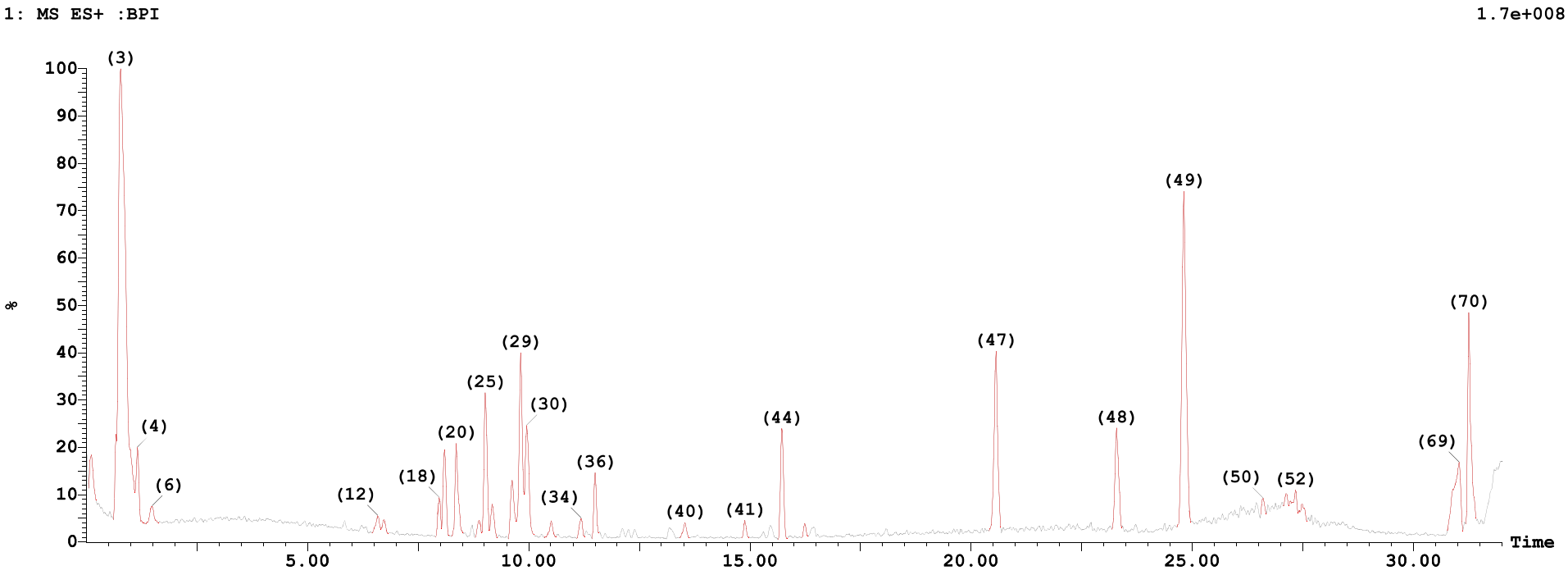
Center for DRUG DISCOVERY RESEARCH and DEVELOPMENT

Openlynx Report -

Sample: 77 Vial:1:A,7 ID:
File:A21 98 Date:01-Mar-2021 Time:16:32:00
Description:K.i

Printed: Sun Mar 07 11:22:28 2021



Peak Number	Time	AreaAbs	Area %Total
1	0.11	1114017.8750	1.14
3	0.77	31786466.0000	32.44
4	1.15	1911046.1250	1.95
6	1.48	658843.1250	0.67
12	6.59	577149.5625	0.59
13	6.73	396076.0938	0.40
18	7.98	802057.6875	0.82
19	8.10	2165250.7500	2.21
20	8.36	2557391.5000	2.61
24	8.88	392499.6563	0.40
25	9.02	3792261.0000	3.87
26	9.17	788109.4375	0.80
28	9.63	1433645.7500	1.46
29	9.82	4733987.0000	4.83

