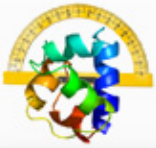

Protein Structure Validation Suite (PSVS)

PSVS report for 75-Sirt1

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PSVS report for 75-Sirt1

Software Environment

Software for structure quality evaluation:

DSSP	DsspCMBI-April-2000
pdbstat	PdbStat-5.9 Version
AutoAssign	Version 2.4.0 (uses only AVS scripts)
RPF analysis	ASDP-1.0
PDB validation	Version 8.061
Verify3D	Version 1.0 corrected by Aneerban
ProsaII	Prosa2003
PROCHECK	Version 3.5.4
MolMol	Version 2K.2

MolProbity programs:

cluster	1999
clashlistcluster	1999 (corrected by Aneerban)
mage	Version 6.35.040409
prekin	Version 6.35.040406
reduce	Version 2.14
probe	Version 2.6

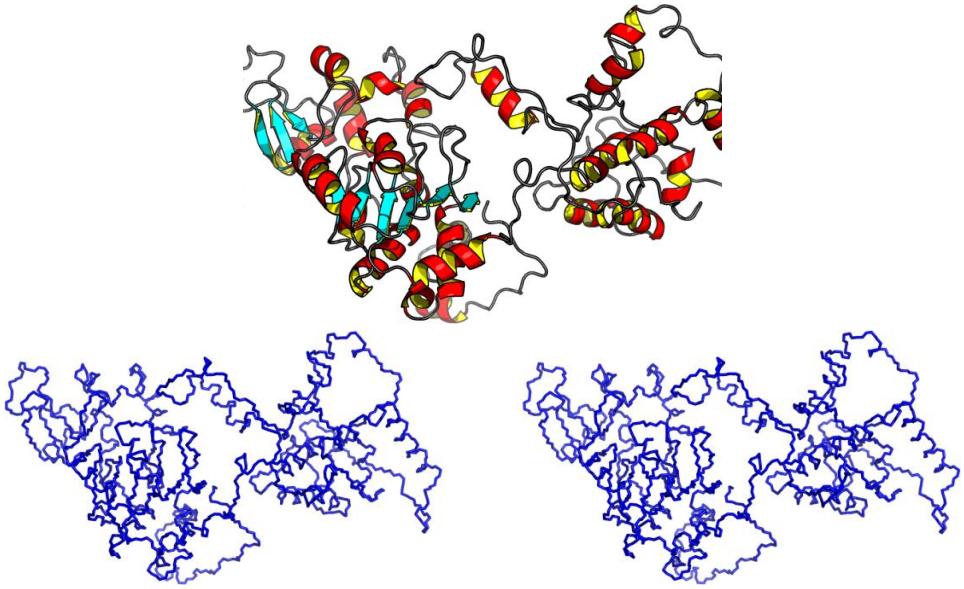
Other Software:

PERL	Version 5.8.0
convert	ImageMagick 5.5.6
ps2pdf	Ghostscript 7.05
htmldoc	v1.9
gnuplot	Version 3.7 patchlevel 3
jpegtopnm	year 2000
pnmcrop	year 2000
pnmtojpeg	year 2000

Structure Quality Analysis for NAME

Analyses performed for all residues.
Procheck analysis,RMSD calculation and structure superimposition are based on: all residues

NESG ID:	NAME
PDB ID:	
Deposition date:	
Common Name:	
Class:	
Length (a.a.):	537
Organism:	
SwissProt / TrEMBL ID:	
# models:	1
Oligomerization:	monomer
Molecular weight:	58785



Secondary Structure Elements:
alpha helices:
beta strands:

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
92.2%	7.8%	0.0%	0.0%

Ramachandran Plot Summary for selected residues[3] from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
98.7%	1.1%	0.2%		

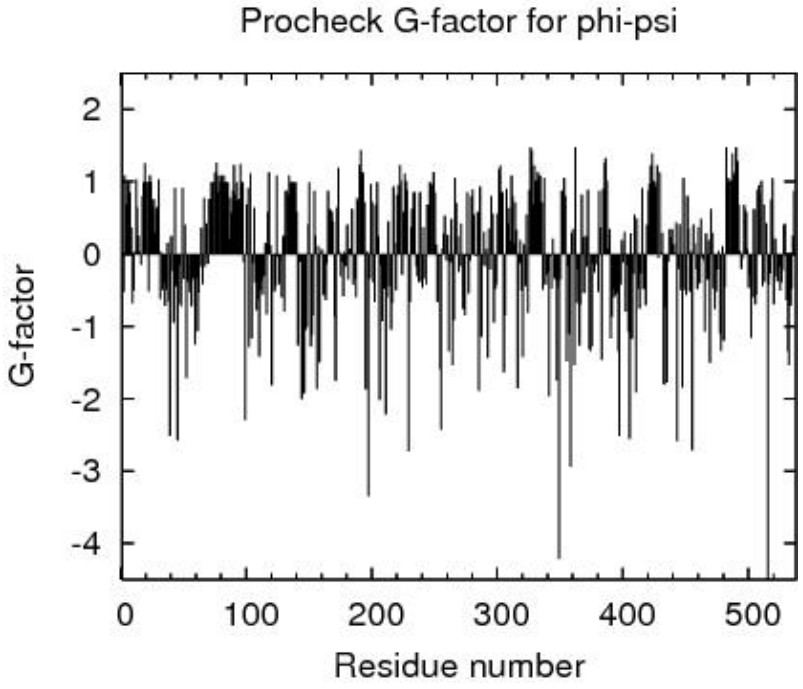
Global quality scores

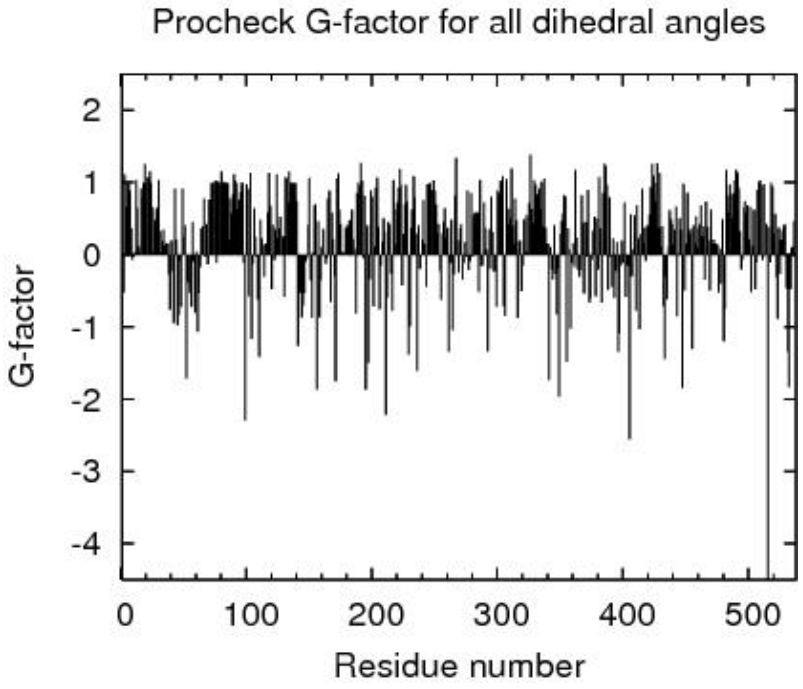
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)[3]*	*Procheck (all)[3]*	*MolProbity Clashscore*
-Raw score	0.36	0.59	-0.01	0.22	4.84
Z-score[1]	-1.61	-0.25	0.28	1.30	0.69

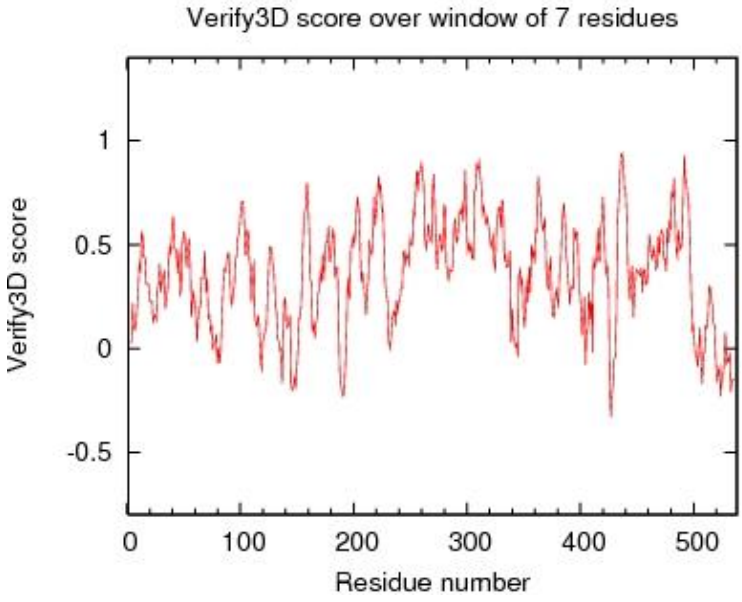
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

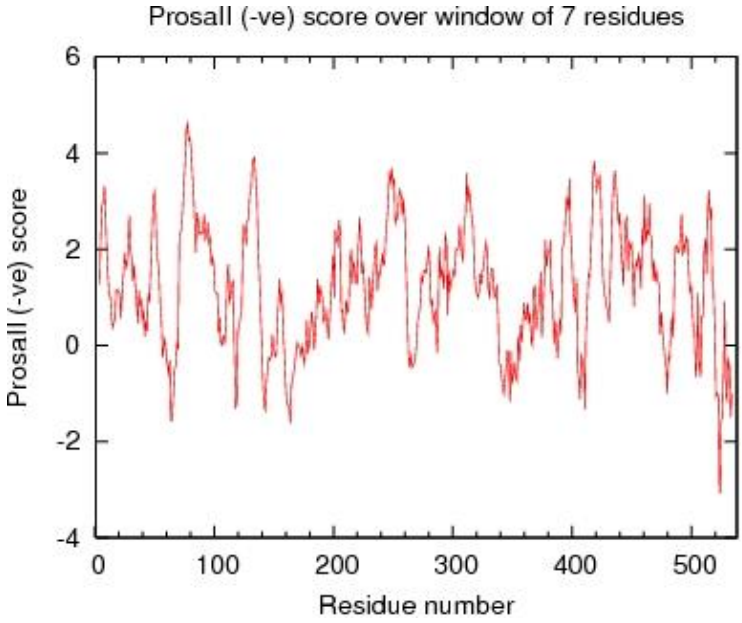
Number of close contacts (within 2.2 Å):	0
RMS deviation for bond angles:	1.3 °
RMS deviation for bond lengths:	0.017 Å

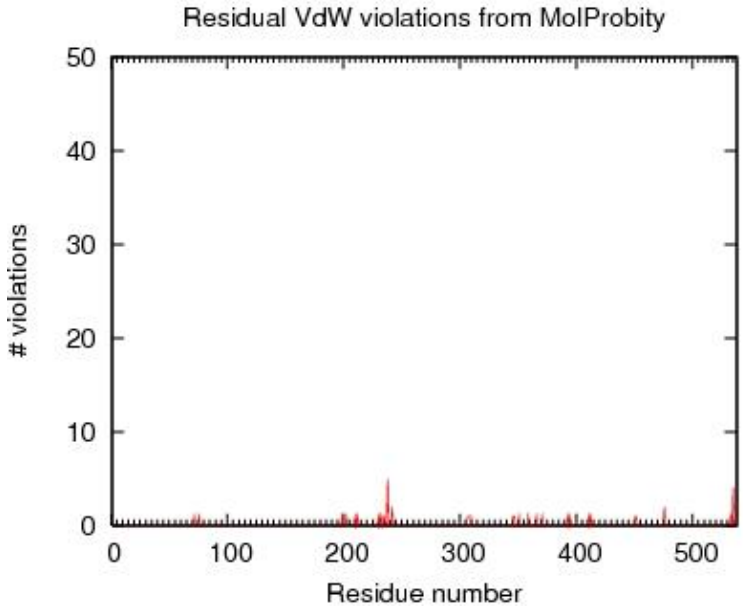
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[3]Selected residues: all

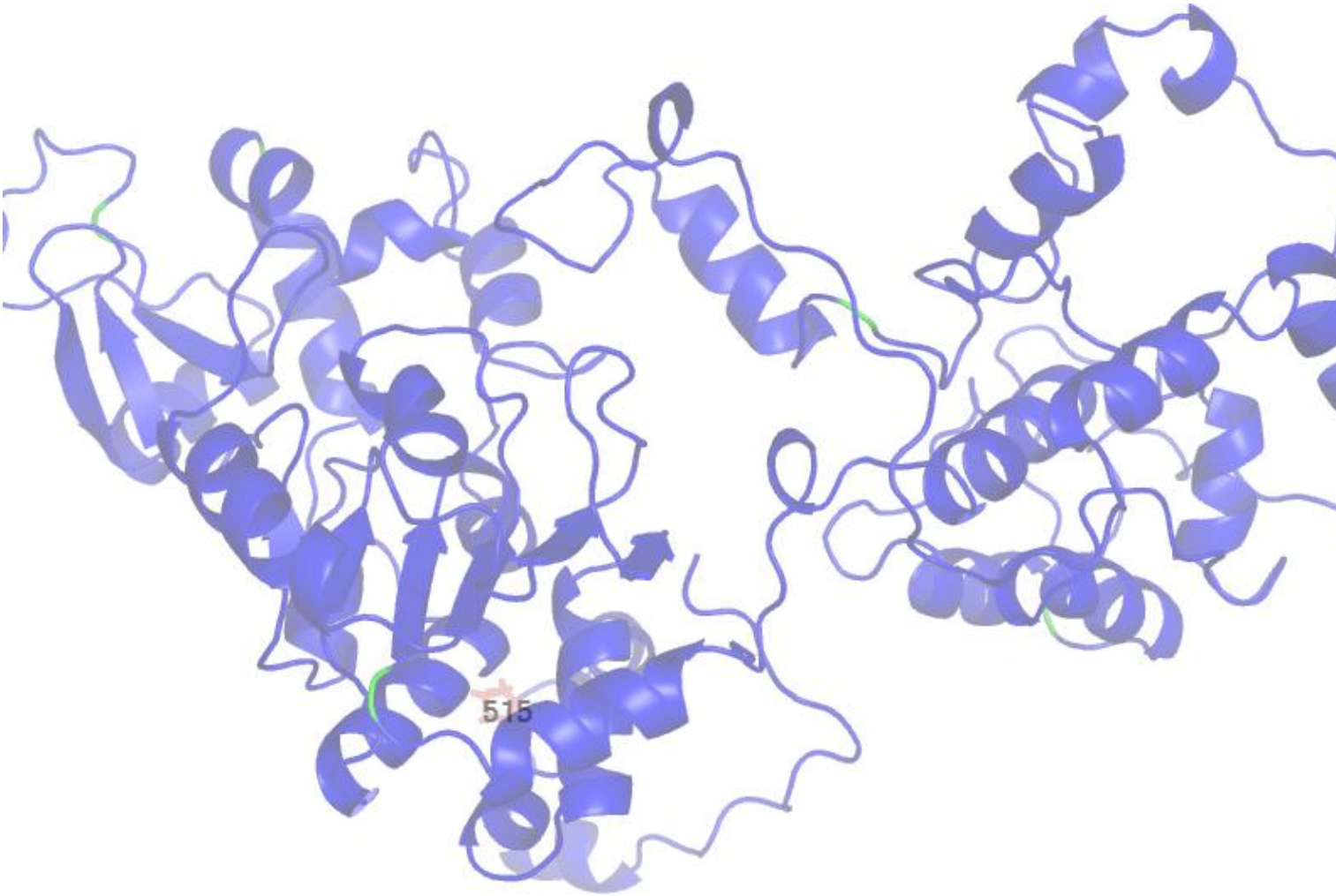

Procheck G-factor for phi-psi
G-factor
2
1
0
-1
-2
-3
-4
0
100
200
300
400
500
Residue number


Procheck G-factor for all dihedral angles
G-factor
2
1
0
-1
-2
-3
-4
0
100
200
300
400
500
Residue number


Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
0
100
200
300
400
500
Residue number


ProsaII (-ve) score over window of 7 residues
ProsaII (-ve) score
6
4
2
0
-2
-4
0
100
200
300
400
500
Residue number





Residue Plot of Ramachandran anlysis(based on data from Richardson Lab's Molprobity)

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Summary of structure quality factors

Analyses performed for all residues.

Total structures computed	currently unknown		
Number of structures used	1		
Structure Quality Factors - overall statistics			
	Mean score	SD	Z-score [g]
Procheck G-factor [e] (phi / psi only)	-0.01	N/A	0.28
Procheck G-factor [e] (all dihedral angles)	0.22	N/A	1.30
Verify3D	0.36	0.0000	-1.61
ProsaII (-ve)	0.59	0.0000	-0.25
MolProbity clashscore	4.84	0.0000	0.69
Ramachandran Plot Summary from Procheck			
Most favoured regions	92.2%		
Additionally allowed regions	7.8%		
Generously allowed regions	0.0%		
Disallowed regions	0.0%		
Ramachandran Plot Statistics from Richardson's lab			
Most favoured regions	98.7%		
Allowed regions	1.1%		
Disallowed regions	0.2%		

[f] Residues selected based on: all residues

Selected residue ranges: all

[g] With respect to mean and standard deviation for for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

Generated using PSVS 1.5

Detailed results of 75-Sirt1 by PSVS

Output from PDBStat

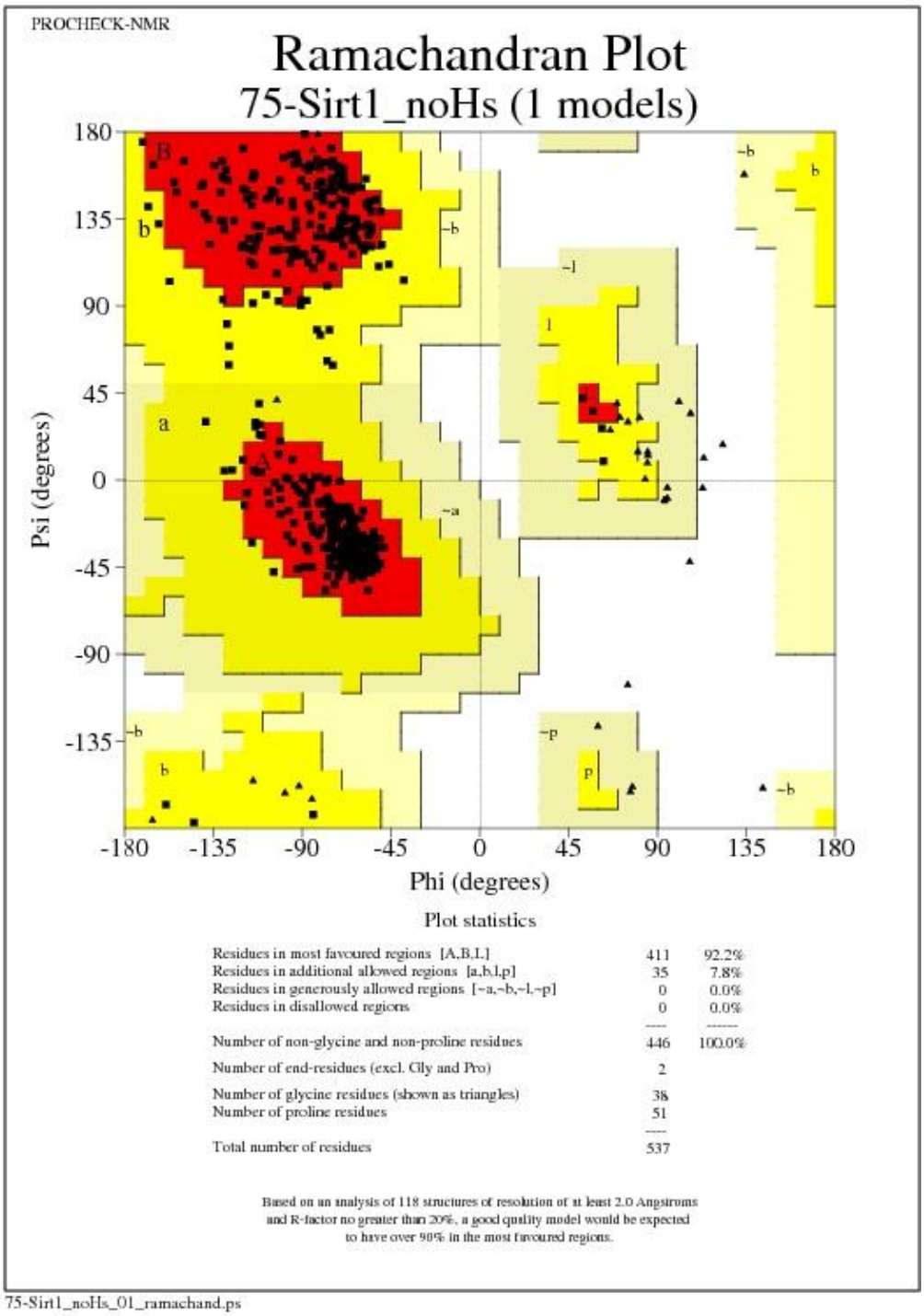
Output from PROCHECK

Ramachandran Plot for all models

Text summary of Ramachandran Plot

```
 +----------<<< P  R  O  C  H  E  C  K     S  U  M  M  A  R  Y  >>>----------+
 |                                                                            |
 | 75-Sirt1_noHs_000.rin   0.0                                  537 residues  |
 |                                                                            |
 | Ramachandran plot:   92.2% core    7.8% allow    0.0% gener    0.0% disall |
 |                                                                            |
+| All Ramachandrans:    3 labelled residues (out of 535)                     |
 | Chi1-chi2 plots:      0 labelled residues (out of 311)                     |
```

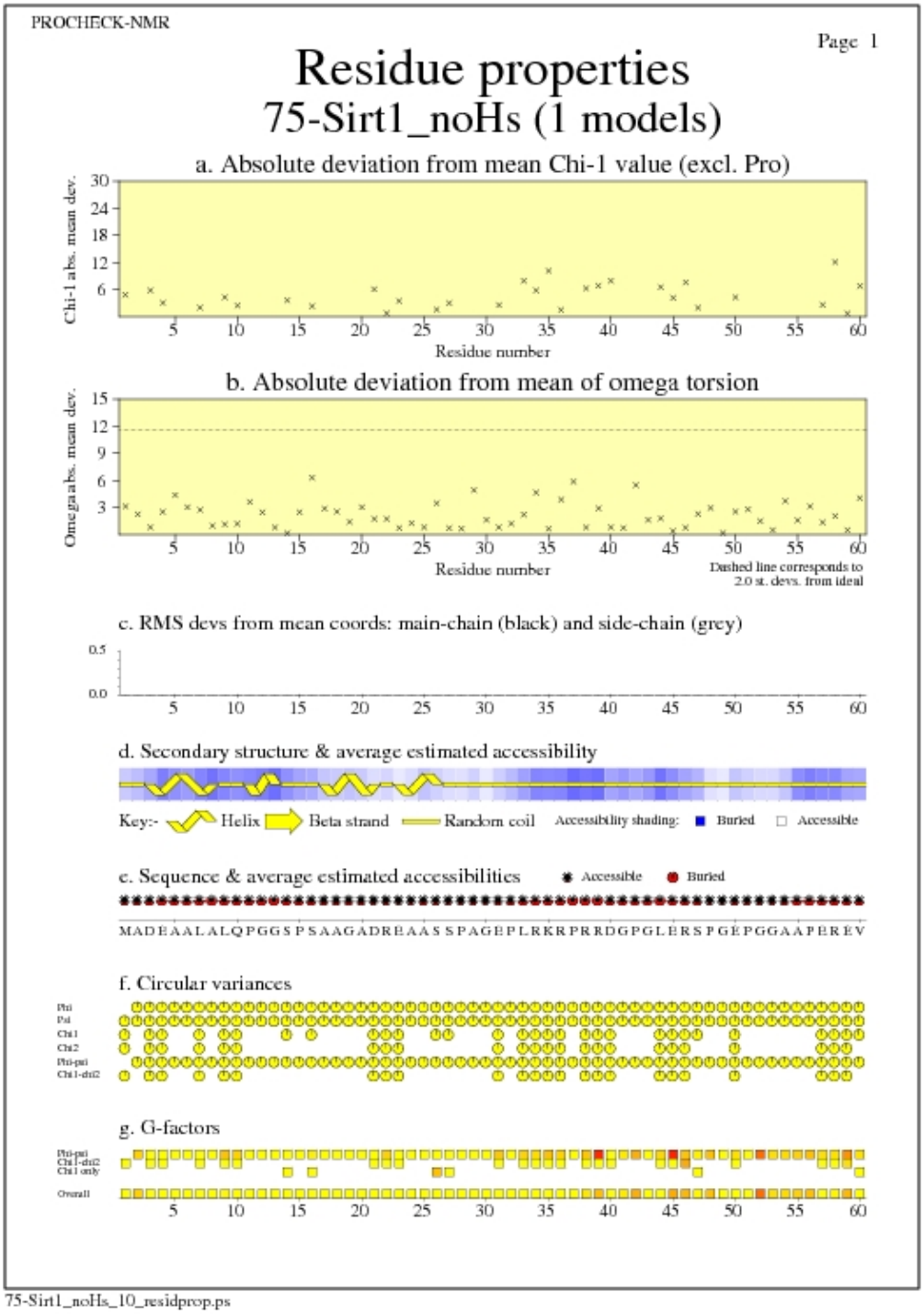
JPEG image for all model Ramachandran Plot



75-Sirt1_noHs_01_ramachand.ps

Residue Properties for all models

JPEG for all model Residue Properties - page $num_n



75-Sirt1_noHs_10_residprop.ps

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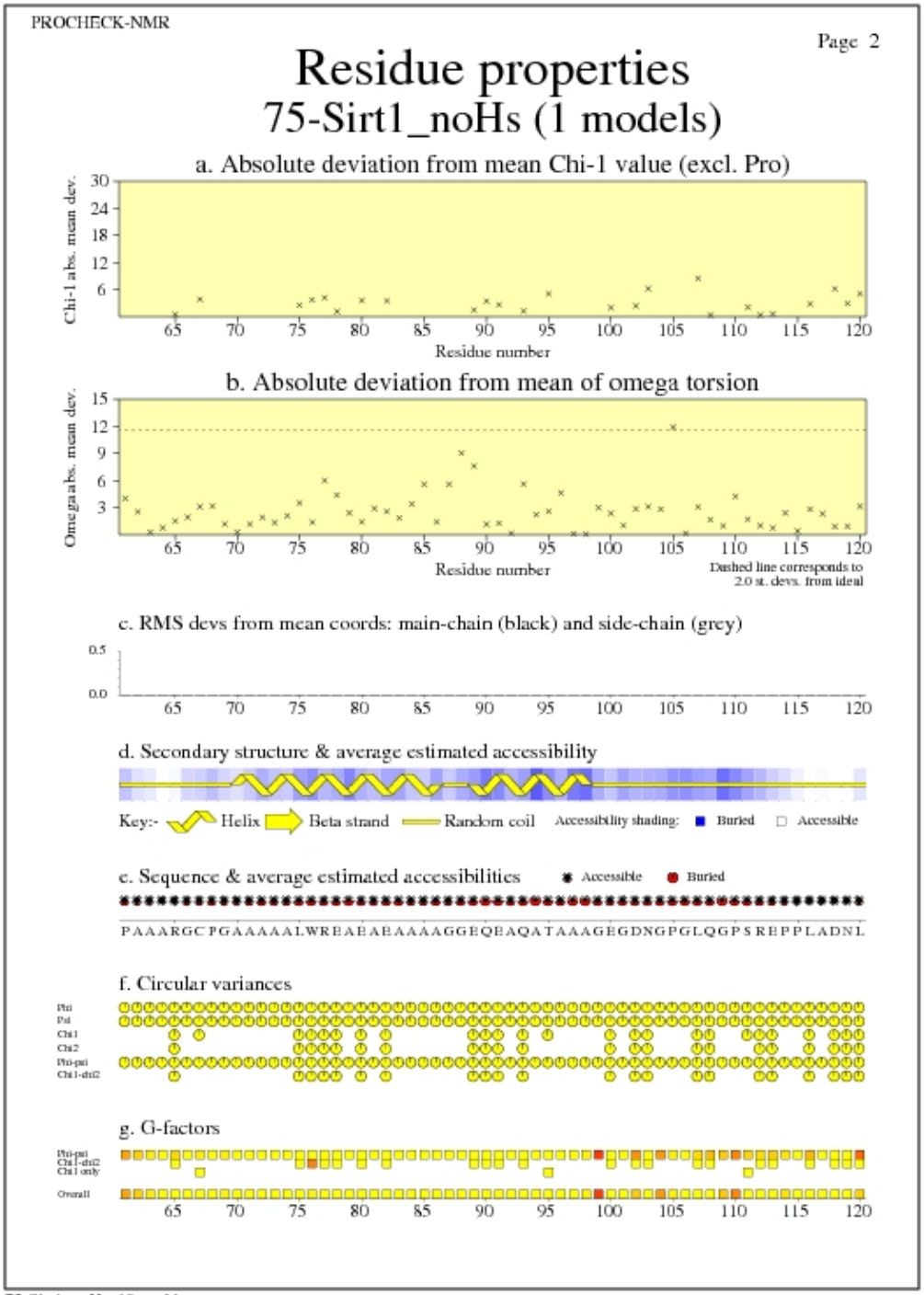

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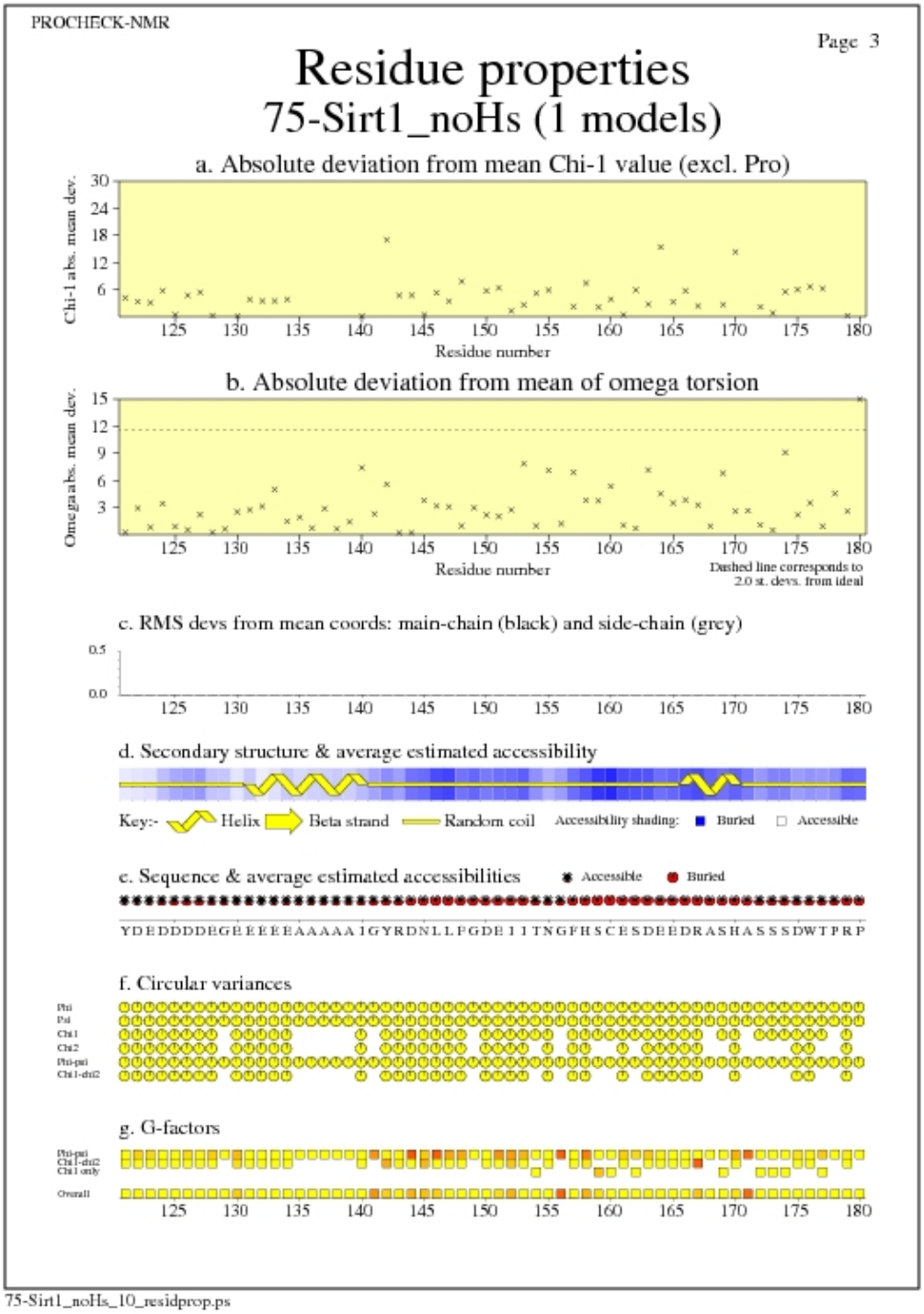

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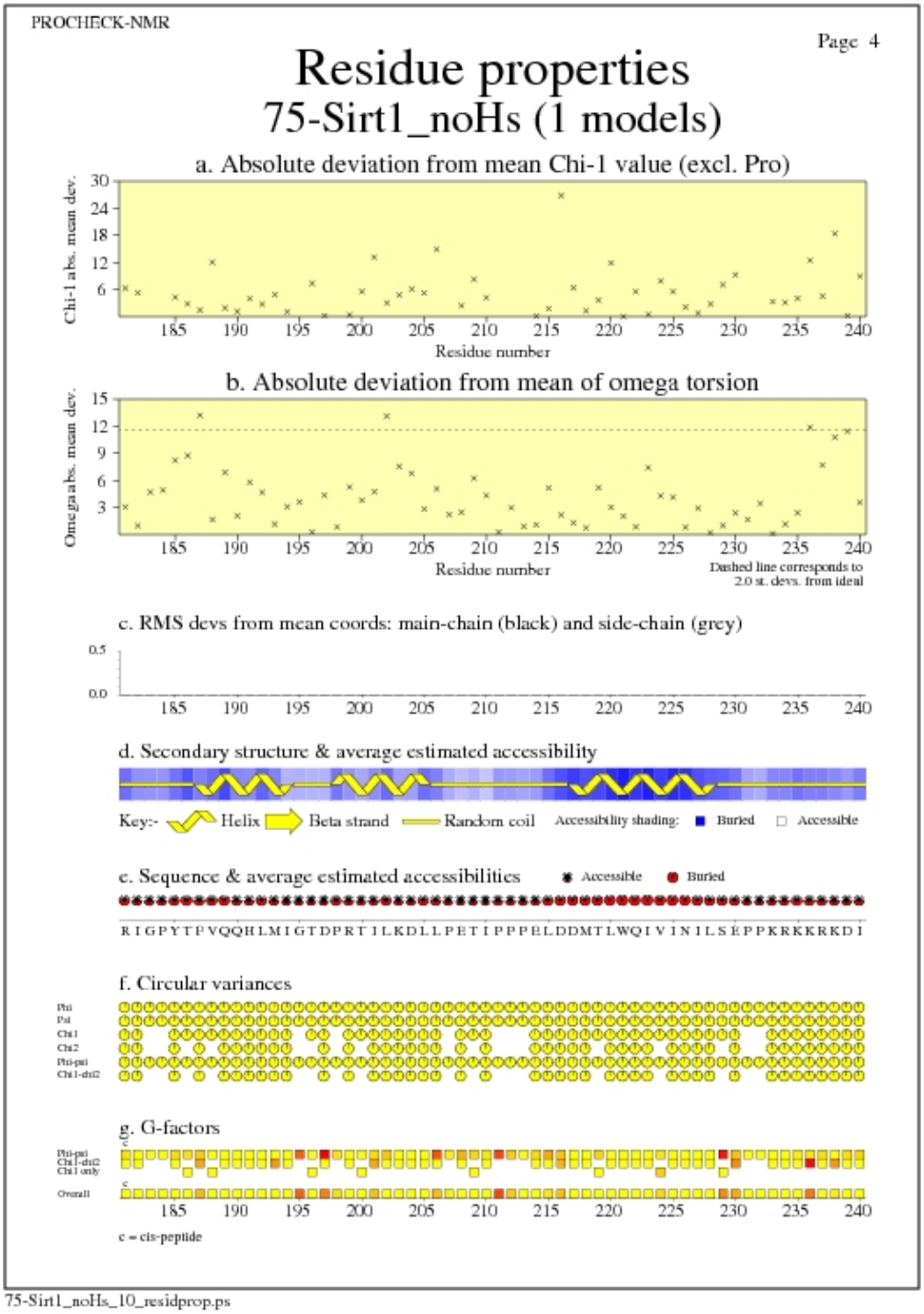

