

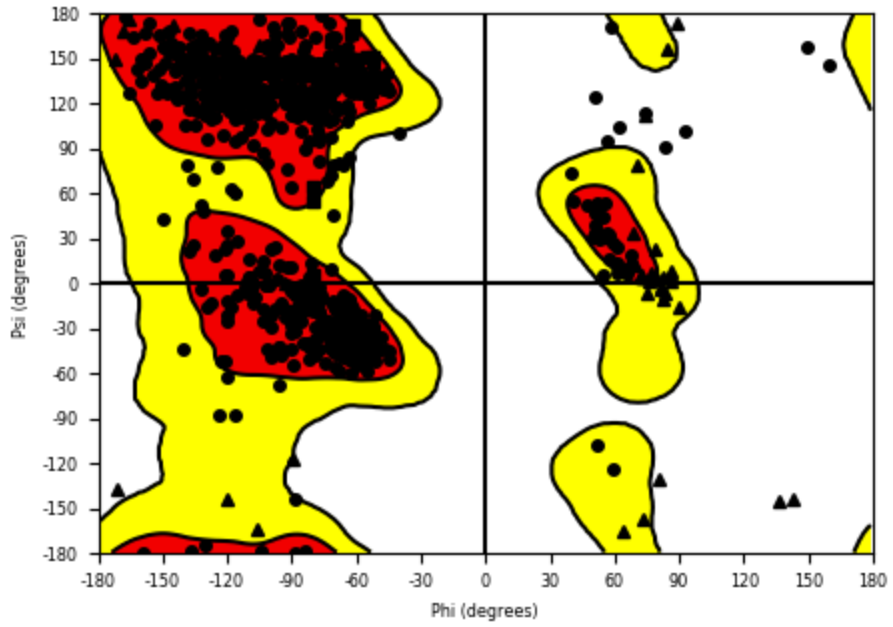
Supplementary Table 1. Interacting residue of IgE-Fab antibody (Chain H & L) with B2D0J5 allergen

Residue	Closest	Distance	Specific Interactions	# HB	# vdW Clash	Surface Complementarity	Buried SASA
A:174:Ile	H:59:Tyr	3.5 A		0	0	0.72	25.50%
A:190:Arg	L:31:Thr L:67:Tyr L:30:Asn	2.9 A 3.6 A 3.7 A	2x hb, 1x clash to L:31:Thr 1x clash to L:67:Tyr	2	2	0.6	80.80%
A:193:Phe				0	0	0.11	26.90%
A:194:Asn	L:67:Tyr L:28:Arg	2.9 A 3.0 A	1x hb to L:28:Arg 1x hb to L:67:Tyr	2	0	0.51	58.90%
A:222:Tyr				0	0	0.1	98.40%
A:223:Leu				0	0	0.1	58.80%
A:224:Ser	H:102:Tyr	3.1 A		0	0	0.48	95.70%
A:225:Pro	H:102:Tyr L:31:Thr L:50:Ala	3.6 A 3.7 A 3.7 A		0	0	0.65	96.30%
A:226:Met	L:32:Tyr H:102:Tyr	3.6 A 3.7 A	1x clash to L:32:Tyr	0	1	0.86	61.10%
A:228:Ala	L:31:Thr L:53:Ser L:50:Ala	3.2 A 3.5 A 3.7 A		0	0	0.73	99.70%