Sample: 77
File:A21 98
Description:K.i

Vial:1:A,7
Date:01-Mar-2021

ID:
Time:16:32:00

Printed: Sun Mar 07 11:22:28 2021

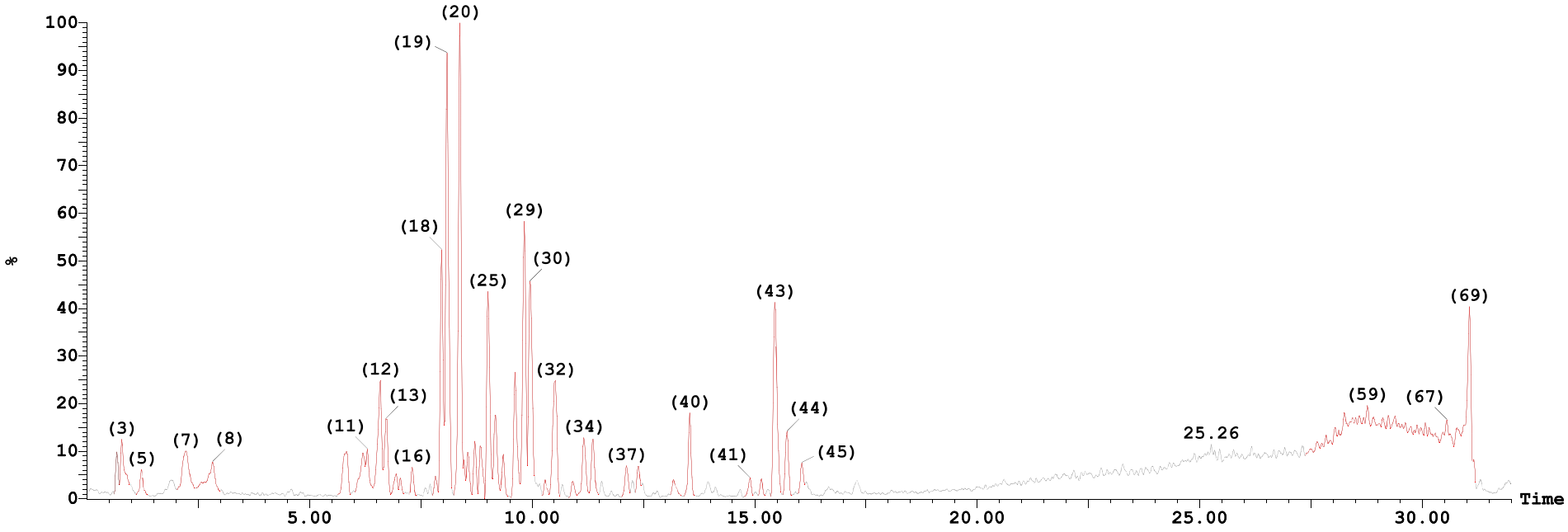
30	9.96	3349827.7500	3.42
32	10.51	481729.3438	0.49
34	11.19	561637.6875	0.57
36	11.50	1411218.8750	1.44
40	13.53	455450.7188	0.46
41	14.89	395022.6250	0.40
44	15.72	3172072.2500	3.24
46	16.24	299066.5938	0.31
47	20.56	5812398.0000	5.93
48	23.29	3342056.5000	3.41
49	24.82	13181537.0000	13.45
50	26.60	383974.8438	0.39
51	27.12	361518.7188	0.37
52	27.33	851184.0000	0.87
53	27.49	572736.3125	0.58
69	31.03	4473581.5000	4.57
70	31.26	5778681.0000	5.90

Openlynx Report -

Sample: 77 Vial:1:A,7 ID:
File:A21 98 Date:01-Mar-2021 Time:16:32:00
Description:K.i

Printed: Sun Mar 07 11:22:28 2021

2: MS ES- :BPI 9.5e+006



Peak Number	Time	AreaAbs	Area %Total
2	0.68	41650.7305	0.49
3	0.78	75226.0313	0.88
5	1.23	40098.3711	0.47
7	2.22	128286.4844	1.50
8	2.83	96522.4609	1.13
9	5.83	116226.4766	1.36
10	6.20	84879.3750	0.99
11	6.30	58150.9805	0.68
12	6.60	213067.3438	2.49
13	6.72	135151.4375	1.58
14	6.94	35152.2422	0.41
15	7.05	18913.4043	0.22
16	7.31	36034.0352	0.42
17	7.83	22579.4609	0.26

Sample: 77 Vial:1:A,7 ID:
File:A21 98 Date:01-Mar-2021 Time:16:32:00
Description:K.i

Printed: Sun Mar 07 11:22:28 2021

18	7.97	256968.7656	3.00
19	8.09	575091.0625	6.72
20	8.38	724580.3750	8.47
21	8.47	28295.2070	0.33
22	8.56	60617.0078	0.71
23	8.71	69412.0156	0.81
24	8.84	86279.0000	1.01
25	9.01	305223.9375	3.57
26	9.18	106232.1250	1.24
27	9.36	51806.8594	0.61
28	9.62	188508.3906	2.20
29	9.83	370693.2813	4.33
30	9.95	317302.4688	3.71
31	10.29	20783.8984	0.24
32	10.52	249557.7969	2.92
33	10.92	23251.9531	0.27
34	11.16	95376.6953	1.11
35	11.37	85686.3281	1.00
37	12.12	45977.2188	0.54
38	12.38	30247.1895	0.35
39	13.18	31592.7949	0.37
40	13.54	118888.5078	1.39
41	14.89	26042.1211	0.30
42	15.15	20796.0430	0.24
43	15.45	368515.9063	4.31
44	15.73	105201.7031	1.23
45	16.06	33724.3672	0.39
54	27.64	49688.4375	0.58
55	27.84	91065.8984	1.06
56	28.04	55482.2500	0.65
57	28.24	169695.0781	1.98
58	28.59	264669.0000	3.09
59	28.76	182338.6250	2.13
60	28.90	211917.3125	2.48
61	29.11	94679.0938	1.11
62	29.23	97642.6250	1.14
63	29.39	452805.7813	5.29
64	29.88	208989.7344	2.44
65	30.07	78988.0156	0.92
66	30.15	227651.7813	2.66
67	30.55	275451.7813	3.22
68	30.78	144205.7656	1.68
69	31.06	455144.0938	5.32

