

Supplementary Table 1.

EntryID	Target	Program Type	Entry	Invalid	Conformers	Accuracy	Convergence	ROG	NOE completeness	DP Score	W packing quality	MP Clash Z-score	MP Clash score (pdb style)	W Ramachandra n appearance	MP Ramachandra n disallowed	PC_NMR ϕ/ψ Z-score	W X Z	PC_NMR dihedral Z-score	Intra-NOEs	Seq-NOEs	Med-NOEs	Long-NOEs	Ambig-NOEs	Queen Information	NOE violations >0.1 Å	NOE violations >0.3 Å	NOE violations >0.5 Å	dihedrals	dihedral violations >1°	dihedral violations >3°	dihedral violations >5°	RDCs
HR2876B	HR2876B		HR2876B		20	0.62	green	73.2	0.93	2.10	0.02	9.06	-1.93	0	-0.04	-0.44	-0.30	699	519	1147	0	66.278	119	11	0	112	81	38	15	0		
255	HR2876B	ARIA	HR2876B_ARIA_c		10	0.72	0.36	green	75.2	0.93	2.09	-0.74	12.36	-1.55	2.1	-0.35	-0.45	-0.53	619	1333	451	942	580	45.138	208	112	53	172	173	91	59	0
256	HR2876B	ARIA	HR2876B_ARIA_cr		10	0.78	0.53	green	75.5	0.93	2.00	-1.32	16.63	-2.24	3.4	-0.98	-0.67	-1.06	627	1340	447	946	609	75.970	315	202	143	172	272	170	138	121
240	HR2876B	ARIA	HR2876B_ARIA_ur		10	0.91	0.58	green	74.4	0.90	2.42	-3.56	27.49	-2.23	1.6	-0.98	-2.37	-1.54	1041	1224	1024	2180	1447	66.538	7755	6749	5793	172	267	175	107	0
241	HR2876B	ARIA	HR2876B_ARIA_ur		10	1.05	0.70	green	74.5	0.91	1.72	-4.18	31.03	-3.06	2.4	-1.77	-2.14	-2.37	1057	1201	1067	2132	1461	80.438	7473	6483	5580	172	497	345	257	121
313	HR2876B	ASDP-CNS	HR2876B_ASDP-CNS_c		20	0.97	0.54	green	66.4	0.92	2.05	-1.70	21.32	-1.82	0.1	-0.59	-1.51	-1.01	493	441	381	759	0	87.979	85	0	0	164	362	116	64	0
278	HR2876B	ASDP-CNS	HR2876B_ASDP-CNS_ur		15	1.00	0.82	green	67.1	0.91	1.35	-0.92	15.57	-2.41	0.1	-0.55	-2.95	-1.42	569	429	440	809	0	75.689	189	9	0	164	422	210	118	120
314	HR2876B	ASDP-Rosetta	HR2876B_ASDP-Rosetta_c		20	0.76	0.38	green	66.8	0.93	2.36	-0.66	4.96	-0.03	0	0.24	5.00	1.12	500	440	387	751	0	94.678	104	36	9	164	198	167	142	0
279	HR2876B	ASDP-Rosetta	HR2876B_ASDP-Rosetta_ur		20	0.88	0.53	green	66.2	0.92	2.04	-0.22	10.32	-0.42	0	0.28	2.86	0.83	569	429	440	809	0	75.689	466	309	221	164	183	118	88	120
244	HR2876B	autonee-Rosetta-alpha	HR2876B_autonee-Rosetta-alpha_ur		10	1.50	1.17	green	1.77	0.99	2.78	-1.36			0.8	-0.59	5.07	0.41	0	0	0	0	0	0	0	0	0	0	0	0	0	0
325	HR2876B	Cheshire	HR2876B_Cheshire_s		10	3.06	3.19	green	0.37		8.21	-3.47				-1.09			0	0	0	0	0	0	0	0	0	0	0	0	0	