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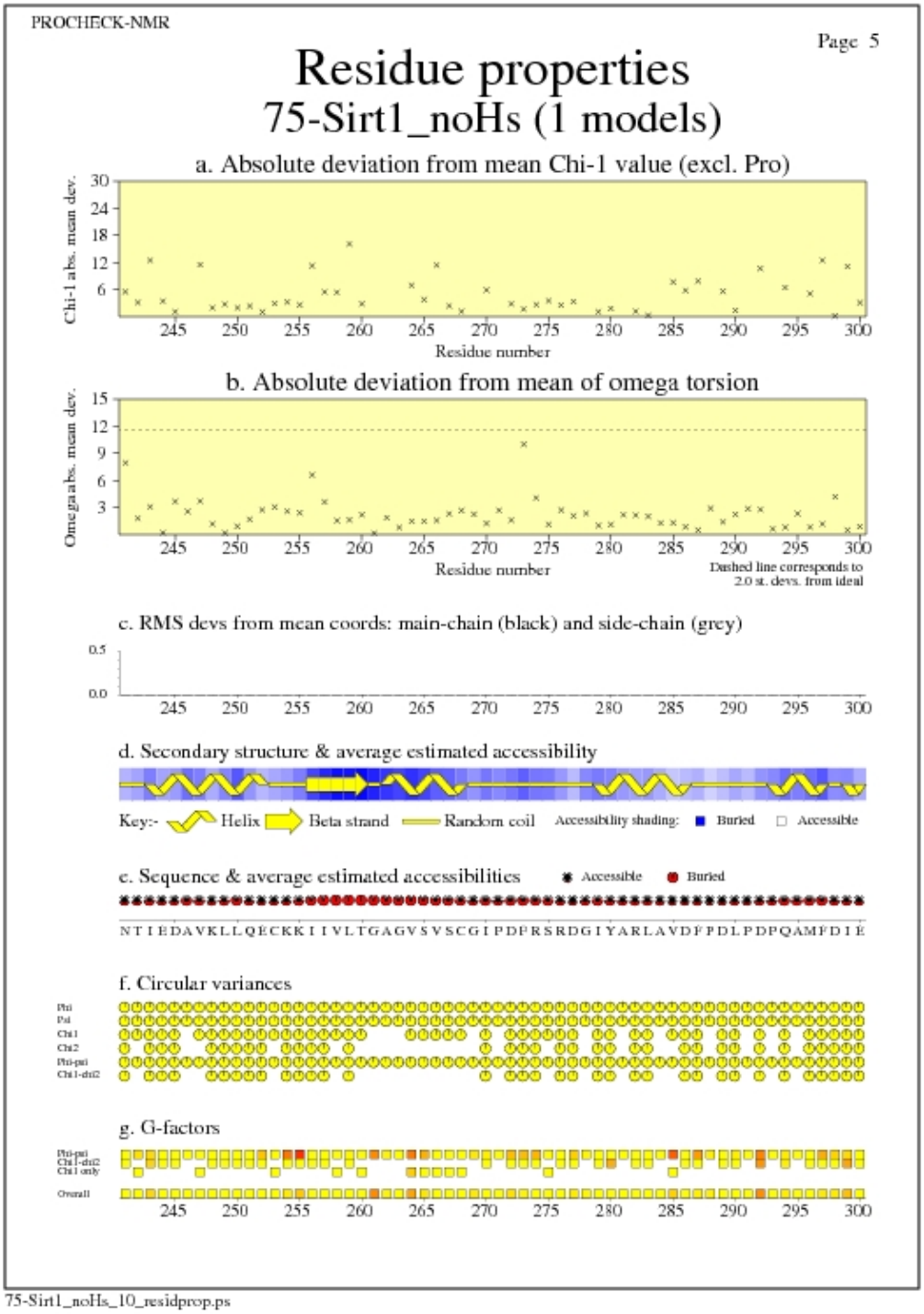

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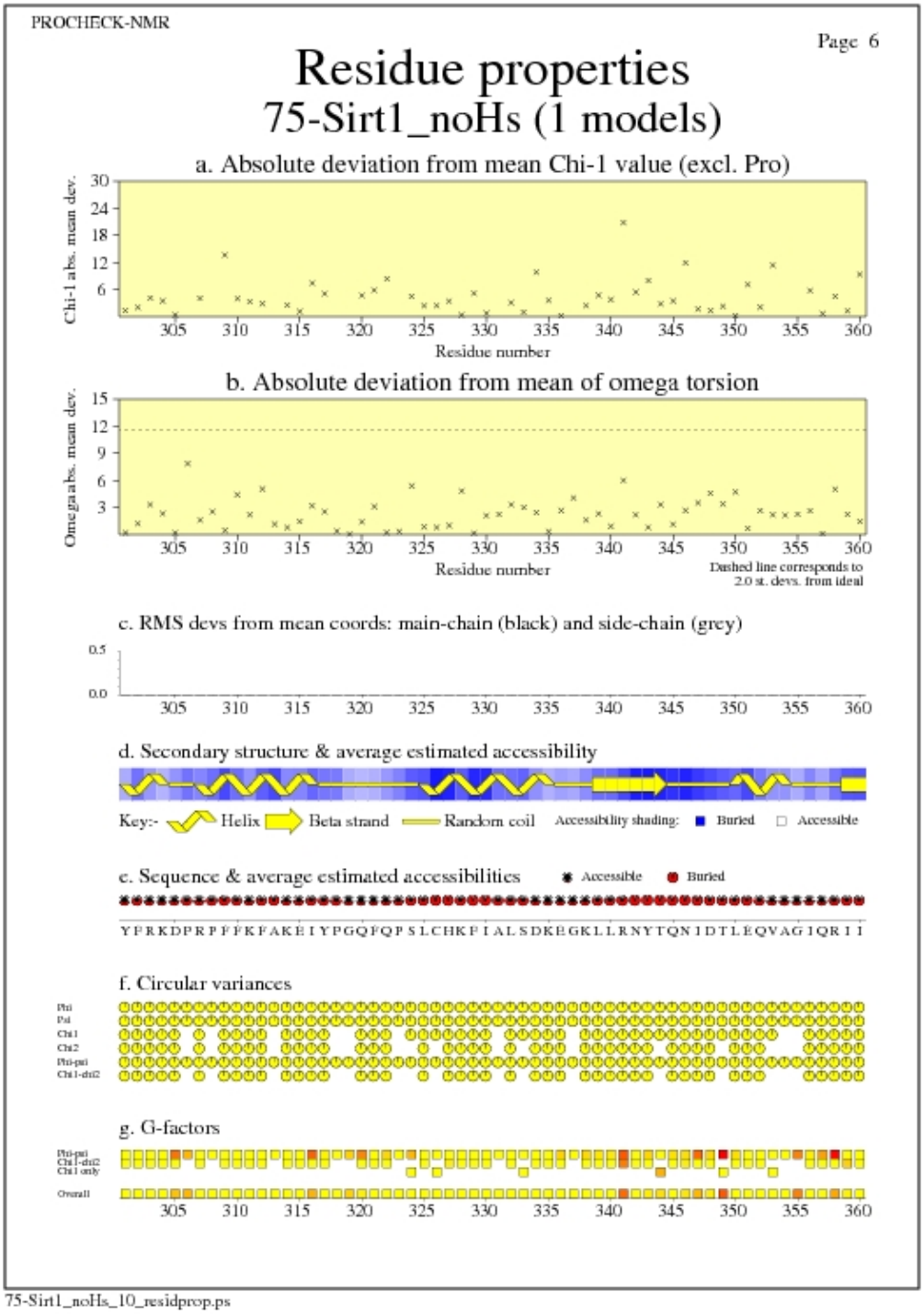

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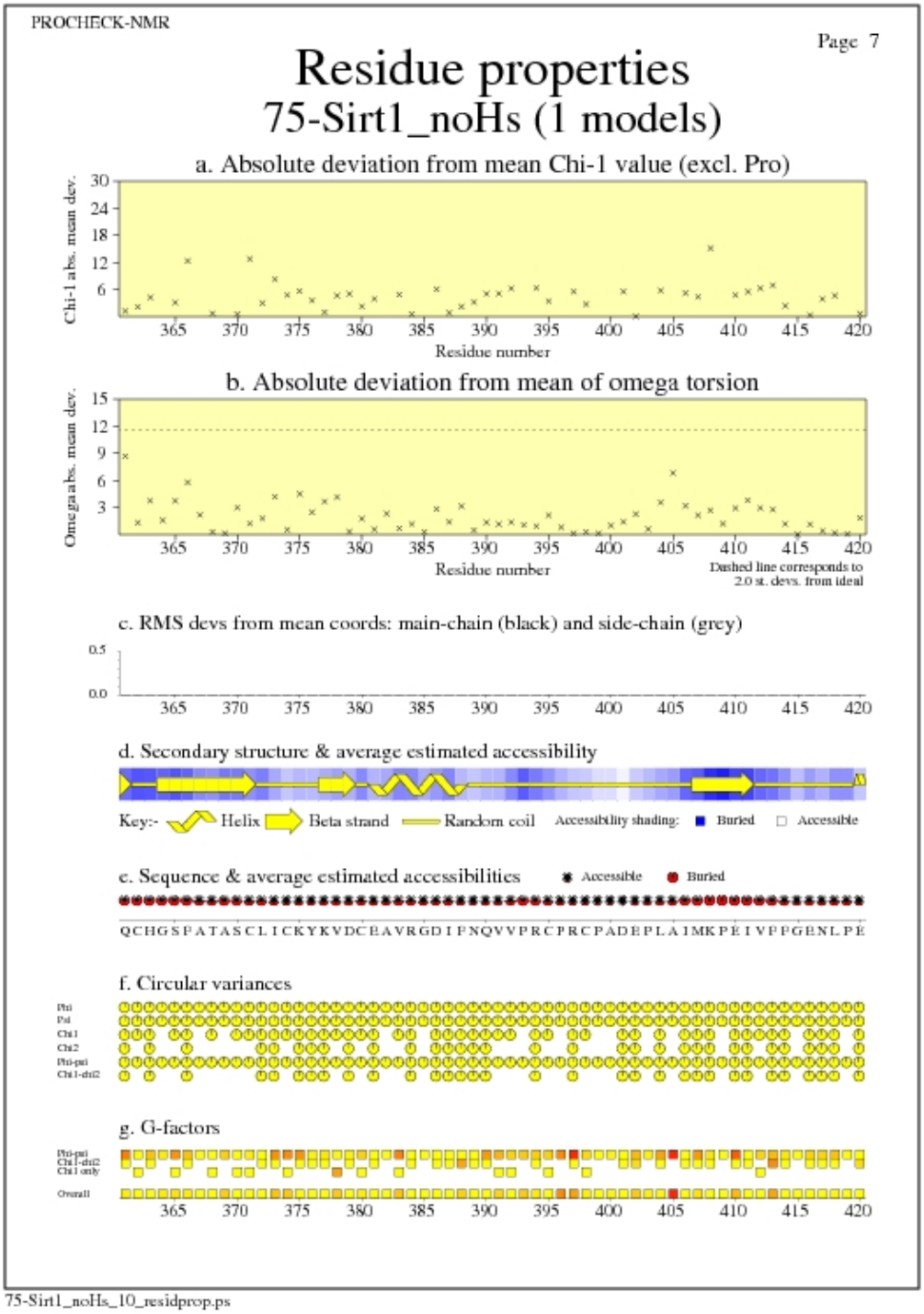

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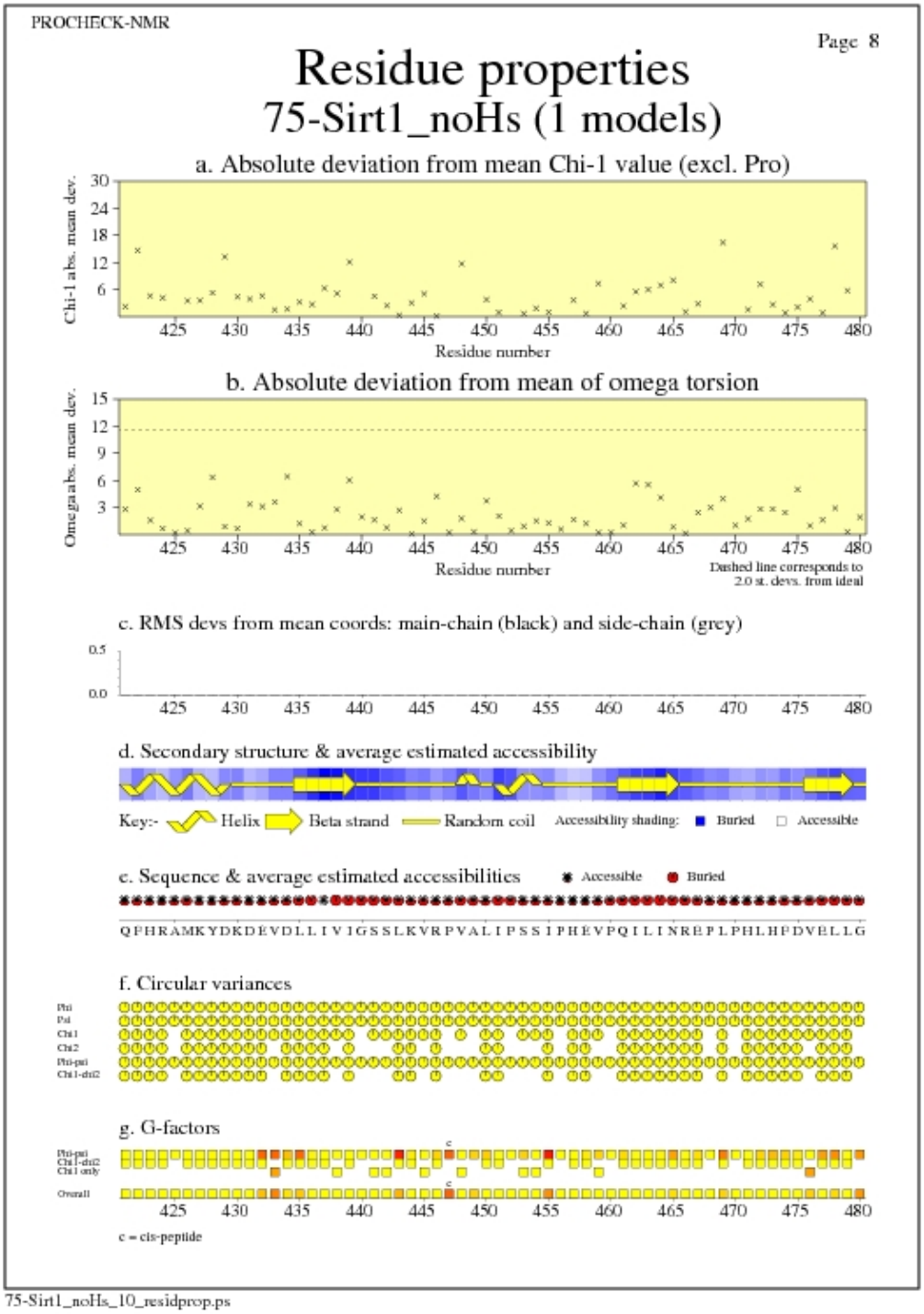

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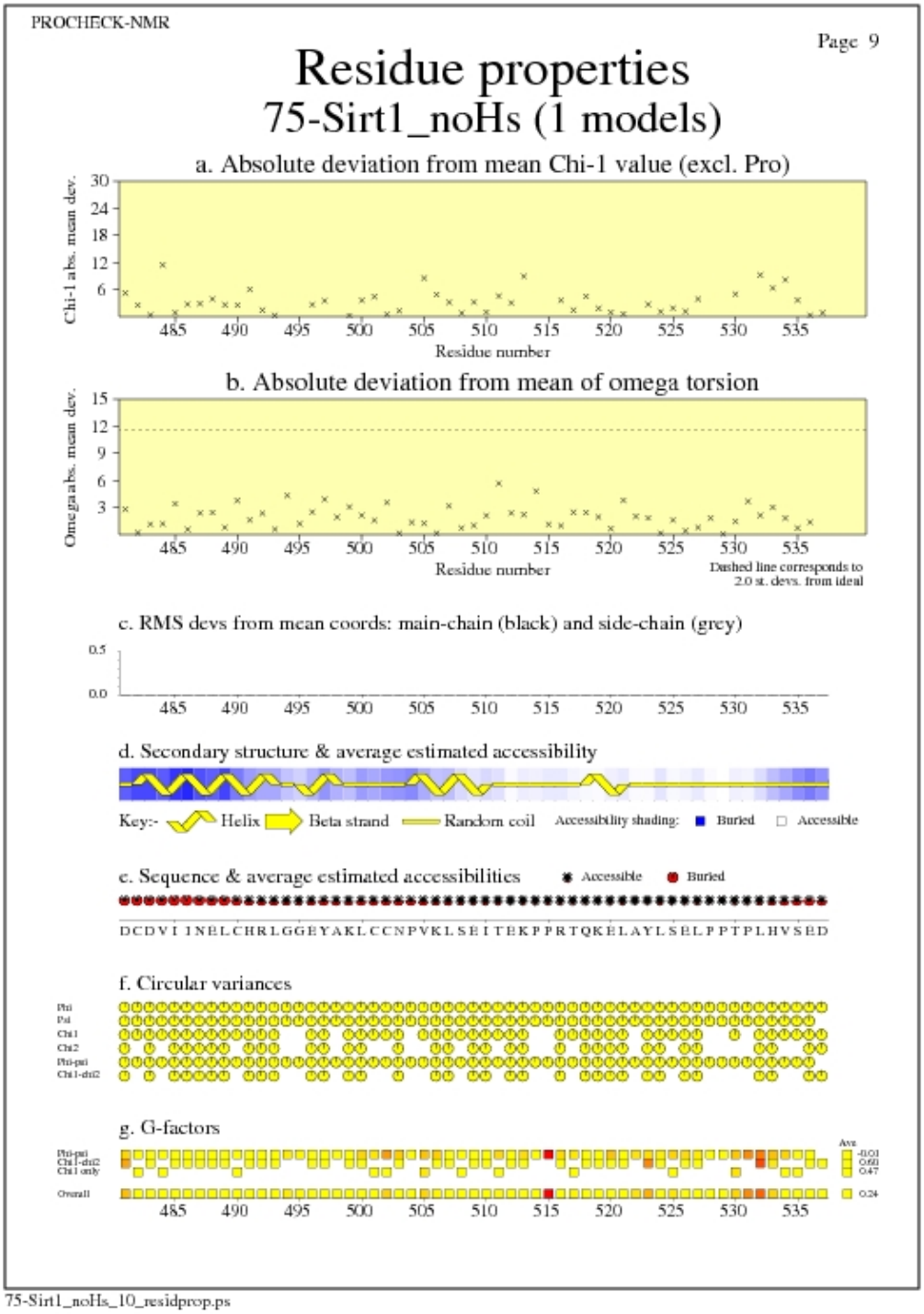
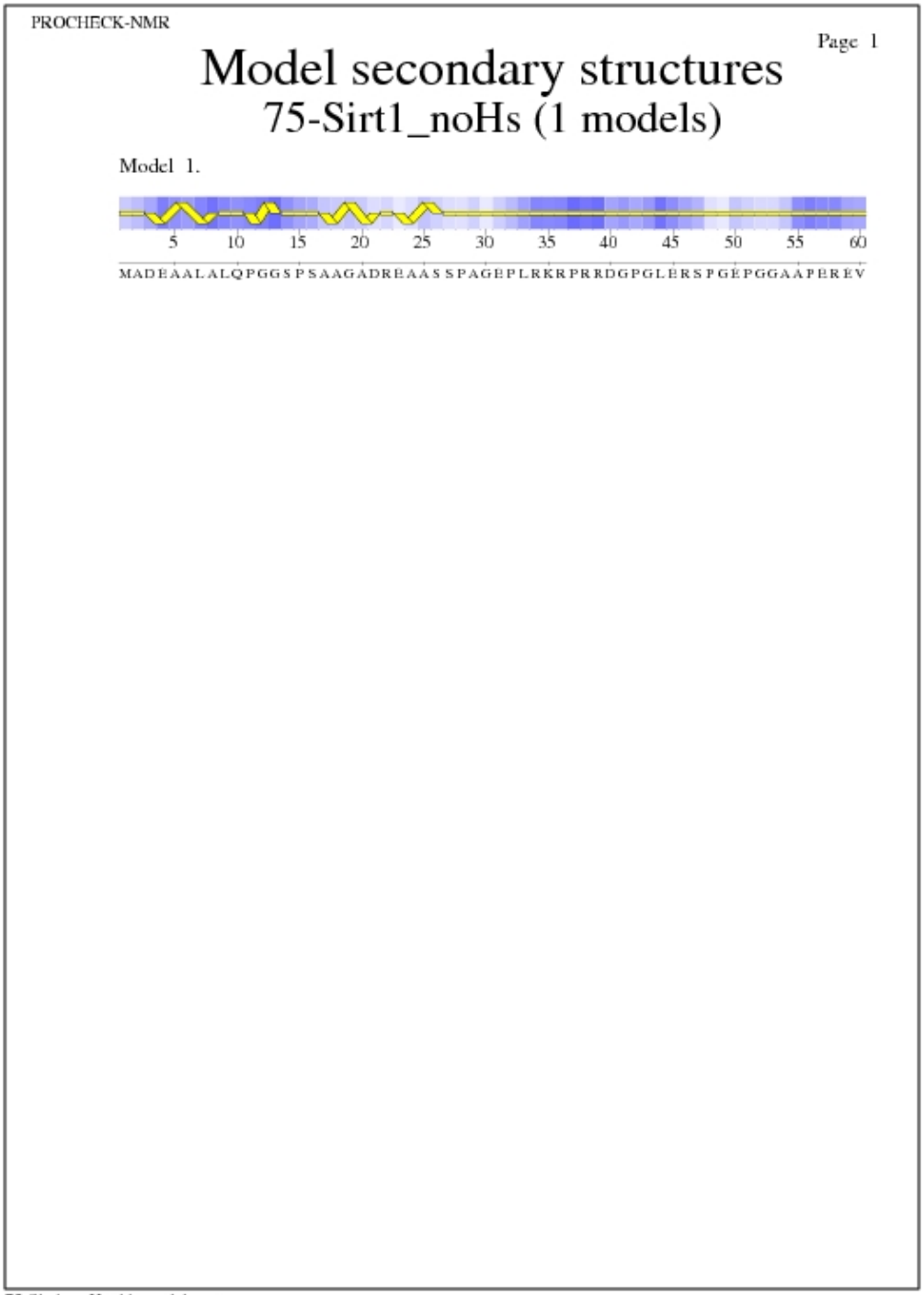
JPEG for all model Residue Properties - page $num_n



75-Sirt1_noHs_10_residprop.ps

Model Secondary Structures from Procheck

JPEG for Model Secondary Structures - page $num_n



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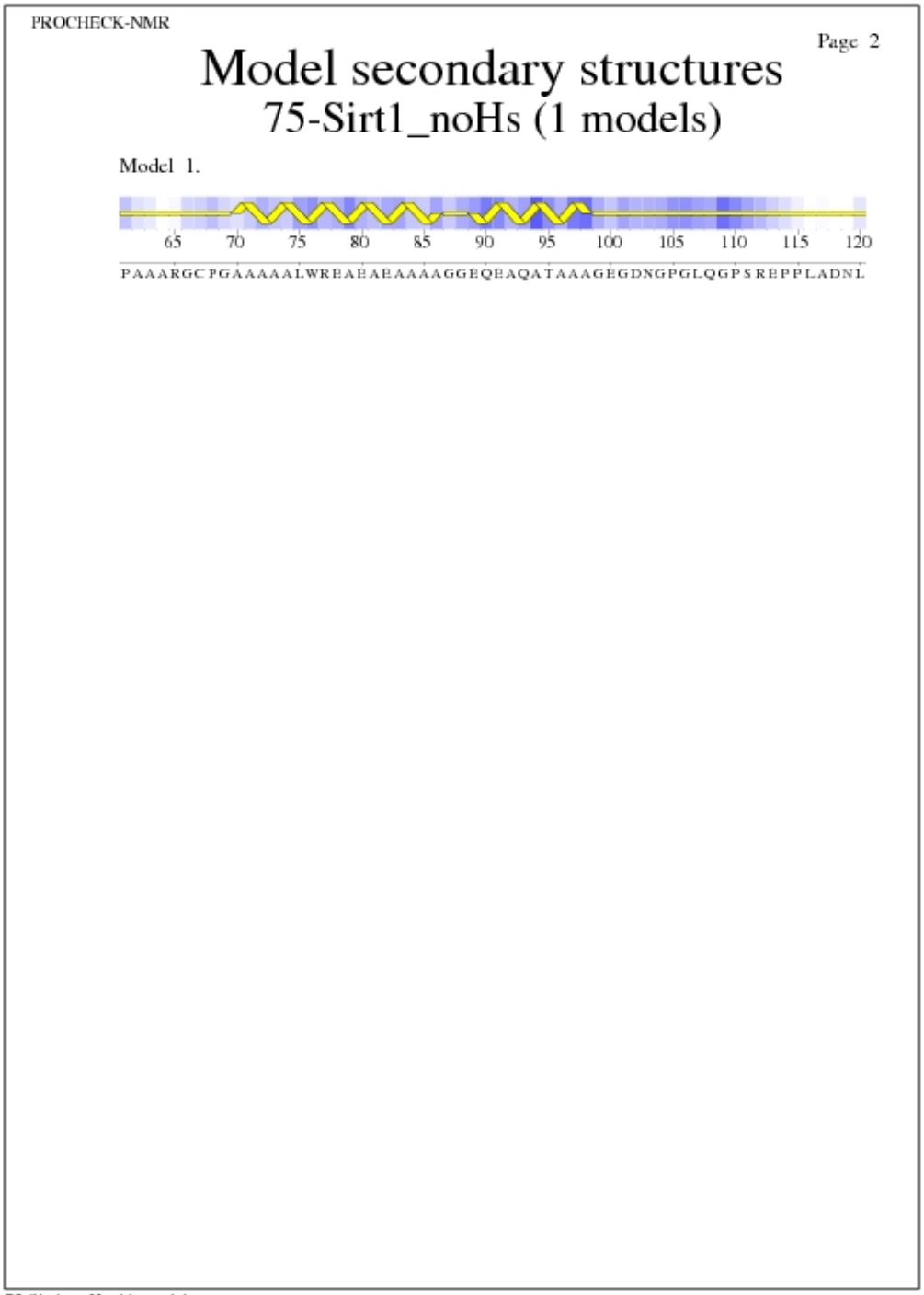

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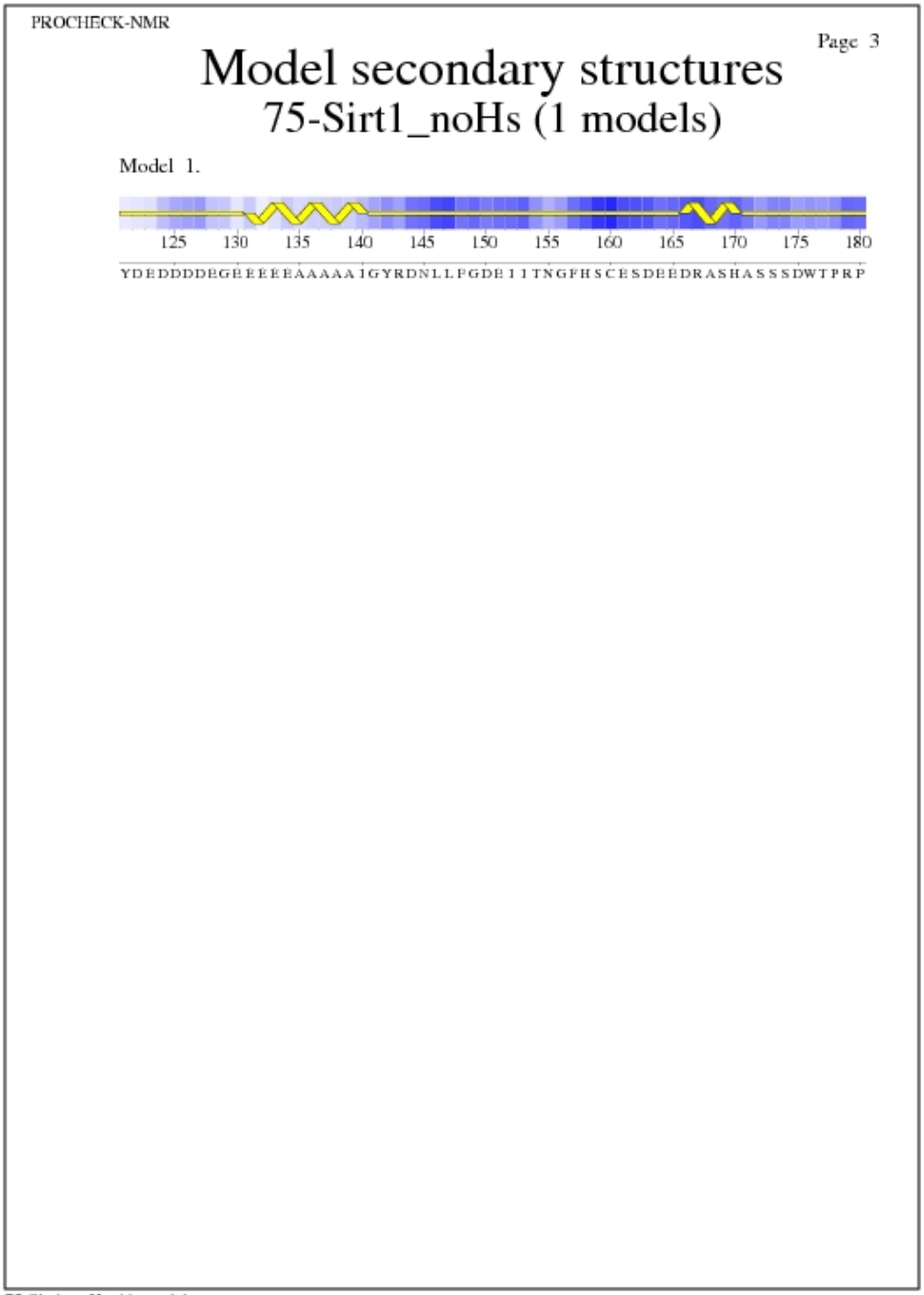

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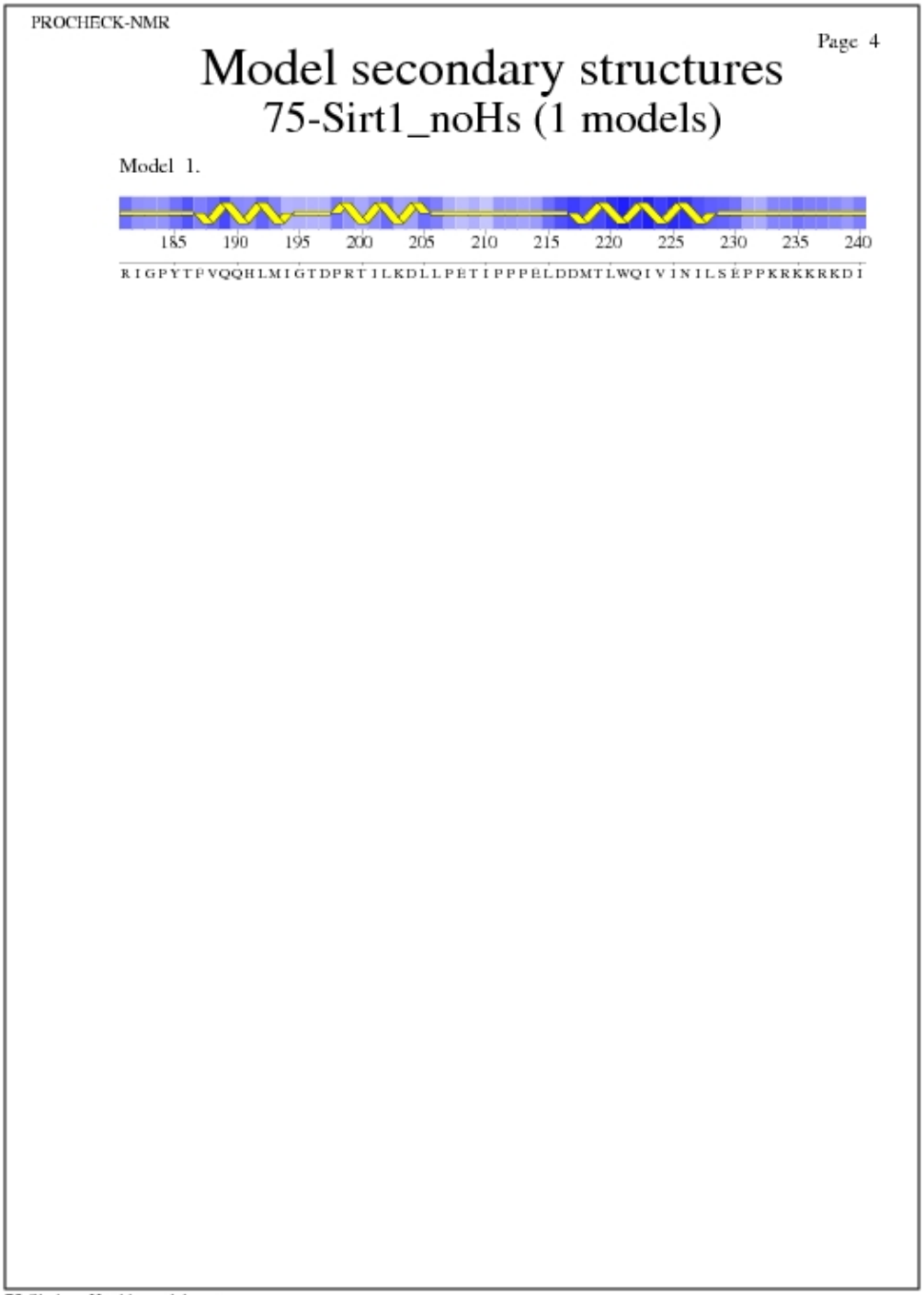

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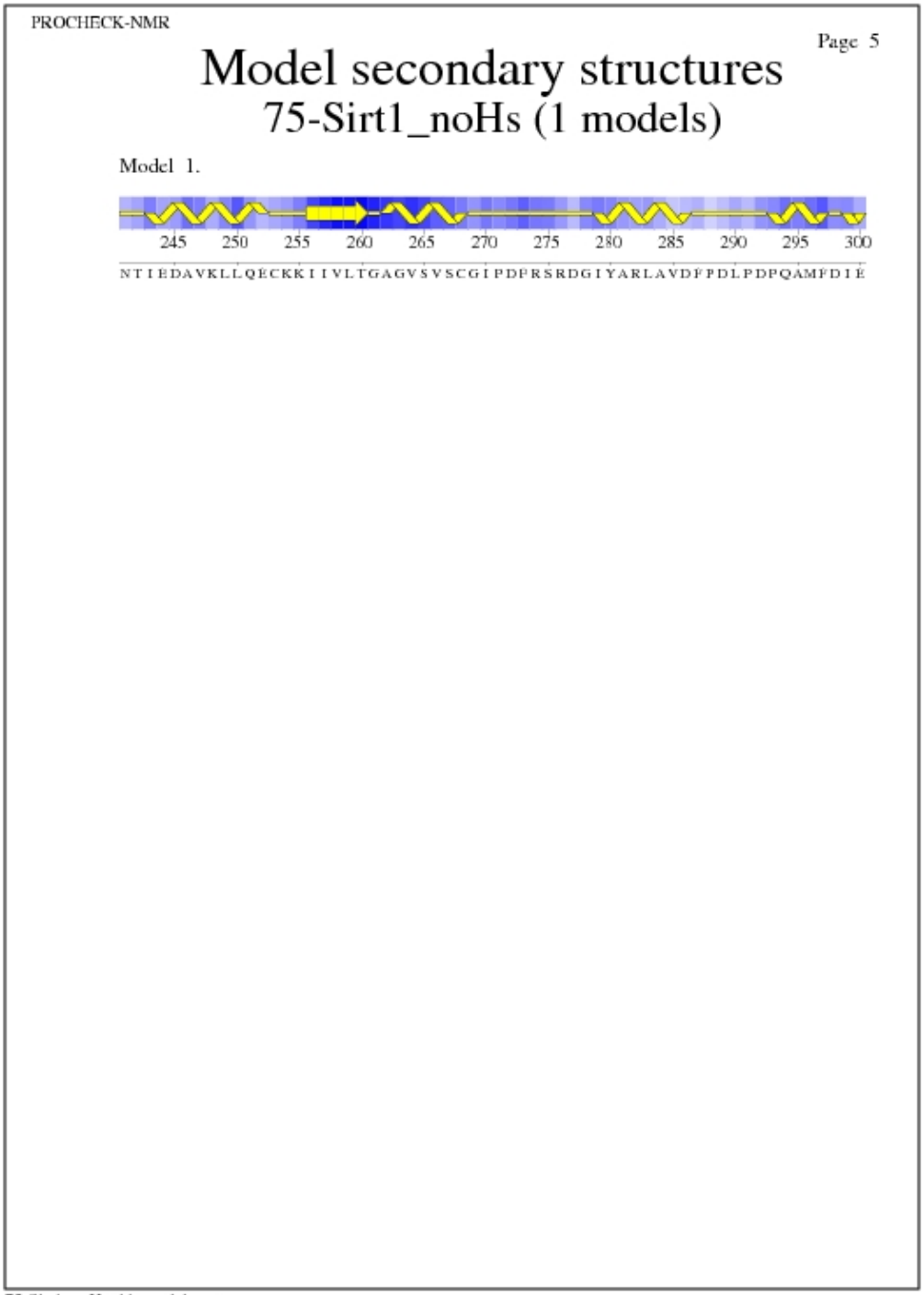

