

Protein Structure Validation Suite (PSVS)

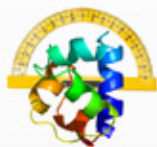


PSVS report for fl-SIRT1

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PSVS report for fl-SIRT1



Protein Structure Validation Suite
(PSVS)



Software Environment

Software for structure quality evaluation:

DSSP	DsspCMBI-April-2000
pdostat	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

MolProbit 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.): 747

Organism:

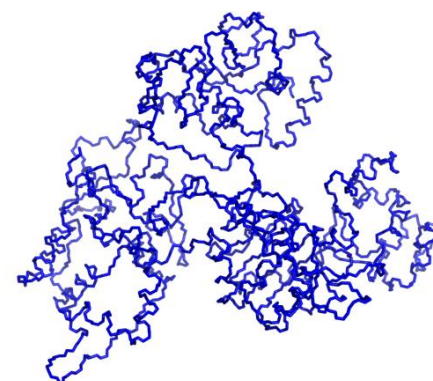
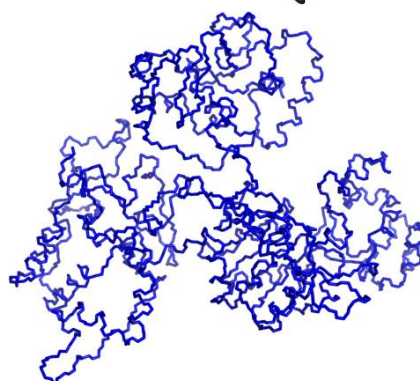
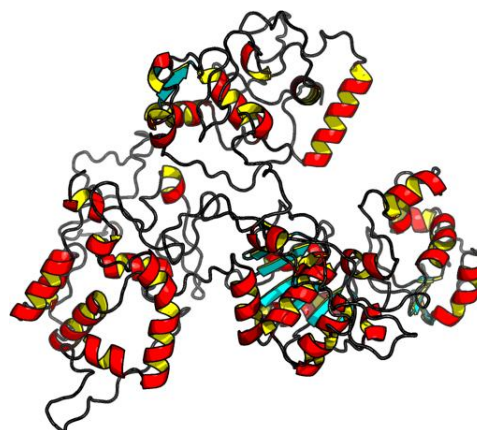
SwissProt /

TrEMBL ID:

models: 1

Oligomerization: monomer

Molecular weight: 81680



Secondary Structure Elements:

alpha helices:

beta strands:

Ramachandran Plot Summary for selected residues³ from Procheck

<i>Most favoured regions</i>	<i>Additionally allowed regions</i>	<i>Generously allowed regions</i>	<i>Disallowed regions</i>
90.3%	9.1%	0.5%	0.2%

Ramachandran Plot Summary for selected residues³ from Richardson Lab's Molprobit

<i>Most favoured regions</i>	<i>Allowed regions</i>	<i>Disallowed regions</i>	View plot	View model summary
97.7%	1.9%	0.4%		

Global quality scores

Program	<i>Verify3D</i>	<i>ProsaII (-ve)</i>	<i>Procheck (phi-psi)³</i>	<i>Procheck (all)³</i>	<i>MolProbit Clashscore</i>
-Raw score	0.35	0.50	-0.08	0.19	8.03
Z-score ¹	-1.77	-0.62	0.00	1.12	0.15

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

Number of close contacts (within 2.2 Å): 0

PSVS Software Environment

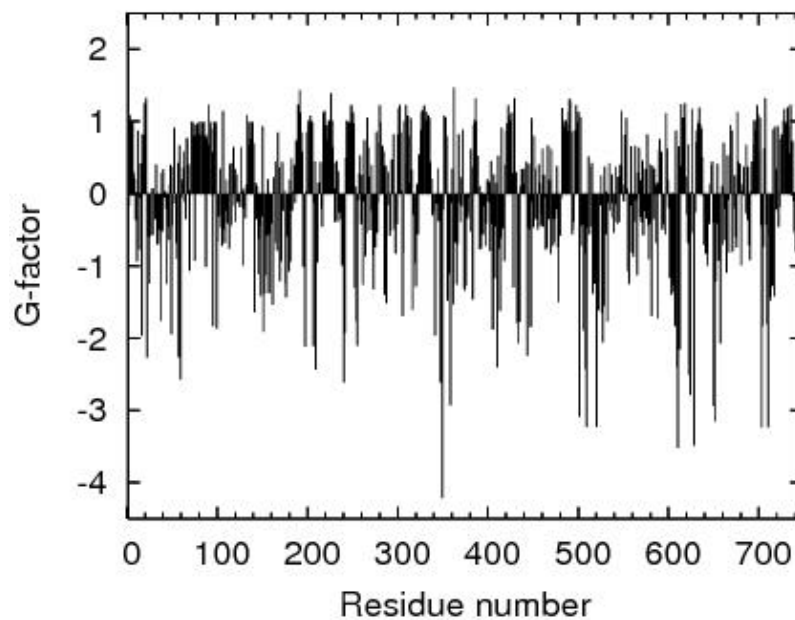
RMS deviation for bond angles: 1.6 °

RMS deviation for bond lengths: 0.017 Å

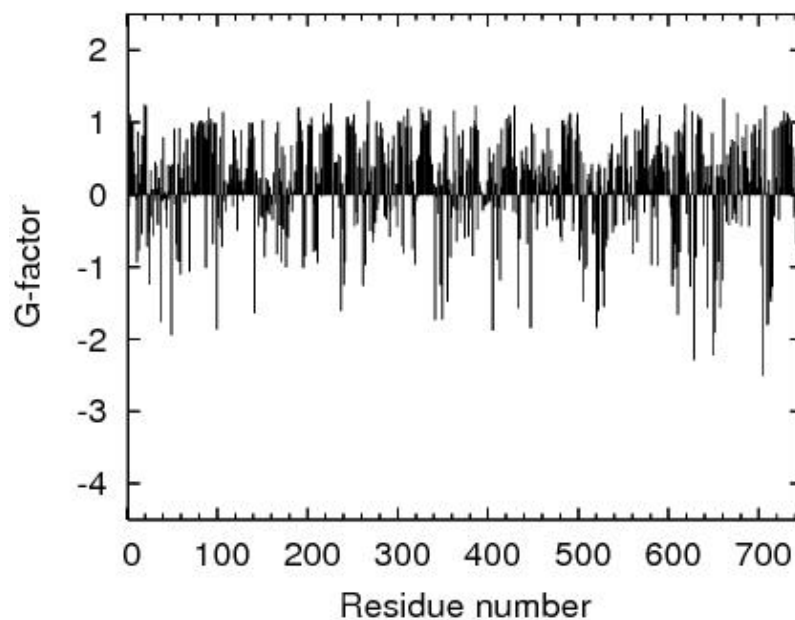
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution ≤ 1.80 Å, R-factor ≤ 0.25 and R-free ≤ 0.28 ; a positive value indicates a 'better' score

³Selected residues: all

Procheck G-factor for phi-psi

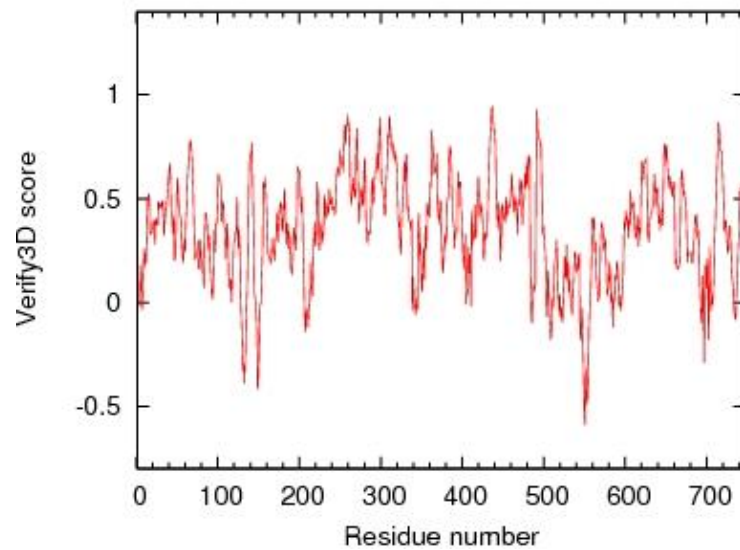


Procheck G-factor for all dihedral angles

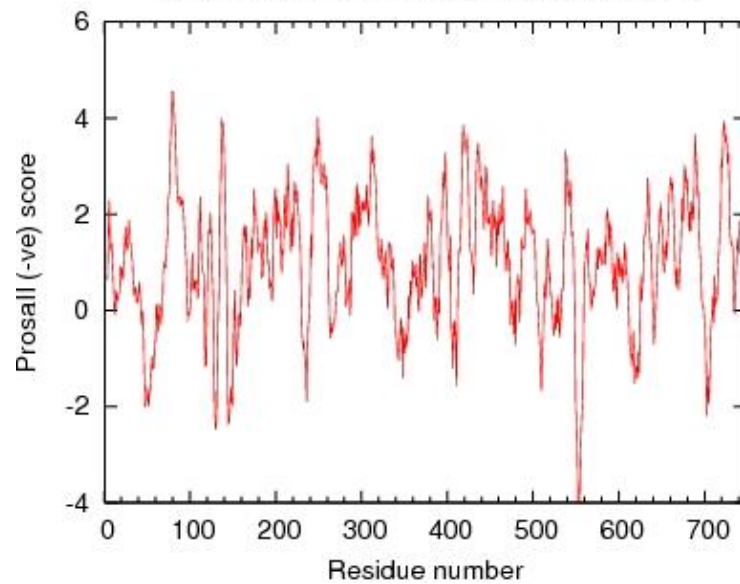


PSVS Software Environment

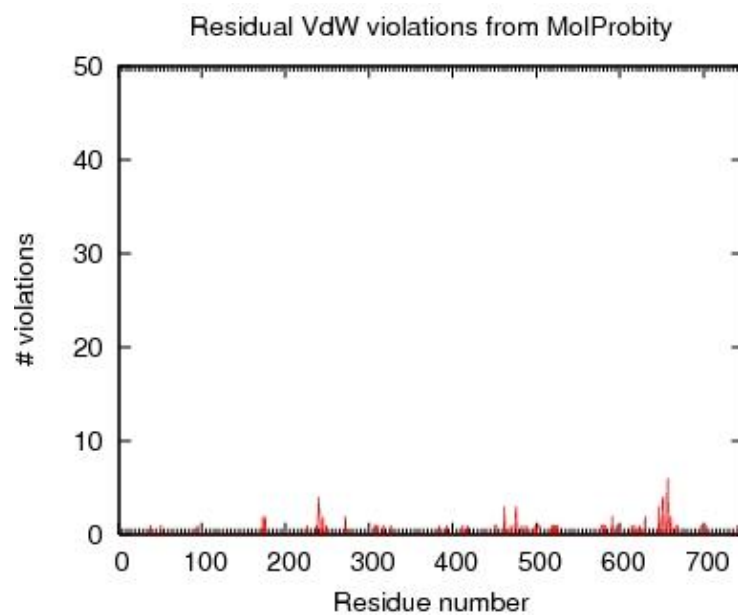
Verify3D score over window of 7 residues

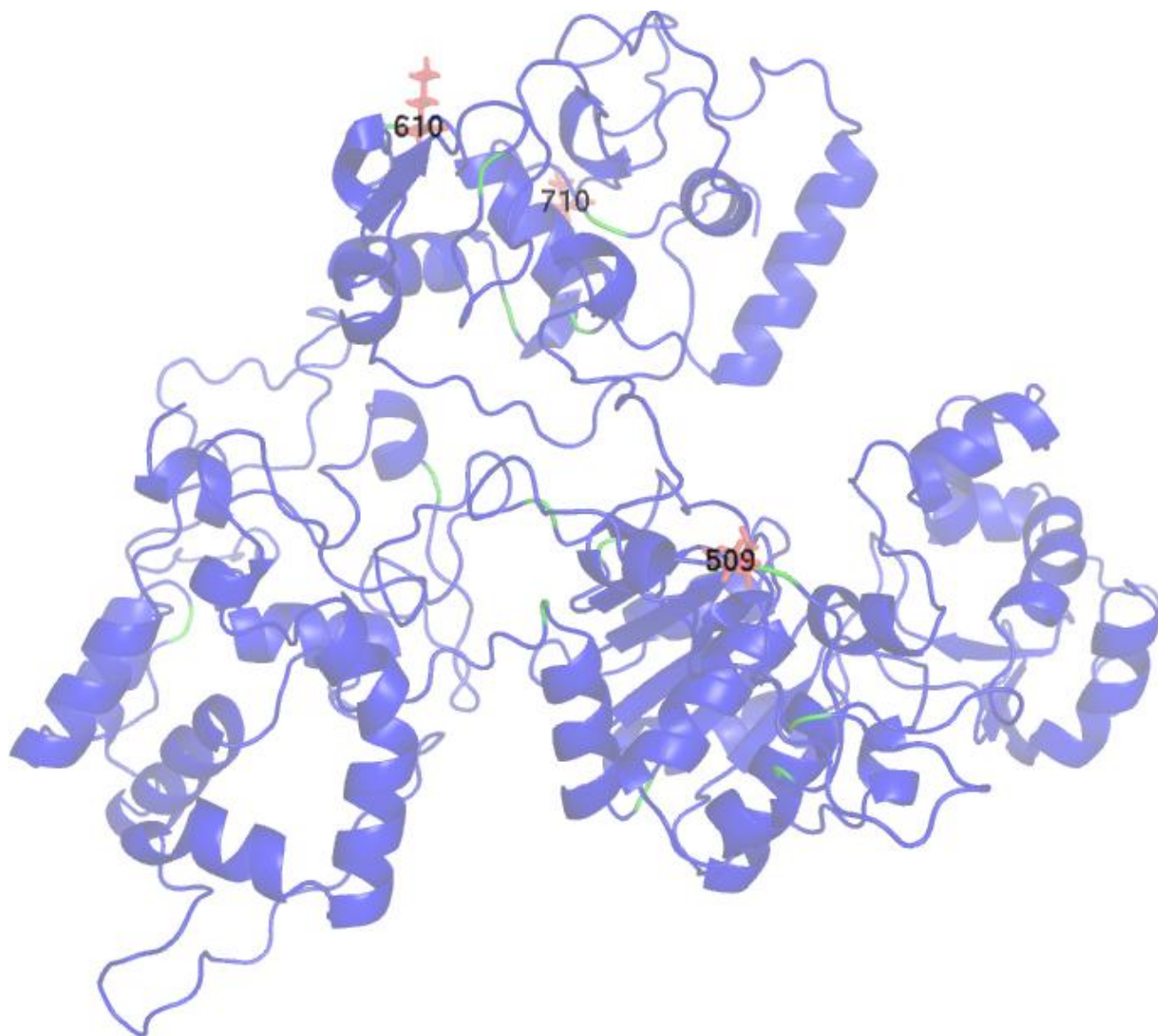


ProsaII (-ve) score over window of 7 residues



PSVS Software Environment





Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobit)

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2. Bowie J U, Luthy R and Eisenberg D, "A Method to Identify Protein Sequences that Fold into a Known Three-Dimensional Structure", Science 253 (1991): 164-169
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PSVS Software Environment

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13. Koradi, R, et al, "MOLMOL: a program for display and analysis of macromolecular structures ", J Mol Graphics 14 (1996): 51-55.
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15. Lovell S C et al, "Structure validation by Calpha geometry: phi,psi and Cbeta deviation" Proteins (2003) 50: 437-450
16. Kabsch W, Sander C, "Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features", Biopolymers (1983) 22: 2577-2637
17. Bagaria, A., Jaravine, V., Huang, Y.J., Montelione, G.T., and Guntert, P. "Protein structure validation by generalized linear model root-mean-square deviation prediction". Protein Sci 21(2012), 229-238.

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)	-0.08	N/A	0.00
Procheck G-factor ^e (all dihedral angles)	0.19	N/A	1.12
Verify3D	0.35	0.0000	-1.77
ProsaII (-ve)	0.50	0.0000	-0.62
MolProbity clashscore	8.03	0.0000	0.15
Ramachandran Plot Summary from Procheck			
Most favoured regions	90.3%		
Additionally allowed regions	9.1%		
Generously allowed regions	0.5%		
Disallowed regions	0.2%		
Ramachandran Plot Statistics from Richardson's lab			
Most favoured regions	97.7%		
Allowed regions	1.9%		
Disallowed regions	0.4%		

^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 fl-SIRT1 by PSVS

Output from PDBStat

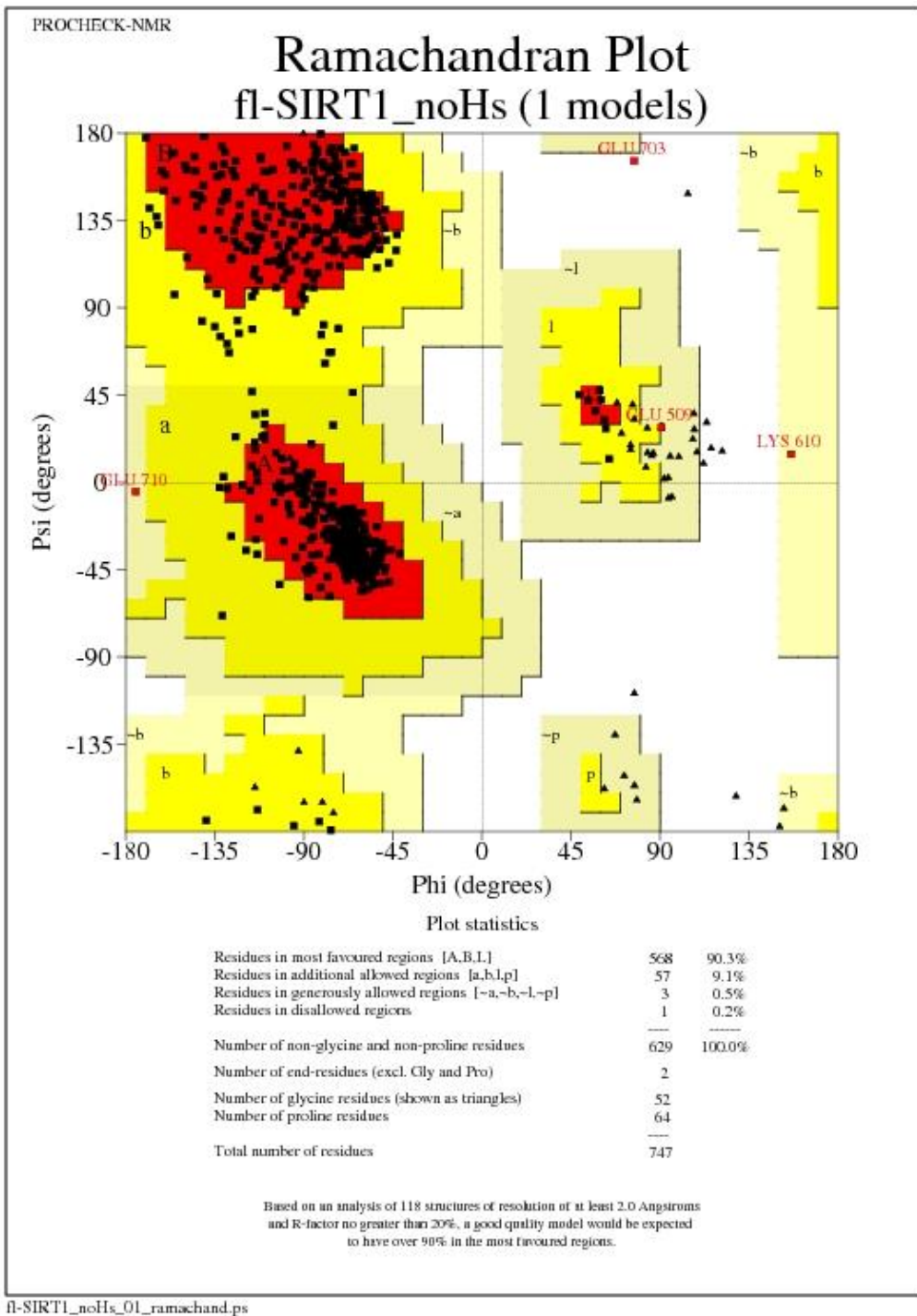
Output from PROCHECK

Ramachandran Plot for all models

Text summary of Ramachandran Plot

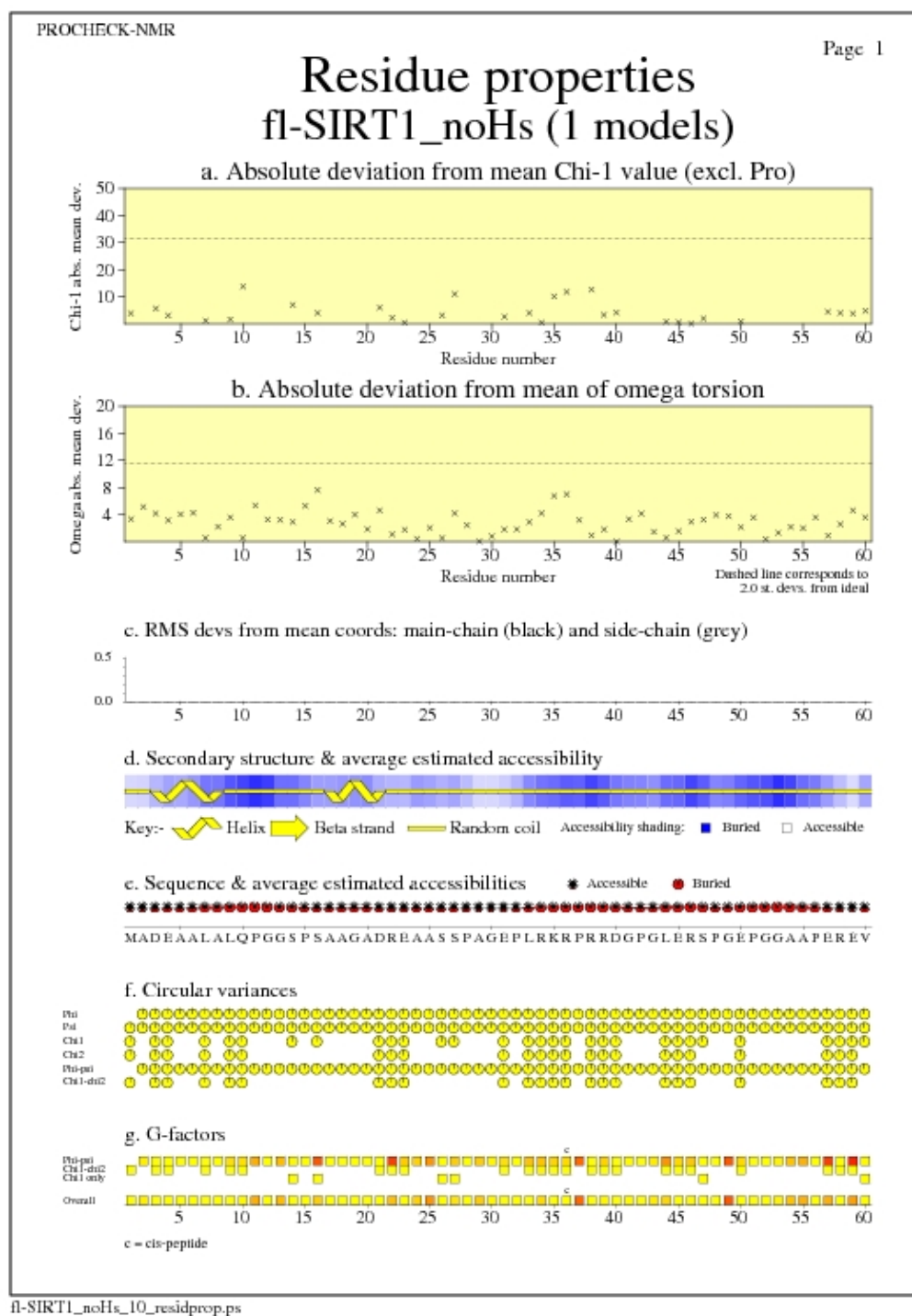
```
+-----<<< P R O C H E C K       S U M M A R Y >>>-----+
|
| fl-SIRT1_noHs_000.rin    0.0                                747 residues |
|
*| Ramachandran plot:    90.3% core    9.1% allow    0.5% gener    0.2% disall |
|
+| All Ramachandrans:    9 labelled residues (out of 745)          |
+| Chi1-chi2 plots:      1 labelled residues (out of 427)          |
```