Sample: 77 Vial:1:A,7 ID:
File:A21 98 Date:01-Mar-2021 Time:16:32:00
Description:K.i

Printed: Sun Mar 07 11:22:28 2021

PUMP

Waters ACQUITY QSM

Solvent A Name:	Water + 0.1 % Formic acid
Solvent B Name:	Methanol+0.1% Formic acid
Solvent C Name:	Methanol 90%+ water10%
Solvent D Name:	Acetonitrile
Low Pressure Limit:	0 psi
High Pressure Limit:	14852 psi
Seal Wash Period:	30.00 min

Gradient

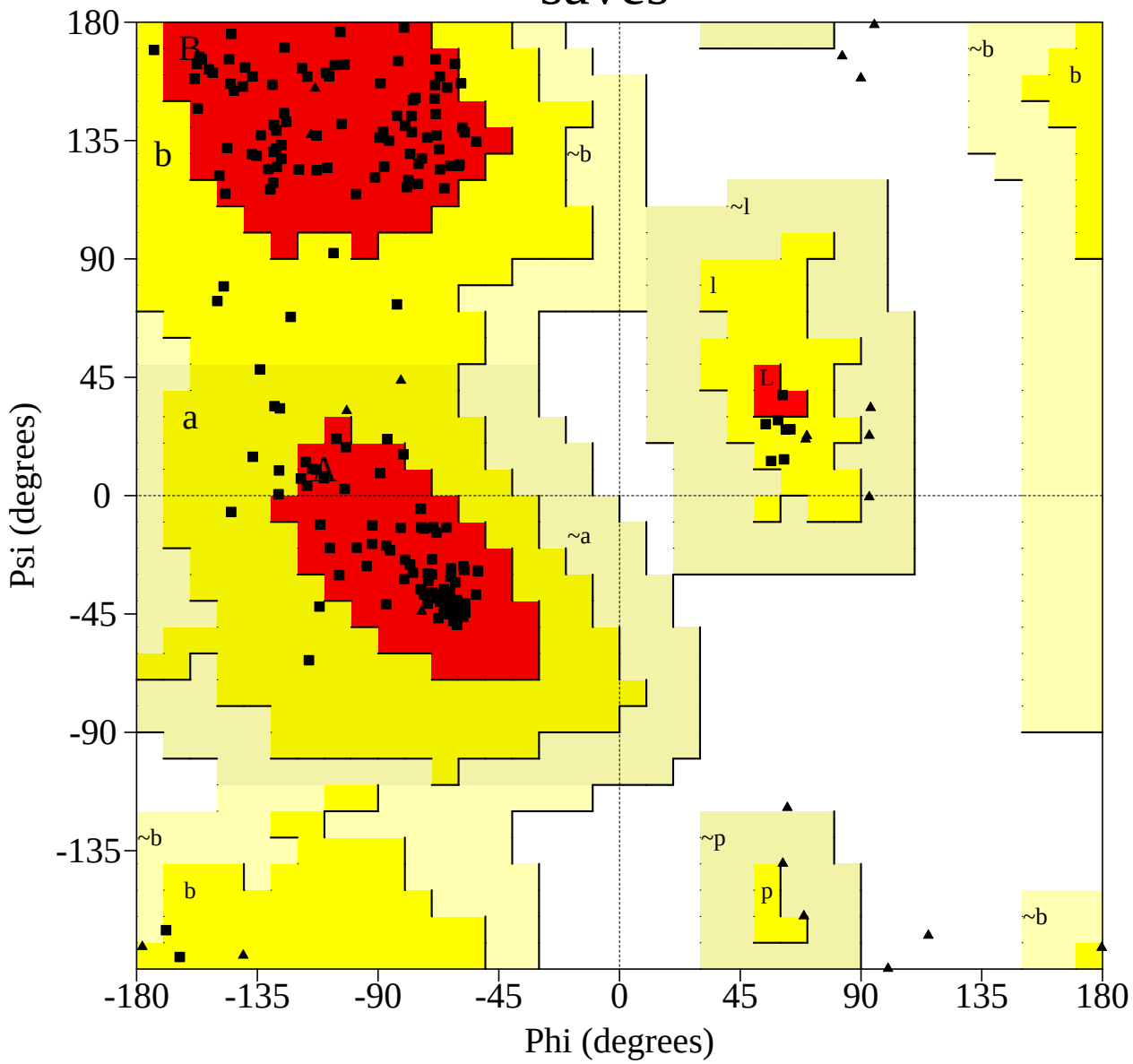
Time (min)	Flow Rate	A%	B%	Curve
Initial	0.200	90.0	0.0	0.0
2.00	0.200	90.0	0.0	0.0
5.00	0.200	70.0	0.0	0.0
15.00	0.200	30.0	0.0	0.0
22.00	0.200	10.0	0.0	0.0
25.00	0.200	10.0	0.0	0.0
26.00	0.200	0.0	0.0	0.0
29.00	0.200	0.0	0.0	0.0
32.00	0.200	90.0	0.0	0.0