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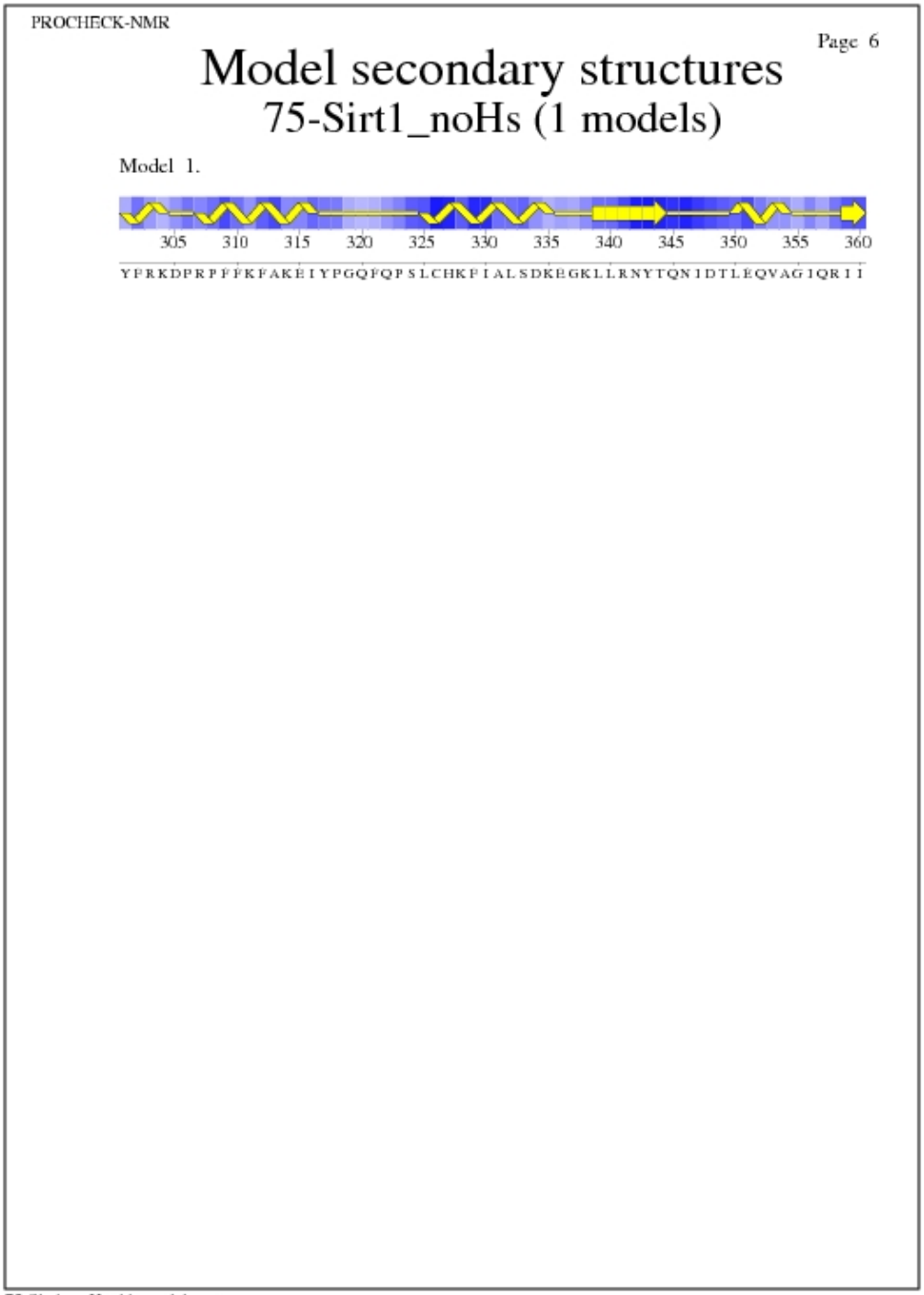

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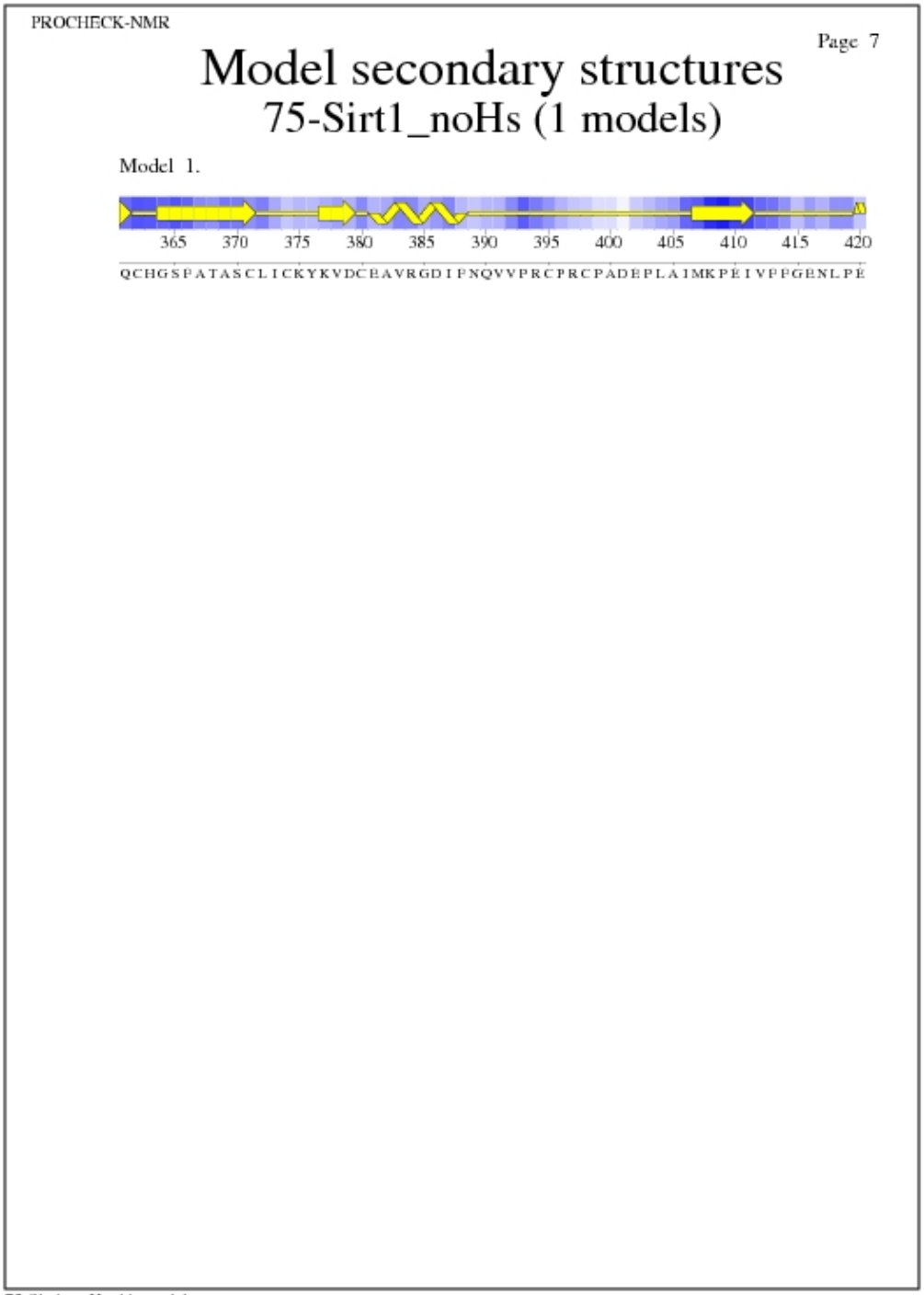

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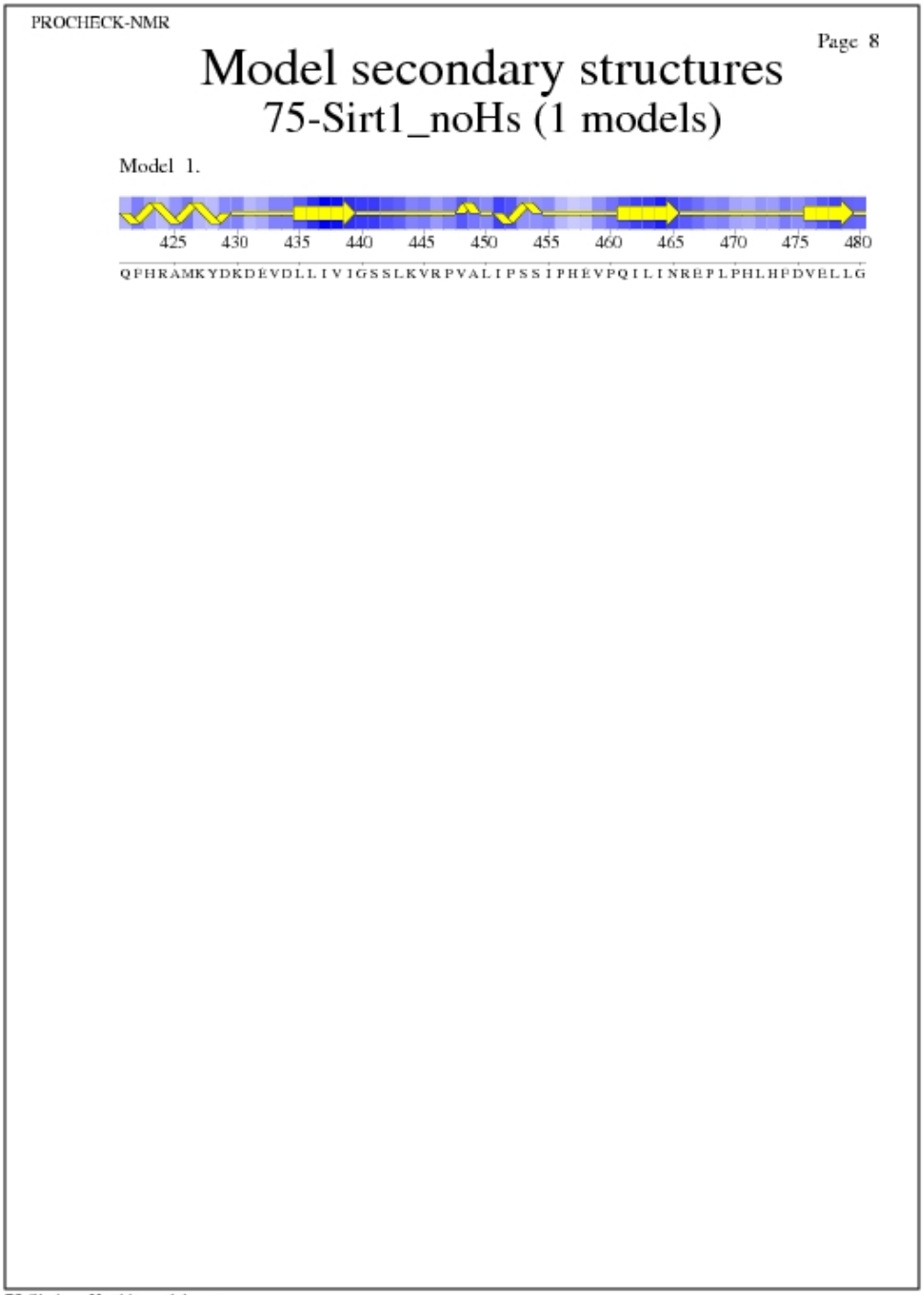
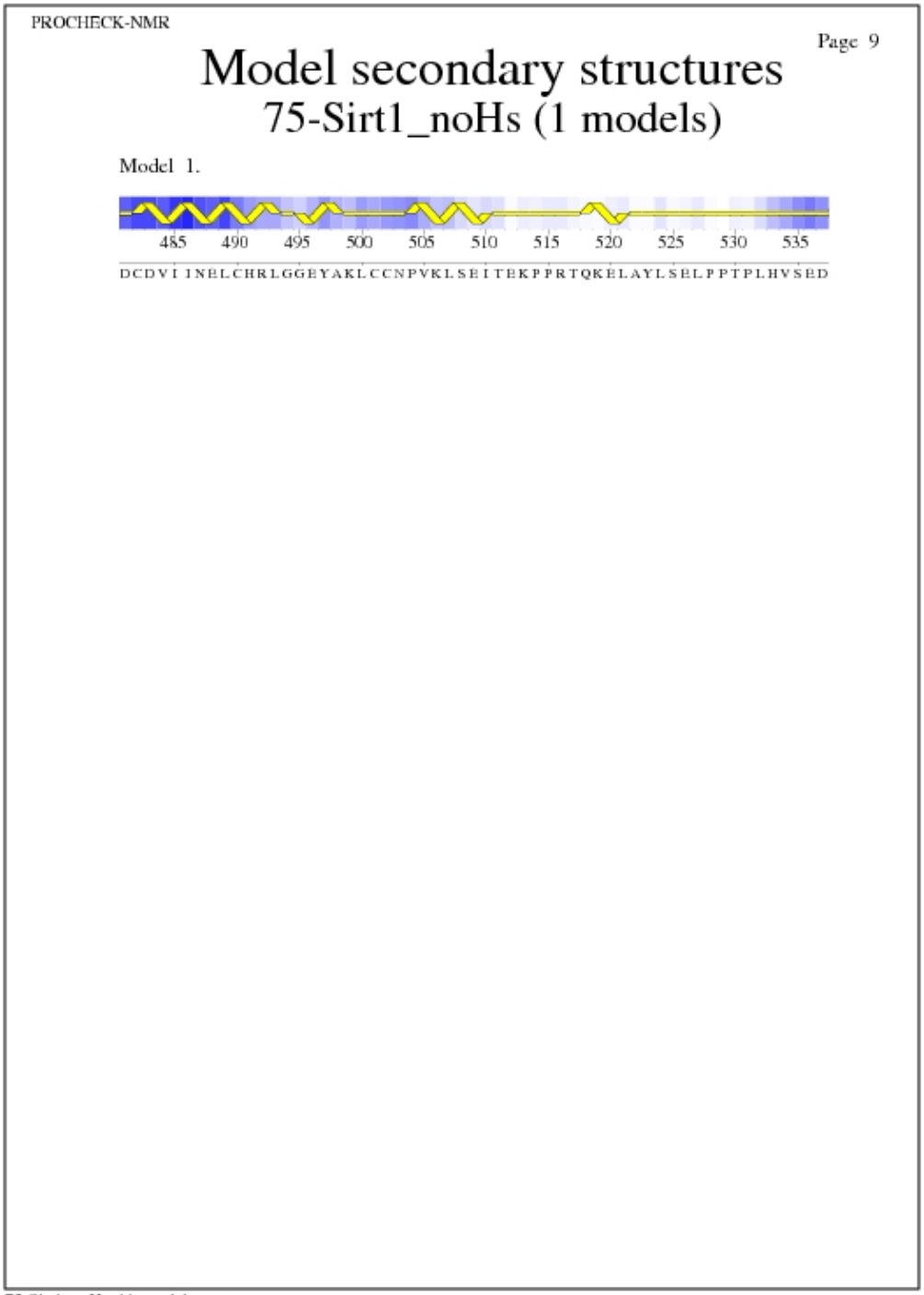
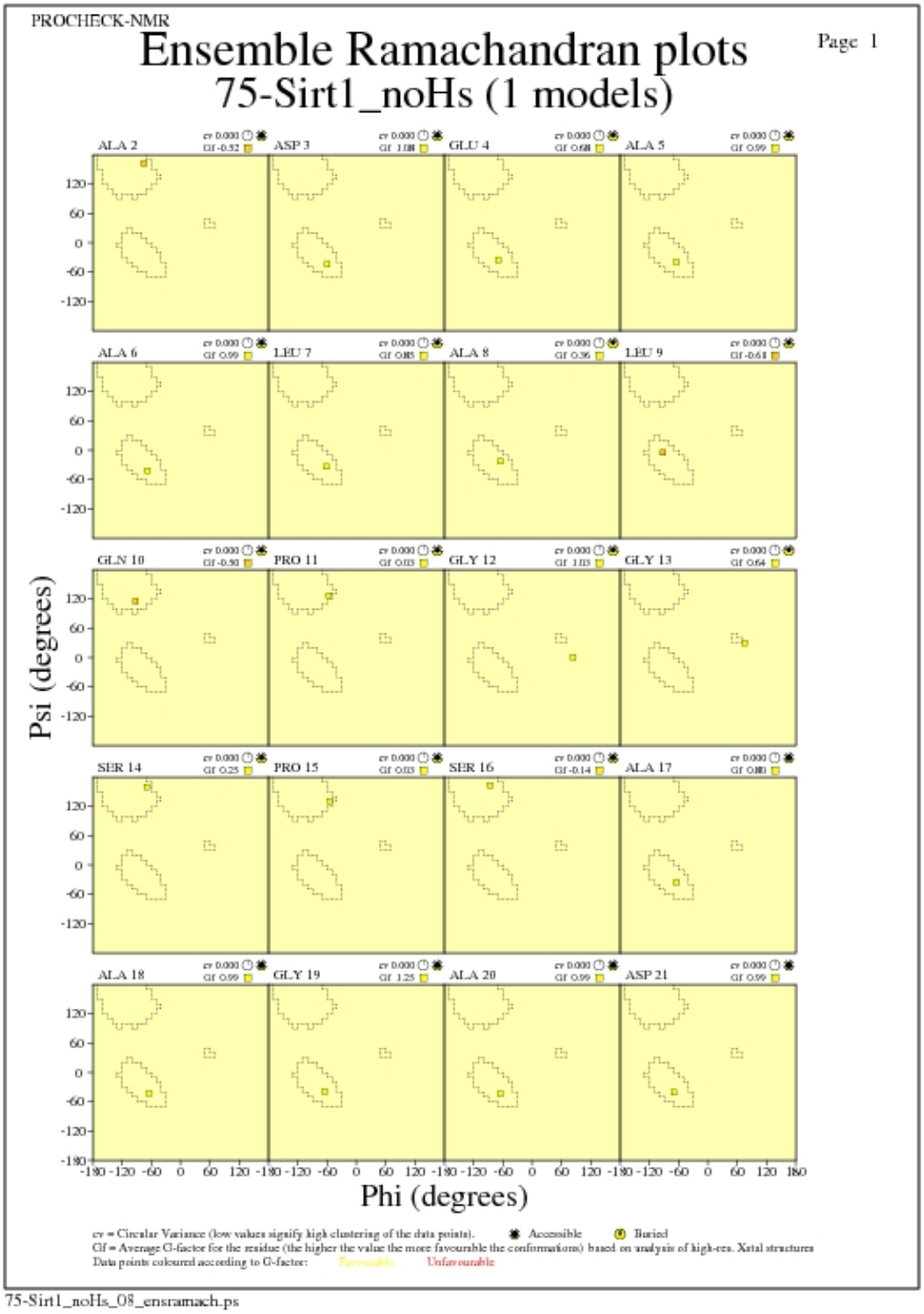


JPEG for Model Secondary Structures - page $num_n



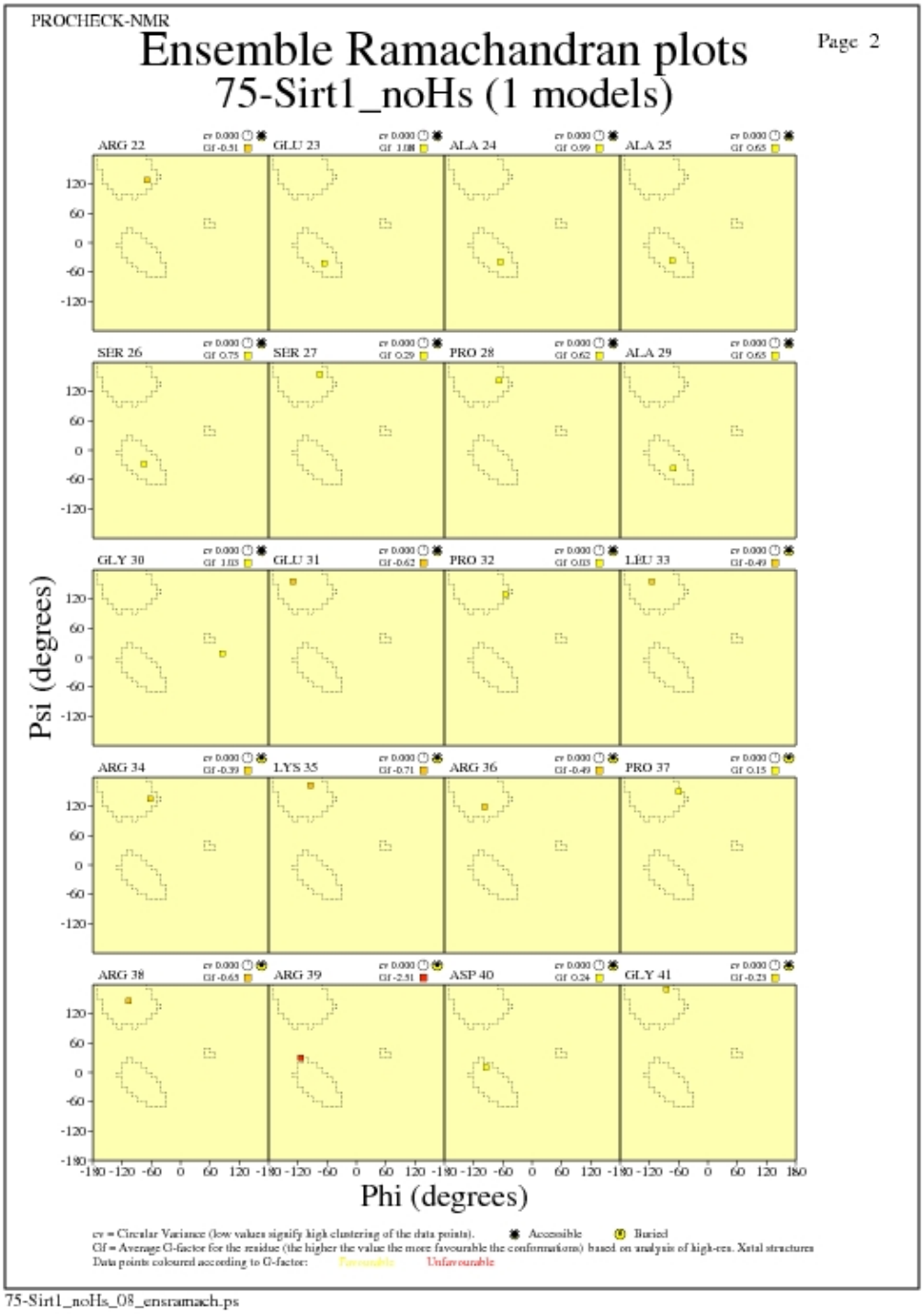
Ramachandran Plots for each residue

JPEG for residue Ramachandran Plots - page $num_n



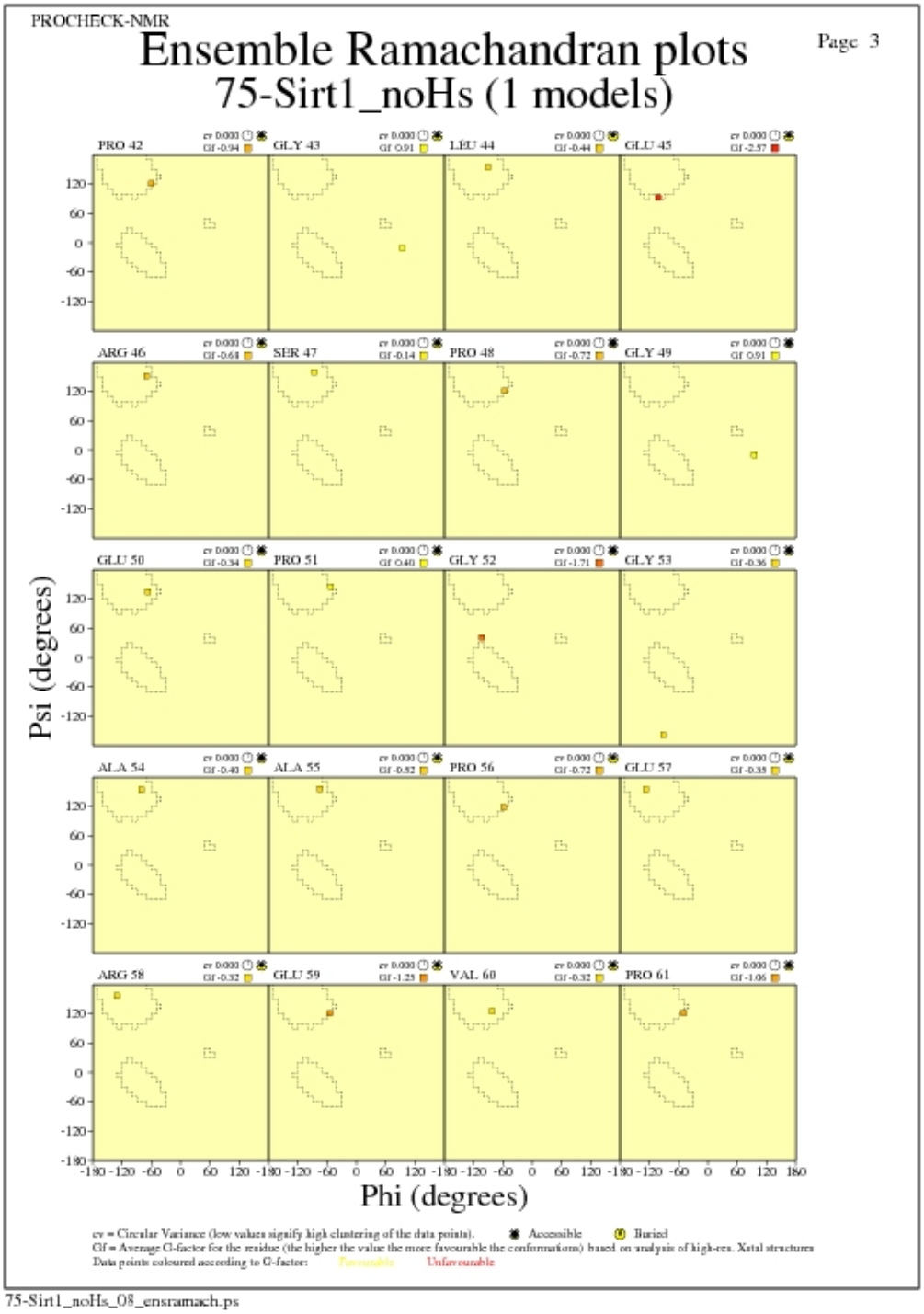
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



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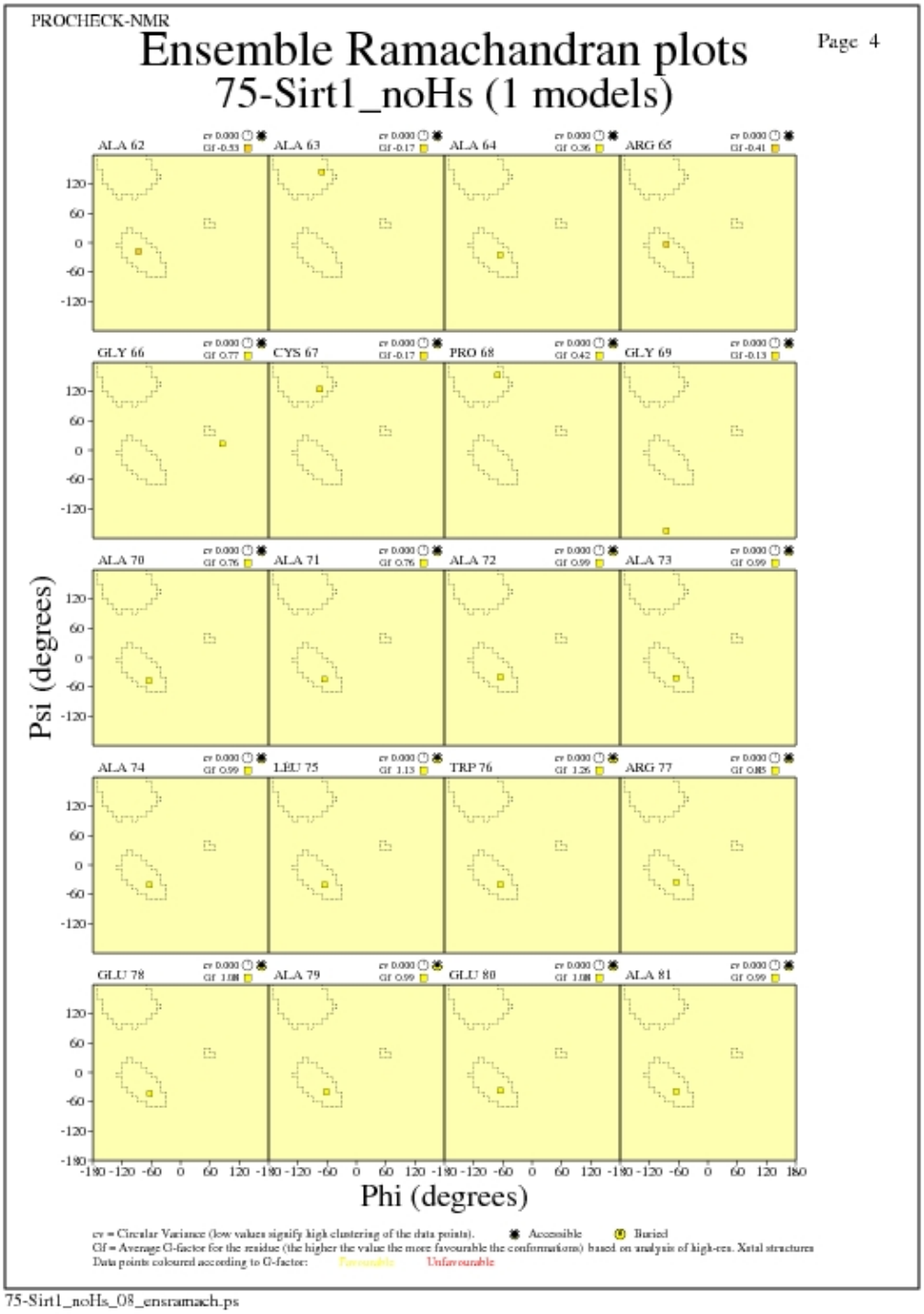
JPEG for residue Ramachandran Plots - page $num_n



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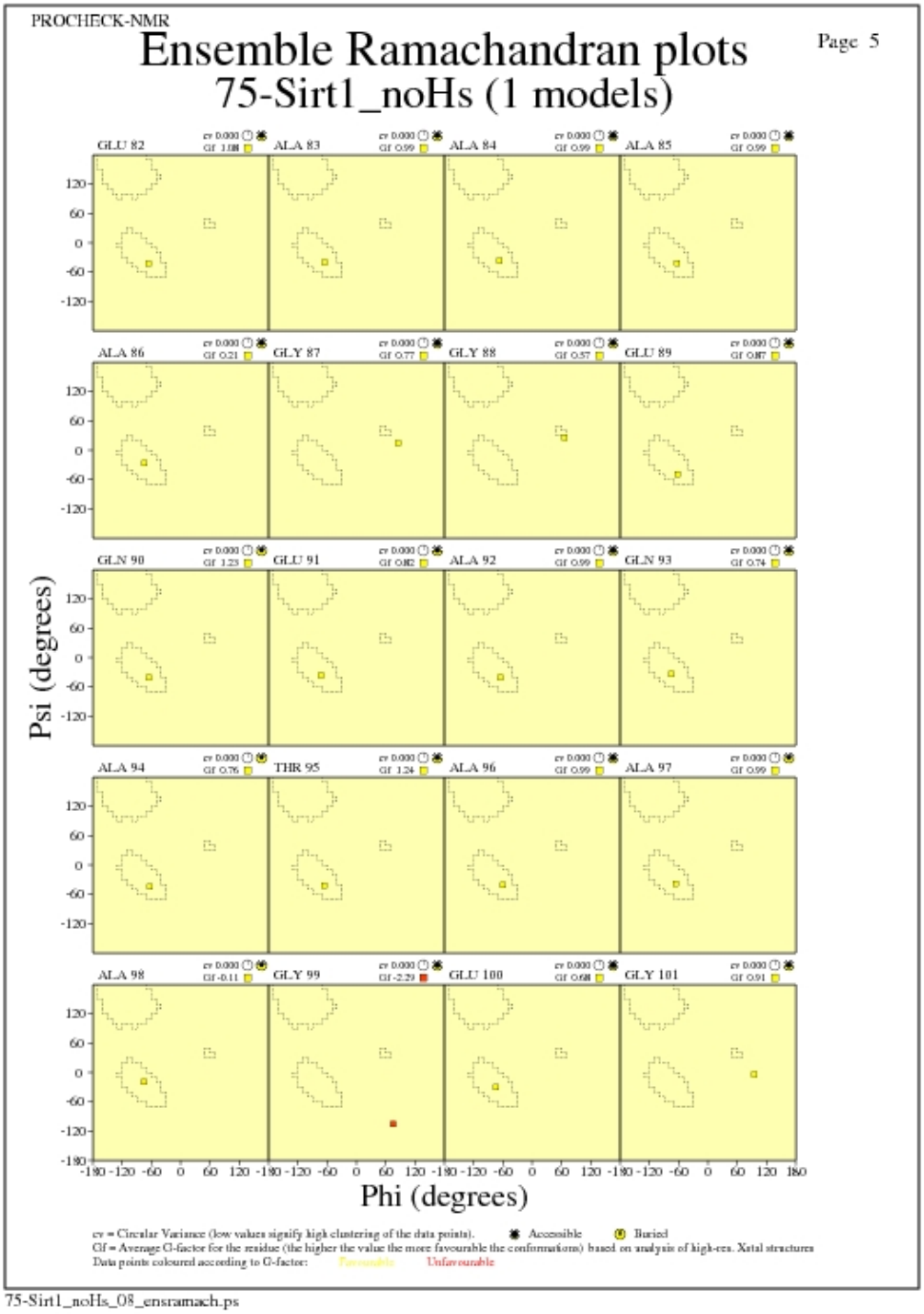
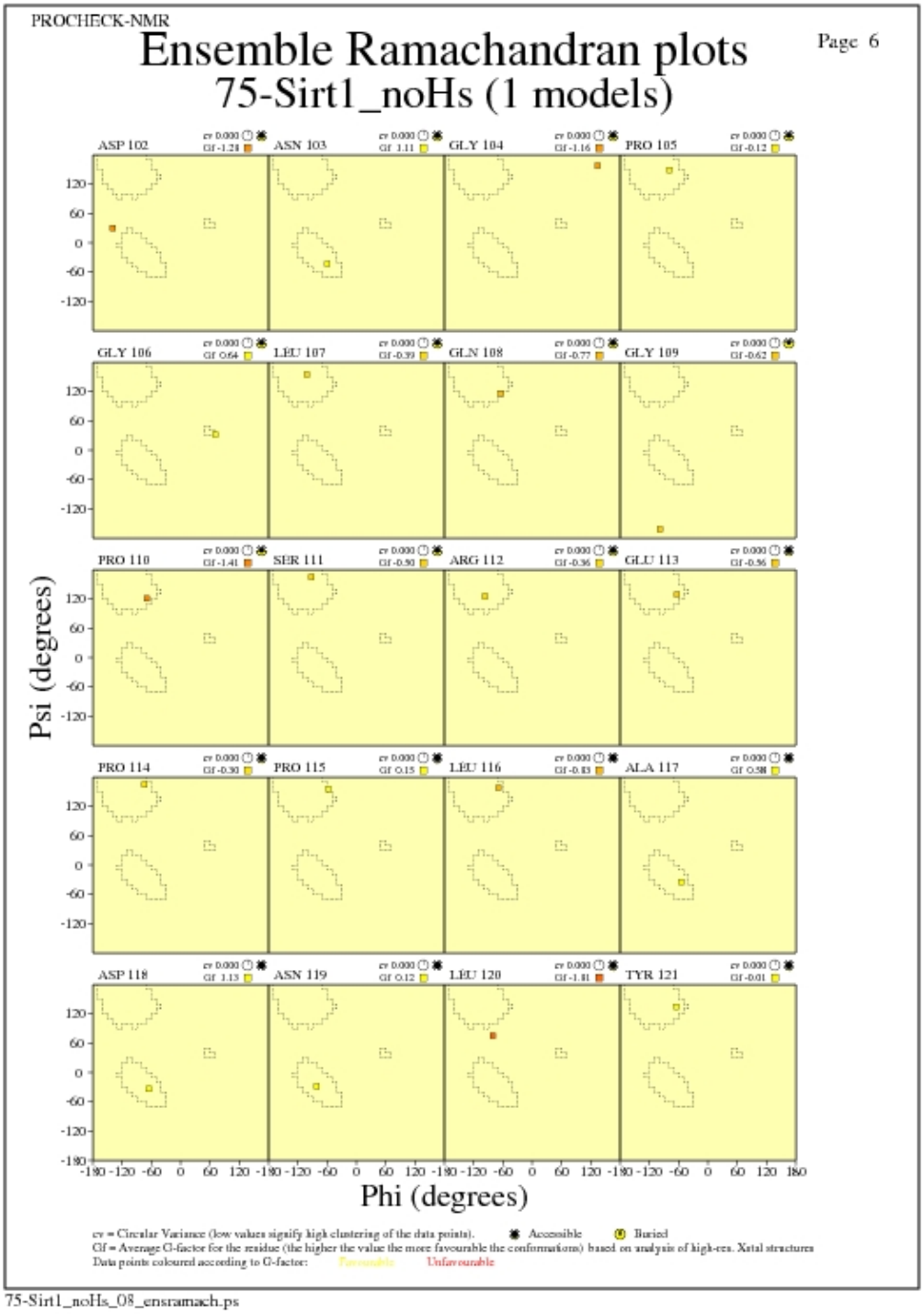
JPEG for residue Ramachandran Plots - page $num_n



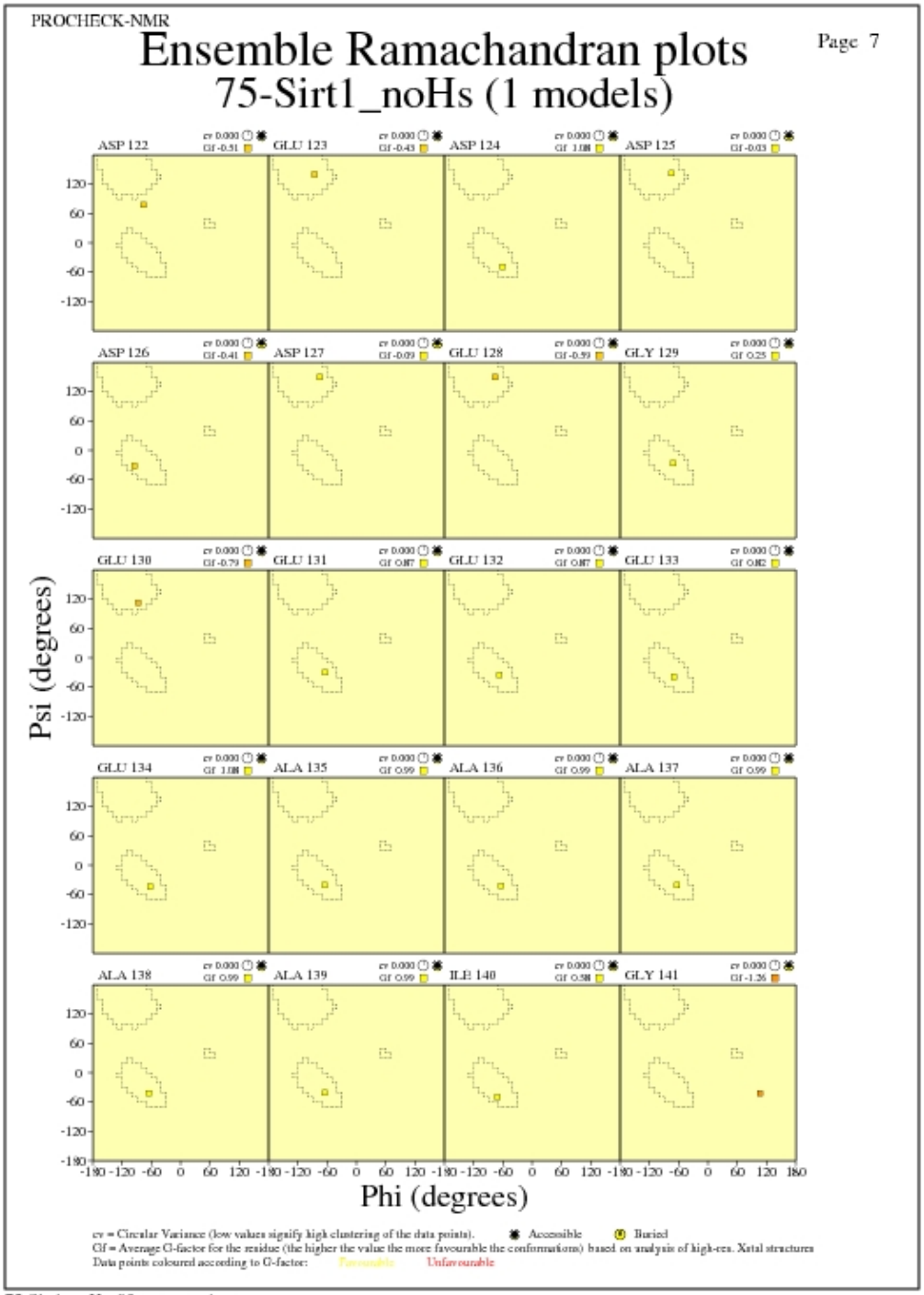
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