JPEG image for all model Ramachandran Plot

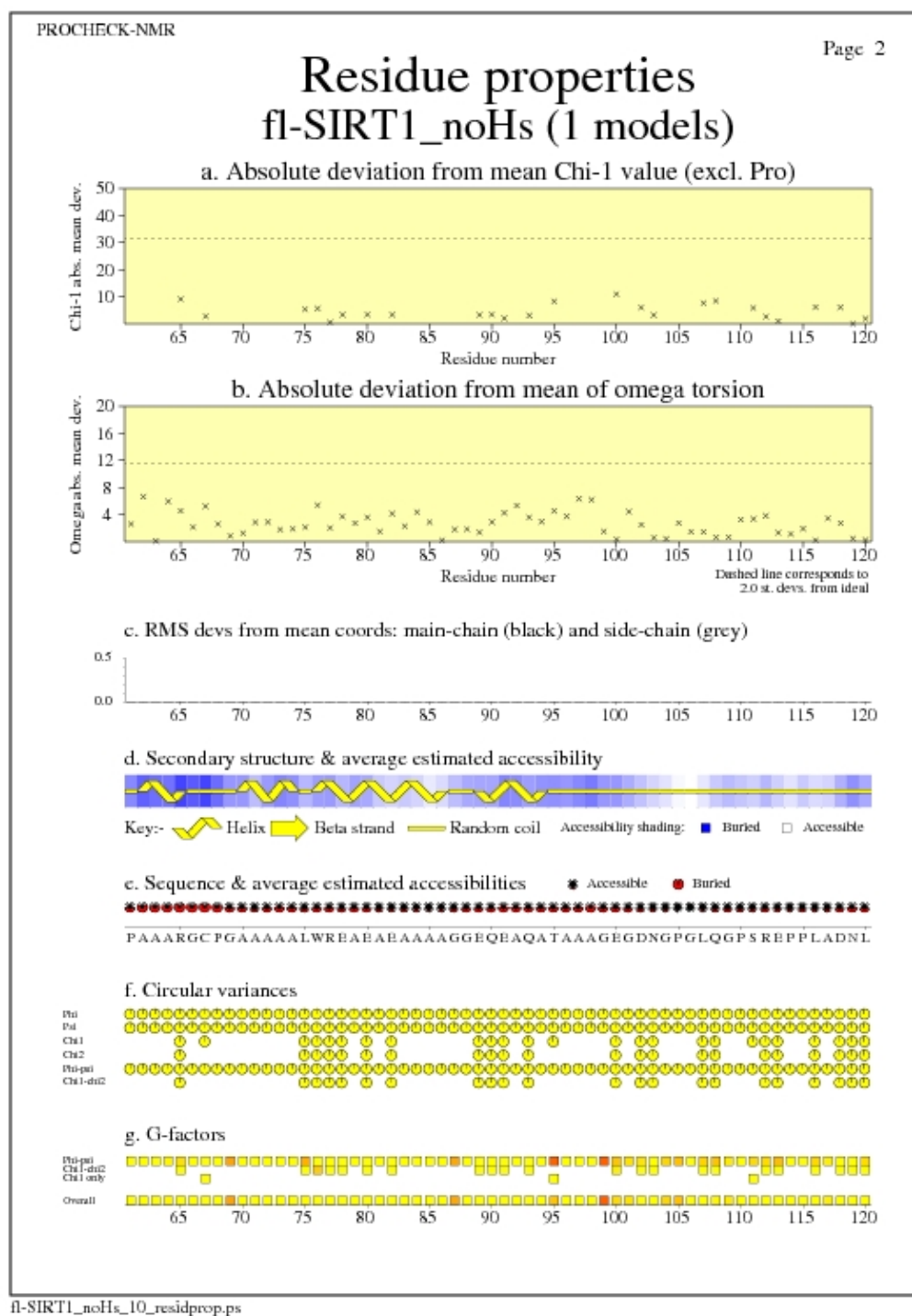


Residue Properties for all models

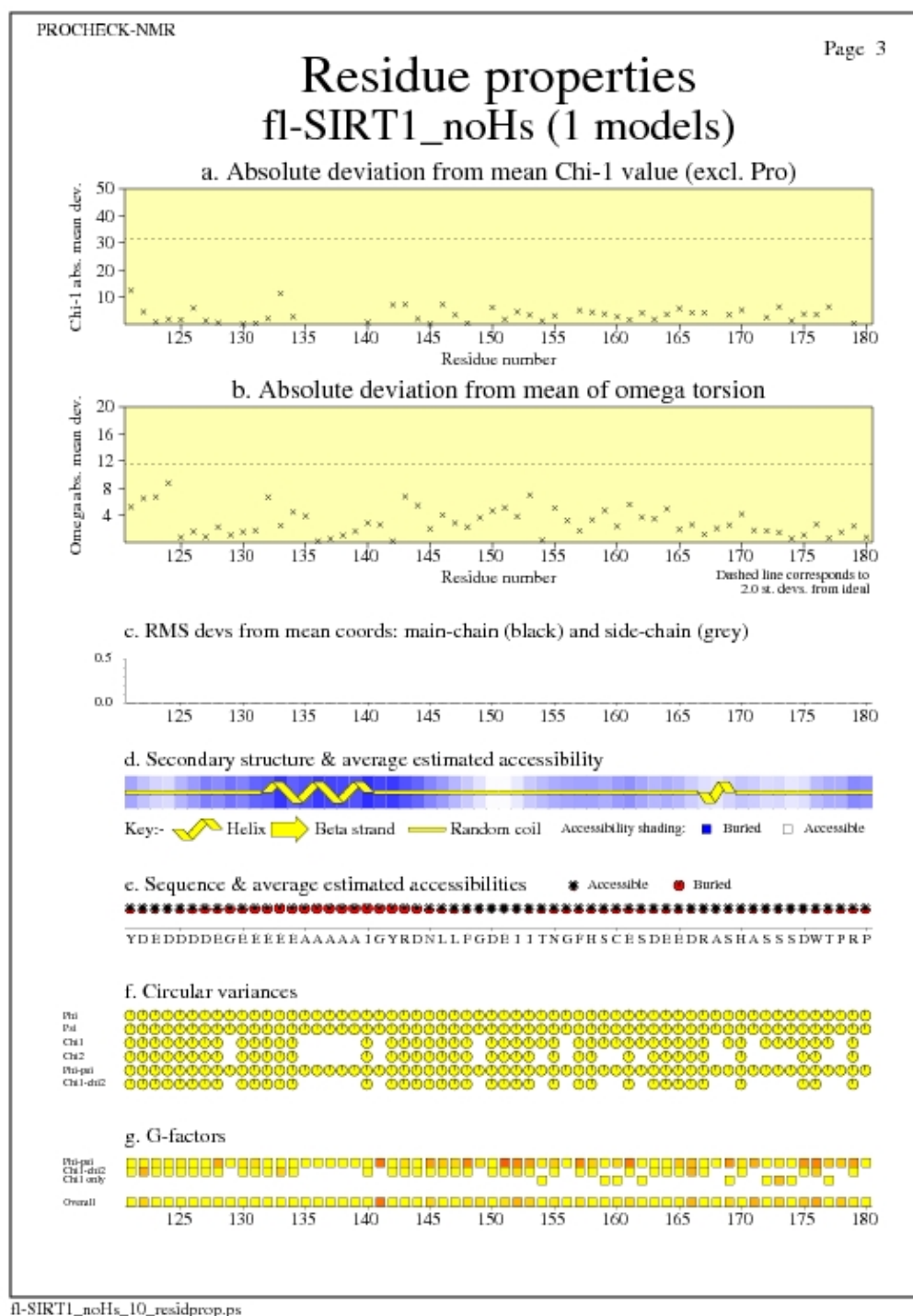
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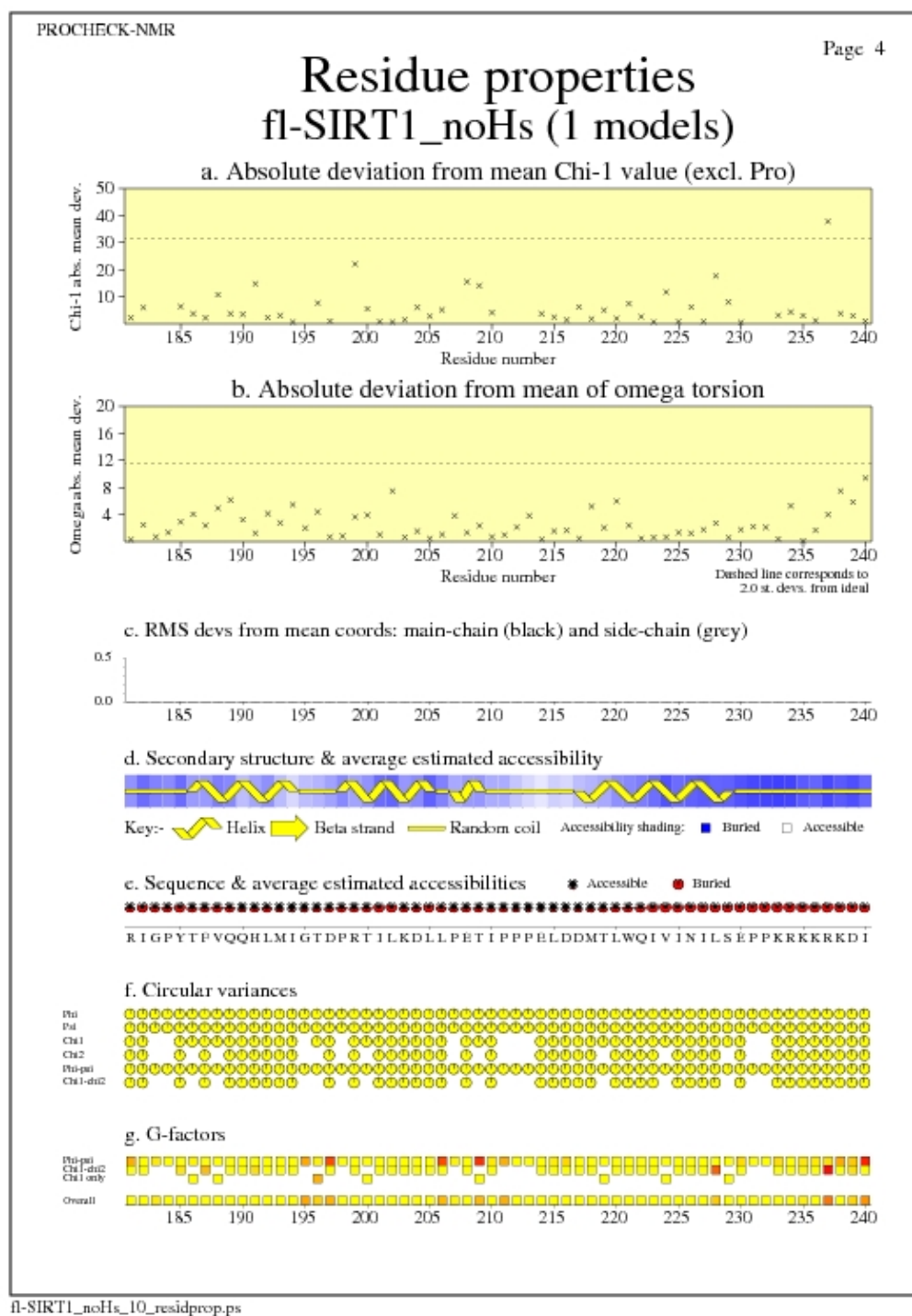
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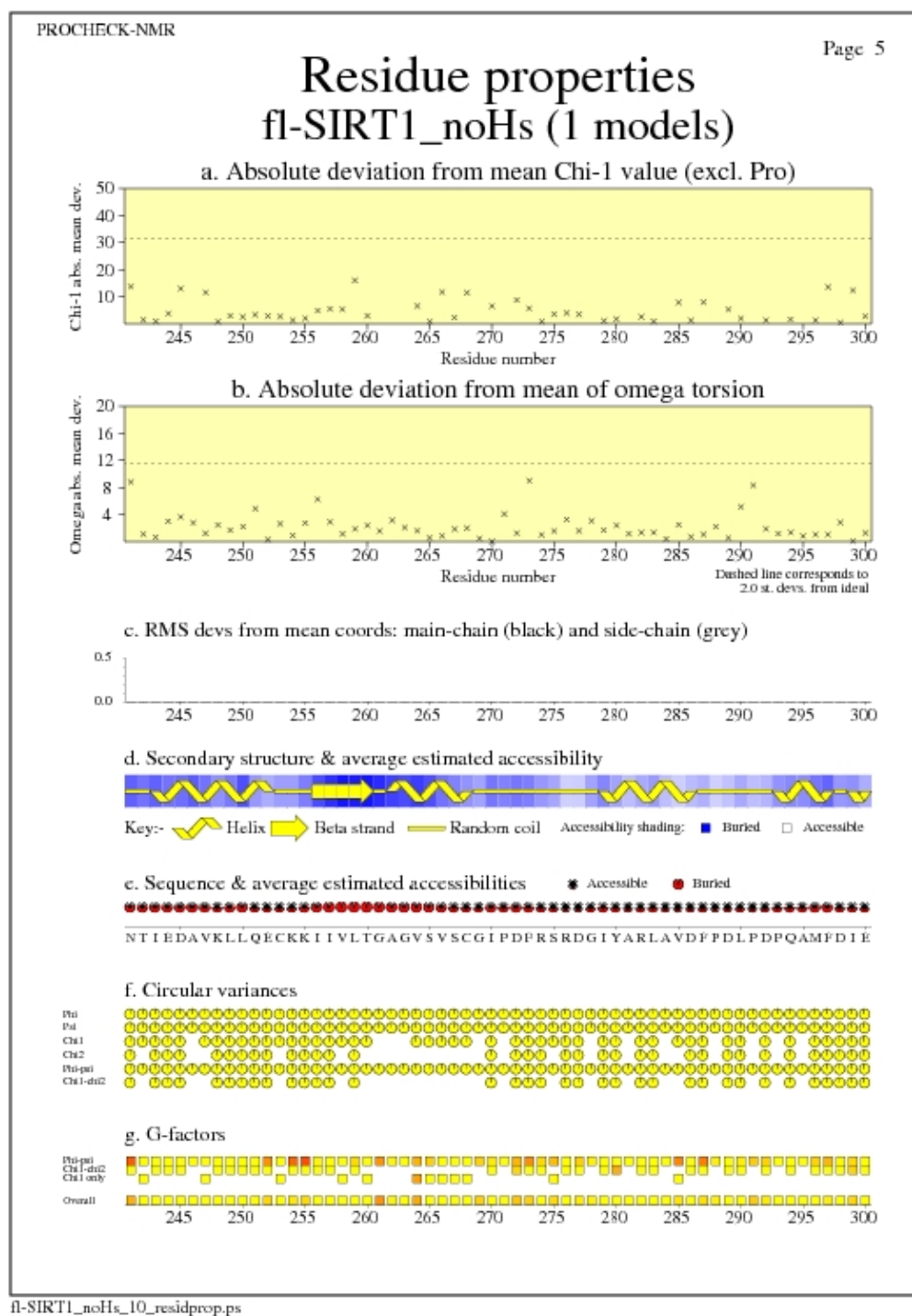
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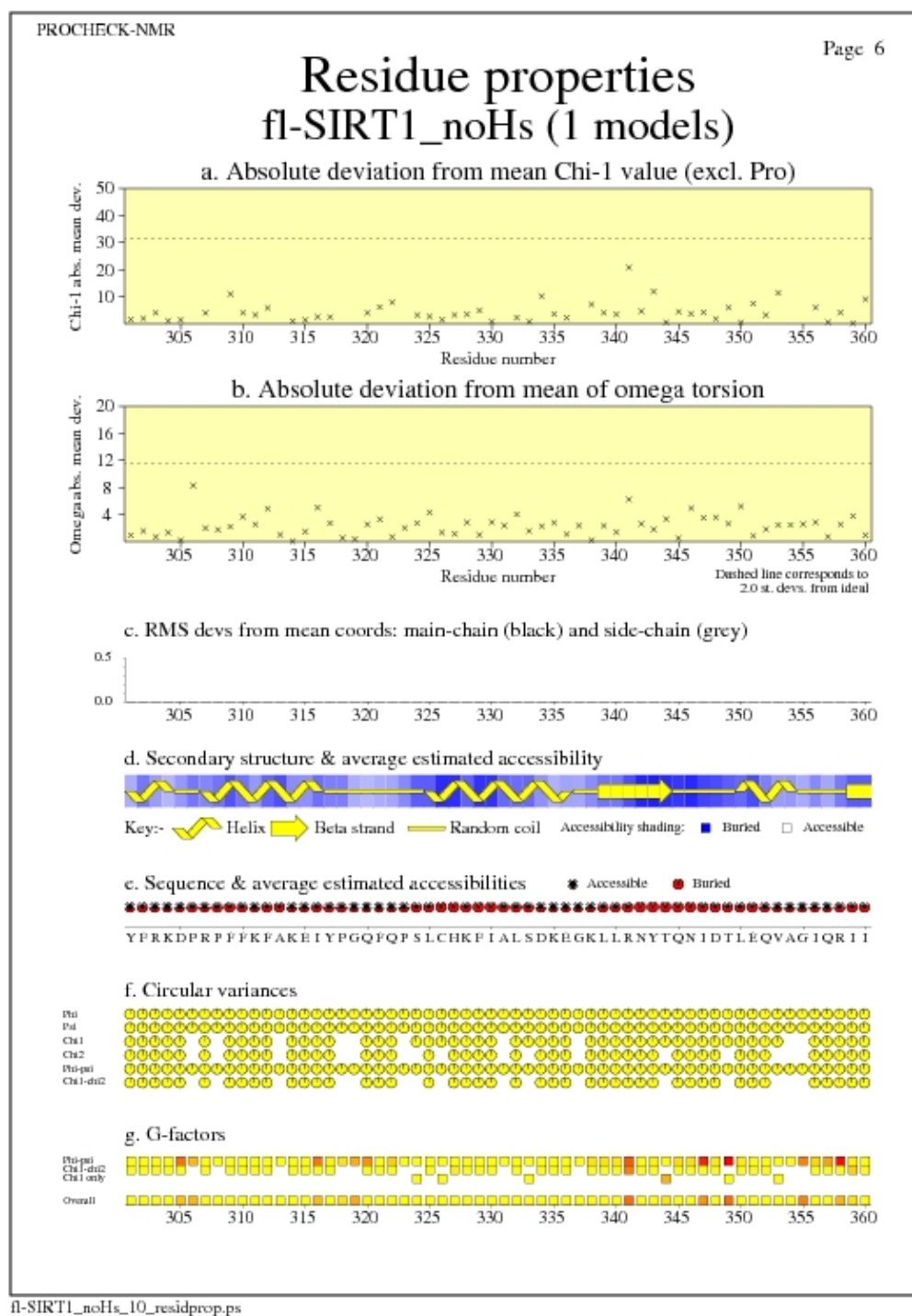
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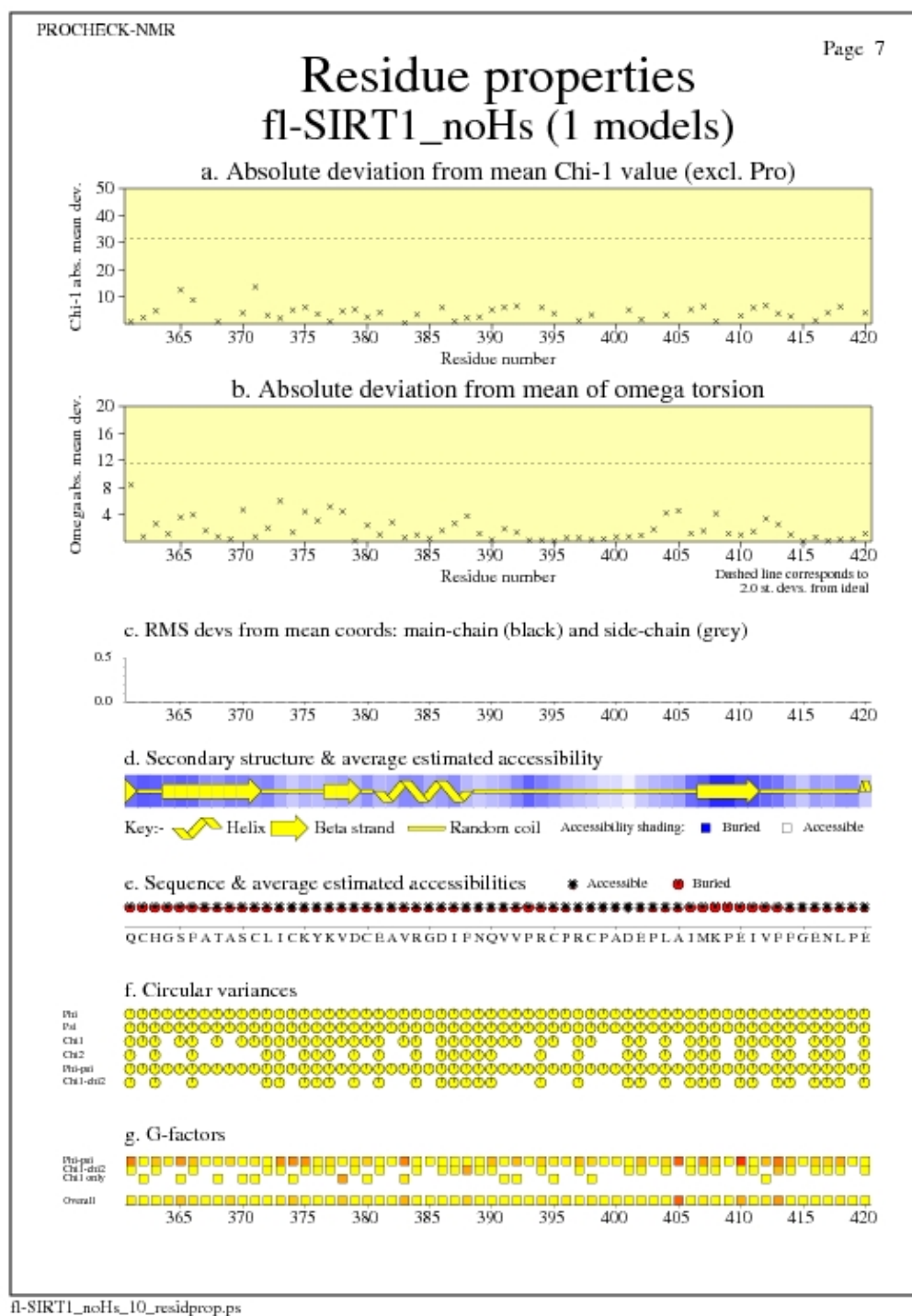
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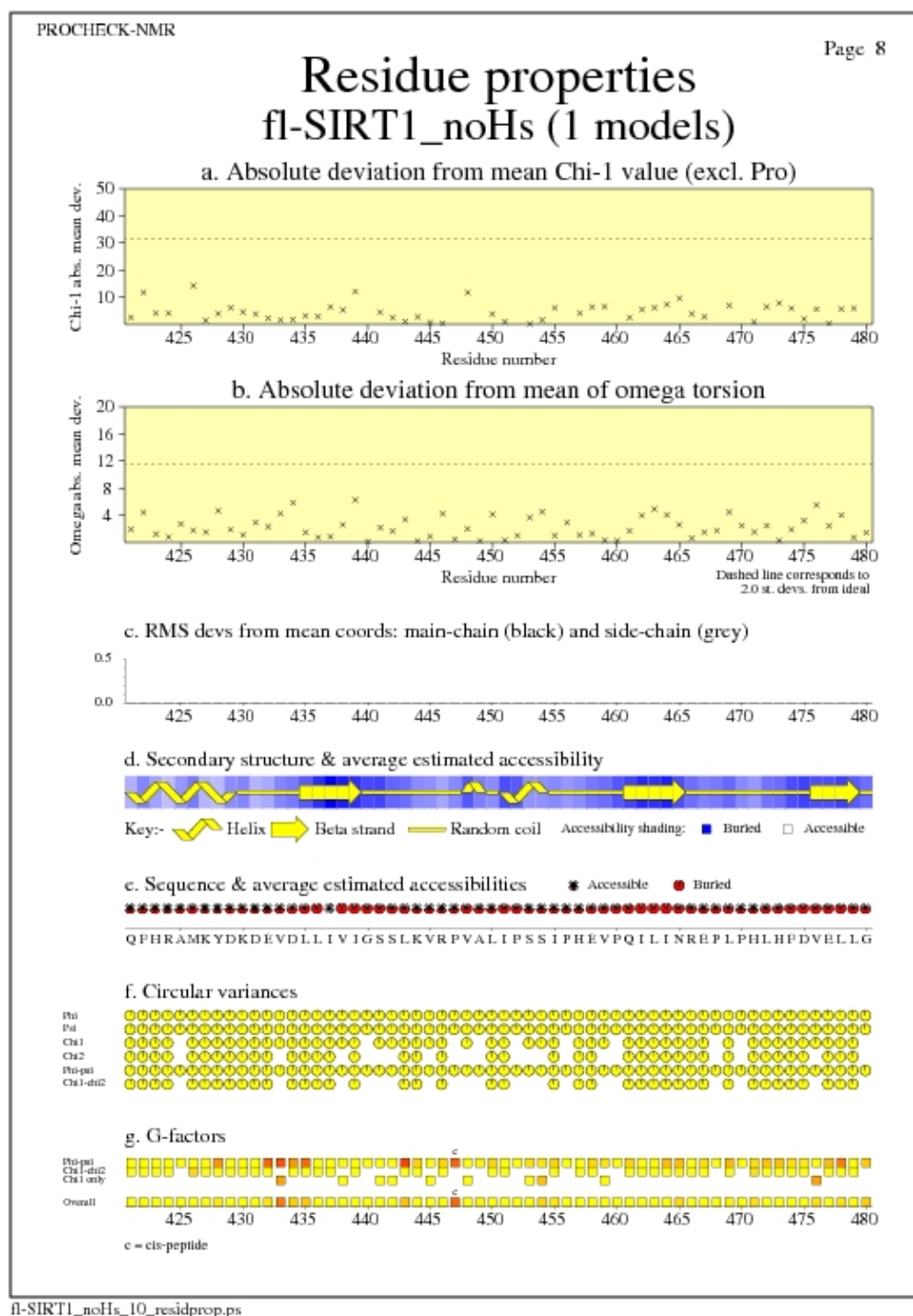
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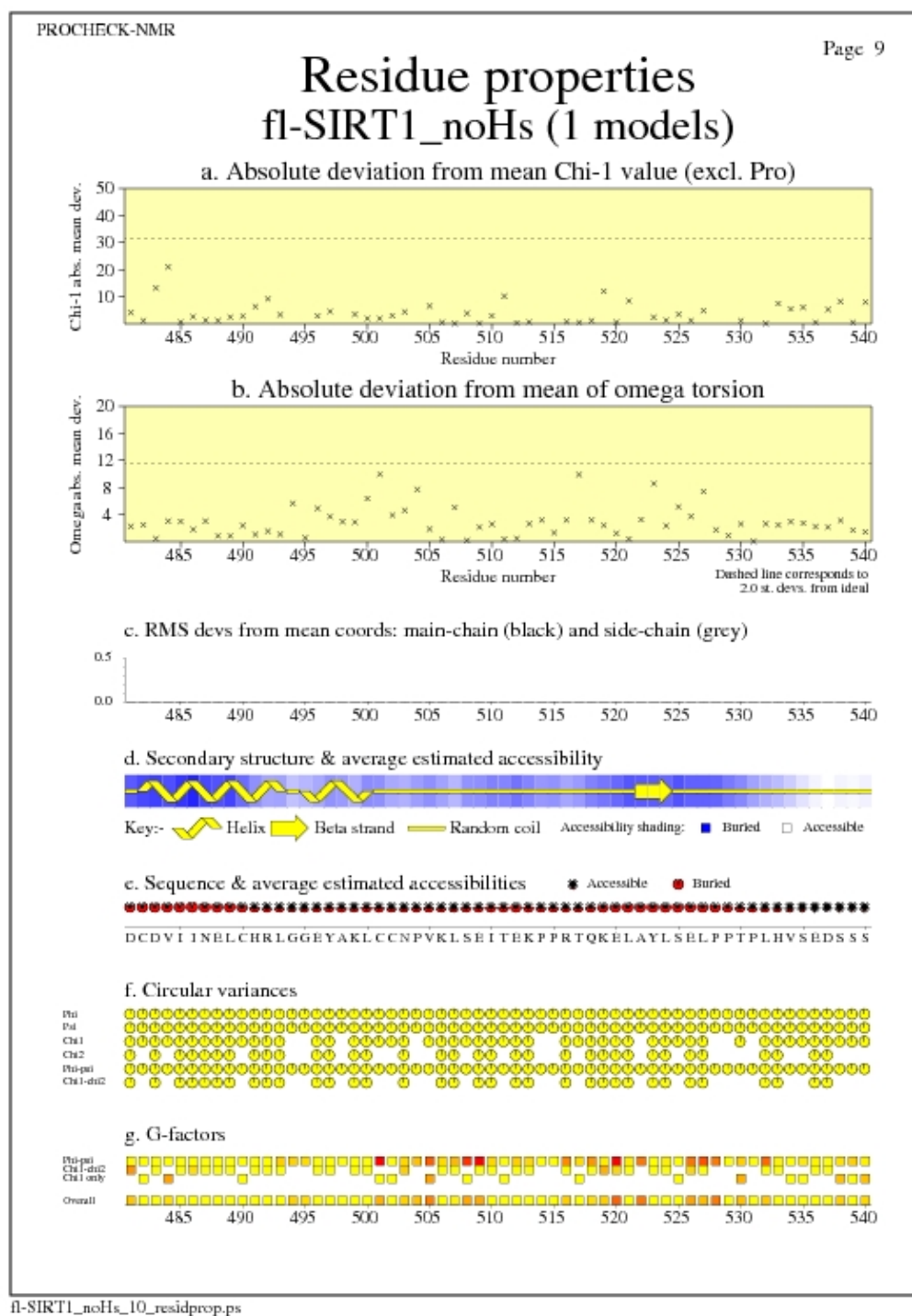
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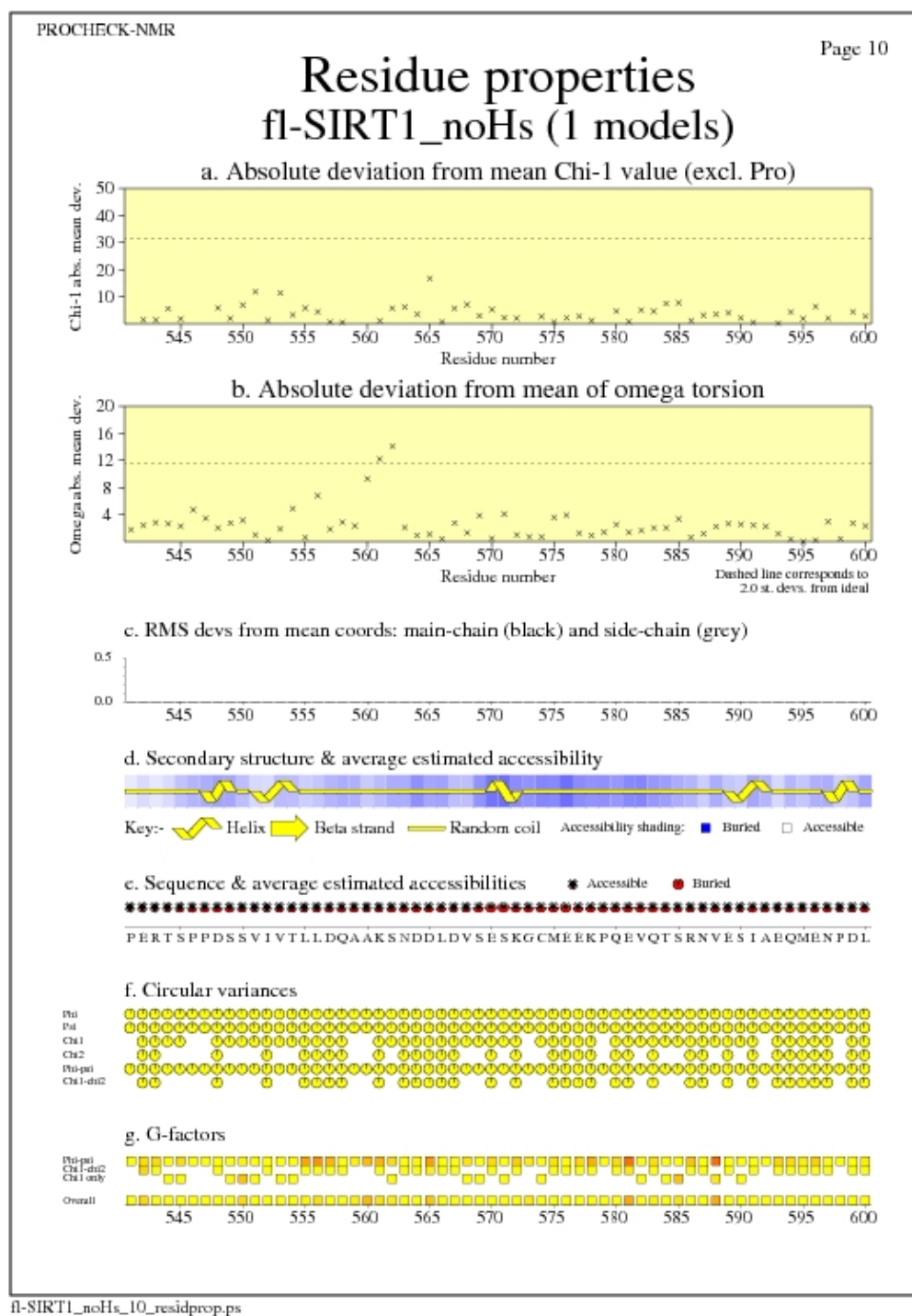
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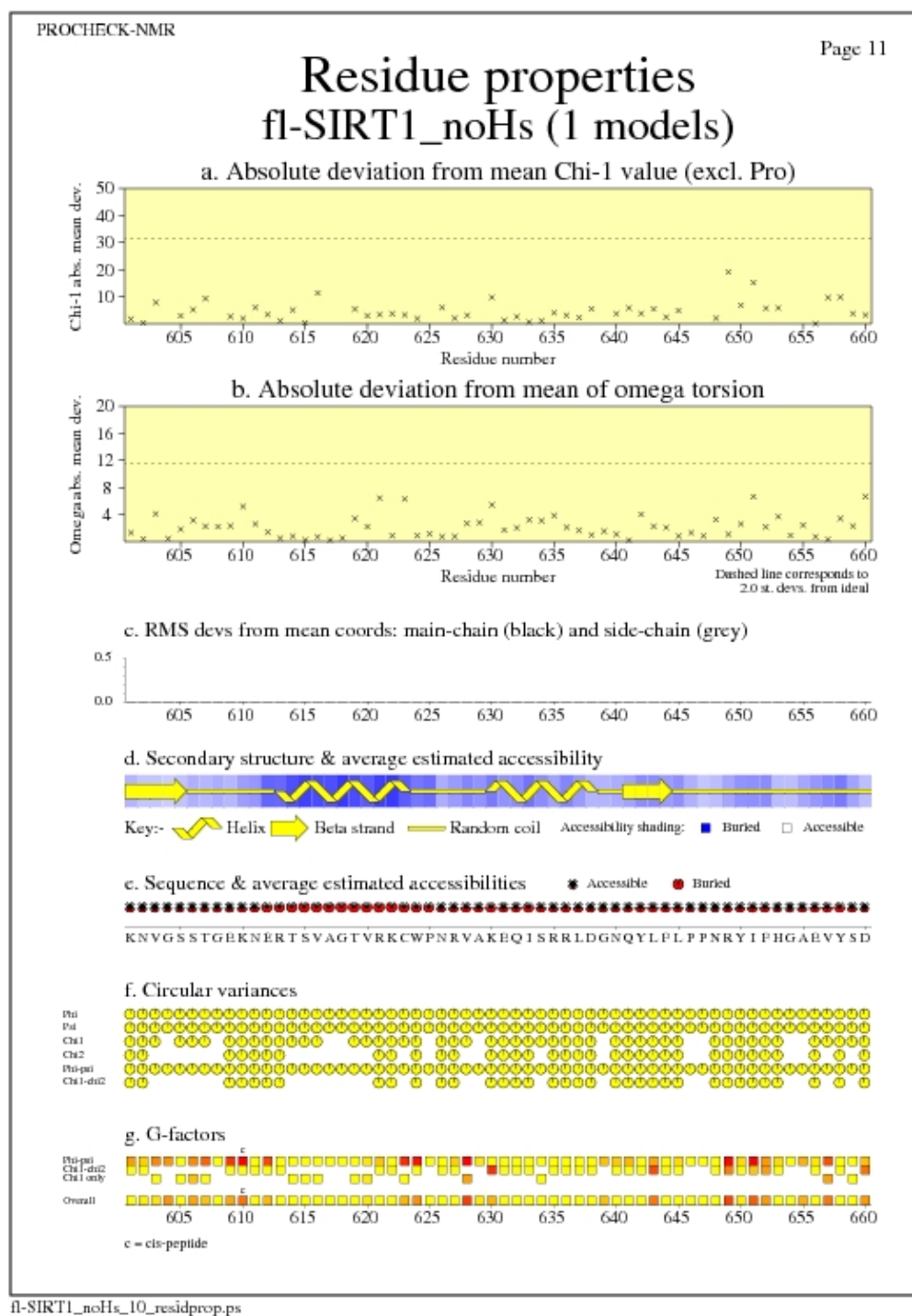
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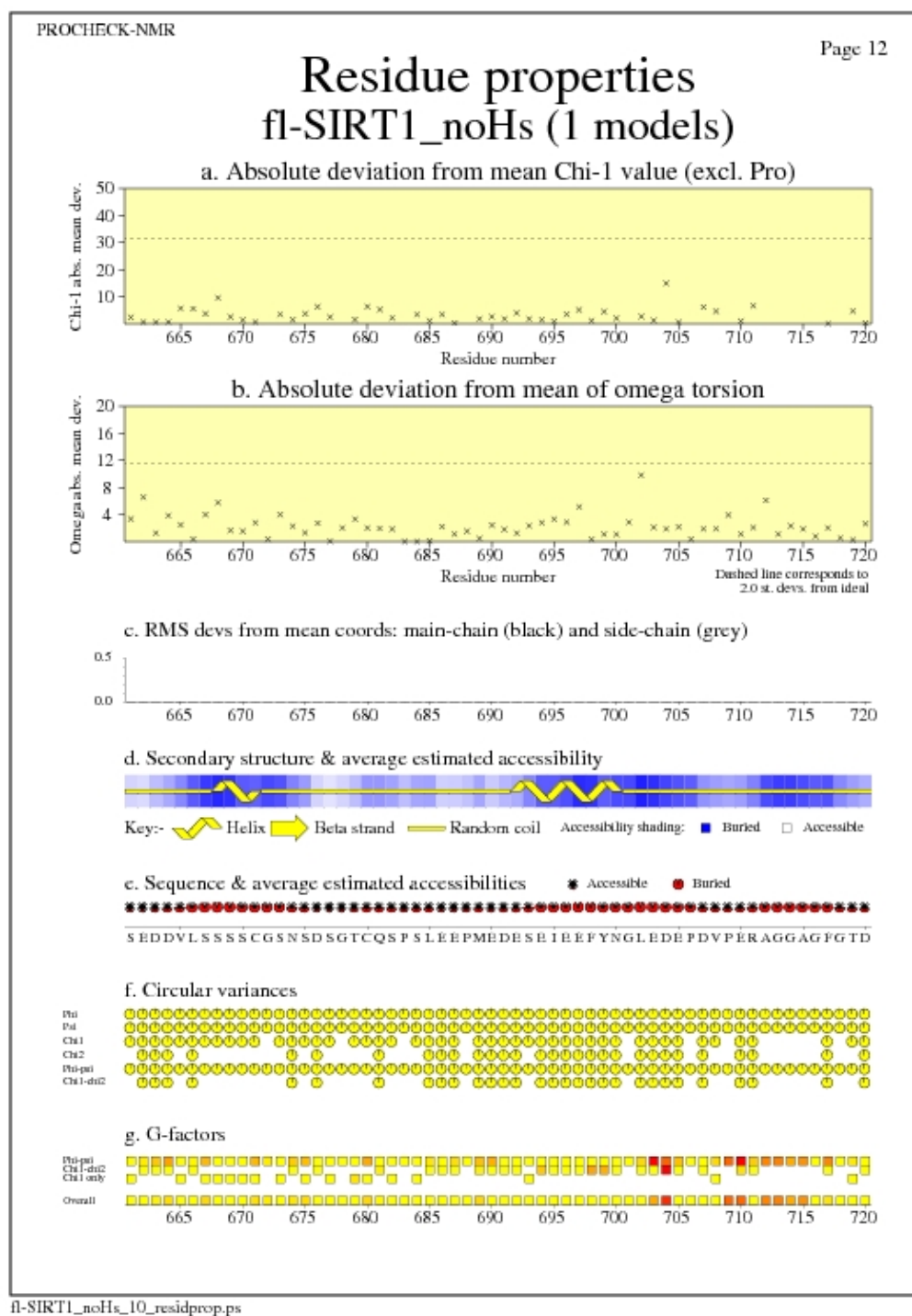
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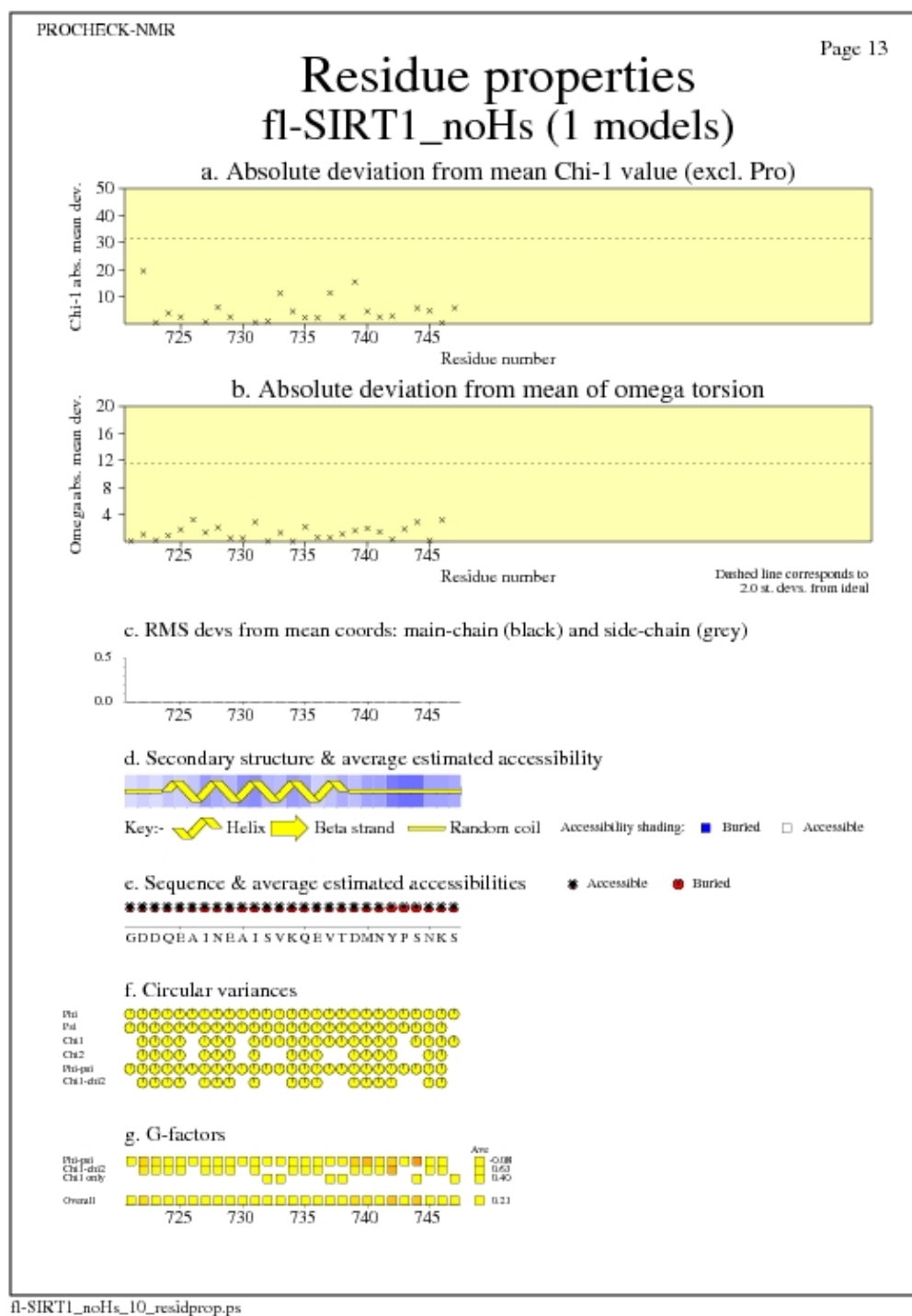
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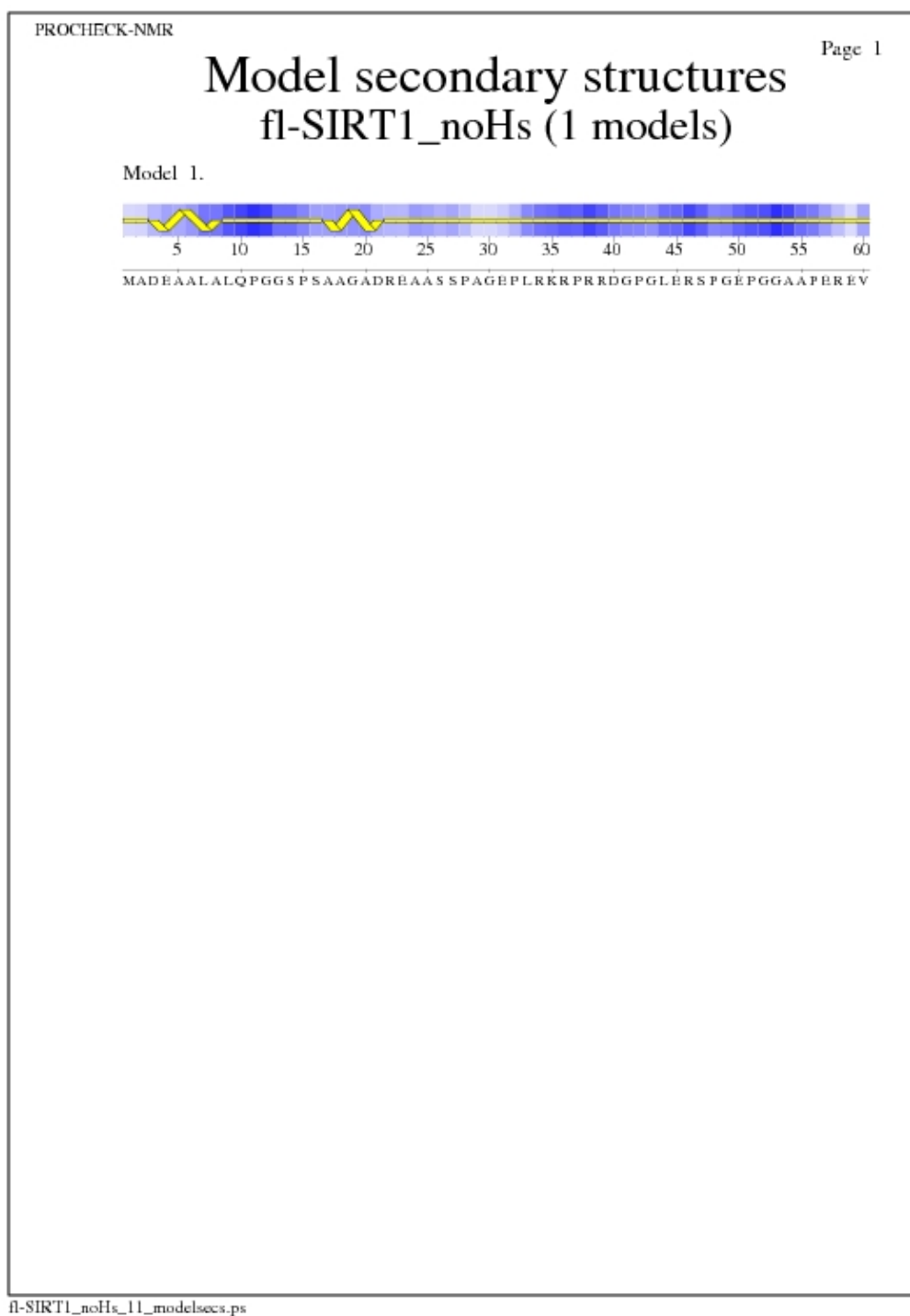


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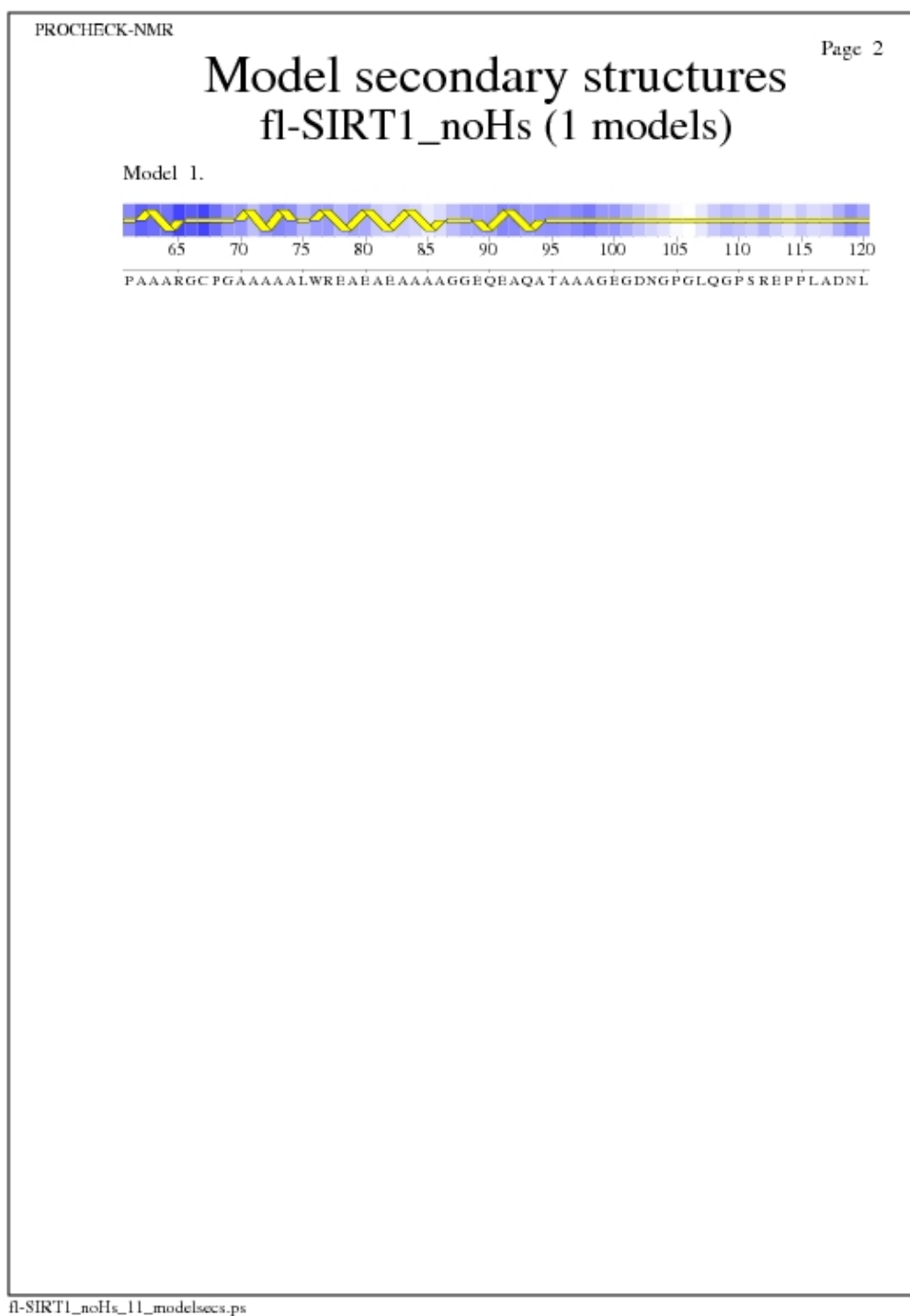