Comment:

PROCHECK

Ramachandran Plot

saves



Plot statistics

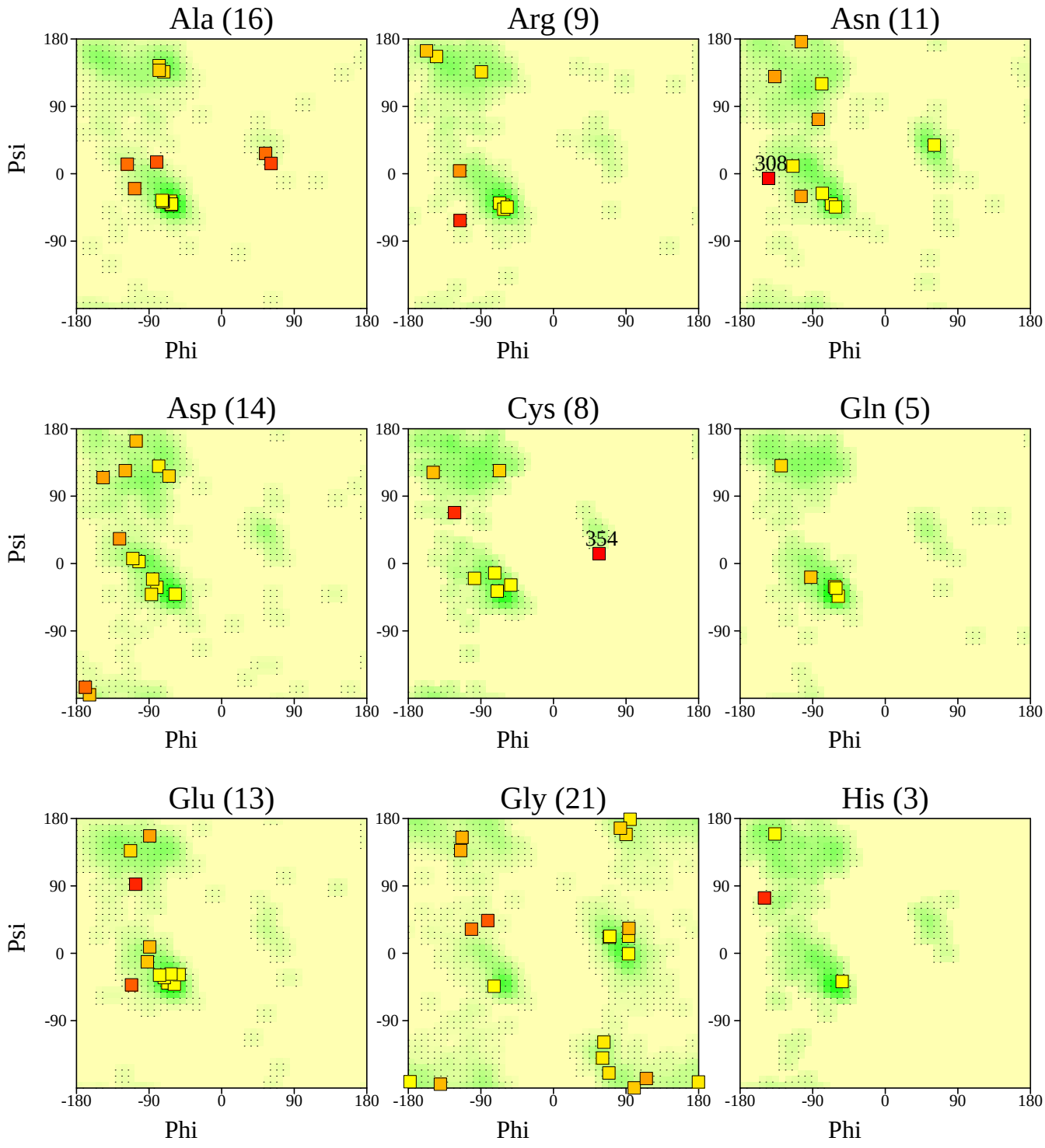
Residues in most favoured regions [A,B,L]	163	87.2%
Residues in additional allowed regions [a,b,l,p]	24	12.8%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%
Residues in disallowed regions	0	0.0%
	----	------
Number of non-glycine and non-proline residues	187	100.0%
Number of end-residues (excl. Gly and Pro)	2	
Number of glycine residues (shown as triangles)	21	
Number of proline residues	7	