A:229:Gly	L:50:Ala L:52:Ser	3.6 A 3.6 A		0	0	0.74	88.70%
A:230:Leu				0	0	0.26	99.30%
A:232:Lyn				0	0	0	6.00%
A:306:Val				0	0	0.22	8.70%
A:308:Thr	H:53:Tyr	3.0 A		0	0	0.84	68.20%
A:309:Tyr	H:55:Ser H:34:Tyr H:53:Tyr H:57:Asn	2.9 A 3.5 A 3.5 A 3.9 A	1x hb to H:55:Ser	1	0	0.75	79.10%
A:310:Gly	H:34:Tyr L:96:Tyr	3.0 A 3.8 A	1x hb to H:34:Tyr	1	0	0.67	61.90%
A:311:Ser	L:92:Leu H:101:Gly L:91:Ser L:96:Tyr L:93:Ser L:94:Ala	2.9 A 3.1 A 3.3 A 3.4 A 3.6 A 3.7 A	1x hb to L:92:Leu	1	0	0.77	82.50%

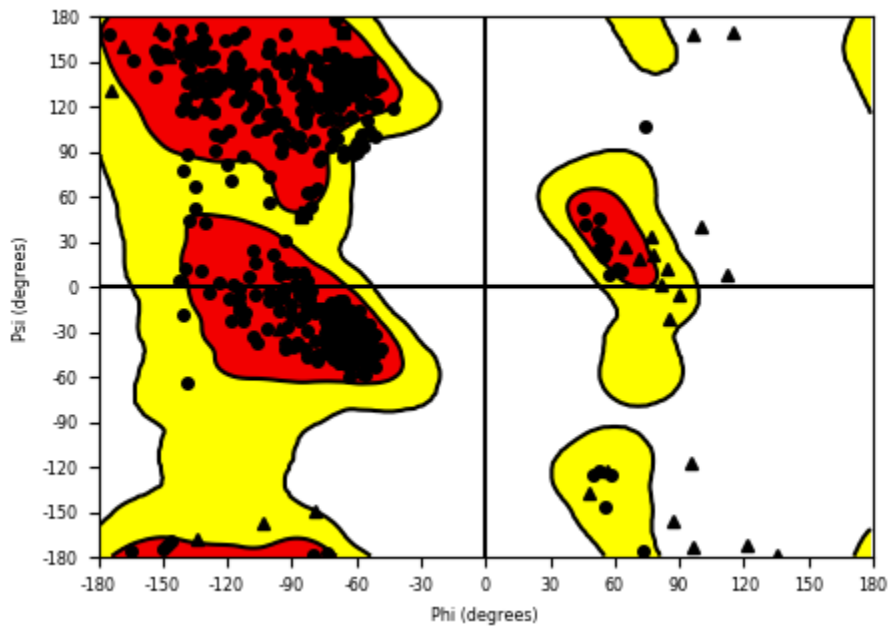
A:312:Asn	L:32:Tyr L:91:Ser H:102:Tyr	3.1 A 3.7 A 4.0 A		0	0	0.76	60.80%
A:313:Pro	H:102:Tyr H:101:Gly	2.9 A 4.0 A		0	0	0.8	90.40%
A:314:Phe	H:102:Tyr	2.8 A	1x hb to H:102:Tyr	1	0	0.8	98.80%
A:315:Ile				0	0	0	100.00%
A:316:Ser	H:100:Asp H:32:Gly	3.0 A 3.0 A	1x hb to H:100:Asp	1	0	0.7	92.40%
