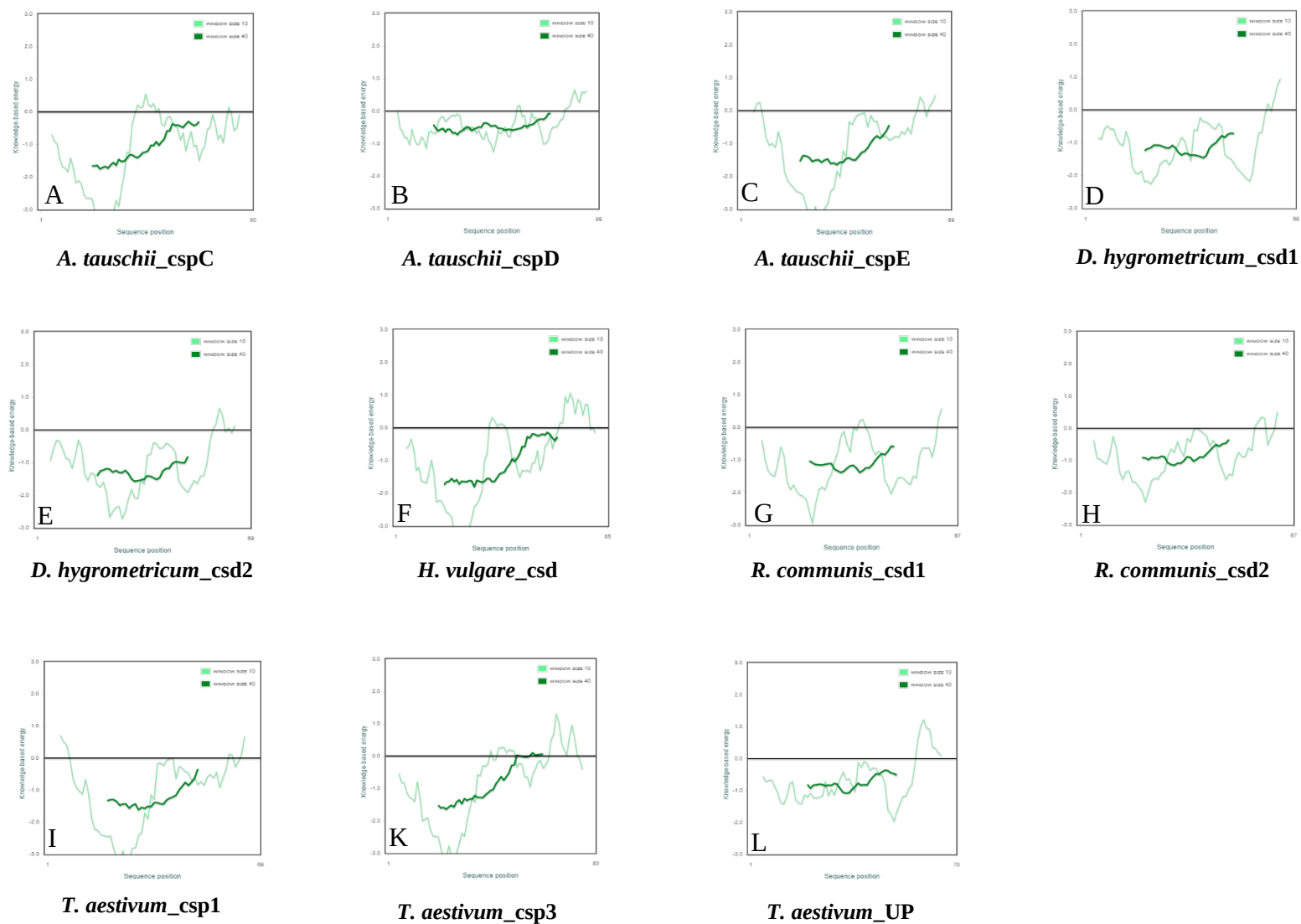


Figure S6: Energy vs. sequence length plots of 3D models. Light green line on the plots shows energy of residues over a range of 10 amino acids and dark green line shows energy of residues over a range of 40 amino acids.