Total number of residues	217	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

Ramachandran plots for all residue types

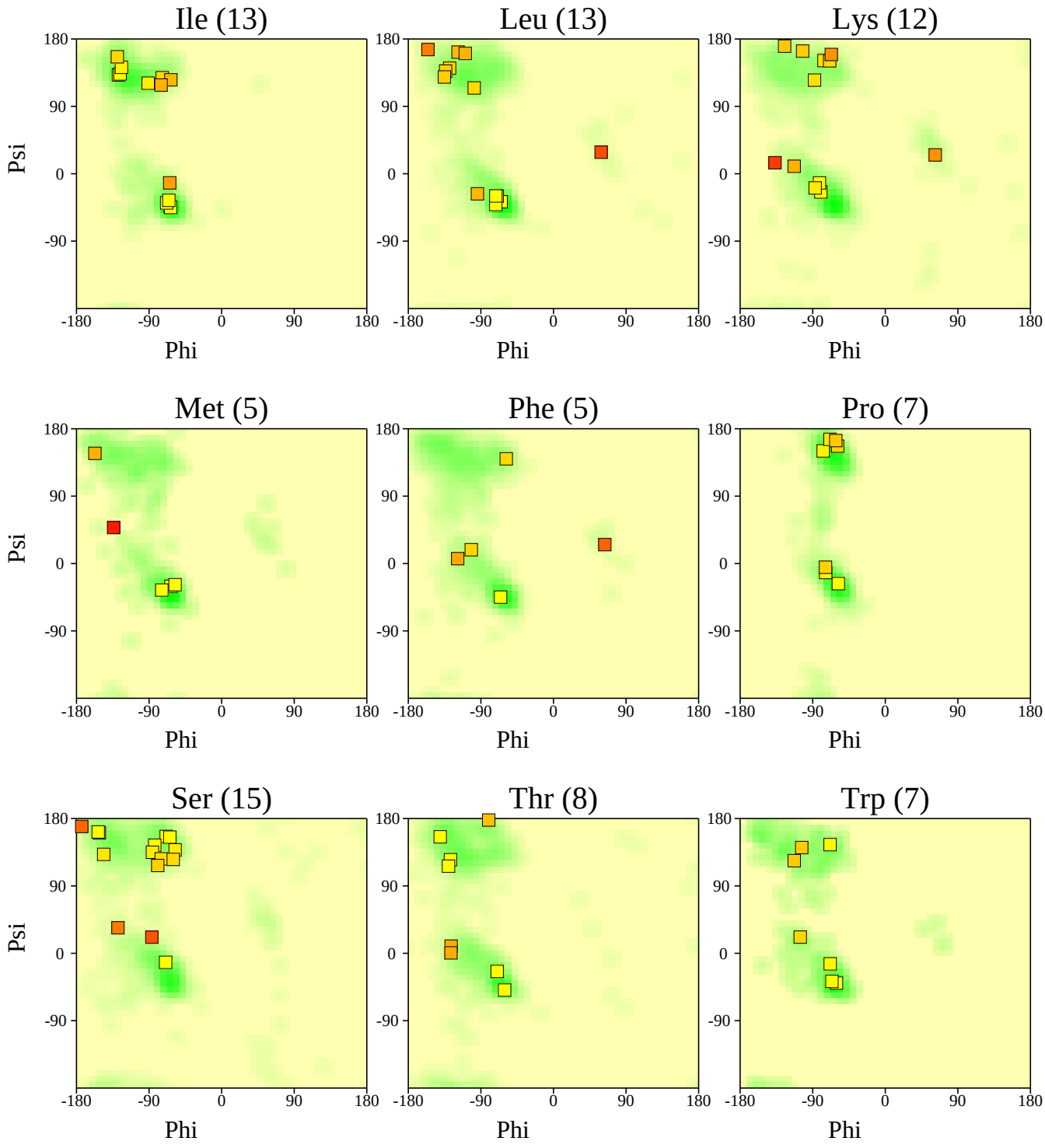
saves



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

Ramachandran plots for all residue types

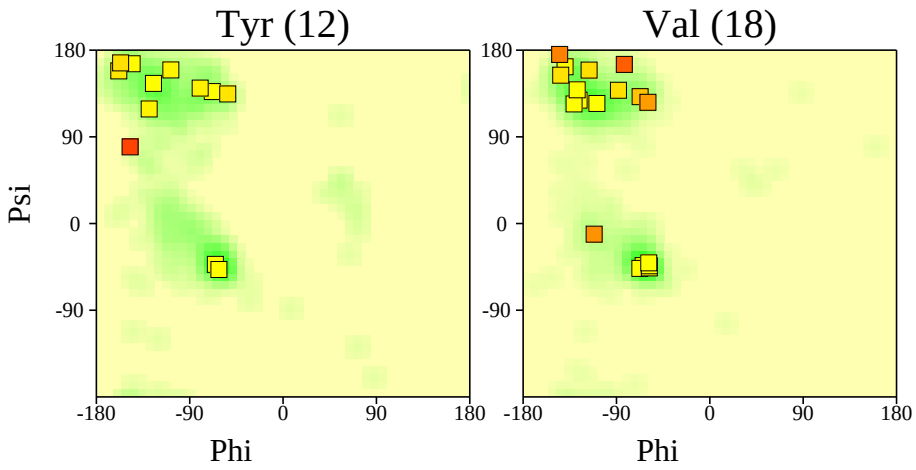
saves



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