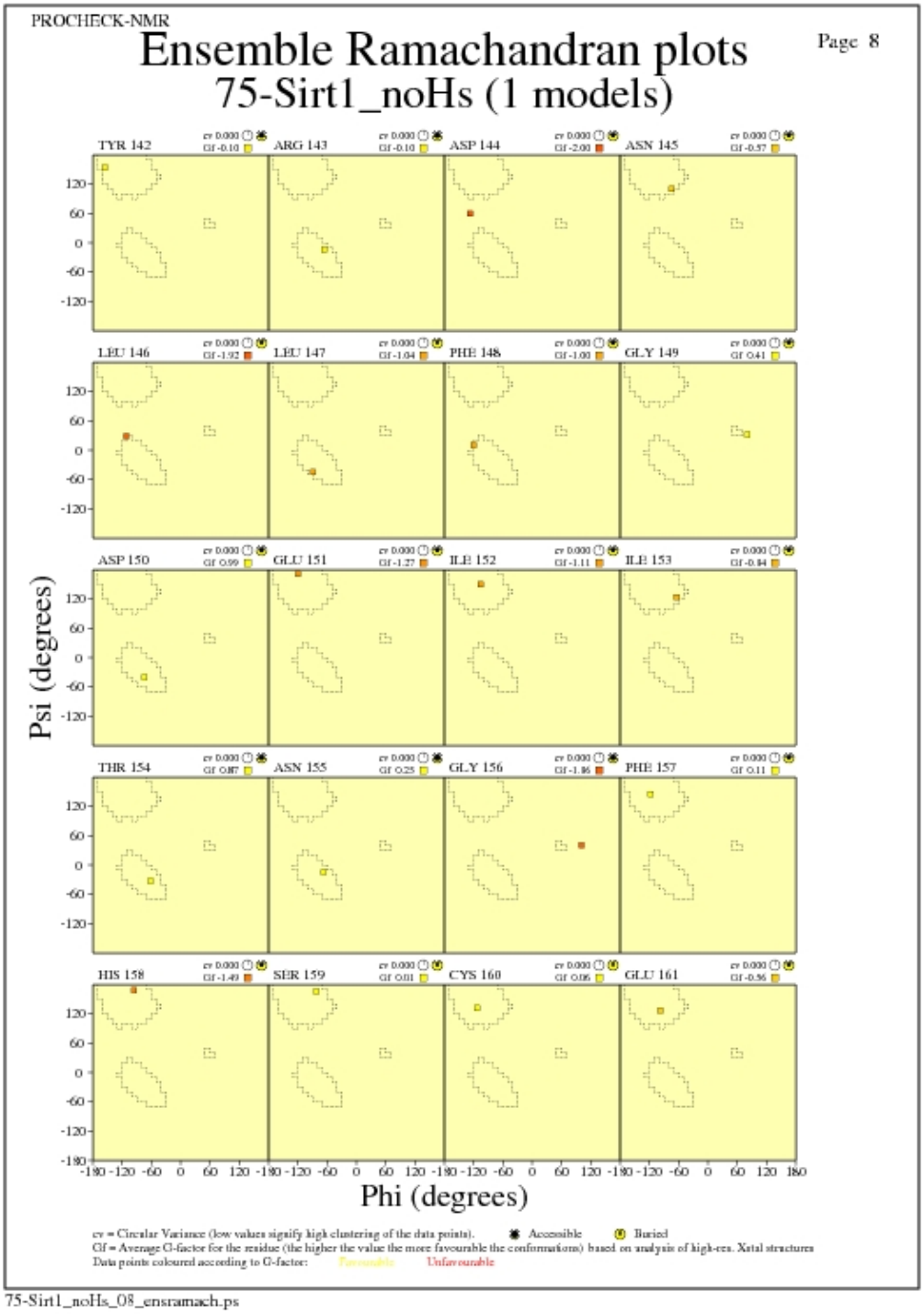
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



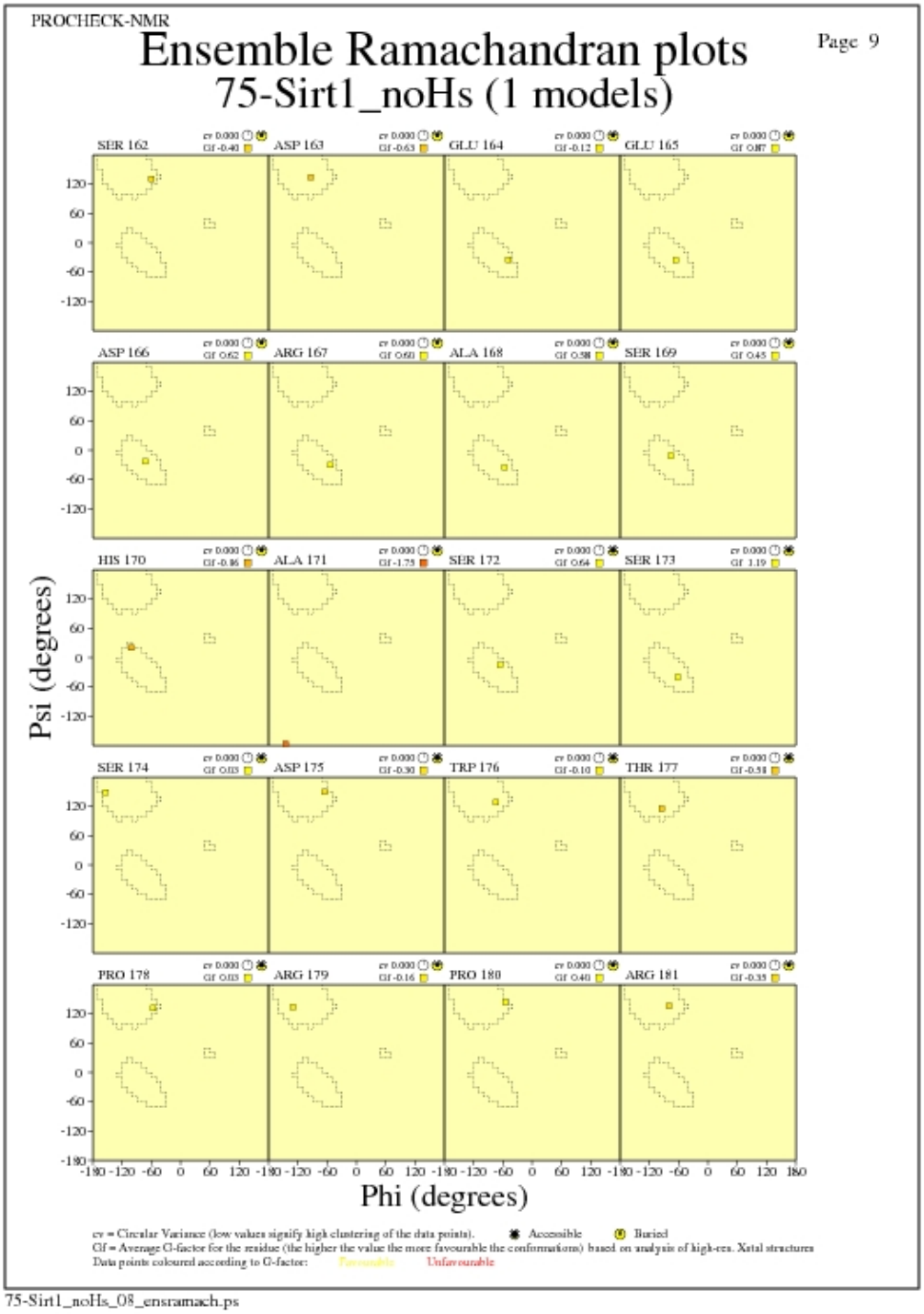
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



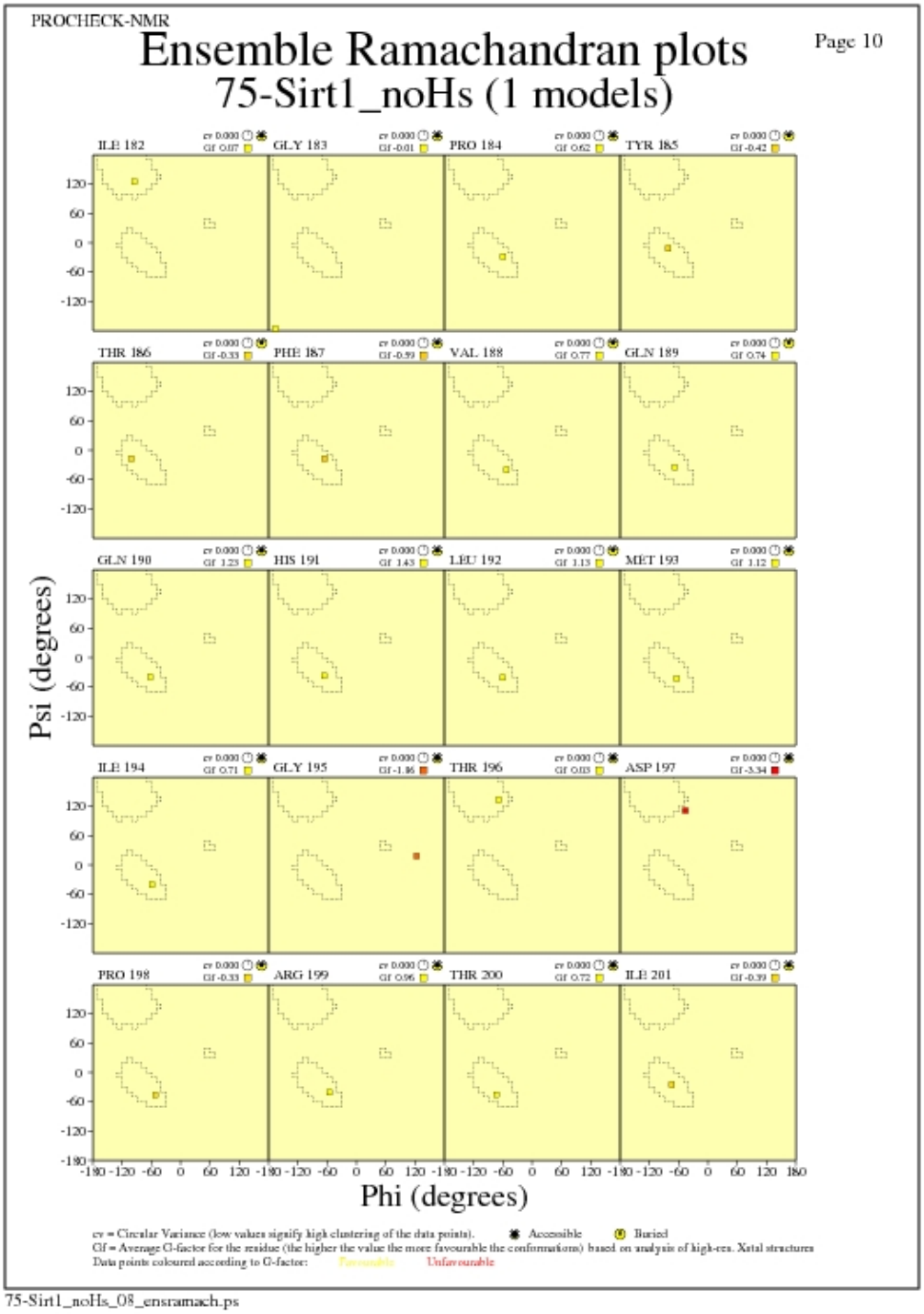
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



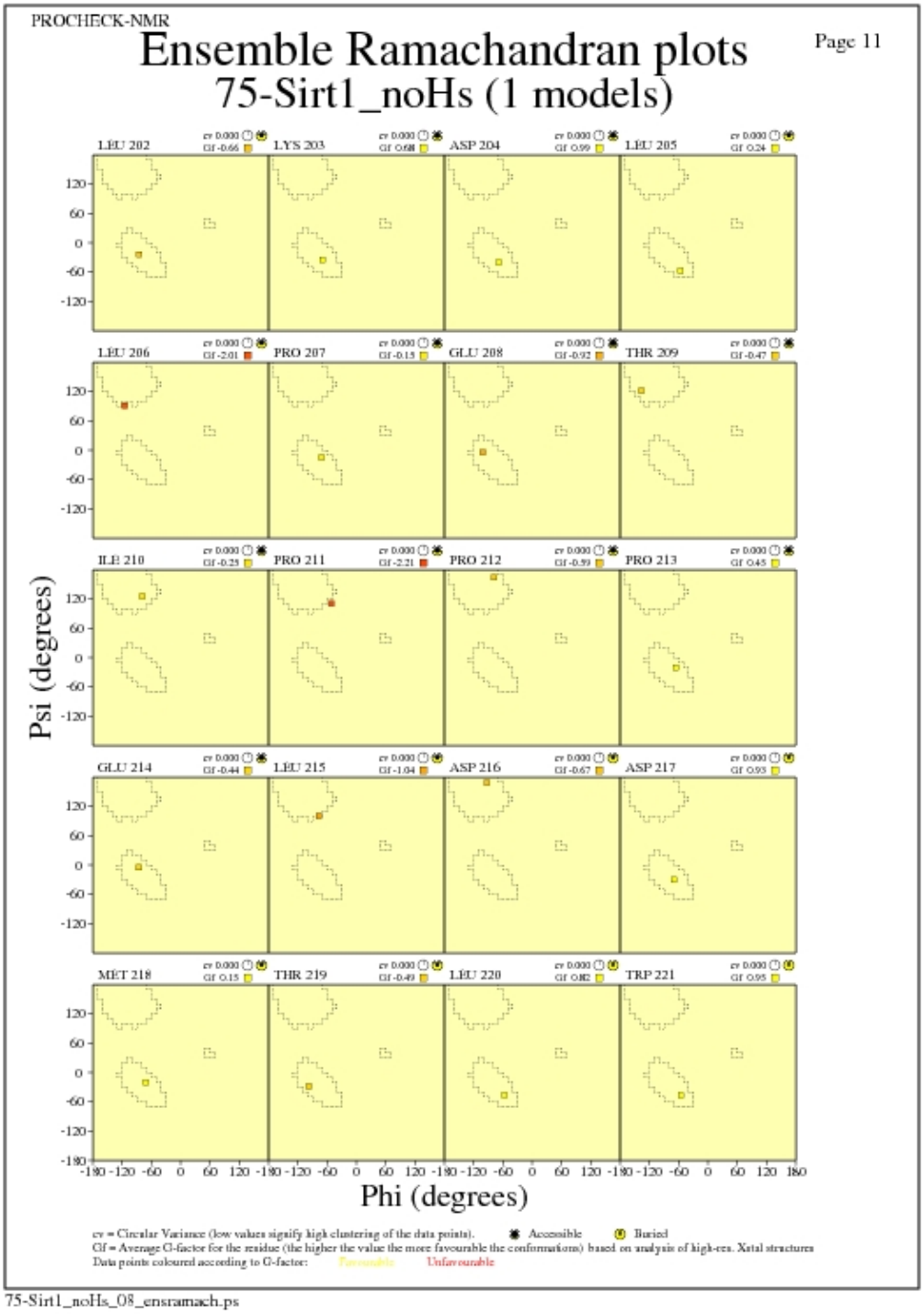
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



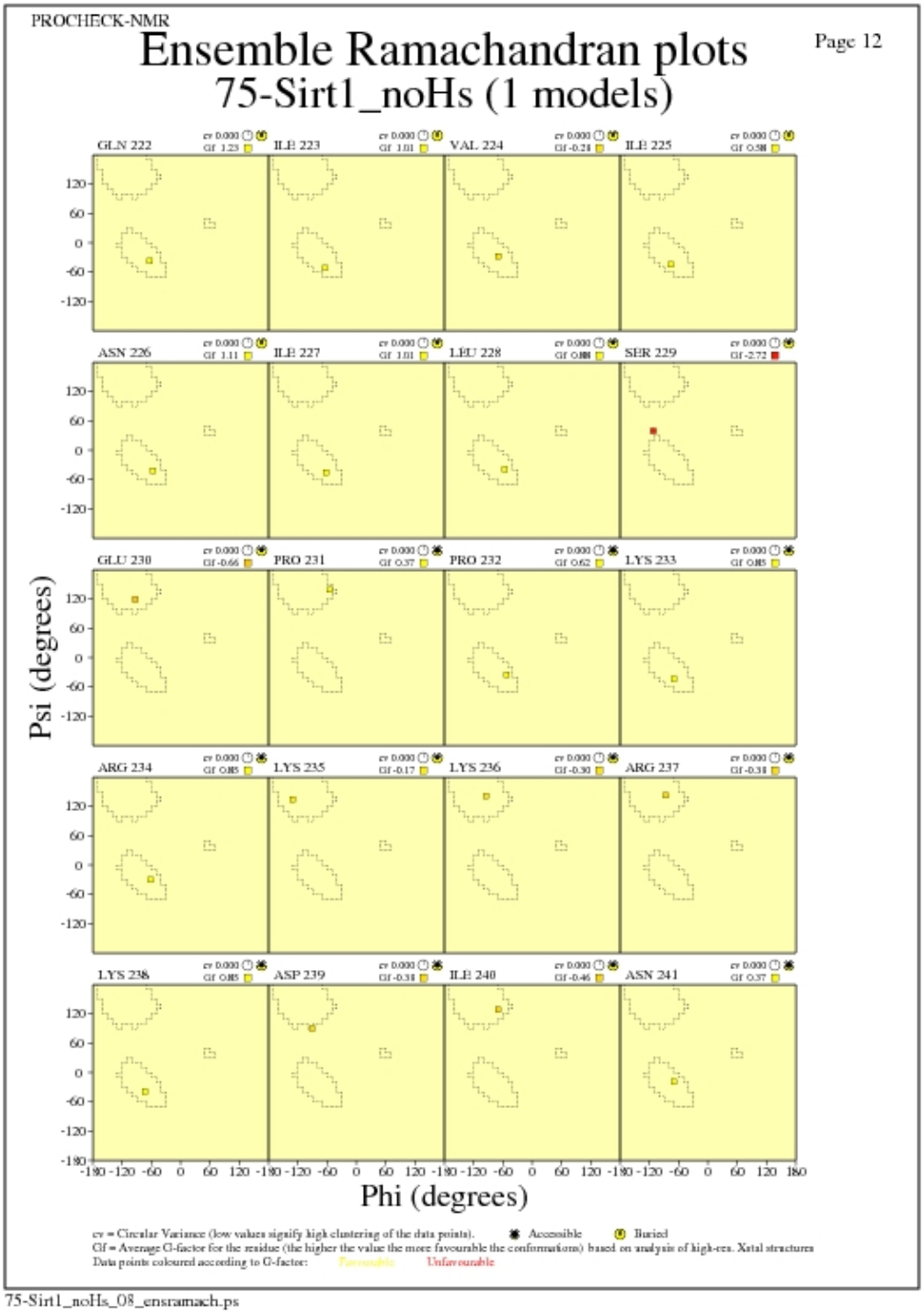
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



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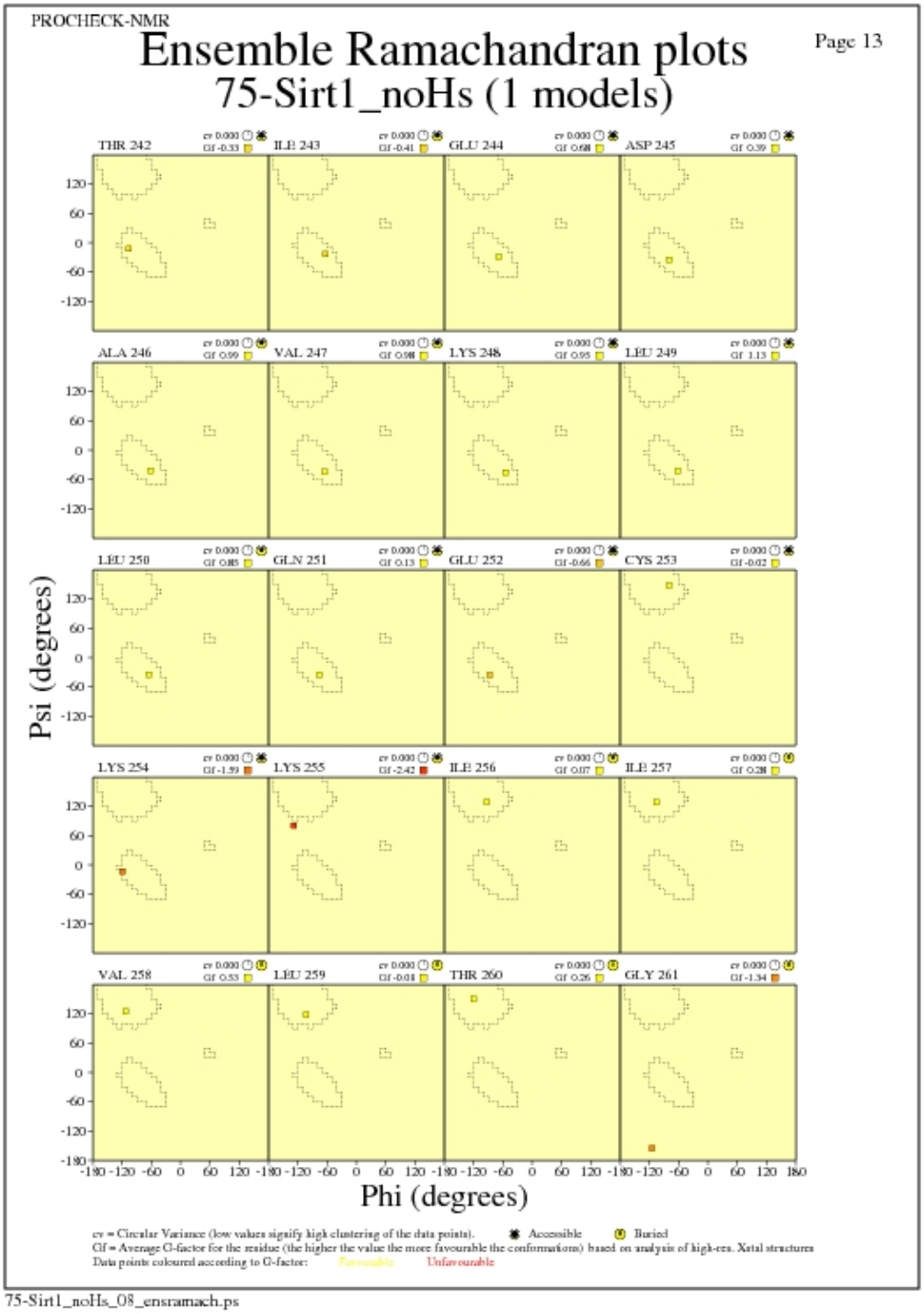
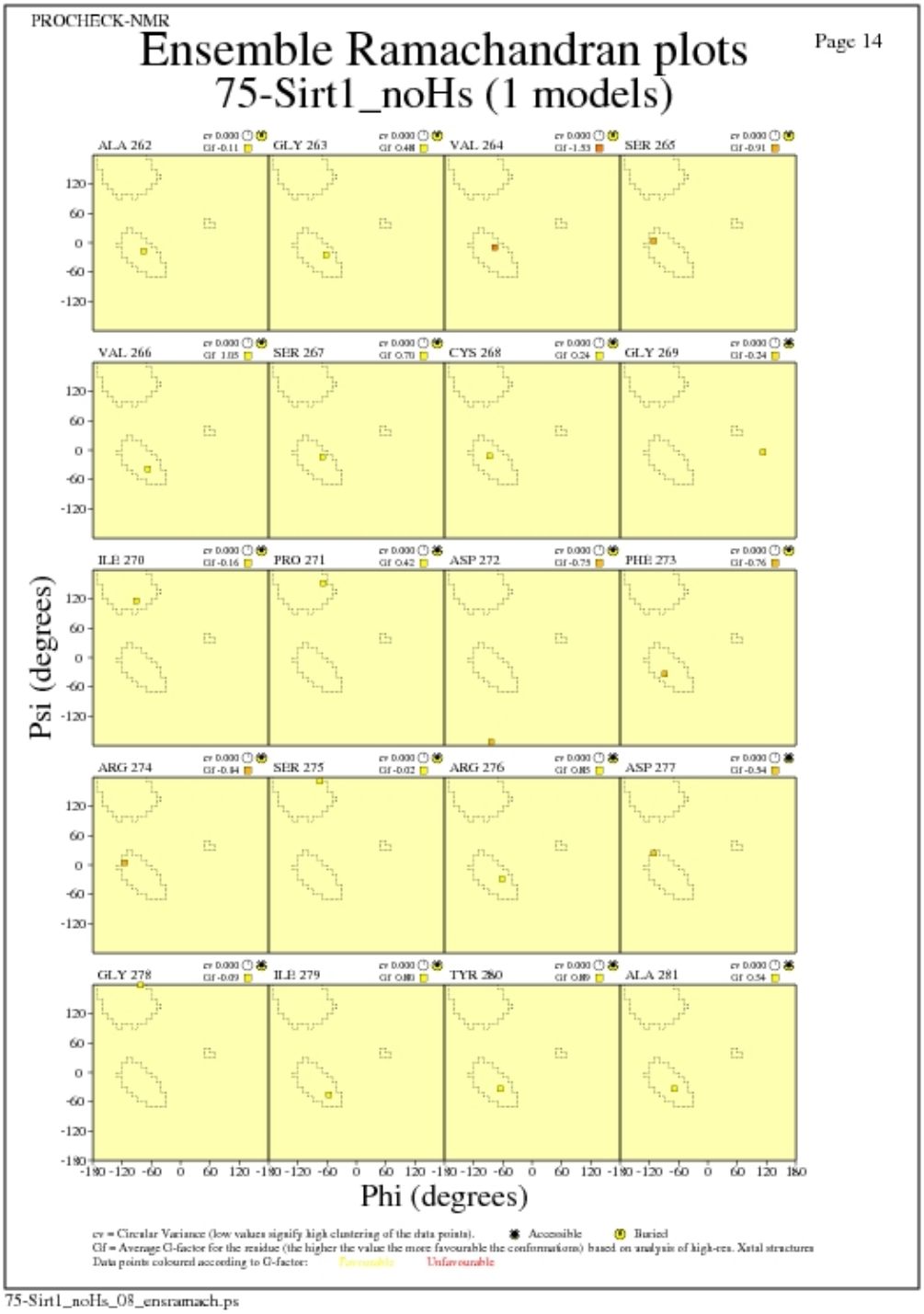
JPEG for residue Ramachandran Plots - page $num_n



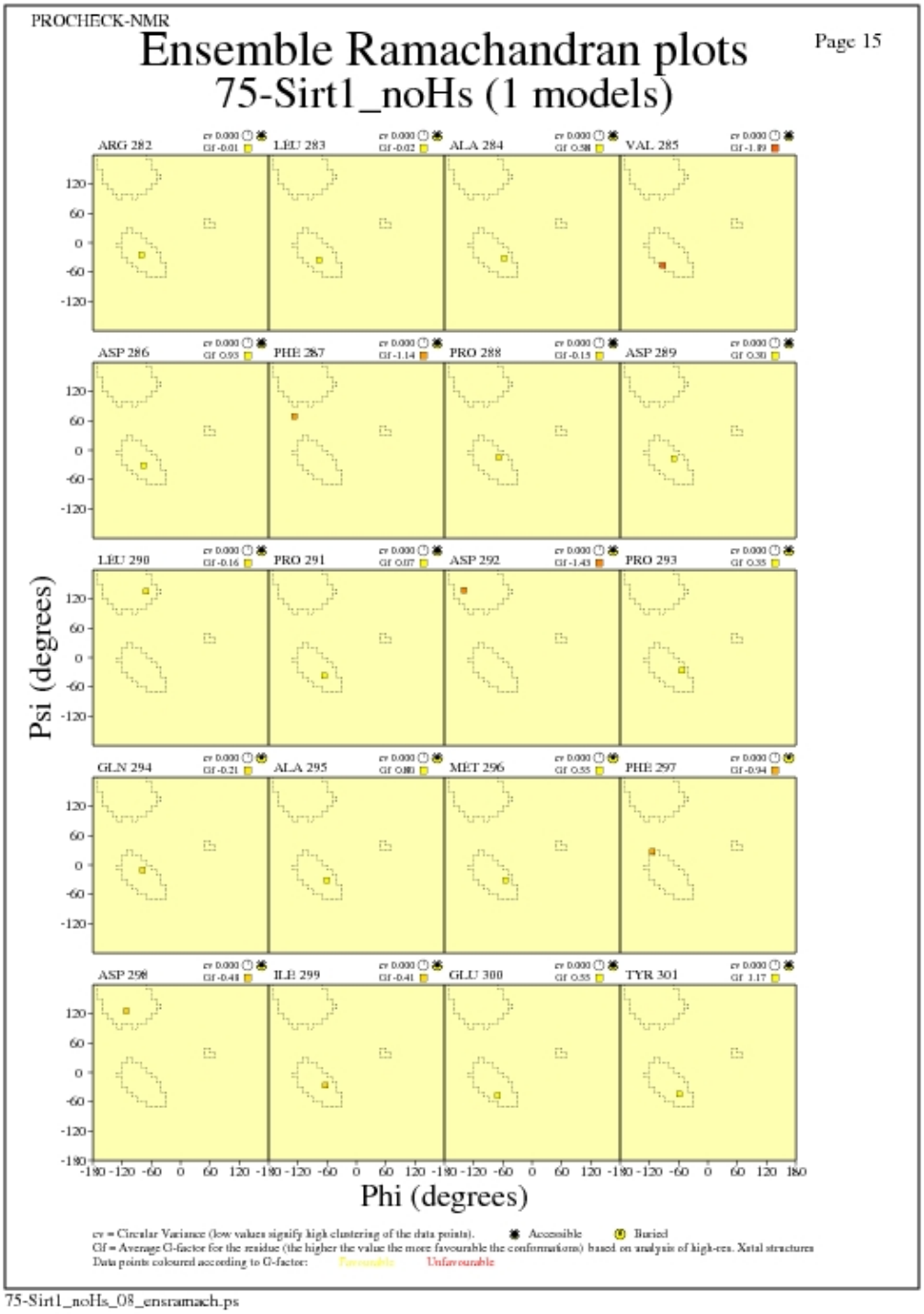
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



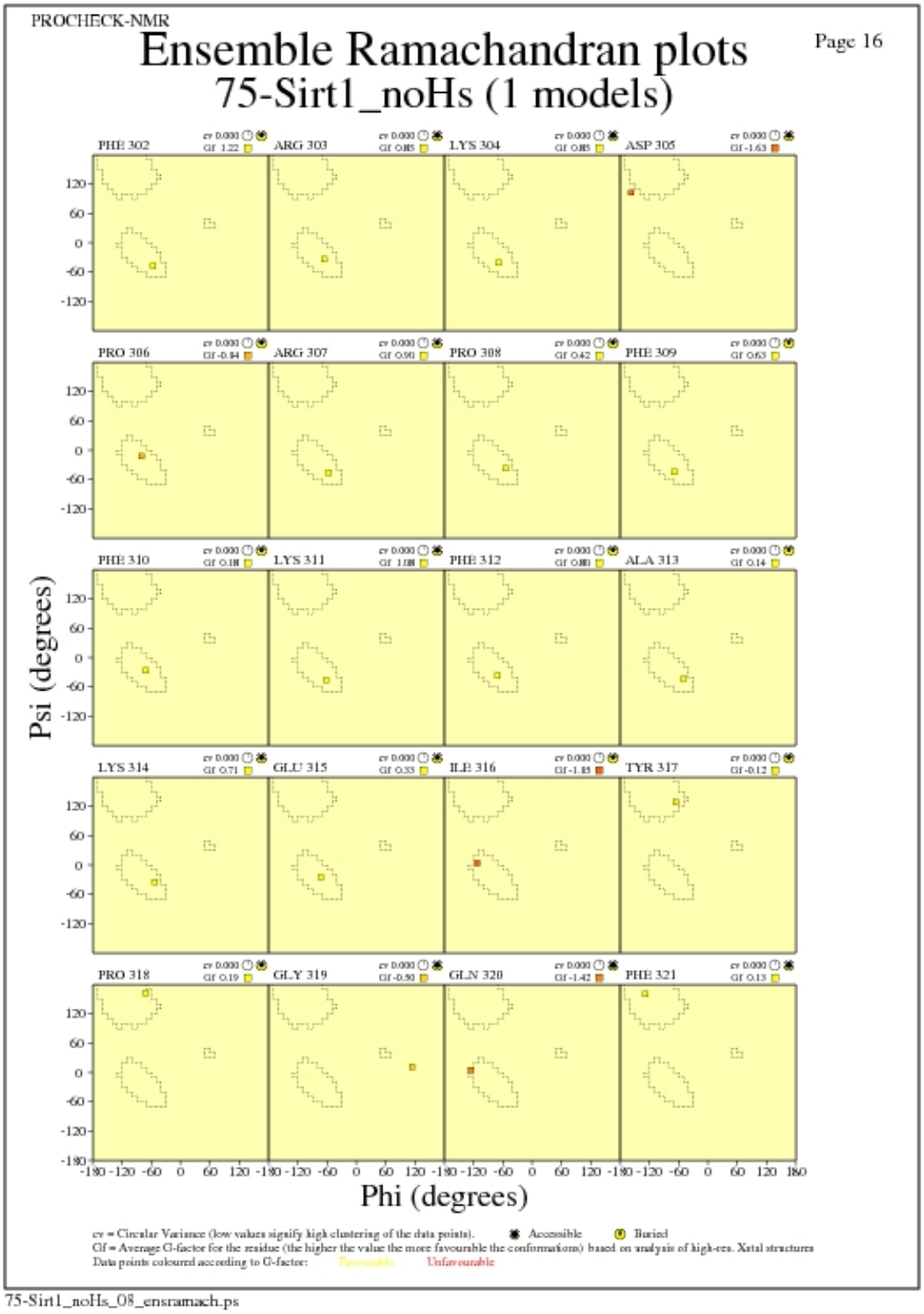
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



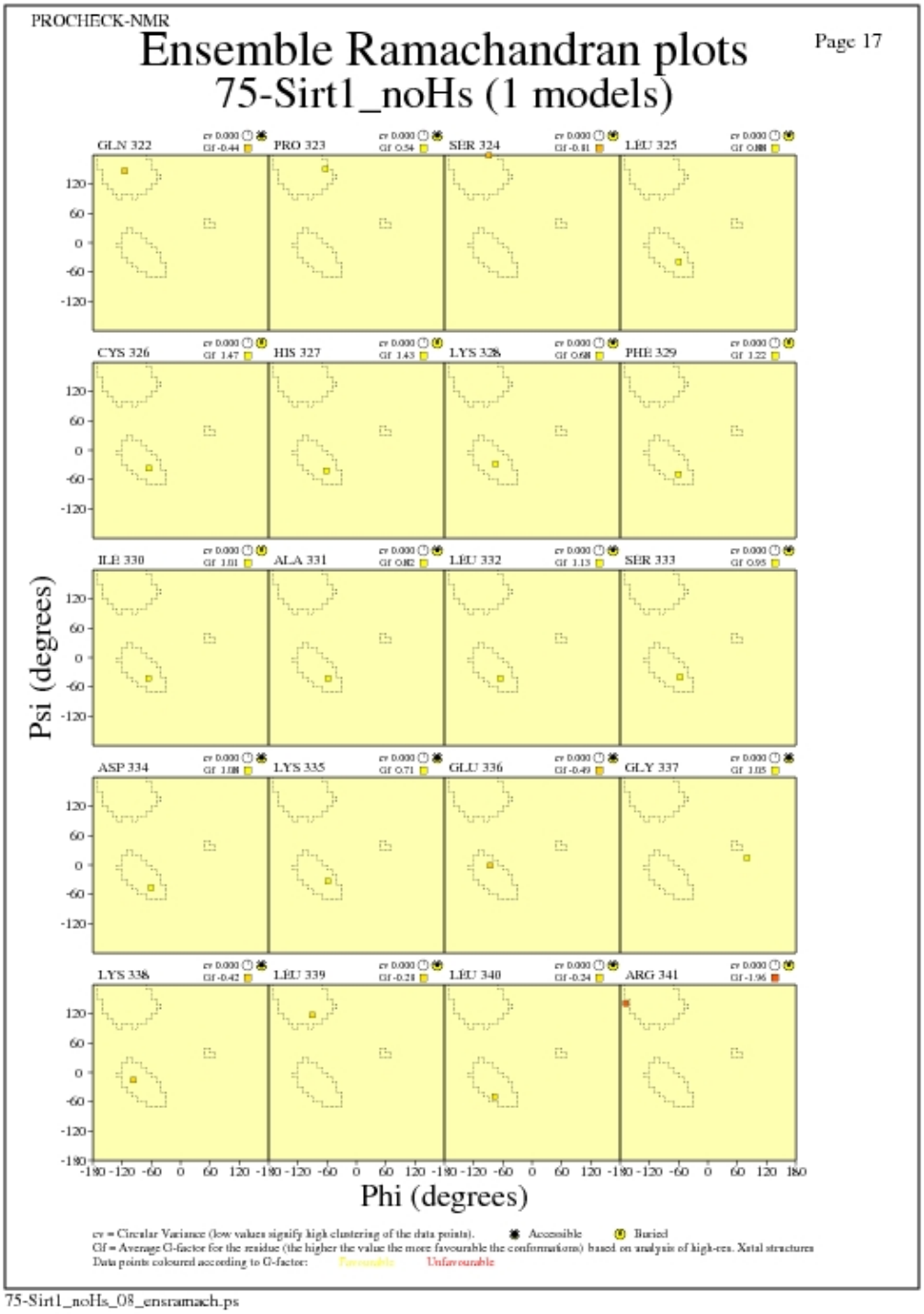
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