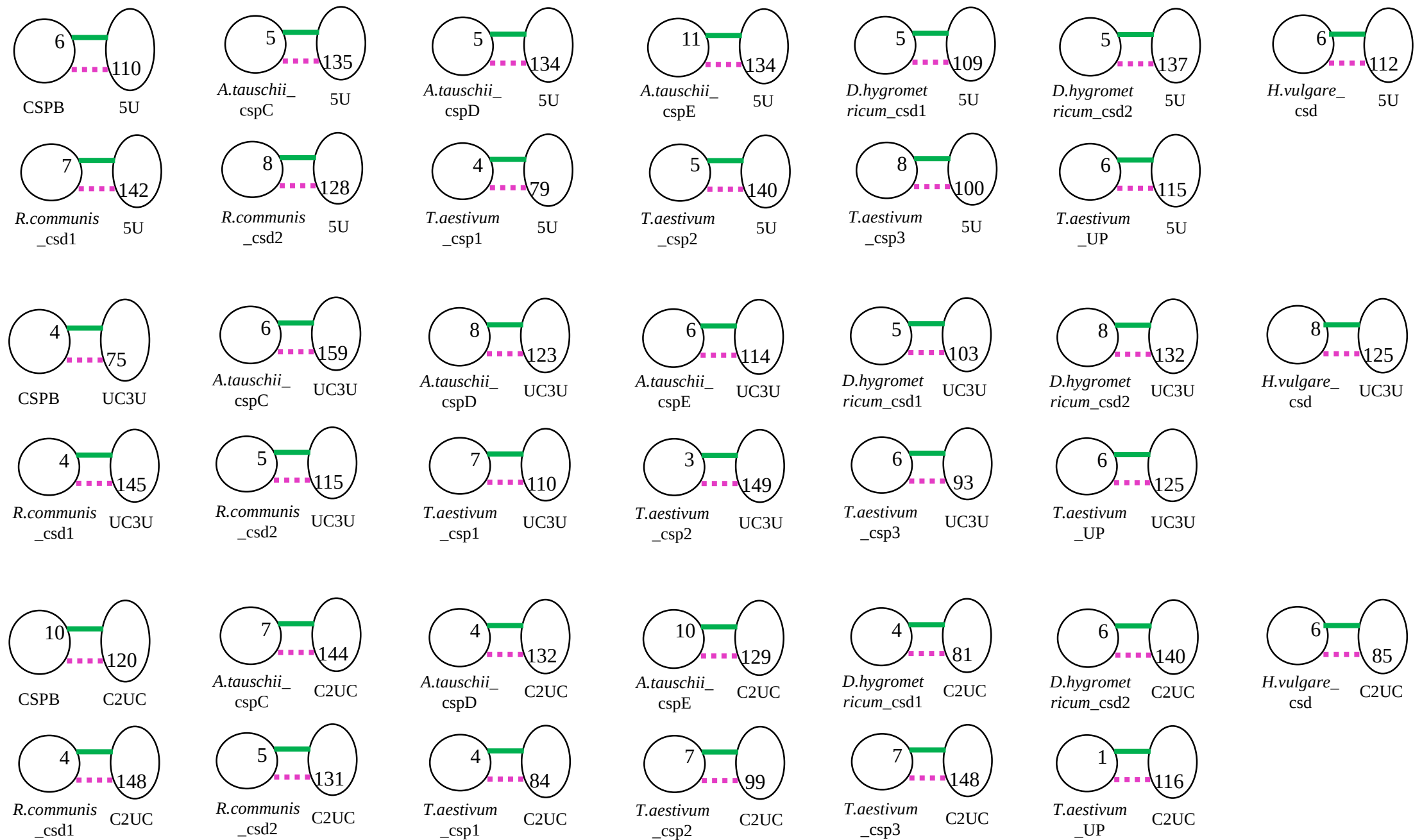


Figure S7: Intermolecular interactions in protein-RNA complexes. Green solid lines indicate hydrogen bond. Purple dotted lines indicate non-bonded interactions. Circular shapes indicate protein molecules and oval shapes indicate RNA molecules.

Table S6: Intermolecular interactions of plant CSPs structure models docked with 5U-RNA

Sr. No.	Name of complex	Residues forming H-bonds	Distance (Å)	Residues making non-bonded contacts
1.	CSPB	OE1 (Gln 59) ← N3 (U1)	2.79	Lys 7, Trp 8, Asn 10, Glu 12, Lys 13, Phe 15, Asp 25, Phe 27, His 29, Ser 31, Arg 56, Gly 57, Pro 58, Gln 59 (Total 110)
		NE (Arg 56) → O2' (U1)	2.87	
		OD2 (Asp 25) ← N3 (U3)	2.81	
		ND2 (Asn 10) → O2 (U4)	2.95	
		NZ (Lys 13) → O2' (U4)	2.96	
		ND2 (Asn 10) → O2' (U5)	3.17	
2.	<i>A.tauschii_cspC</i>	N (Gln 57) → O2' (U1)	2.98	Lys 8, Trp 9, Asn 11, Lys 14, Phe 16, Phe 18, Asp 27, Phe 29, Val 30, His 31, Gly 56, Gln 57, Lys 58, Pro 60, Ser 61, Ala 62, Val 63 (Total 135)
		OG (Ser 61) ← O2' (U1)	2.78	
		O (Ala 62) ← N3 (U1)	3.04	
		OD2 (Asp 27) ← N3 (U3)	2.82	
		OD1 (Asn 11) ← N3 (U4)	3.00	
3.	<i>A.tauschii_cspD</i>	NE2 (His 60) → O4 (U2)	3.15	Lys 7, Gly 8, Asn 10, Lys 13, Phe 17, Glu 25, Asp 26, Phe 28, His 30, Tyr 31, Gly 55, Pro 56, Lys 57, Gly 58, Leu 59, His 60 (Total 135)
		NZ (Lys 57) → O2' (U3)	3.08	
		O (Leu 59) ← N3 (U3)	3.04	
		N (Asn 10) → O2 (U4)	3.17	
		ND2 (Asn 10) → O2' (U4)	3.00	
4.	<i>A.tauschii_cspE</i>	OG (Ser 62) → O2 (U1)	2.83	Lys 9, Trp 10, Asn 12, Lys 15, Phe 17, Phe 19, Asp 28, Phe 30, His 32, Ser 34, Gly 57, Ala 58, Lys 59, Gly 60, Pro 61, Ser 62 (Total 134)
		N (Ala 58) → O4 (U2)	3.01	
		NZ (Lys 59) → O2' (U2)	3.11	
		N (Gly 60) → O4 (U2)	3.17	
		O (Pro 61) ← N3 (U2)	3.13	
		NZ (Lys 9) → O2 (U3)	2.95	
		NE1 (Trp 10) → O2 (U3)	3.11	
		OD2 (Asp 28) ← N3 (U3)	2.83	
		OD1 (Asn 12) ← N3 (U4)	2.84	
		OD1 (Asn 12) ← O2' (U5)	2.89	
		ND2 (Asn 12) → O2' (U5)	3.06	
5.	<i>D.hygrometricum_csd1</i>	OD2 (Asp 28) ← N3 (U2)	3.08	Trp 11, Asn 13, Ala 15, Lys 16, Phe 18, Asp 28, Phe 30, His 32, Pro 58, Lys 59, Leu 61, Gln 62 (Total 109)
		ND2 (Asn 13) → O4 (U4)	3.31	
		O (Ala 15) ← N3 (U4)	3.28	
		NZ (Lys 16) → O5' (U4)	3.14	
		NZ (Lys 16) → O4' (U4)	2.86	
6.	<i>D.hygrometricum_csd2</i>	N (Lys 59) → O2 (U1)	3.07	Trp 11, Asn 13, Lys 16, Phe 18, Phe 20, Asp 28, Phe 30, Gln 58, Lys 59, Gly 60, Leu 61, Gln 62 (Total 137)
		N (Leu 61) → O4 (U2)	3.23	
		NE1 (Trp 11) → O2 (U3)	3.11	
		OD2 (Asp 28) ← N3 (U3)	2.73	
		NZ (Lys 16) → O2' (U4)	3.08	
7.	<i>H. vulgare_csd</i>	NZ (Lys 11) → O4 (U1)	2.94	Lys 11, Trp 12, Lys 17, Phe 19, Phe 21, Lys 29, Asp 30, Phe 32, His 34, Gln 57, Gly 59, Lys 61, Gly 62, Pro 63, Ser 64, Ala 65 (Total 112)
		NZ (Lys 29) → O5' (U1)	3.01	
		NE2 (His 34) → O2 (U3)	2.98	
		OG (Ser 64) ← O2' (U4)	2.96	
		N (Ala 65) → O2 (U4)	3.04	
		NE2 (Gln 57) → O2' (U5)	2.91	
				Contd...