326	HR2876B	Cheshire-YAPP	HR2876B_Cheshire-YAPP_c		50	0.80	0.46	orange	0.93	0.60	19.36	-5.16				-6.86			0	0	0	0	0	0	0	0	0	0	0	0	0	
262	HR2876B	Cheshire-YAPP	HR2876B_Cheshire-YAPP_u		100	1.00	0.48	orange	0.91	1.52	-10.04	30.71	-3.21		1.6	-1.57	-7.20	-4.91	0	0	0	0	0	0	0	0	0	0	0	0	0	0
283	HR2876B	CS-HM-Rosetta	HR2876B_CS-HM-Rosetta_sr		1	2.30		orange			-1.72		-2.19			6.46			0	0	0	0	0	0	0	0	0	0	0	0	0	
259	HR2876B	CYANA	HR2876B_CYANA_c		20	0.71	0.38	green	76.1	0.93	1.79	0.67	5.13	-2.57	0.1	-1.02	-4.08	-2.31	675	592	525	1184	0	90.712	22	0	0	0	0	0	0	0
227	HR2876B	Ponderosa	HR2876B_Ponderosa_r		20	1.29	0.11	orange	0.89	0.52	-2.24	23.86	-0.55		1	-0.35	-6.03	-2.42	577	482	380	795	0	67.914	64	0	0	316	513	417	366	0
239	HR2876B	UNIO	HR2876B_UNIO_r		20	1.05	0.58	orange	64.8	0.89	0.27	-5.09	36.05	-4.78	0.4	-2.52	-6.63	-5.14	462	435	265	579	0	66.952	238	51	27	274	1092	956	851	0
238	HR2876B	UNIO	HR2876B_UNIO_u		20	1.03	0.45	red	55.8	0.87	0.84	-12.88	75.19	-5.56	3.1	-3.62	-6.74	-6.39	795	405	617	1228	0	88.163	521	134	82	274	1279	1091	958	0
HR2876C	HR2876C		HR2876C		20	0.97	0.54	green	68.0	0.89	2.41	-6.13	20.75	-1.70	0	0.32	-0.39	0.34	744	648	739	907	0	54.959	105	2	0	124	302	78	7	0
303	HR2876C	ARIA	HR2876C_ARIA_cr		15	1.05	0.12	green	63.5	0.90	2.39	-1.23	20.13	-1.32	2.8	-0.39	-0.70	-0.47	431	1008	451	500	325	54.387	94	19	12	140	251	175	152	95
304	HR2876C	ARIA	HR2876C_ARIA_cr(10-97)		15	1.05	0.12	green	63.5	0.90	2.39	-1.23	20.13	-1.32	2.8	-0.39	-0.70	-0.47	431	1008	451	500	325	54.387	94	19	12	140	240	164	142	95
296	HR2876C	ARIA	HR2876C_ARIA_ur		15	0.81	0.42	green	61.4	0.86	3.18	-2.23	26.59	-0.18	0.1	-0.04	-0.42	-0.18	664	936	688	795	440	72.045	1434	478	169	140	280	159	141	95
307	HR2876C	ASDP-Rosetta	HR2876C_ASDP-Rosetta_cr		20	0.76	0.51	green	62.2	0.89	2.91	-0.02	8.87	0.93	0	0.79	3.91	1.77	529	425	515	506	0	82.340	1311	426	111	158	200	121	85	0
301	HR2876C	ASDP-Rosetta	HR2876C_ASDP-Rosetta_ur		20	1.41	0.65	green	58.2	0.83	1.93	-1.20	15.18	-0.07	0	0.67	2.08	1.12	569	393	507	443	0	80.670	1299	557	229	158	334	251	184	0
288	HR2876C	autonee-Rosetta-alpha	HR2876C_autonee-Rosetta-alpha_ur		10	1.16	0.79	green	0.85	3.18	0.92	3.69	0.45	0	0	0.79	6.20	2.19	0	0	0	0	0	0	0	0	0	0	0	0	0	0
310	HR2876C	BE-metadynamics	HR2876C_BE-metadynamics_s		28	1.68	1.66	green	0.77	0.70	1.13	2.35	-3.97		0.4	-1.06	-4.91	-2.07	0	0	0	0	0	0	0	0	0	0	0	0	0	