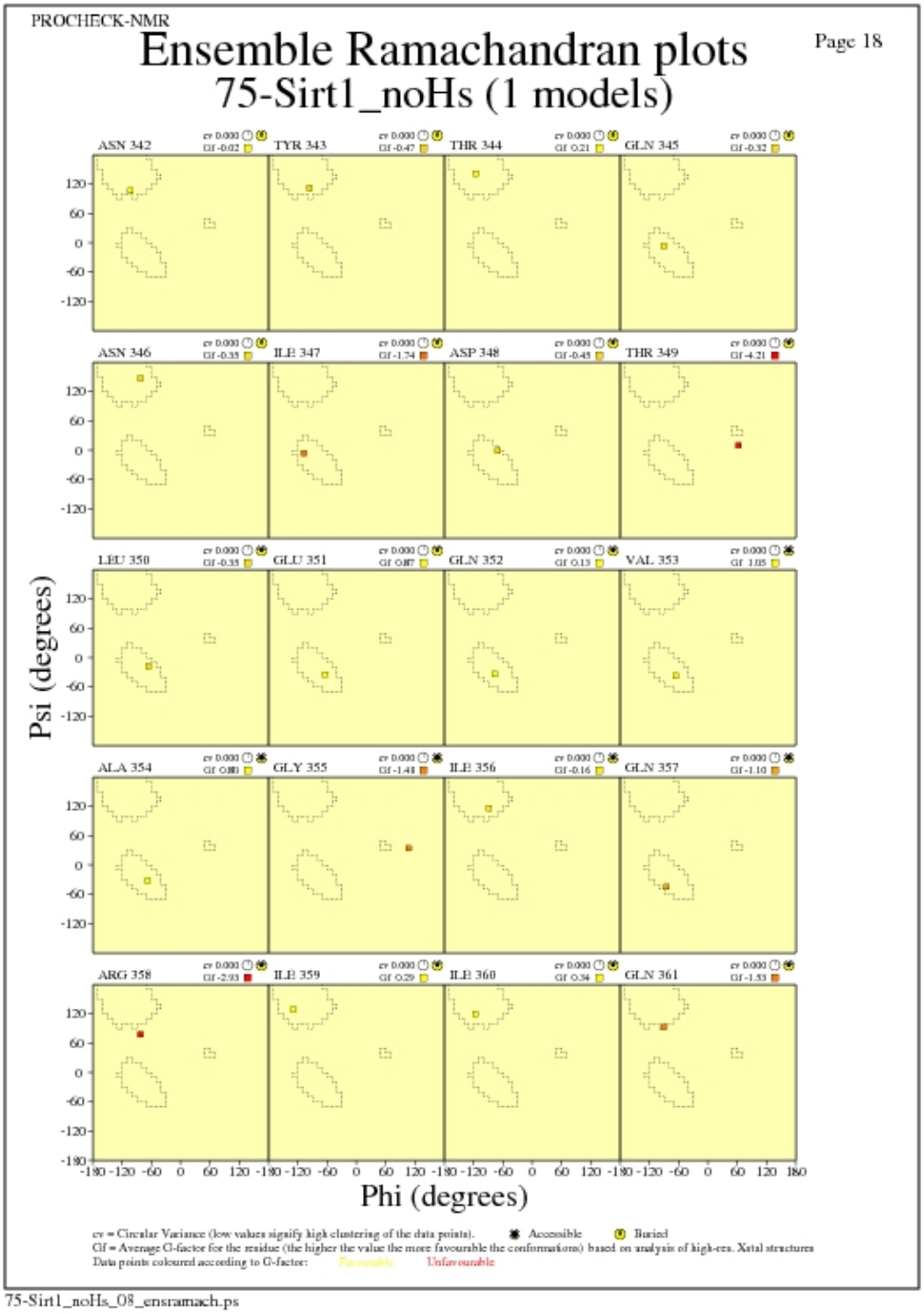
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



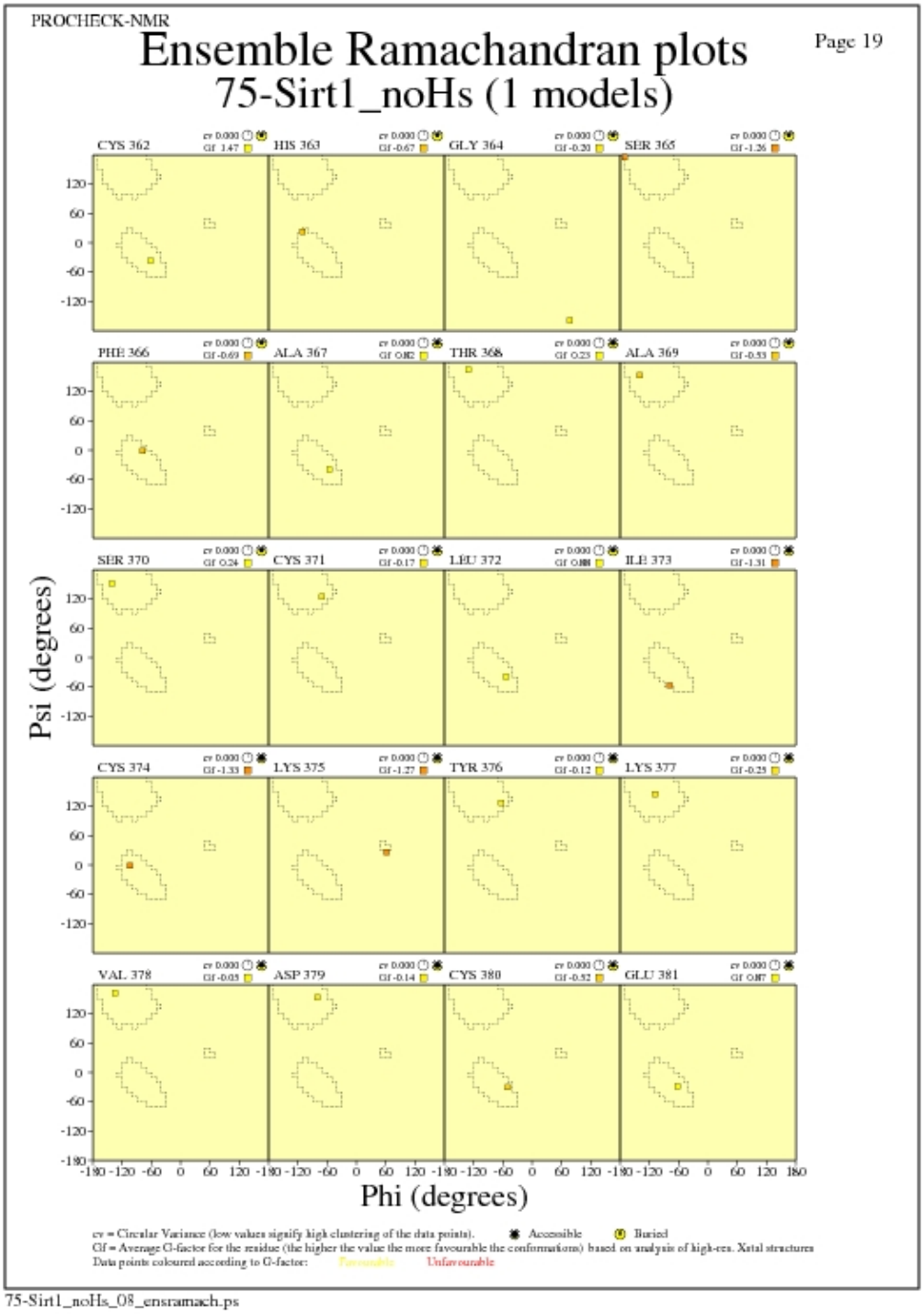
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



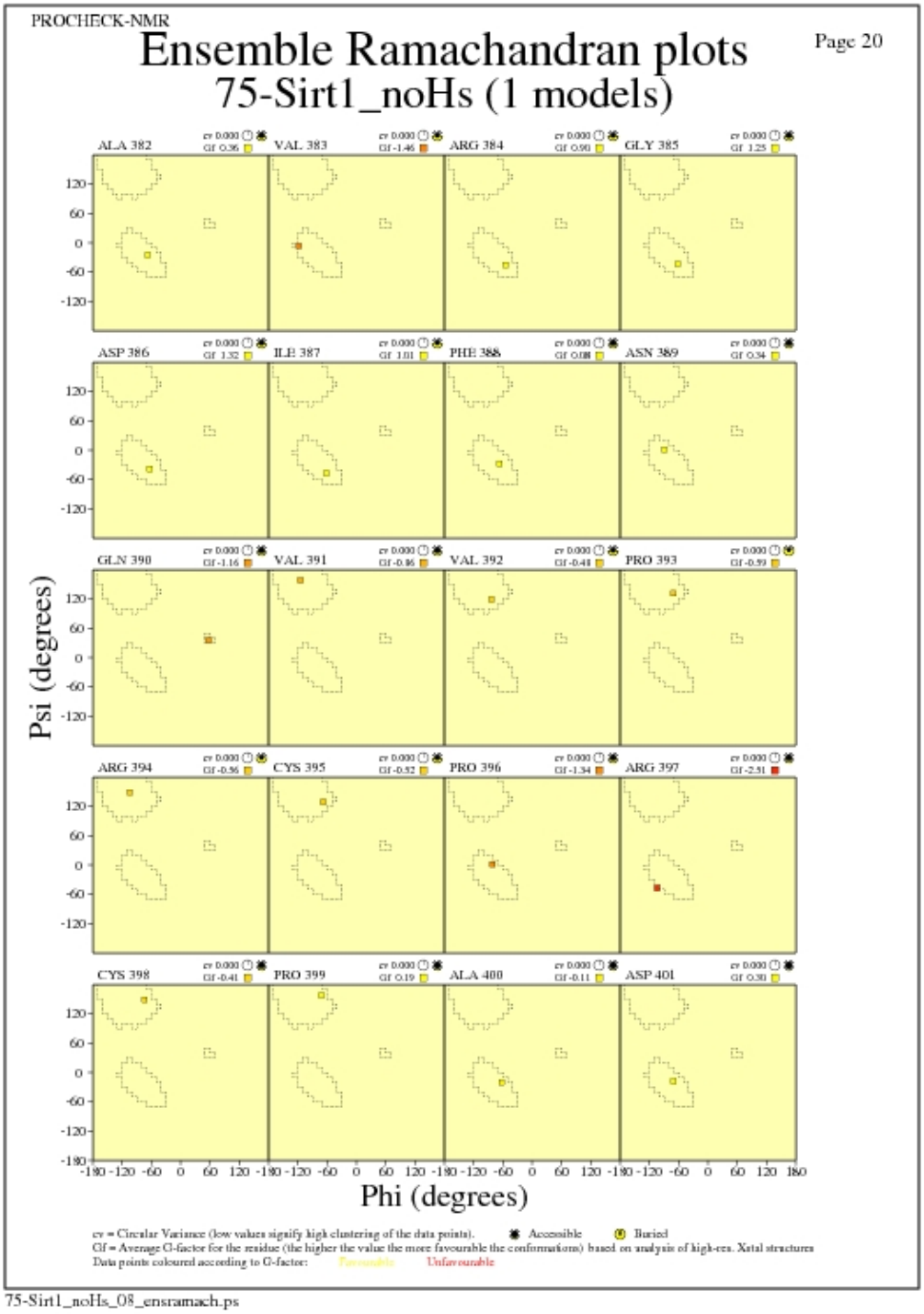
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



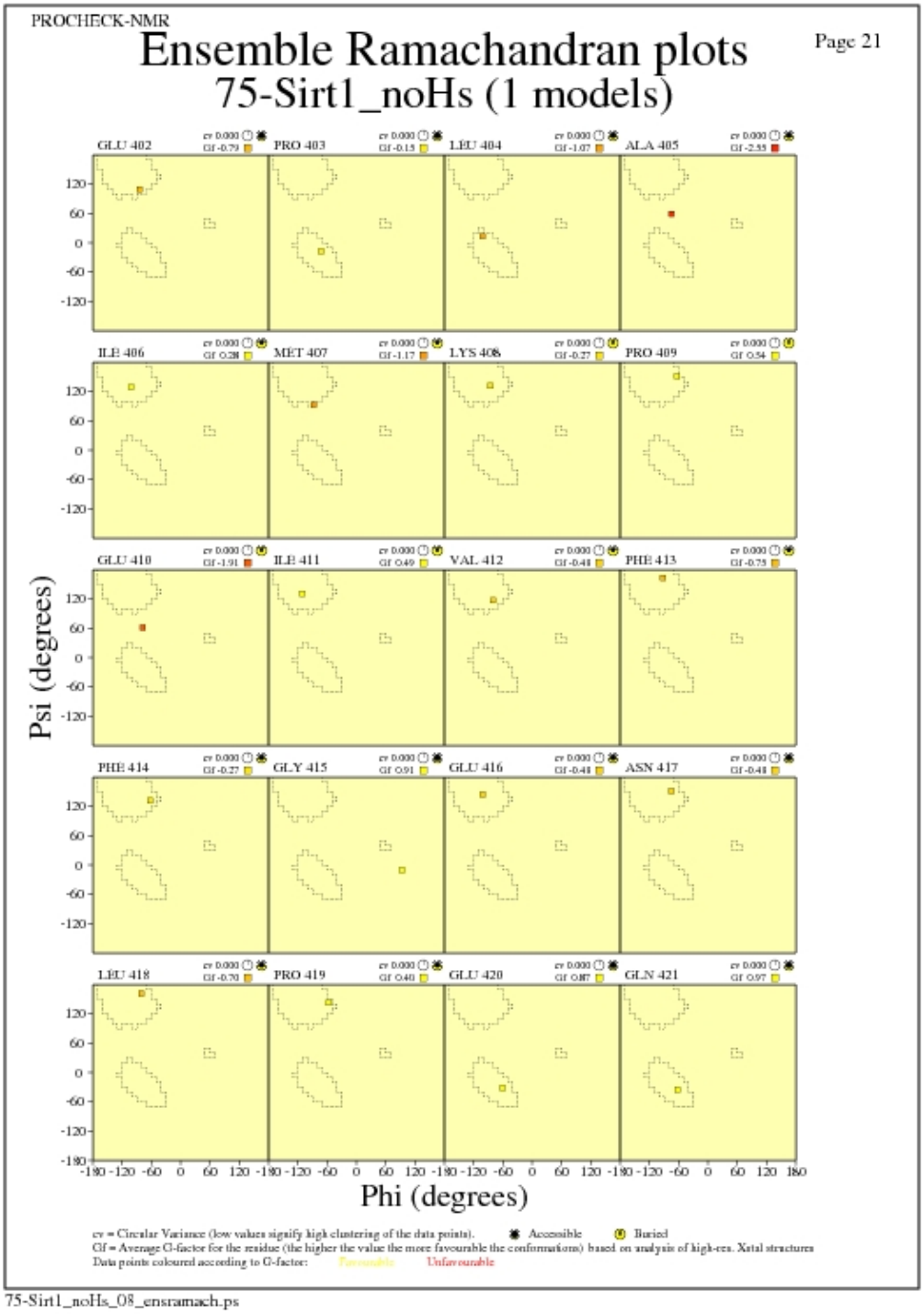
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



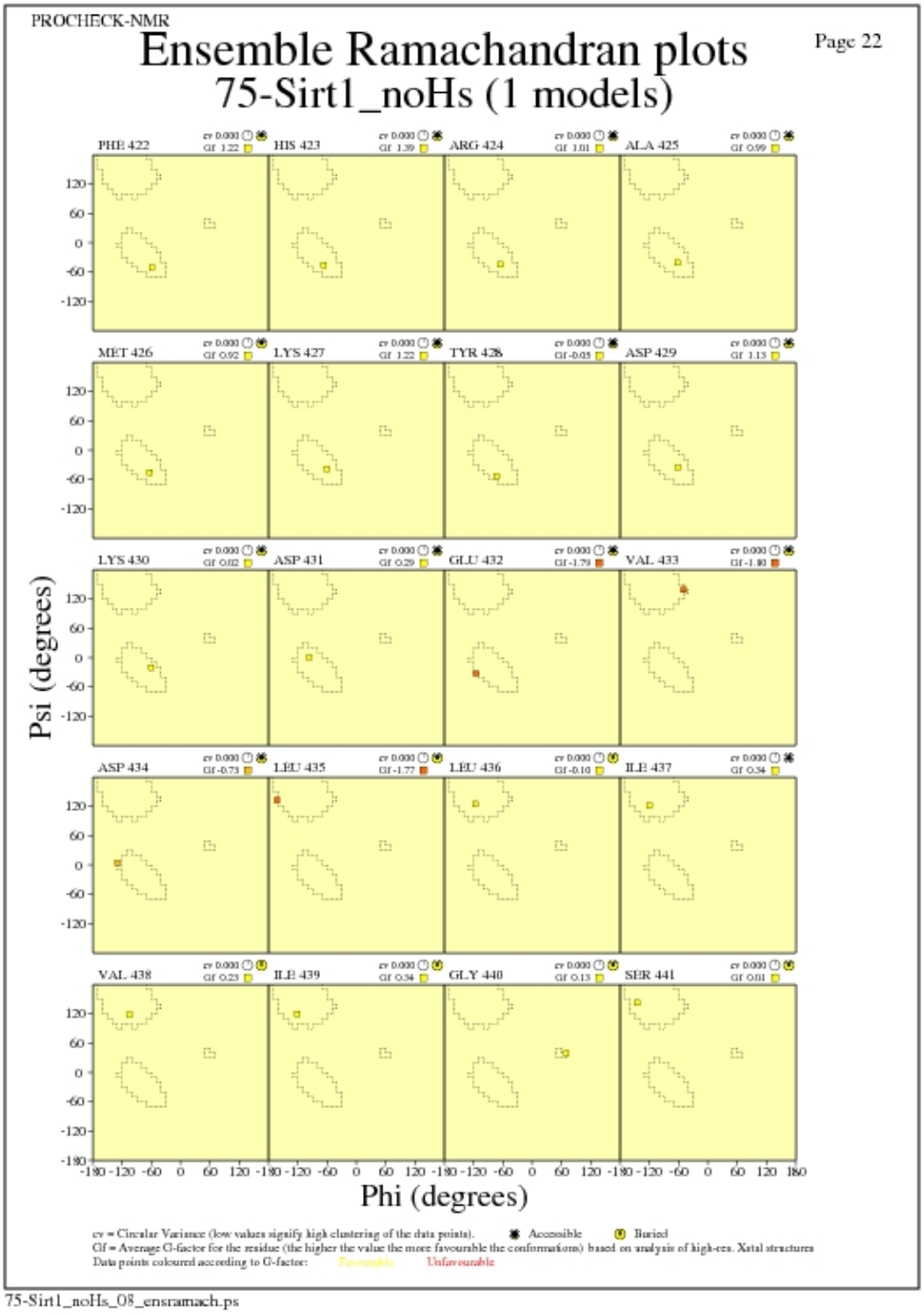
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



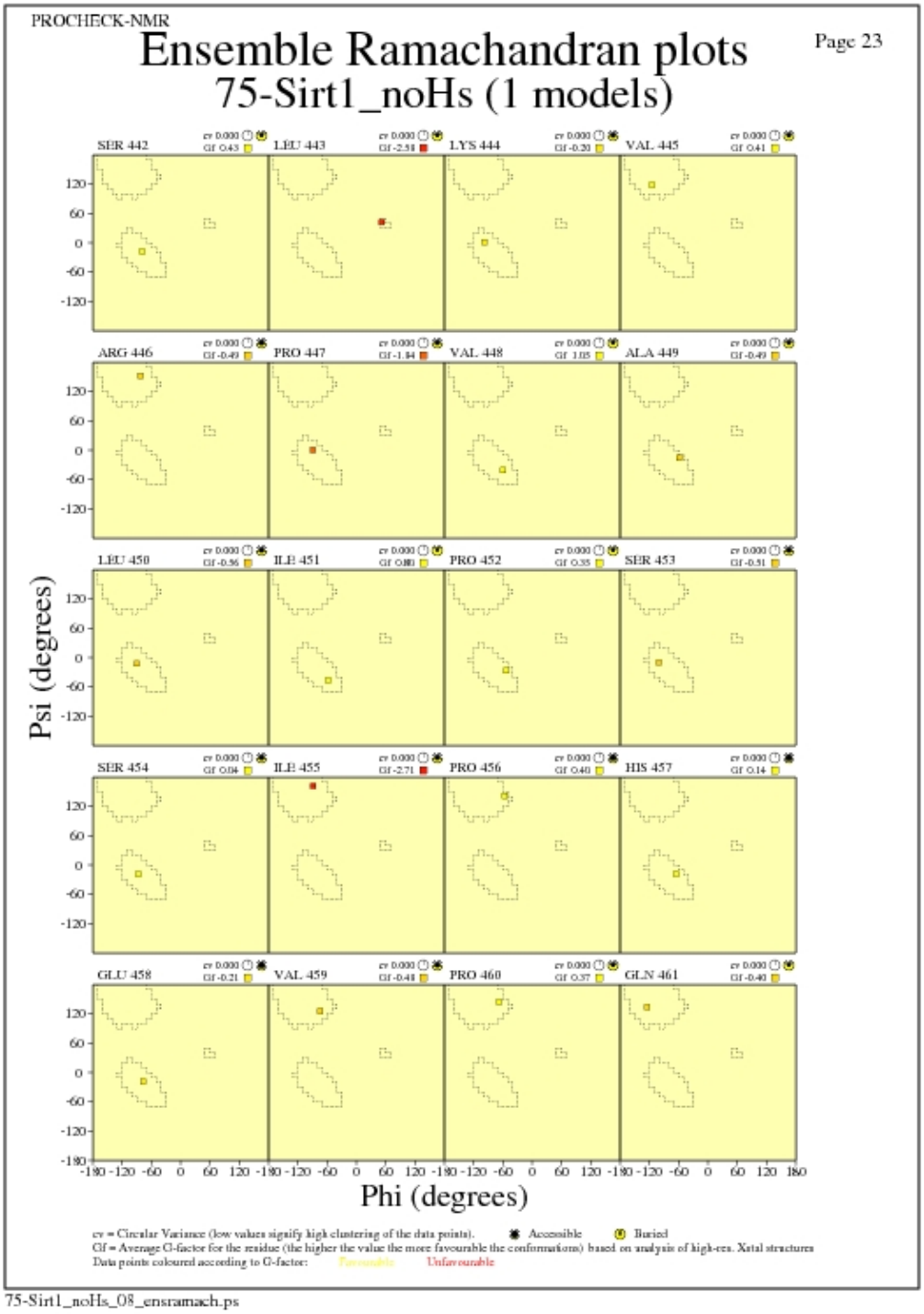
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



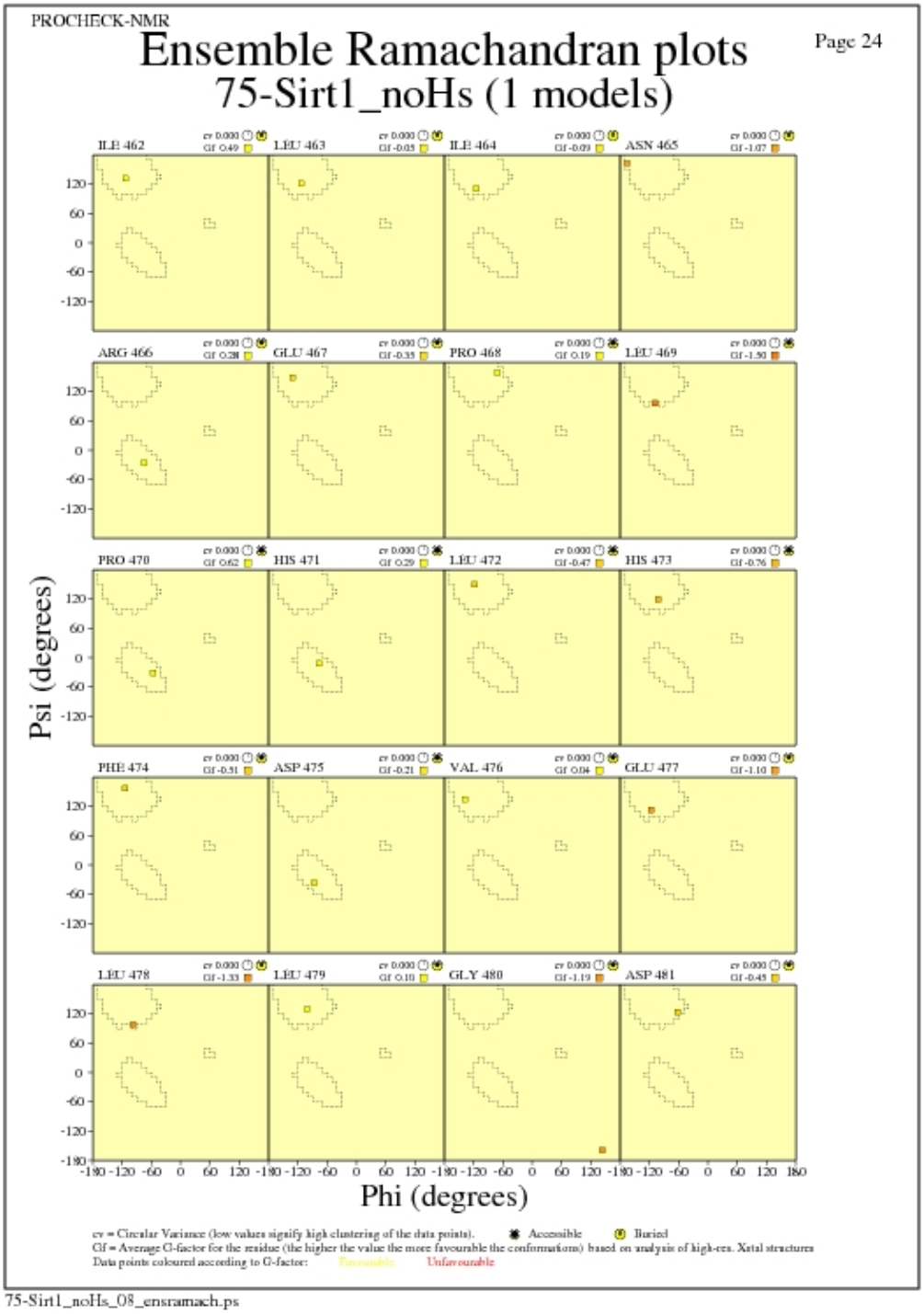
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



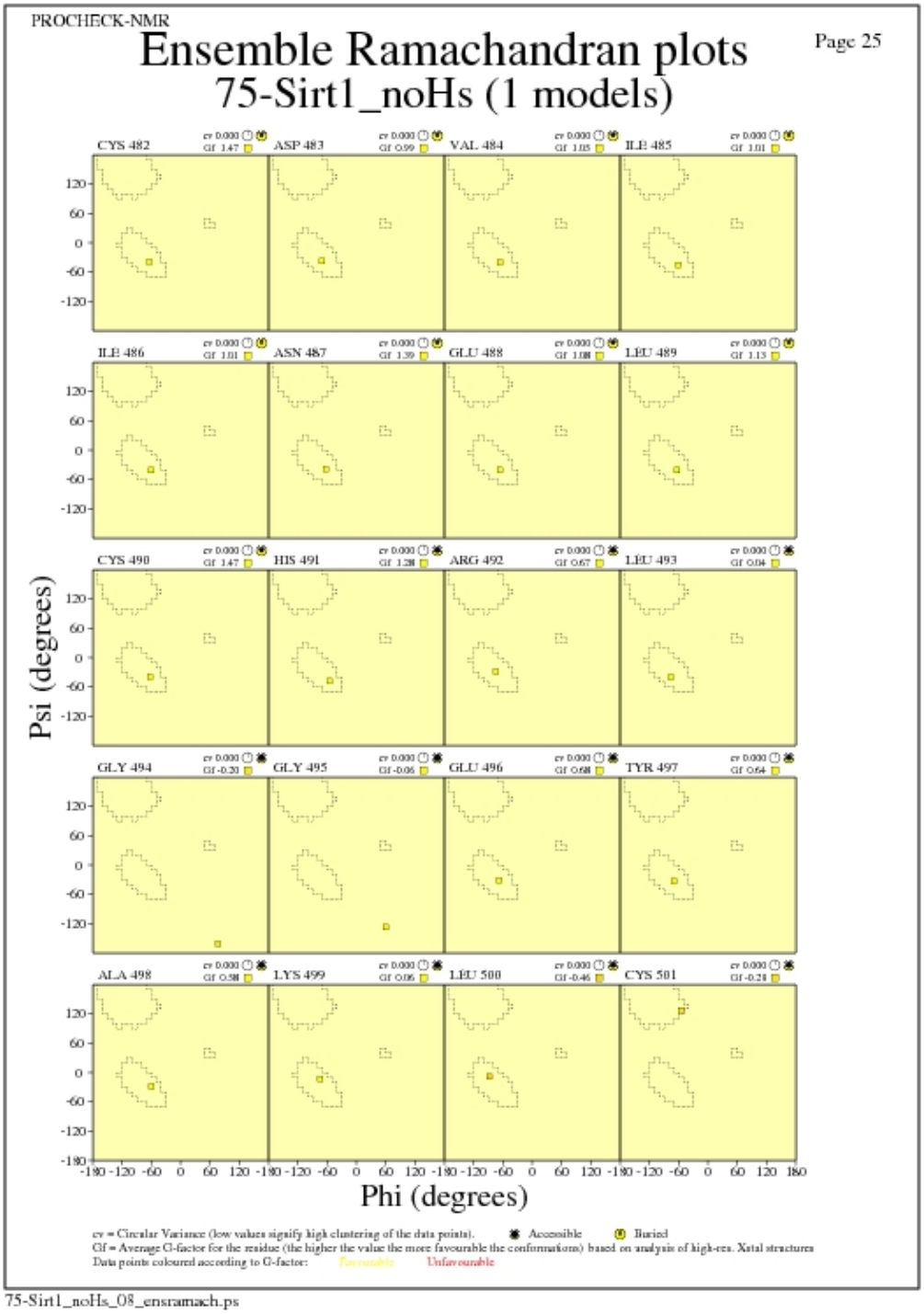
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



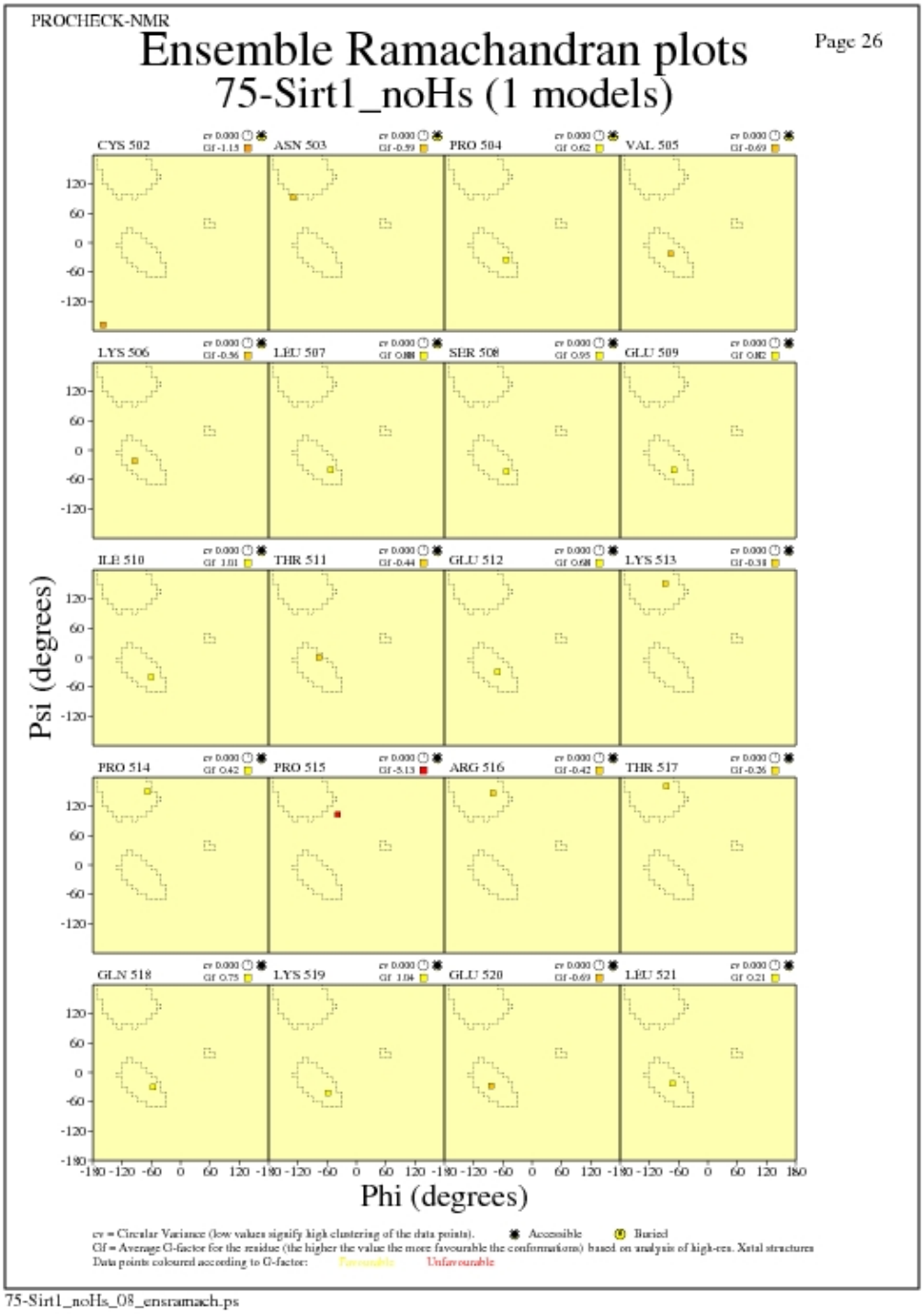
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



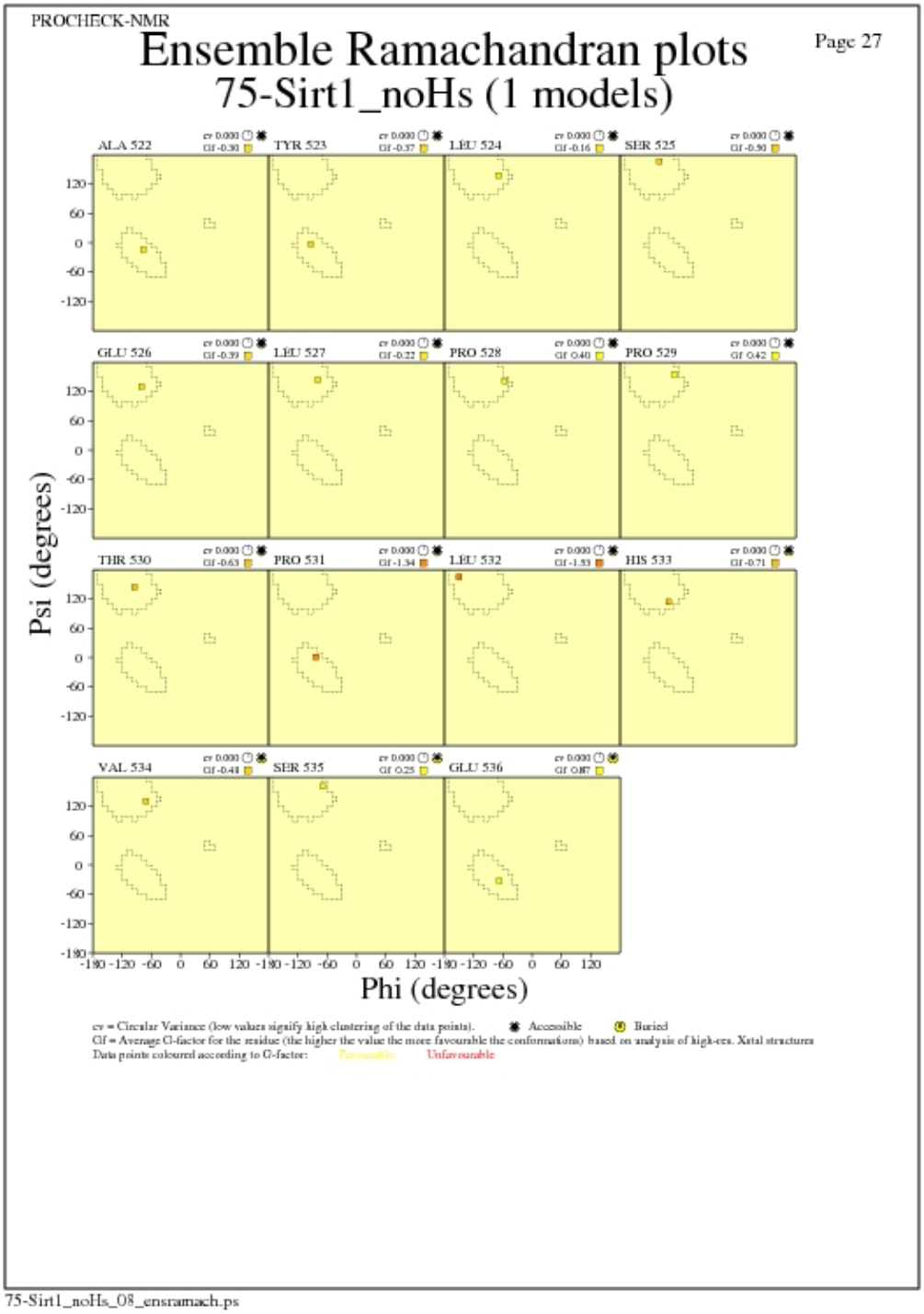
75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n