A:317:Asn	H:33:Tyr	3.0 A	1x hb to H:33:Tyr	1	0	0.46	98.50%
A:321:Asn				0	0	0	6.10%
A:322:Ile				0	0	0.34	15.90%
A:325:Asn	H:33:Tyr H:98:Arg H:105:Asp L:55:Gln	2.9 A 3.0 A 3.5 A 3.9 A	1x clash to H:33:Tyr 1x hb, 2x clash to H:98:Arg	1	3	0.68	77.30%
A:326:Gly	L:56:Ser L:55:Gln	3.1 A 3.3 A	1x hb to L:56:Ser	1	0	0.88	90.10%
A:327:Gln	H:100:Asp H:105:Asp L:49:Tyr L:55:Gln	2.8 A 3.3 A 3.7 A 3.9 A		0	0	0.78	93.00%
A:328:Val	L:49:Tyr	2.9 A		0	0	0.69	91.30%
A:329:Tyr	L:53:Ser L:52:Ser L:49:Tyr	3.0 A 3.1 A 3.5 A	1x hb to L:52:Ser	1	0	0.69	85.80%
A:330:Asp				0	0	0.32	50.70%
A:430:Ile	L:56:Ser	2.9 A	1x hb to L:56:Ser	1	0	0.94	45.50%
A:432:Lys	L:58:Val L:60:Ser L:54:Leu L:59:Pro	2.8 A 3.0 A 3.2 A 3.8 A	2x clash to L:54:Leu 1x hb to L:58:Val 1x hb to L:60:Ser	2	2	0.47	51.20%
A:556:Leu				0	0	0	7.00%
