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Genetic control of grain amino acid composition in a UK soft wheat mapping population

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Supplementary tables

Supplementary table 1. Broad sense heritability estimates, kendall correlation coefficients for traits across both environments, and within and between environments average genomic prediction accuracies (as Pearson correlation coefficients). Heritability estimates and genomic prediction performed on transformed data, kendall correlation coefficients performed on non-transformed data.

Traits	h^2	r	Within environment GP r			Between environments GP r		
			H18	H19	Mean	H18 train	H19 train	Mean
Amino acids								
Ala	0.37	0.00	0.26	0.29	0.27	0.24	0.24	0.24
Asn	0.60	0.34	0.36	0.48	0.42	0.35	0.33	0.34
Asp	0.82	0.51	0.59	0.52	0.55	0.51	0.55	0.53
Glu	0.61	0.33	0.34	0.33	0.33	0.25	0.26	0.25
Gln	0.69	0.30	0.47	0.55	0.51	0.45	0.43	0.44
Gly	0.00	-0.12	0.06	0.22	0.14	0.17	0.12	0.15
Iso	0.71	0.39	0.48	0.48	0.48	0.42	0.44	0.43
Leu	0.35	0.18	0.14	0.19	0.17	0.13	0.13	0.13
Lys	0.45	0.15	0.00	0.20	0.10	0.09	0.10	0.10
Phe	0.34	0.17	0.17	0.31	0.24	0.09	0.07	0.08
Ser	0.00	-0.14	0.11	0.40	0.25	0.20	0.15	0.17
Tyr	0.00	-0.23	0.16	0.12	0.14	0.08	0.10	0.09
Functional traits								
Area	0.91	0.63	0.61	0.67	0.64	0.61	0.58	0.59
Length	0.96	0.77	0.71	0.77	0.74	0.73	0.72	0.73
Width	0.84	0.55	0.53	0.47	0.50	0.43	0.40	0.41
Diameter	0.90	0.60	0.62	0.56	0.59	0.57	0.57	0.57
KHI	0.85	0.58	0.46	0.50	0.48	0.41	0.40	0.41
Weight	0.89	0.59	0.58	0.54	0.56	0.53	0.53	0.53
HFN	0.64	0.34	0.51	0.33	0.42	0.35	0.37	0.36

Supplementary table 2. Multi-environment QTL for measured amino acids. Chr. (Chromosome), Pos. (Position), QTL x E (QTL by environment interaction).

Trait	Single trait linkage analysis (H18 and H19)							H18					H19				
	Marker	Chr.	cM	Mb p	$-\log_{10}(p)$	QTL x E	Ratio	Effect	S.E.	High value	p	% Expl.	Effect	S.E.	High value	p	% Expl.
Asparagine	WC.0221262	4B	114.47	601	5.96	yes	4.34	0.041	0.020	Robigus	0.040	2.6	0.178	0.034	Robigus	<0.001	14.8
Log _e alanine	WC.0218011	1A2	27.3	593	5.10	yes	0.34	0.065	0.016	Claire	<0.001	10.9	0.022	0.015	Robigus	0.159	1
	WC.0223839	7B	211.2	719	5.03	no	1.00	0.052	0.012	Robigus	<0.001	7.1	0.052	0.012	Robigus	<0.001	5.7
Aspartic acid	WC.0218489	1B	54.4	530	5.40	no	1.00	0.123	0.027	Claire	<0.001	8	0.123	0.027	Claire	<0.001	5.9
	WC.0214359	3A2	2.3	738	7.95	yes	1.68	0.118	0.029	Robigus	<0.001	7.3	0.198	0.033	Robigus	<0.001	15.3
	WC.0221037	4A	148.8	703	8.08	no	1.00	0.154	0.027	Claire	<0.001	12.6	0.154	0.027	Claire	<0.001	9.3
	WC.0227146	4D	48.8	16	3.70	no	1.00	0.102	0.028	Claire	<0.001	5.5	0.102	0.028	Claire	<0.001	4.1
Log _e glutamate	WC.0221329	4B	100.8	518	4.27	yes	2.41	0.034	0.013	Robigus	0.011	3.7	0.082	0.019	Robigus	<0.001	10.1
Log _e glutamine	WC.0218486	1B	117.93	660	2.16	yes	9.91	0.011	0.038	Robigus	0.760	0.1	0.109	0.038	Robigus	0.004	4.9
	WC.0221302	4B	103.7	547	3.50	no	1.00	0.105	0.029	Robigus	<0.001	5.4	0.105	0.029	Robigus	<0.001	4.5
	WC.0228471	6B	19.7	25	5.09	no	1.00	0.129	0.029	Claire	<0.001	8.2	0.129	0.029	Claire	<0.001	6.7
Glycine	WC.0218011	1A2	27.3	593	5.37	yes	0.53	0.017	0.004	Claire	<0.001	9.6	0.009	0.003	Robigus	0.005	4.3
	WC.0226796	4B	155.2	327	4.26	no	1.00	0.010	0.002	Robigus	<0.001	3.2	0.010	0.002	Robigus	<0.001	5.3
-1/Isoleucine	WC.0221386	4B	94.3	172	7.31	yes	5.10	0.161	0.120	Robigus	0.180	1	0.821	0.151	Robigus	<0.001	14.1
	WC.0223785	7B	211.2	717	3.60	no	1.00	0.421	0.115	Robigus	<0.001	6.8	0.421	0.115	Robigus	<0.001	3.7
Log _e lysine	WC.0218011	1A2	27.3	593	4.95	yes	0.38	0.064	0.014	Claire	<0.001	12.1	0.024	0.011	Claire	0.038	2.6
Phenylalanine	WC.0220622	3B1	78.1	116	3.83	yes	1.80	0.005	0.002	Robigus	0.001	6.2	0.009	0.003	Robigus	0.002	5.6
Log _e serine	WC.0226730	4B	123.8	632	3.39	yes	2.33	0.033	0.031	Claire	0.279	0.7	0.077	0.020	Robigus	<0.001	7.9