Table S6: Intermolecular interactions of plant CSPs structure models docked with 5U-RNA

Sr. No.	Name of complex	Residues forming H-bonds	Distance (Å)	Residues making non-bonded contacts
8..	<i>R.communis_csd1</i>	NE2 (His 30) → O5' (U1)	2.97	Lys 7, Trp 8, Phe 9, Asn 10, Ser 12, Lys 13, Phe 15, Asp 26, Phe 28, His 30, Ser 32, Gly 55, Pro 56, Lys 57, Gly 58. Lys 59, Gln 60 (Total 142)
		NE2 (His 30) ← O5' (U1)	2.97	
		NE1 (Trp 8) → O2 (U3)	3.27	
		OD1 (Asp26) ← N3 (U3)	3.14	
		ND2 (Asn 10) → O2 (U4)	3.01	
		ND2 (Asn 10) → O2' (U4)	2.74	
		NZ (Lys 13) → O3' (U4)	3.33	
9.	<i>R.communis_csd2</i>	O (Lys 13) ← N3 (U3)	2.87	Trp 8, Lys 13, Phe 15, Phe 17, Asp 26, Phe 28, His 30, Ser 32, Glu 33, Lys 53, Met 54, Gly 55, Pro 56, Lys 57, Gly 58, Gln 60 (Total 128)
		OG (Ser 32) ← N3 (U4)	2.80	
		NZ (Lys 53) → O2 (U4)	2.93	
		NZ (Lys 53) → O2' (U4)	2.87	
		O (Met 54) ← O2' (U4)	2.93	
		OE1 (Gln 60) ← O2' (U4)	3.10	
		NE2 (Gln 60) → O2 (U4)	2.94	
10.	<i>T. aestivum_csp1</i>	NZ (Lys 53) → O4' (U5)	2.95	Lys 9, Trp 10, Asn 12, Ser 14, Lys 15, Phe 17, Phe 19, Asp 28, Phe 30, His 32, Pro 61, Ser 62 (Total 79)
		OD2 (Asp 28) ← N3 (U3)	3.21	
		NZ (Lys 15) → O2' (U4)	3.10	
		NZ (Lys 15) → O3' (U4)	3.07	
11.	<i>T. aestivum_csp2</i>	OG (Ser 14) ← O3' (U5)	2.99	Trp 10, , Phe 11, Asn 12, Glu 13, Ser 14, Lys 15, Gly 16, Phe 17, Phe 19, Asp 28, Phe 30, His 32, , Phe 33, , Phe 41, Lys 42, Gly 57, Thr 58, Lys 59, Gly 60, Pro 61, Thr 62 (Total 140)
		O (Lys 15) ← O3' (U1)	2.82	
		O (Lys 15) ← O5' (U2)	3.18	
		NE2 (His 32) → O4' (U2)	2.73	
		N (Gly 60) → O2 (U3)	2.89	
12.	<i>T. aestivum_csp3</i>	O (Gly 60) ← N3 (U3)	2.73	Lys 8, Trp 9, Asn 11, Lys 14, Phe 16, Phe 18, Asp 27, Phe 29, His 31, Lys 58, Pro 60, Ser 61 (Total 100)
		NZ (Lys 58) → O2 (U1)	3.11	
		NZ (Lys 58) → O4 (U2)	3.05	
		OG (Ser 61) → O4 (U2)	2.69	
		NZ (Lys 8) → O2 (U3)	2.95	
		NE1 (Trp 9) → O2 (U3)	3.27	
		N (Asp 27) ← O4 (U3)	3.08	
		OD2 (Asp 27) → N3 (U3)	2.79	
13.	<i>T. aestivum_UP</i>	NZ (Lys 14) → O2' (U4)	2.93	Lys 10, Ser 11, Asn 13, Lys 16, Phe 18, Leu 20, Asp 29, Phe 31, His 33, , Phe 34, Arg 35, Lys 60, Gly 61, Met 62, Gln 63 (Total 115)
		NE2 (His 33) → O4' (U1)	3.23	
		NH2 (Arg 35) → O4 (U2)	3.26	
		OE1 (Gln 63) ← N3 (U2)	3.06	
		O (Met 62) ← N3 (U3)	2.96	
		NZ (Lys 16) → O2' (U4)	3.07	
		NZ (Lys 16) → O3' (U4)	2.92	