A:557:Asn	H:27:Ser H:26:Gly H:30:Ser H:31:Gly	2.8 A 3.3 A 3.4 A 3.8 A	1x hb to H:27:Ser	1	0	0.72	66.30%
H:1:Val				0	0	0	9.50%
H:25:Gly				0	0	0	8.30%
H:26:Gly	A:557:Asn	3.3 A		0	0	0	41.20%
H:27:Ser	A:557:Asn	2.8 A	1x hb to A:557:Asn	1	0	0.72	24.30%
H:30:Ser	A:557:Asn	3.4 A		0	0	0.86	44.20%

H:31:Gly	A:557:Asn	3.8 A		0	0	0.27	93.00%
H:32:Gly	A:316:Ser	3.0 A		0	0	0.58	95.20%
H:33:Tyr	A:325:Asn A:317:Asn	2.9 A 3.0 A	1x hb to A:317:Asn 1x clash to A:325:Asn	1	1	0.48	89.80%
H:34:Tyr	A:310:Gly A:309:Tyr	3.0 A 3.5 A	1x hb to A:310:Gly	1	0	0.69	87.20%
H:53:Tyr	A:308:Thr A:309:Tyr	3.0 A 3.5 A		0	0	0.84	90.50%
H:55:Ser	A:309:Tyr	2.9 A	1x hb to A:309:Tyr	1	0	0.91	17.70%
H:57:Asn	A:309:Tyr	3.9 A		0	0	0.52	30.10%
H:59:Tyr	A:174:Ile	3.5 A		0	0	0.67	34.10%
H:98:Arg	A:325:Asn	3.0 A	1x hb, 2x clash to A:325:Asn	1	2	0.55	88.20%