309	HR2876C	Cheshire	HR2876C_Cheshire_s		10	1.84	1.32	green	2.05	-1.70	19.03	-2.14			0.6	-0.04	-0.68	0.06	0	0	0	0	0	0	0	0	0	0	0	0	0	0
308	HR2876C	Cheshire-YAPP	HR2876C_Cheshire-YAPP_c		50	1.05	0.56	red	0.90	1.68	-5.08	32.06	-5.05		1.3	-2.36	-7.62	-5.03	0	0	0	0	0	0	0	0	0	0	0	0	0	0
300	HR2876C	Cheshire-YAPP	HR2876C_Cheshire-YAPP_u		50	2.07	1.14	red	0.85	0.01	-10.58	58.46	-7.18		4.9	-4.48	-7.74	-7.69	0	0	0	0	0	0	0	0	0	0	0	0	0	0
291	HR2876C	CS-HM-Rosetta	HR2876C_CS-HM-Rosetta_sr		11	1.40	0.86	green	0.81	1.93	0.89	3.85	-0.18		0.7	-0.28	6.08	0.83	0	0	0	0	0	0	0	0	0	0	0	0	0	0
285	HR2876C	CS-HM-Rosetta	HR2876C_CS-HM-Rosetta_ur		11	1.88	0.42	green	1.99	0.99	3.80	-3.50			0	0.12	6.31	1.24	0	0	0	0	0	0	0	0	0	0	0	0	0	0
286	HR2876C	CS-Rosetta	HR2876C_CS-Rosetta_s		10	0.86	0.82	green	3.07	-0.19	6.57	-0.01			0	0.75	5.75	1.89	0	0	0	0	0	0	0	0	0	0	0	0	0	0
287	HR2876C	CS-Rosetta3	HR2876C_CS-Rosetta3_s		6	1.00	0.85	green	2.70	0.55	5.91	0.01			0	0.59	6.62	1.83	0	0	0	0	0	0	0	0	0	0	0	0	0	0
302	HR2876C	CYANA	HR2876C_CYANA_c		20	0.84	0.34	green	71.0	0.89	1.83	-0.20	12.37	-2.52	0	-0.16	-5.42	-1.60	739	607	735	940	0	73.930	64	0	0	0	0	0	0	
297	HR2876C	CYANA	HR2876C_CYANA_u		20	0.97	0.30	orange	66.8	0.87	1.49	-2.03	21.89	-4.40	2.6	-1.65	-6.15	-3.61	724	615	690	879	0	74.135	111	0	0	0	0	0	0	0
305	HR2876C	I-TASSER	HR2876C_I-TASSER_c		1	1.32		green	86.2	0.82	-1.14	-1.19	18.17	-0.50	0	0.04	-3.21	-1.30	1781	2253	1792	2011	275	89.898	216	75	28	138	32	24	16	0
298	HR2876C	I-TASSER	HR2876C_I-TASSER_ur		1	1.11		green	86.3	0.76	-1.66	-0.03	10.38	-2.06	2.3	-0.94	-2.24	-2.07	1867	1660	1970	2259	181	95.111	246	121	71	138	57	42	37	0
284	HR2876C	Ponderosa	HR2876C_Ponderosa_r		20	0.95	0.17	orange	0.83	1.64	-2.66	27.68	-1.14	0	-0.04	-7.22	-2.72	526	428	419	326	0	31.966	3829	2463	1688	307	863	733	621	0	
293	HR2876C	UNIO	HR2876C_UNIO_r		20	1.32	0.63	orange	48.0	0.86	1.03	-3.52	34.99	-5.13	0.1	-1.81	-6.94	-4.67	404	406	314	348	0	55.568	332	167	108	259	1218	1017	907	0
294	HR2876C	UNIO	HR2876C_UNIO_u		20	1.12	0.50	red	57.7	0.86	0.84	-7.89	64.62	-6.04	0.3	-2.91	-7.24	-5.62														