Model Secondary Structures from Proccheck

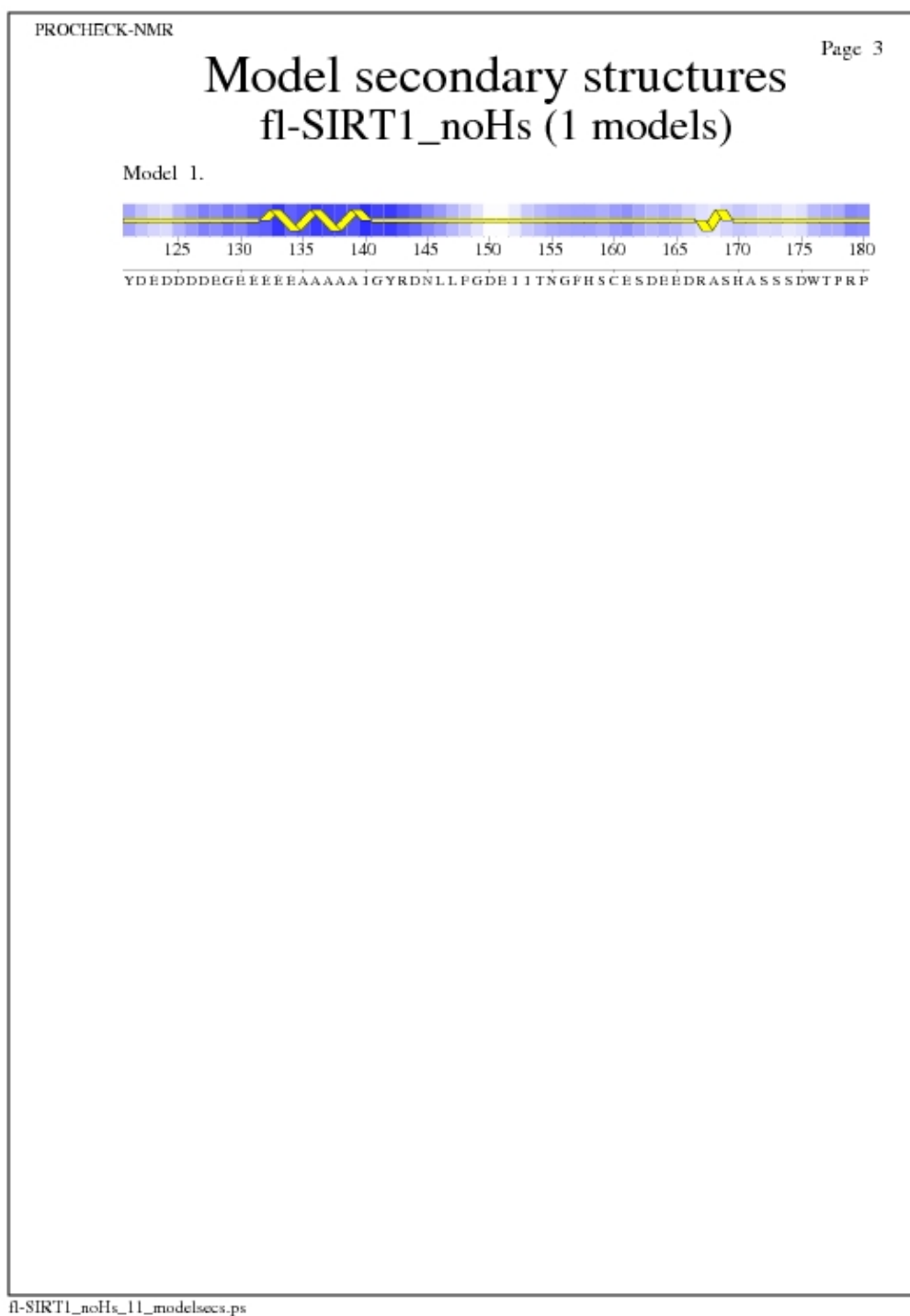
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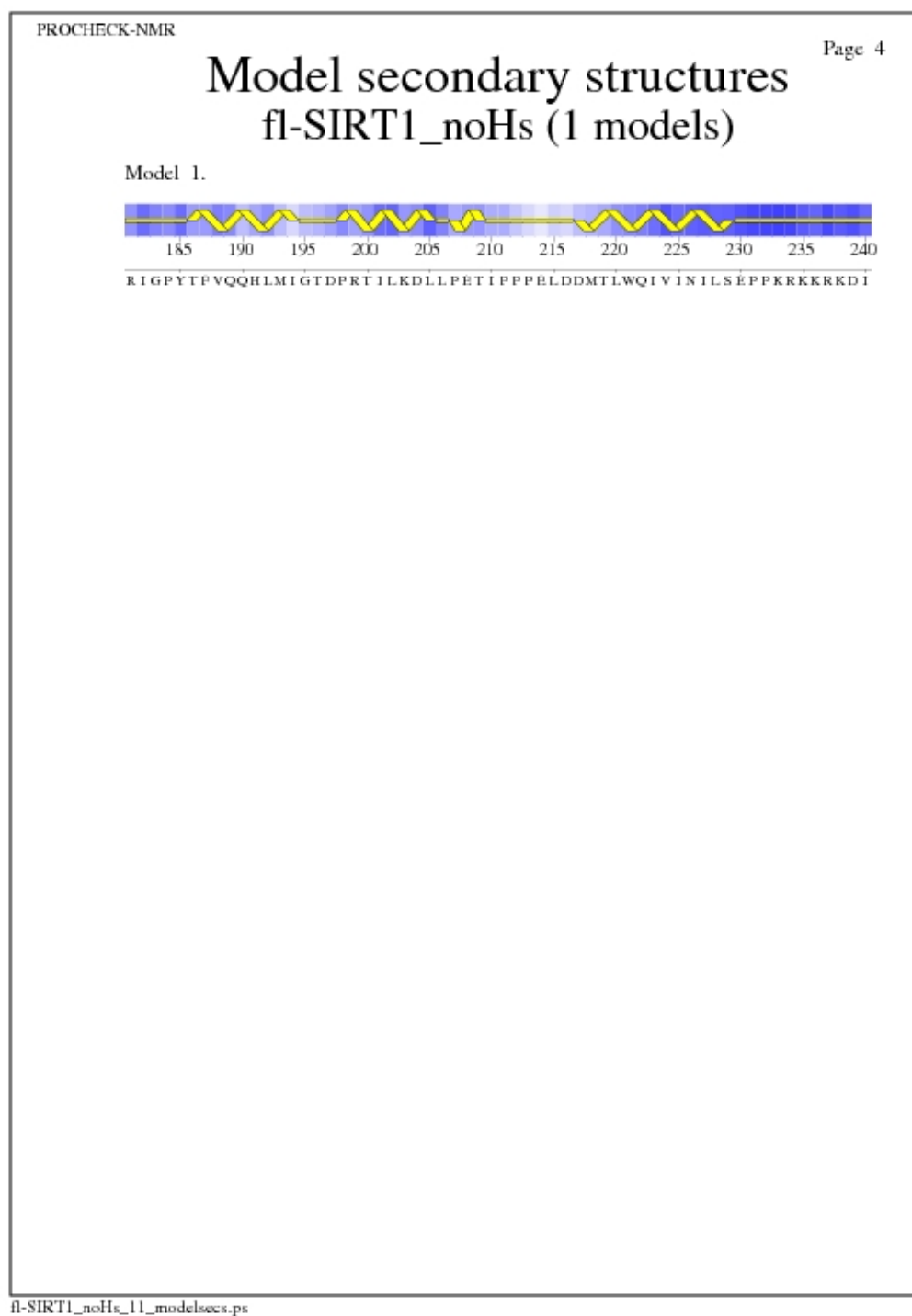
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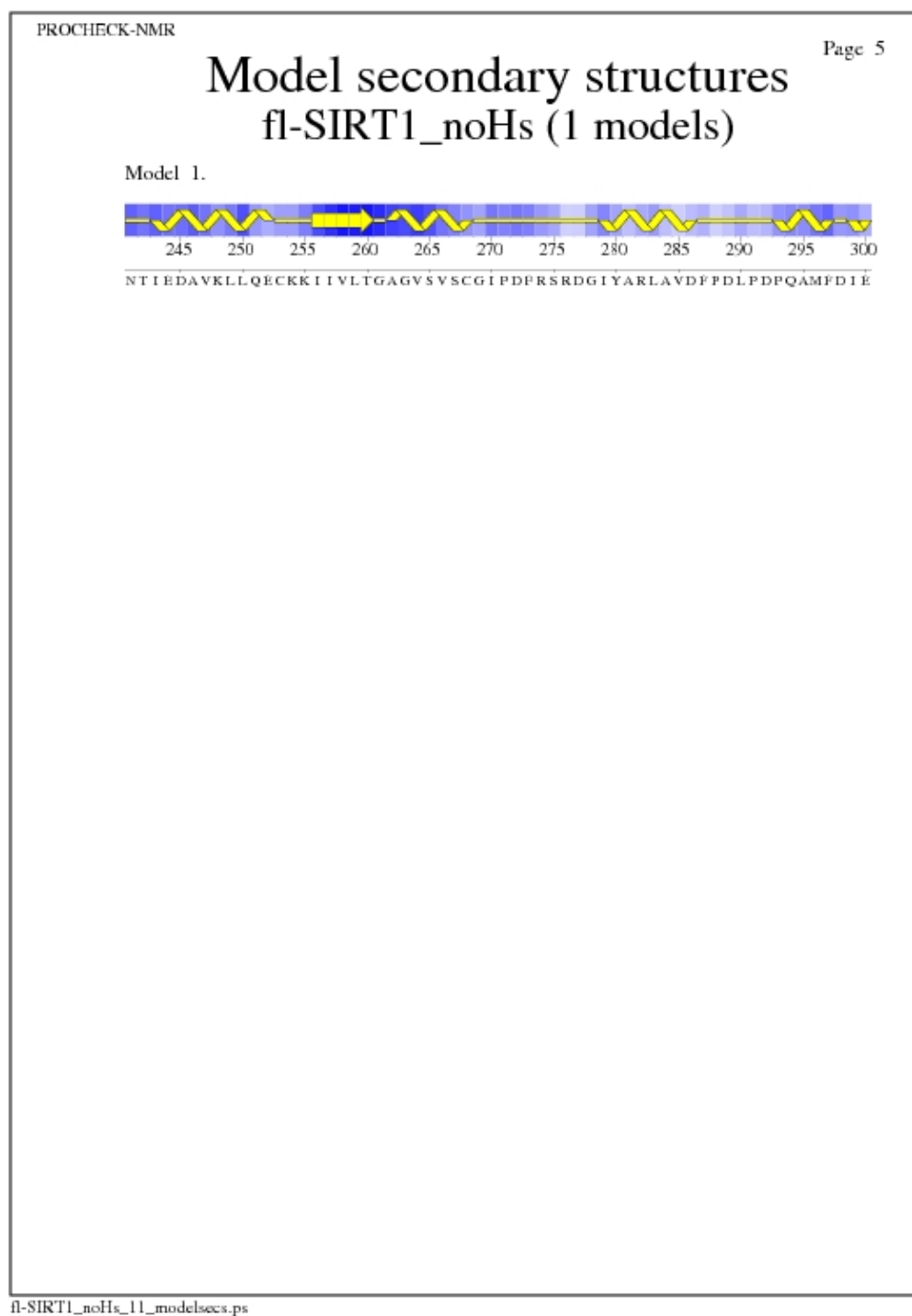
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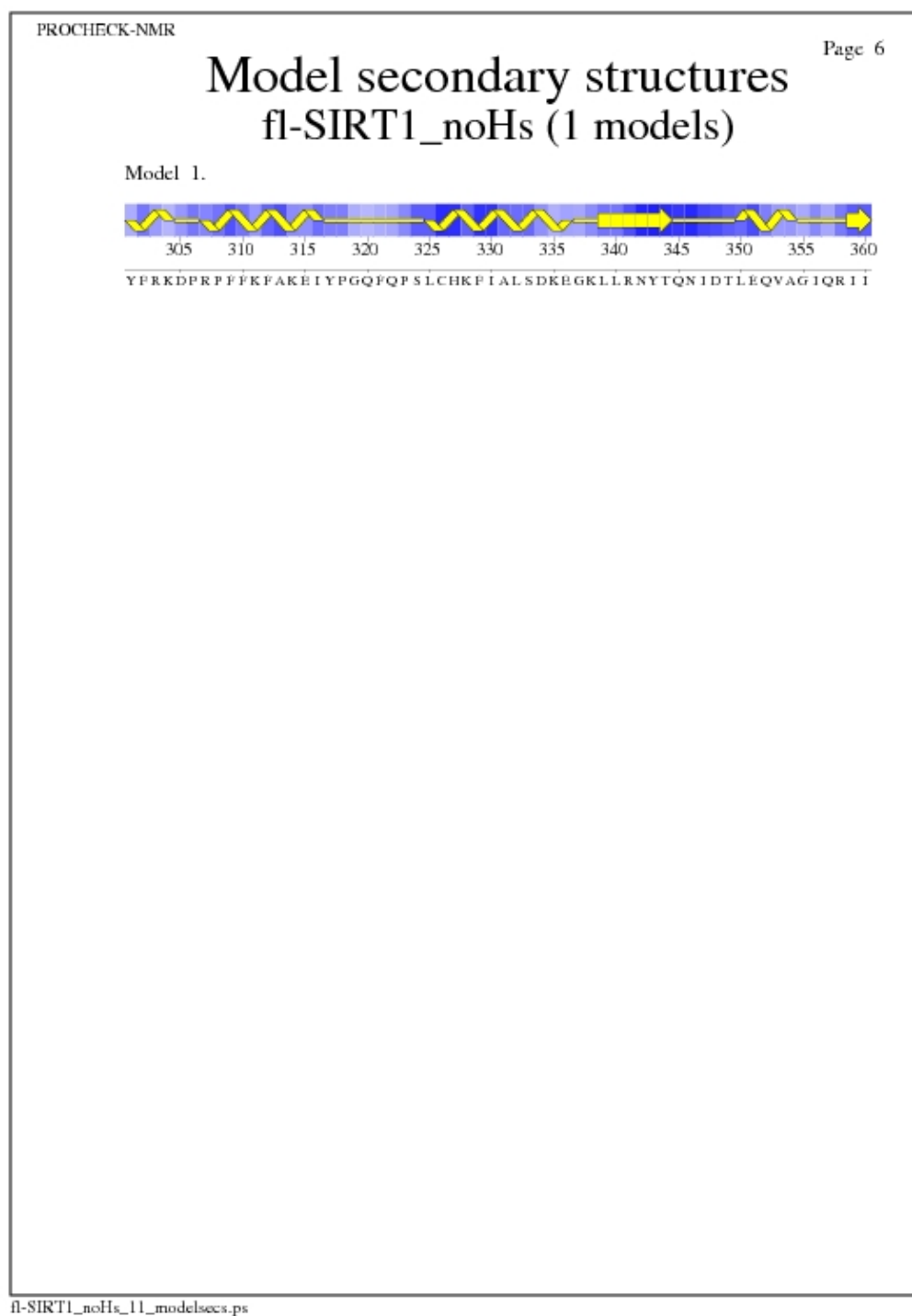
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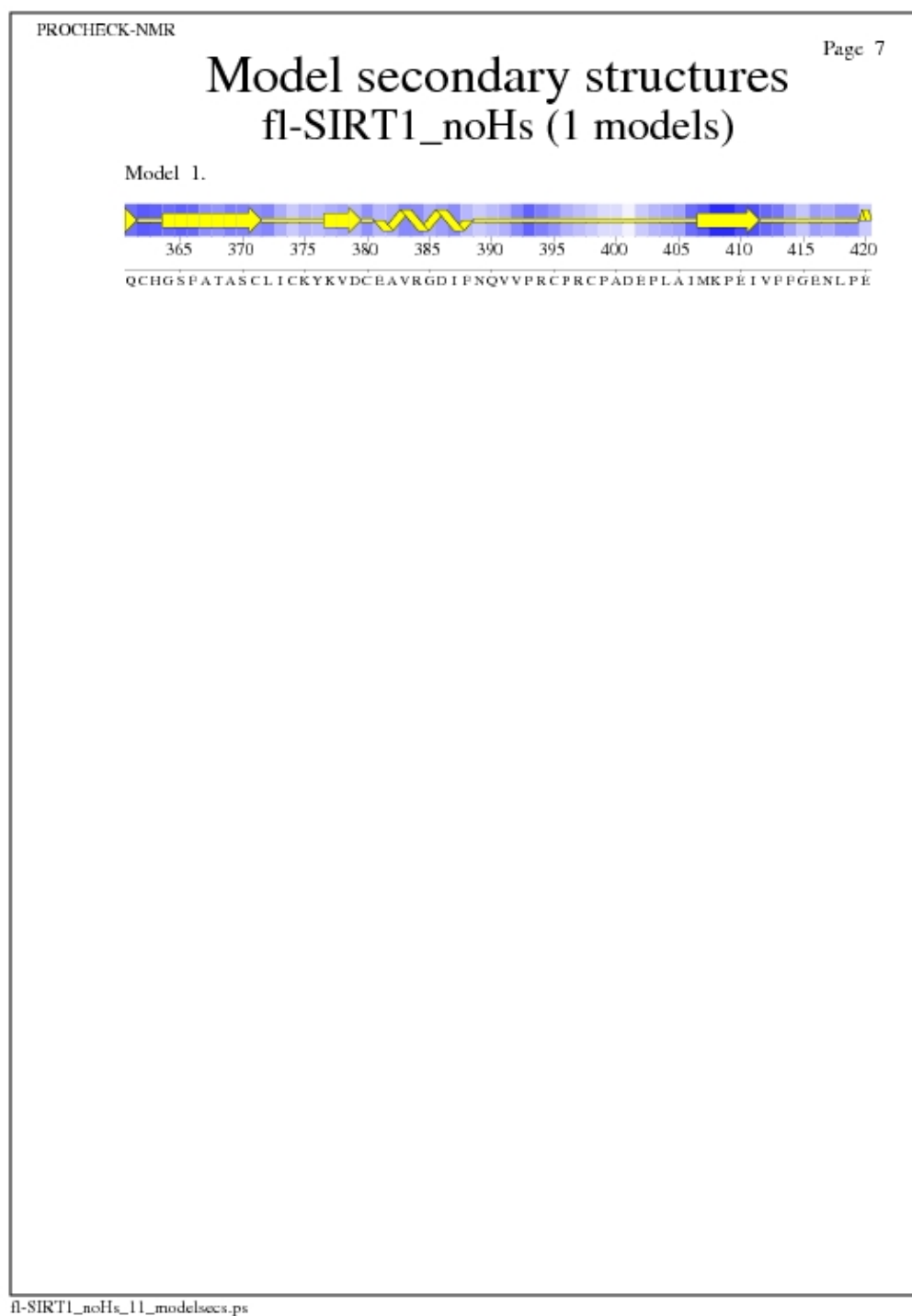
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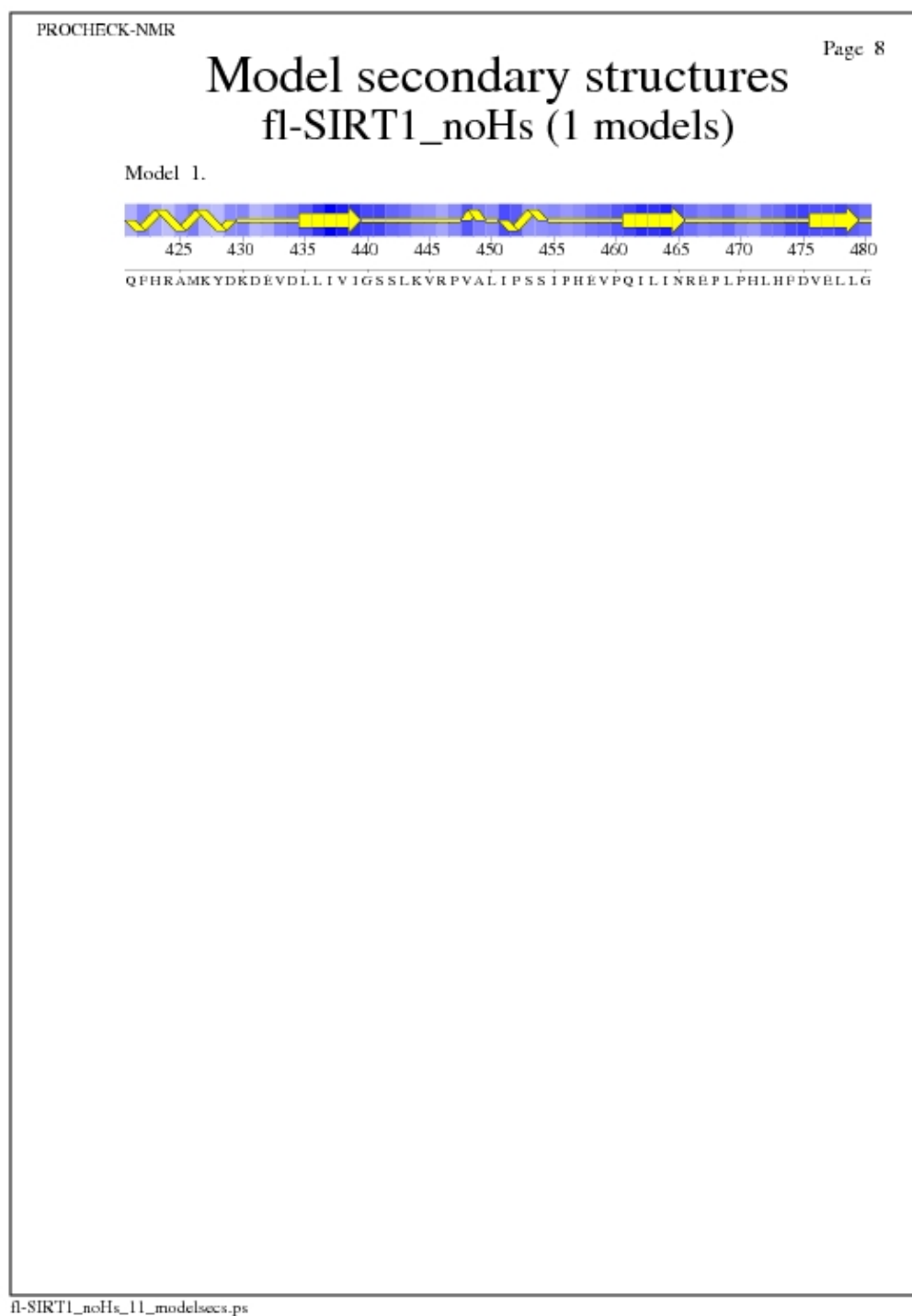
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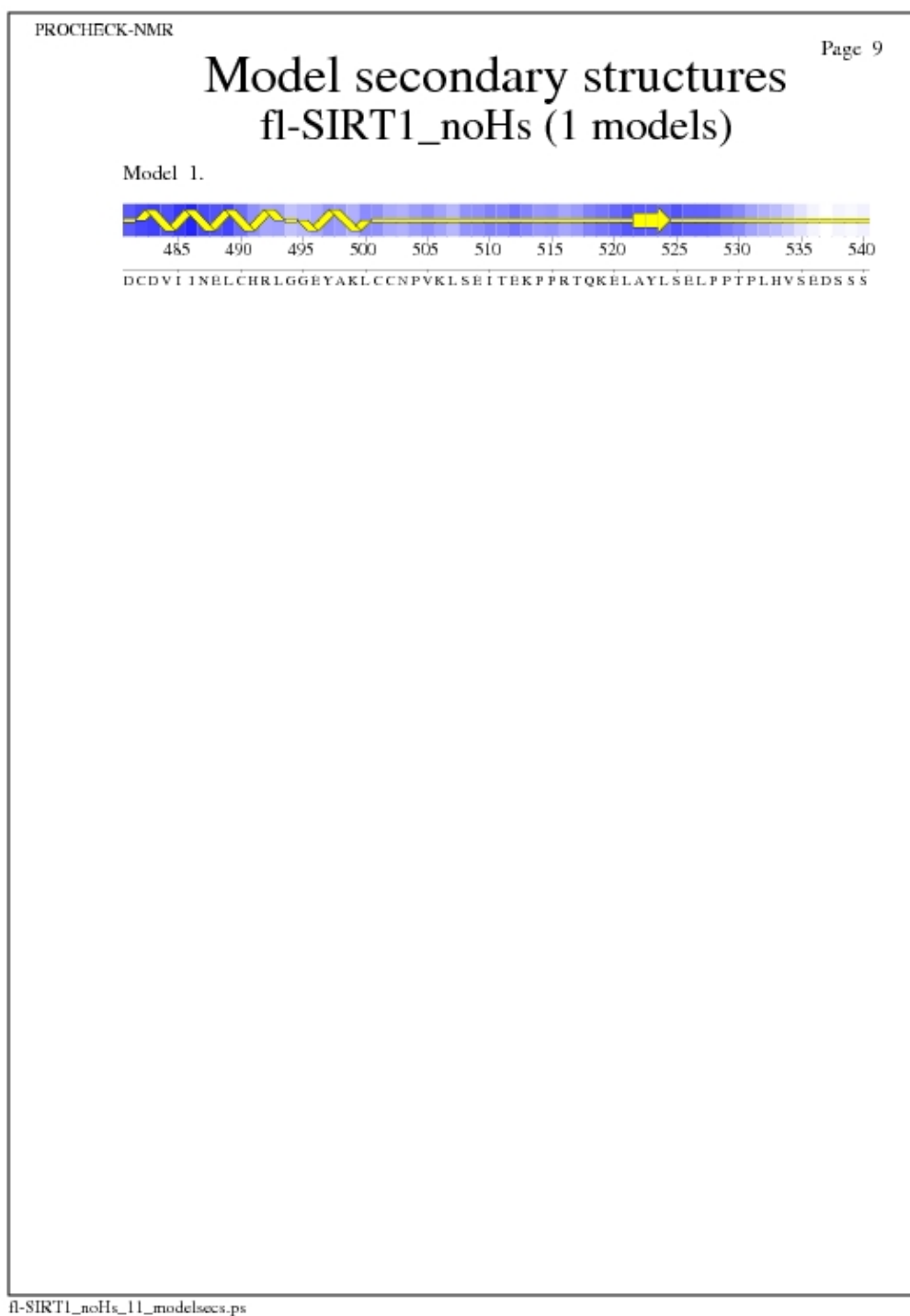
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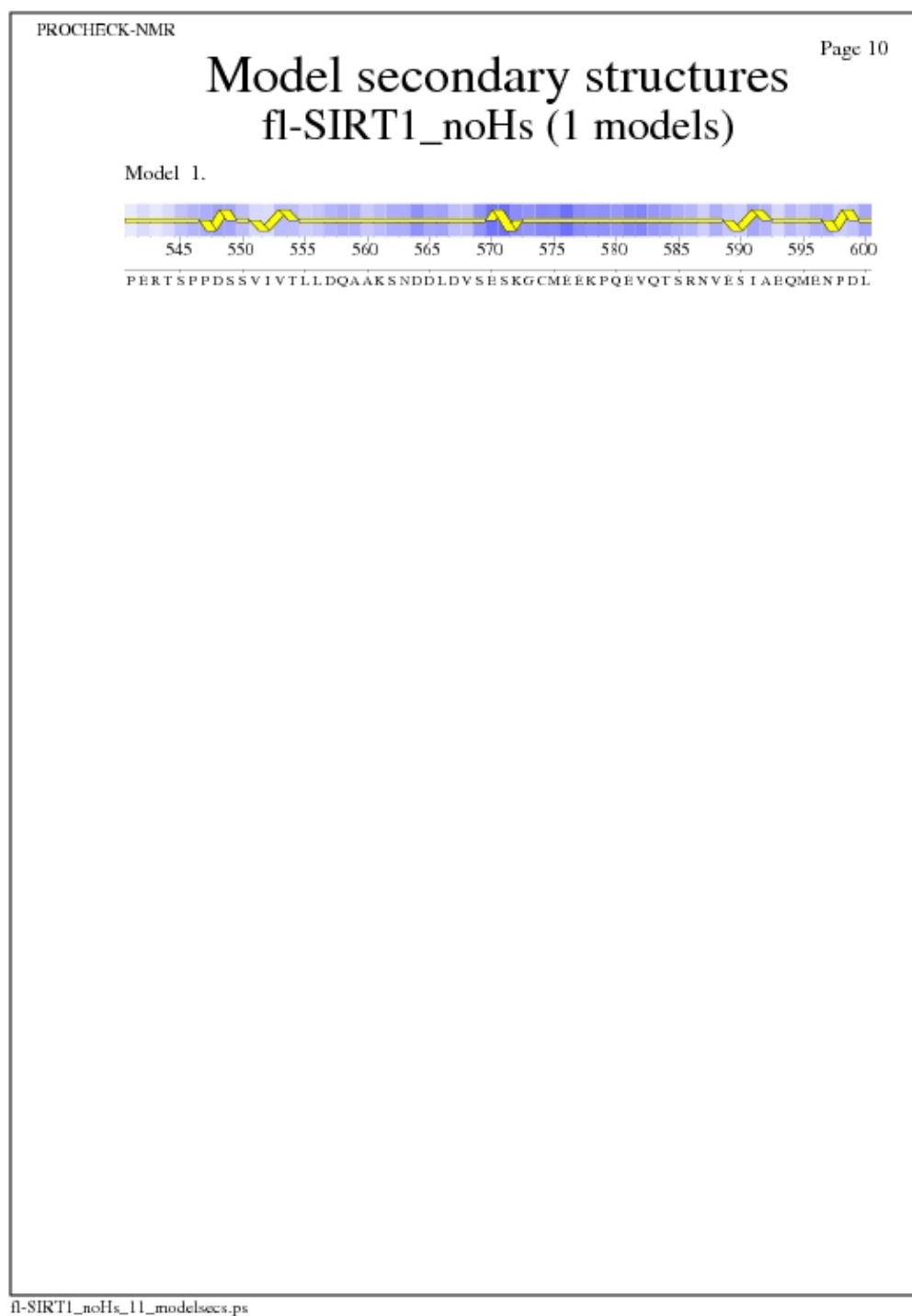
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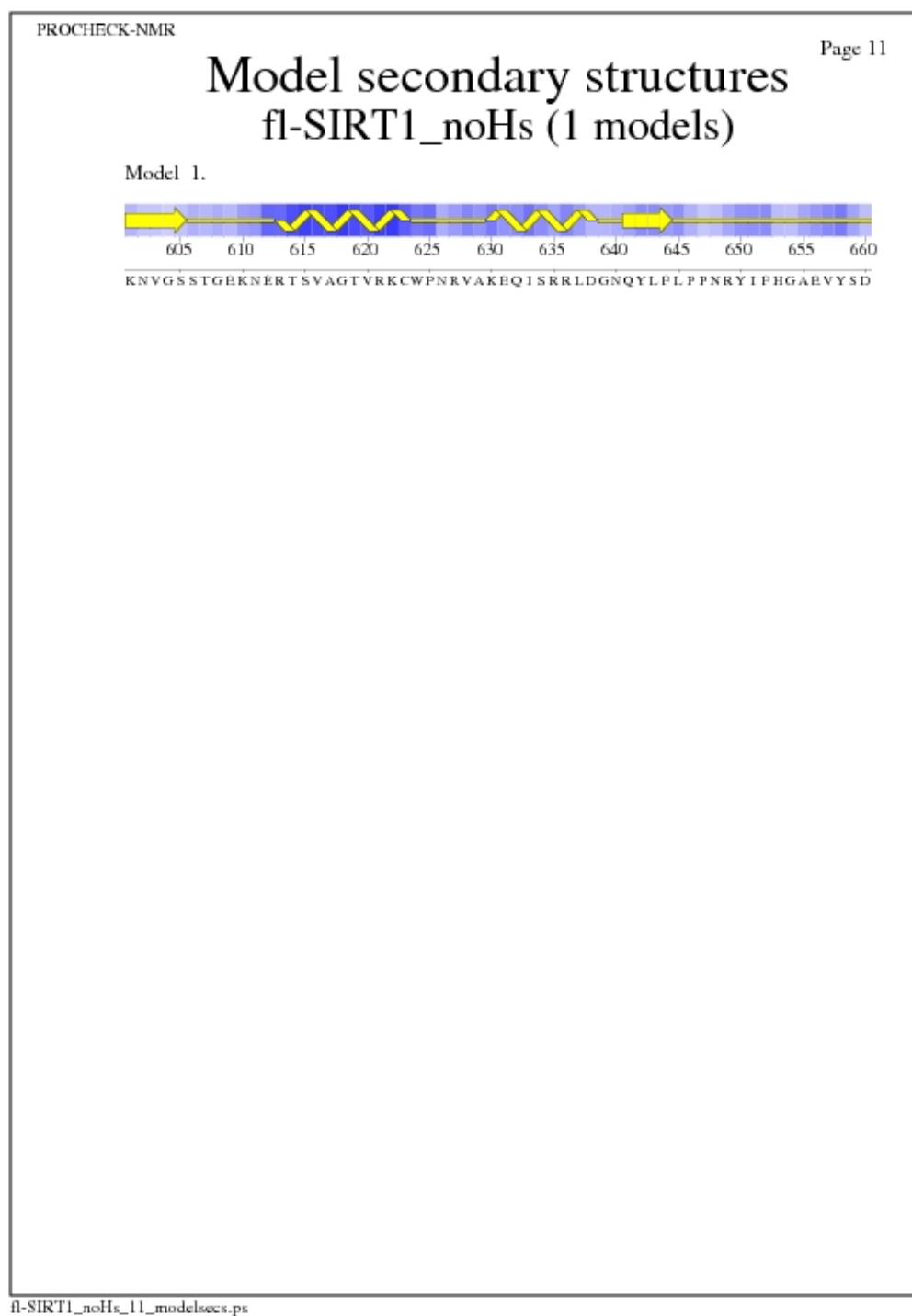
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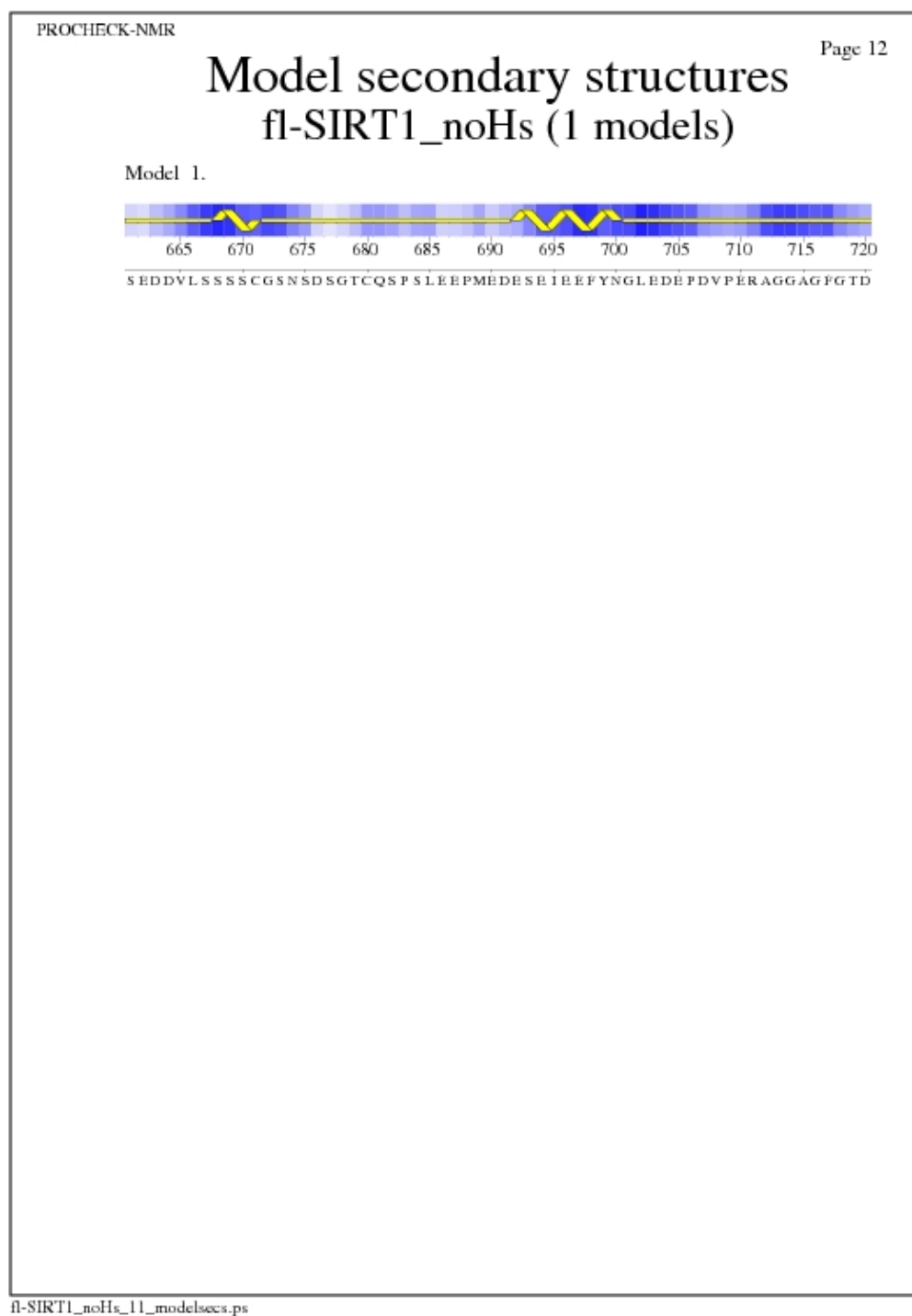
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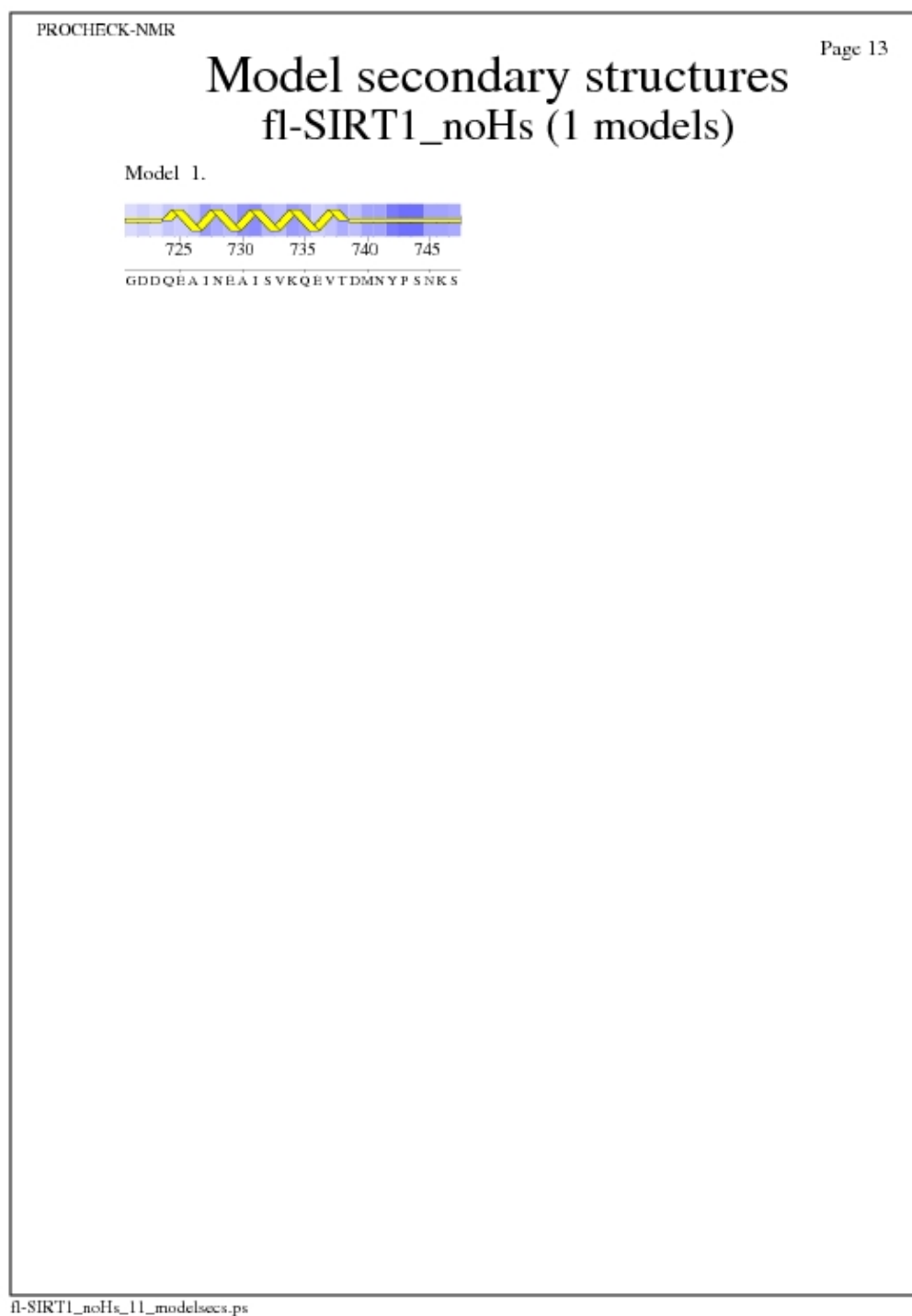
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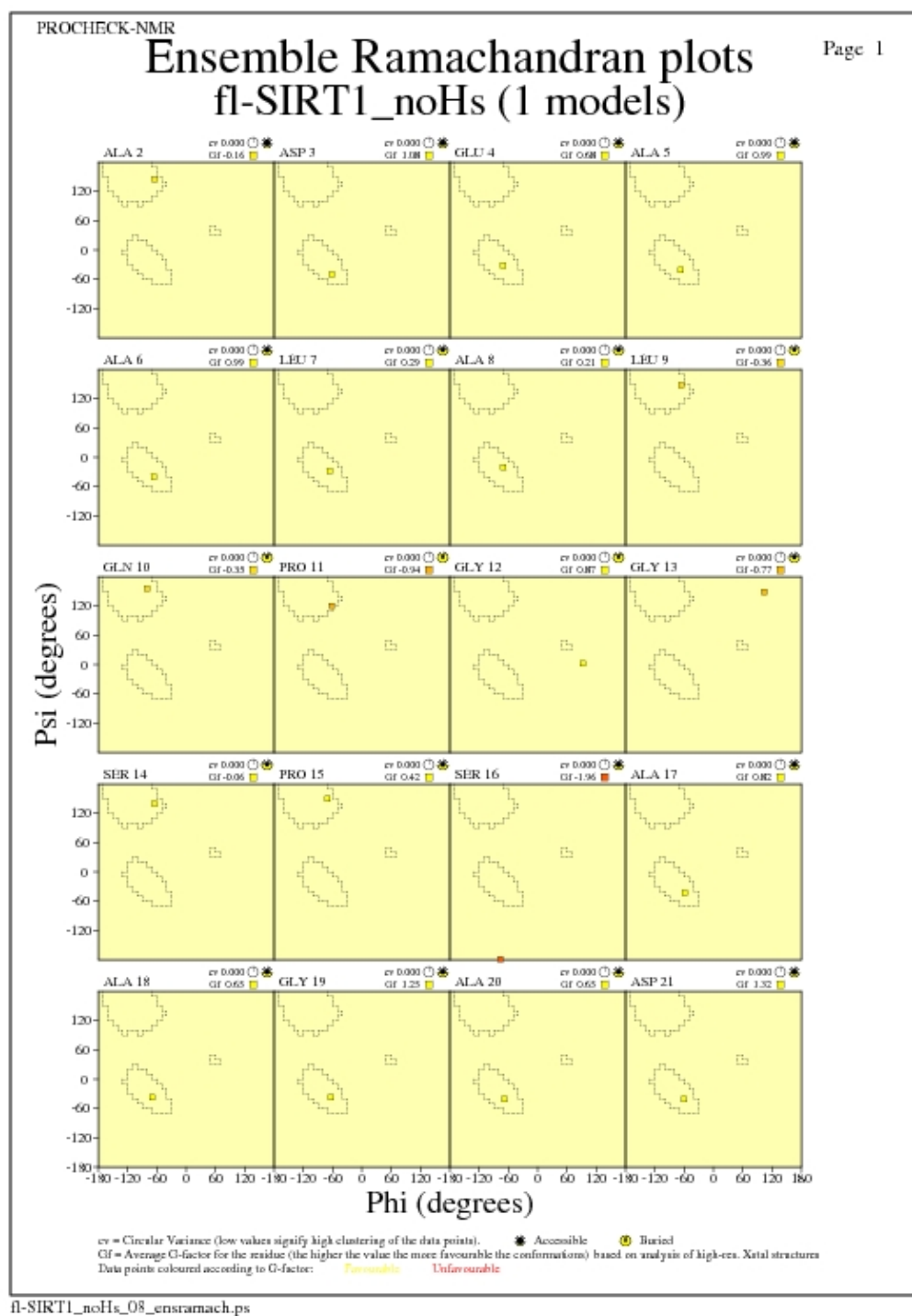


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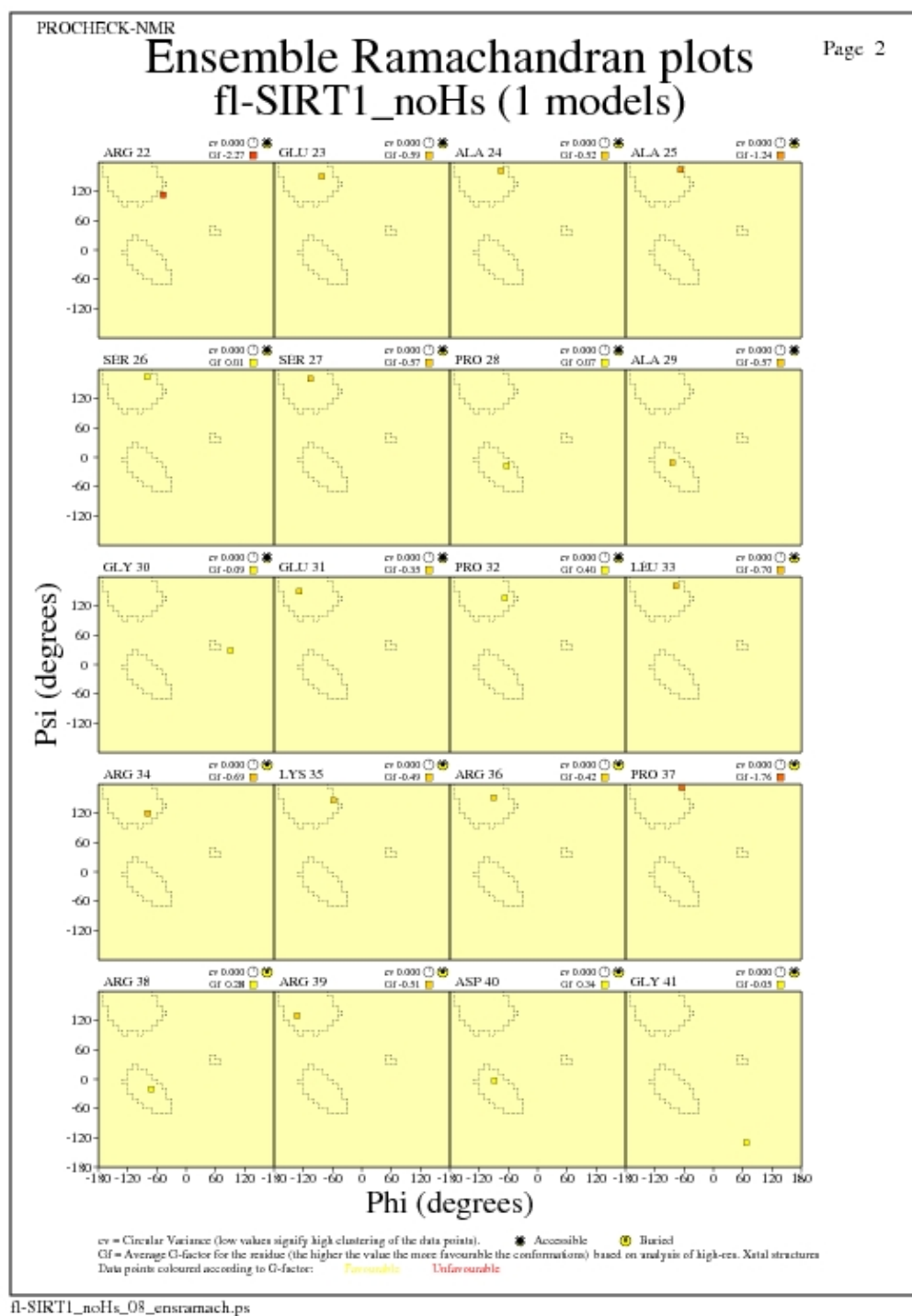