75-Sirt1_noHs_08_ensramach.ps

JPEG for residue Ramachandran Plots - page $num_n

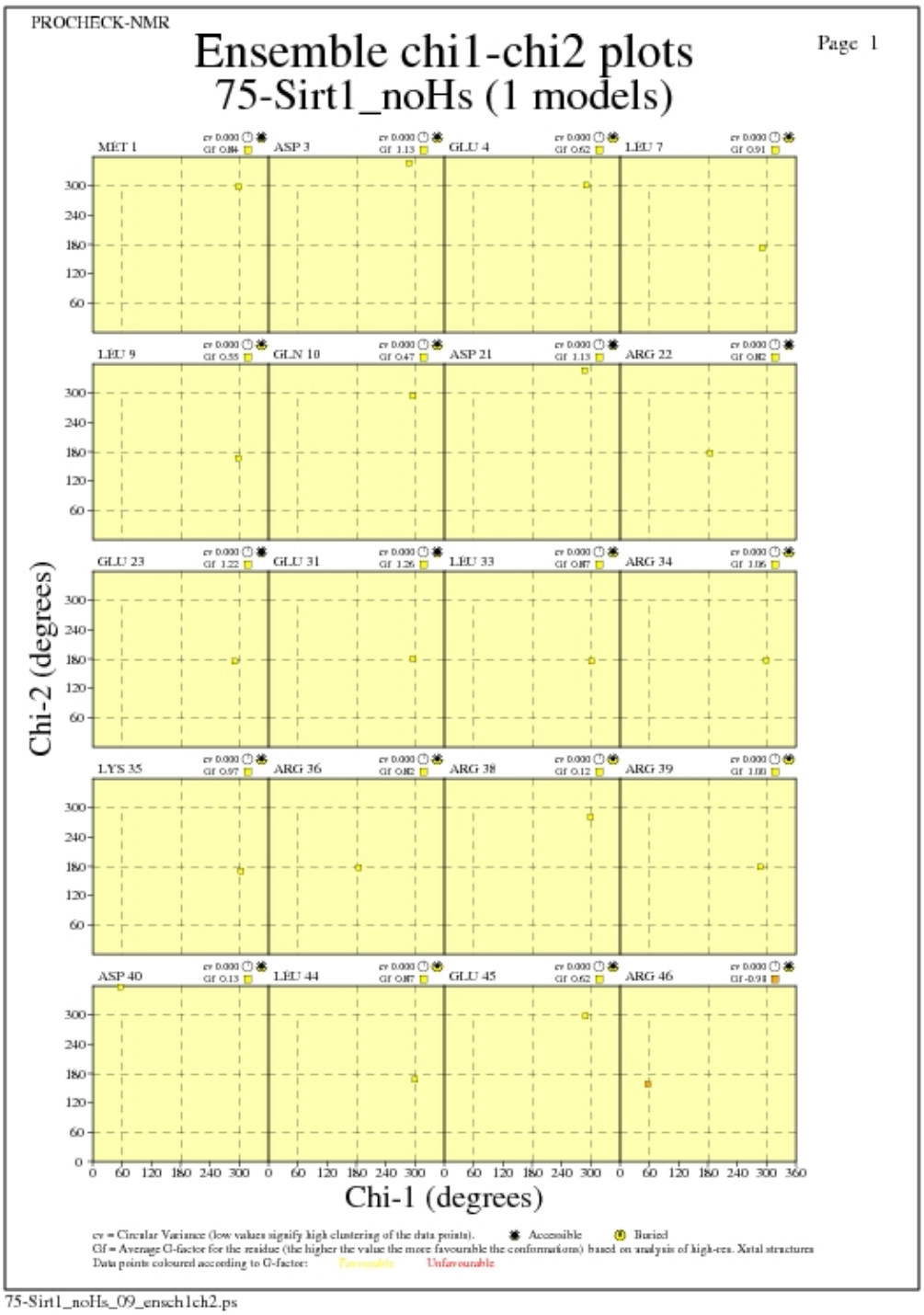


75-Sirt1_noHs_08_ensramach.ps

Ramachandran analysis for each residue from Molprobity

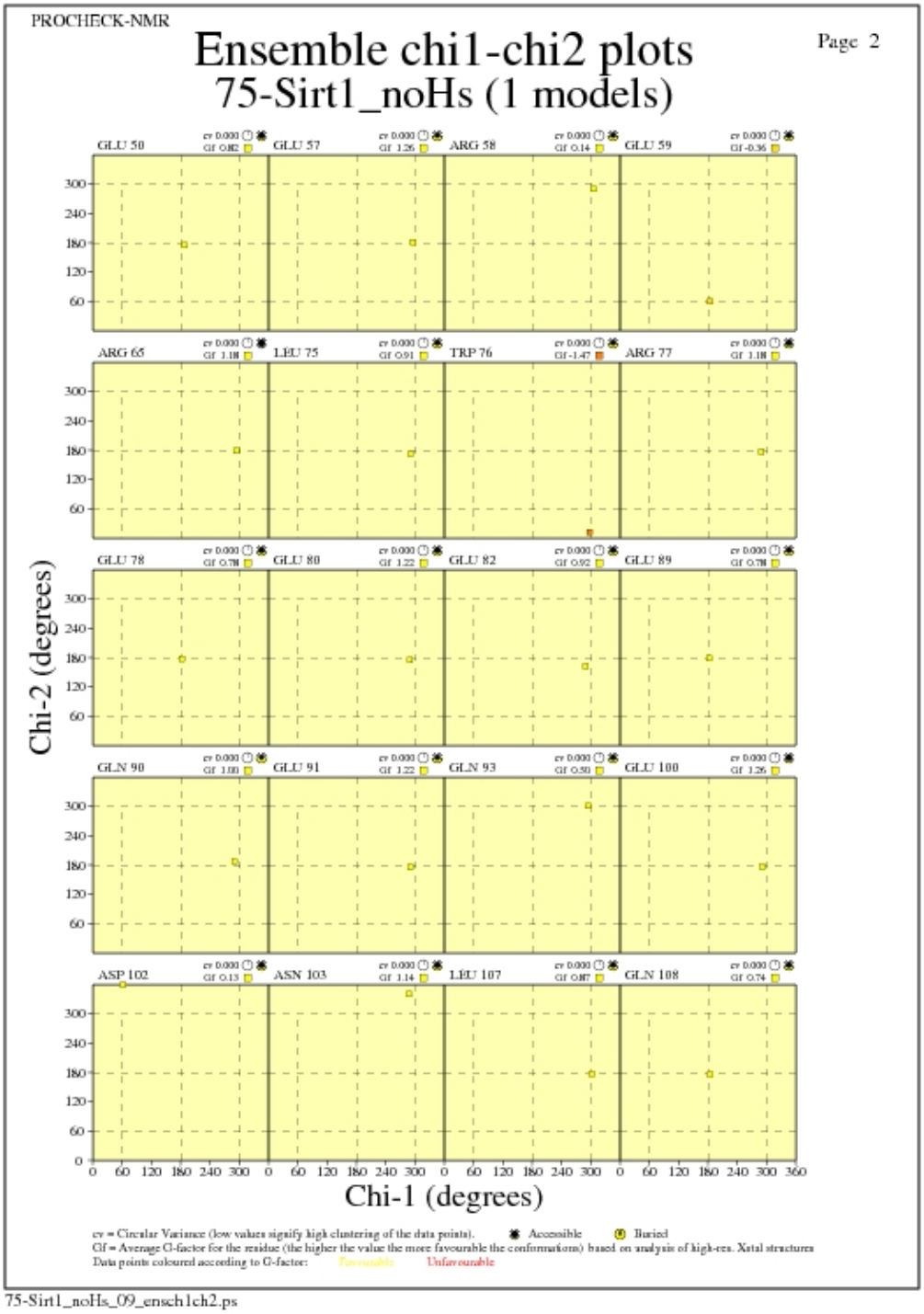
Chi1-Chi2 Plots for each residue

JPEG for residue Chi1-Chi2 Plots - page $num_n



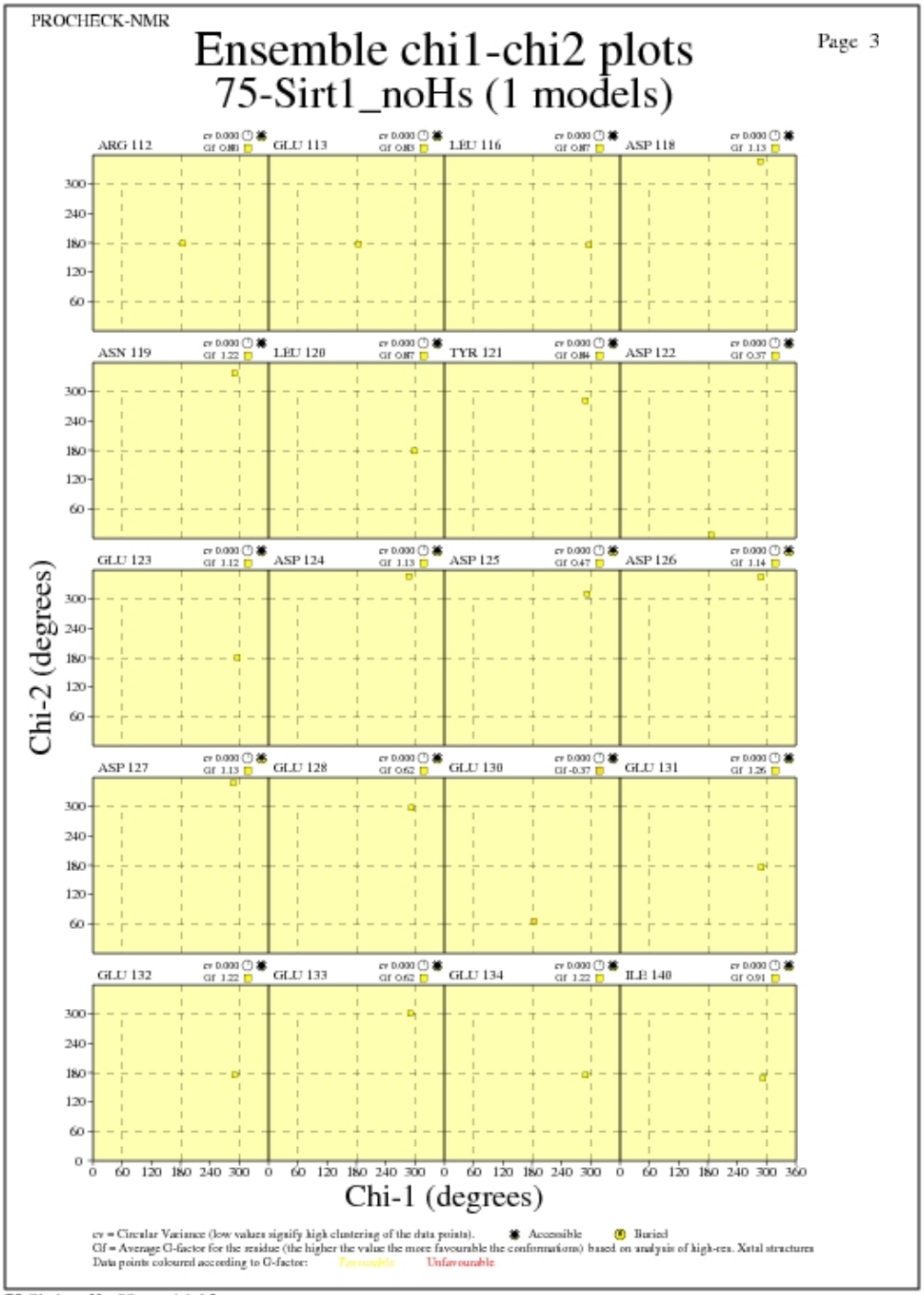
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



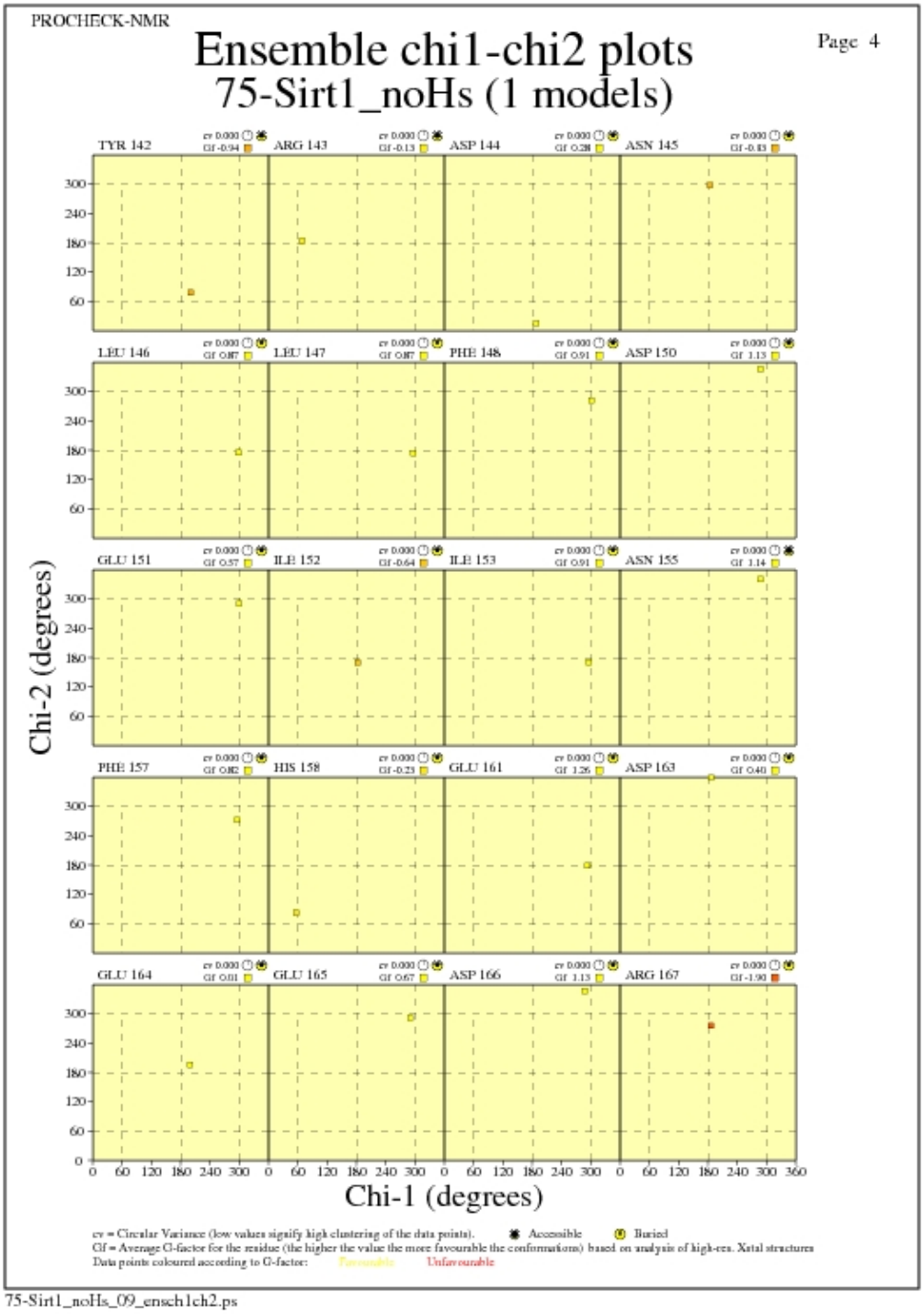
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



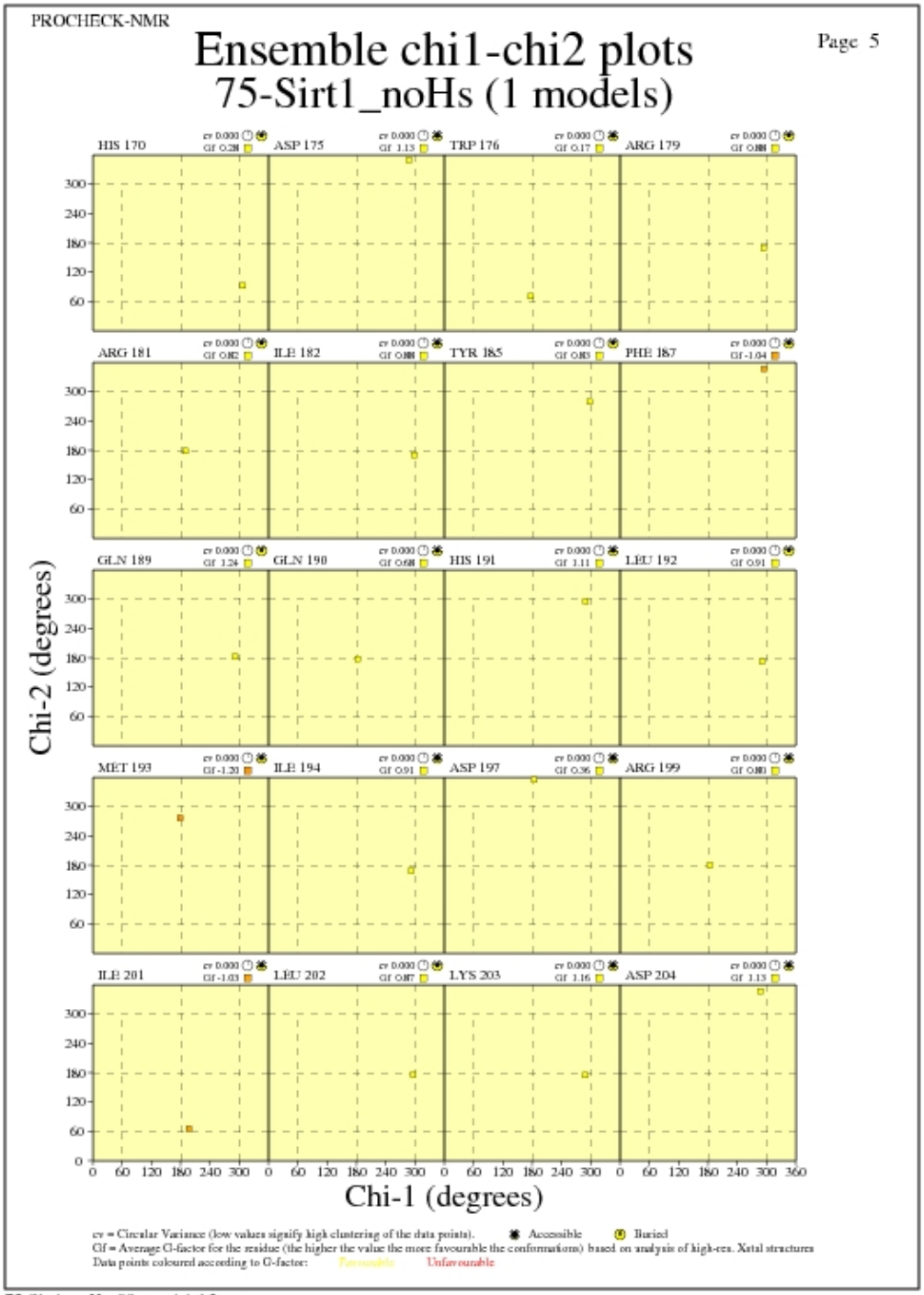
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



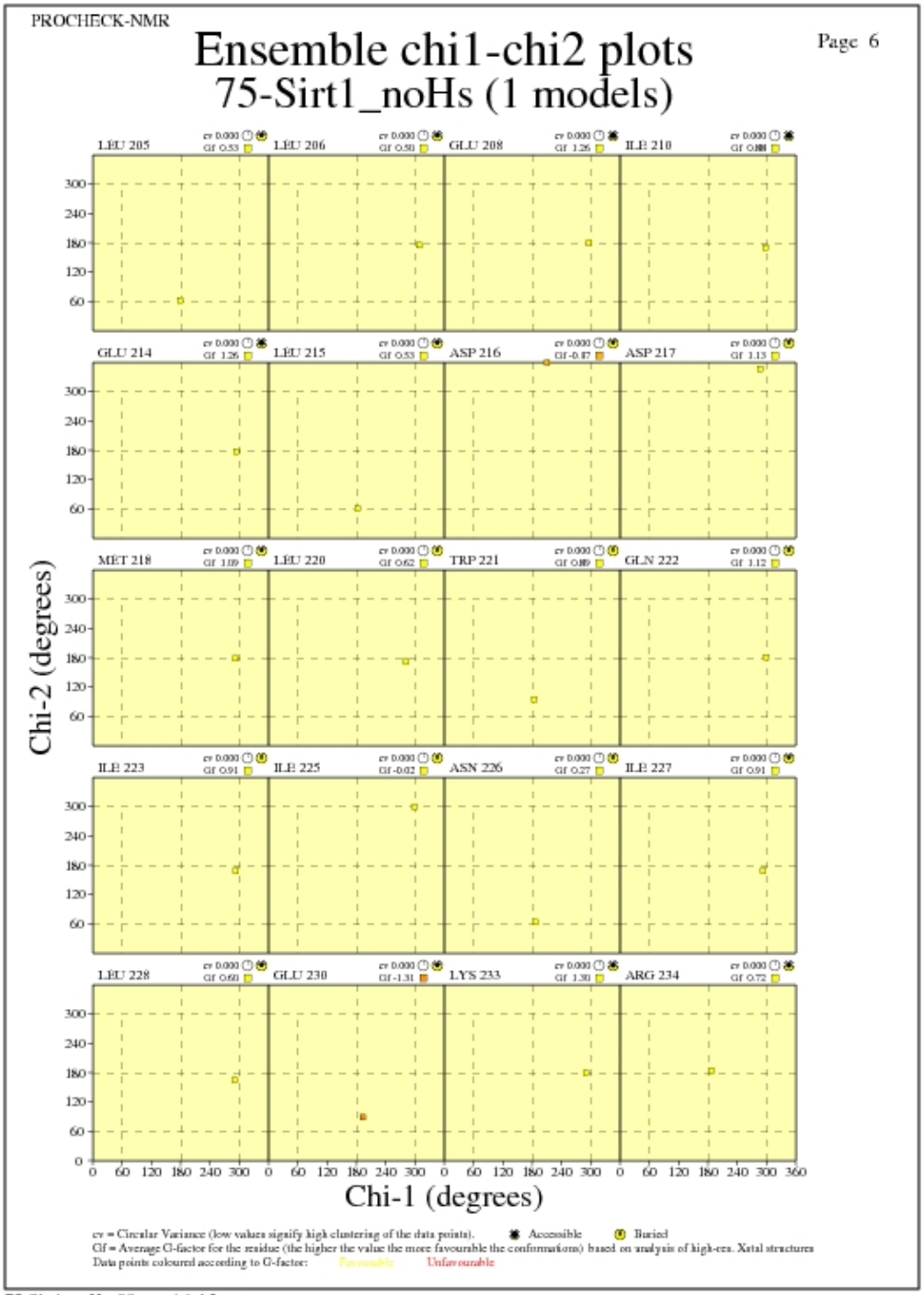
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



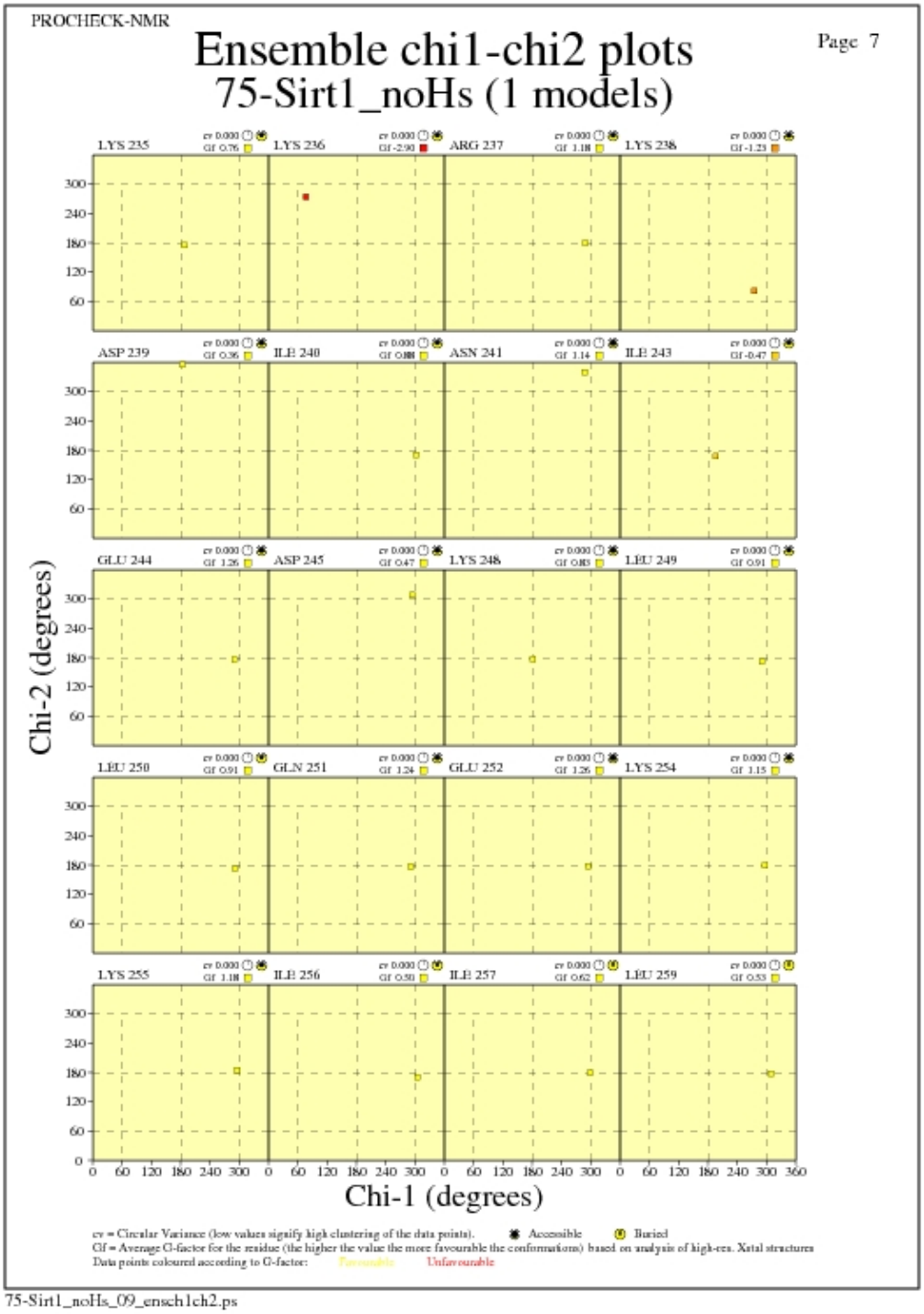
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



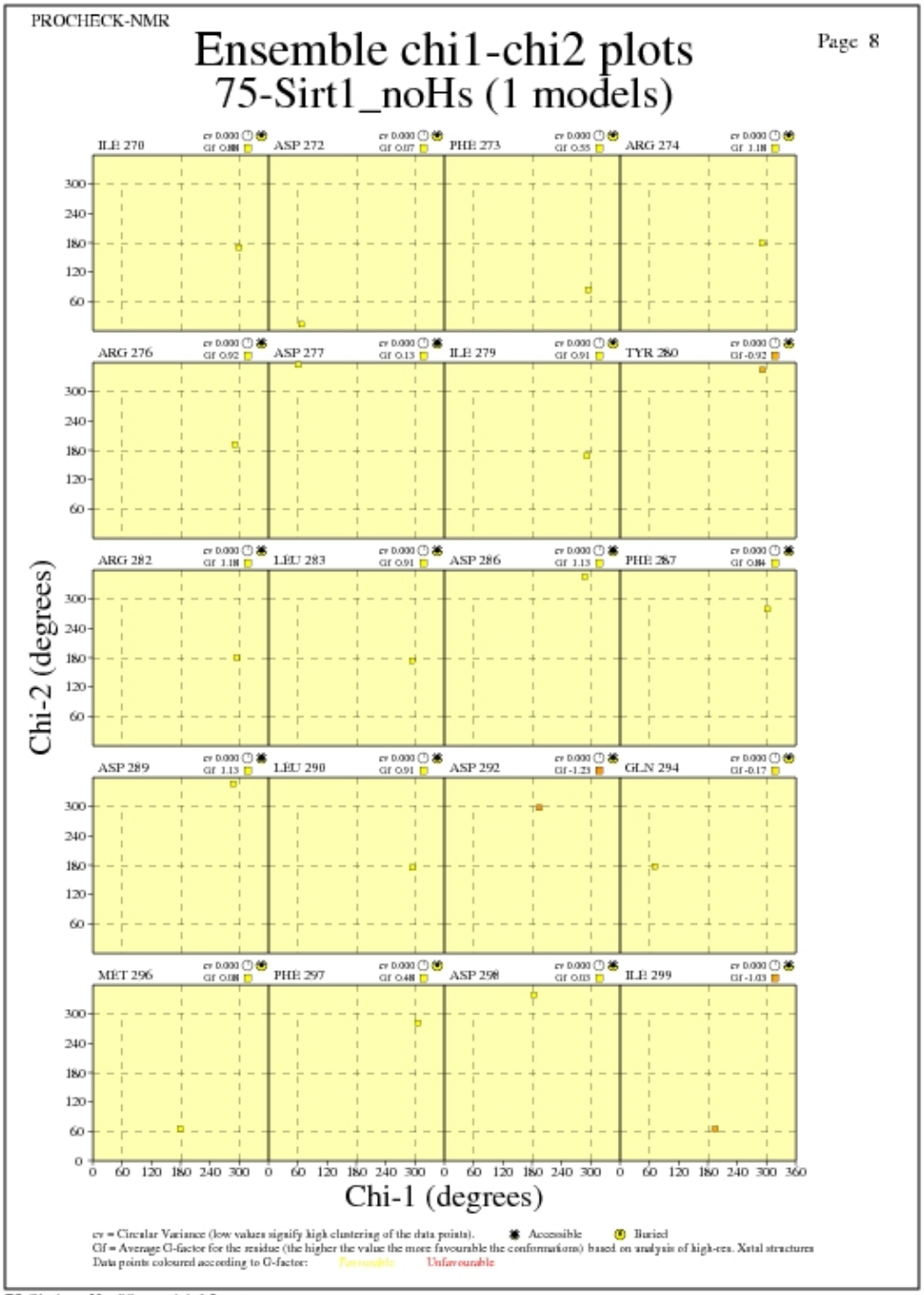
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



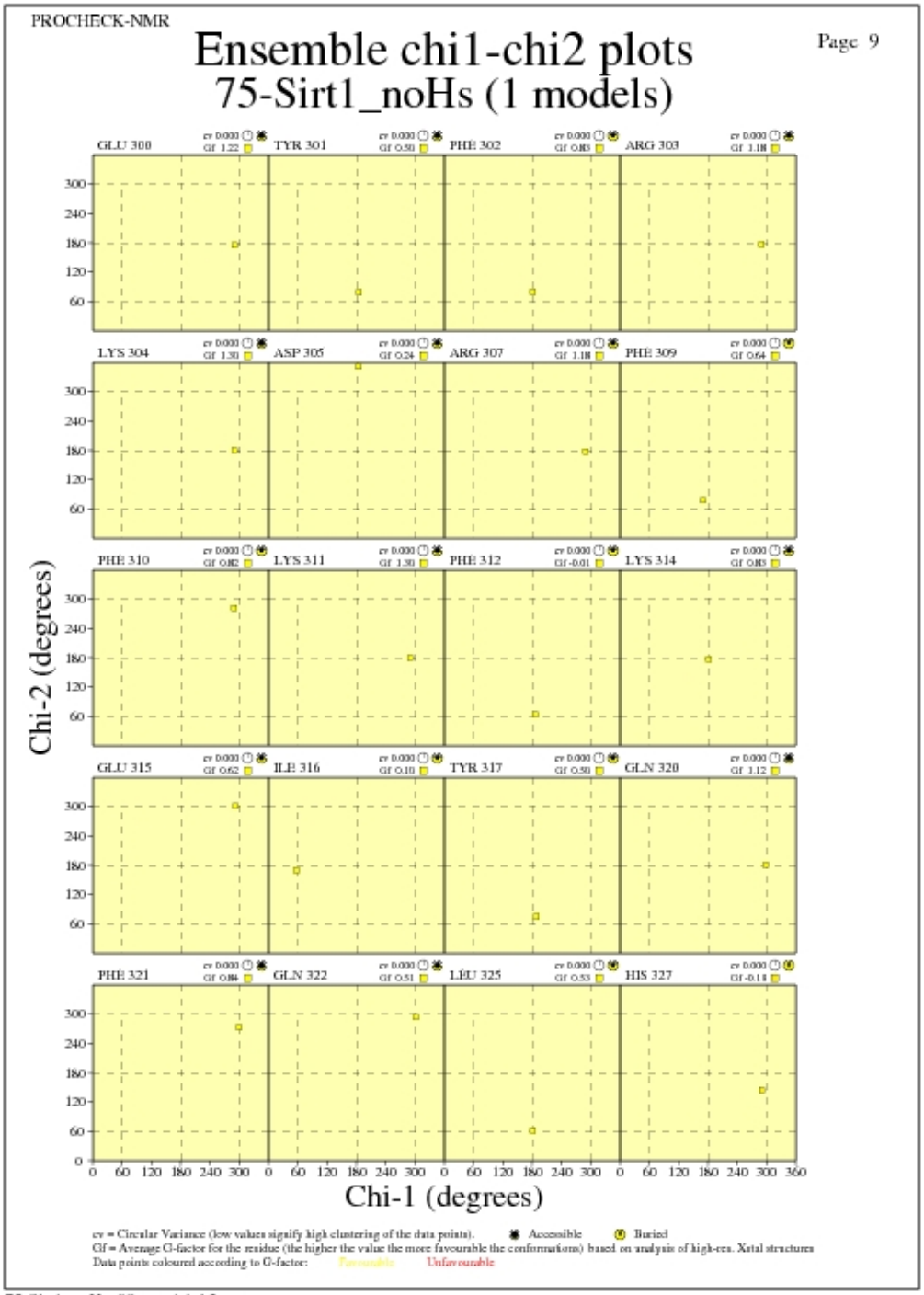
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



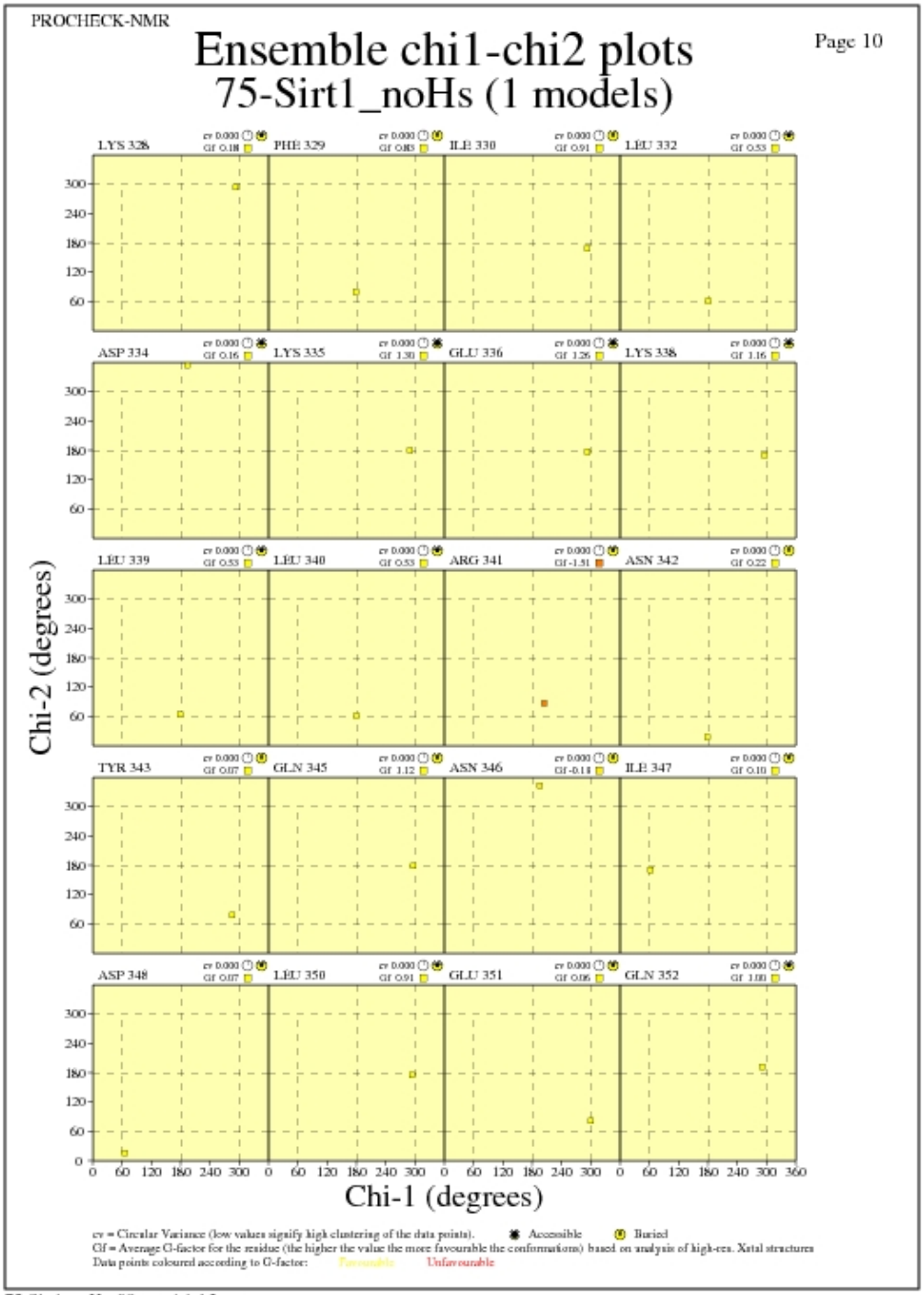
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