Table S7: Intermolecular interactions of plant CSPs structure models docked with UC3U-RNA

Sr. No.	Name of complex	Residues forming H-bonds	Distance (Å)	Residues making non-bonded contacts
1.	CSPB	O (Arg 56) ← N4 (C2)	2.92	Lys 7, Trp 8, Asn 10, Lys 13, Phe 15, Phe 17, Asp 24, Asp 25, Phe 27, Arg 56, Gly 57, Pro 58, Gln 59 (Total 75)
		NZ (Lys 13) → O2' (U3)	3.00	
		NZ (Lys 13) → O3' (U3)	3.01	
		NZ (Lys 7) → O2' (U4)	3.33	
2.	<i>A.tauschii_cspC</i>	OE1 (Gln 57) ← O2' (U1)	2.72	Trp 9, Asn 11, Ser 13, Lys 14, Gly 15, Phe 16, Phe 18, Asp 27, Phe 29, His 31, Gln 57, Lys 58, Gly 59, Pro 60, Ser 61, (Total 159)
		N (Lys 58) → O4' (U1)	2.87	
		NZ (Lys 14) → O2 (C2)	2.84	
		NZ (Lys 14) → O2' (C2)	2.97	
		NE2 (His 31) ← O2' (U4)	3.23	
		NE2 (His 31) ← O2' (U4)	3.23	
3.	<i>A.tauschii_cspD</i>	NZ (Lys 57) → O2' (C2)	3.07	Lys 7, Gly 8, Asn 10, Lys 13, Tyr 15, Phe 17, Glu 25, Asp 26, Phe 28, His 30, Gly 55, Pro 56, Lys 57, Gly 58, Leu 59, His 60 (Total 123)
		N (Gly 58) ← N3 (C2)	3.32	
		NZ (Lys 7) → O2 (U3)	3.07	
		N (Asp 26) → O4 (U3)	3.17	
		O (Gly 8) ← N3 (U4)	2.82	
		NZ (Lys 13) → O2' (U4)	3.00	
		NZ (Lys 13) → O3' (U4)	2.83	
		OH (Tyr 15) ← O2' (U4)	2.69	
4.	<i>A.tauschii_cspE</i>	O (Gly 60) ← N4 (C2)	2.84	Lys 9, Trp 10, Asn 12, Lys 15, Phe 17, Phe 19, Asp 28, Phe 30, His 32, Ala 58, Lys 59, Gly 60, Pro 61, Ser 62 (Total 114)
		O (Pro 61) ← N4 (C2)	3.13	
		OG (Ser 62) ← N4 (C2)	2.82	
		NZ (Lys 9) → O2 (U3)	3.00	
		OD2 (Asp 28) ← N3 (U3)	2.71	
		ND2 (Asn 12) → O3' (U5)	2.96	
5.	<i>D.hygrometricum_csd1</i>	O (Ala 15) ← O2' (U1)	3.24	Lys 10, Trp 11, Asn 13, Ala 15, Lys 16, Phe 18, Gly 19, Phe 20, Asp 28, Phe 30, Phe 41, Pro 58, Lys 59, Gln 62 (Total 103)
		NZ (Lys 16) → O2' (C2)	2.94	
		NE2 (Gln 62) → O2 (U3)	3.06	
		NZ (Lys 10) → O2' (U5)	3.21	
		OD2 (Asp 28) ← N3 (U5)	2.69	
6.	<i>D.hygrometricum_csd2</i>	NE2 (Gln 58) → O5' (U1)	3.00	Lys 10, Trp 11, Asn 13, Lys 16, Phe 18, Phe 20, Asp 28, Phe 30, His 32, Arg 34, Gln 58, Lys 59, Gly 60, Leu 61, Gln 62 (Total 132)
		OE1 (Gln 62) ← N3 (U1)	3.16	
		O (Lys 59) ← N4 (C2)	2.79	
		NZ (Lys 10) → O2 (U3)	3.15	
		NE1 (Trp 11) → O4' (U3)	3.28	
		OD2 (Asp 28) ← N3 (U3)	2.75	
		NZ (Lys 16) → O2' (U4)	3.20	
		NZ (Lys 16) → O3' (U4)	3.23	

Contd...