Ramachandran Plots for each residue

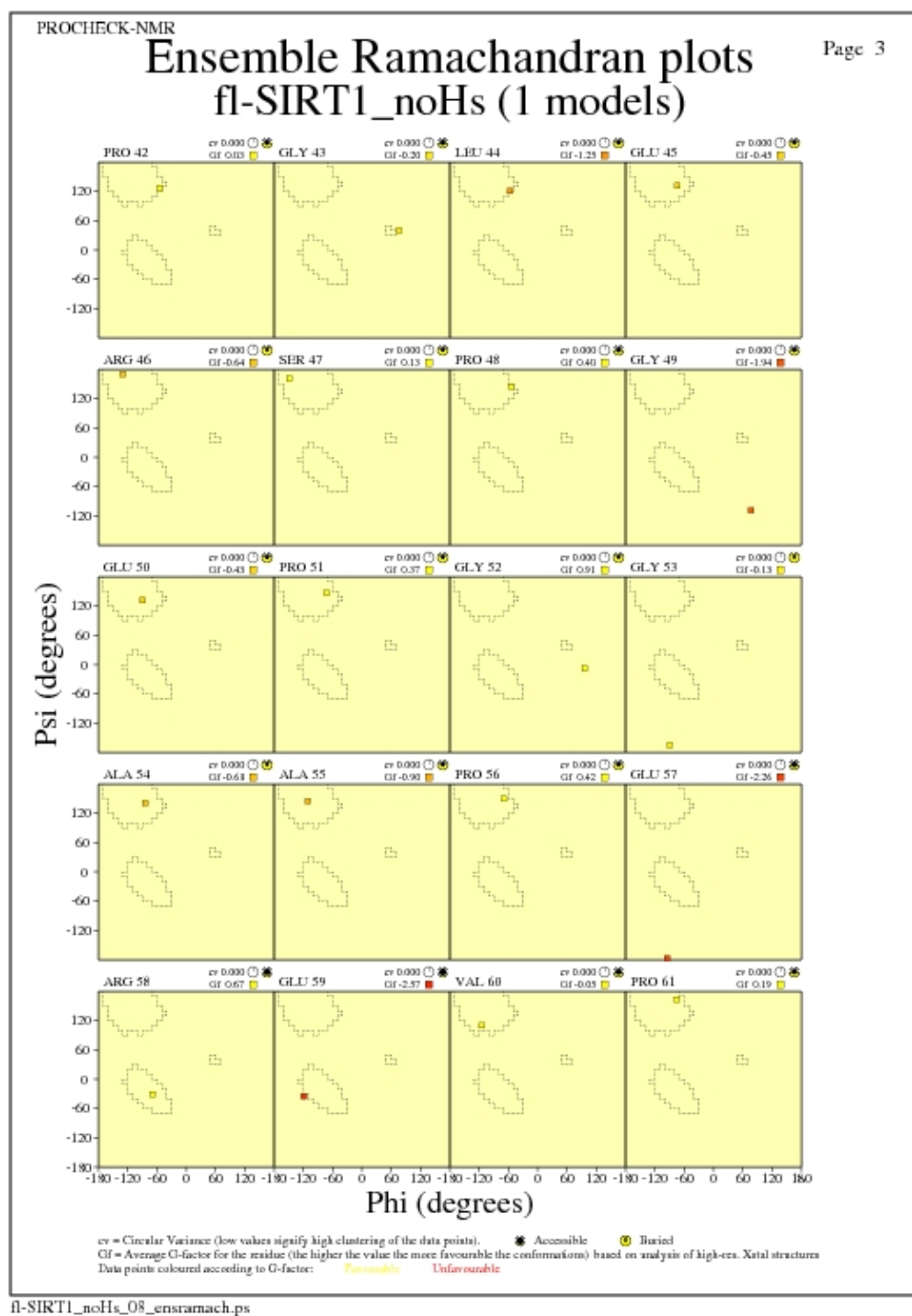
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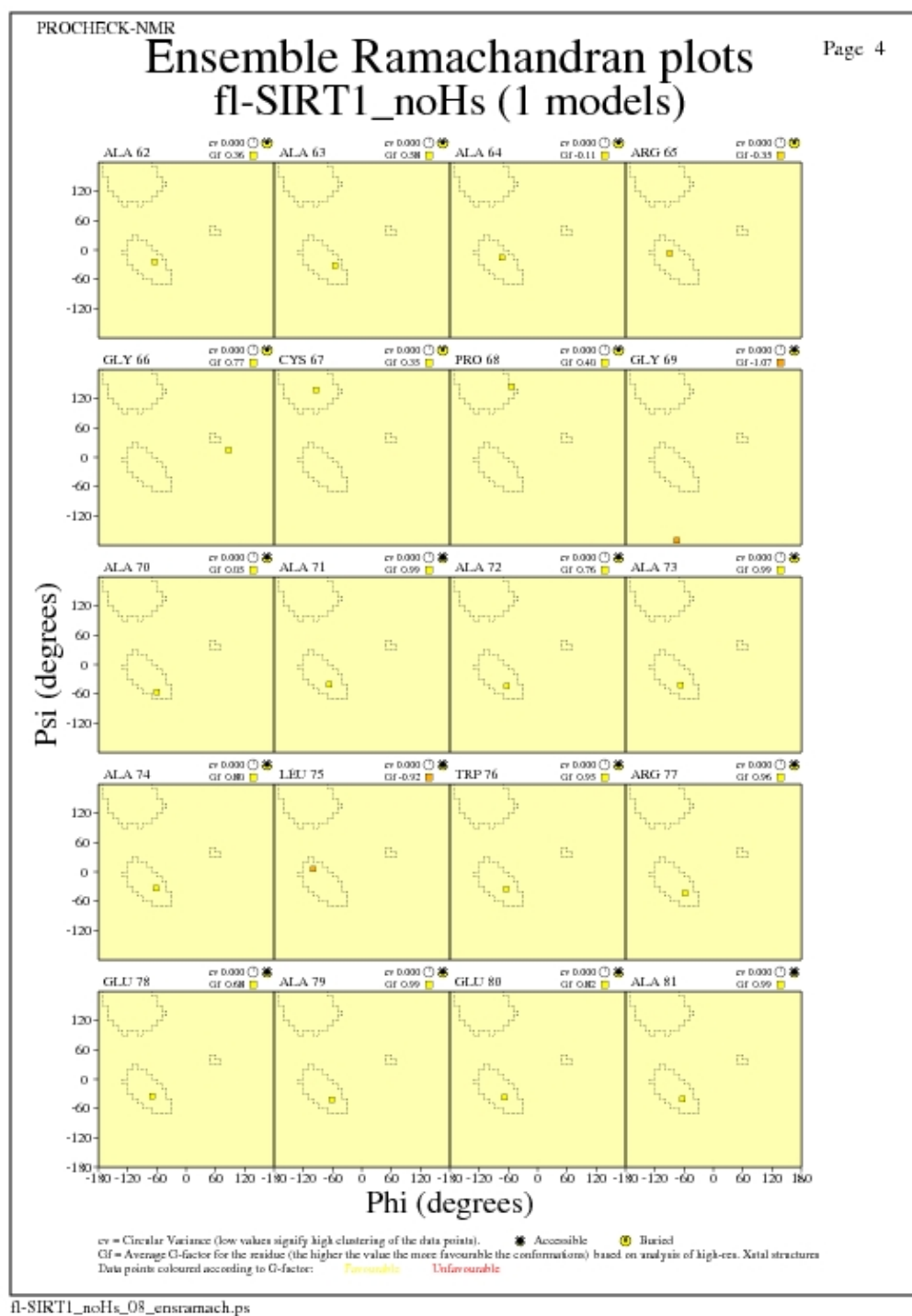
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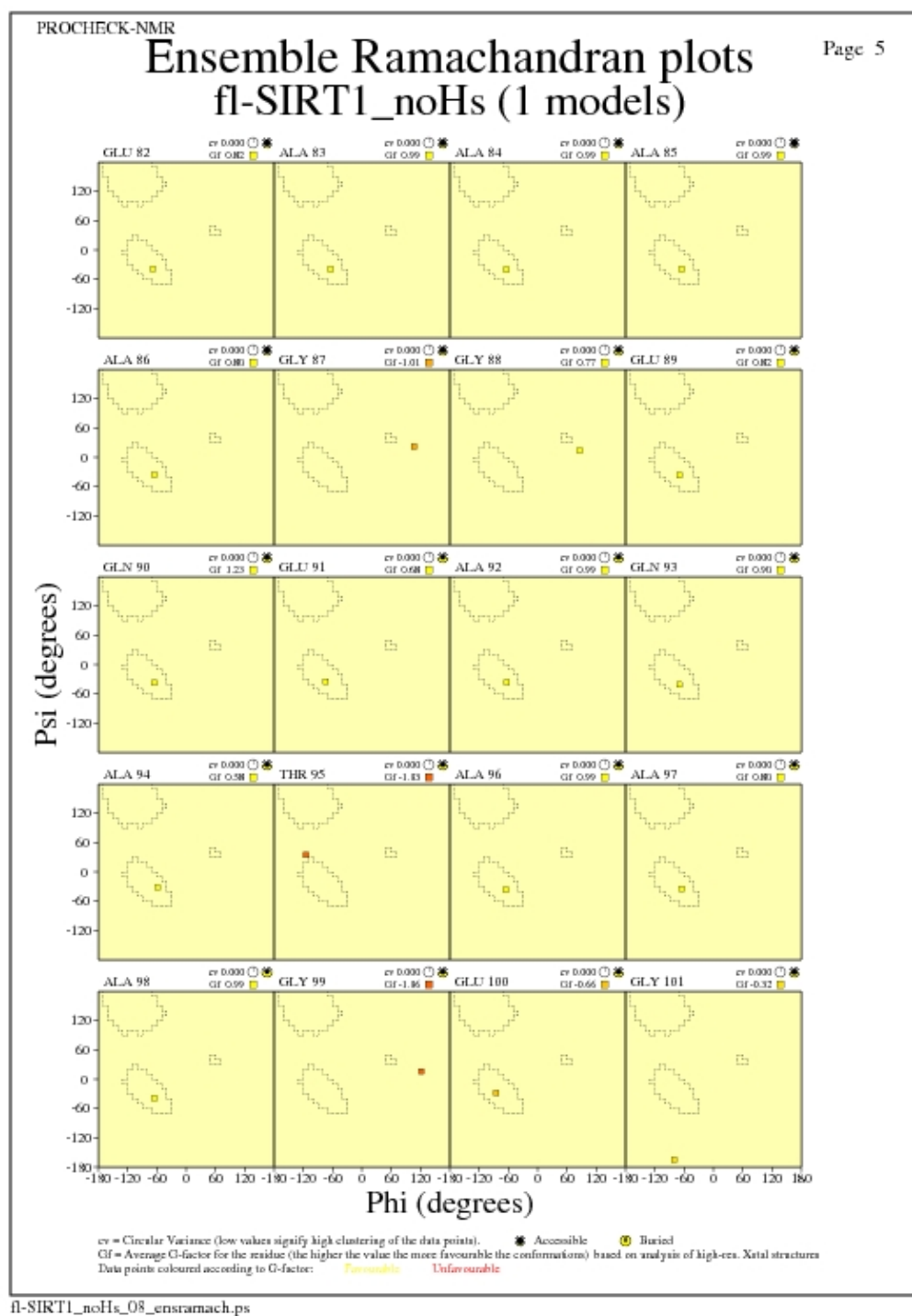
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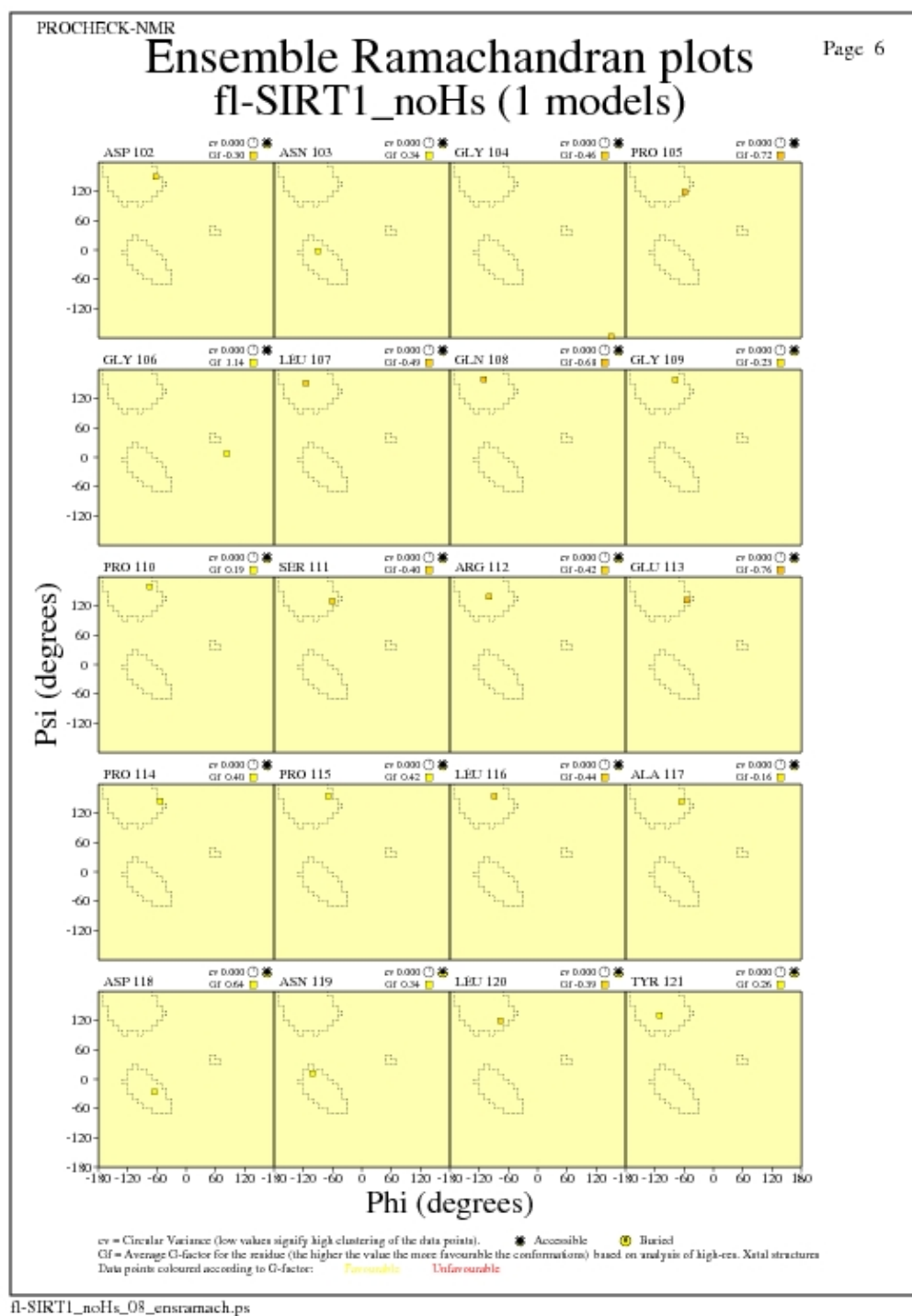
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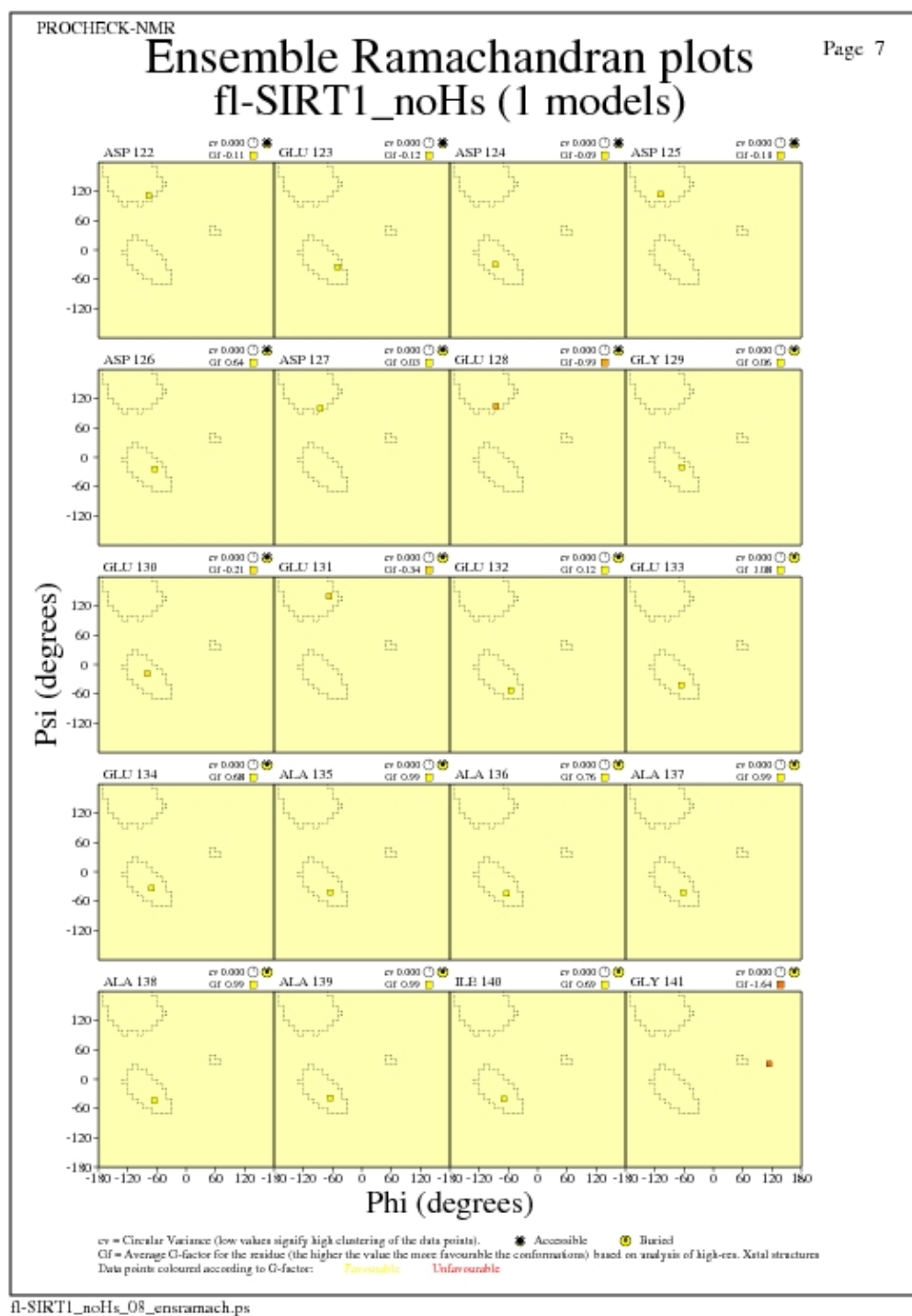
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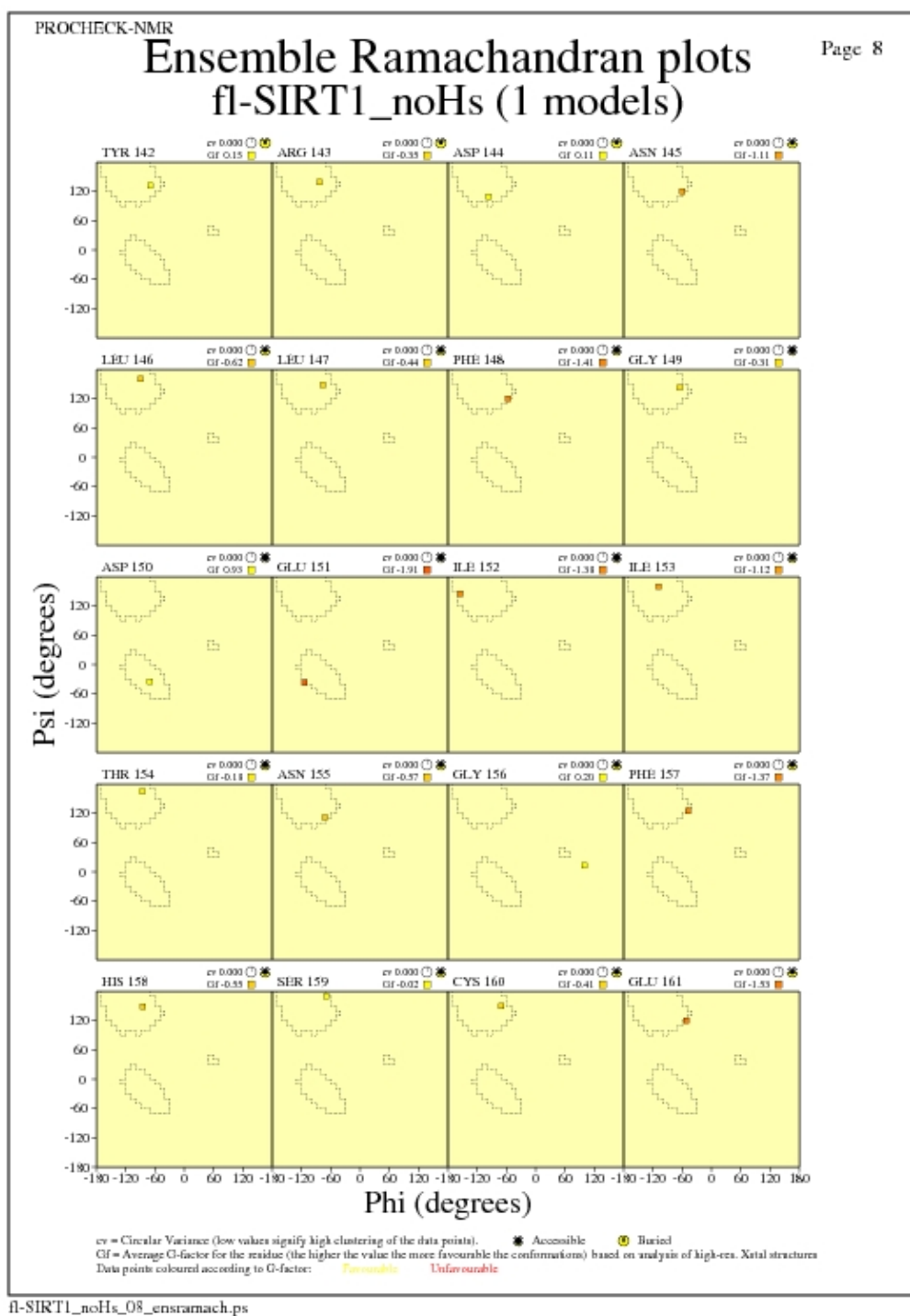
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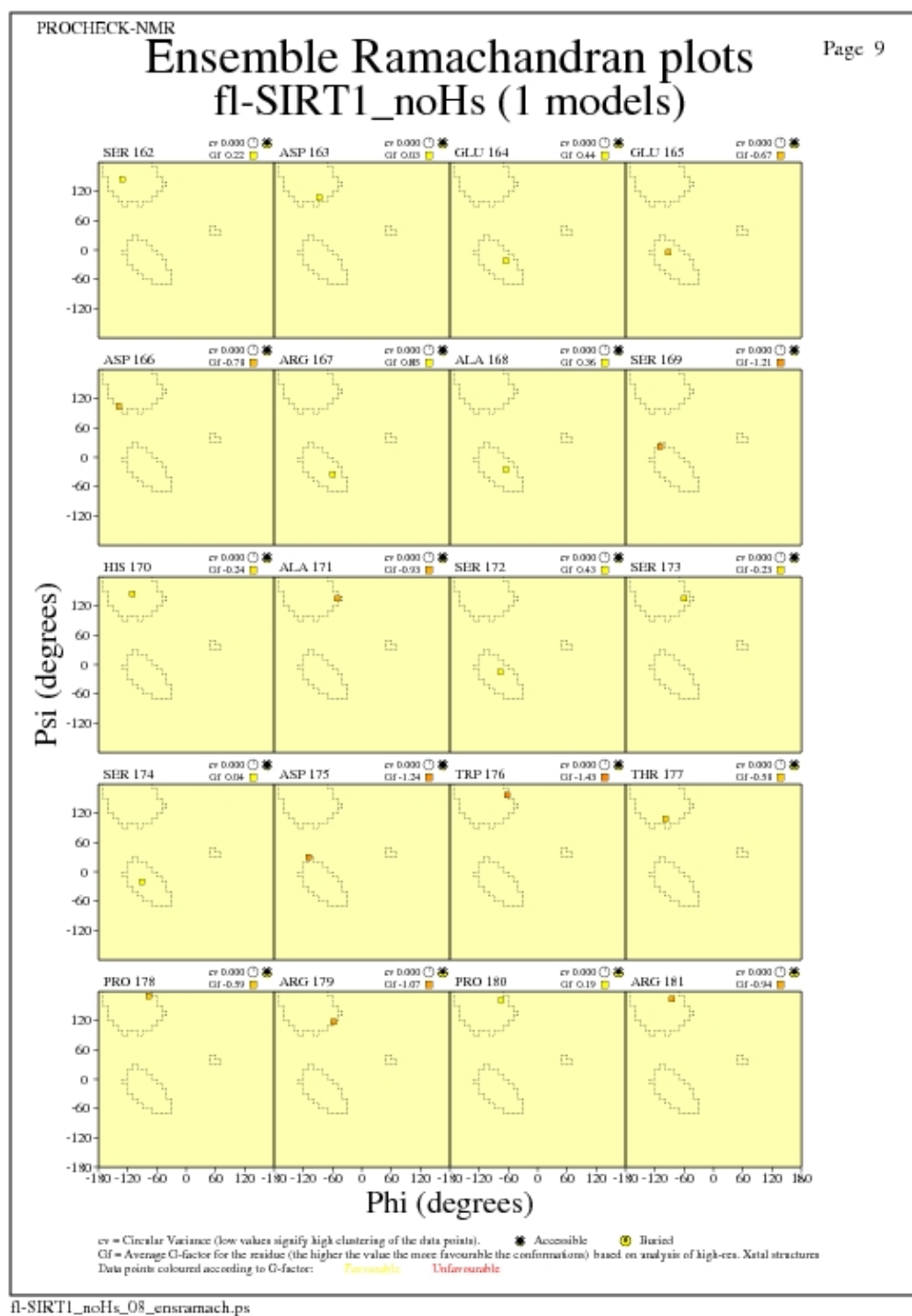
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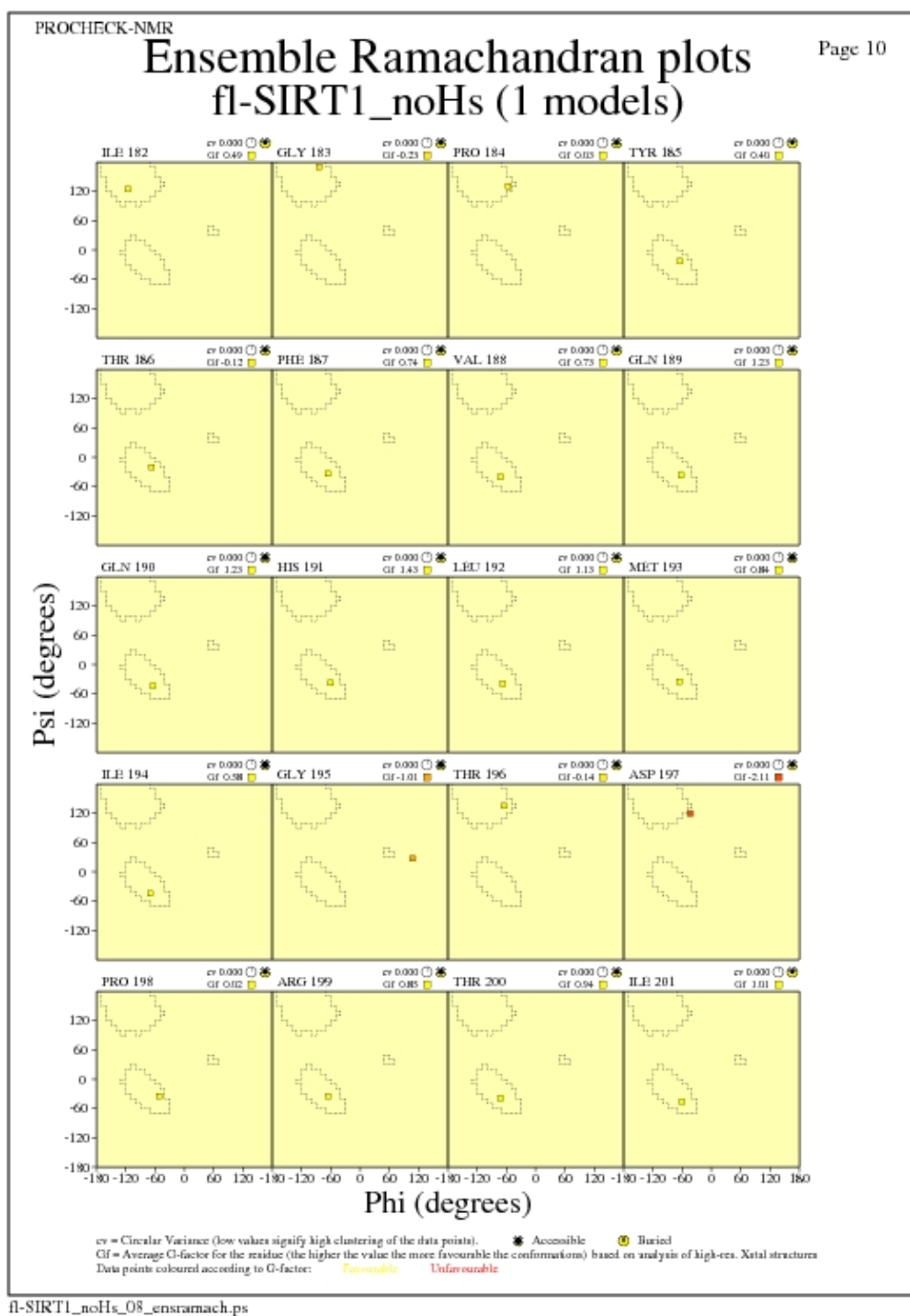
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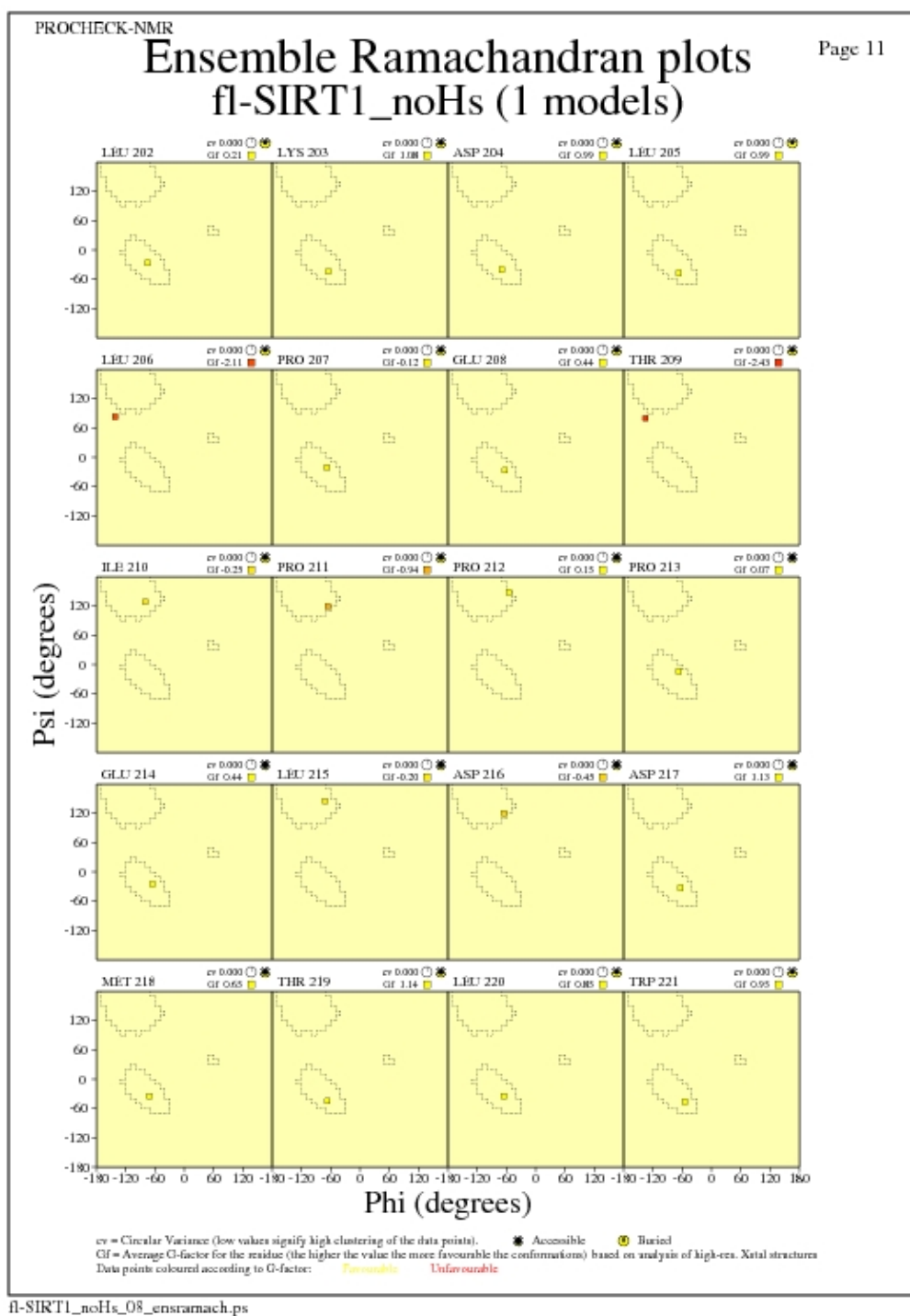
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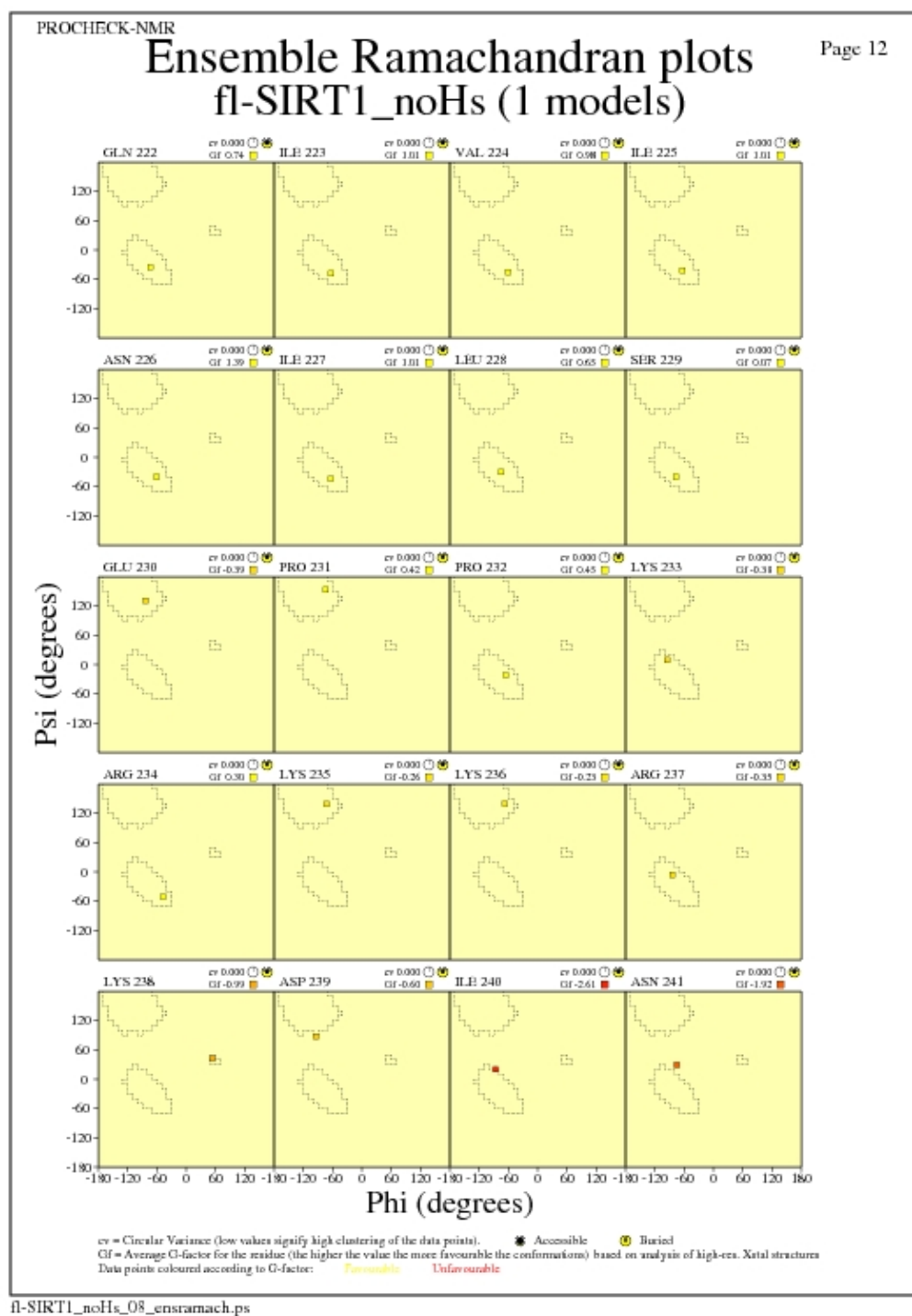
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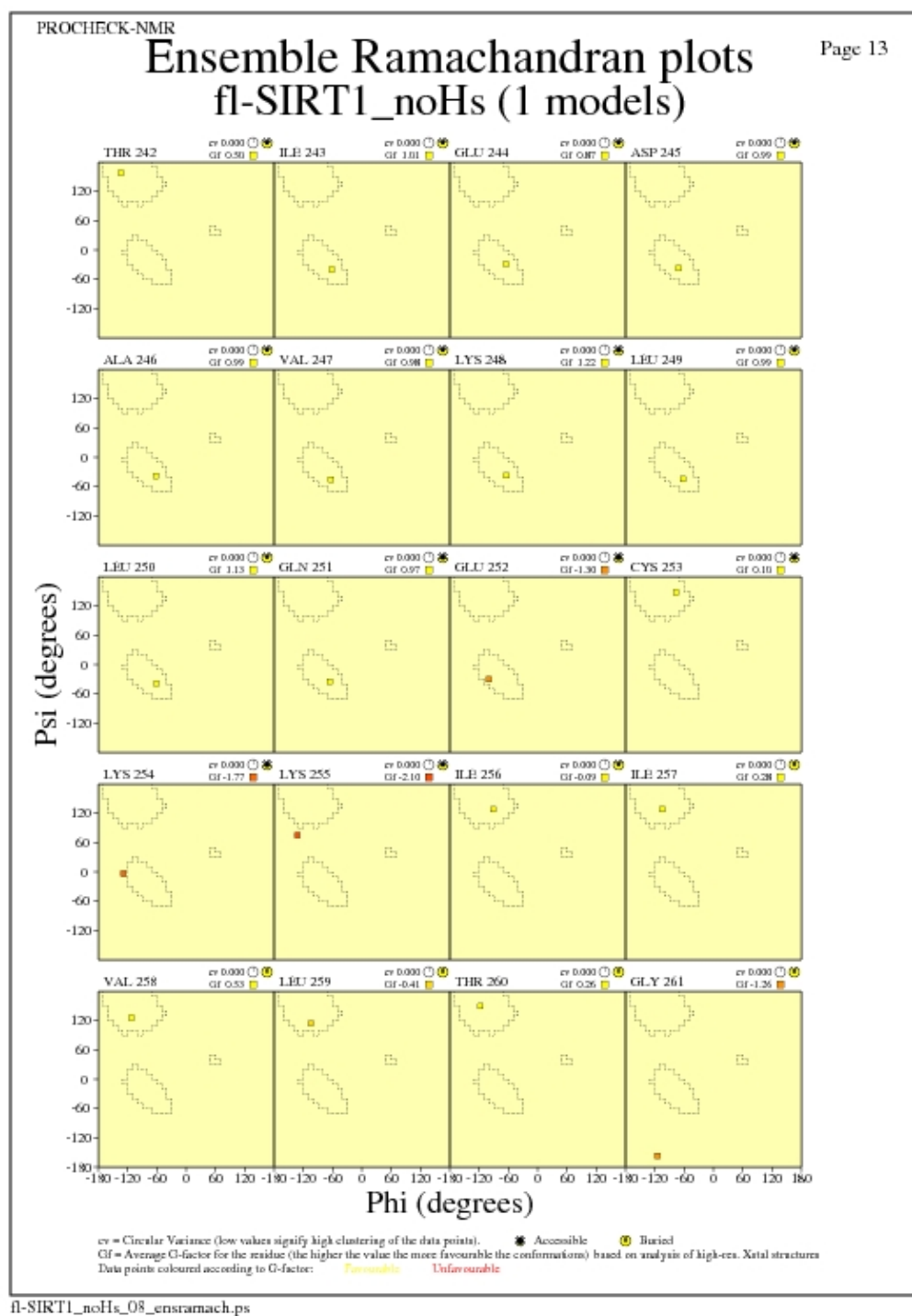
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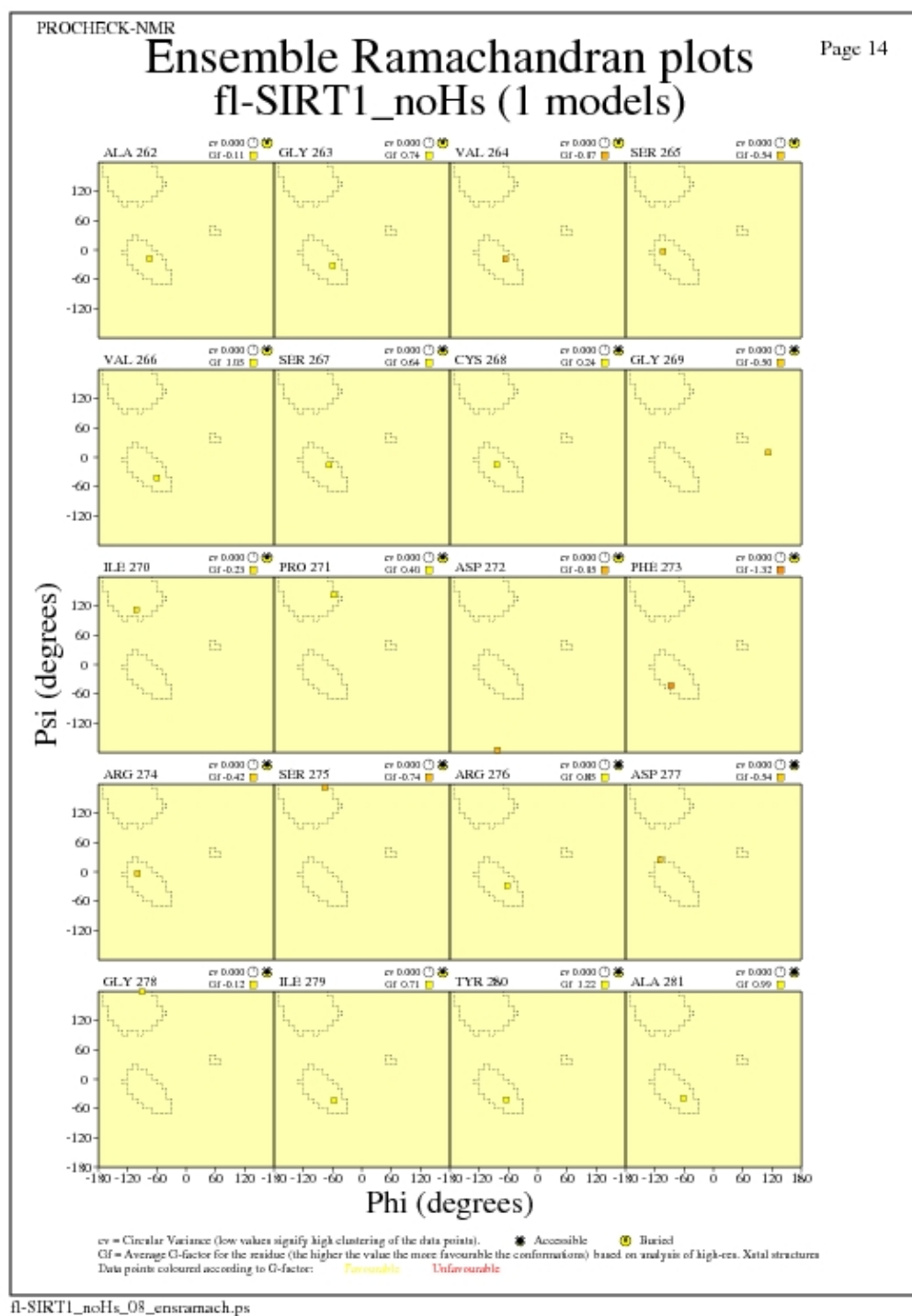
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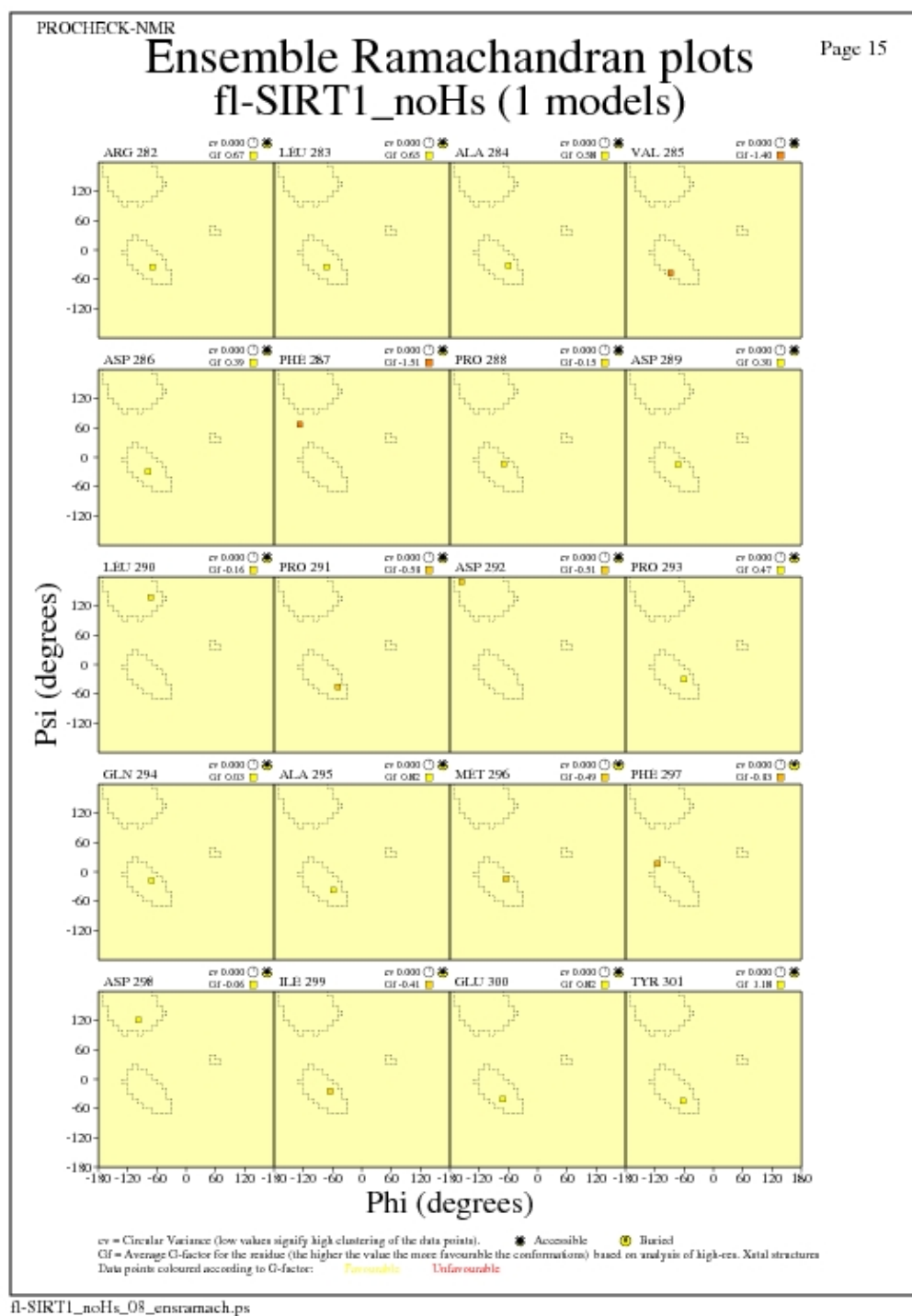
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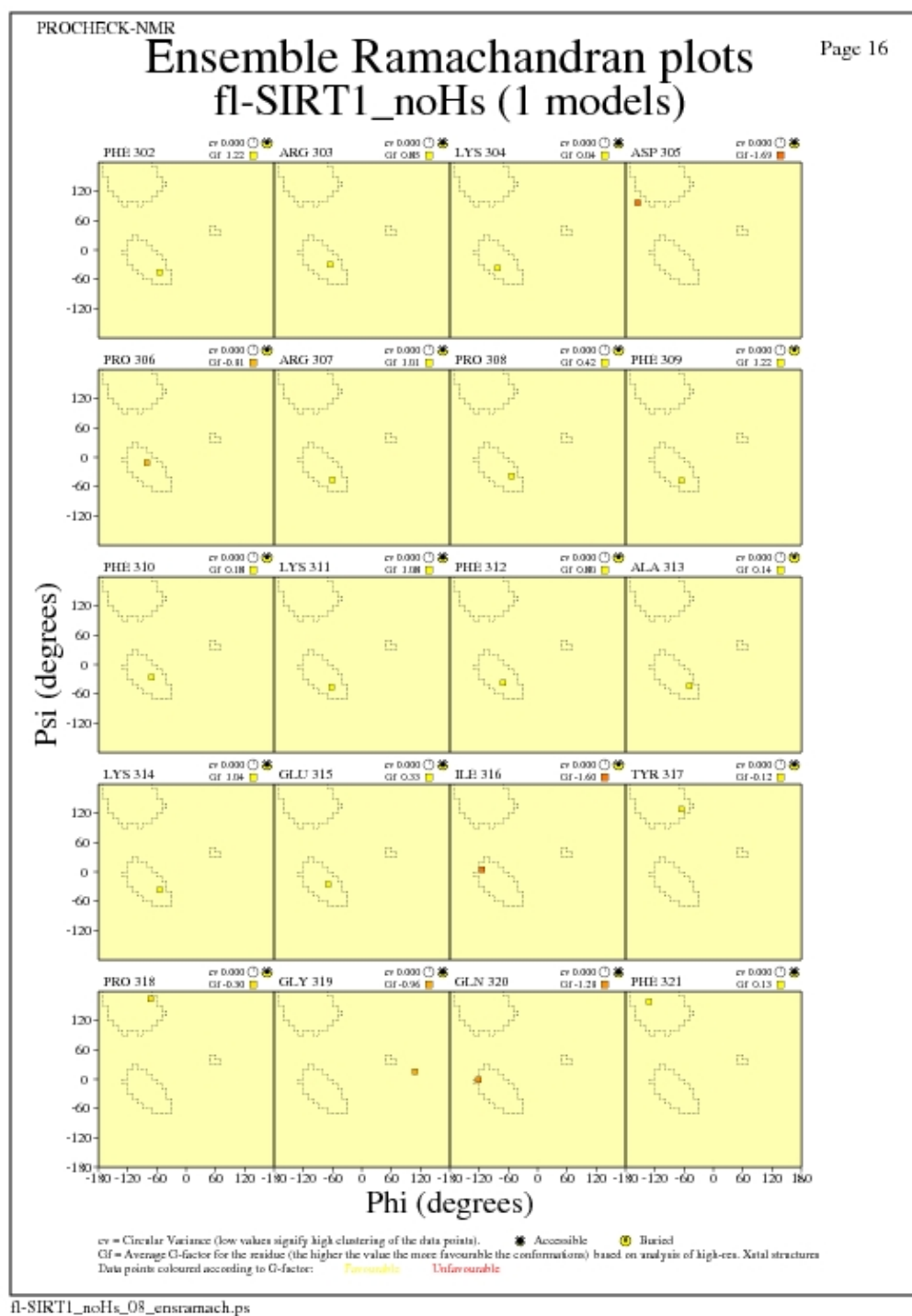
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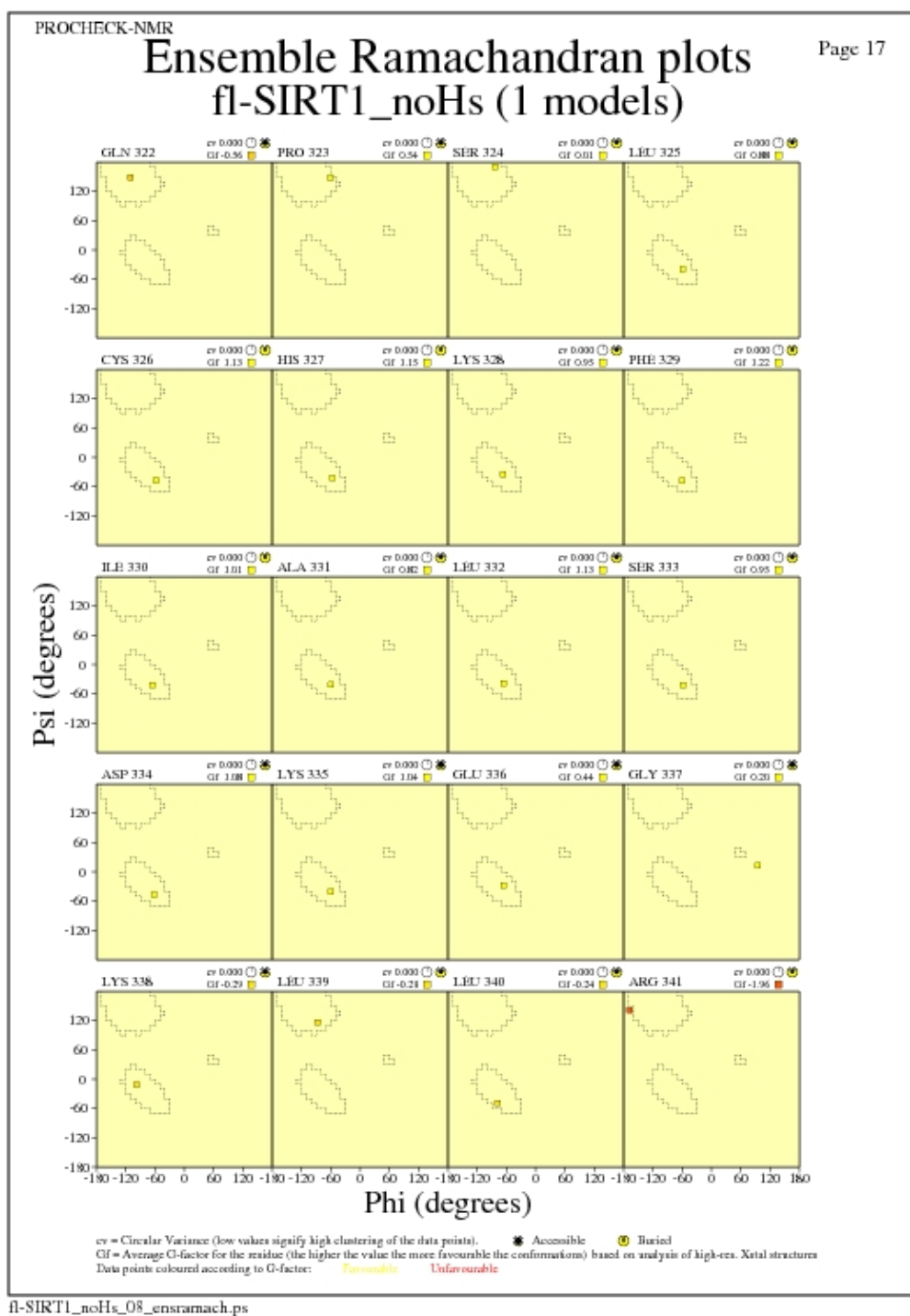
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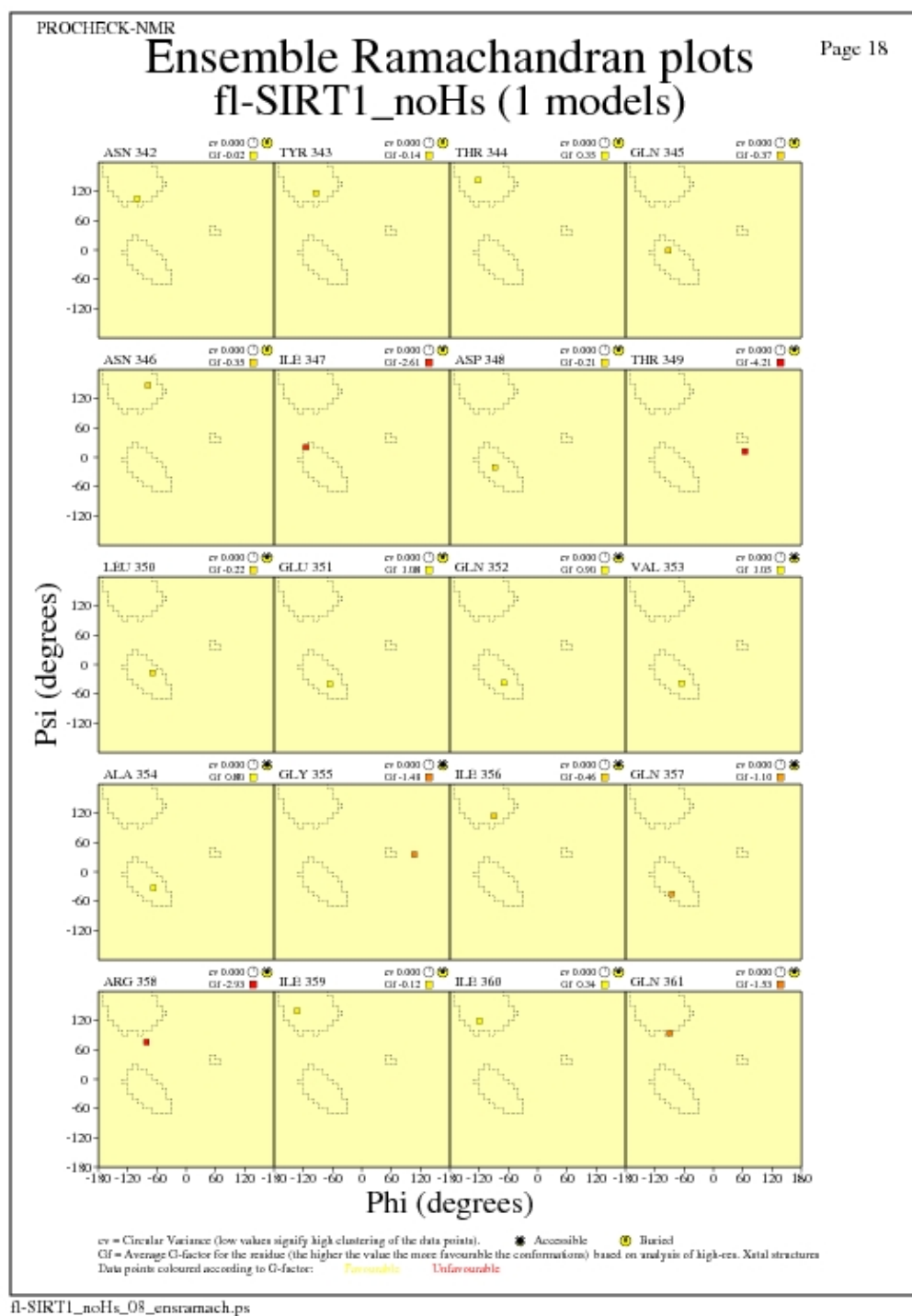
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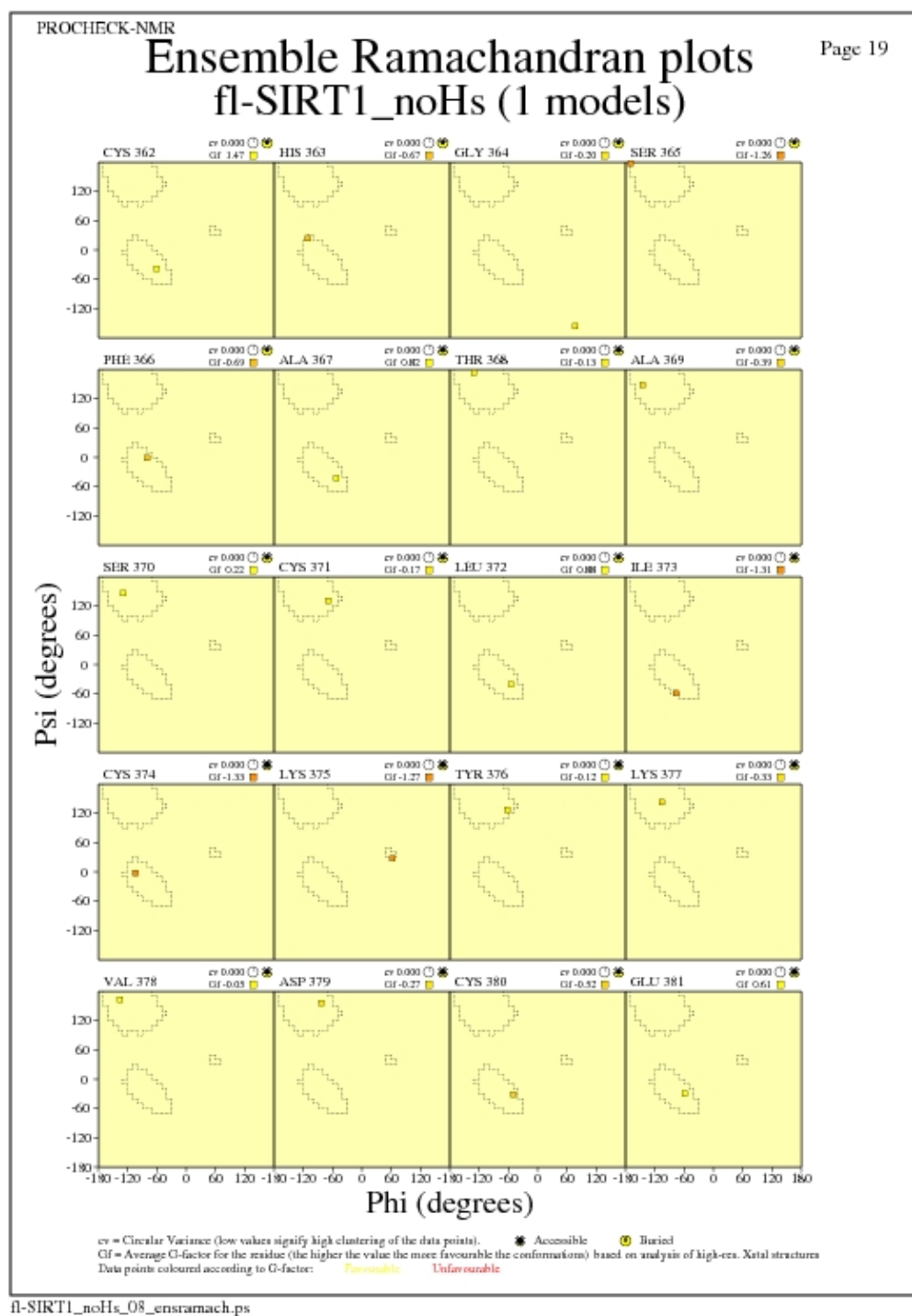
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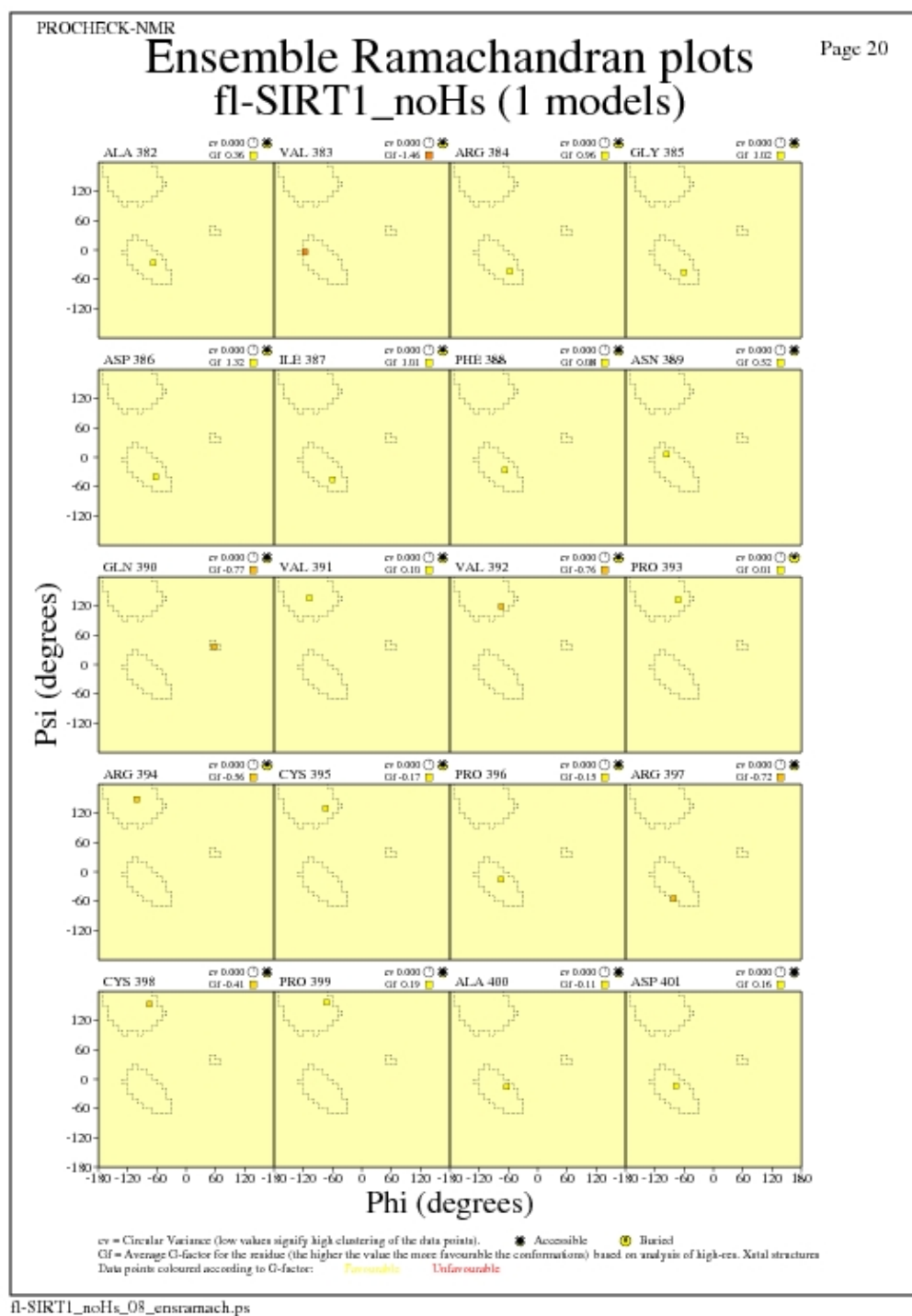
JPEG for residue Ramachandran Plots - page \$num_n