H:100:Asp	A:327:Gln A:316:Ser	2.8 A 3.0 A	1x hb to A:316:Ser	1	0	0.8	89.50%
H:101:Gly	A:311:Ser A:313:Pro	3.1 A 4.0 A		0	0	0.76	90.30%
H:102:Tyr	A:314:Phe A:313:Pro A:224:Ser A:225:Pro A:226:Met A:312:Asn	2.8 A 2.9 A 3.1 A 3.6 A 3.7 A 4.0 A	1x hb to A:314:Phe	1	0	0.83	95.00%
H:103:Thr				0	0	0.18	59.80%
H:105:Asp	A:327:Gln A:325:Asn	3.3 A 3.5 A		0	0	0.73	74.30%
H:106:Ile				0	0	0.3	29.10%
L:28:Arg	A:194:Asn	3.0 A	1x hb to A:194:Asn	1	0	0.94	11.60%
L:30:Asn	A:190:Arg	3.7 A		0	0	0.74	29.60%
L:31:Thr	A:190:Arg A:228:Ala A:225:Pro	2.9 A 3.2 A 3.7 A	2x hb, 1x clash to A:190:Arg	2	1	0.54	94.10%
L:32:Tyr	A:312:Asn A:226:Met	3.1 A 3.6 A	1x clash to A:226:Met	0	1	0.53	84.20%
L:34:Asn				0	0	0.06	0.00%
L:46:Leu				0	0	0.23	0.00%
L:49:Tyr	A:328:Val A:329:Tyr A:327:Gln	2.9 A 3.5 A 3.7 A		0	0	0.48	98.00%