Supplementary table 3. Multi-environment QTL for selected grain traits. Chr. (Chromosome), Pos. (Position), QTL x E (QTL by environment interaction).

Trait	Single trait linkage analysis (H18 and H19)							H18					H19				
	Marker	Chr.	cM	Mbp	$-\log_{10}(p)$	QTLx E	Ratio	Effect	High value	S.E.	P	% Expl.	Effect	High value	S.E.	P	% Expl.
Log _e KHI	WC.022103 7	4A	148.8	703	8.26	yes	1.41	0.03 2	Robigus	0.00 6	<0.00 1	14.8	0.04 5	Robigus	0.00 8	<0.00 1	14.7
	WC.022674 1	4B	110.8	594	4.30	yes	2.06	0.01 7	Robigus	0.00 6	0.002	4.2	0.03 5	Robigus	0.00 8	<0.00 1	8.6
	WC.022275 4	6A	83.22	108	6.09	yes	4.40	0.00 5	Claire	0.00 6	0.377	0.4	0.02 2	Robigus	0.00 8	0.007	3.4
	WC.022867 8	7A	152.1 7	539	4.45	no	1.00	0.02 4	Claire	0.00 6	<0.00 1	8.1	0.02 4	Claire	0.00 6	<0.00 1	4.1
Area	WC.021744 1	2A	70.8	176	7.48	yes	1.43	0.32 5	Robigus	0.08 0	<0.00 1	7.4	0.46 4	Robigus	0.08 0	<0.00 1	15.8
	WC.022093 8	4A	149.7	709	2.22	no	1.00	0.20 8	Claire	0.07 6	0.006	3	0.20 8	Claire	0.07 6	0.006	3.2
	WC.019322 8	7A	158.0 9	610	4.94	no	1.00	0.36 0	Robigus	0.08 2	<0.00 1	9.1	0.36 0	Robigus	0.08 2	<0.00 1	9.5
Length	WC.022513 0	2A	67.2	166	8.15	no	1.00	0.07 7	Robigus	0.01 3	<0.00 1	9.6	0.07 7	Robigus	0.01 3	<0.00 1	9.1
	WC.021286 4	3A1	92.1	63	4.86	no	1.00	0.05 8	Robigus	0.01 3	<0.00 1	5.5	0.05 8	Robigus	0.01 3	<0.00 1	5.1
	WC.022595 2	3B1	128.8	739	7.18	no	1.00	0.07 2	Claire	0.01 3	<0.00 1	8.5	0.07 2	Claire	0.01 3	<0.00 1	8
	WC.022111 9	4A	149.7	702	7.12	yes	1.91	0.03 4	Claire	0.01 4	0.019	1.8	0.06 5	Claire	0.01 4	<0.00 1	6.5
	WC.022193 2	5A1	0.6	1	9.23	no	1.00	0.08 4	Robigus	0.01 4	<0.00 1	11.4	0.08 4	Robigus	0.01 4	<0.00 1	10.7
	WC.022341 3	7A	171.6	641	7.23	no	1.00	0.07 2	Robigus	0.01 3	<0.00 1	8.4	0.07 2	Robigus	0.01 3	<0.00 1	7.9
	WC.022240 6	7B	40.6	34	7.35	yes	1.54	0.04 8	Claire	0.01 4	0.001	3.7	0.07 4	Claire	0.01 4	<0.00 1	8.4
Width	WC.021744 1	2A	72.25	176	4.88	no	1.00	0.03 1	Robigus	0.00 7	<0.00 1	6.1	0.03 1	Robigus	0.00 7	<0.00 1	6.9
	WC.009549 7	2B	120.7 8	545	4.04	yes	3.44	0.00 9	Claire	0.00 8	0.257	0.5	0.03 1	Claire	0.00 8	<0.00 1	7.1
	WC.022714 6	4D	48.8	16	5.98	no	1.00	0.03 5	Robigus	0.00 7	<0.00 1	8	0.03 5	Robigus	0.00 7	<0.00 1	8.9
	WC.022819 4	6A	86.1	127	7.35	yes	0.59	0.04 4	Robigus	0.00 8	<0.00 1	12.9	0.02 6	Robigus	0.00 8	0.001	4.9
	WC.022884	7A	174.8	641	3.04	no	1.00	0.02	Robigus	0.00	0.001	3.8	0.02	Robigus	0.00	0.001	4.2