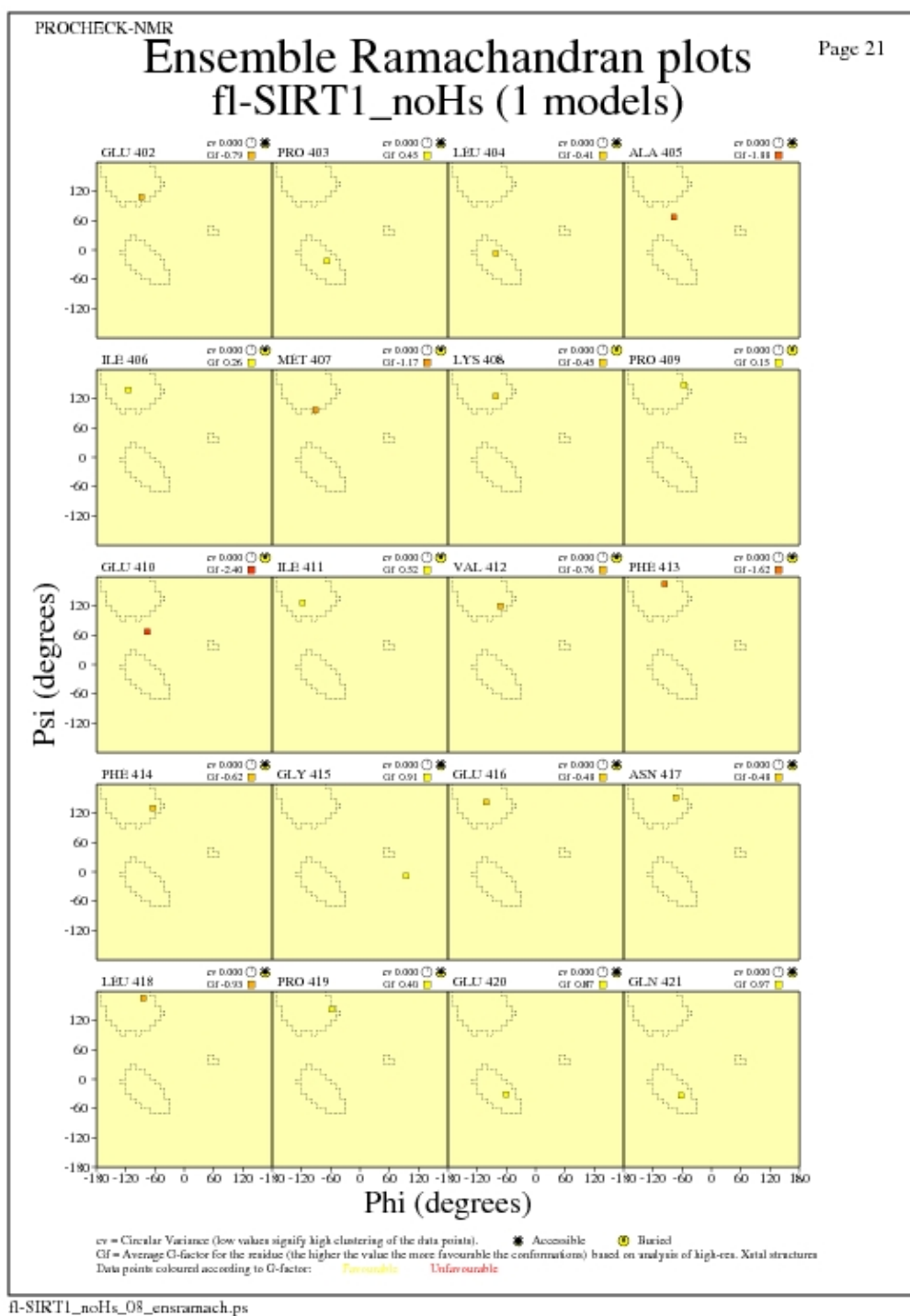
JPEG for residue Ramachandran Plots - page \$num_n



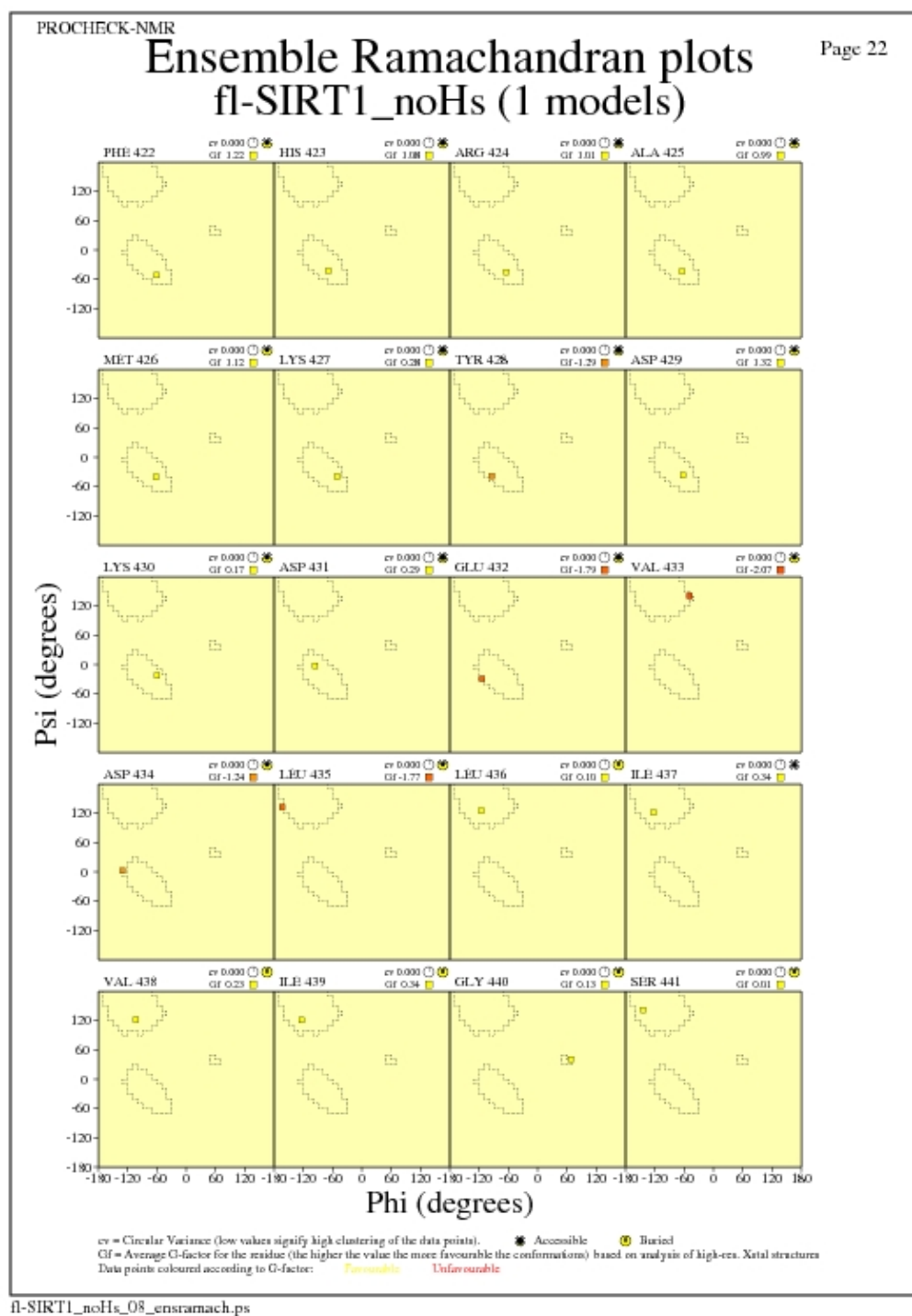
JPEG for residue Ramachandran Plots - page \$num_n



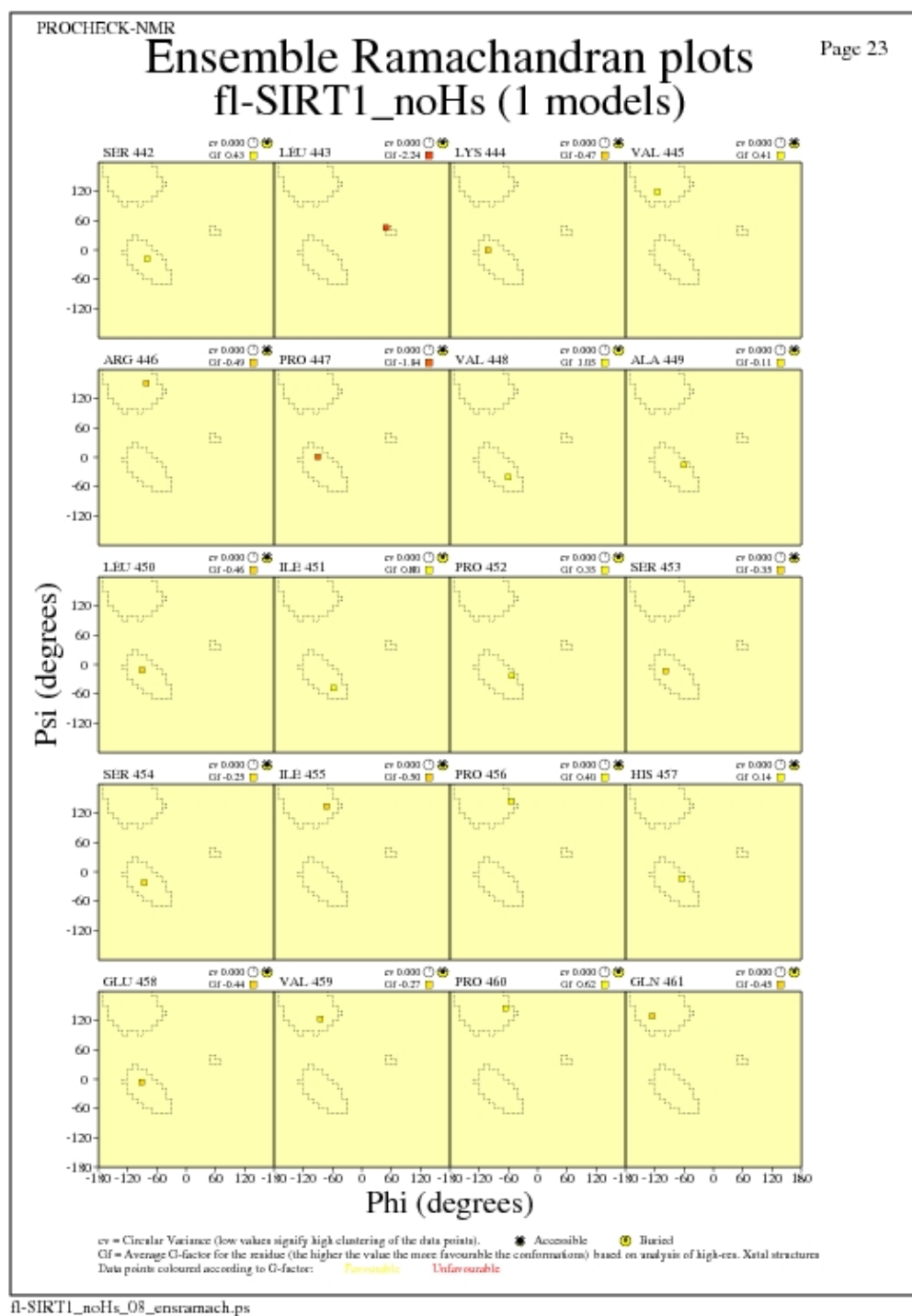
JPEG for residue Ramachandran Plots - page \$num_n



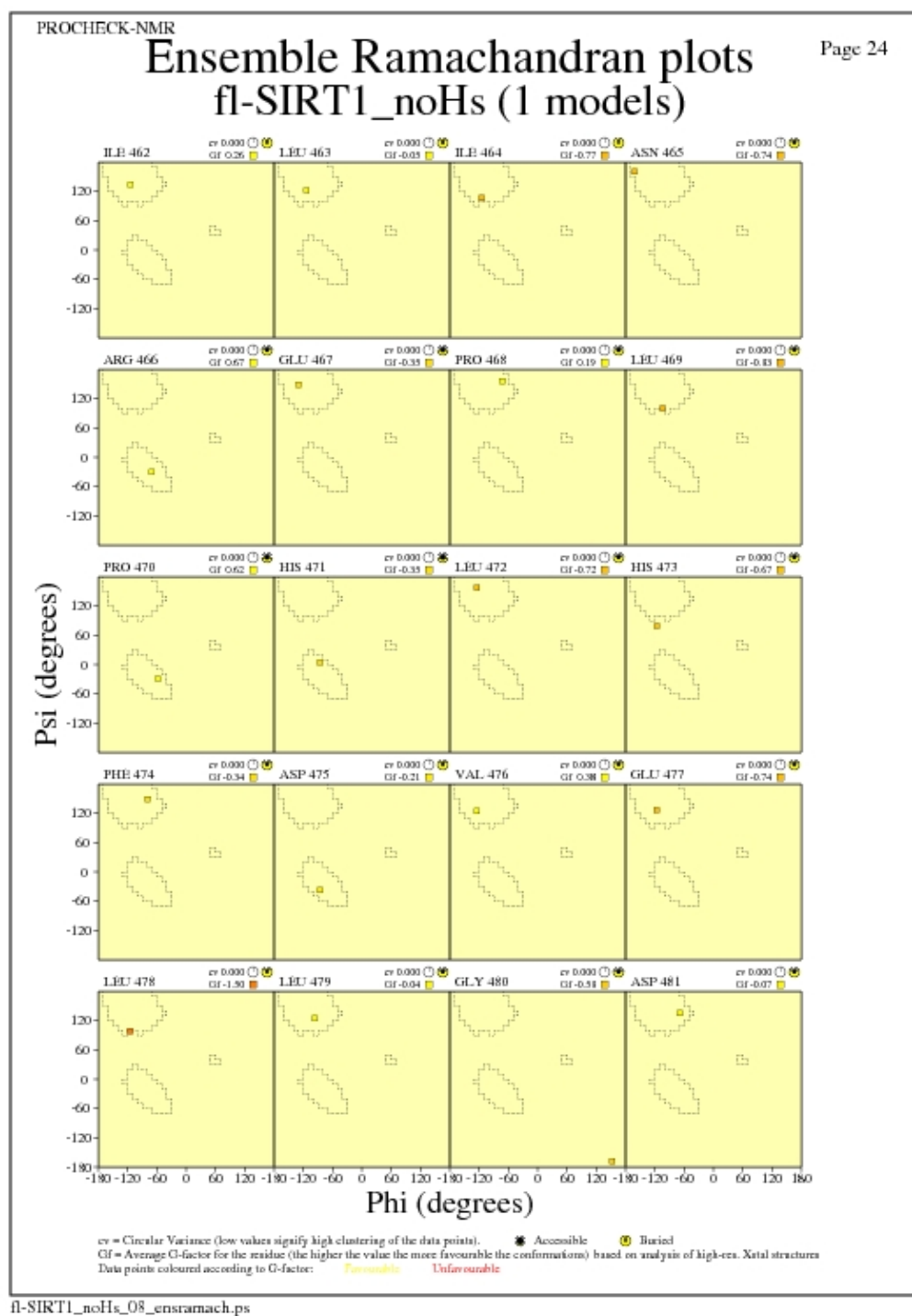
JPEG for residue Ramachandran Plots - page \$num_n



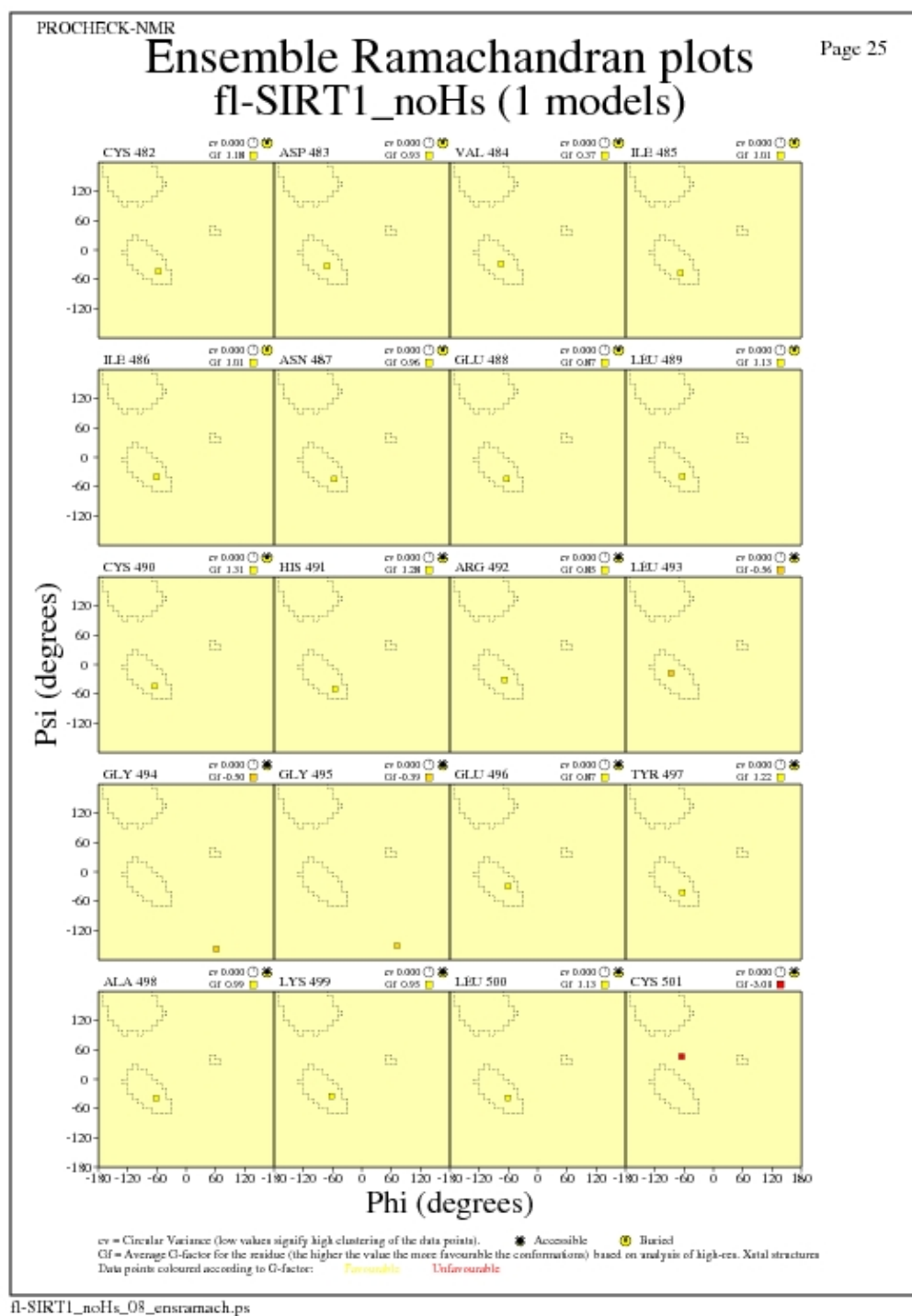
JPEG for residue Ramachandran Plots - page \$num_n



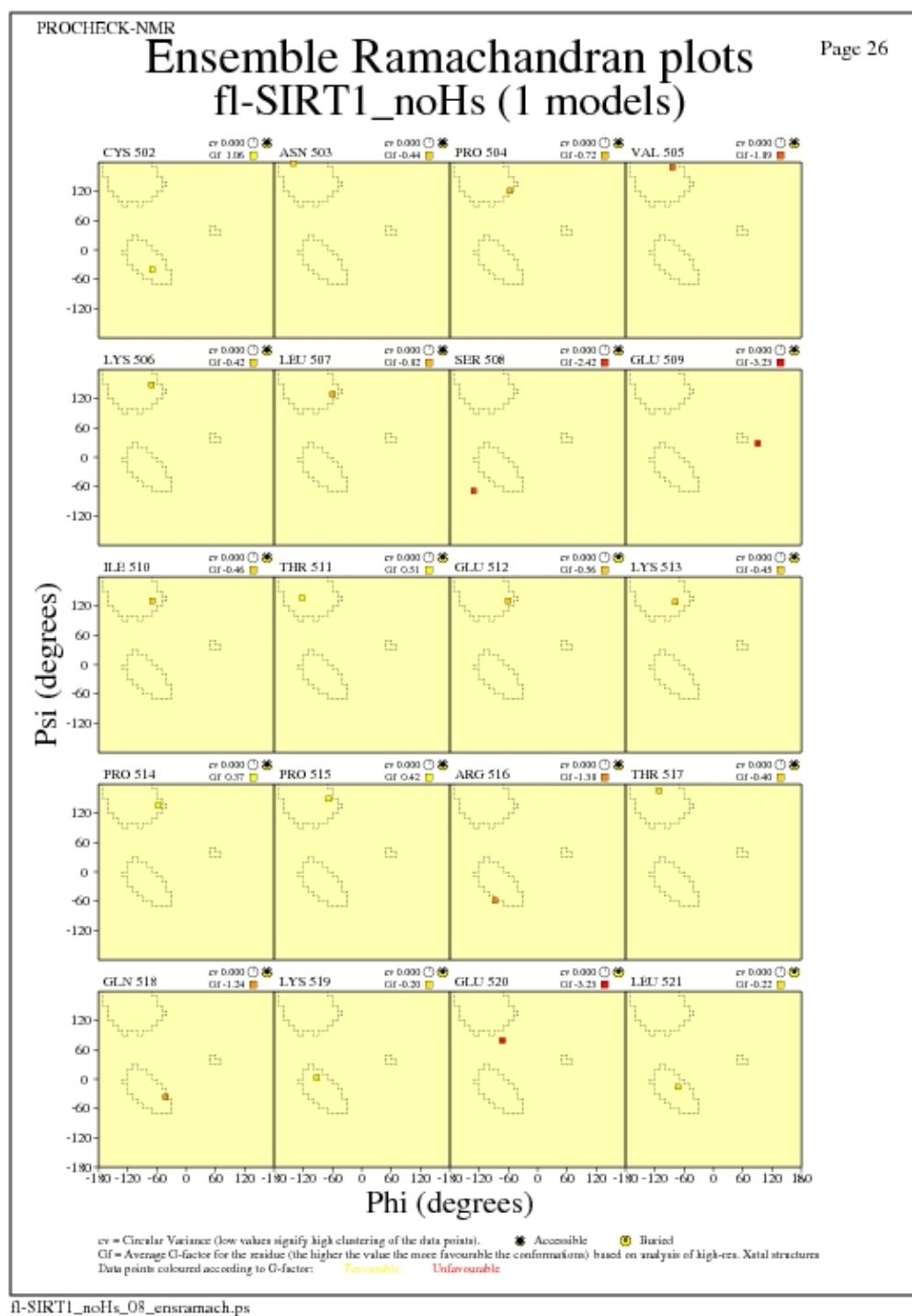
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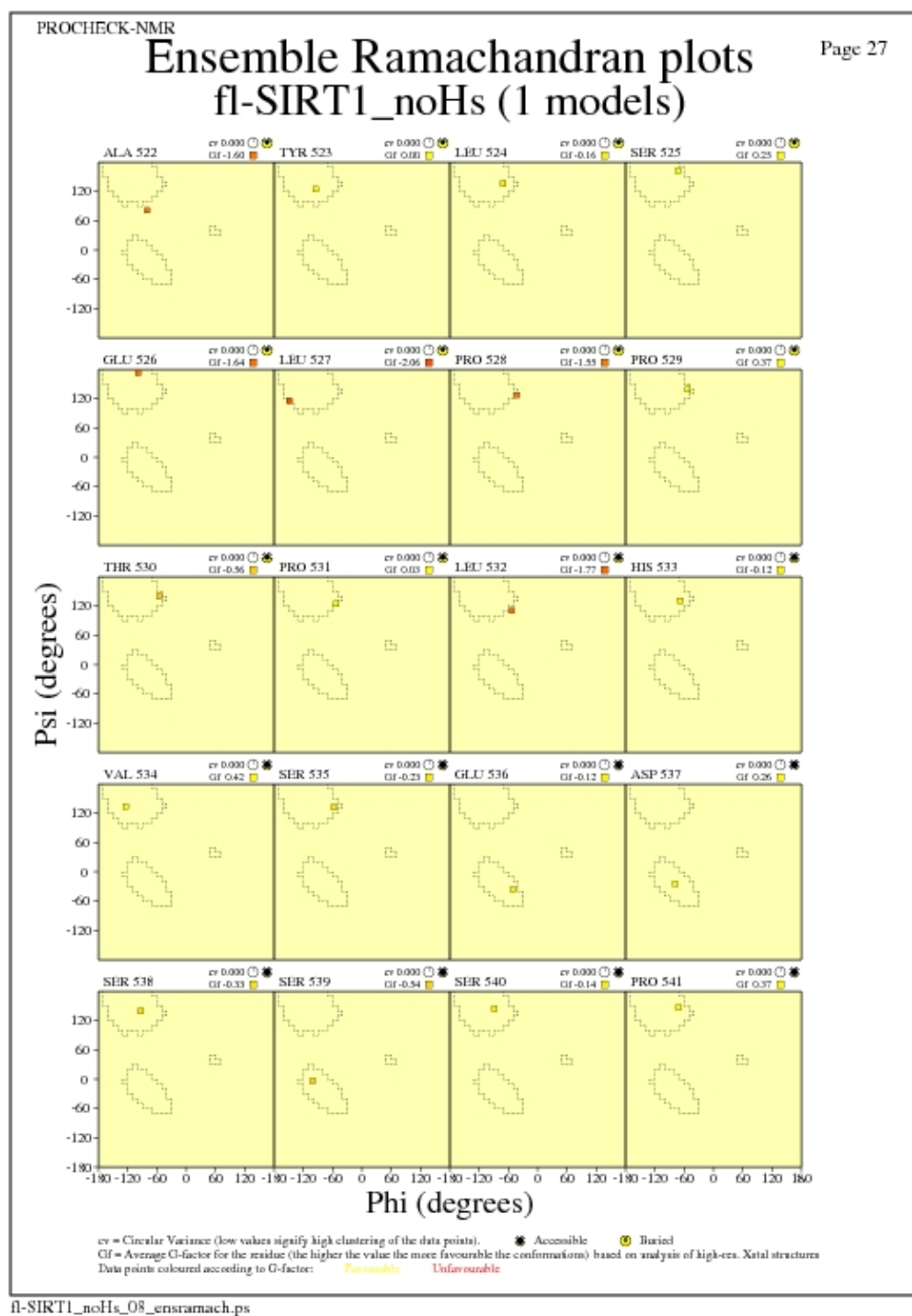
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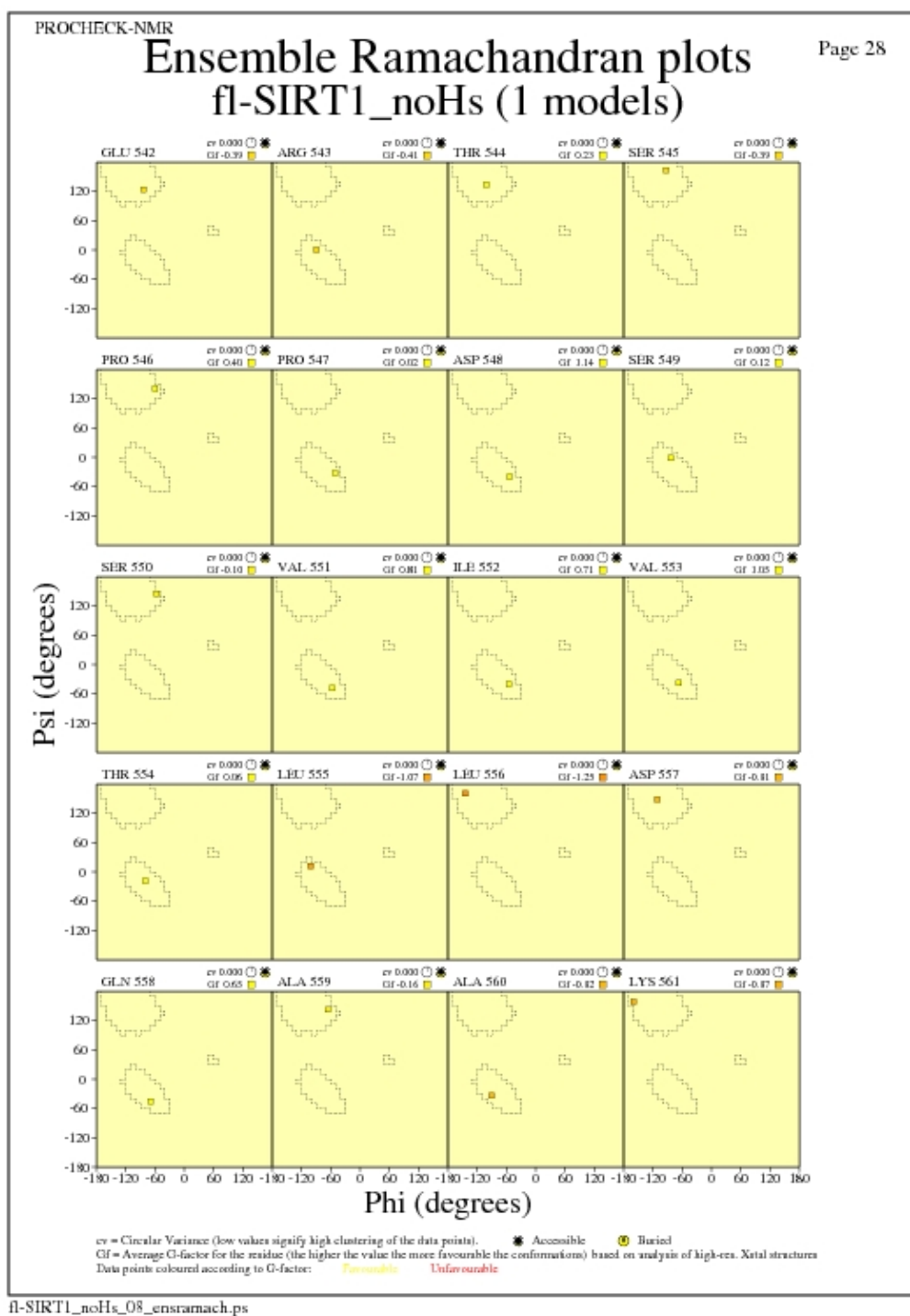
JPEG for residue Ramachandran Plots - page \$num_n



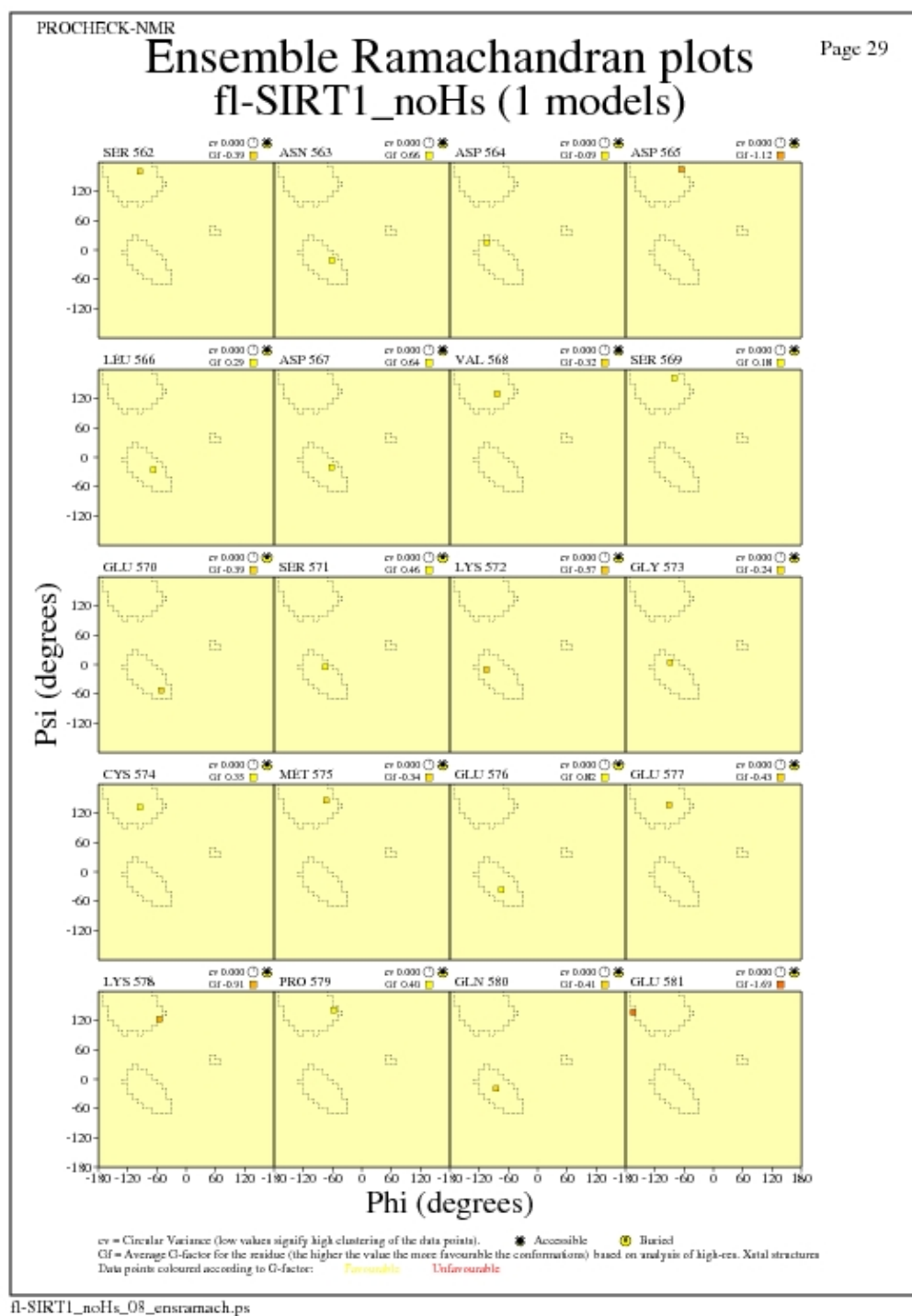
JPEG for residue Ramachandran Plots - page \$num_n



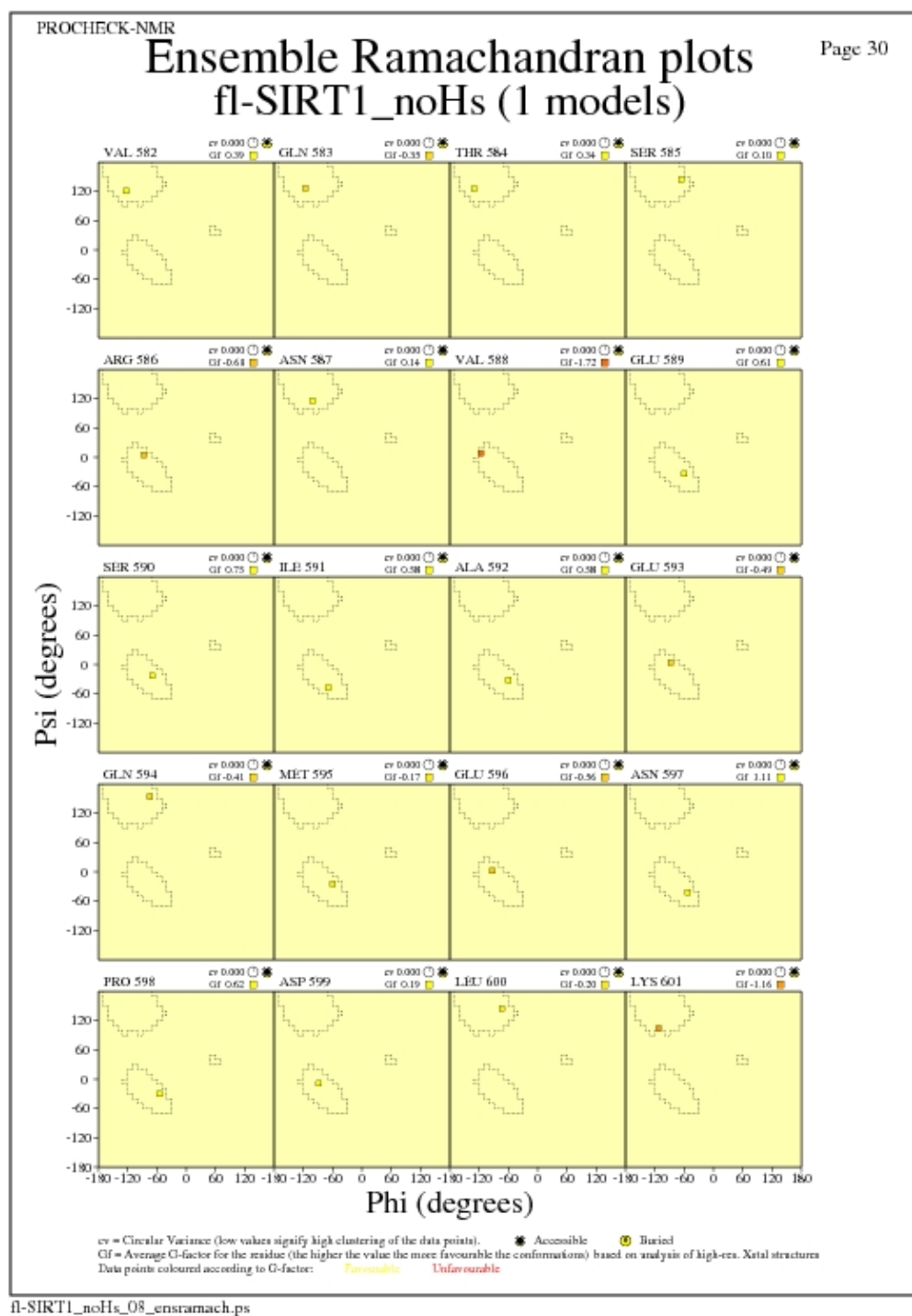
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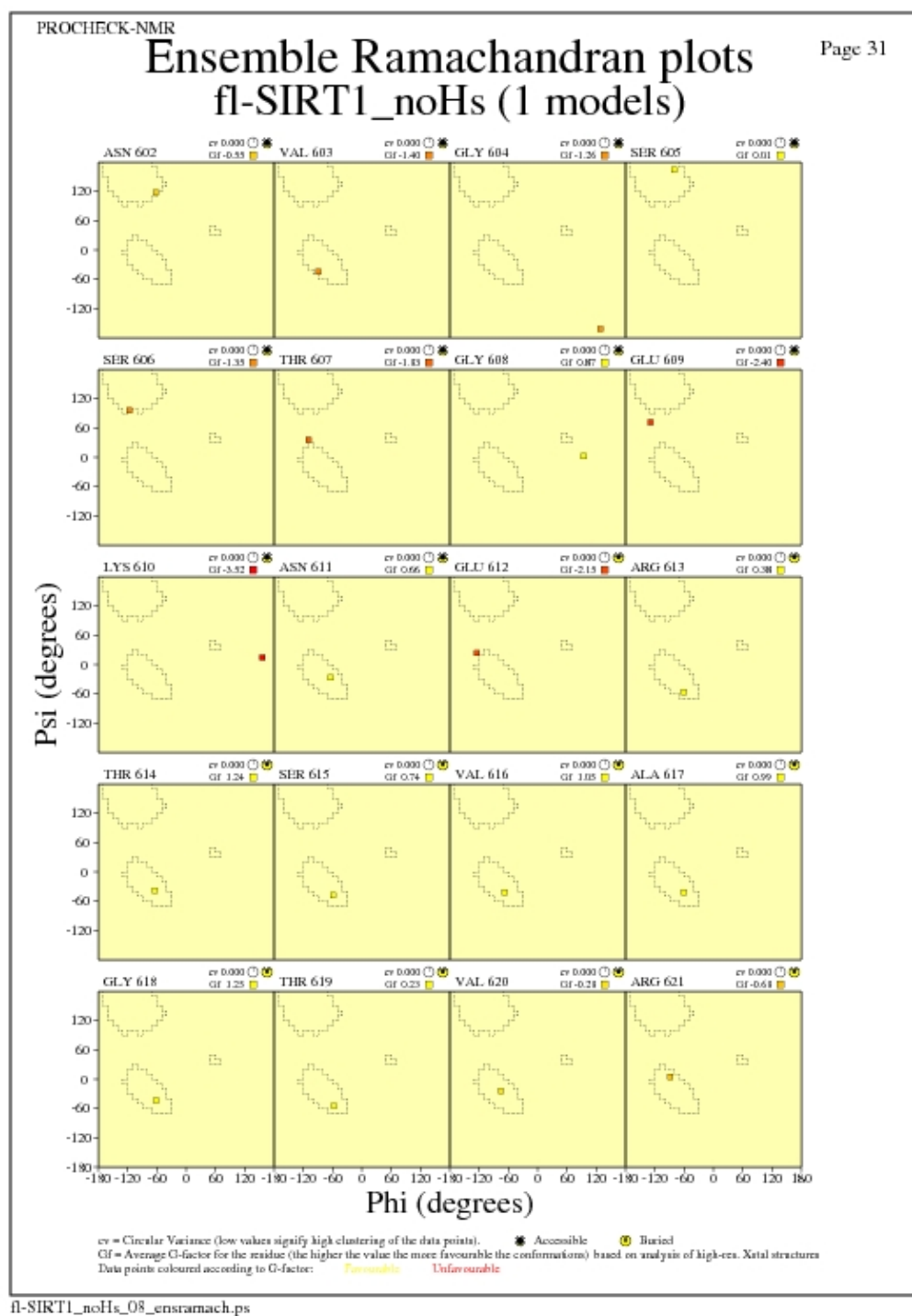
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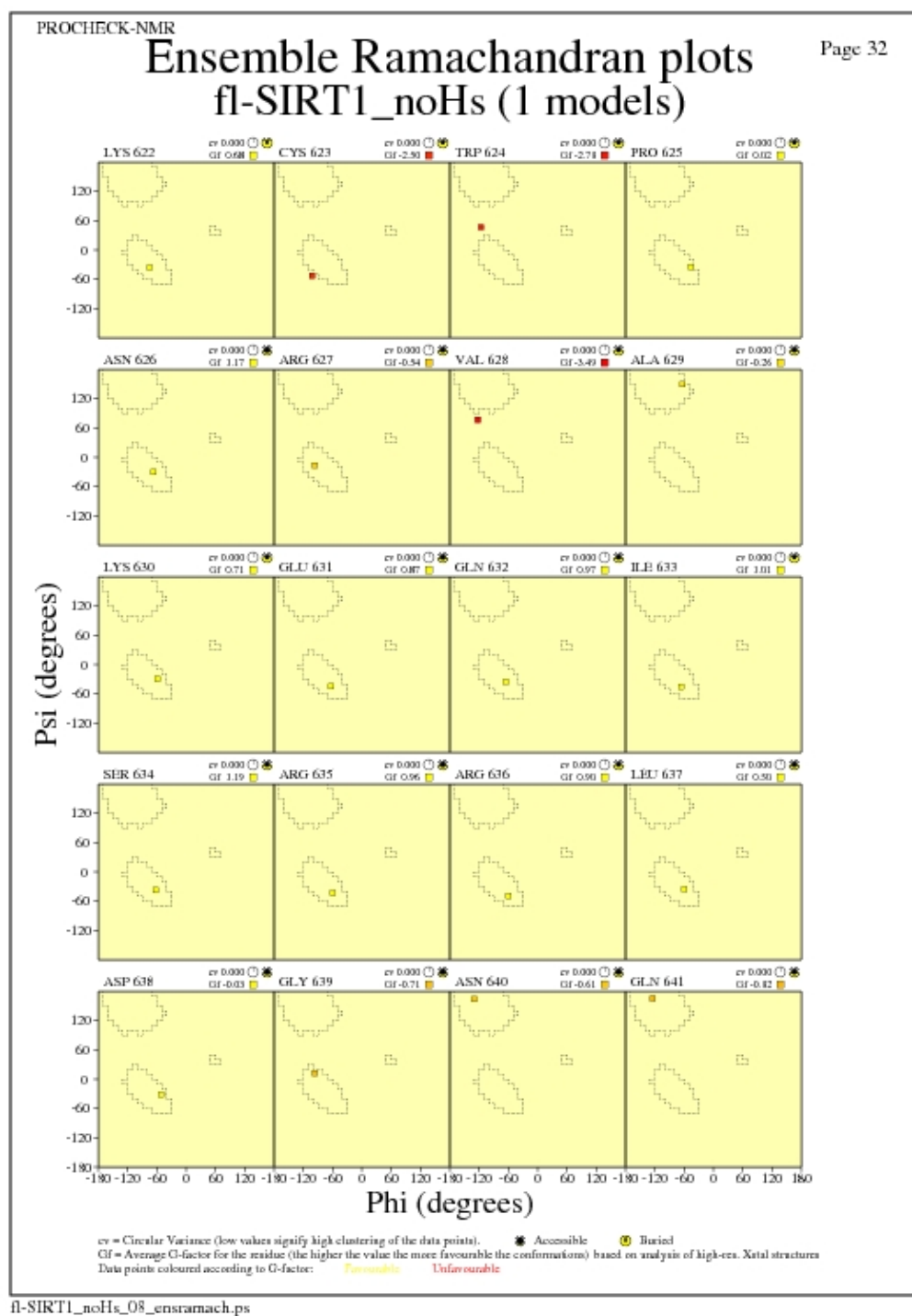
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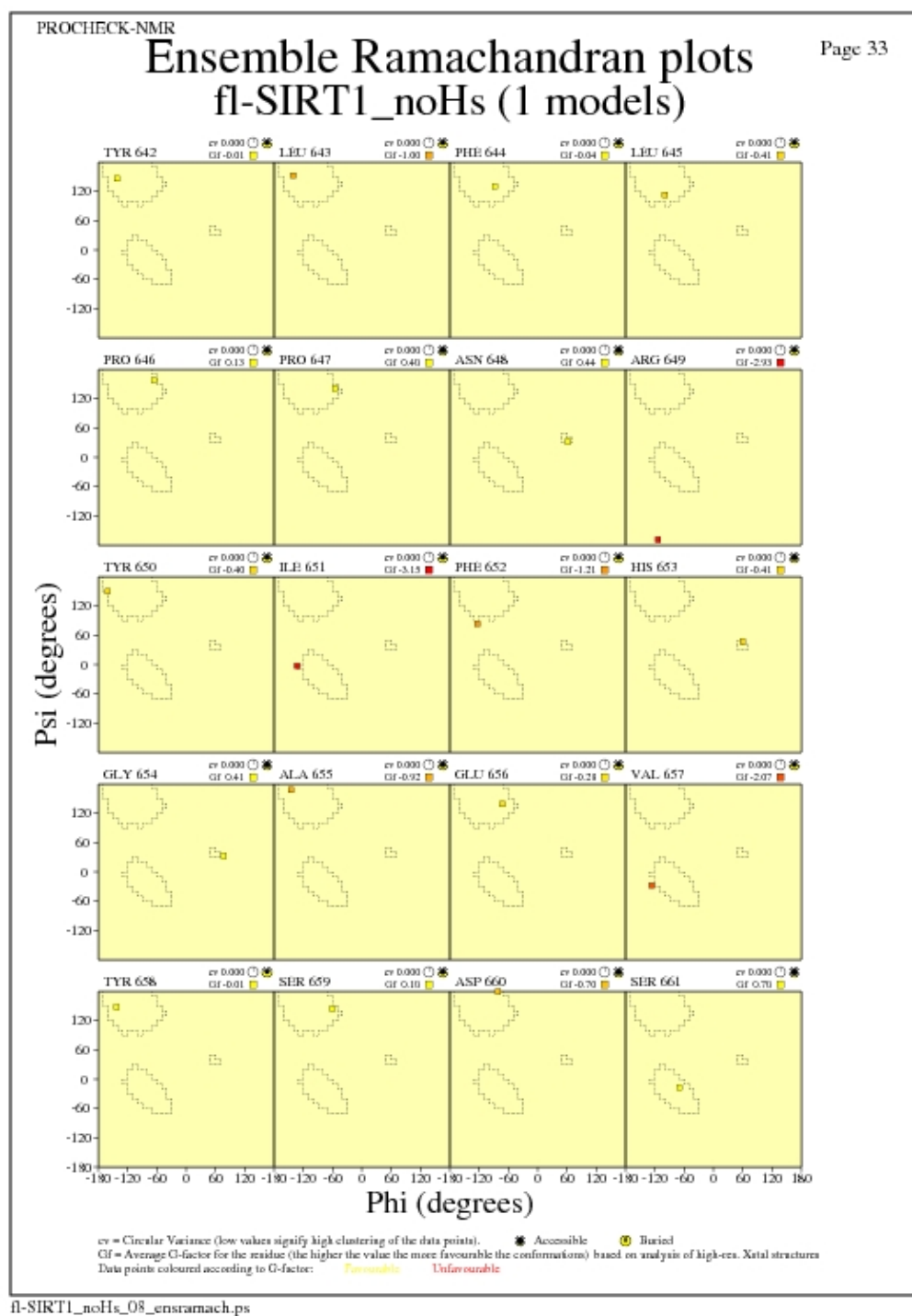
JPEG for residue Ramachandran Plots - page \$num_n