EntryID	Target	Program Type	Entry	Invalid	Conformers	Accuracy	Convergence	ROG	NOE completeness	DP Score	WI packing quality	MP Clash Z-score	MP Clash score (pdb-style)	WI Ramachandran appearance	MP % Ramachandran disallowed	PC_NMR Φ/ψ Z-score	WI χ Z-score	PC_NMR dihedral Z-score	Intra-NOEs	Seq-NOEs	Med-NOEs	Long-NOEs	Ambig-NOEs	Queen Information	NOE violations > 0.1 Å	NOE violations > 0.3 Å	NOE violations > 0.5 Å	dihedrals	dihedral violations > 1°	dihedral violations > 3°	dihedral violations > 5°	RDCs		
ST322	ST322		ST322		20	1.91	0.57	green	63.4	0.81	2.38	-0.06	12.63	-4.23	0	-2.91	-3.68	-4.02	280	320	137	371	0	32.415	252	1	0	70	28	0	0			
225	ST322	ARIA	ST322_ARIA_c		10	2.19	0.51	green	52.0	0.73	3.13	-1.08	17.35	-1.60	0.2	-2.12	-0.58	-2.66	218	694	111	232	893	31.127	249	148	87	78	244	128	97	0		
333	ST322	ARIA	ST322_ARIA_u	TRUE	10	9.27	2.02	orange	62.4	0.51	-4.23		63.77	-5.92		-5.54		742	741	716	1789	2074	105.501	13546	11966	10478	78	557	364	254	0			
229	ST322	ASDP-CNS	ST322_ASDP-CNS_c		20	1.91	0.67	red	62.7	0.80	1.05	-0.75	19.92	-2.66	0.1	-2.71	-7.79	-6.62	213	284	105	258	0	43.591	42	11	1	92	368	171	91	0		
222	ST322	ASDP-CNS	ST322_ASDP-CNS_u		20	2.85	1.43	red	48.8	0.77	0.07	-1.08	21.45	-2.71	0	-1.49	-7.76	-5.14	237	247	79	143	0	39.702	52	2	0	92	399	249	155	0		
230	ST322	ASDP-Rosetta	ST322_ASDP-Rosetta_c		20	1.49	0.81	green	61.5	0.81	2.48	-0.71	17.73	-0.50	0	-1.30	3.58	-1.06	213	284	105	258	0	43.591	175	52	10	92	266	195	130	0		
223	ST322	ASDP-Rosetta	ST322_ASDP-Rosetta_u		20	2.28	1.50	green	48.0	0.79	1.96	0.03	9.89	0.66	0	-0.47	5.35	0.06	237	247	79	143	0	39.702	189	75	14	92	275	225	177	0		
220	ST322	autonee-Rosetta-alpha	ST322_autonee-Rosetta-alpha_u		10	4.34	0.44	green			1.69	1.41	0.00	0.62	1.7	-1.30	5.83	-0.06	0	0	0	0	0				0	0	0	0	116	104	84	0
231	ST322	Cheshire	ST322_Cheshire_s		10	1.30	0.82	green			0.70	4.47	0.65	4.39	-3.14	0.5	-2.40	0.01	-2.13	0	0	0	0				0	0	0	190	174	158	0	
224	ST322	CYANA	ST322_CYANA_c		20	2.83	0.50	orange	60.6	0.77	1.73	0.79	6.41	-3.34	1.1	-3.38	-6.44	-5.32	278	296	132	329	0	38.716	7	0	0	0	337	294	238	0		
221	ST322	Ponderosa	ST322_Ponderosa_r		20	3.69	0.25	orange			0.59	-0.14	-2.12	32.37	-0.38	0.1	-1.46	-5.92	-0.02	231	178	74	81	0	14.679	74	0	0	211	329	286	244	0	
YR313A	YR313A		YR313A		20		0.97	green	61.2	0.87	2.70	-0.58	12.18	-2.87	0	-0.55	-1.31	-0.59	631	743	413	754	0	49.414	74	1	0	122	130	37	3	0		