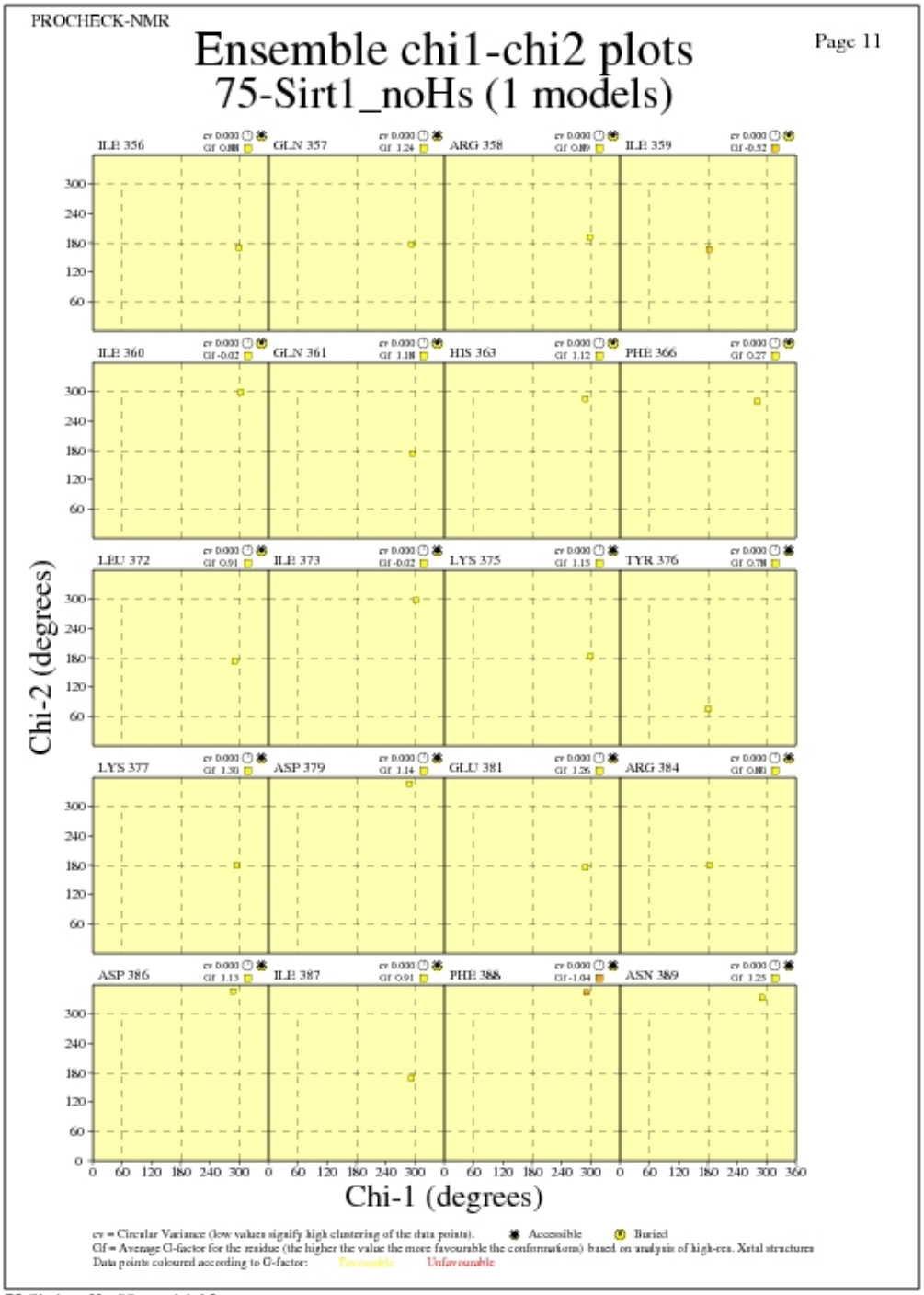
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



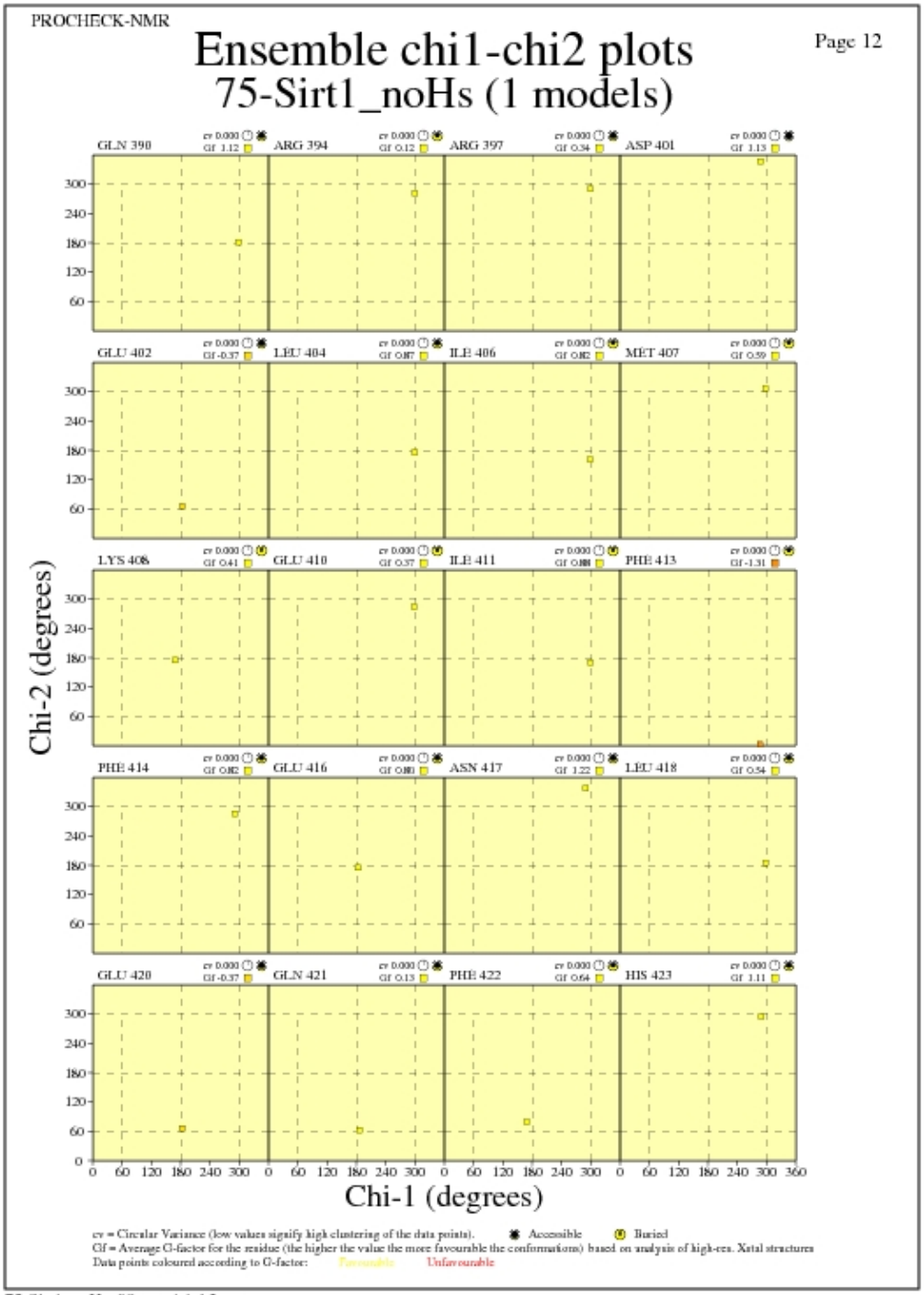
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



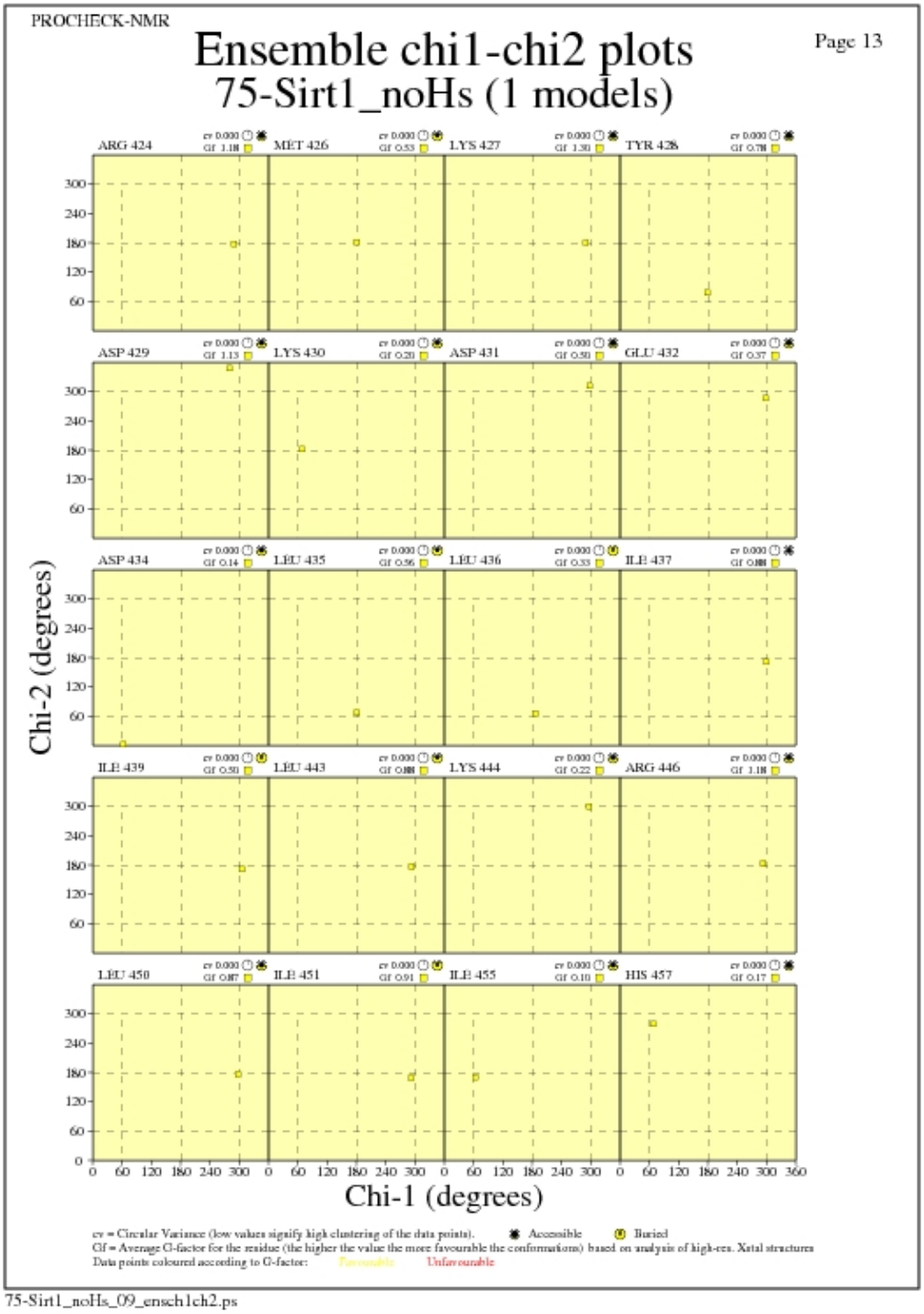
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



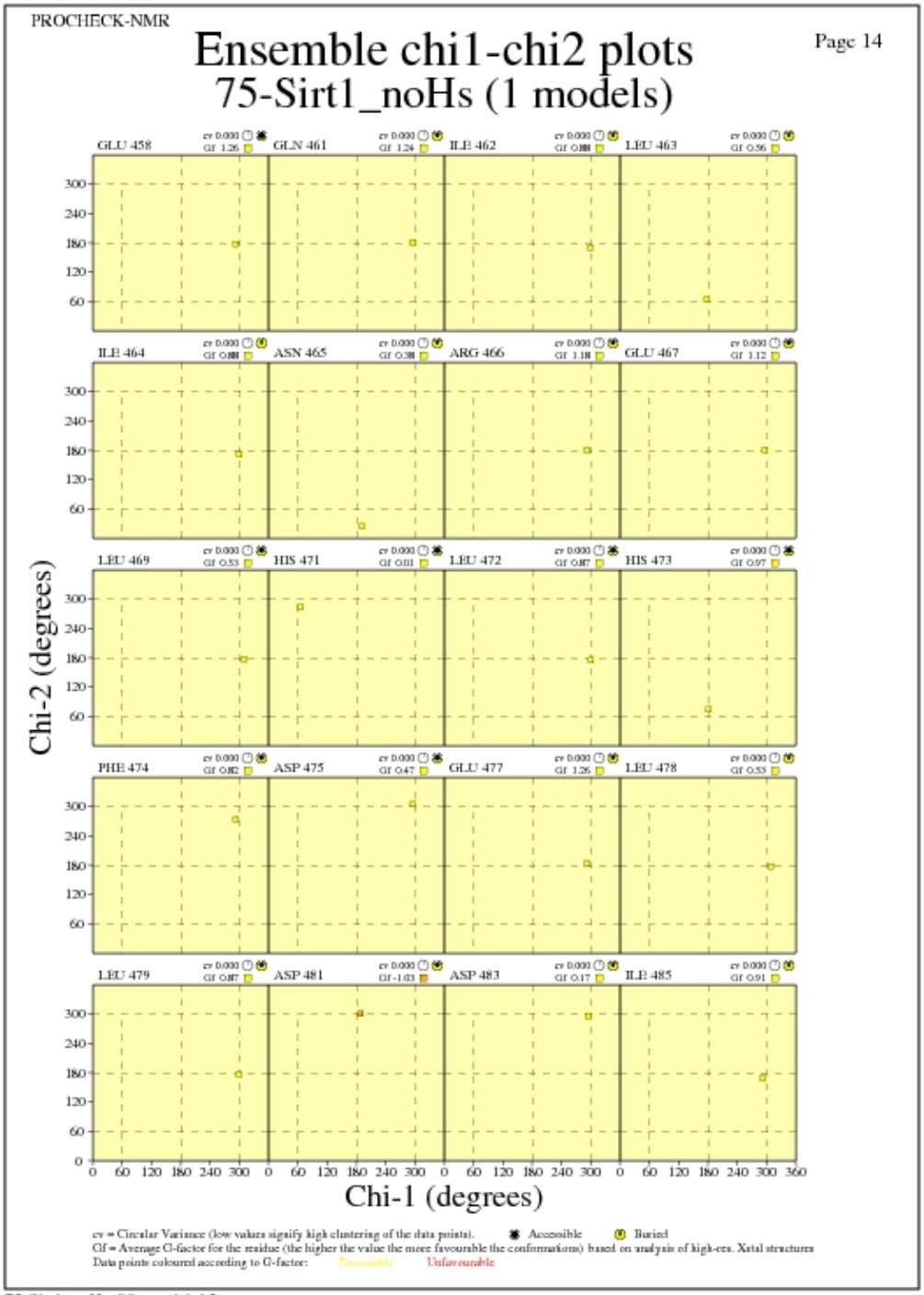
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



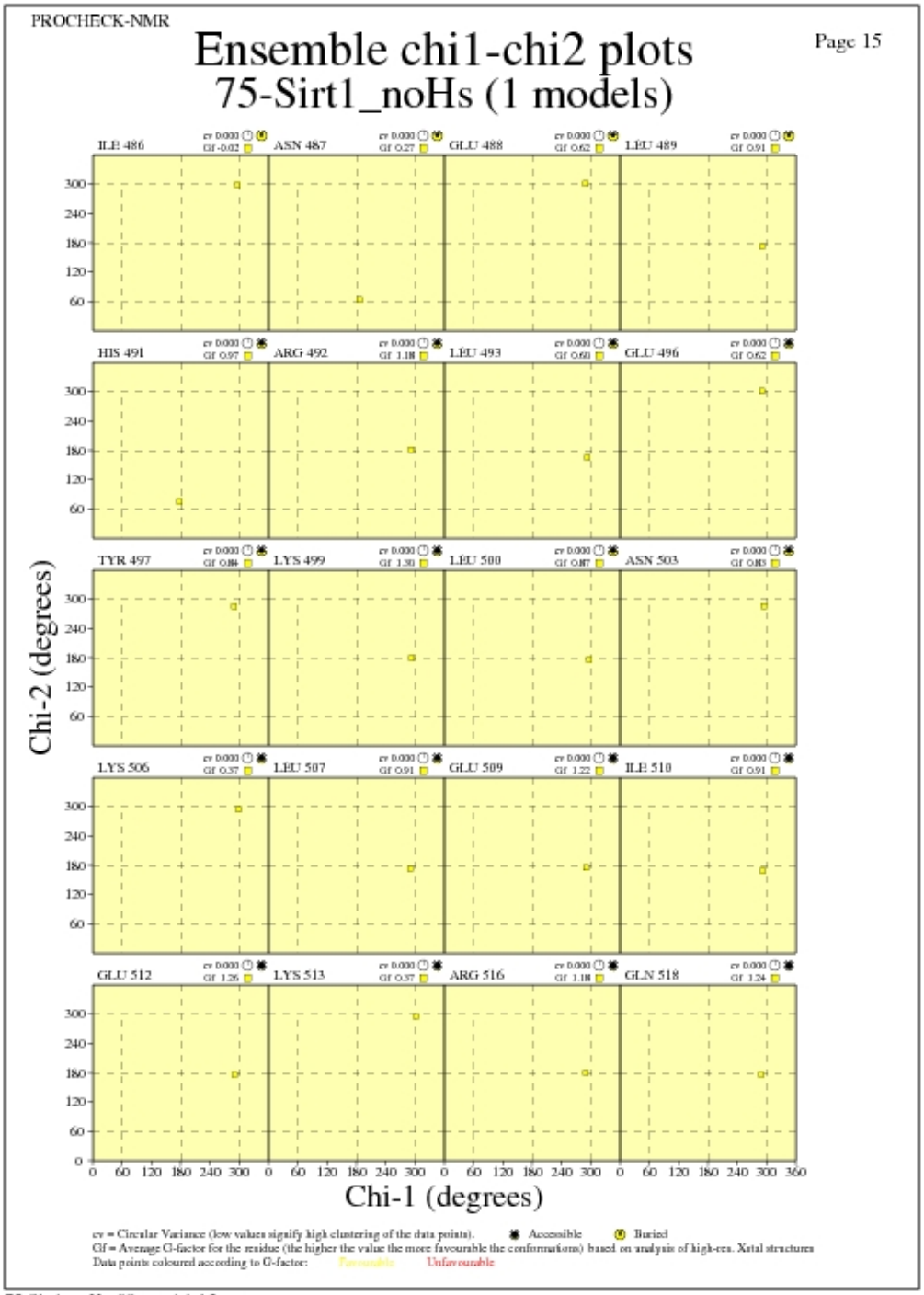
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



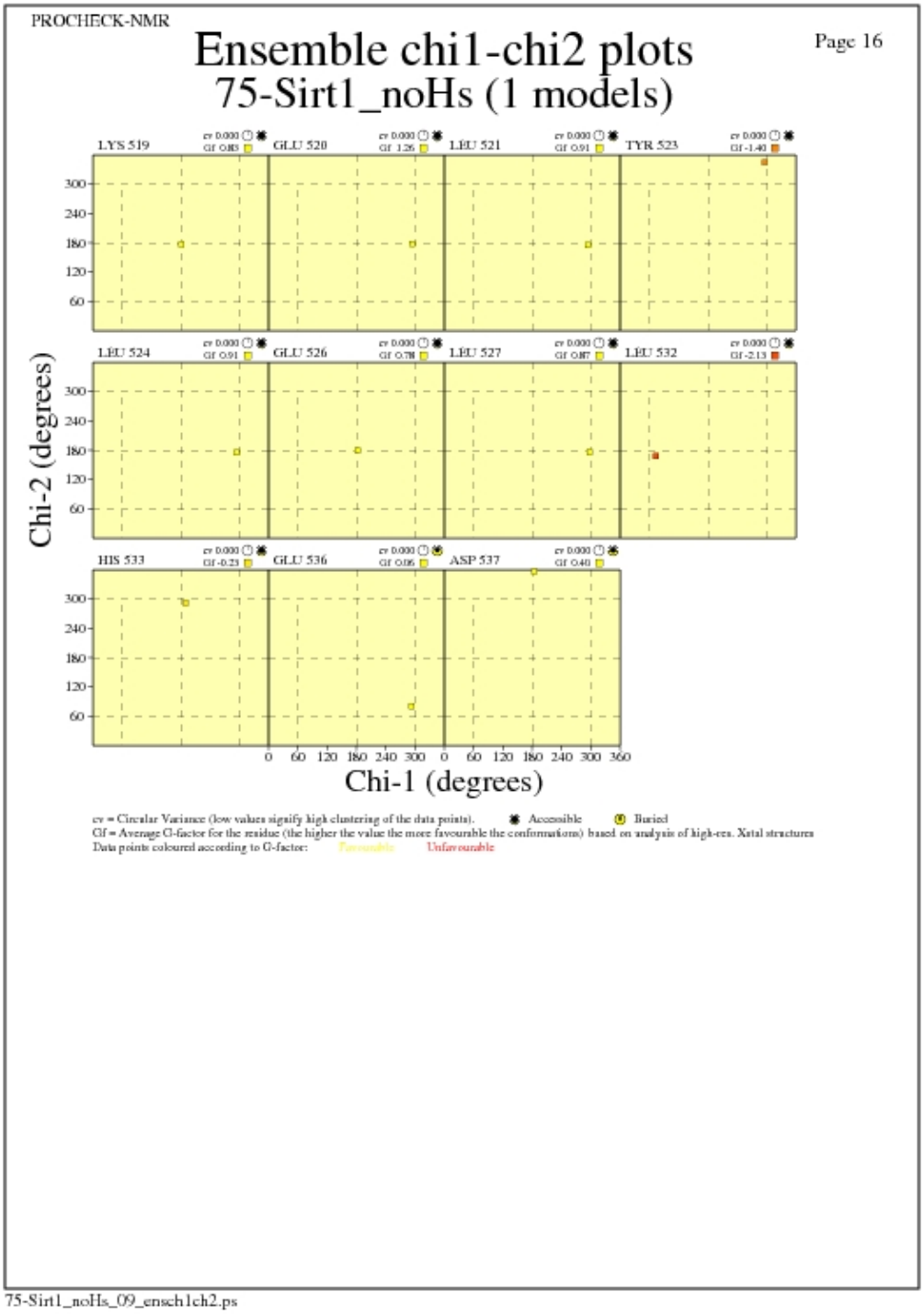
75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



75-Sirt1_noHs_09_ensch1ch2.ps

JPEG for residue Chi1-Chi2 Plots - page $num_n



75-Sirt1_noHs_09_ensch1ch2.ps

Procheck G-factors for phi-psi for each residue

JPEG image for residue phi-psi G-factors

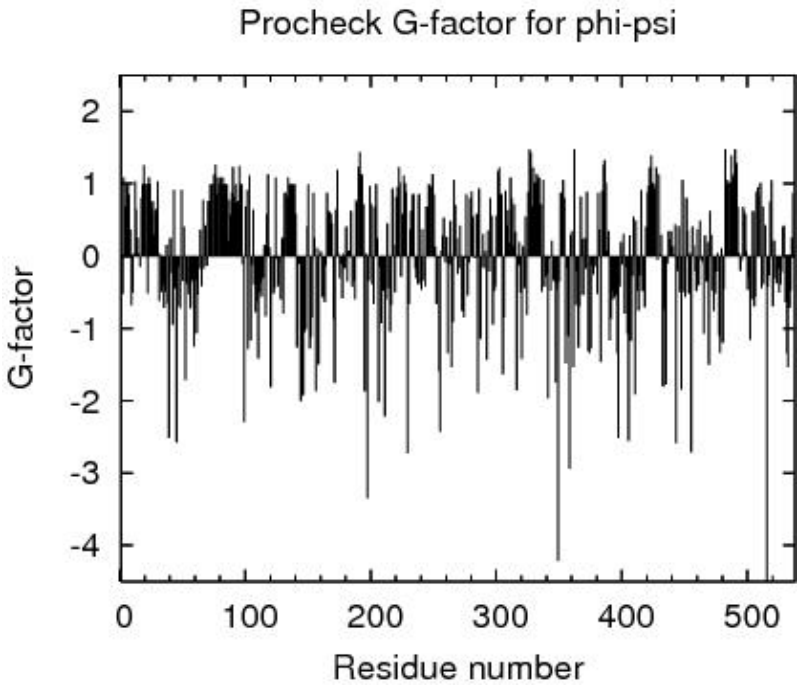


Table of Procheck G-factors for phi-psi for ordered residues

```
#phipsi_gfactor
#Residue\Model  average
2       -0.52
3       1.08
4       0.68
5       0.99
6       0.99
7       0.85
8       0.36
9       -0.68
10      -0.50
11      0.03
12      1.03
13      0.64
14      0.25
15      0.03
16      -0.14
17      0.80
18      0.99
19      1.25
20      0.99
21      0.99
22      -0.51
23      1.08
24      0.99
25      0.65
26      0.75
27      0.29
28      0.62
29      0.65
30      1.03
31      -0.62
32      0.03
33      -0.49
34      -0.39
```

35	-0.71
36	-0.49
37	0.15
38	-0.65
39	-2.51
40	0.24
41	-0.23
42	-0.94
43	0.91
44	-0.44
45	-2.57
46	-0.68
47	-0.14
48	-0.72
49	0.91
50	-0.34
51	0.40
52	-1.71
53	-0.36
54	-0.40
55	-0.52
56	-0.72
57	-0.35
58	-0.32
59	-1.25
60	-0.32
61	-1.06
62	-0.53
63	-0.17
64	0.36
65	-0.41
66	0.77
67	-0.17
68	0.42
69	-0.13
70	0.76
71	0.76
72	0.99
73	0.99
74	0.99
75	1.13
76	1.26
77	0.85
78	1.08
79	0.99
80	1.08
81	0.99
82	1.08
83	0.99
84	0.99
85	0.99
86	0.21
87	0.77
88	0.57
89	0.87
90	1.23
91	0.82
92	0.99
93	0.74
94	0.76
95	1.24
96	0.99

97	0.99
98	-0.11
99	-2.29
100	0.68
101	0.91
102	-1.28
103	1.11
104	-1.16
105	-0.12
106	0.64
107	-0.39
108	-0.77
109	-0.62
110	-1.41
111	-0.50
112	-0.36
113	-0.56
114	-0.30
115	0.15
116	-0.83
117	0.58
118	1.13
119	0.12
120	-1.81
121	-0.01
122	-0.51
123	-0.43
124	1.08
125	-0.03
126	-0.41
127	-0.09
128	-0.59
129	0.25
130	-0.79
131	0.87
132	0.87
133	0.82
134	1.08
135	0.99
136	0.99
137	0.99
138	0.99
139	0.99
140	0.58
141	-1.26
142	-0.10
143	-0.10
144	-2.00
145	-0.57
146	-1.92
147	-1.04
148	-1.00
149	0.41
150	0.99
151	-1.27
152	-1.11
153	-0.84
154	0.87
155	0.25
156	-1.86
157	0.11
158	-1.49

159	0.01
160	0.06
161	-0.56
162	-0.40
163	-0.63
164	-0.12
165	0.87
166	0.62
167	0.60
168	0.58
169	0.45
170	-0.86
171	-1.75
172	0.64
173	1.19
174	0.03
175	-0.30
176	-0.10
177	-0.58
178	0.03
179	-0.16
180	0.40
181	-0.35
182	0.07
183	-0.01
184	0.62
185	-0.42
186	-0.33
187	-0.59
188	0.77
189	0.74
190	1.23
191	1.43
192	1.13
193	1.12
194	0.71
195	-1.86
196	0.03
197	-3.34
198	-0.33
199	0.96
200	0.72
201	-0.39
202	-0.66
203	0.68
204	0.99
205	0.24
206	-2.01
207	-0.15
208	-0.92
209	-0.47
210	-0.25
211	-2.21
212	-0.59
213	0.45
214	-0.44
215	-1.04
216	-0.67
217	0.93
218	0.15
219	-0.49
220	0.82

221	0.95
222	1.23
223	1.01
224	-0.28
225	0.58
226	1.11
227	1.01
228	0.88
229	-2.72
230	-0.66
231	0.37
232	0.62
233	0.85
234	0.85
235	-0.17
236	-0.30
237	-0.38
238	0.85
239	-0.38
240	-0.46
241	0.37
242	-0.33
243	-0.41
244	0.68
245	0.39
246	0.99
247	0.98
248	0.95
249	1.13
250	0.85
251	0.13
252	-0.66
253	-0.02
254	-1.59
255	-2.42
256	0.07
257	0.28
258	0.53
259	-0.08
260	0.26
261	-1.34
262	-0.11
263	0.48
264	-1.53
265	-0.91
266	1.05
267	0.70
268	0.24
269	-0.24
270	-0.16
271	0.42
272	-0.75
273	-0.76
274	-0.84
275	-0.02
276	0.85
277	-0.54
278	-0.09
279	0.80
280	0.89
281	0.54
282	-0.01

283	-0.02
284	0.58
285	-1.89
286	0.93
287	-1.14
288	-0.15
289	0.30
290	-0.16
291	0.07
292	-1.43
293	0.35
294	-0.21
295	0.80
296	0.55
297	-0.94
298	-0.48
299	-0.41
300	0.55
301	1.17
302	1.22
303	0.85
304	0.85
305	-1.63
306	-0.84
307	0.90
308	0.42
309	0.63
310	0.18
311	1.08
312	0.80
313	0.14
314	0.71
315	0.33
316	-1.85
317	-0.12
318	0.19
319	-0.50
320	-1.42
321	0.13
322	-0.44
323	0.54
324	-0.81
325	0.88
326	1.47
327	1.43
328	0.68
329	1.22
330	1.01
331	0.82
332	1.13
333	0.95
334	1.08
335	0.71
336	-0.49
337	1.05
338	-0.42
339	-0.28
340	-0.24
341	-1.96
342	-0.02
343	-0.47
344	0.21

345	-0.32
346	-0.35
347	-1.74
348	-0.45
349	-4.21
350	-0.35
351	0.87
352	0.13
353	1.05
354	0.80
355	-1.48
356	-0.16
357	-1.10
358	-2.93
359	0.29
360	0.34
361	-1.53
362	1.47
363	-0.67
364	-0.20
365	-1.26
366	-0.69
367	0.82
368	0.23
369	-0.53
370	0.24
371	-0.17
372	0.88
373	-1.31
374	-1.33
375	-1.27
376	-0.12
377	-0.25
378	-0.05
379	-0.14
380	-0.52
381	0.87
382	0.36
383	-1.46
384	0.90
385	1.25
386	1.32
387	1.01
388	0.08
389	0.34
390	-1.16
391	-0.86
392	-0.48
393	-0.59
394	-0.56
395	-0.52
396	-1.34
397	-2.51
398	-0.41
399	0.19
400	-0.11
401	0.30
402	-0.79
403	-0.15
404	-1.07
405	-2.55
406	0.28

407	-1.17
408	-0.27
409	0.54
410	-1.91
411	0.49
412	-0.48
413	-0.75
414	-0.27
415	0.91
416	-0.48
417	-0.48
418	-0.70
419	0.40
420	0.87
421	0.97
422	1.22
423	1.39
424	1.01
425	0.99
426	0.92
427	1.22
428	-0.05
429	1.13
430	0.02
431	0.29
432	-1.79
433	-1.80
434	-0.73
435	-1.77
436	-0.10
437	0.34
438	0.23
439	0.34
440	0.13
441	0.01
442	0.43
443	-2.58
444	-0.20
445	0.41
446	-0.49
447	-1.84
448	1.05
449	-0.49
450	-0.56
451	0.80
452	0.35
453	-0.51
454	0.04
455	-2.71
456	0.40
457	0.14
458	-0.21
459	-0.48
460	0.37
461	-0.40
462	0.49
463	-0.05
464	-0.09
465	-1.07
466	0.28
467	-0.35
468	0.19

469	-1.50
470	0.62
471	0.29
472	-0.47
473	-0.76
474	-0.51
475	-0.21
476	0.04
477	-1.10
478	-1.33
479	0.10
480	-1.19
481	-0.45
482	1.47
483	0.99
484	1.05
485	1.01
486	1.01
487	1.39
488	1.08
489	1.13
490	1.47
491	1.28
492	0.67
493	0.04
494	-0.20
495	-0.06
496	0.68
497	0.64
498	0.58
499	0.06
500	-0.46
501	-0.28
502	-1.15
503	-0.59
504	0.62
505	-0.69
506	-0.56
507	0.88
508	0.95
509	0.82
510	1.01
511	-0.44
512	0.68
513	-0.38
514	0.42
515	-5.13
516	-0.42
517	-0.26
518	0.75
519	1.04
520	-0.69
521	0.21
522	-0.30
523	-0.37
524	-0.16
525	-0.50
526	-0.39
527	-0.22
528	0.40
529	0.42
530	-0.63

```
531     -1.34
532     -1.53
533     -0.71
534     -0.48
535     0.25
536     0.87
#Reported_Model_Average -0.011
#Overall_Average_Reported       -0.011
```

Procheck G-factors for all dihedral angles for each residue

JPEG image for residue all dihedral G-factors

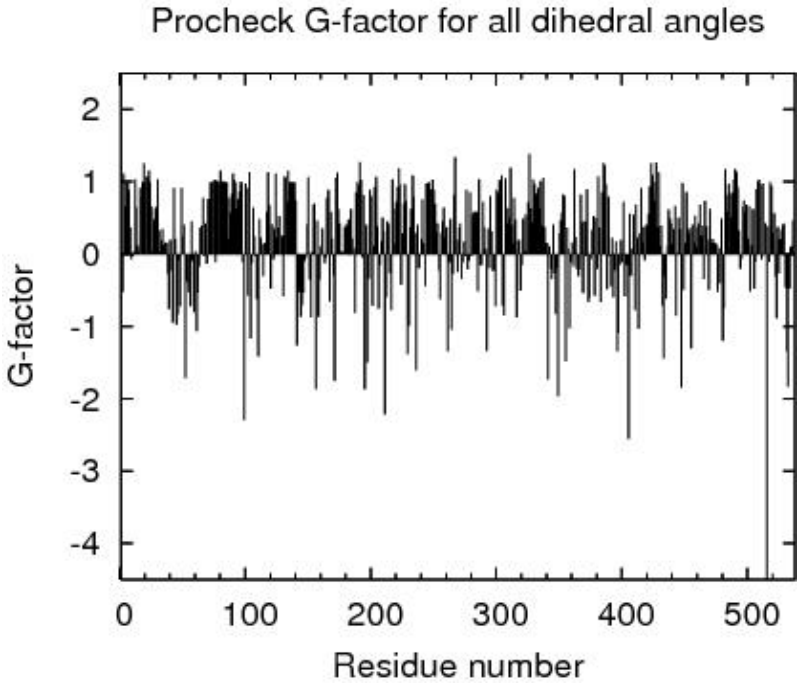


Table of Procheck G-factors for all dihedrals for ordered residues

```
#alldih_gfactor
#Residue\Model  average
1       0.84
2       -0.52
3       1.11
4       0.65
5       0.99
6       0.99
7       0.88
8       0.36
9       -0.07
10      -0.02
11      0.03
12      1.03
13      0.64
14      0.11
15      0.03
16      0.91
17      0.80
18      0.99
```

19	1.25
20	0.99
21	1.06
22	0.16
23	1.15
24	0.99
25	0.65
26	0.02
27	0.47
28	0.62
29	0.65
30	1.03
31	0.32
32	0.03
33	0.19
34	0.34
35	0.13
36	0.16
37	0.15
38	-0.27
39	-0.76
40	0.19
41	-0.23
42	-0.94
43	0.91
44	0.21
45	-0.97
46	-0.83
47	-0.08
48	-0.72
49	0.91
50	0.24
51	0.40
52	-1.71
53	-0.36
54	-0.40
55	-0.52
56	-0.72
57	0.45
58	-0.09
59	-0.80
60	0.04
61	-1.06
62	-0.53
63	-0.17
64	0.36
65	0.39
66	0.77
67	-0.02
68	0.42
69	-0.13
70	0.76
71	0.76
72	0.99
73	0.99
74	0.99
75	1.02
76	-0.11
77	1.01
78	0.93
79	0.99
80	1.15

81	0.99
82	1.00
83	0.99
84	0.99
85	0.99
86	0.21
87	0.77
88	0.57
89	0.83
90	1.11
91	1.02
92	0.99
93	0.62
94	0.76
95	0.86
96	0.99
97	0.99
98	-0.11
99	-2.29
100	0.97
101	0.91
102	-0.57
103	1.13
104	-1.16
105	-0.12
106	0.64
107	0.24
108	-0.02
109	-0.62
110	-1.41
111	0.48
112	0.22
113	0.13
114	-0.30
115	0.15
116	0.02
117	0.58
118	1.13
119	0.67
120	-0.47
121	0.41
122	-0.07
123	0.35
124	1.11
125	0.22
126	0.36
127	0.52
128	0.02
129	0.25
130	-0.58
131	1.07
132	1.05
133	0.72
134	1.15
135	0.99
136	0.99
137	0.99
138	0.99
139	0.99
140	0.74
141	-1.26
142	-0.52

143	-0.12
144	-0.86
145	-0.70
146	-0.53
147	-0.09
148	-0.04
149	0.41
150	1.06
151	-0.35
152	-0.87
153	0.03
154	0.68
155	0.69
156	-1.86
157	0.46
158	-0.86
159	-0.35
160	0.10
161	0.35
162	-0.01
163	-0.12
164	-0.05
165	0.77
166	0.88
167	-0.65
168	0.58
169	0.21
170	-0.29
171	-1.75
172	1.05
173	1.12
174	0.62
175	0.42
176	0.03
177	0.03
178	0.03
179	0.36
180	0.40
181	0.24
182	0.47
183	-0.01
184	0.62
185	0.21
186	0.08
187	-0.81
188	0.85
189	0.99
190	0.95
191	1.27
192	1.02
193	-0.04
194	0.81
195	-1.86
196	0.40
197	-1.49
198	-0.33
199	0.88
200	0.80
201	-0.71
202	0.11
203	0.92
204	1.06