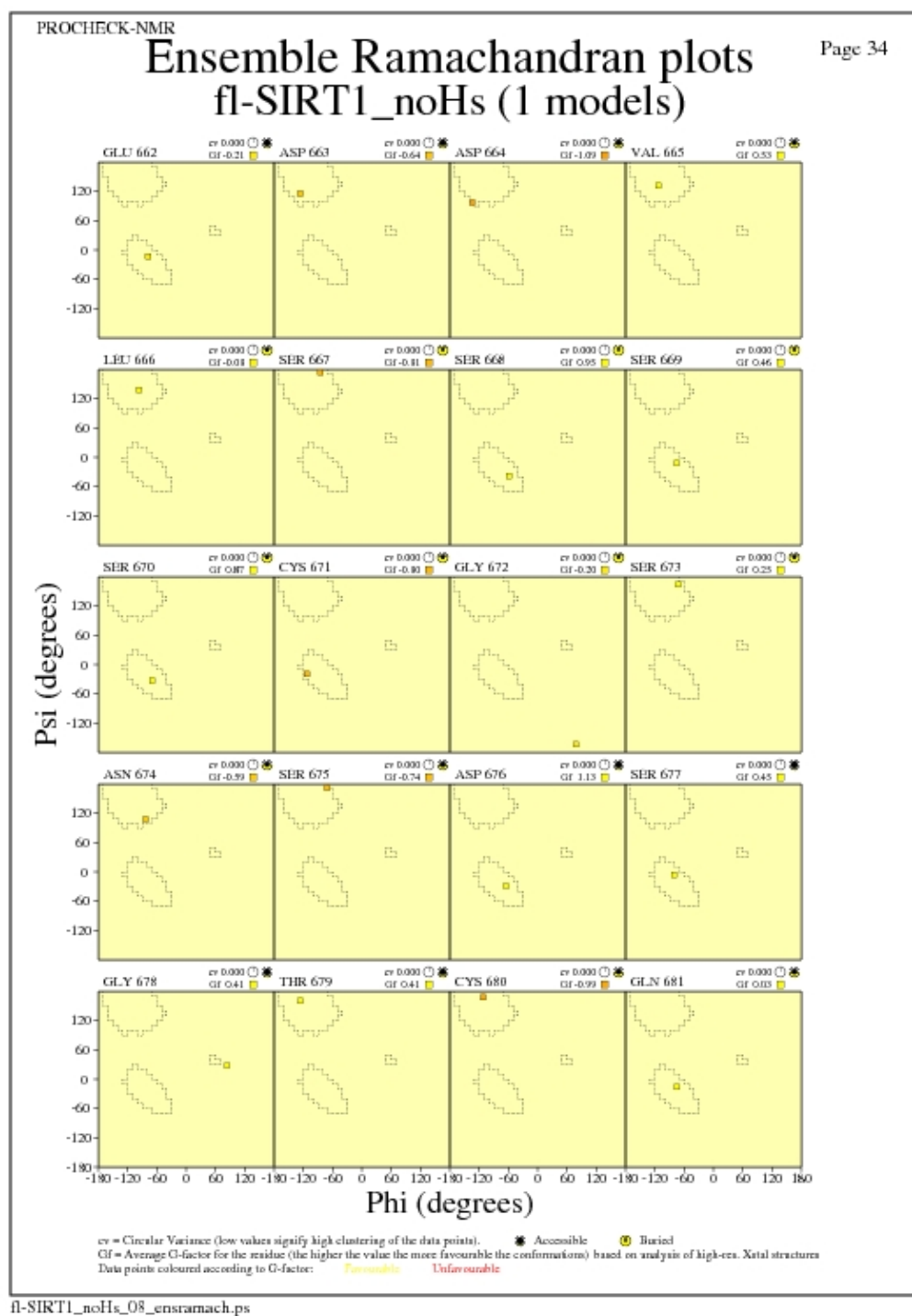
JPEG for residue Ramachandran Plots - page \$num_n



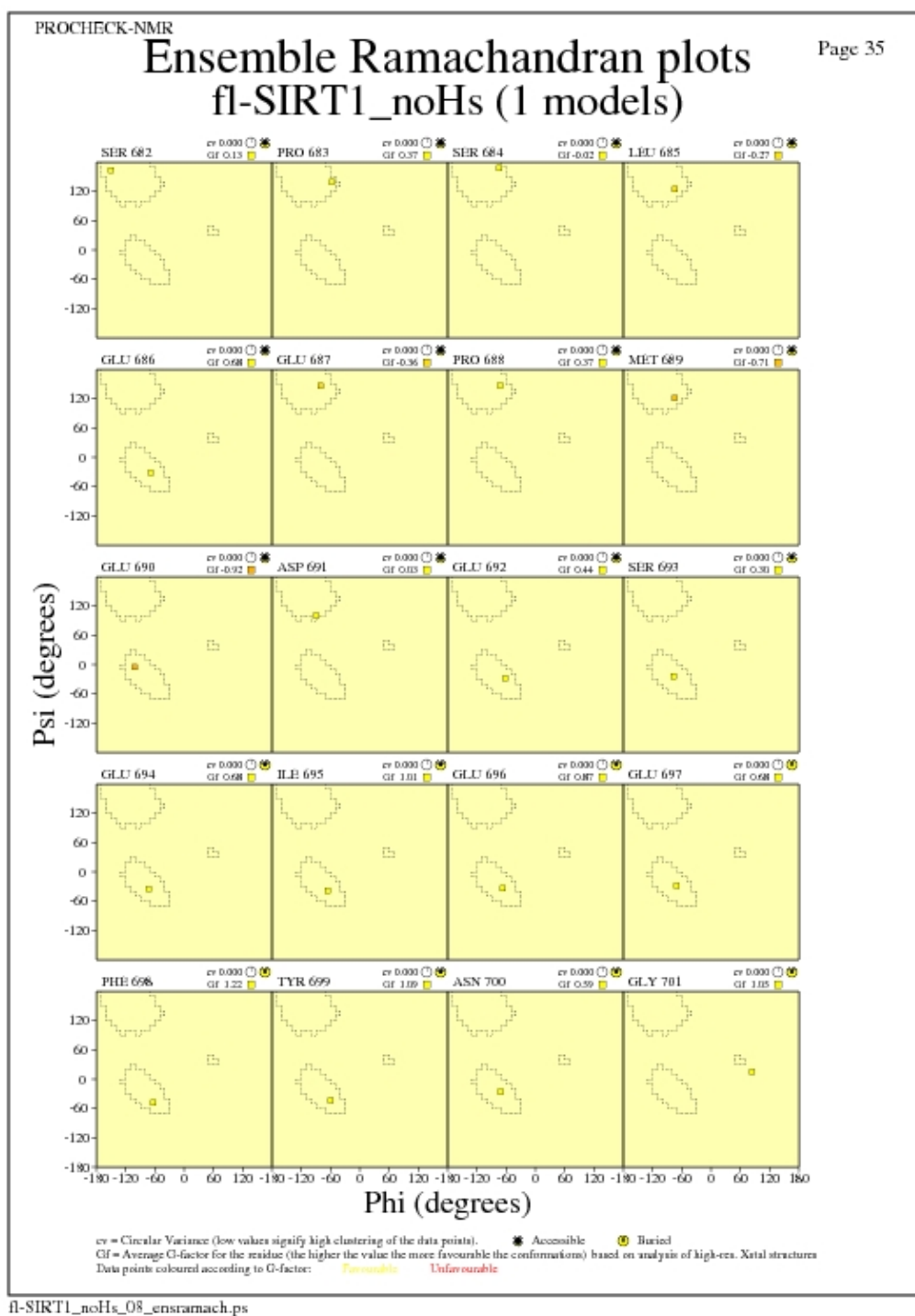
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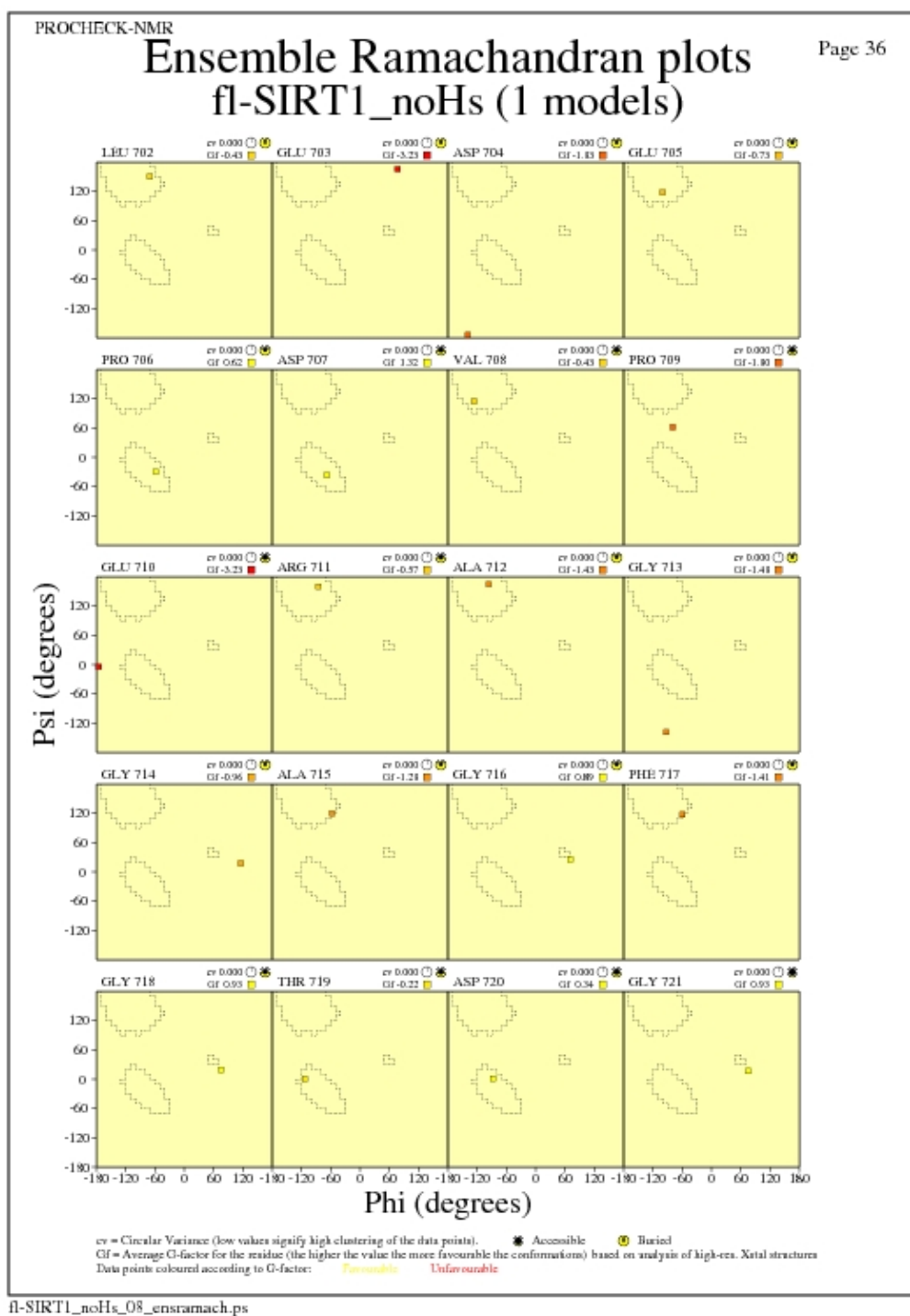
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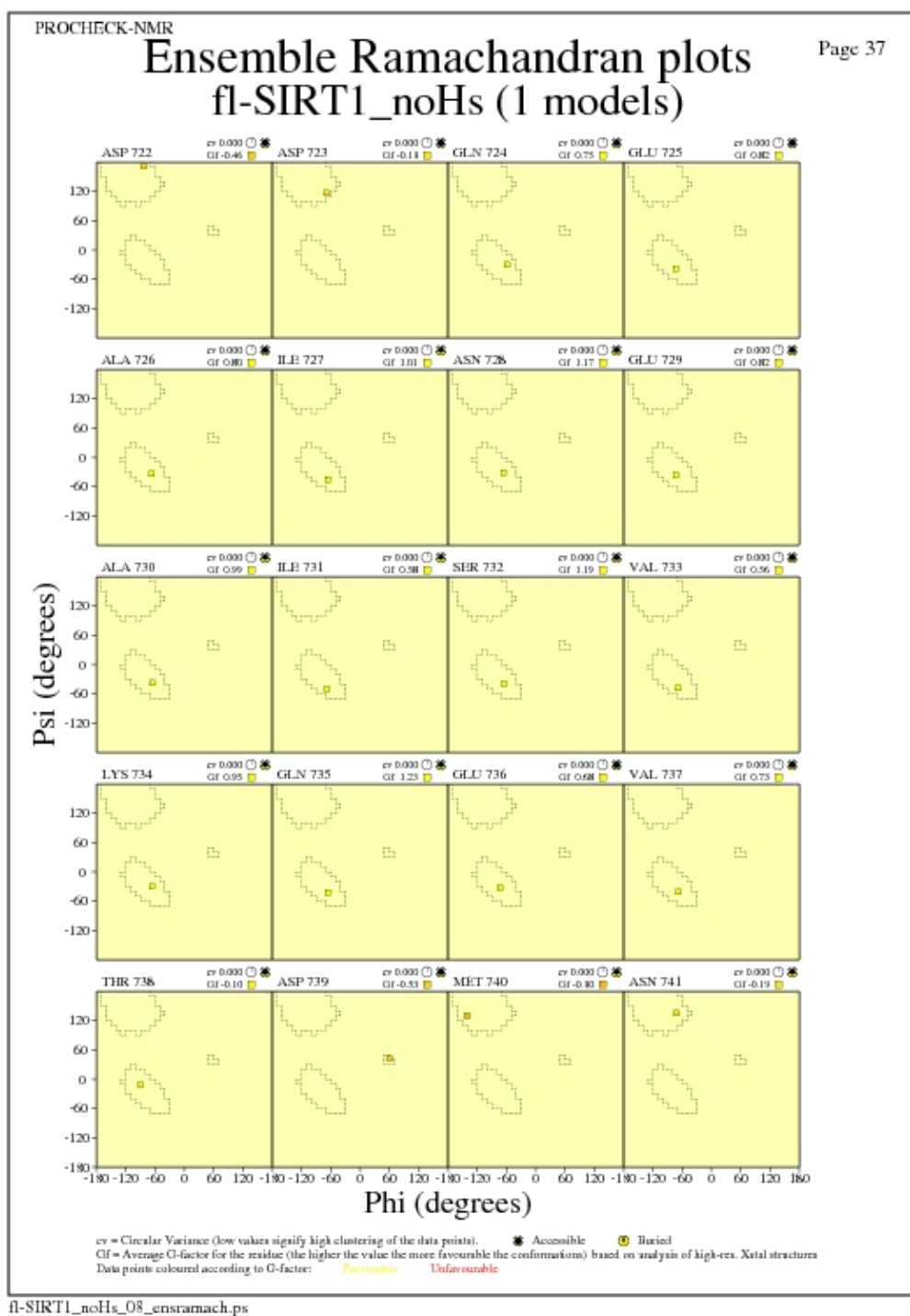
JPEG for residue Ramachandran Plots - page \$num_n



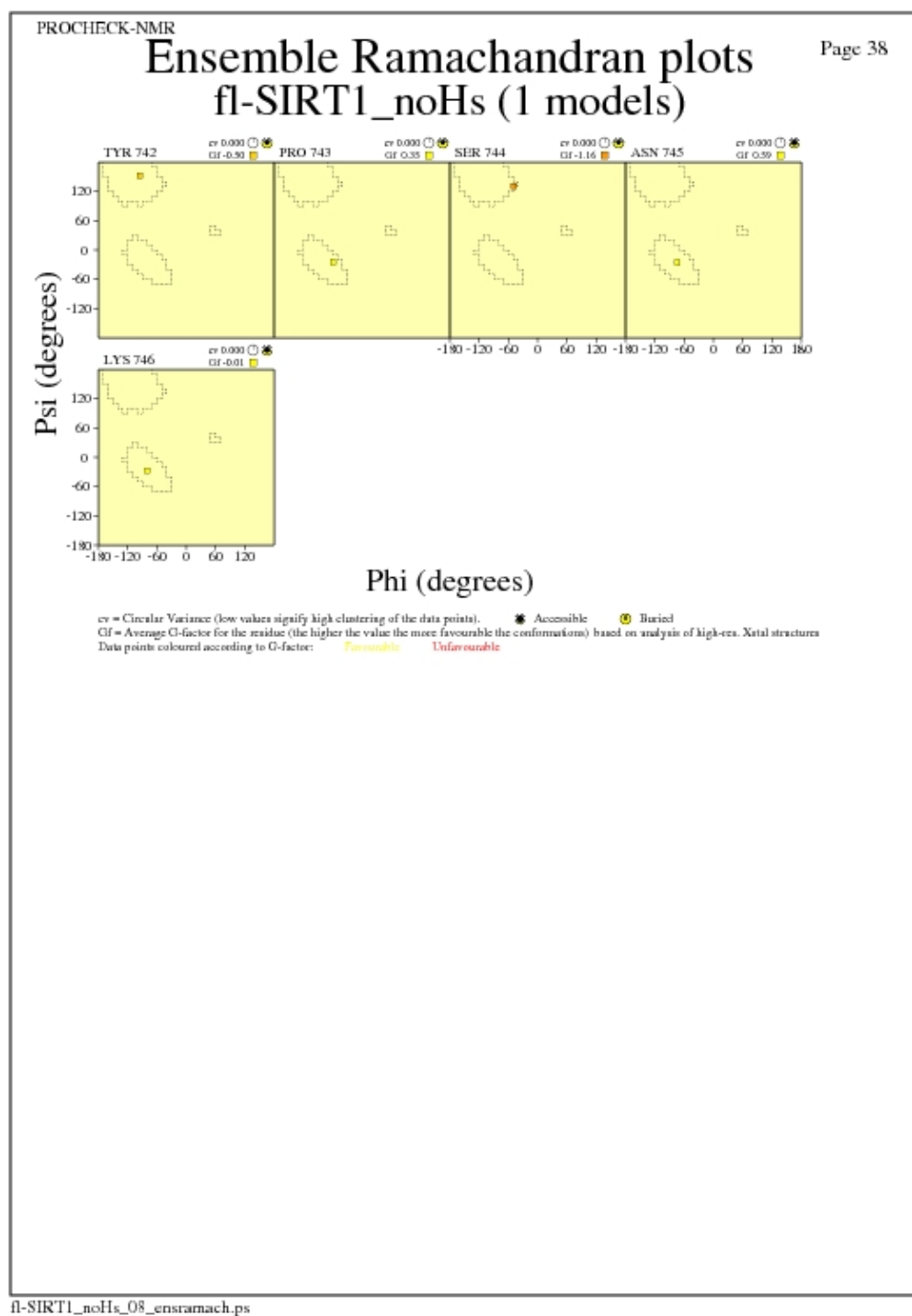
JPEG for residue Ramachandran Plots - page \$num_n



JPEG for residue Ramachandran Plots - page \$num_n



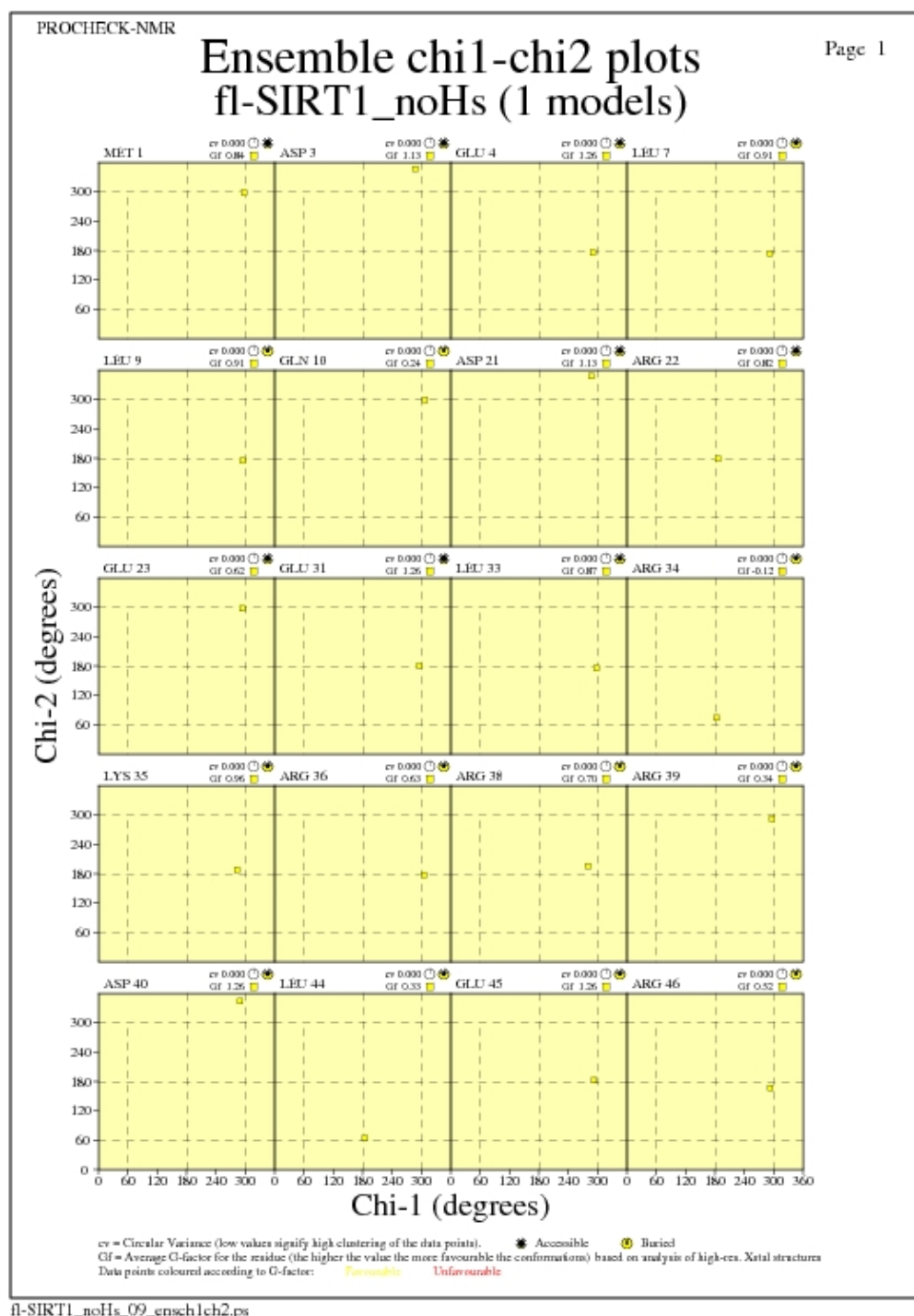
JPEG for residue Ramachandran Plots - page \$num_n



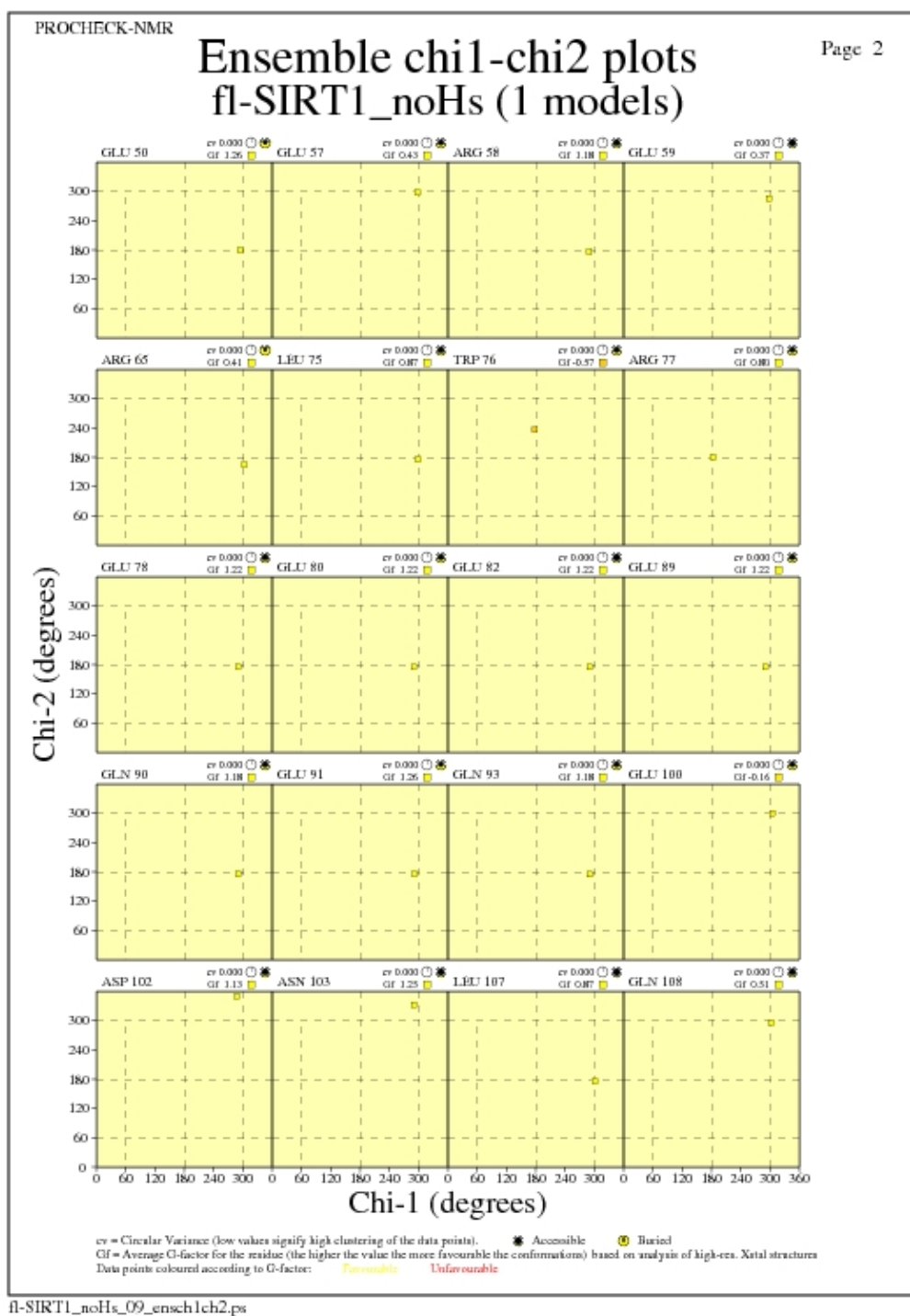
Ramachandran analysis for each residue from Molprobit

Chi1-Chi2 Plots for each residue

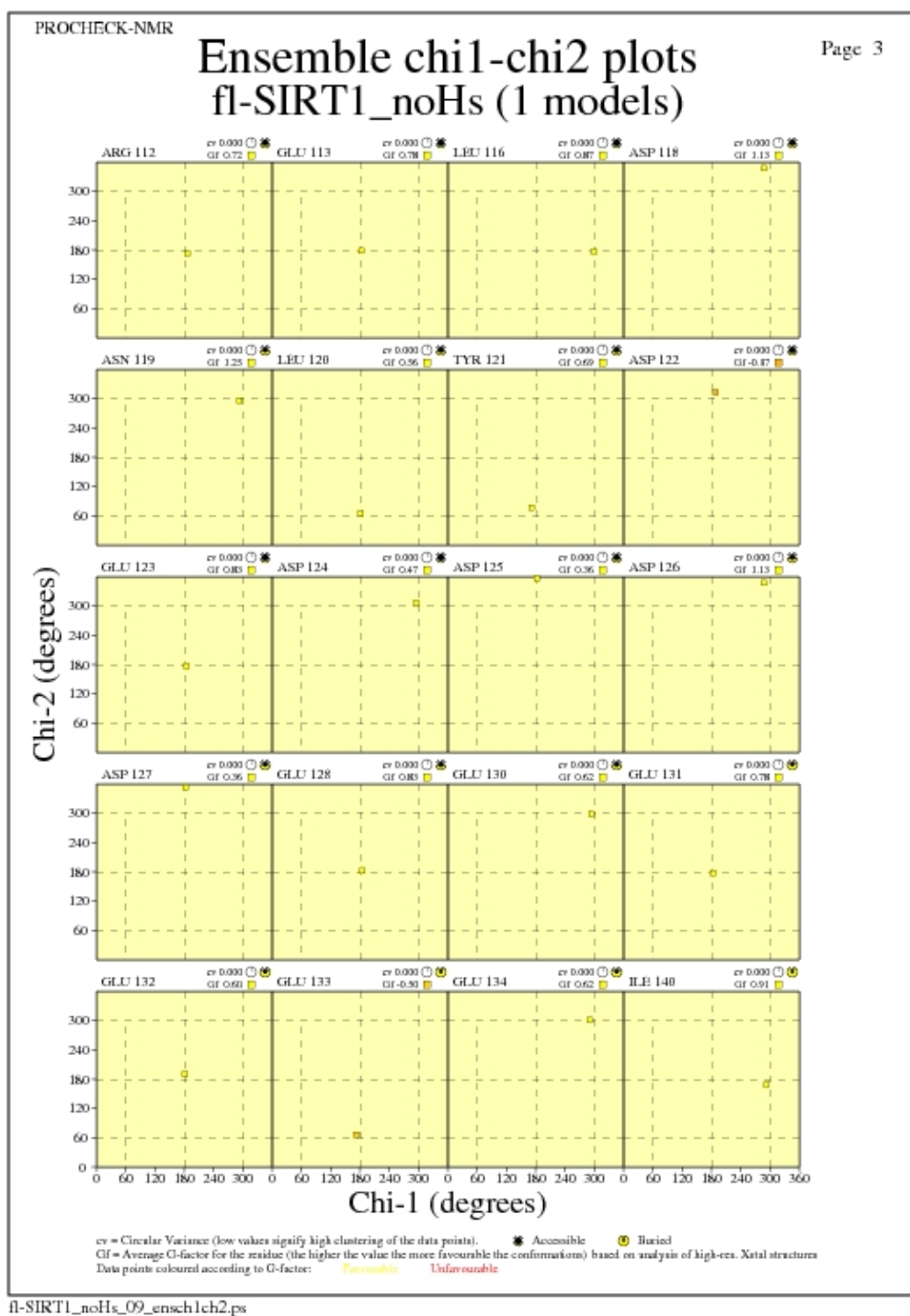
JPEG for residue Chi1-Chi2 Plots - page \$num_n



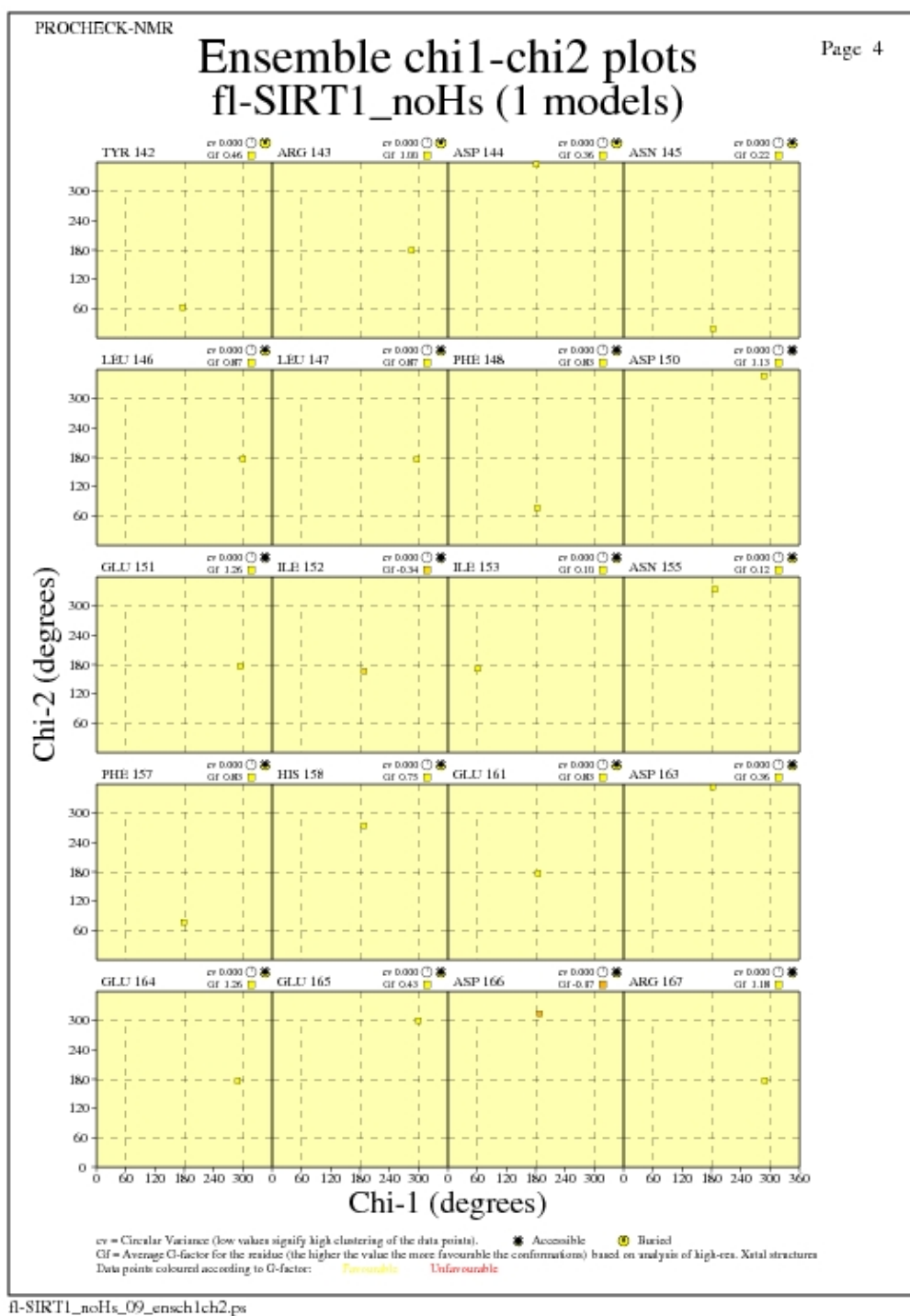
JPEG for residue Chi1-Chi2 Plots - page \$num_n



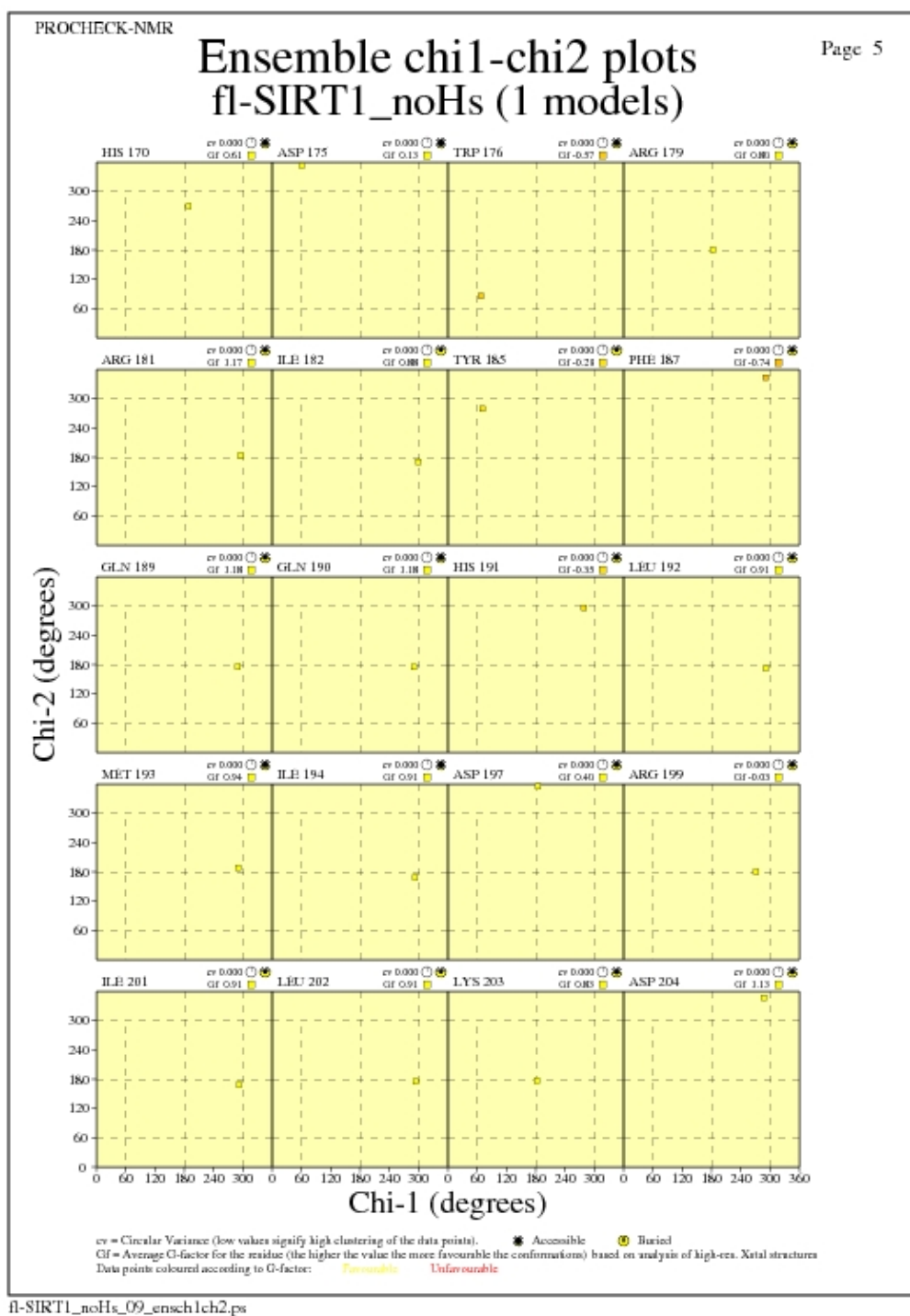
JPEG for residue Chi1-Chi2 Plots - page \$num_n



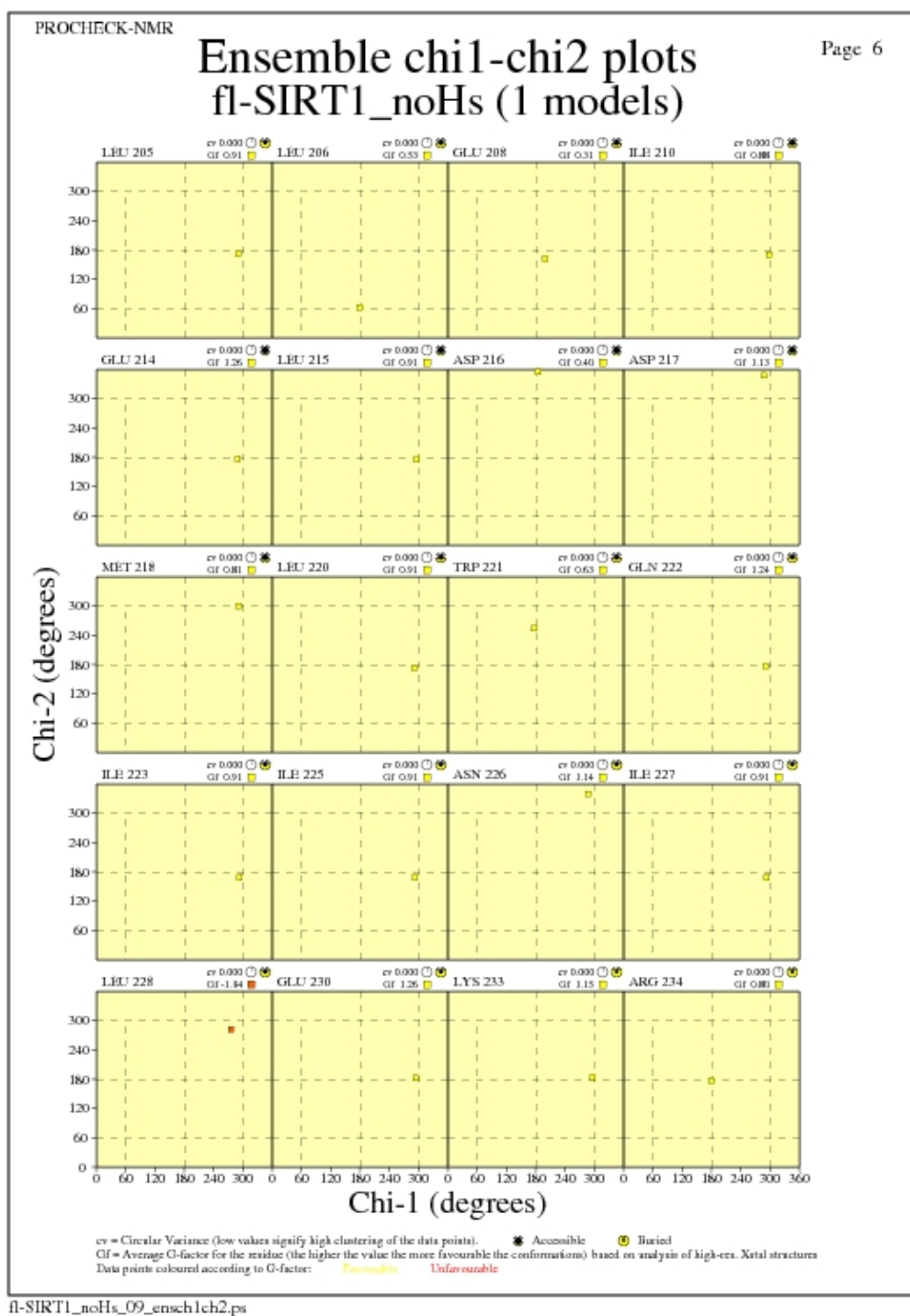
JPEG for residue Chi1-Chi2 Plots - page \$num_n