Table S7: Intermolecular interactions of plant CSPs structure models docked with UC3U-RNA				
Sr. No.	Name of complex	Residues forming H-bonds	Distance (Å)	Residues making non-bonded contacts
7.	<i>H. vulgare_csd</i>	NZ (Lys 11) → O4 (U1)	2.87	Lys 11, Trp 12, Phe 19, Phe 21, Lys 29, Asp 30, Phe 32, Val 33, His 34, Ala 37, Gln 57, Gly 59, Gln 60, Lys 61, Gly 62, Pro 63, Ser 64, Ala 65 (Total 125)
		O (Asp 30) ← O2' (U1)	2.98	
		NZ (Lys 61) → O5' (U3)	3.06	
		O (Phe 32) ← N3 (U4)	2.88	
		N (His 34) → O4 (U4)	3.05	
		O (Gly 62) → O3' (U4)	3.18	
		O (Pro 63) ← O2' (U4)	3.18	
		NE2 (Gln 57) → O2' (U5)	2.97	
8.	<i>R.communis_csd1</i>	NE2 (His 30) → O1P (C2)	3.07	Trp 8, Asp 11, Ser 12, Lys 13, Gly 14, Phe 15, Phe 17, Asp 26, Phe 28, His 30, Phe 31, Ser 32, Gly 55, Lys 57, Gly 58. Lys 59, Gln 60 (Total 145)
		NE2 (Gln 60) → N3 (C2)	3.17	
		N (Gly 55) → O4 (U3)	3.11	
		O (Lys 59) ← N3 (U3)	3.16	
9.	<i>R.communis_csd2</i>	NZ (Lys 7) → O5' (U1)	3.13	Lys 7, Trp 8, Lys 13, Phe 15, Phe 17, Glu 25, Asp 26, Phe 28, His 30, Gly 55, Pro 56, Lys 57, Gly 58, Lys 59, Gln 60 (Total 115)
		O (Asp 26) ← N3 (U1)	2.97	
		N (Lys 59) → O4 (U1)	3.04	
		O (Gly 58) ← N4 (C2)	3.17	
		NZ (Lys 57) → O4' (U3)	3.13	
10.	<i>T. aestivum_csp1</i>	O (Pro 61) ← N4 (C2)	3.20	Lys 9, Trp 10, Phe 11, Asn 12, Glu 13, Ser 14, Lys 15, Phe 17, Phe 19, Lys 27, Asp 28, Phe 30, His 32, Gly 60, Pro 61, Ser 62 (Total 110)
		OD2 (Asp 28) ← N3 (U3)	2.82	
		ND2 (Asn 12) → O2' (U4)	2.92	
		O (Phe 11) ← O2' (U5)	3.34	
		OD1 (Asn 12) ← O3' (U5)	3.31	
		OG (Ser 14) → O3' (U5)	2.85	
		OG (Ser 14) ← O3' (U5)	2.85	
11.	<i>T. aestivum_csp2</i>	O (Glu 13) ← O2' (U1)	3.22	Trp 10, Glu 13, Ser 14, Lys 15, Gly 16, Phe 17, Phe 19, Asp 28, Phe 30, His 32, , Phe 33, Ser 34, Phe 41, Lys 42, Gly 57, Thr 58, Lys 59, Gly 60, Thr 62 (Total 149)
		NE2 (His 32) → O4' (C2)	3.04	
		O (Asp 28) ← N3 (U4)	3.20	
12.	<i>T. aestivum_csp3</i>	NZ (Lys 58) → O4 (U1)	2.83	Lys 8, Trp 9, Asn 11, Lys 14, Phe 18, Asp 27, Phe 29, His 31, Lys 58, Gly 59, Pro 60, Ser 61 (Total 93)
		NZ (Lys 8) → O2 (U3)	3.08	
		NE1 (Trp 9) → O4' (U3)	3.12	
		NE1 (Trp 9) → O2 (U3)	3.19	
		OD2 (Asp 27) ← N3 (U3)	2.74	
		NZ (Lys 14) → O2' (U4)	2.91	
13.	<i>T. aestivum_UP</i>	N (Lys 60) → O2 (U1)	3.14	Lys 10, Ser 11, Asn 13, Lys 16, Phe 18, Gly 19, Leu 20, Asp 29, Phe 31, His 33, Gly 58, Gln 59, Lys 60, Gly 61, Met 62, Gln 63 (Total 125)
		OE1 (Gln 63) ← O2' (U1)	3.32	
		NE2 (His 33) → O2P (C2)	3.07	
		O (Ser 11) ← O2' (U4)	2.89	
		OD1 (Asp 29) ← N3 (U4)	2.83	
		NZ (Lys 10) → O2' (U5)	3.21	

Table S8: Intermolecular interactions of plant CSPs structure models docked with C2UC-RNA