253	YR313A	ARIA	YR313A_ARIA_c		10	1.12	0.50	green	62.0	0.84	2.93	-0.93	16.27	-1.25	1	-0.63	-0.77	-0.83	608	1495	354	655	575	28.782	372	230	105	174	163	115	78	0		
254	YR313A	ARIA	YR313A_ARIA_cr		10	1.39	0.64	green	61.3	0.83	2.42	-1.03	16.66	-3.21	0	-1.26	-0.49	-1.24	602	1500	346	616	545	47.096	386	218	123	174	417	235	154	112		
334	YR313A	ARIA	YR313A_ARIA_ur	TRUE	10	14.85	12.74	orange	68.4	0.59	-2.40		34.83	-8.83		-9.20		822	1408	464	106	519	28.661	3931	3217	2629	174	1139	840	643	112			
315	YR313A	ASDP-CNS	YR313A_ASDP-CNS_c		20	1.81	0.74	green	54.6	0.80	2.33	-2.64	27.03	-2.08	0.1	-1.06	-2.78	-2.01	478	555	297	484	0	79.991	105	4	0	198	412	146	51	0		
276	YR313A	ASDP-CNS	YR313A_ASDP-CNS_u		19	1.44	1.11	green	51.4	0.84	2.48	-1.42	20.02	-2.24	0.1	-0.55	-3.12	-1.36	506	529	297	455	0	60.701	124	7	0	198	519	202	99	0		
316	YR313A	ASDP-Rosetta	YR313A_ASDP-Rosetta_c		20	1.75	1.06	green	60.0	0.83	2.82	-0.18	10.02	-0.19	0	0.20	4.65	1.06	487	558	301	475	0	77.327	259	82	25	198	211	149	103	0		
277	YR313A	ASDP-Rosetta	YR313A_ASDP-Rosetta_u		20	1.45	0.75	green	48.3	0.84	2.97	-0.11	9.98	-0.03	0.1	0.12	4.07	0.83	506	529	297	455	0	60.701	395	306	241	198	139	90	66	0		
285	YR313A	autonee-Rosetta-alpha	YR313A_autonee-Rosetta-alpha_ur		10	1.20	0.75	green			3.83	0.83	3.82	-0.90	0	-0.04	6.40	1.30	0	0	0	0	0				0	0	0	0	169	138	112	0
327	YR313A	Cheshire	YR313A_Cheshire_s		11	2.04		green			-1.21			-3.28			-1.84		0	0	0	0	0				0	0	40	34	31	0		
328	YR313A	Cheshire-YAPP	YR313A_Cheshire-YAPP_c		50	1.12	0.80	red			0.86	1.10		31.19	-5.86		-7.11		0	0	0	0	0				0	0	0	0	2989	2628	2301	0
261	YR313A	Cheshire-YAPP	YR313A_Cheshire-YAPP_u		100	1.73	1.53	orange			0.82	1.14	-6.95	21.30	-3.19	1.5	-0.63	-7.88	-4.44	0	0	0	0				0	0	0	0	1605	1123	821	0
282	YR313A	CS-HM-Rosetta	YR313A_CS-HM-Rosetta_sr		1	2.17		orange			-0.37	0.64	5.19	-2.72	0	-1.02	6.03	0.06	0	0	0	0				0	0	0	31	22	16	0		
260	YR313A	CYANA	YR313A_CYANA_c		20	1.21	0.67	green	64.3	0.86	1.84	0.96	3.70	-2.88	0.3	-1.46	-4.65	-2.78	626	324	389	778	0	82.907	51	0	0	0	545	424	338	0		
228	YR313A	Ponderosa	YR313A_Ponderosa_r		20	1.67	0.12	green			0.78	-3.21	27.18	-0.80	0	-0.43	-6.48	-2.90	638	723	426	737	0	73.187	14	2	0	412	586	523	440	0		
237	YR313A	UNIO	YR313A_UNIO_r		20	2.94	1.81	red	40.7	0.82	-0.24	-2.71	24.38	-4.85	0.1	-1.46	-7.07	-4.49	291	529	102	192	0	27.243	264	77	47	314	1315	1177	1031	0		