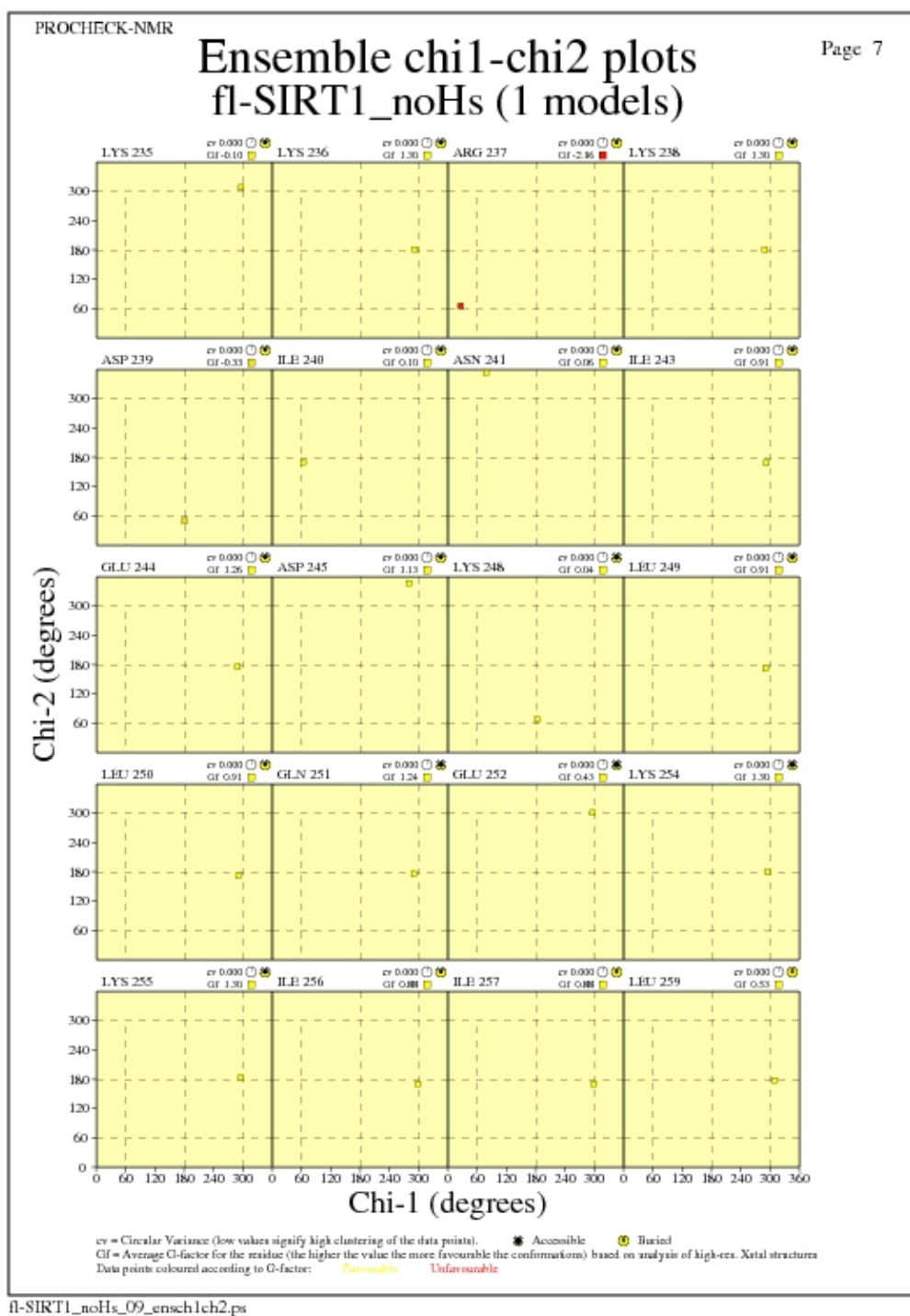
JPEG for residue Chi1-Chi2 Plots - page \$num_n



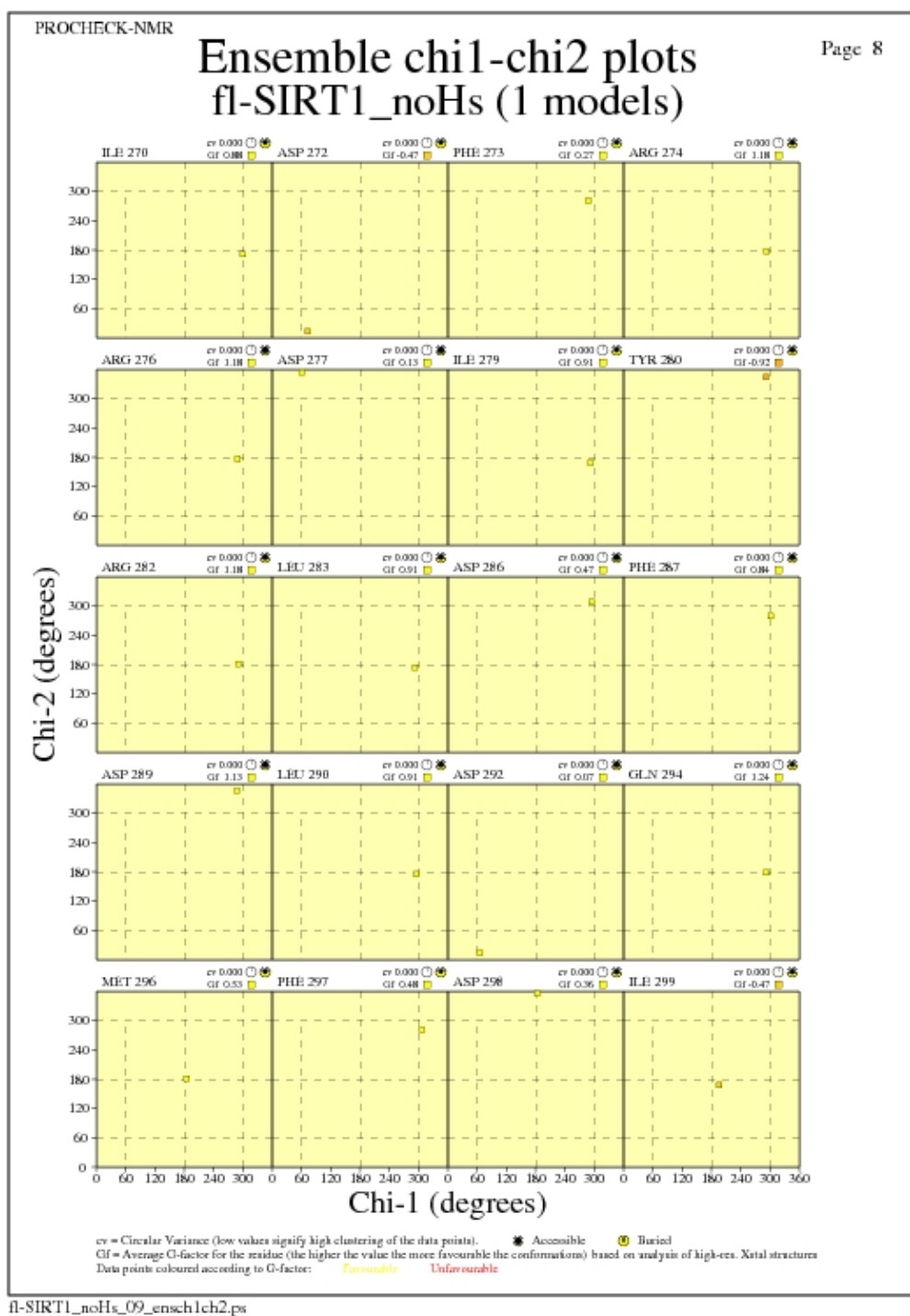
JPEG for residue Chi1-Chi2 Plots - page \$num_n



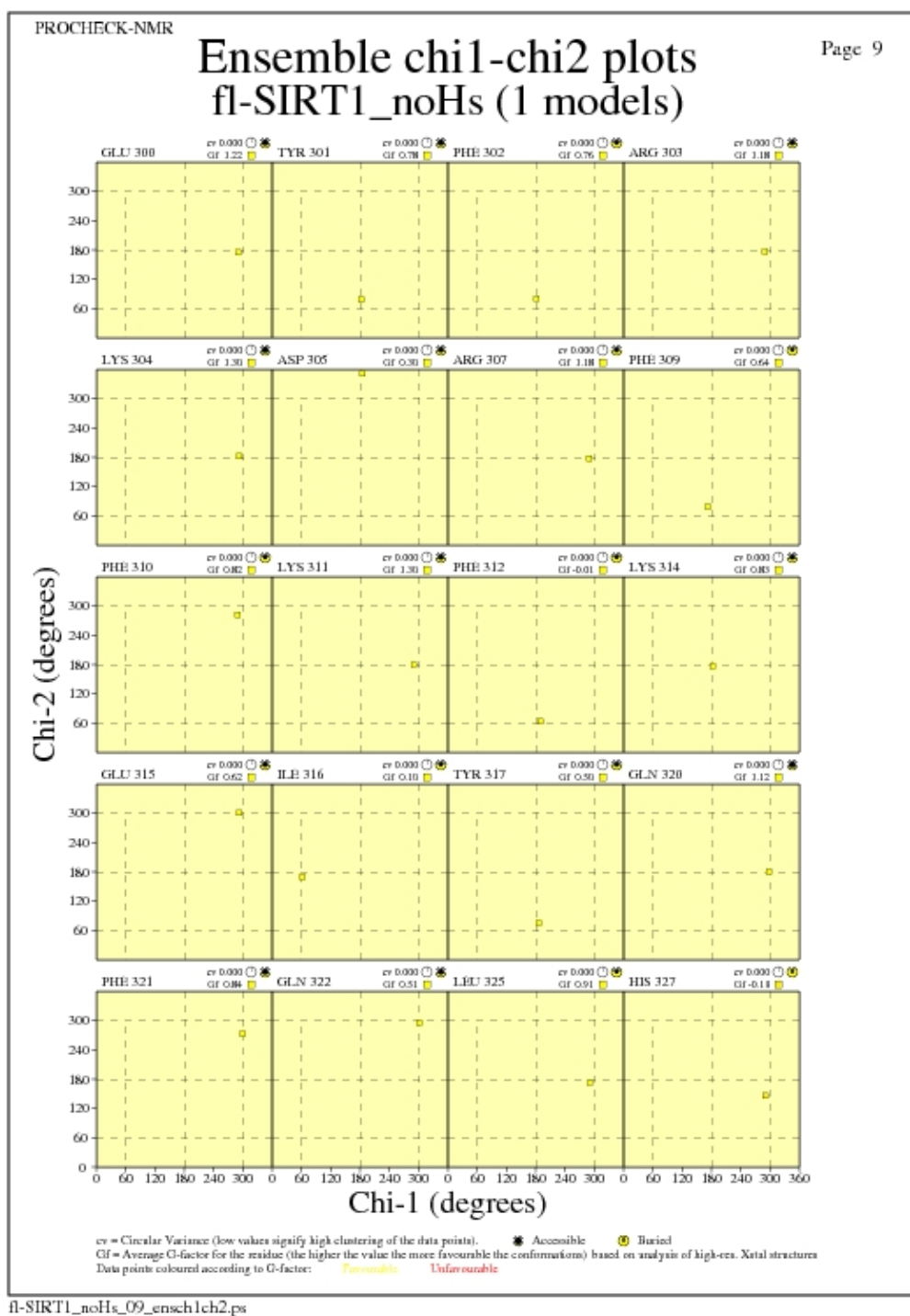
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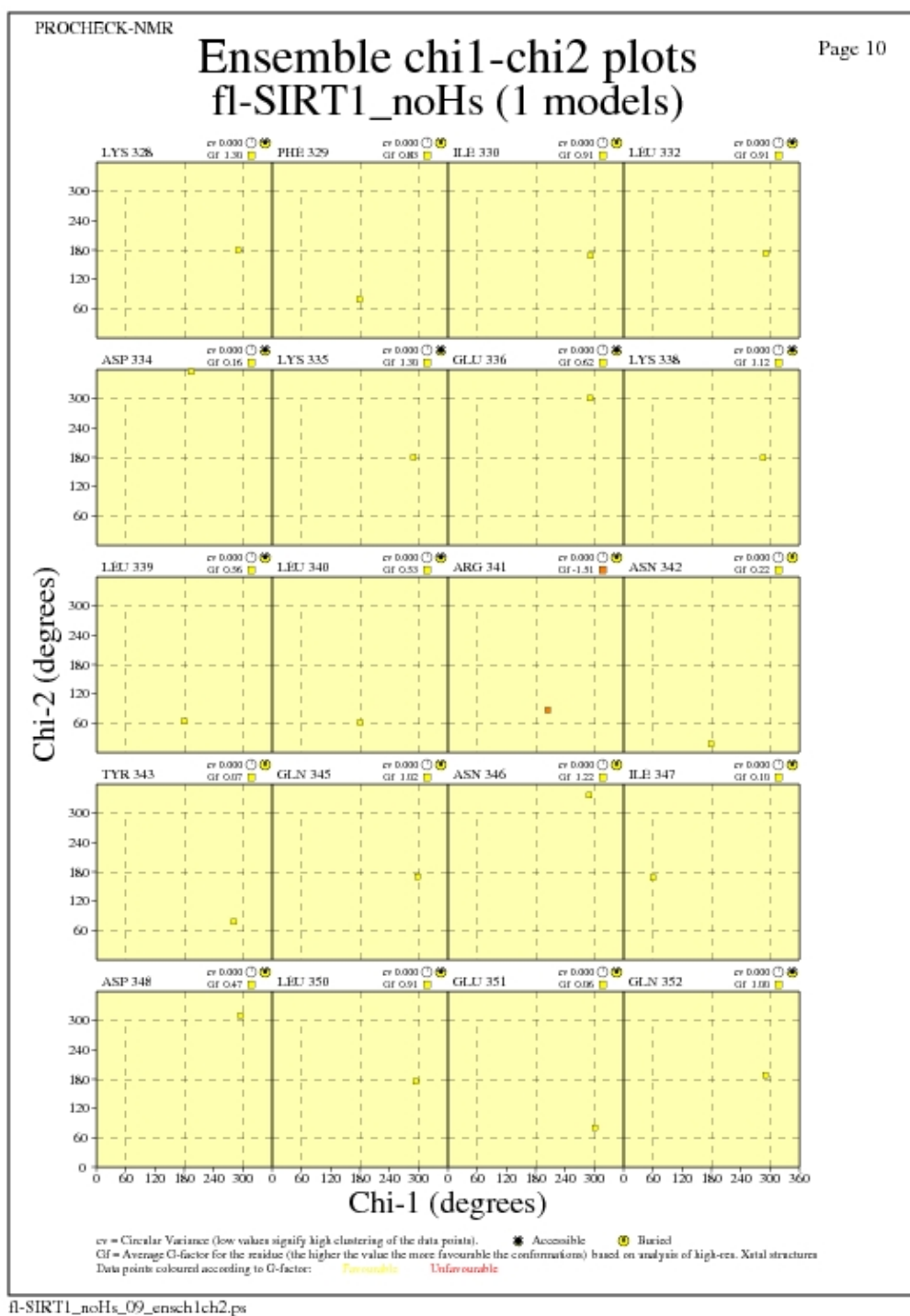
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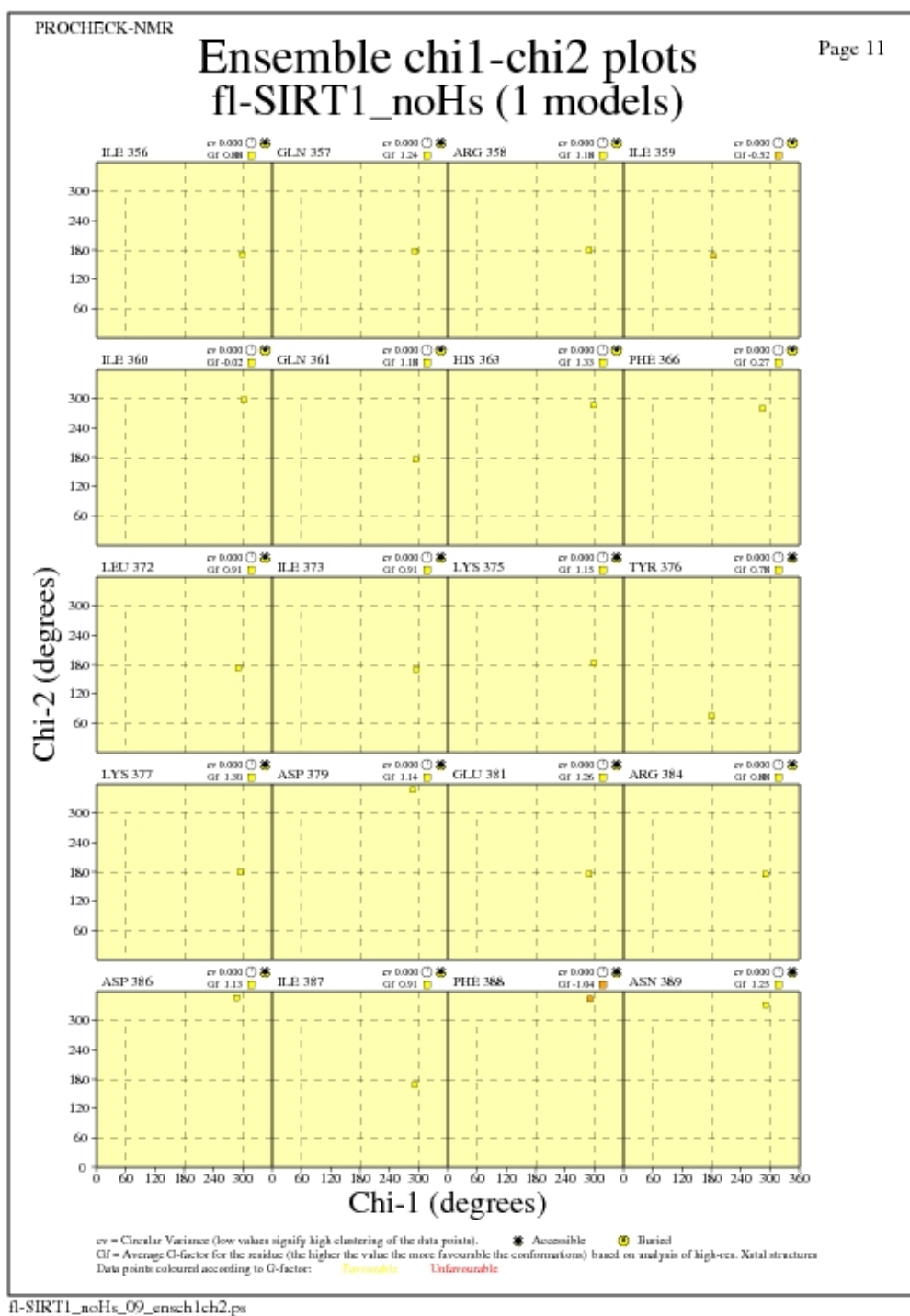
JPEG for residue Chi1-Chi2 Plots - page \$num_n



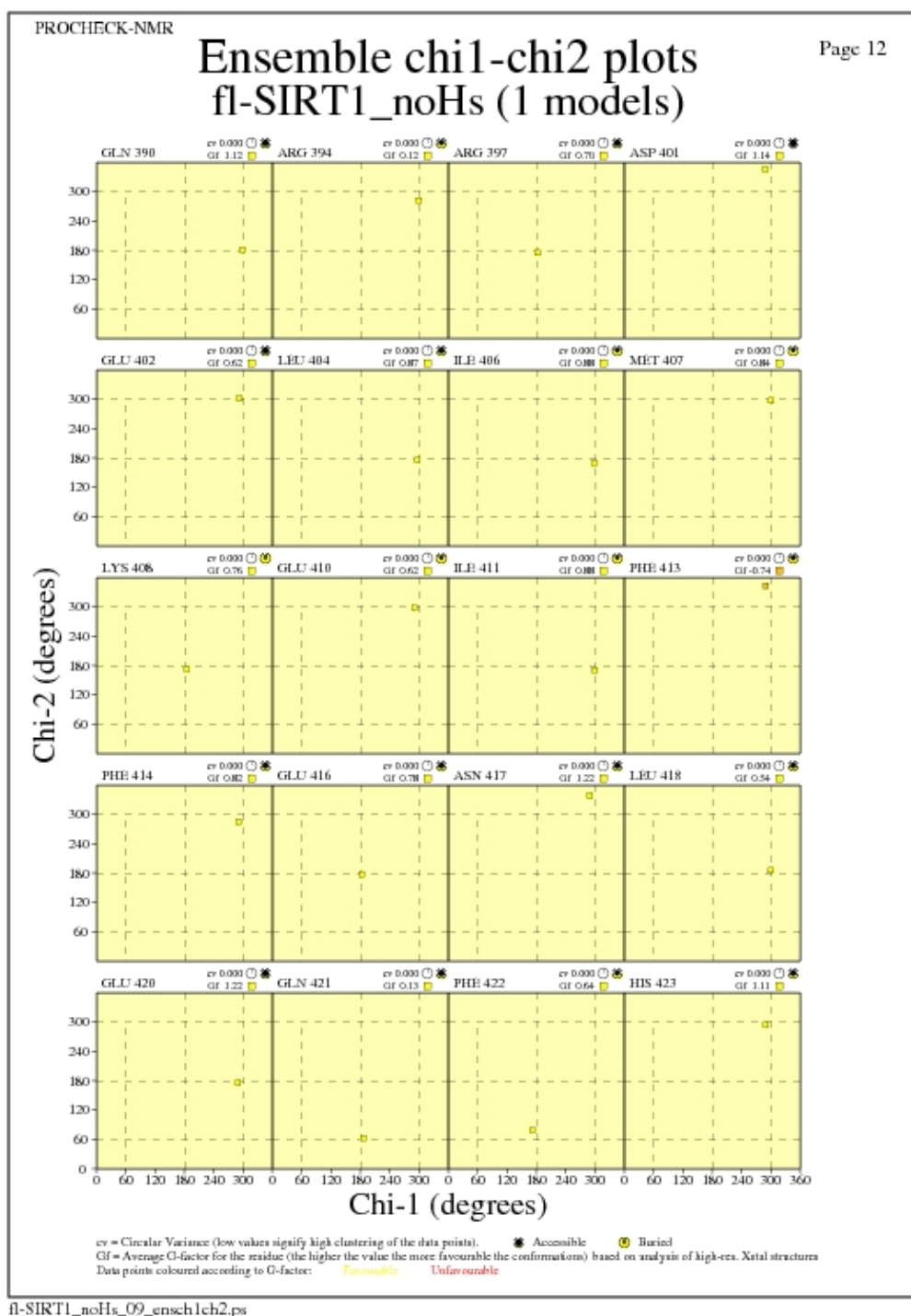
JPEG for residue Chi1-Chi2 Plots - page \$num_n



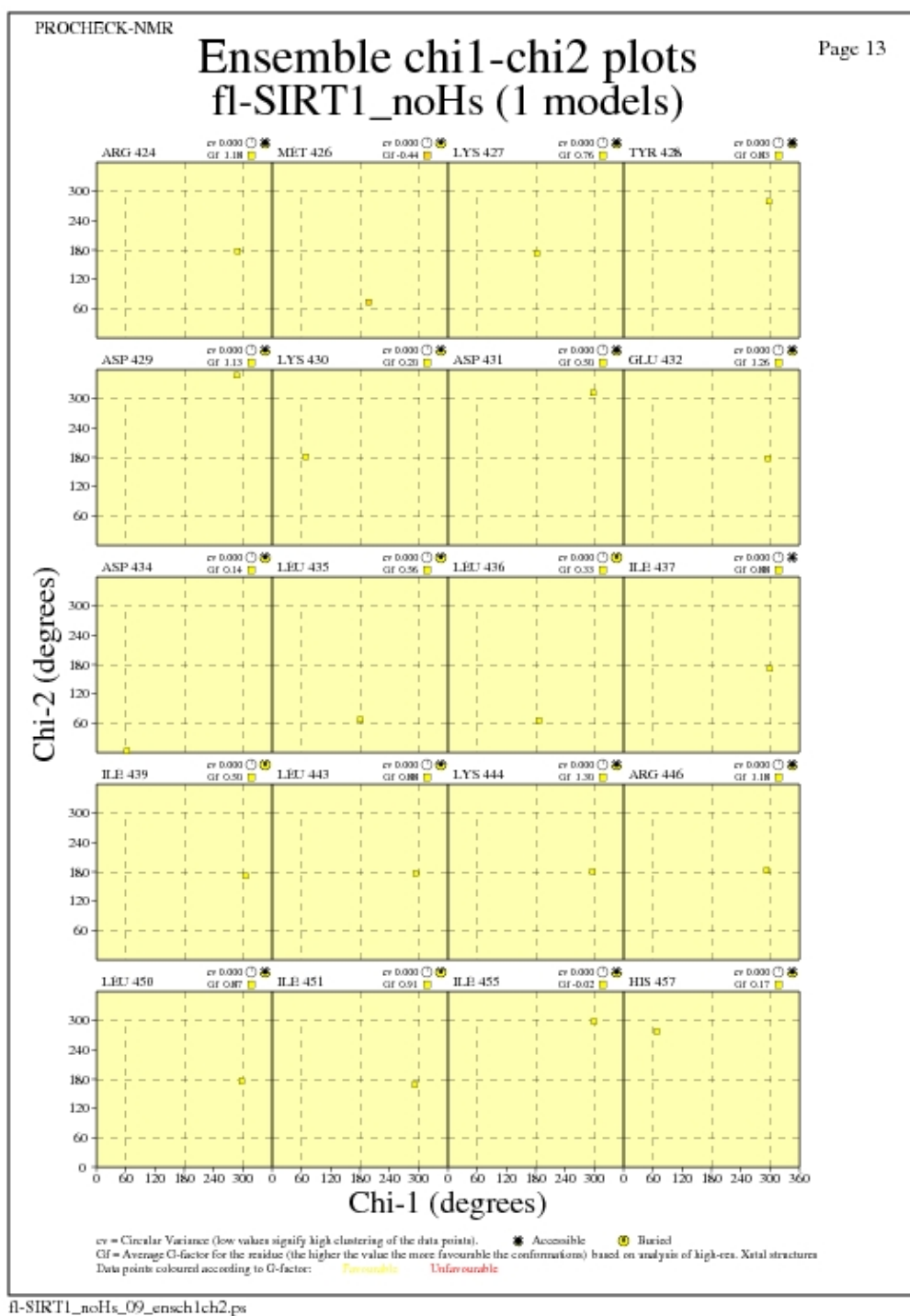
JPEG for residue Chi1-Chi2 Plots - page \$num_n



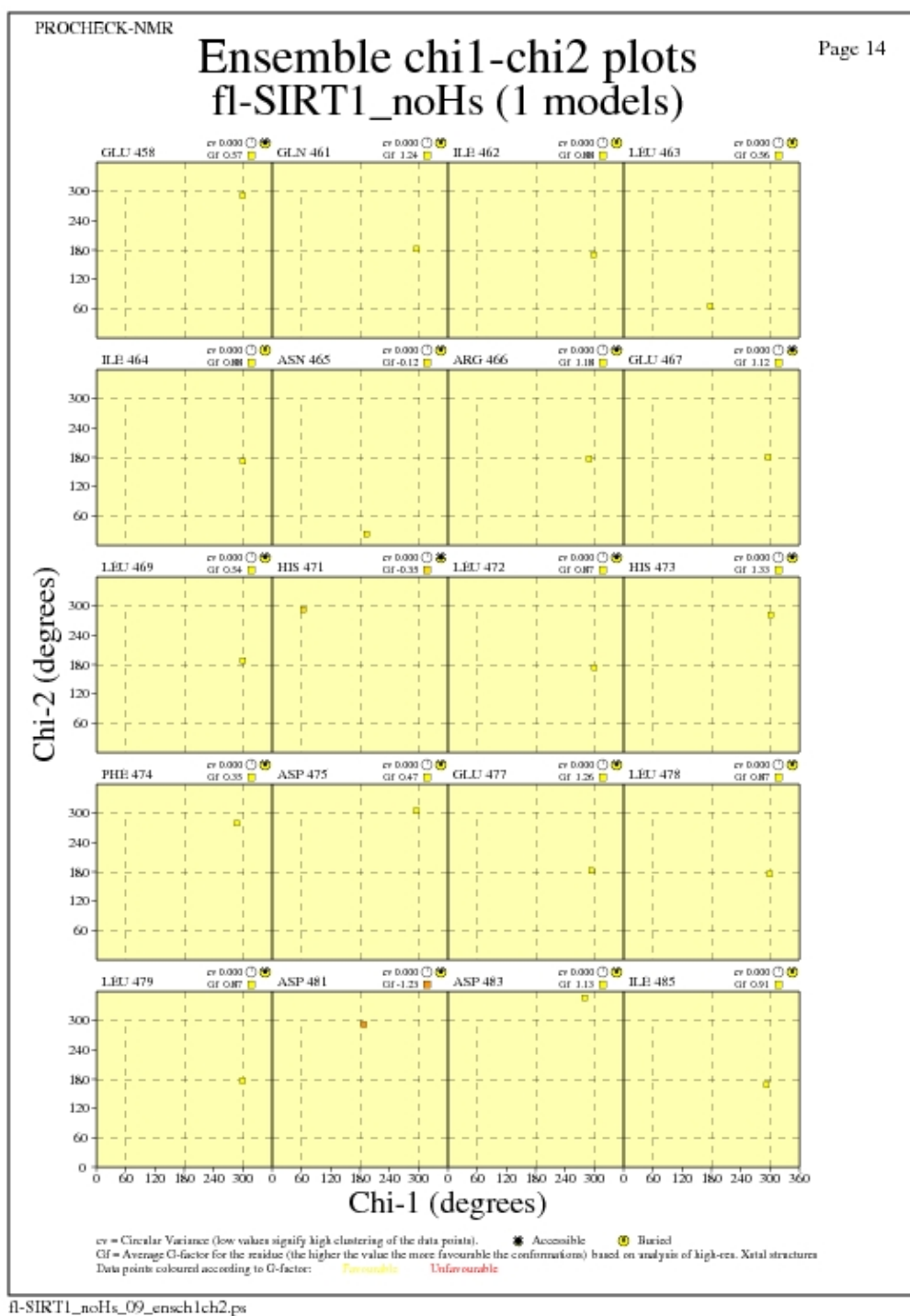
JPEG for residue Chi1-Chi2 Plots - page \$num_n



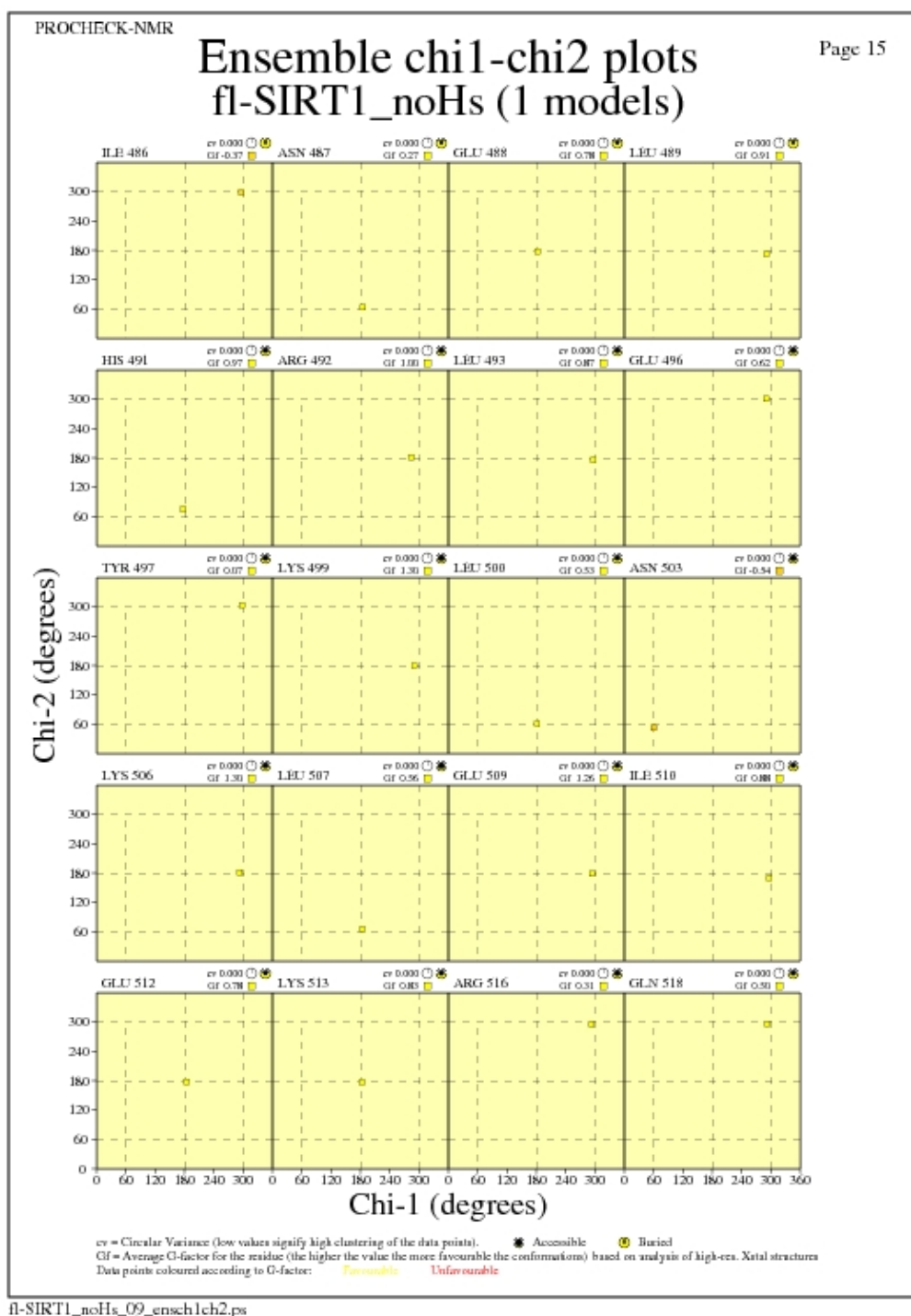
JPEG for residue Chi1-Chi2 Plots - page \$num_n



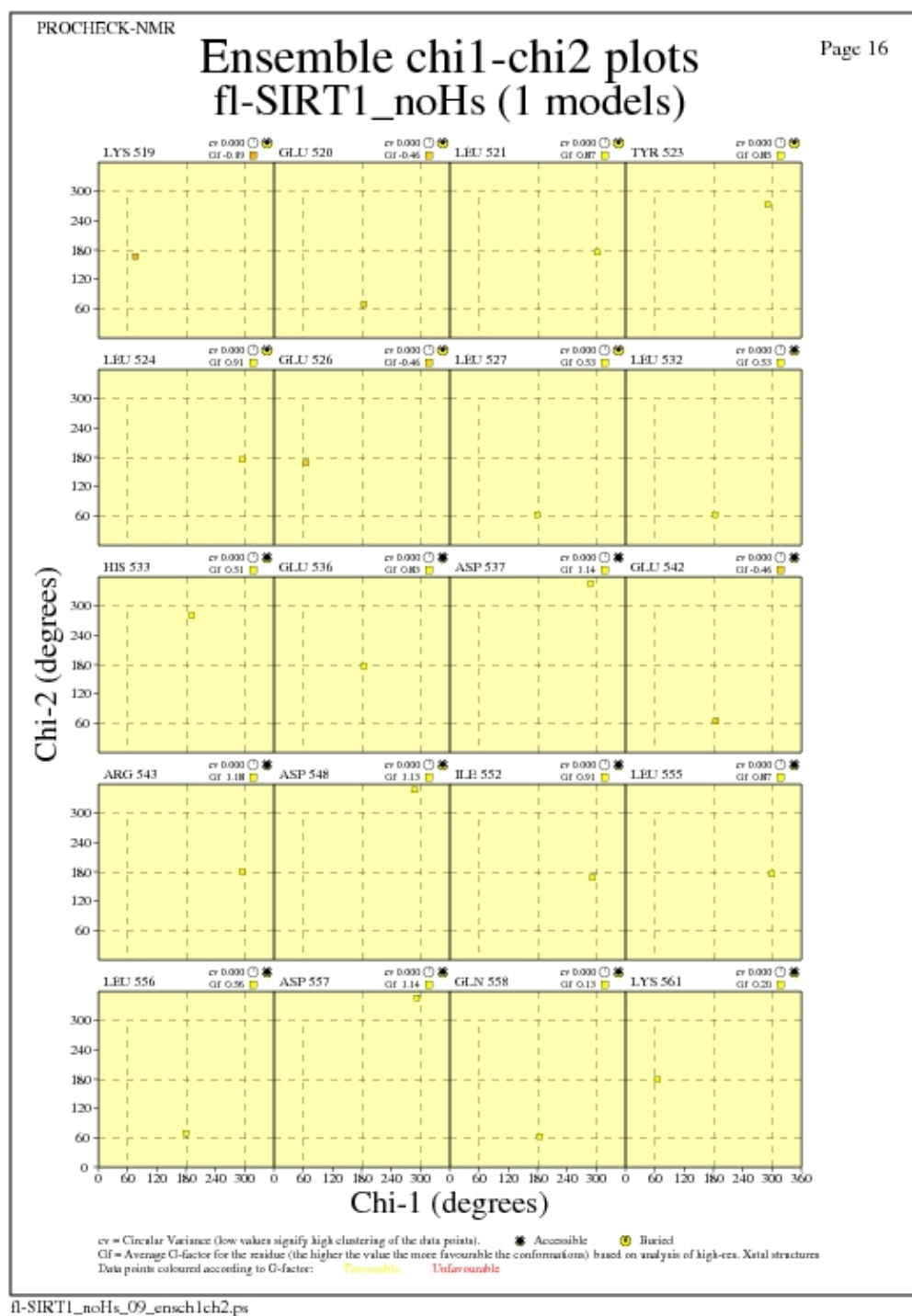
JPEG for residue Chi1-Chi2 Plots - page \$num_n



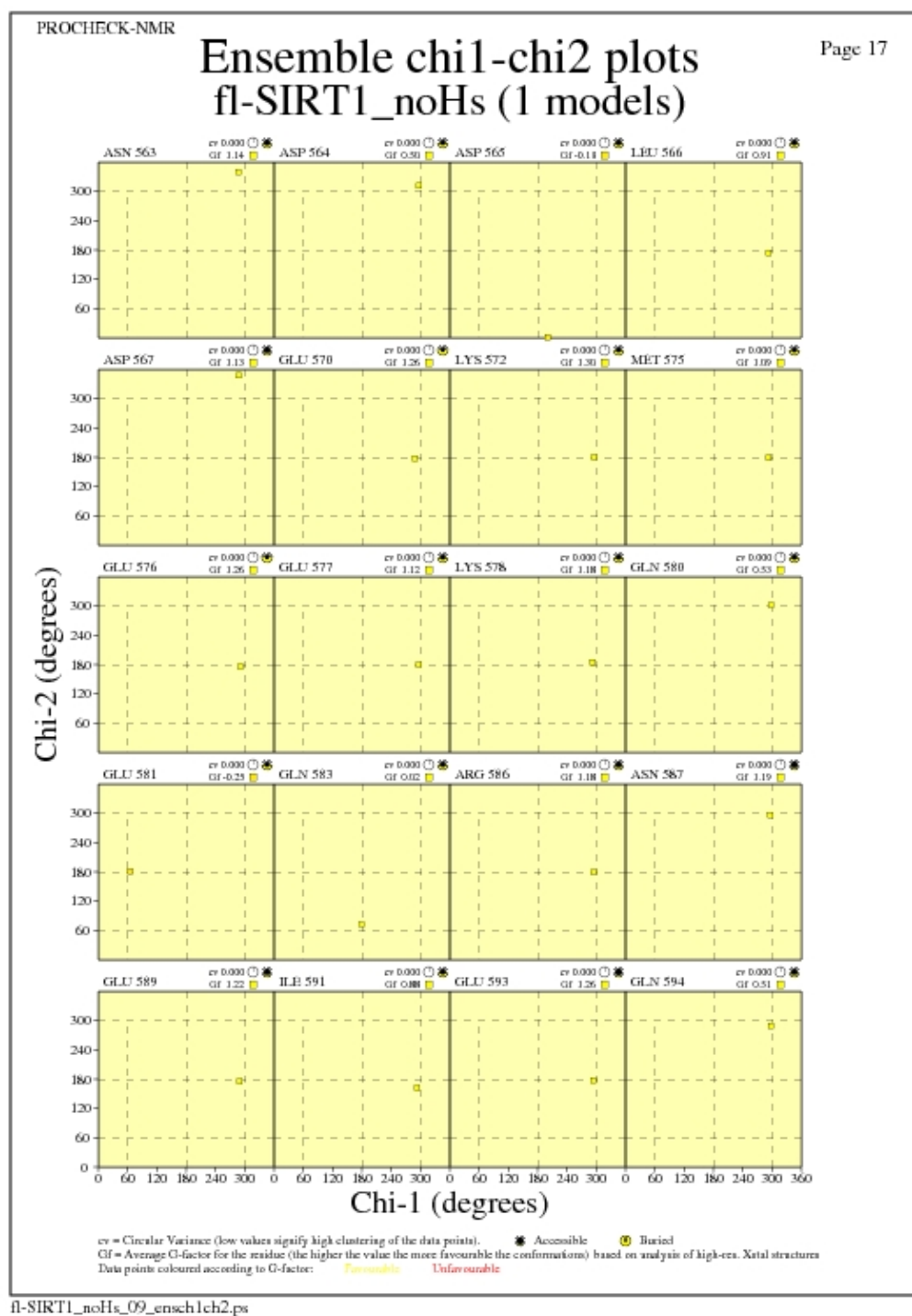
JPEG for residue Chi1-Chi2 Plots - page \$num_n