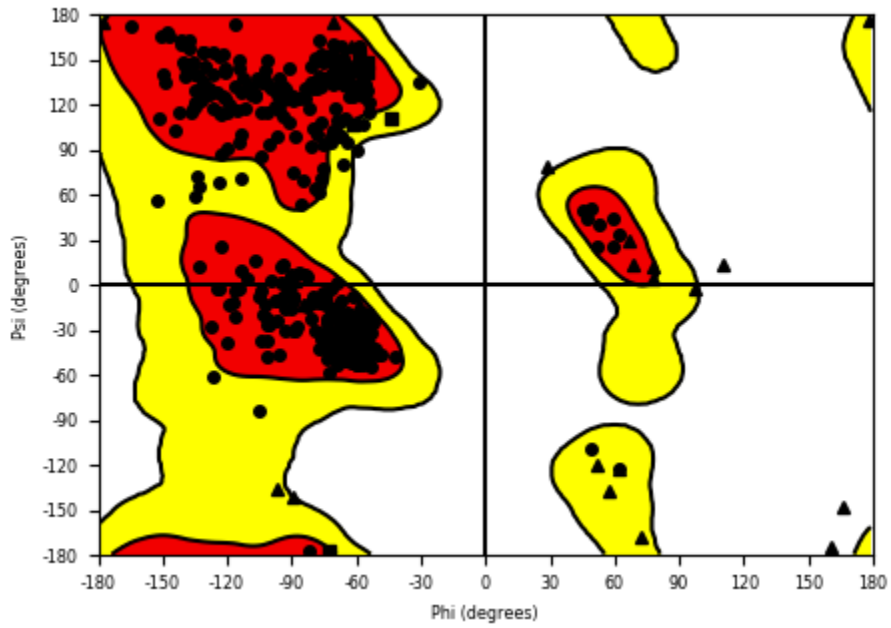
L:50:Ala	A:229:Gly A:225:Pro A:228:Ala	3.6 A 3.7 A 3.7 A		0	0	0.7	99.10%
L:52:Ser	A:329:Tyr A:229:Gly	3.1 A 3.6 A	1x hb to A:329:Tyr	1	0	0.81	55.40%
L:53:Ser	A:329:Tyr A:228:Ala	3.0 A 3.5 A		0	0	0.7	100.00%
L:54:Leu	A:432:Lys	3.2 A	2x clash to A:432:Lys	0	2	0.27	70.70%
L:55:Gln	A:326:Gly A:325:Asn A:327:Gln	3.3 A 3.9 A 3.9 A		0	0	0.78	89.70%
L:56:Ser	A:430:Ile A:326:Gly	2.9 A 3.1 A	1x hb to A:326:Gly 1x hb to A:430:Ile	2	0	0.91	75.30%
L:57:Gly				0	0	0.33	12.50%
L:58:Val	A:432:Lys	2.8 A	1x hb to A:432:Lys	1	0	0.37	72.70%
L:59:Pro	A:432:Lys	3.8 A		0	0	0	2.10%
L:60:Ser	A:432:Lys	3.0 A	1x hb to A:432:Lys	1	0	0.79	20.50%
L:67:Tyr	A:194:Asn A:190:Arg	2.9 A 3.6 A	1x clash to A:190:Arg 1x hb to A:194:Asn	1	1	0.38	54.80%
L:91:Ser	A:311:Ser A:312:Asn	3.3 A 3.7 A		0	0	0.75	96.40%