	9 WC.021252 8	7B	107.2	641	4.60	yes	0.11	4 0.02 8	Robigus	7 0.00 8	<0.00 1	5.2	4 0.00 3	Robigus	7 0.00 8	0.732	0.1
Diameter	WC.021744 1	2A	72.25	176	3.62	no	1.00	0.03 0	Robigus	0.00 8	<0.00 1	3.1	0.03 0	Robigus	0.00 8	<0.00 1	3.2
	WC.022615 4	3B1	81.6	237	9.72	no	1.00	0.05 1	Claire	0.00 8	<0.00 1	8.9	0.05 1	Claire	0.00 8	<0.00 1	9.4
	WC.022686 8	4B	82.5	32	18.53	no	1.00	0.07 2	Claire	0.00 8	<0.00 1	17.7	0.07 2	Claire	0.00 8	<0.00 1	18.7
	WC.022714 6	4D	48.8	16	7.84	no	1.00	0.04 7	Robigus	0.00 8	<0.00 1	7.6	0.04 7	Robigus	0.00 8	<0.00 1	8.1
	WC.022185 9	5A2	2.3	30	5.62	no	1.00	0.03 8	Claire	0.00 8	<0.00 1	5	0.03 8	Claire	0.00 8	<0.00 1	5.2
	WC.021295 7	6A	99.37	499	8.73	no	1.00	0.05 0	Robigus	0.00 8	<0.00 1	8.4	0.05 0	Robigus	0.00 8	<0.00 1	8.8
	WC.022240 6	7B	40.6	34	4.43	no	1.00	0.03 4	Claire	0.00 8	<0.00 1	3.9	0.03 4	Claire	0.00 8	<0.00 1	4.1
	Weight	WC.021744 1	2A	72.25	176	6.45	no	1.00	0.93 6	Robigus	0.18 4	<0.00 1	8.4	0.93 6	Robigus	0.18 4	<0.00 1
WC.022957 1		2B	9.37	12	3.18	no	1.00	0.62 9	Claire	0.18 5	0.001	3.8	0.62 9	Claire	0.18 5	0.001	4.4
WC.022686 8		4B	82.5	32	9.25	no	1.00	1.12 7	Claire	0.18 2	<0.00 1	12.2	1.12 7	Claire	0.18 2	<0.00 1	14.1
WC.021295 7		6A	99.37	499	8.28	no	1.00	1.08 5	Robigus	0.18 6	<0.00 1	11.3	1.08 5	Robigus	0.18 6	<0.00 1	13.1
-1/(500- HFN)	WC.018890 4	4A	147.1	733	8.24	no	1.00	0.00 1	Robigus	0.00 0	<0.00 1	11.5	0.00 1	Robigus	0.00 0	<0.00 1	10.3
	WC.022714 9	4D	56.9	17	10.92	yes	0.00	0.00 1	Robigus	0.00 0	<0.00 1	23.5	0.00 0	Robigus	0.00 0	<0.00 1	5.6
Heading date	WC.022661 6	4A	130.3	632	4.14	no	1.00	0.25 8	Claire	0.06 5	<0.00 1	8.6	0.25 8	Claire	0.06 5	<0.00 1	2.2
	WC.022177 4	5A3	104.9	706	4.51	yes	3.88	0.14 6	Claire	0.06 5	0.024	2.8	0.56 6	Claire	0.12 4	<0.00 1	10.5
Plant height	WC.022686 8	4B	82.5	32	17.98	no	1.00	3.92 1	Claire	0.44 4	<0.00 1	19.8	3.92 1	Claire	0.44 4	<0.00 1	20.7
	WC.021305 1	4D	56.9	17	28.97	yes	1.16	4.64 7	Robigus	0.47 1	<0.00 1	27.8	5.37 6	Robigus	0.47 1	<0.00 1	38.9
Grain yield	WC.022757 1	7B	16.5	328	5.62	yes	0.66	0.35 4	Robigus	0.07 0	<0.00 1	13.9	0.23 5	Robigus	0.07 0	0.001	6.2

Supplementary table 4. Sources of variation related to asparagine and falling number screened in this study in the Claire x Robigus mapping population. Chr. (chromosome).