Sr. No.	Name of complex	Residues forming H-bonds	Distance (Å)	Residues making non-bonded contacts
1.	CSPB	NE2 (His 29) → O5' (C2)	2.88	Lys 7, Trp 8, Asn 10, Lys 13, Phe 15, Phe 17, Asp 25, Phe 27, His 29, Arg 56, Gly 57, Pro 58, Gln 59 (Total 120)
		NE2 (His 29) ← O5' (C2)	2.88	
		NE (Arg 56) → O2' (C2)	2.90	
		NH2 (Arg 56) → O2' (C2)	3.11	
		NE2 (Gln 59) → O4 (U3)	2.99	
		NZ (Lys 7) → O2 (U4)	2.95	
		NE1 (Trp 8) → O2 (U4)	3.24	
		OD2 (Asp 25) ← N3 (U4)	2.80	
		ND2 (Asn 10) → O2 (C5)	2.92	
		NZ (Lys 13) → O2' (C5)	3.13	
2.	<i>A.tauschii_cspC</i>	OG (Ser 61) → O2' (C2)	2.97	Lys 8, Trp 9, Asn 11, Lys 14, Phe 16, Phe 18, Asp 27, Phe 29, His 31, Gly 56, Gln 57, Lys 58, Pro 60, Ser 61, Ala 62, Val 63 (Total 144)
		OG (Ser 61) ← O2' (C2)	2.97	
		O (Asp 27) ← N3 (U3)	2.96	
		NZ (Lys 8) → O4 (U4)	3.03	
		NZ (Lys 14) → O3' (U4)	2.94	
		NZ (Lys 13) → O5' (C5)	3.30	
		NZ (Lys 13) → O4' (C5)	3.27	
3.	<i>A.tauschii_cspD</i>	ND2 (Asn 10) → O2 (C2)	2.94	Lys 7, Gly 8, Phe 9, Asn 10, Lys 13, Tyr 15, Phe 17, Glu 25, Asp 26, Phe 28, His 30, Gly 55, Pro 56, Lys 57, Gly 58, Leu 59, His 60 (Total 132)
		NZ (Lys 13) → O2' (C2)	3.02	
		O (Asp 26) ← O2' (C5)	2.96	
		N (Leu 59) → O2' (C5)	2.98	
4.	<i>A.tauschii_cspE</i>	NZ (Lys 9) → O5' (C2)	2.90	Lys 9, Trp 10, Asn 12, Lys 15, Phe 17, Phe 19, Asp 28, Phe 30, His 32, Gly 57, Ala 58, Lys 59, Gly 60, Pro 61, Ser 62 (Total 129)
		NZ (Lys 9) → O4' (C2)	3.27	
		NE1 (Trp 10) → O4' (C2)	3.05	
		OD2 (Asp 28) ← O5' (C2)	2.58	
		NE2 (His 32) → O4' (U4)	3.06	
		N (Ala 58) → O3' (C5)	2.88	
		N (Lys 59) → O3' (C5)	3.02	
		N (Gly 60) → O3' (C5)	2.87	
		O (Gly 60) ← O2' (C5)	3.11	
		OG (Ser 62) ← O2' (U5)	2.74	
5.	<i>D.hygrometricum_csd1</i>	NE2 (Gln 62) → O2 (C2)	2.80	Lys 10, Trp 11, Asn 13, Lys 16, Phe 18, Phe 20, Asp 28, Phe 30, Pro 58, Phe 41, Pro 58, Lys 59, Leu 61, Gln 62 (Total 81)
		O (Asp 28) ← N3 (U3)	3.21	
		N (Leu 61) → O4 (U3)	3.20	
		NZ (Lys 10) → O4 (U4)	3.03	
6.	<i>D.hygrometricum_csd2</i>	NE2 (Gln 58) → O2' (C2)	3.05	Lys 10, Trp 11, Asn 13, Lys 16, Phe 18, Phe 20, Asp 28, Phe 30, His 32, Gln 58, Lys 59, Gly 60, Leu 61, Gln 62 (Total 140)
		N (Leu 61) → O4 (U3)	3.11	
		NZ (Lys 10) → O2 (U4)	3.13	
		NE1 (Trp 11) → O2 (U4)	3.09	
		OD2 (Asp 28) ← N3 (U4)	2.75	
		ND2 (Asn 13) → O2' (C5)	2.88	

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Table S8: Intermolecular interactions of plant CSPs structure models docked with C2UC-RNA