Ramachandran plots for all residue types

saves

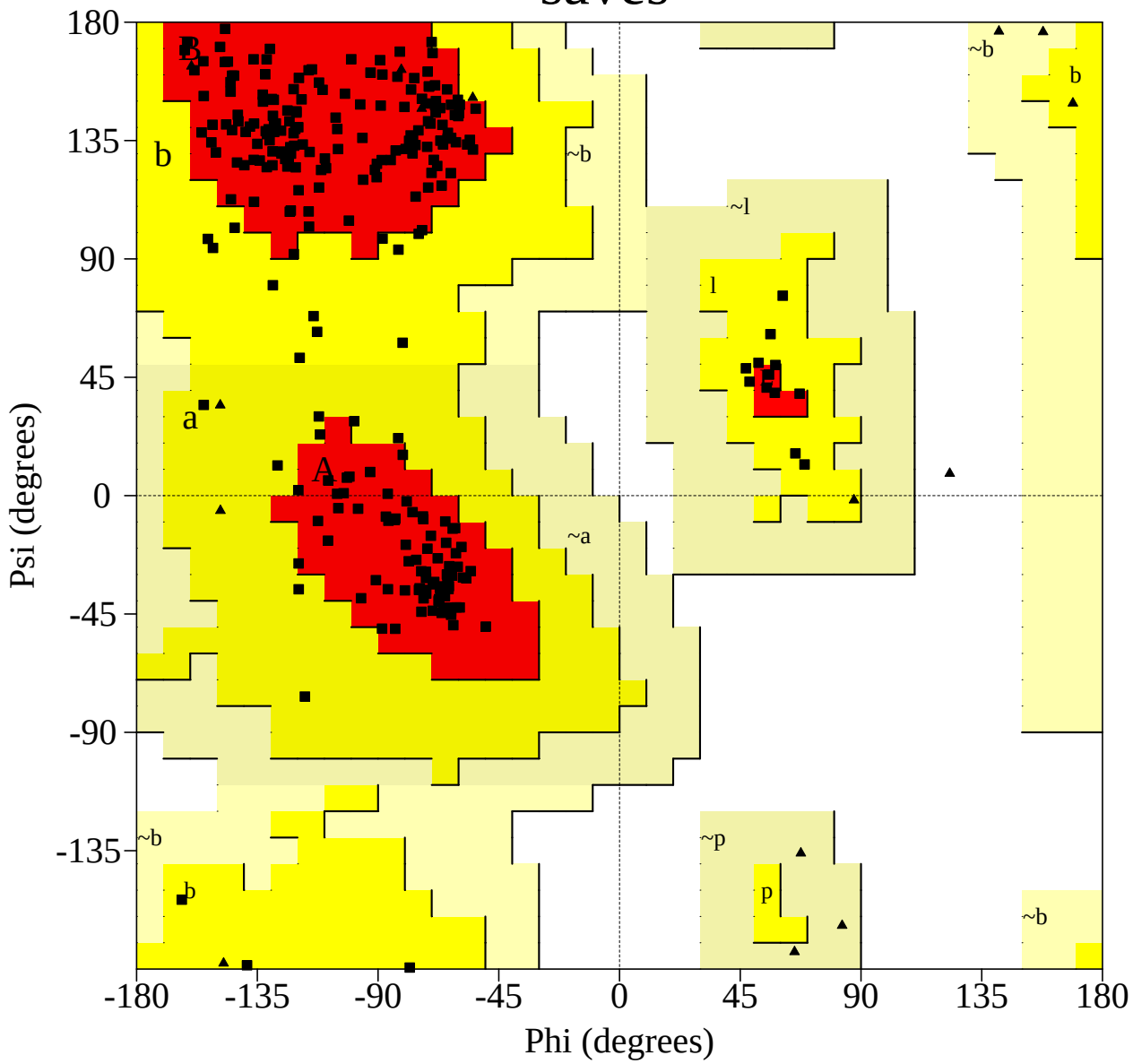


Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

Ramachandran Plot

saves



Plot statistics

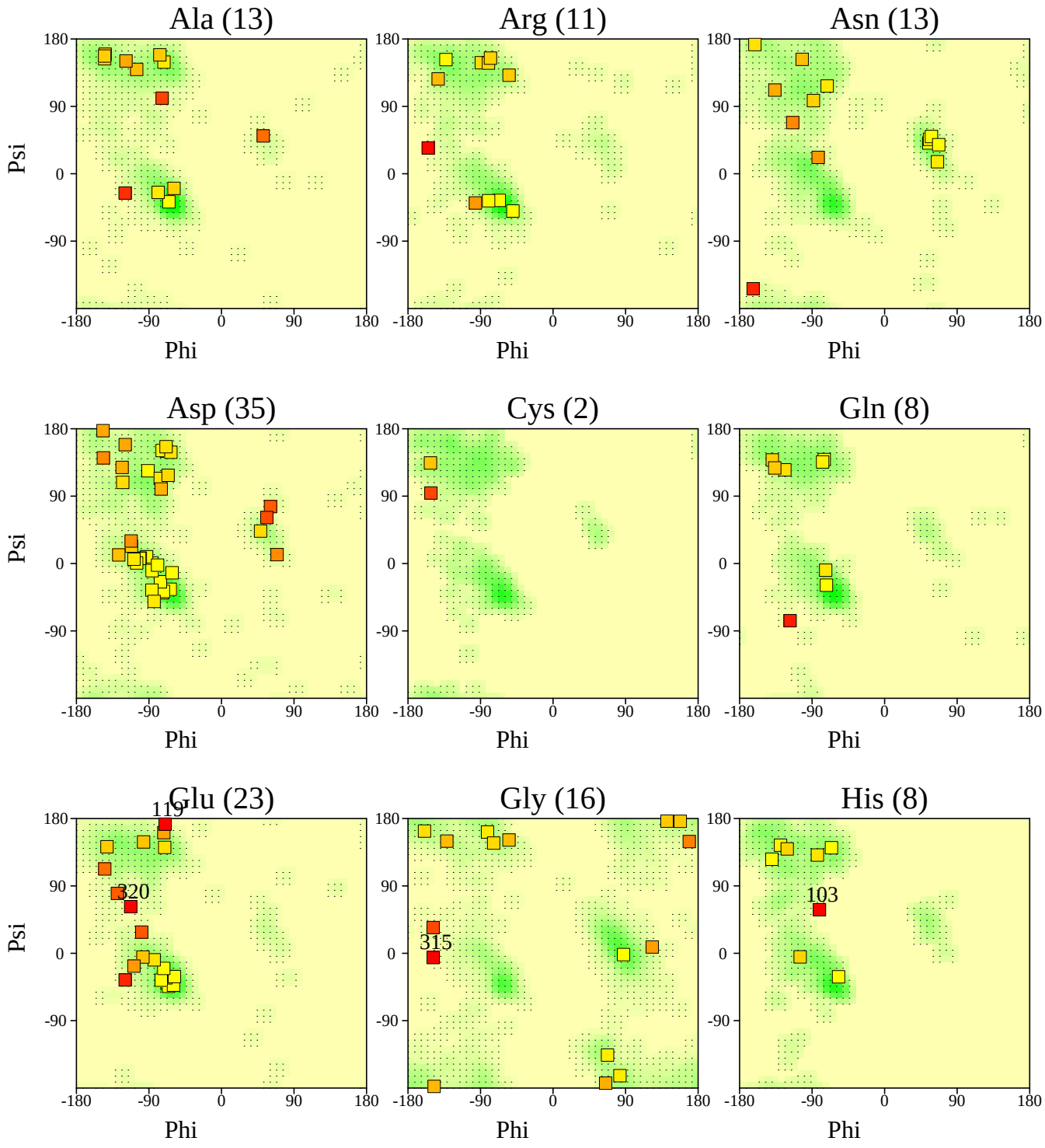
Residues in most favoured regions [A,B,L]	227	88.7%
Residues in additional allowed regions [a,b,l,p]	29	11.3%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%
Residues in disallowed regions	0	0.0%
	----	------
Number of non-glycine and non-proline residues	256	100.0%
Number of end-residues (excl. Gly and Pro)	2	
Number of glycine residues (shown as triangles)	16	
Number of proline residues	17	

Total number of residues	291	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