Source of variation	Claire	Robigus	Chr.	Reference
ASN-B2 PAV	Absent	Absent	3B	Oddy et al., 2021
ASN-B1	Non-functional	Functional	5B	Oddy et al., 2021
ASN-A3.1	Non-functional	Non-functional	1A	Oddy et al., 2021
Rht-B1	Rht-B1a (WT)	Rht-B1b (Dwarf)	4B	Wilkinson et al., 2020
Rht-D1	Rht-D1b (Dwarf)	Rht-D1a (WT)	4D	Wilkinson et al., 2020
<i>T. dicoccoides</i> introgression	Absent	Present	4A	Przewieslik-Allen et al., 2021
TaMKK3A	A	A	4A	Shorinola et al., 2016
PM19-A1 promoter InDel	Deletion	Deletion	4A	Shorinola et al., 2016

Supplementary table 5. List of UK winter wheat varieties separated by *Rht-B1* allele status.

Type	Rht-B1 WT	Rht-B1 DWARF	
G1	Avalon Cadenza Crusoe Gallant Hereward	Malacca Shamrock Skyfall Solstice Spark	
G2	Bonham Charger Cordiale Cubanita Einstein	Evoke Podium Rialto Shango Sterling	Cashel
G3	Claire Cocoon Croft Delphi Diego	Invicta Scout Tuxedo Warrior Weaver	Icon Monterey Robigus Torch Zulu
G4 - Hard	Badger Buster Dickens Duxford Evolution	Icebreaker Kielder Relay Savannah	Gator Goldengun Oakley Santiago Solace
G4 - Soft	Alchemy Cougar Denman Horatio Lancaster	Leeds Revelation Rowan Twister Viscount	Myriad Panacea

Supplementary table 6. REML analysis of factors influencing asparagine content in field trials from 2011 – 2012 and 2012 – 2013.

Fixed term	Wald statistic	d.f.	Wald/d.f.	chi pr
Year	125.04	1	125.04	<0.001
Rht_B1	0.17	1	0.17	0.676
ASN_B2	3.49	1	3.49	0.062
Treatment	125.4	1	125.4	<0.001
Year.Rht_B1	2.79	1	2.79	0.095
Year.ASN_B2	0.07	1	0.07	0.796
Rht_B1.ASN_B2	0.73	1	0.73	0.393
Year.Treatment	84.24	1	84.24	<0.001
Rht_B1.Treatment	3.09	1	3.09	0.079
ASN_B2.Treatment	6.57	1	6.57	0.010
Year.Rht_B1.ASN_B2	0.02	1	0.02	0.877
Rht_B1.ASN_B2.Variety	92.97	58	1.6	0.002
Year.Rht_B1.Treatment	3.34	1	3.34	0.068
Year.ASN_B2.Treatment	7.01	1	7.01	0.008
Rht_B1.ASN_B2.Treatment	0.73	1	0.73	0.394
Year.Rht_B1.ASN_B2.Variety	7.35	7	1.05	0.393
Year.Rht_B1.ASN_B2.Treatment	1.55	1	1.55	0.213
Rht_B1.ASN_B2.Variety.Treatment	64.83	58	1.12	0.251
Year.Rht_B1.ASN_B2.Variety.Treat ment	6.54	7	0.93	0.478

Supplementary table 7. Physical locations of the HFN and Asn QTL in varieties Chinese Spring and Robigus.

Trait	Chr.	Location	Peak (Mbp)	Lower CI (Mbp)	Upper CI (Mbp)	QTL size (bp)	No. of genes
HF N	4A	CS	733	691	745	54,058,906	824
Asn	4B	CS	601	533	632	96,765,195	754
Lys	1A	CS	593	590	594	4,471,109	50

Supplementary table 8. Physical location of the lysine QTL in the wheat pangenome (chromosome level assemblies) and gene content.

Genome	Chr	Lower CI	Upper CI	QTL size	No. of genes
IWGSC	1A	590	594	4,471,109	50
Arinalrfor	1A	598	603	4,559,393	55
Jagger	1A	592	596	4,481,576	60
Julius	NA	NA	NA	NA	NA
Lancer	1A	591	595	4,548,456	59
Landmark	1A	593	595	2,101,319	38
Mace	1A	586	591	4,477,846	55
SY Mattis	1A	596	601	4,560,453	66
Norin61	1A	589	594	4,645,175	58
Stanley	scaffold_v3_2071	5	NA	NA	NA