L:92:Leu	A:311:Ser	2.9 A	1x hb to A:311:Ser	1	0	0.65	30.00%
L:93:Ser	A:311:Ser	3.6 A		0	0	0.82	12.80%
L:94:Ala	A:311:Ser	3.7 A		0	0	0.8	27.70%
L:96:Tyr	A:311:Ser A:310:Gly	3.4 A 3.8 A		0	0	0.65	98.10%



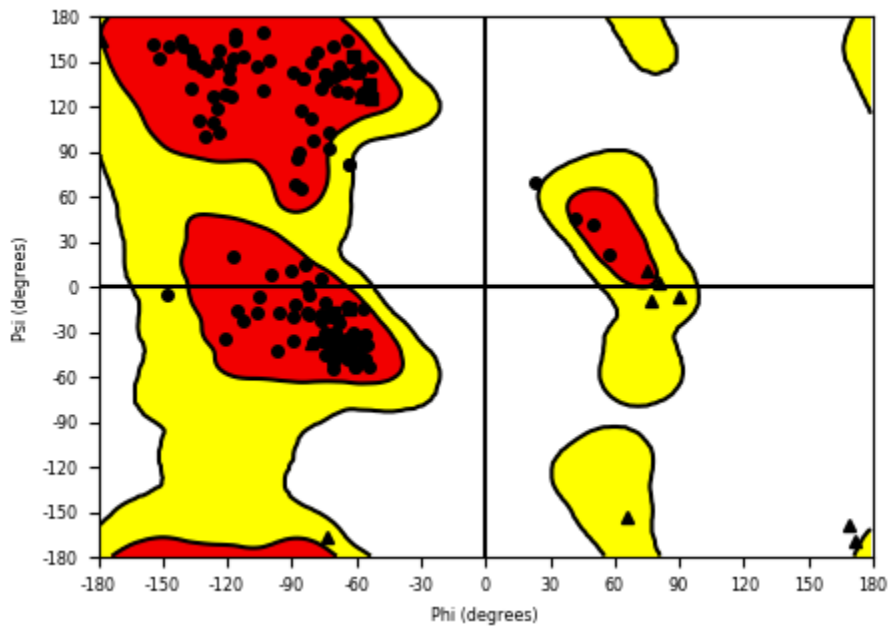
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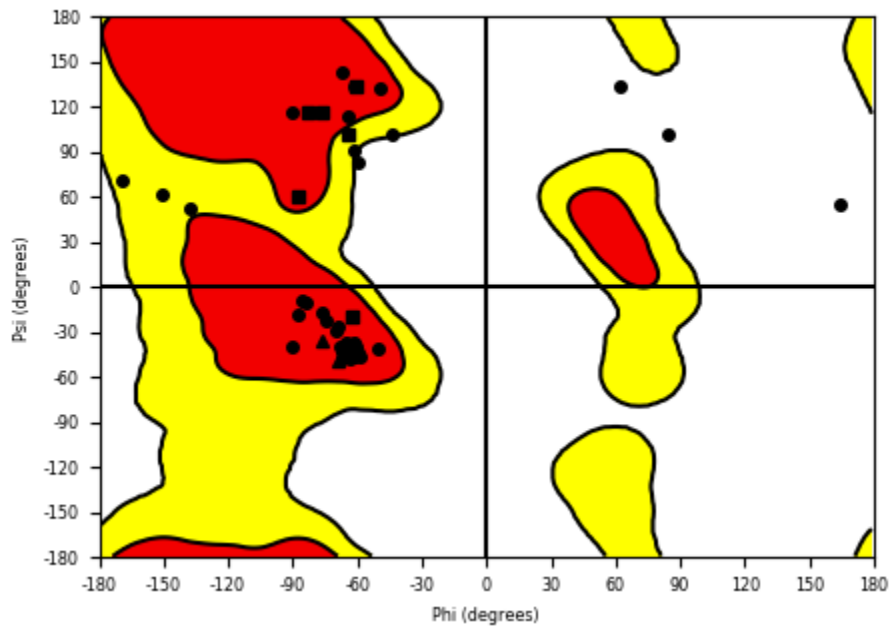
B2D0J5



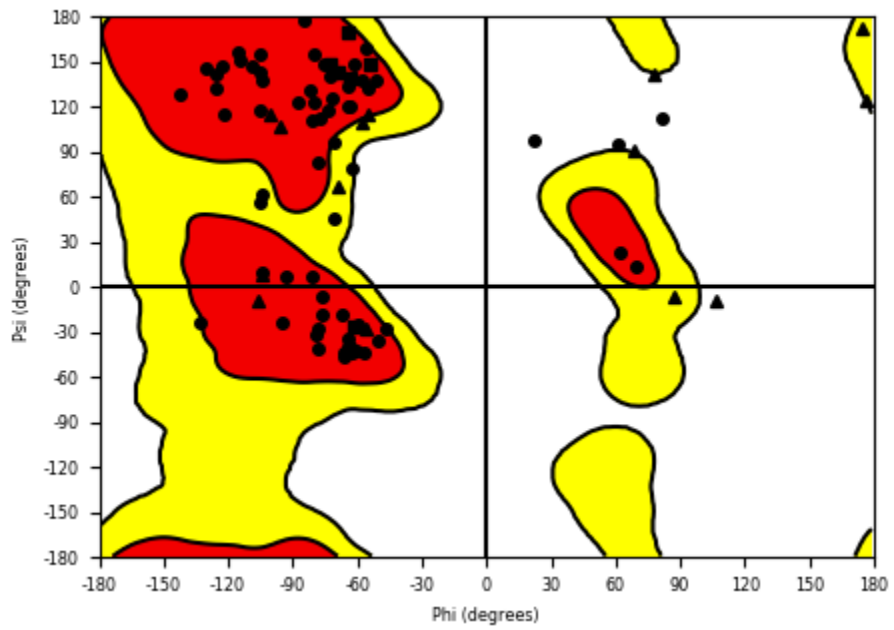
C9WMM5



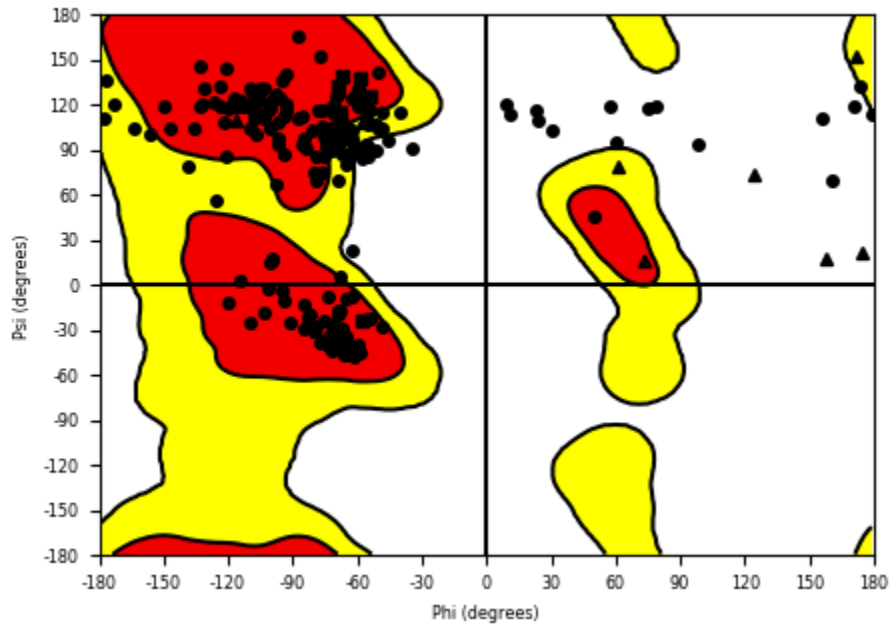
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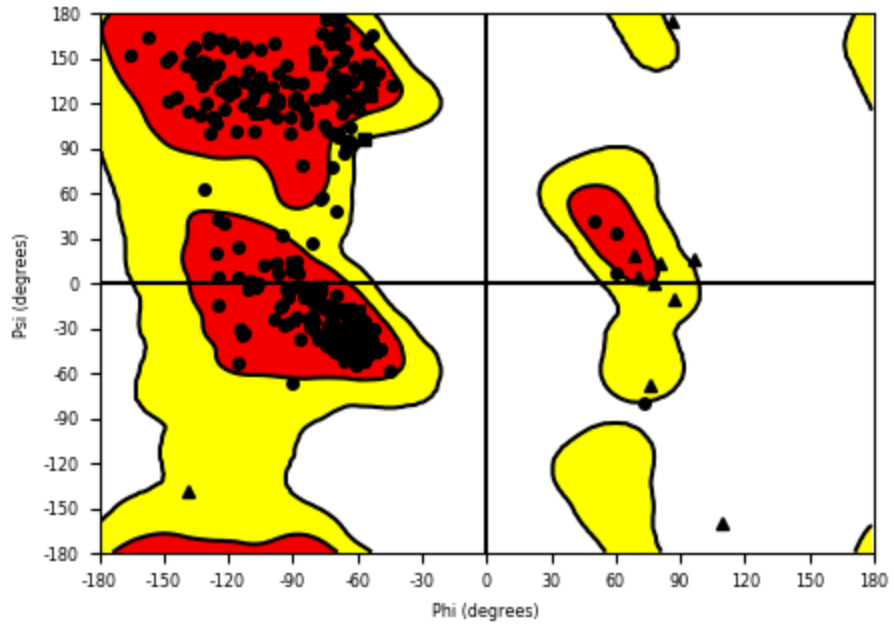
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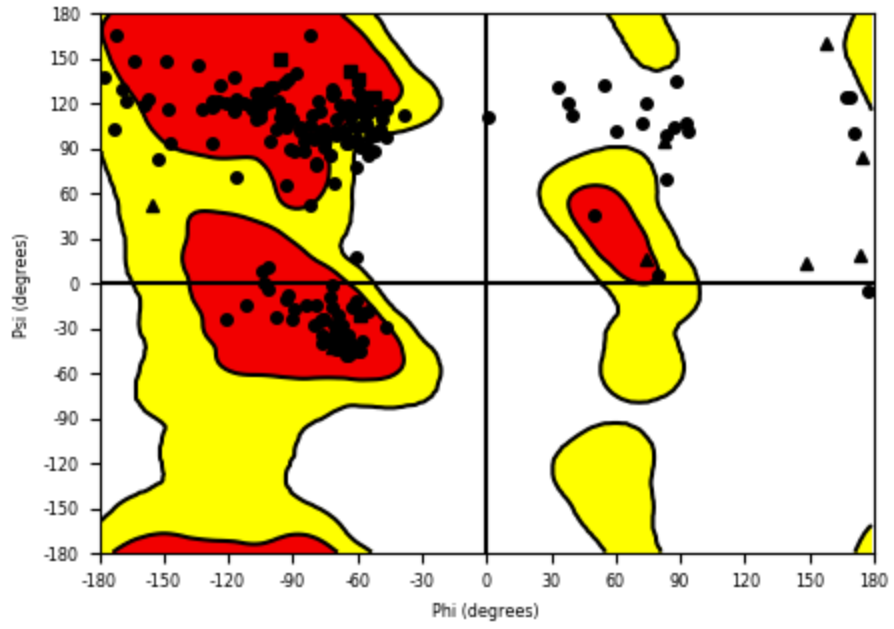
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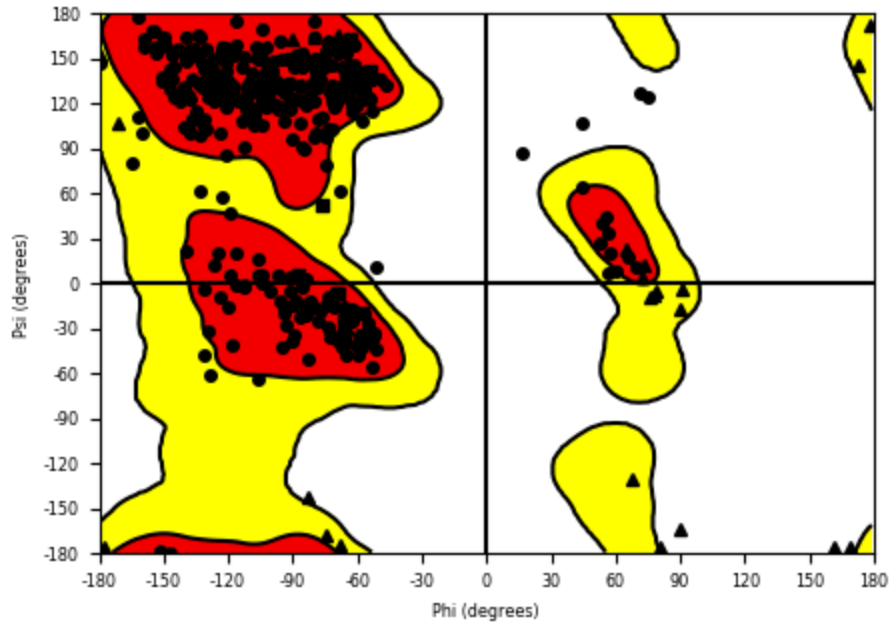
Q5BLY4



Q5BLY5



Q5EF78



Q8MQS8

Supplementary Figure 1. Ramachandran plots of modeled allergens proteins