Ramachandran plots for all residue types

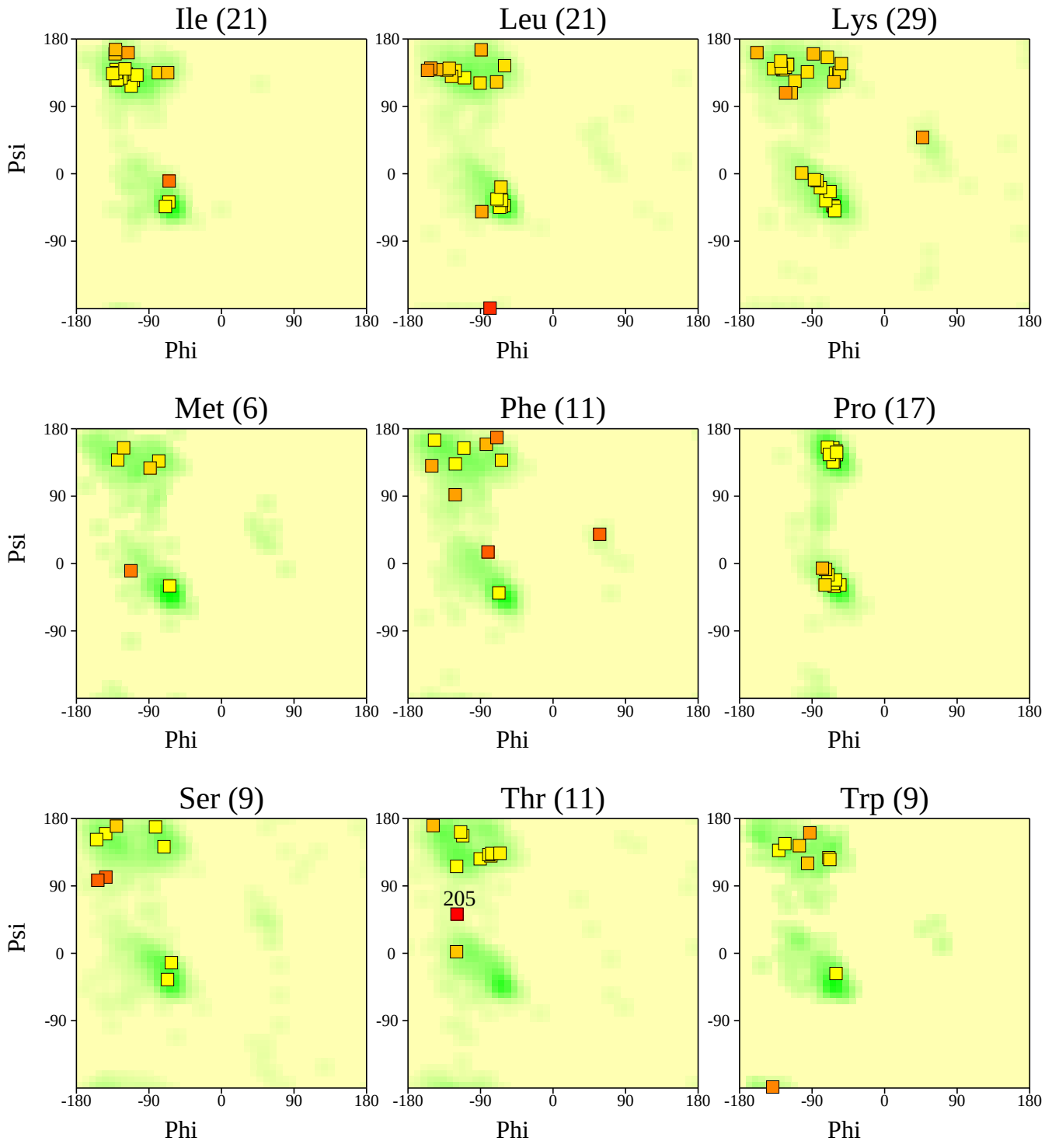
saves



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

Ramachandran plots for all residue types

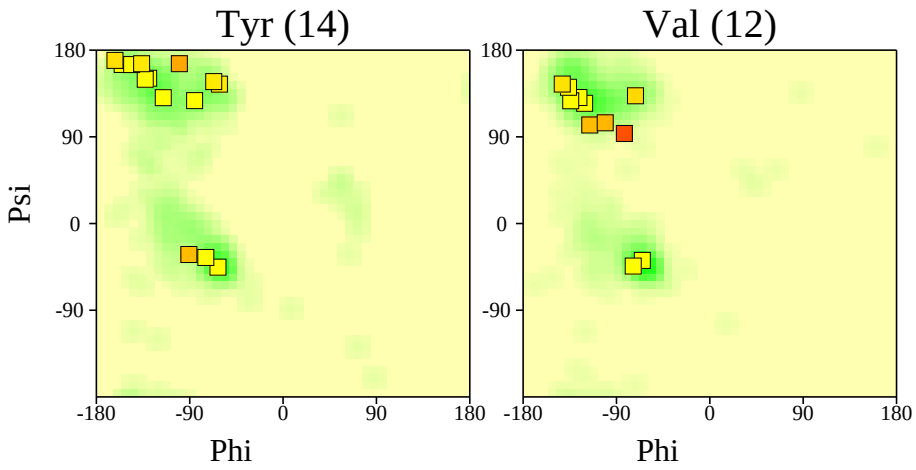
saves



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

Ramachandran plots for all residue types

saves



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.