Sr. No.	Name of complex	Residues forming H-bonds	Distance (Å)	Residues making non-bonded contacts
7.	<i>H. vulgare_csd</i>	OD2 (Asp 30) ← O5' (C2)	2.71	Lys 11, Trp 12, Asn 14, Phe 19, Phe 21, Asp 30, Phe 32, His 34, Lys 61, Gly 62, Pro 63, Ser 64, Ala 65 (Total 85)
		ND2 (Asn 14) → O4 (U3)	3.35	
		N (Gly 62) → O3' (C5)	3.19	
		O (Gly 62) ← O2' (C5)	3.08	
		OG (Ser 64) ← O2' (C5)	3.10	
		N (Ala 65) → O2 (C5)	3.11	
8.	<i>R.communis_csd1</i>	NE2 (His 30) → O3' (C2)	3.24	Trp 8, Phe 9, Asn 10, Asp 11, Ser 12, Lys 13, Gly 14, Phe 15, Gly 16, Phe 17, Asp 26, Leu 27, Phe 28, His 30, Phe 31, Glu 54, Gly 55, Pro 56, Lys 57, Gly 58, Lys 59, Gln 60 (Total 148)
		NE2 (His 30) → O5' (U3)	2.83	
		NE2 (His 30) ← O5' (U3)	2.83	
		O (Asp 26) ← N4 (C5)	3.10	
9.	<i>R.communis_csd2</i>	NE2 (Gln 60) → O2 (C2)	2.98	Lys 7, Trp 8, Asn 10, Phe 15, Phe 17, Asp 26, Phe 28, His 30, Gly 55, Pro 56, Lys 57, Gly 58, Lys 59, Gln 60 (Total 131)
		O (Lys 59) ← N3 (U3)	3.09	
		NZ (Lys 7) → O2 (U4)	3.18	
		OD2 (Asp 26) ← N3 (U4)	3.23	
		ND2 (Asn 10) → O2 (C5)	3.03	
10.	<i>T. aestivum_csp1</i>	O (Pro 61) ← N3 (U3)	3.14	Lys 9, Trp 10, Asn 12, Phe 17, Phe 19, Lys 27, Asp 28, Phe 30, His 32, Pro 61, Ser 62 (Total 84)
		OG (Ser 62) → O4 (U3)	2.92	
		NZ (Lys 9) → O2 (U4)	3.06	
		NZ (Lys 27) → O4 (U4)	3.00	
11.	<i>T. aestivum_csp2</i>	NE1 (Trp 10) → O4' (C2)	2.86	Lys 9, Trp 10, Asn 12, Lys 15, Phe 17, Phe 19, Asp 28, Phe 30, His 32, Gly 57, Thr 58, Lys 59, Gly 60, Pro 61, Thr 62 (Total 99)
		ND2 (Asn 12) → O2 (U3)	2.86	
		NZ (Lys 15) → O2' (U3)	2.98	
		N (Thr 58) → O3' (C5)	3.20	
		N (Lys 59) → O3' (C5)	2.91	
		O (Gly 60) ← O2' (C5)	2.99	
		OG1 (Thr 62) → O2 (C5)	2.82	
12.	<i>T. aestivum_csp3</i>	NZ (Lys 58) → O4 (U3)	3.02	Lys 8, Trp 9, Phe 10, Asn 11, Lys 14, Gly 15, Phe 16, Gly 17, Phe 18, Asp 27, Phe 29, His 31, Phe 32, Glu 45, Lys 58, Gly 59, Pro 60, Ser 61 (Total 148)
		OG (Ser 61) → O4 (U3)	2.75	
		NZ (Lys 8) → O2 (U4)	2.99	
		NE1 (Trp 9) → O4' (U4)	2.88	
		OD2 (Asp 27) ← N3 (U4)	2.83	
		ND2 (Asn 11) → O2 (C5)	3.07	
		OE1 (Glu 45) ← N4 (C5)	2.66	
13.	<i>T. aestivum_UP</i>	OD2 (Asp 29) ← N4 (C5)	2.90	Lys 10, Ser 11, Lys 16, Phe 18, Gly 19, Leu 20, Asp 29, Phe 31, His 33, Arg 35, Gln 57, Gly 58, Gln 59, Lys 60, Gly 61, Met 62, Gln 63 (Total 116)