205	0.38
206	-0.75
207	-0.15
208	0.17
209	0.50
210	0.31
211	-2.21
212	-0.59
213	0.45
214	0.41
215	-0.26
216	-0.77
217	1.03
218	0.62
219	0.14
220	0.72
221	0.92
222	1.18
223	0.96
224	-0.42
225	0.28
226	0.69
227	0.96
228	0.74
229	-1.38
230	-0.99
231	0.37
232	0.62
233	1.08
234	0.79
235	0.29
236	-1.60
237	0.40
238	-0.19
239	-0.01
240	0.21
241	0.75
242	0.15
243	-0.44
244	0.97
245	0.43
246	0.99
247	0.79
248	0.89
249	1.02
250	0.88
251	0.69
252	0.30
253	0.42
254	-0.22
255	-0.62
256	0.29
257	0.45
258	0.64
259	0.22
260	0.37
261	-1.34
262	-0.11
263	0.48
264	-1.04
265	-0.27
266	0.82

267	1.33
268	0.19
269	-0.24
270	0.36
271	0.42
272	-0.34
273	-0.11
274	0.17
275	-0.02
276	0.88
277	-0.21
278	-0.09
279	0.85
280	-0.02
281	0.54
282	0.58
283	0.45
284	0.58
285	-0.51
286	1.03
287	-0.15
288	-0.15
289	0.72
290	0.37
291	0.07
292	-1.33
293	0.35
294	-0.19
295	0.80
296	0.31
297	-0.23
298	-0.23
299	-0.72
300	0.88
301	0.83
302	1.02
303	1.01
304	1.08
305	-0.70
306	-0.84
307	1.04
308	0.42
309	0.63
310	0.50
311	1.19
312	0.40
313	0.14
314	0.77
315	0.47
316	-0.87
317	0.19
318	0.19
319	-0.50
320	-0.15
321	0.48
322	0.04
323	0.54
324	0.03
325	0.71
326	1.38
327	0.63
328	0.43

329	1.03
330	0.96
331	0.82
332	0.83
333	0.91
334	0.62
335	1.00
336	0.39
337	1.05
338	0.37
339	0.13
340	0.15
341	-1.73
342	0.10
343	-0.20
344	-0.34
345	0.40
346	-0.26
347	-0.82
348	-0.19
349	-1.96
350	0.28
351	0.46
352	0.57
353	0.82
354	0.80
355	-1.48
356	0.36
357	0.07
358	-1.02
359	-0.11
360	0.16
361	-0.17
362	1.17
363	0.23
364	-0.20
365	-0.30
366	-0.21
367	0.82
368	0.43
369	-0.53
370	0.45
371	-0.02
372	0.89
373	-0.66
374	-0.60
375	-0.06
376	0.33
377	0.52
378	-0.57
379	0.50
380	-0.20
381	1.07
382	0.36
383	-0.66
384	0.85
385	1.25
386	1.23
387	0.96
388	-0.48
389	0.79
390	-0.02

391	-0.44
392	0.22
393	-0.59
394	-0.22
395	0.17
396	-1.34
397	-1.08
398	-0.14
399	0.19
400	-0.11
401	0.72
402	-0.58
403	-0.15
404	-0.10
405	-2.55
406	0.55
407	-0.29
408	0.07
409	0.54
410	-0.77
411	0.68
412	0.22
413	-1.03
414	0.28
415	0.91
416	0.16
417	0.37
418	-0.08
419	0.40
420	0.25
421	0.55
422	0.93
423	1.25
424	1.09
425	0.99
426	0.73
427	1.26
428	0.37
429	1.13
430	0.11
431	0.39
432	-0.71
433	-1.44
434	-0.30
435	-0.61
436	0.11
437	0.61
438	0.49
439	0.42
440	0.13
441	0.34
442	0.66
443	-0.85
444	0.01
445	0.50
446	0.34
447	-1.84
448	0.98
449	-0.49
450	0.15
451	0.85
452	0.35

453	0.28
454	0.35
455	-1.30
456	0.40
457	0.16
458	0.53
459	0.09
460	0.37
461	0.42
462	0.68
463	0.25
464	0.39
465	-0.34
466	0.73
467	0.38
468	0.19
469	-0.49
470	0.62
471	0.15
472	0.20
473	0.10
474	0.15
475	0.13
476	-0.52
477	0.08
478	-0.40
479	0.49
480	-1.19
481	-0.74
482	1.17
483	0.58
484	0.82
485	0.96
486	0.50
487	0.83
488	0.85
489	1.02
490	1.17
491	1.13
492	0.92
493	0.32
494	-0.20
495	-0.06
496	0.65
497	0.74
498	0.58
499	0.68
500	0.21
501	0.66
502	-0.51
503	0.12
504	0.62
505	-0.47
506	-0.10
507	0.89
508	1.00
509	1.02
510	0.96
511	-0.07
512	0.97
513	-0.01
514	0.42

```
515     -5.13
516     0.38
517     -0.10
518     0.99
519     0.94
520     0.29
521     0.56
522     -0.30
523     -0.88
524     0.37
525     -0.26
526     0.20
527     0.33
528     0.40
529     0.42
530     -0.46
531     -1.34
532     -1.83
533     -0.47
534     0.09
535     0.11
536     0.46
537     0.40
#Reported_Model_Average 0.219
#Overall_Average_Reported       0.219
```

Output from Verify3D

Verify3D Score over a window of $winsize_s residues

JPEG image for Verify3D Score

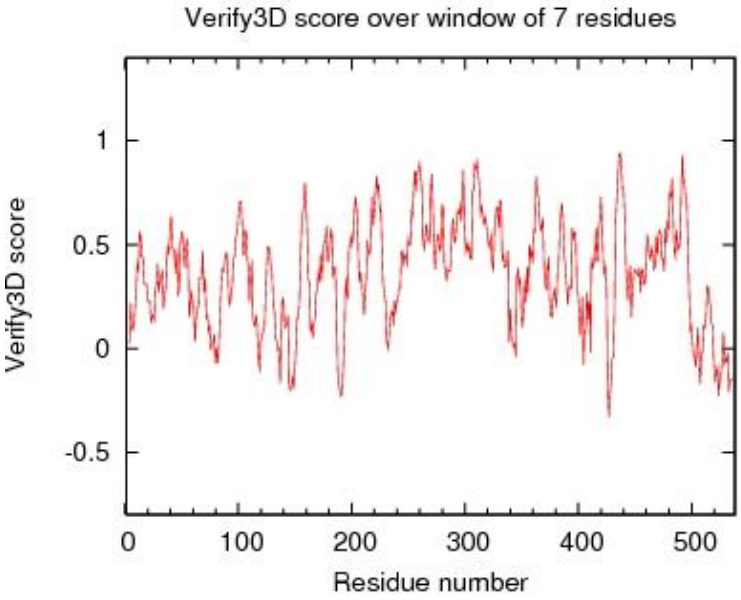


Table of Verify3D scores for ordered residues across all models

```
#verify3d
#Residue\Model  only_model
1       -0.83
```

```
2       0.14
3       0.34
4       0.28
5       0.49
6       0.49
7       -0.68
8       0.49
9       -0.68
10      0.25
11      0.44
12      1.10
13      1.10
14      0.17
15      0.25
16      0.59
17      0.14
18      -0.25
19      1.10
20      0.14
21      0.23
22      0.24
23      0.04
24      0.14
25      -0.25
26      0.34
27      0.34
28      0.25
29      0.14
30      1.10
31      0.28
32      0.44
33      -0.68
34      0.71
35      0.47
36      0.24
37      -0.11
38      0.71
39      0.71
40      0.34
41      1.10
42      0.25
43      1.10
44      0.29
45      -0.46
46      0.71
47      0.17
48      0.44
49      1.10
50      -0.46
51      0.44
52      1.10
53      1.10
54      0.14
55      -0.25
56      0.64
57      0.28
58      0.71
59      0.28
60      -0.74
61      0.64
62      0.14
63      0.14
```

```
64      0.14
65      -0.41
66      1.10
67      -0.35
68      0.64
69      1.10
70      0.14
71      0.14
72      0.49
73      -0.25
74      0.14
75      -0.68
76      1.12
77      -0.41
78      0.28
79      -0.25
80      0.04
81      0.14
82      -0.46
83      0.14
84      0.14
85      -0.25
86      0.14
87      1.10
88      1.10
89      0.28
90      0.10
91      0.28
92      0.14
93      0.25
94      0.49
95      0.08
96      0.14
97      0.49
98      0.49
99      1.10
100     0.28
101     1.10
102     0.23
103     0.51
104     1.10
105     0.64
106     1.10
107     -0.68
108     0.25
109     1.10
110     0.44
111     0.17
112     0.24
113     0.04
114     0.44
115     0.44
116     -0.68
117     0.14
118     0.23
119     0.51
120     -0.68
121     -0.43
122     0.23
123     0.28
124     0.23
125     0.51
```

```
126     0.51
127     0.51
128     0.28
129     1.10
130     0.28
131     0.04
132     0.04
133     0.28
134     -0.59
135     0.14
136     0.14
137     0.14
138     -0.25
139     0.14
140     -0.94
141     1.10
142     1.25
143     0.24
144     -0.83
145     -0.26
146     0.29
147     -0.68
148     -1.29
149     1.10
150     0.34
151     -0.46
152     -0.54
153     0.81
154     0.08
155     -0.26
156     1.10
157     0.71
158     1.04
159     0.59
160     1.29
161     0.28
162     0.59
163     0.51
164     -0.46
165     -0.46
166     0.51
167     -0.44
168     0.49
169     0.17
170     1.04
171     -0.25
172     0.34
173     0.59
174     0.17
175     0.23
176     1.12
177     0.08
178     0.64
179     0.71
180     0.64
181     0.71
182     -0.94
183     1.10
184     0.64
185     1.14
186     0.55
187     -0.84
```

```
188     1.00
189     -0.87
190     -0.57
191     -1.21
192     0.77
193     0.23
194     -0.94
195     1.10
196     0.08
197     0.51
198     0.64
199     0.24
200     0.08
201     0.81
202     1.06
203     0.47
204     0.23
205     1.06
206     1.06
207     0.44
208     0.28
209     0.08
210     -0.94
211     0.59
212     0.64
213     0.44
214     0.04
215     1.06
216     0.51
217     0.34
218     0.23
219     0.55
220     0.77
221     1.62
222     0.10
223     0.93
224     1.00
225     0.81
226     0.09
227     0.93
228     0.77
229     0.17
230     -0.46
231     -0.11
232     0.44
233     -0.10
234     -0.44
235     0.47
236     0.47
237     0.24
238     0.08
239     0.51
240     -0.54
241     0.41
242     0.08
243     0.81
244     0.28
245     0.51
246     0.49
247     0.66
248     0.47
249     -0.33
```

```
250     1.06
251     0.25
252     0.28
253     1.29
254     0.47
255     0.47
256     0.81
257     0.93
258     1.00
259     1.06
260     0.55
261     1.10
262     0.49
263     1.10
264     0.66
265     0.59
266     -0.74
267     0.17
268     1.29
269     1.10
270     0.81
271     0.44
272     0.51
273     1.04
274     0.71
275     0.17
276     -0.41
277     0.23
278     1.10
279     0.93
280     1.14
281     0.14
282     0.24
283     1.06
284     0.14
285     -0.80
286     0.51
287     1.04
288     0.44
289     0.23
290     1.06
291     0.44
292     0.51
293     0.64
294     0.25
295     0.49
296     0.91
297     1.40
298     0.34
299     0.81
300     0.04
301     1.14
302     1.40
303     -0.88
304     0.47
305     0.51
306     0.64
307     0.24
308     0.64
309     1.40
310     1.40
311     0.47
```

```
312     1.40
313     0.49
314     0.47
315     0.28
316     0.93
317     0.52
318     0.64
319     1.10
320     0.25
321     0.71
322     -0.03
323     0.59
324     0.17
325     0.77
326     1.29
327     -0.61
328     0.47
329     1.40
330     0.93
331     0.49
332     0.77
333     0.59
334     0.34
335     0.47
336     -0.59
337     1.10
338     0.08
339     0.77
340     0.77
341     0.71
342     -2.61
343     0.52
344     0.08
345     0.10
346     0.51
347     0.81
348     0.34
349     0.08
350     0.77
351     -0.46
352     0.25
353     -0.74
354     0.49
355     1.10
356     0.93
357     -0.03
358     0.71
359     -0.54
360     0.81
361     0.10
362     1.29
363     0.54
364     1.10
365     0.59
366     1.40
367     0.14
368     0.08
369     0.49
370     0.17
371     1.29
372     0.77
373     -0.28
```

374	-0.35
375	-0.10
376	1.25
377	0.47
378	-0.09
379	0.23
380	-0.35
381	0.28
382	0.14
383	1.00
384	0.24
385	1.10
386	0.51
387	0.93
388	0.71
389	0.41
390	0.25
391	-0.74
392	0.66
393	-0.07
394	0.24
395	1.29
396	0.44
397	0.24
398	1.29
399	0.25
400	0.14
401	0.23
402	-0.59
403	0.25
404	-0.33
405	0.49
406	0.81
407	0.91
408	-2.12
409	0.59
410	0.28
411	0.93
412	-0.40
413	1.40
414	-0.84
415	1.10
416	0.28
417	0.41
418	1.06
419	0.64
420	0.28
421	0.25
422	1.40
423	1.04
424	-0.41
425	-0.25
426	0.23
427	0.47
428	-0.43
429	-1.97
430	0.08
431	0.23
432	0.28
433	1.00
434	0.51
435	1.06

```
436     1.06
437     0.93
438     1.00
439     0.93
440     1.10
441     0.17
442     0.17
443     1.06
444     0.08
445     -0.74
446     0.24
447     0.64
448     1.00
449     0.49
450     -0.68
451     0.93
452     -0.07
453     0.34
454     0.59
455     0.93
456     0.44
457     -0.41
458     0.04
459     0.66
460     0.44
461     0.10
462     0.93
463     0.77
464     0.93
465     -0.26
466     0.24
467     0.28
468     0.44
469     0.77
470     0.25
471     1.04
472     0.77
473     -0.41
474     1.04
475     0.51
476     0.66
477     -0.59
478     1.06
479     0.29
480     1.10
481     0.51
482     1.29
483     0.34
484     0.66
485     0.93
486     0.93
487     -0.26
488     -0.59
489     1.06
490     1.29
491     0.20
492     0.71
493     1.06
494     1.10
495     1.10
496     0.28
497     1.14
```

```
498     -0.25
499     0.47
500     -0.33
501     -0.35
502     -0.35
503     0.41
504     0.64
505     -0.74
506     0.47
507     -0.68
508     0.34
509     0.28
510     -0.94
511     0.08
512     0.28
513     0.47
514     0.25
515     0.25
516     0.71
517     0.08
518     -0.03
519     -0.10
520     0.28
521     -0.33
522     0.14
523     -0.43
524     -0.68
525     0.34
526     0.04
527     -0.68
528     0.25
529     0.25
530     0.08
531     0.25
532     -0.68
533     0.20
534     -0.80
535     0.59
536     -1.13
537     0.51
#Reported_Model_Average 0.356
#Overall_Average_Reported       0.356
```

Output from Prosall

Prosall Score over a window of $winsize_s residues

JPEG image for Prosall Score

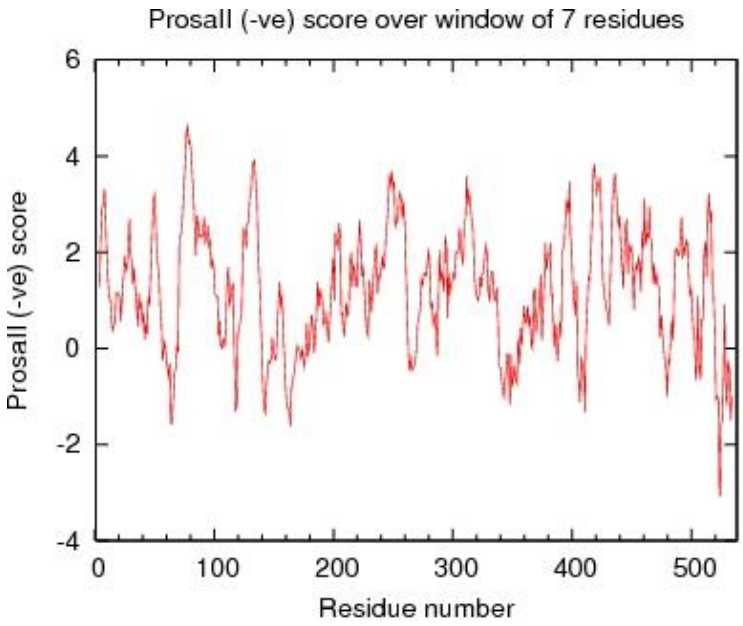


Table of Verify3D scores for ordered residues across all models

```
#verify3d
#Residue\Model  only_model
1       -0.83
2       0.14
3       0.34
4       0.28
5       0.49
6       0.49
7       -0.68
8       0.49
9       -0.68
10      0.25
11      0.44
12      1.10
13      1.10
14      0.17
15      0.25
16      0.59
17      0.14
18      -0.25
19      1.10
20      0.14
21      0.23
22      0.24
23      0.04
24      0.14
25      -0.25
26      0.34
27      0.34
28      0.25
29      0.14
30      1.10
31      0.28
32      0.44
33      -0.68
34      0.71
35      0.47
```

```
36      0.24
37      -0.11
38      0.71
39      0.71
40      0.34
41      1.10
42      0.25
43      1.10
44      0.29
45      -0.46
46      0.71
47      0.17
48      0.44
49      1.10
50      -0.46
51      0.44
52      1.10
53      1.10
54      0.14
55      -0.25
56      0.64
57      0.28
58      0.71
59      0.28
60      -0.74
61      0.64
62      0.14
63      0.14
64      0.14
65      -0.41
66      1.10
67      -0.35
68      0.64
69      1.10
70      0.14
71      0.14
72      0.49
73      -0.25
74      0.14
75      -0.68
76      1.12
77      -0.41
78      0.28
79      -0.25
80      0.04
81      0.14
82      -0.46
83      0.14
84      0.14
85      -0.25
86      0.14
87      1.10
88      1.10
89      0.28
90      0.10
91      0.28
92      0.14
93      0.25
94      0.49
95      0.08
96      0.14
97      0.49
```

98	0.49
99	1.10
100	0.28
101	1.10
102	0.23
103	0.51
104	1.10
105	0.64
106	1.10
107	-0.68
108	0.25
109	1.10
110	0.44
111	0.17
112	0.24
113	0.04
114	0.44
115	0.44
116	-0.68
117	0.14
118	0.23
119	0.51
120	-0.68
121	-0.43
122	0.23
123	0.28
124	0.23
125	0.51
126	0.51
127	0.51
128	0.28
129	1.10
130	0.28
131	0.04
132	0.04
133	0.28
134	-0.59
135	0.14
136	0.14
137	0.14
138	-0.25
139	0.14
140	-0.94
141	1.10
142	1.25
143	0.24
144	-0.83
145	-0.26
146	0.29
147	-0.68
148	-1.29
149	1.10
150	0.34
151	-0.46
152	-0.54
153	0.81
154	0.08
155	-0.26
156	1.10
157	0.71
158	1.04
159	0.59

```
160     1.29
161     0.28
162     0.59
163     0.51
164     -0.46
165     -0.46
166     0.51
167     -0.44
168     0.49
169     0.17
170     1.04
171     -0.25
172     0.34
173     0.59
174     0.17
175     0.23
176     1.12
177     0.08
178     0.64
179     0.71
180     0.64
181     0.71
182     -0.94
183     1.10
184     0.64
185     1.14
186     0.55
187     -0.84
188     1.00
189     -0.87
190     -0.57
191     -1.21
192     0.77
193     0.23
194     -0.94
195     1.10
196     0.08
197     0.51
198     0.64
199     0.24
200     0.08
201     0.81
202     1.06
203     0.47
204     0.23
205     1.06
206     1.06
207     0.44
208     0.28
209     0.08
210     -0.94
211     0.59
212     0.64
213     0.44
214     0.04
215     1.06
216     0.51
217     0.34
218     0.23
219     0.55
220     0.77
221     1.62
```

```
222     0.10
223     0.93
224     1.00
225     0.81
226     0.09
227     0.93
228     0.77
229     0.17
230     -0.46
231     -0.11
232     0.44
233     -0.10
234     -0.44
235     0.47
236     0.47
237     0.24
238     0.08
239     0.51
240     -0.54
241     0.41
242     0.08
243     0.81
244     0.28
245     0.51
246     0.49
247     0.66
248     0.47
249     -0.33
250     1.06
251     0.25
252     0.28
253     1.29
254     0.47
255     0.47
256     0.81
257     0.93
258     1.00
259     1.06
260     0.55
261     1.10
262     0.49
263     1.10
264     0.66
265     0.59
266     -0.74
267     0.17
268     1.29
269     1.10
270     0.81
271     0.44
272     0.51
273     1.04
274     0.71
275     0.17
276     -0.41
277     0.23
278     1.10
279     0.93
280     1.14
281     0.14
282     0.24
283     1.06
```

```
284     0.14
285     -0.80
286     0.51
287     1.04
288     0.44
289     0.23
290     1.06
291     0.44
292     0.51
293     0.64
294     0.25
295     0.49
296     0.91
297     1.40
298     0.34
299     0.81
300     0.04
301     1.14
302     1.40
303     -0.88
304     0.47
305     0.51
306     0.64
307     0.24
308     0.64
309     1.40
310     1.40
311     0.47
312     1.40
313     0.49
314     0.47
315     0.28
316     0.93
317     0.52
318     0.64
319     1.10
320     0.25
321     0.71
322     -0.03
323     0.59
324     0.17
325     0.77
326     1.29
327     -0.61
328     0.47
329     1.40
330     0.93
331     0.49
332     0.77
333     0.59
334     0.34
335     0.47
336     -0.59
337     1.10
338     0.08
339     0.77
340     0.77
341     0.71
342     -2.61
343     0.52
344     0.08
345     0.10
```

```
346     0.51
347     0.81
348     0.34
349     0.08
350     0.77
351     -0.46
352     0.25
353     -0.74
354     0.49
355     1.10
356     0.93
357     -0.03
358     0.71
359     -0.54
360     0.81
361     0.10
362     1.29
363     0.54
364     1.10
365     0.59
366     1.40
367     0.14
368     0.08
369     0.49
370     0.17
371     1.29
372     0.77
373     -0.28
374     -0.35
375     -0.10
376     1.25
377     0.47
378     -0.09
379     0.23
380     -0.35
381     0.28
382     0.14
383     1.00
384     0.24
385     1.10
386     0.51
387     0.93
388     0.71
389     0.41
390     0.25
391     -0.74
392     0.66
393     -0.07
394     0.24
395     1.29
396     0.44
397     0.24
398     1.29
399     0.25
400     0.14
401     0.23
402     -0.59
403     0.25
404     -0.33
405     0.49
406     0.81
407     0.91
```

```
408     -2.12
409     0.59
410     0.28
411     0.93
412     -0.40
413     1.40
414     -0.84
415     1.10
416     0.28
417     0.41
418     1.06
419     0.64
420     0.28
421     0.25
422     1.40
423     1.04
424     -0.41
425     -0.25
426     0.23
427     0.47
428     -0.43
429     -1.97
430     0.08
431     0.23
432     0.28
433     1.00
434     0.51
435     1.06
436     1.06
437     0.93
438     1.00
439     0.93
440     1.10
441     0.17
442     0.17
443     1.06
444     0.08
445     -0.74
446     0.24
447     0.64
448     1.00
449     0.49
450     -0.68
451     0.93
452     -0.07
453     0.34
454     0.59
455     0.93
456     0.44
457     -0.41
458     0.04
459     0.66
460     0.44
461     0.10
462     0.93
463     0.77
464     0.93
465     -0.26
466     0.24
467     0.28
468     0.44
469     0.77
```

```
470     0.25
471     1.04
472     0.77
473     -0.41
474     1.04
475     0.51
476     0.66
477     -0.59
478     1.06
479     0.29
480     1.10
481     0.51
482     1.29
483     0.34
484     0.66
485     0.93
486     0.93
487     -0.26
488     -0.59
489     1.06
490     1.29
491     0.20
492     0.71
493     1.06
494     1.10
495     1.10
496     0.28
497     1.14
498     -0.25
499     0.47
500     -0.33
501     -0.35
502     -0.35
503     0.41
504     0.64
505     -0.74
506     0.47
507     -0.68
508     0.34
509     0.28
510     -0.94
511     0.08
512     0.28
513     0.47
514     0.25
515     0.25
516     0.71
517     0.08
518     -0.03
519     -0.10
520     0.28
521     -0.33
522     0.14
523     -0.43
524     -0.68
525     0.34
526     0.04
527     -0.68
528     0.25
529     0.25
530     0.08
531     0.25
```

```
532     -0.68
533     0.20
534     -0.80
535     0.59
536     -1.13
537     0.51
#Reported_Model_Average 0.356
#Overall_Average_Reported       0.356
```

Output from MolProbity

VdW violations from MAGE

JPEG image for MAGE VdW violation

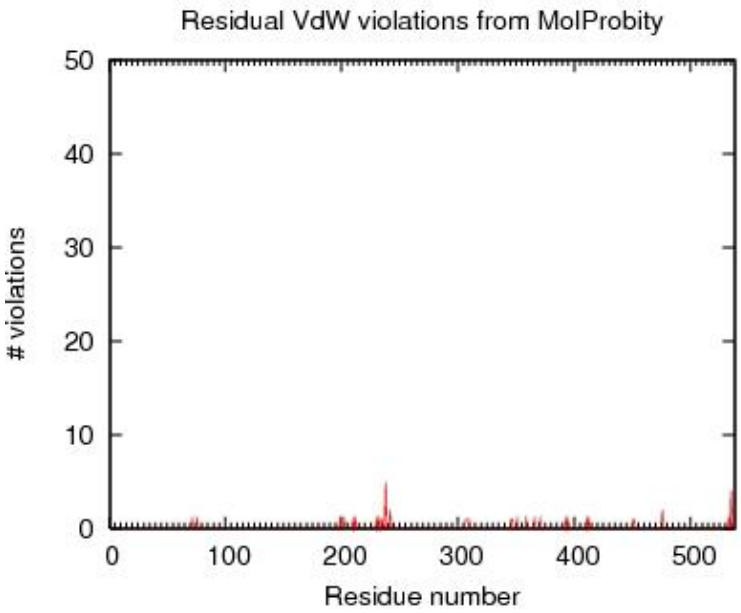


Table of MAGE VdW violations for ordered residues across all models

```
#mage_clash
#Residue\Model  only_model
1.000   0
2.000   0
3.000   0
4.000   0
5.000   0
6.000   0
7.000   0
8.000   0
9.000   0
10.000  0
11.000  0
12.000  0
13.000  0
14.000  0
15.000  0
16.000  0
17.000  0
18.000  0
```

```
19.000  0
20.000  0
21.000  0
22.000  0
23.000  0
24.000  0
25.000  0
26.000  0
27.000  0
28.000  0
29.000  0
30.000  0
31.000  0
32.000  0
33.000  0
34.000  0
35.000  0
36.000  0
37.000  0
38.000  0
39.000  0
40.000  0
41.000  0
42.000  0
43.000  0
44.000  0
45.000  0
46.000  0
47.000  0
48.000  0
49.000  0
50.000  0
51.000  0
52.000  0
53.000  0
54.000  0
55.000  0
56.000  0
57.000  0
58.000  0
59.000  0
60.000  0
61.000  0
62.000  0
63.000  0
64.000  0
65.000  0
66.000  0
67.000  0
68.000  0
69.000  0
70.000  0
71.000  0
72.000  1
73.000  0
74.000  0
75.000  0
76.000  1
77.000  0
78.000  0
79.000  0
80.000  0
```

```
81.000  0
82.000  0
83.000  0
84.000  0
85.000  0
86.000  0
87.000  0
88.000  0
89.000  0
90.000  0
91.000  0
92.000  0
93.000  0
94.000  0
95.000  0
96.000  0
97.000  0
98.000  0
99.000  0
100.000 0
101.000 0
102.000 0
103.000 0
104.000 0
105.000 0
106.000 0
107.000 0
108.000 0
109.000 0
110.000 0
111.000 0
112.000 0
113.000 0
114.000 0
115.000 0
116.000 0
117.000 0
118.000 0
119.000 0
120.000 0
121.000 0
122.000 0
123.000 0
124.000 0
125.000 0
126.000 0
127.000 0
128.000 0
129.000 0
130.000 0
131.000 0
132.000 0
133.000 0
134.000 0
135.000 0
136.000 0
137.000 0
138.000 0
139.000 0
140.000 0
141.000 0
142.000 0
```

```
143.000 0
144.000 0
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535.000 4
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#Reported_Model_Average 0.074
#Overall_Average_Reported       0.074
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List of bad contacts calculated by MAGE

```
/farm/software/bin/probe

:  4130:  238 LYS  CG  :  535 SER  CB  :   -1.620:       10
:  4130:  238 LYS  CG  :  535 SER  CA  :   -1.515:       10
:  4130:  238 LYS  CD  :  535 SER  CB  :   -1.192:       10
:  4130:  535 SER  N   :  238 LYS  CG  :   -0.771:       10
:  4130:  238 LYS  O   :  533 HIS  CE1 :   -0.615:       10

:  4130:  476 VAL  CG2 :  242 THR  OG1 :   -0.735:        5
:  4130:  476 VAL  CG2 :  242 THR  CB  :   -0.520:        5

:  4130:  235 LYS  O   :  232 PRO  O   :   -0.561:       10

:  4130:  234 ARG  CD  :  230 GLU  OE1 :   -0.557:        5

:  4130:  452 PRO  CD  :  451 ILE  N   :   -0.549:        0

:  4130:  359 ILE  CD1 :  351 GLU  CB  :   -0.535:        0

:  4130:  371 CYS  SG  :  395 CYS  SG  :   -0.495:        0

:  4130:  413 PHE  CZ  :  309 PHE  CE1 :   -0.446:        0

:  4130:  310 PHE  CE2 :  393 PRO  CD  :   -0.436:        0

:  4130:  346 ASN  OD1 :  347 ILE  N   :   -0.434:        0

:  4130:  308 PRO  CD  :  307 ARG  N   :   -0.426:        0

:  4130:  210 ILE  O   :  212 PRO  CD  :   -0.417:        5

:  4130:   72 ALA  O   :   76 TRP  CD1 :   -0.412:        5

:  4130:  199 ARG  O   :  203 LYS  CG  :   -0.411:        5
```

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:  4130:  411 ILE  CD1 :  366 PHE  CE1 :   -0.403:        0
#sum2 ::4.84 clashscore : 4.84 clashscore B
```

Output from PDB validation software

Summary from PDB validation

Jan. 29, 14:10:11 2017

Greetings,

[Text modified to reflect that this was run under PSVS - Aneerban Bhattacharya: Dec 2005]

The following checks were made on :

DISTANCES AND ANGLES

We have checked your intra and intermolecular distances and angles with the procedures currently in place at PDB:

==> The following solvent molecules are further away than 3.5 Angstroms from macromolecule atoms which are available for hydrogen bonding in the asymmetric unit.

none

The coordinates for water molecules which could be translated back into the asymmetric unit are listed. If you do not indicate otherwise we will replace the solvent coordinates in the entry with the ones below:

none

==> Close contacts in same asymmetric unit. Distances smaller than 2.2 Angstroms are considered as close contacts.

Chain	Atom	Res	Seq		Chain	Atom	Res	Seq	Symm_Code	Distance
	CG	LYS	238	-		CB	SER	535	(1, 5, 5, 5)	Dist = 1.86
	CG	LYS	238	-		CA	SER	535	(1, 5, 5, 5)	Dist = 1.96

==> Close contacts based on crystal symmetry. Distances smaller than 2.2 Angstroms are considered as close contacts.

none

==> Bond and angle checks are performed by first computing the average rms error for all bonds and angles relative to standard values for nucleotide units [L. Clowney et al., Geometric Parameters in Nucleic Acids: Nitrogenous Bases, J.Am.Chem.Soc. 1996, 118, 509-518; A. Gelbin et al., Geometric Parameters in Nucleic Acids: Sugar and Phosphate Constituents, J.Am.Chem.Soc. 1996, 118, 519-529] and amino acid units [R.A. Engh and R. Huber, Accurate Bond and Angle Parameters for X-ray protein structure refinement, Acta Crystallogr. 1991, A47, 392-400]. Any bond or angle which deviates from the

dictionary values by more than six times this computed rms error is identified as an outlier.

*** Covalent Bond Lengths:

The RMS deviation for covalent bonds relative to the standard dictionary is 0.017 Angstroms

The following table contains a list of the covalent bonds greater than 6.0*RMSD.

Deviation	Residue Name	Chain ID	Sequence Number	AT1	-	AT2	Bond Distance	Dictionary Value
0.137	PRO		11	CG	-	CD	1.640	1.503
0.143	PRO		15	CG	-	CD	1.646	1.503
0.143	PRO		32	CG	-	CD	1.646	1.503
0.116	PRO		42	CG	-	CD	1.619	1.503
0.134	PRO		48	CG	-	CD	1.637	1.503
0.132	PRO		51	CG	-	CD	1.635	1.503
0.123	PRO		56	CG	-	CD	1.626	1.503
0.171	PRO		61	CG	-	CD	1.674	1.503
0.121	PRO		105	CG	-	CD	1.624	1.503
0.122	PRO		114	CG	-	CD	1.625	1.503
0.136	PRO		178	CG	-	CD	1.639	1.503
0.123	PRO		180	CG	-	CD	1.626	1.503
0.198	PRO		198	CG	-	CD	1.701	1.503
0.195	PRO		211	CG	-	CD	1.698	1.503
0.141	PRO		212	CG	-	CD	1.644	1.503
0.134	PRO		231	CG	-	CD	1.637	1.503
0.173	PRO		232	CG	-	CD	1.676	1.503
0.150	PRO		293	CG	-	CD	1.653	1.503
0.121	PRO		306	CG	-	CD	1.624	1.503
0.172	PRO		308	CG	-	CD	1.675	1.503
0.109	PRO		318	CG	-	CD	1.612	1.503
0.158	PRO		396	CG	-	CD	1.661	1.503
0.120	PRO		419	CG	-	CD	1.623	1.503
0.200	PRO		447	CG	-	CD	1.703	1.503
0.150	PRO		452	CG	-	CD	1.653	1.503
0.125	PRO		456	CG	-	CD	1.628	1.503
0.154	PRO		470	CG	-	CD	1.657	1.503
0.169	PRO		504	CG	-	CD	1.672	1.503
0.205	PRO		515	CG	-	CD	1.708	1.503
0.126	PRO		528	CG	-	CD	1.629	1.503
0.166	PRO		531	CG	-	CD	1.669	1.503

*** Covalent Angle Values:

The RMS deviation for covalent angles relative to the standard dictionary is 1.3 degrees.

The following table contains a list of the covalent bond angles greater than 6.0*RMSD.

Deviation	Residue	Chain	Sequence	AT1	-	AT2	-	AT3	Bond	Dictionary

	Name	ID	Number						Angle	Value
-8.5	PRO		61	CB	-	CG	-	CD	97.6	106.1
-7.7	CYS		67	N	-	CA	-	CB	102.8	110.5
-7.7	CYS		160	N	-	CA	-	CB	102.8	110.5
-9.6	PRO		198	CB	-	CG	-	CD	96.5	106.1
-9.5	PRO		211	CB	-	CG	-	CD	96.6	106.1
-8.6	PRO		232	CB	-	CG	-	CD	97.5	106.1
-7.7	CYS		253	N	-	CA	-	CB	102.8	110.5
-7.7	CYS		268	N	-	CA	-	CB	102.8	110.5
8.3	ARG		274	N	-	CA	-	C	119.5	111.2
-8.6	PRO		308	CB	-	CG	-	CD	97.5	106.1
-7.8	CYS		326	N	-	CA	-	CB	102.7	110.5
-7.8	CYS		362	N	-	CA	-	CB	102.7	110.5
-7.7	CYS		371	N	-	CA	-	CB	102.8	110.5
-7.7	CYS		374	N	-	CA	-	CB	102.8	110.5
-7.8	CYS		380	N	-	CA	-	CB	102.7	110.5
-7.8	CYS		395	N	-	CA	-	CB	102.7	110.5
-7.9	PRO		396	CB	-	CG	-	CD	98.2	106.1
-7.7	CYS		398	N	-	CA	-	CB	102.8	110.5
-9.7	PRO		447	CB	-	CG	-	CD	96.4	106.1
-7.8	PRO		470	CB	-	CG	-	CD	98.3	106.1
-7.7	CYS		482	N	-	CA	-	CB	102.8	110.5
-7.7	CYS		490	N	-	CA	-	CB	102.8	110.5
-7.7	CYS		501	N	-	CA	-	CB	102.8	110.5
-7.7	CYS		502	N	-	CA	-	CB	102.8	110.5
-8.3	PRO		504	CB	-	CG	-	CD	97.8	106.1
-9.9	PRO		515	CB	-	CG	-	CD	96.2	106.1
-8.3	PRO		531	CB	-	CG	-	CD	97.8	106.1

TORSION ANGLES

The torsion angle distributions have been checked. The postscript file of the conformation rings showing the torsion angle distributions will be sent in a separate E-mail message.

CHIRALITY

The chirality has been checked and there are no incorrect carbon chiral centers. Some of O1P and O2P atoms do not follow the convention defined in the standard IUBMB nomenclature (Liebecq, C. Compendium of Biochemical Nomenclature and Related Documents, 2nd ed.; Portland Press: London and Chapel Hill, 1992). If you do not indicate otherwise, we will switch the labels of O1P and O2P as shown below.

Chain	Residue Name	Residue Number	Chiral Center	Chiral Neighbor	Original Atom Name
	PRO	61	CG	2HG	
	PRO	198	CG	2HG	
	PRO	211	CG	2HG	
	PRO	232	CG	2HG	
	PRO	308	CG	2HG	
	PRO	504	CG	2HG	
	PRO	515	CG	2HG	

OTHER IMPORTANT ISSUES

==> Please check carefully REMARKS 3 and 200 and fill in the parameters as appropriate.

```
75-Sirt1.pdb: Missing KEYWDS records

75-Sirt1.pdb: Missing TITLE record
```