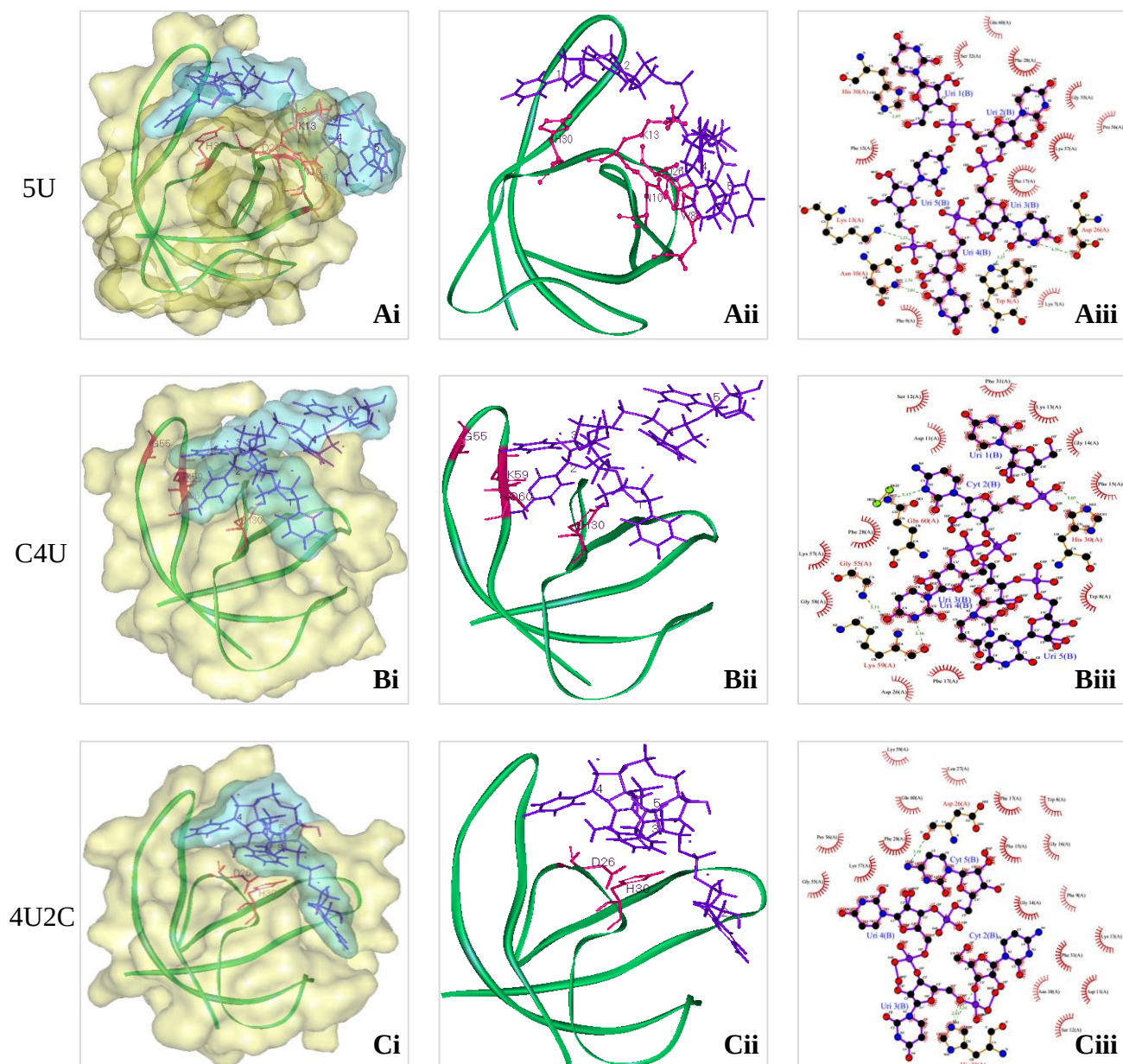


Figure S8: Docking and molecular interactions of *R. communis*-csd1 with three different RNA molecules. **A.** with 5U RNA **B.** with UC3U RNA, and **C.** with C2UC RNA; **i.** molecular surface representation of *R. communis*-csd1-RNA complexes **ii.** ribbon representation of protein and stick representation of RNA molecules. Side chains of interacting residues of protein are shown as sticks in pink color. **iii.** 2-D plots of respective CSP-RNA interactions.

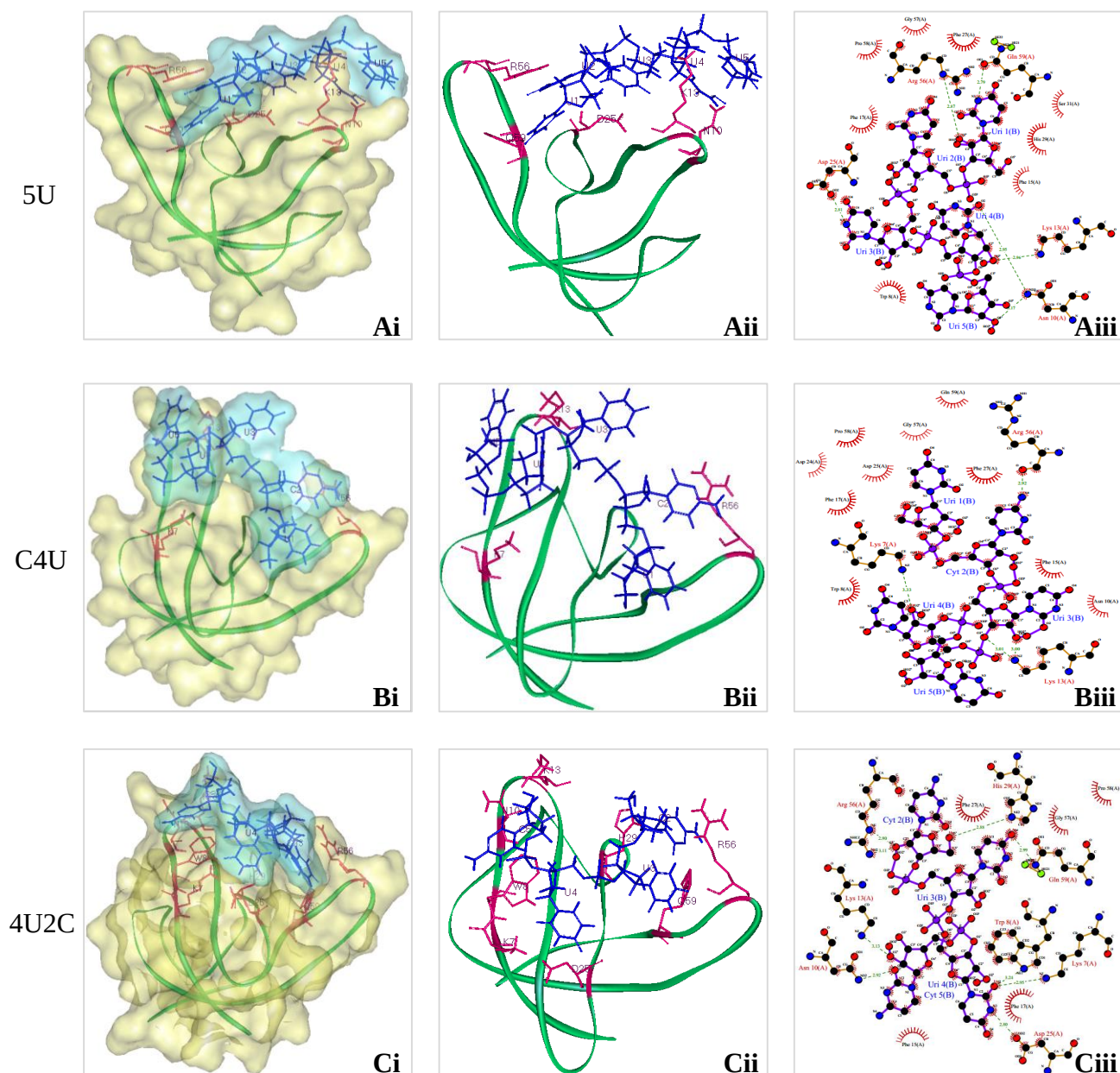


Figure S9: Docking and molecular interactions of CSPB with three different RNA molecules. **A.** with 5U RNA **B.** with UC3U RNA, and **C.** with C2UC RNA; **i.** molecular surface representation of CSPB-RNA complexes **ii.** ribbon representation of protein and stick representation of RNA molecules. Side chains of interacting residues of protein are shown as sticks in pink color. **iii.** 2-D plots of respective CSP-RNA interactions.