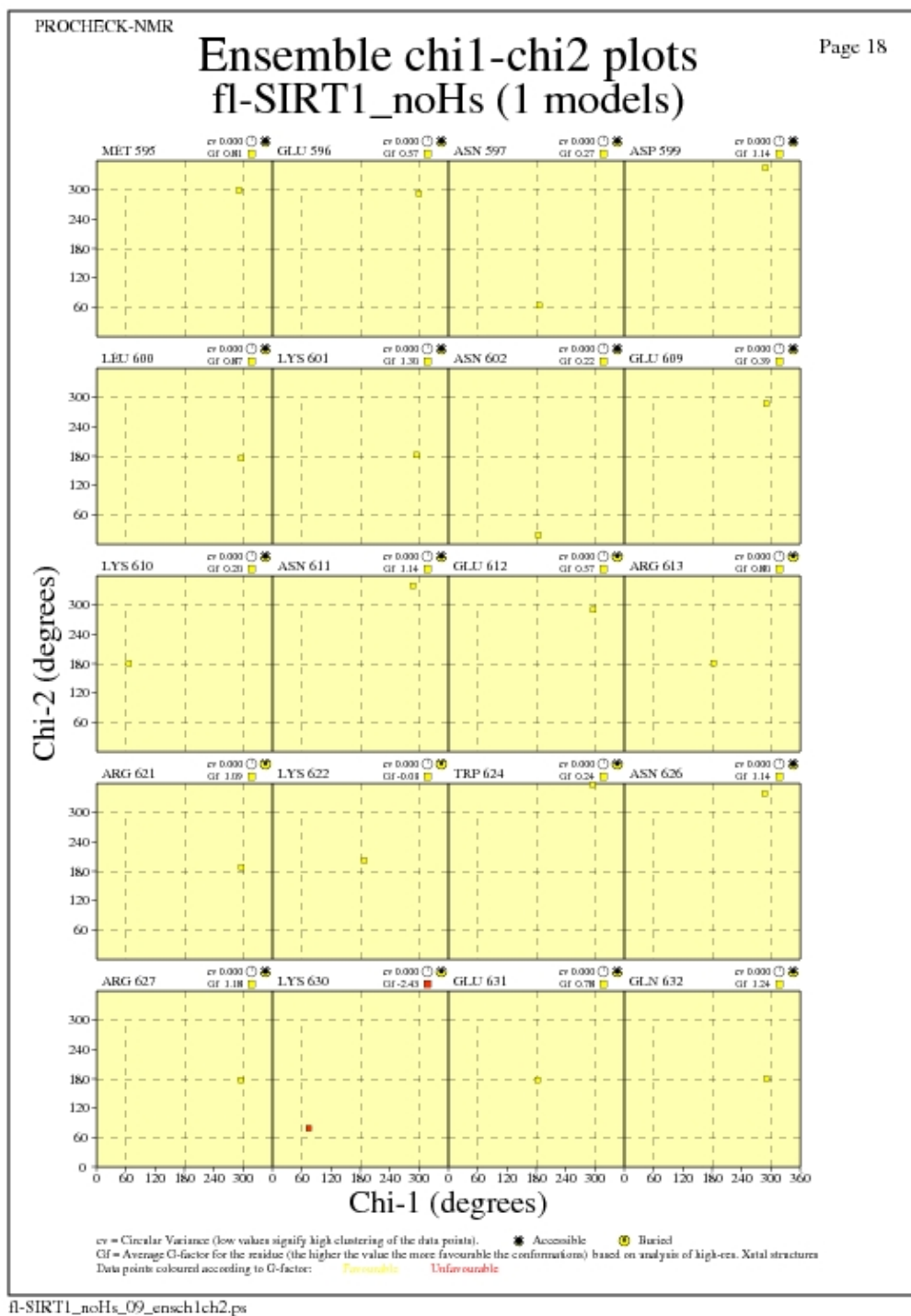
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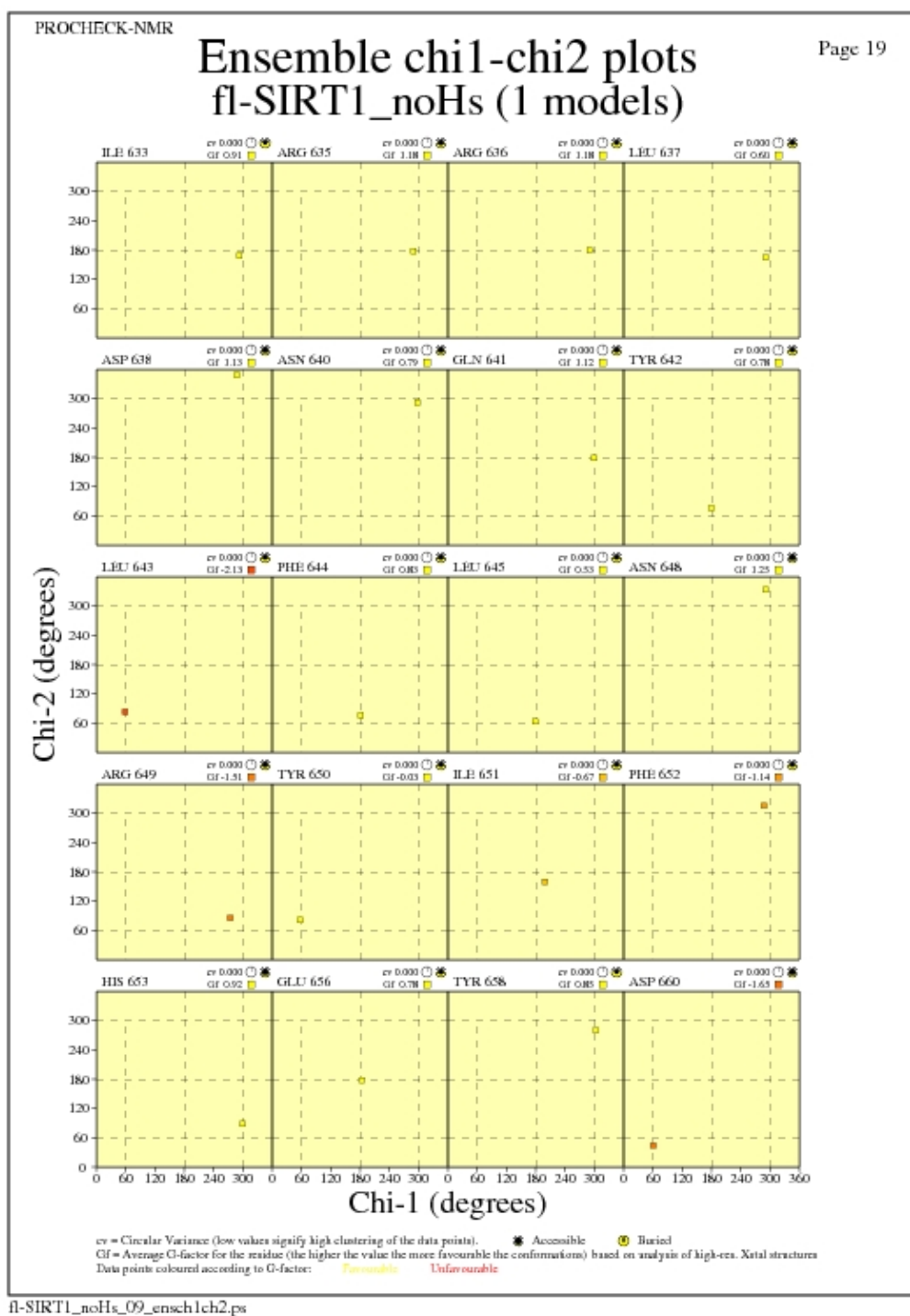
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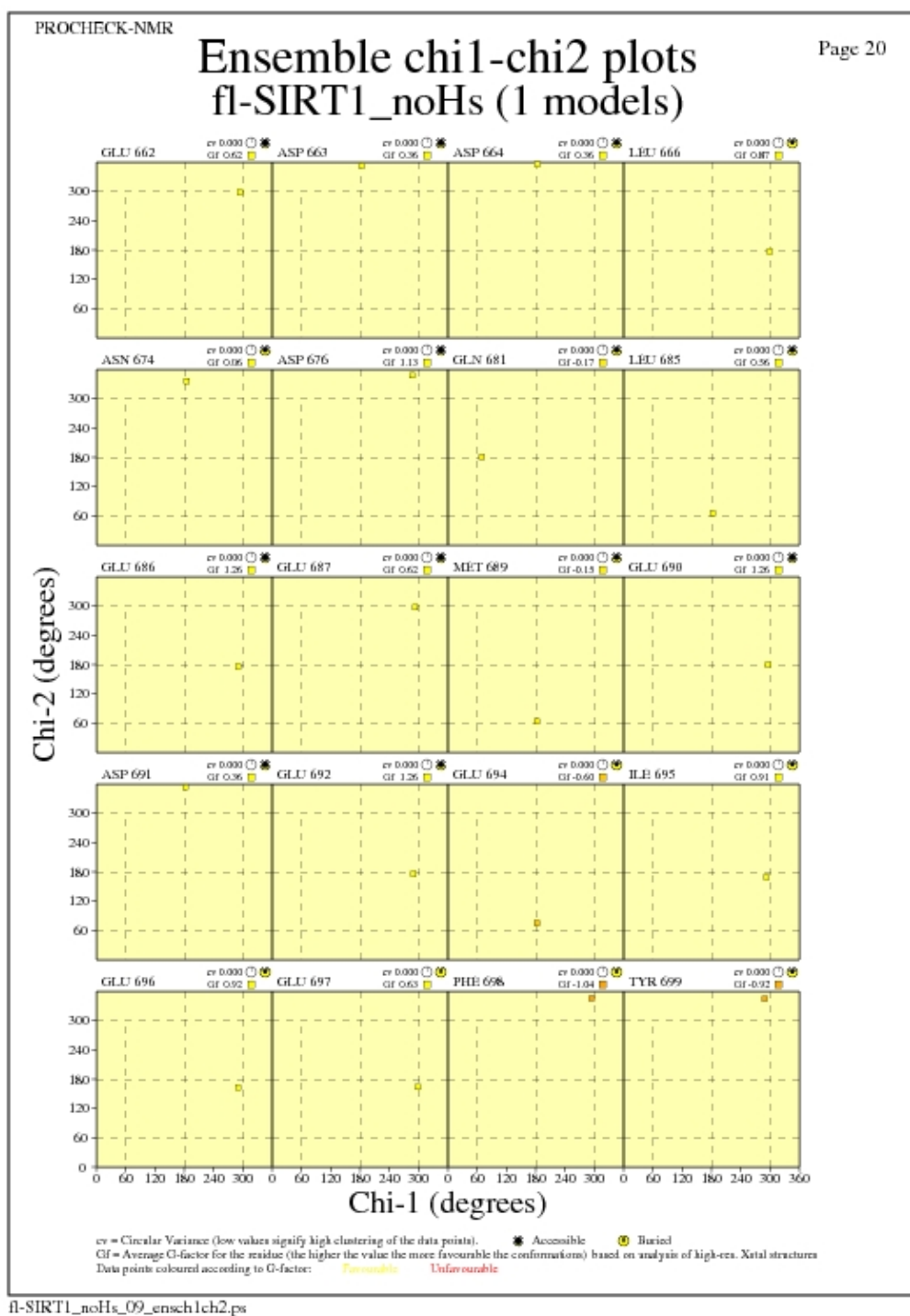
JPEG for residue Chi1-Chi2 Plots - page \$num_n



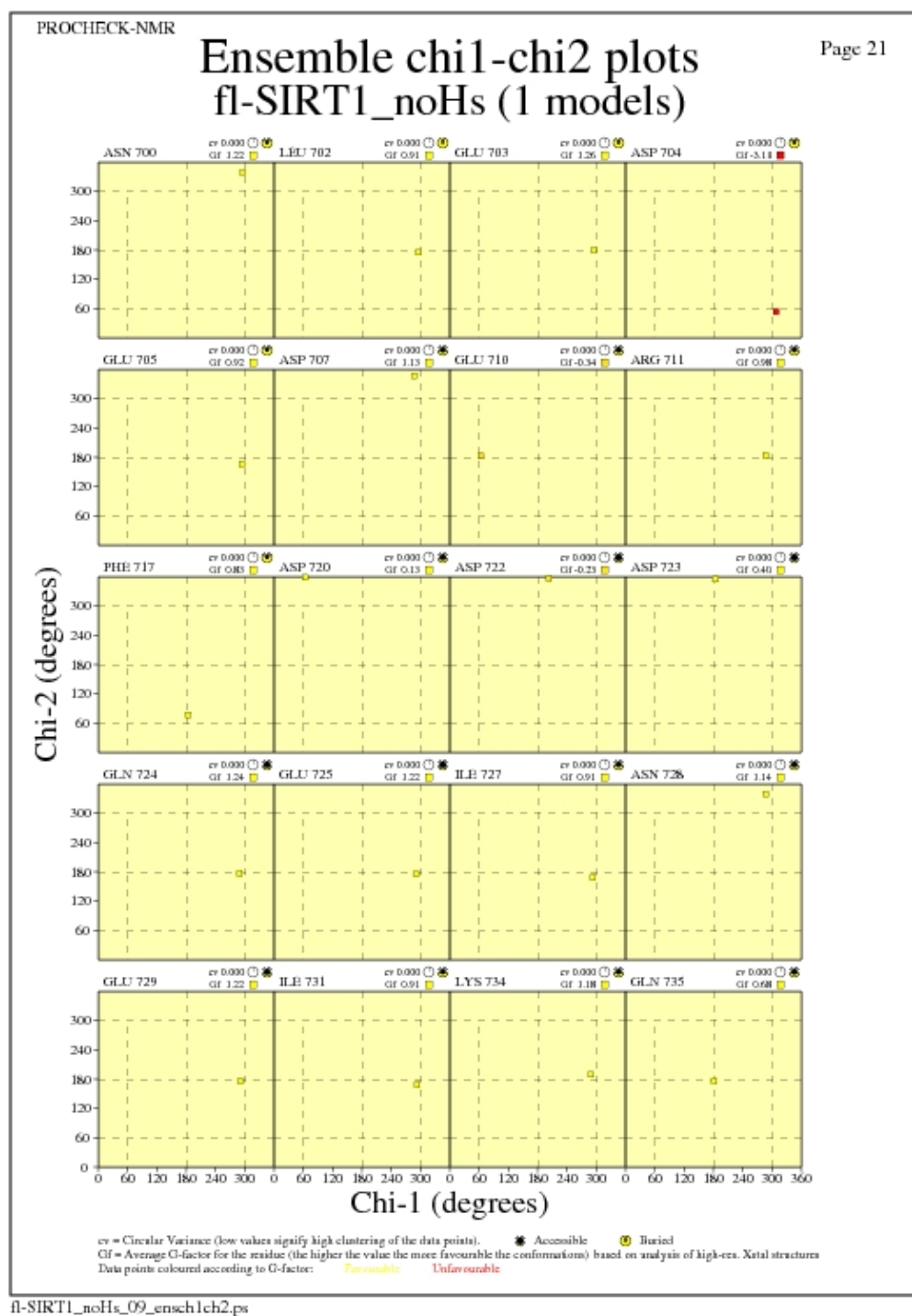
JPEG for residue Chi1-Chi2 Plots - page \$num_n



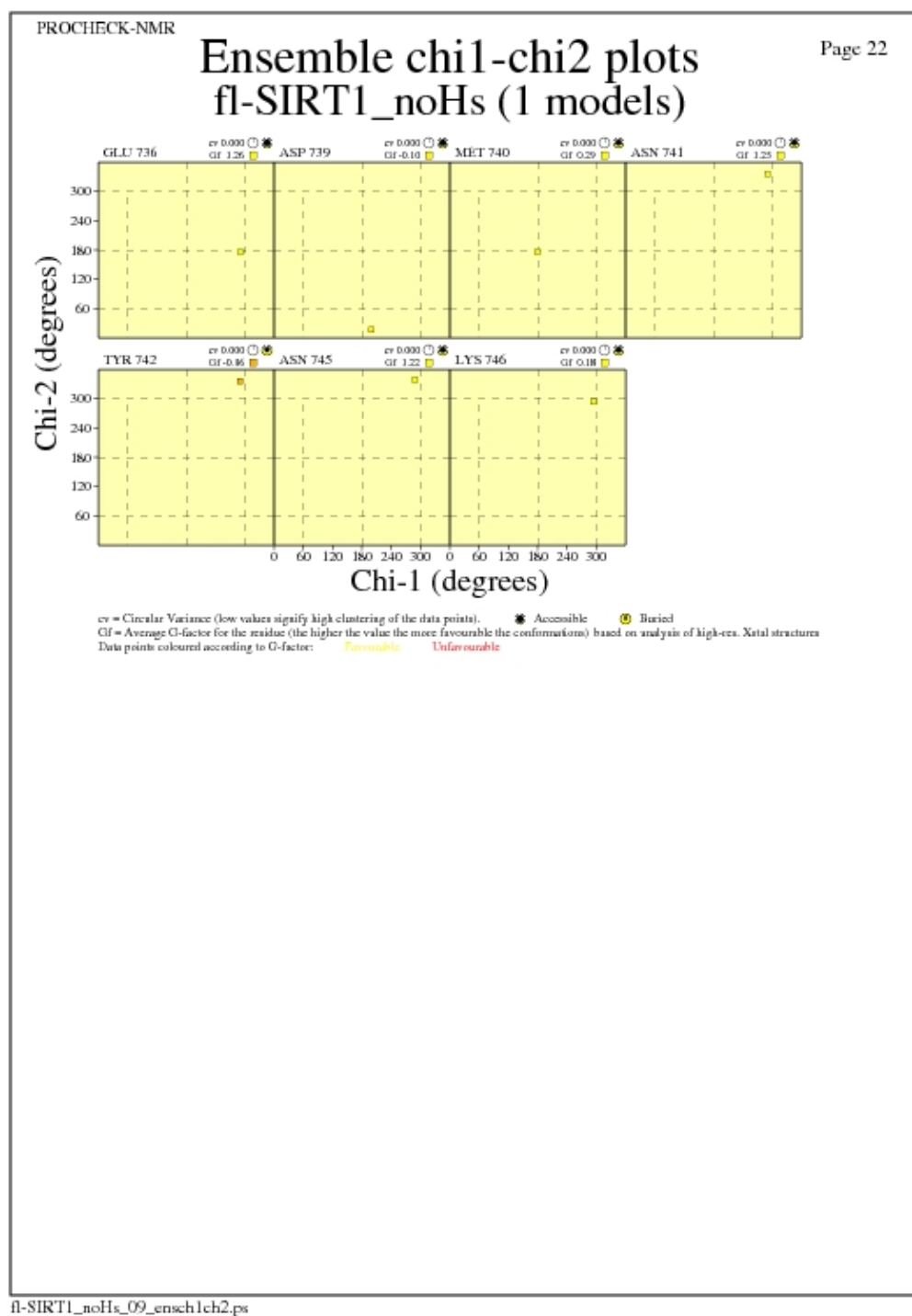
JPEG for residue Chi1-Chi2 Plots - page \$num_n



JPEG for residue Chi1-Chi2 Plots - page \$num_n



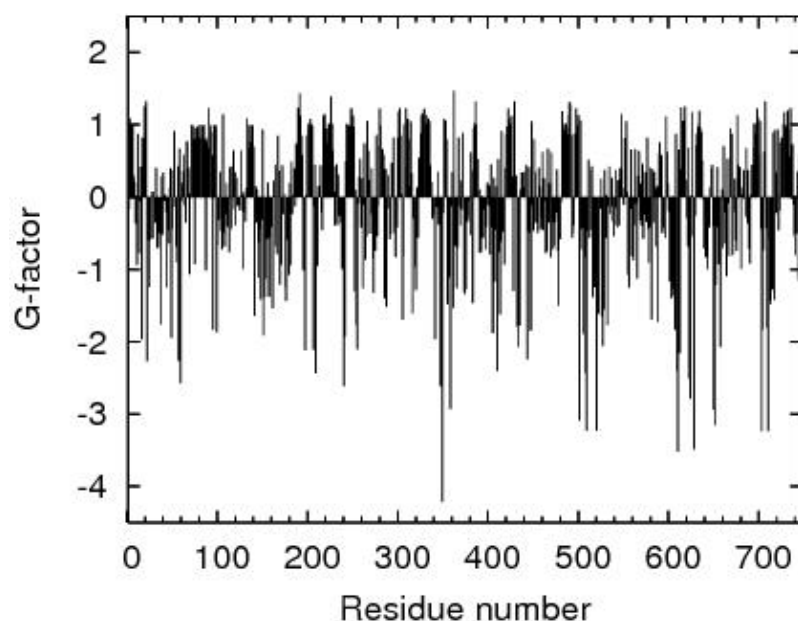
JPEG for residue Chi1-Chi2 Plots - page \$num_n



Procheck G-factors for phi-psi for each residue

JPEG image for residue phi-psi G-factors

Procheck G-factor for phi-psi

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

```
#phipsi_gfactor
#Residue\Model  average
2      -0.16
3       1.08
4       0.68
5       0.99
6       0.99
7       0.29
8       0.21
9      -0.36
10     -0.35
11     -0.94
12      0.87
13     -0.77
14     -0.06
15      0.42
16     -1.96
17      0.82
18      0.65
19      1.25
20      0.65
21      1.32
22     -2.27
23     -0.59
24     -0.52
25     -1.24
26      0.01
27     -0.57
28      0.07
29     -0.57
30     -0.09
31     -0.35
32      0.40
33     -0.70
34     -0.69
```


PSVS Software Environment

35	-0.49
36	-0.42
37	-1.76
38	0.28
39	-0.51
40	0.34
41	-0.05
42	0.03
43	-0.20
44	-1.25
45	-0.45
46	-0.64
47	0.13
48	0.40
49	-1.94
50	-0.43
51	0.37
52	0.91
53	-0.13
54	-0.68
55	-0.90
56	0.42
57	-2.26
58	0.67
59	-2.57
60	-0.05
61	0.19
62	0.36
63	0.58
64	-0.11
65	-0.35
66	0.77
67	0.35
68	0.40
69	-1.07
70	0.05
71	0.99
72	0.76
73	0.99
74	0.80
75	-0.92
76	0.95
77	0.96
78	0.68
79	0.99
80	0.82
81	0.99
82	0.82
83	0.99
84	0.99
85	0.99
86	0.80
87	-1.01
88	0.77
89	0.82
90	1.23
91	0.68
92	0.99
93	0.90
94	0.58
95	-1.83
96	0.99

PSVS Software Environment

97	0.80
98	0.99
99	-1.86
100	-0.66
101	-0.32
102	-0.30
103	0.34
104	-0.46
105	-0.72
106	1.14
107	-0.49
108	-0.68
109	-0.23
110	0.19
111	-0.40
112	-0.42
113	-0.76
114	0.40
115	0.42
116	-0.44
117	-0.16
118	0.64
119	0.34
120	-0.39
121	0.26
122	-0.11
123	-0.12
124	-0.09
125	-0.18
126	0.64
127	0.03
128	-0.99
129	0.06
130	-0.21
131	-0.34
132	0.12
133	1.08
134	0.68
135	0.99
136	0.76
137	0.99
138	0.99
139	0.99
140	0.69
141	-1.64
142	0.15
143	-0.35
144	0.11
145	-1.11
146	-0.62
147	-0.44
148	-1.41
149	-0.31
150	0.93
151	-1.91
152	-1.38
153	-1.12
154	-0.18
155	-0.57
156	0.20
157	-1.37
158	-0.55

PSVS Software Environment

159	-0.02
160	-0.41
161	-1.53
162	0.22
163	0.03
164	0.44
165	-0.67
166	-0.78
167	0.85
168	0.36
169	-1.21
170	-0.24
171	-0.93
172	0.43
173	-0.23
174	0.04
175	-1.24
176	-1.43
177	-0.58
178	-0.59
179	-1.07
180	0.19
181	-0.94
182	0.49
183	-0.23
184	0.03
185	0.40
186	-0.12
187	0.74
188	0.73
189	1.23
190	1.23
191	1.43
192	1.13
193	0.84
194	0.58
195	-1.01
196	-0.14
197	-2.11
198	0.02
199	0.85
200	0.94
201	1.01
202	0.21
203	1.08
204	0.99
205	0.99
206	-2.11
207	-0.12
208	0.44
209	-2.43
210	-0.25
211	-0.94
212	0.15
213	0.07
214	0.44
215	-0.20
216	-0.45
217	1.13
218	0.65
219	1.14
220	0.85

PSVS Software Environment

221	0.95
222	0.74
223	1.01
224	0.98
225	1.01
226	1.39
227	1.01
228	0.65
229	0.07
230	-0.39
231	0.42
232	0.45
233	-0.38
234	0.30
235	-0.26
236	-0.23
237	-0.35
238	-0.99
239	-0.60
240	-2.61
241	-1.92
242	0.50
243	1.01
244	0.87
245	0.99
246	0.99
247	0.98
248	1.22
249	0.99
250	1.13
251	0.97
252	-1.30
253	0.10
254	-1.77
255	-2.10
256	-0.09
257	0.28
258	0.53
259	-0.41
260	0.26
261	-1.26
262	-0.11
263	0.74
264	-0.87
265	-0.54
266	1.05
267	0.64
268	0.24
269	-0.50
270	-0.23
271	0.40
272	-0.85
273	-1.32
274	-0.42
275	-0.74
276	0.85
277	-0.54
278	-0.12
279	0.71
280	1.22
281	0.99
282	0.67

PSVS Software Environment

283	0.65
284	0.58
285	-1.40
286	0.39
287	-1.51
288	-0.15
289	0.30
290	-0.16
291	-0.58
292	-0.51
293	0.47
294	0.03
295	0.82
296	-0.49
297	-0.83
298	-0.06
299	-0.41
300	0.82
301	1.18
302	1.22
303	0.85
304	0.04
305	-1.69
306	-0.81
307	1.01
308	0.42
309	1.22
310	0.18
311	1.08
312	0.80
313	0.14
314	1.04
315	0.33
316	-1.60
317	-0.12
318	-0.30
319	-0.96
320	-1.28
321	0.13
322	-0.56
323	0.54
324	0.01
325	0.88
326	1.13
327	1.15
328	0.95
329	1.22
330	1.01
331	0.82
332	1.13
333	0.95
334	1.08
335	1.04
336	0.44
337	0.20
338	-0.29
339	-0.28
340	-0.24
341	-1.96
342	-0.02
343	-0.14
344	0.35

PSVS Software Environment

345	-0.37
346	-0.35
347	-2.61
348	-0.21
349	-4.21
350	-0.22
351	1.08
352	0.90
353	1.05
354	0.80
355	-1.48
356	-0.46
357	-1.10
358	-2.93
359	-0.12
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	-0.13
369	-0.39
370	0.22
371	-0.17
372	0.88
373	-1.31
374	-1.33
375	-1.27
376	-0.12
377	-0.33
378	-0.05
379	-0.27
380	-0.52
381	0.61
382	0.36
383	-1.46
384	0.96
385	1.02
386	1.32
387	1.01
388	0.08
389	0.52
390	-0.77
391	0.10
392	-0.76
393	0.01
394	-0.56
395	-0.17
396	-0.15
397	-0.72
398	-0.41
399	0.19
400	-0.11
401	0.16
402	-0.79
403	0.45
404	-0.41
405	-1.88
406	0.26

PSVS Software Environment

407	-1.17
408	-0.45
409	0.15
410	-2.40
411	0.52
412	-0.76
413	-1.62
414	-0.62
415	0.91
416	-0.48
417	-0.48
418	-0.93
419	0.40
420	0.87
421	0.97
422	1.22
423	1.08
424	1.01
425	0.99
426	1.12
427	0.28
428	-1.29
429	1.32
430	0.17
431	0.29
432	-1.79
433	-2.07
434	-1.24
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	-2.24
444	-0.47
445	0.41
446	-0.49
447	-1.84
448	1.05
449	-0.11
450	-0.46
451	0.80
452	0.35
453	-0.35
454	-0.25
455	-0.50
456	0.40
457	0.14
458	-0.44
459	-0.27
460	0.62
461	-0.45
462	0.26
463	-0.05
464	-0.77
465	-0.74
466	0.67
467	-0.35
468	0.19

PSVS Software Environment

469	-0.83
470	0.62
471	-0.35
472	-0.72
473	-0.67
474	-0.34
475	-0.21
476	0.38
477	-0.74
478	-1.50
479	-0.04
480	-0.58
481	-0.07
482	1.18
483	0.93
484	0.37
485	1.01
486	1.01
487	0.96
488	0.87
489	1.13
490	1.31
491	1.28
492	0.85
493	-0.56
494	-0.50
495	-0.39
496	0.87
497	1.22
498	0.99
499	0.95
500	1.13
501	-3.08
502	1.06
503	-0.44
504	-0.72
505	-1.89
506	-0.42
507	-0.82
508	-2.42
509	-3.23
510	-0.46
511	0.51
512	-0.56
513	-0.45
514	0.37
515	0.42
516	-1.38
517	-0.40
518	-1.24
519	-0.20
520	-3.23
521	-0.22
522	-1.60
523	0.00
524	-0.16
525	0.25
526	-1.64
527	-2.06
528	-1.55
529	0.37
530	-0.56

PSVS Software Environment

531	0.03
532	-1.77
533	-0.12
534	0.42
535	-0.23
536	-0.12
537	0.26
538	-0.33
539	-0.54
540	-0.14
541	0.37
542	-0.39
543	-0.41
544	0.23
545	-0.39
546	0.40
547	0.02
548	1.14
549	0.12
550	-0.10
551	0.81
552	0.71
553	1.05
554	0.06
555	-1.07
556	-1.25
557	-0.81
558	0.65
559	-0.16
560	-0.82
561	-0.87
562	-0.39
563	0.66
564	-0.09
565	-1.12
566	0.29
567	0.64
568	-0.32
569	0.18
570	-0.39
571	0.46
572	-0.57
573	-0.24
574	0.35
575	-0.34
576	0.82
577	-0.43
578	-0.91
579	0.40
580	-0.41
581	-1.69
582	0.39
583	-0.35
584	0.34
585	0.10
586	-0.68
587	0.14
588	-1.72
589	0.61
590	0.75
591	0.58
592	0.58

PSVS Software Environment

593	-0.49
594	-0.41
595	-0.17
596	-0.56
597	1.11
598	0.62
599	0.19
600	-0.20
601	-1.16
602	-0.55
603	-1.40
604	-1.26
605	0.01
606	-1.35
607	-1.83
608	0.87
609	-2.40
610	-3.52
611	0.66
612	-2.15
613	0.38
614	1.24
615	0.74
616	1.05
617	0.99
618	1.25
619	0.23
620	-0.28
621	-0.68
622	0.68
623	-2.50
624	-2.78
625	0.02
626	1.17
627	-0.54
628	-3.49
629	-0.26
630	0.71
631	0.87
632	0.97
633	1.01
634	1.19
635	0.96
636	0.90
637	0.50
638	-0.03
639	-0.71
640	-0.61
641	-0.82
642	-0.01
643	-1.00
644	-0.04
645	-0.41
646	0.13
647	0.40
648	0.44
649	-2.93
650	-0.40
651	-3.15
652	-1.21
653	-0.41
654	0.41

PSVS Software Environment

655	-0.92
656	-0.28
657	-2.07
658	-0.01
659	0.10
660	-0.70
661	0.70
662	-0.21
663	-0.64
664	-1.09
665	0.53
666	-0.08
667	-0.81
668	0.95
669	0.46
670	0.87
671	-0.80
672	-0.20
673	0.25
674	-0.59
675	-0.74
676	1.13
677	0.45
678	0.41
679	0.41
680	-0.99
681	0.03
682	0.13
683	0.37
684	-0.02
685	-0.27
686	0.68
687	-0.36
688	0.37
689	-0.71
690	-0.92
691	0.03
692	0.44
693	0.30
694	0.68
695	1.01
696	0.87
697	0.68
698	1.22
699	1.09
700	0.59
701	1.05
702	-0.43
703	-3.23
704	-1.83
705	-0.73
706	0.62
707	1.32
708	-0.43
709	-1.80
710	-3.23
711	-0.57
712	-1.43
713	-1.48
714	-0.96
715	-1.28
716	0.89

717	-1.41
718	0.93
719	-0.22
720	0.34
721	0.93
722	-0.46
723	-0.18
724	0.75
725	0.82
726	0.80
727	1.01
728	1.17
729	0.82
730	0.99
731	0.58
732	1.19
733	0.56
734	0.95
735	1.23
736	0.68
737	0.73
738	-0.10
739	-0.53
740	-0.80
741	-0.19
742	-0.50
743	0.35
744	-1.16
745	0.59
746	-0.01
#Reported_Model_Average -0.075	
#Overall_Average_Reported -0.075	

Procheck G-factors for all dihedral angles for each residue

JPEG image for residue all dihedral G-factors

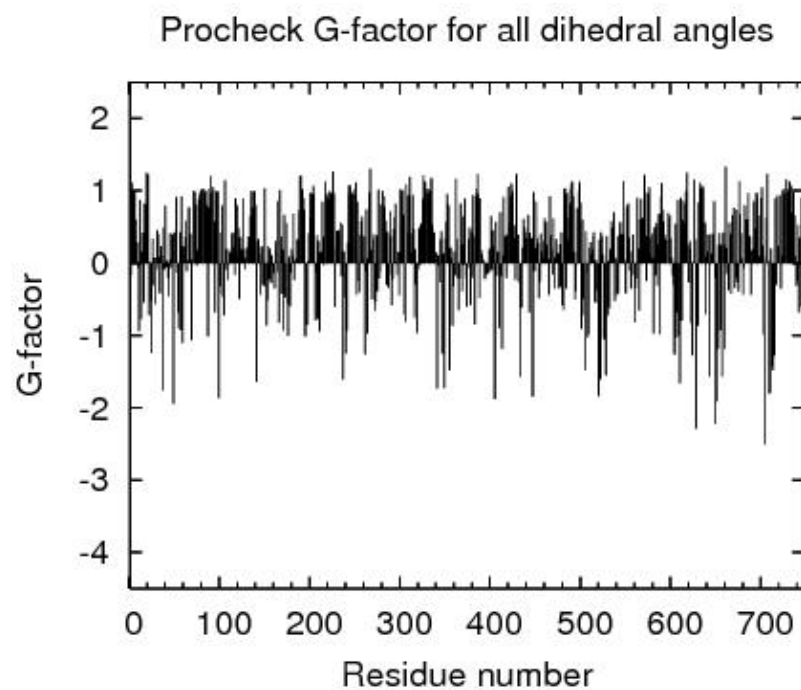


Table of Procheck G-factors for all dihedrals for ordered residues

```

#alldih_gfactor
#Residue\Model  average
1      0.84
2     -0.16
3      1.11
4      0.97
5      0.99
6      0.99
7      0.60
8      0.21
9      0.28
10     -0.06
11     -0.94
12      0.87
13     -0.77
14      0.16
15      0.42
16     -0.54
17      0.82
18      0.65
19      1.25
20      0.65
21      1.23
22     -0.72
23      0.01
24     -0.52
25     -1.24
26      0.34
27     -0.30
28      0.07
29     -0.57
30     -0.09
31      0.45
32      0.40
33      0.09
34     -0.41
35      0.23
36      0.11
37     -1.76
38      0.49
39     -0.08
40      0.80
41     -0.05
42      0.03
43     -0.20
44     -0.46
45      0.41
46     -0.06
47      0.05
48      0.40
49     -1.94
50      0.42
51      0.37
52      0.91
53     -0.13
54     -0.68
55     -0.90
56      0.42
57     -0.92
58      0.92

```

PSVS Software Environment

59	-1.10
60	0.23
61	0.19
62	0.36
63	0.58
64	-0.11
65	0.03
66	0.77
67	0.24
68	0.40
69	-1.07
70	0.05
71	0.99
72	0.76
73	0.99
74	0.80
75	-0.03
76	0.19
77	0.88
78	0.95
79	0.99
80	1.02
81	0.99
82	1.02
83	0.99
84	0.99
85	0.99
86	0.80
87	-1.01
88	0.77
89	1.02
90	1.20
91	0.97
92	0.99
93	1.04
94	0.58
95	-0.68
96	0.99
97	0.80
98	0.99
99	-1.86
100	-0.41
101	-0.32
102	0.42
103	0.79
104	-0.46
105	-0.72
106	1.14
107	0.19
108	-0.09
109	-0.23
110	0.19
111	-0.01
112	0.15
113	0.01
114	0.40
115	0.42
116	0.22
117	-0.16
118	0.89
119	0.80
120	0.09

PSVS Software Environment

121	0.48
122	-0.49
123	0.36
124	0.19
125	0.09
126	0.89
127	0.19
128	-0.08
129	0.06
130	0.20
131	0.22
132	0.36
133	0.29
134	0.65
135	0.99
136	0.76
137	0.99
138	0.99
139	0.99
140	0.80
141	-1.64
142	0.30
143	0.33
144	0.23
145	-0.44
146	0.13
147	0.22
148	-0.29
149	-0.31
150	1.03
151	-0.32
152	-0.86
153	-0.51
154	0.23
155	-0.22
156	0.20
157	-0.27
158	0.10
159	-0.02
160	-0.14
161	-0.35
162	0.30
163	0.19
164	0.85
165	-0.12
166	-0.82
167	1.01
168	0.36
169	-0.42
170	0.19
171	-0.93
172	0.66
173	-0.47
174	0.55
175	-0.56
176	-1.00
177	0.09
178	-0.59
179	-0.13
180	0.19
181	0.11
182	0.68

PSVS Software Environment

183	-0.23
184	0.03
185	0.06
186	0.32
187	0.00
188	0.73
189	1.20
190	1.20
191	0.54
192	1.02
193	0.89
194	0.74
195	-1.01
196	-0.51
197	-0.85
198	0.02
199	0.41
200	0.61
201	0.96
202	0.56
203	0.96
204	1.06
205	0.95
206	-0.79
207	-0.12
208	0.38
209	-0.77
210	0.31
211	-0.94
212	0.15
213	0.07
214	0.85
215	0.36
216	-0.03
217	1.13
218	0.73
219	0.95
220	0.88
221	0.79
222	0.99
223	0.96
224	0.95
225	0.96
226	1.26
227	0.96
228	-0.60
229	0.22
230	0.44
231	0.42
232	0.45
233	0.38
234	0.55
235	-0.18
236	0.53
237	-1.60
238	0.16
239	-0.47
240	-1.25
241	-0.93
242	0.28
243	0.96
244	1.07

PSVS Software Environment

245	1.06
246	0.99
247	0.95
248	0.63
249	0.95
250	1.02
251	1.11
252	-0.43
253	0.85
254	-0.24
255	-0.40
256	0.39
257	0.58
258	0.64
259	0.06
260	0.37
261	-1.26
262	-0.11
263	0.74
264	-0.97
265	0.06
266	0.98
267	1.30
268	0.19
269	-0.50
270	0.32
271	0.40
272	-0.66
273	-0.53
274	0.38
275	-0.39
276	1.01
277	-0.21
278	-0.12
279	0.81
280	0.15
281	0.99
282	0.92
283	0.78
284	0.58
285	-0.30
286	0.43
287	-0.33
288	-0.15
289	0.72
290	0.37
291	-0.58
292	-0.22
293	0.47
294	0.63
295	0.82
296	0.02
297	-0.17
298	0.15
299	-0.44
300	1.02
301	0.98
302	0.99
303	1.01
304	0.67
305	-0.70
306	-0.81

PSVS Software Environment

307	1.09
308	0.42
309	0.93
310	0.50
311	1.19
312	0.40
313	0.14
314	0.94
315	0.47
316	-0.75
317	0.19
318	-0.30
319	-0.96
320	-0.08
321	0.48
322	-0.02
323	0.54
324	0.45
325	0.89
326	1.21
327	0.49
328	1.12
329	1.03
330	0.96
331	0.82
332	1.02
333	1.00
334	0.62
335	1.17
336	0.53
337	0.20
338	0.42
339	0.14
340	0.15
341	-1.73
342	0.10
343	-0.04
344	-0.26
345	0.32
346	0.43
347	-1.25
348	0.13
349	-1.72
350	0.34
351	0.57
352	0.95
353	0.82
354	0.80
355	-1.48
356	0.21
357	0.07
358	-0.87
359	-0.32
360	0.16
361	-0.17
362	1.17
363	0.33
364	-0.20
365	-0.65
366	-0.21
367	0.82
368	0.25

PSVS Software Environment

369	-0.39
370	0.64
371	-0.02
372	0.89
373	-0.20
374	-0.60
375	-0.06
376	0.33
377	0.49
378	-0.57
379	0.43
380	-0.20
381	0.94
382	0.36
383	-0.85
384	0.92
385	1.02
386	1.23
387	0.96
388	-0.48
389	0.89
390	0.18
391	0.12
392	0.05
393	0.01
394	-0.22
395	-0.02
396	-0.15
397	-0.01
398	-0.14
399	0.19
400	-0.11
401	0.65
402	-0.09
403	0.45
404	0.23
405	-1.88
406	0.57
407	-0.17
408	0.16
409	0.15
410	-0.89
411	0.70
412	-0.18
413	-1.18
414	0.10
415	0.91
416	0.15
417	0.37
418	-0.20
419	0.40
420	1.05
421	0.55
422	0.93
423	1.10
424	1.09
425	0.99
426	0.34
427	0.52
428	-0.23
429	1.23
430	0.18

PSVS Software Environment

431	0.39
432	-0.26
433	-1.57
434	-0.55
435	-0.61
436	0.21
437	0.61
438	0.49
439	0.42
440	0.13
441	0.34
442	0.66
443	-0.68
444	0.42
445	0.34
446	0.34
447	-1.84
448	0.98
449	-0.11
450	0.21
451	0.85
452	0.35
453	0.27
454	-0.48
455	-0.26
456	0.40
457	0.16
458	0.07
459	0.30
460	0.62
461	0.39
462	0.57
463	0.25
464	0.05
465	-0.43
466	0.92
467	0.38
468	0.19
469	-0.15
470	0.62
471	-0.35
472	0.07
473	0.33
474	0.00
475	0.13
476	-0.35
477	0.26
478	-0.32
479	0.42
480	-0.58
481	-0.65
482	1.02
483	1.03
484	-0.35
485	0.96
486	0.32
487	0.62
488	0.83
489	1.02
490	1.09
491	1.13
492	0.92

PSVS Software Environment

493	0.15
494	-0.50
495	-0.39
496	0.75
497	0.65
498	0.99
499	1.12
500	0.83
501	-0.90
502	0.60
503	-0.49
504	-0.72
505	-1.48
506	0.44
507	-0.13
508	-1.02
509	-0.98
510	0.21
511	0.28
512	0.11
513	0.19
514	0.37
515	0.42
516	-0.54
517	0.04
518	-0.37
519	-0.54
520	-1.84
521	0.32
522	-1.60
523	0.42
524	0.37
525	0.11
526	-1.05
527	-0.77
528	-1.55
529	0.37
530	-0.72
531	0.03
532	-0.62
533	0.19
534	0.58
535	0.49
536	0.36
537	0.70
538	-0.52
539	0.06
540	-0.43
541	0.37
542	-0.42
543	0.39
544	0.56
545	0.13
546	0.40
547	0.02
548	1.13
549	0.04
550	-0.41
551	0.77
552	0.81
553	0.82
554	0.35

PSVS Software Environment

555	-0.10
556	-0.35
557	0.16
558	0.39
559	-0.16
560	-0.82
561	-0.34
562	-0.21
563	0.90
564	0.20
565	-0.65
566	0.60
567	0.89
568	0.38
569	0.62
570	0.43
571	1.22
572	0.37
573	-0.24
574	0.97
575	0.38
576	1.04
577	0.35
578	0.13
579	0.40
580	0.06
581	-0.97
582	0.49
583	-0.17
584	0.55
585	-0.31
586	0.25
587	0.67
588	-0.98
589	0.92
590	1.10
591	0.73
592	0.58
593	0.39
594	0.05
595	0.32
596	0.00
597	0.69
598	0.62
599	0.66
600	0.34
601	0.07
602	-0.17
603	-0.30
604	-1.26
605	0.54
606	-1.03
607	-0.68
608	0.87
609	-1.00
610	-1.66
611	0.90
612	-0.79
613	0.59
614	0.86
615	0.55
616	0.82

PSVS Software Environment

617	0.99
618	1.25
619	0.26
620	-0.26
621	0.20
622	0.30
623	-0.82
624	-1.27
625	0.02
626	1.15
627	0.32
628	-2.29
629	-0.26
630	-0.86
631	0.83
632	1.11
633	0.96
634	1.03
635	1.07
636	1.04
637	0.55
638	0.55
639	-0.71
640	0.09
641	0.15
642	0.39
643	-1.57
644	0.40
645	0.06
646	0.13
647	0.40
648	0.85
649	-2.22
650	-0.21
651	-1.91
652	-1.18
653	0.25
654	0.41
655	-0.92
656	0.25
657	-1.57
658	0.42
659	0.24
660	-1.18
661	1.33
662	0.20
663	-0.14
664	-0.37
665	0.56
666	0.40
667	-0.42
668	0.66
669	0.67
670	0.76
671	-0.34
672	-0.20
673	0.73
674	-0.26
675	-0.39
676	1.13
677	0.67
678	0.41

PSVS Software Environment

679	0.06
680	-0.43
681	-0.07
682	0.80
683	0.37
684	0.60
685	0.14
686	0.97
687	0.13
688	0.37
689	-0.43
690	0.17
691	0.19
692	0.85
693	0.48
694	0.04
695	0.96
696	0.90
697	0.66
698	0.09
699	0.08
700	0.90
701	1.05
702	0.24
703	-0.98
704	-2.51
705	0.09
706	0.62
707	1.23
708	0.03
709	-1.80
710	-1.78
711	0.20
712	-1.43
713	-1.48
714	-0.96
715	-1.28
716	0.89
717	-0.29
718	0.93
719	0.03
720	0.23
721	0.93
722	-0.35
723	0.11
724	0.99
725	1.02
726	0.80
727	0.96
728	1.15
729	1.02
730	0.99
731	0.74
732	1.12
733	0.69
734	1.06
735	0.95
736	0.97
737	0.66
738	0.10
739	-0.31
740	-0.25


```

741      0.53
742     -0.68
743      0.35
744     -0.60
745      0.90
746      0.08
747     -0.03
#Reported_Model_Average 0.192
#Overall_Average_Reported      0.192

```

Output from Verify3D

Verify3D Score over a window of \$wsize_s residues

JPEG image for Verify3D Score

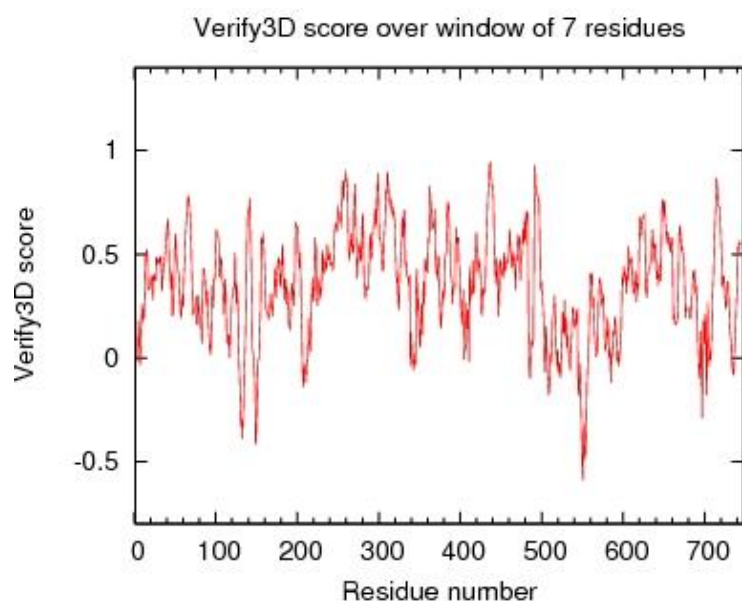


Table of Verify3D scores for ordered residues across all models

```

#verify3d
#Residue\Model  only_model
1      -0.83
2      -0.25
3       0.23
4      -0.59
5       0.14
6       0.49
7       0.77
8       0.49
9      -0.68
10     -0.87
11     -0.07
12      1.10
13      1.10
14      0.17
15      0.64
16      0.34
17      0.14

```

PSVS Software Environment

18	0.14
19	1.10
20	-0.25
21	0.23
22	0.71
23	0.28
24	0.49
25	0.14
26	0.34
27	0.59
28	0.25
29	0.49
30	1.10
31	0.28
32	0.25
33	0.29
34	0.71
35	0.08
36	0.71
37	-0.11
38	0.71
39	0.71
40	0.34
41	1.10
42	0.44
43	1.10
44	0.29
45	0.28
46	-0.44
47	0.17
48	0.44
49	1.10
50	-0.46
51	0.44
52	1.10
53	1.10
54	0.49
55	-0.25
56	0.64
57	-0.59
58	0.24
59	0.28
60	0.66
61	0.44
62	0.49
63	0.14
64	0.49
65	0.71
66	1.10
67	1.29
68	0.64
69	1.10
70	0.14
71	0.14
72	0.14
73	0.49
74	0.14
75	-0.68
76	1.12
77	0.24
78	0.28
79	0.49

PSVS Software Environment

80	-0.46
81	0.14
82	0.28
83	0.49
84	0.14
85	0.14
86	-0.25
87	1.10
88	1.10
89	0.28
90	0.25
91	-0.46
92	-0.25
93	0.25
94	0.14
95	0.55
96	-0.25
97	0.14
98	0.49
99	1.10
100	-0.46
101	1.10
102	0.51
103	0.51
104	1.10
105	0.25
106	1.10
107	-0.68
108	-0.03
109	1.10
110	0.44
111	0.34
112	0.24
113	0.04
114	0.25
115	0.25
116	-0.68
117	0.14
118	0.23
119	0.51
120	-0.68
121	1.25
122	0.51
123	0.04
124	0.23
125	0.51
126	0.51
127	0.51
128	-0.46
129	1.10
130	-0.46
131	-1.13
132	-0.46
133	-0.46
134	-0.46
135	-0.25
136	0.49
137	0.49
138	0.14
139	0.49
140	0.81
141	1.10

PSVS Software Environment

142	1.25
143	0.71
144	0.51
145	0.51
146	-0.68
147	-1.14
148	-0.84
149	1.10
150	0.23
151	0.04
152	-1.63
153	-0.28
154	0.08
155	0.41
156	1.10
157	1.04
158	1.04
159	0.59
160	-0.35
161	0.28
162	0.17
163	0.34
164	0.28
165	0.28
166	0.51
167	-0.41
168	0.14
169	0.34
170	1.04
171	-0.25
172	0.34
173	0.17
174	0.34
175	0.23
176	1.12
177	0.08
178	0.44
179	0.71
180	0.44
181	0.24
182	-0.54
183	1.10
184	0.64
185	1.25
186	0.08
187	-0.84
188	1.00
189	-0.57
190	0.25
191	1.04
192	1.06
193	-0.83
194	-0.94
195	1.10
196	0.55
197	0.51
198	0.64
199	0.71
200	0.08
201	0.93
202	1.06
203	0.47

PSVS Software Environment

204	0.51
205	-0.33
206	0.29
207	0.64
208	-1.13
209	0.55
210	-0.94
211	-0.07
212	0.44
213	0.25
214	0.04
215	-0.33
216	0.51
217	0.51
218	-0.83
219	0.08
220	1.06
221	1.12
222	0.25
223	-0.28
224	1.00
225	0.81
226	-0.26
227	-0.54
228	0.77
229	0.59
230	0.28
231	0.64
232	0.59
233	0.08
234	0.71
235	0.08
236	0.47
237	0.71
238	0.47
239	0.51
240	0.93
241	0.09
242	0.08
243	0.81
244	0.28
245	0.51
246	0.49
247	0.66
248	0.47
249	1.06
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

PSVS Software Environment

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	0.23
287	1.04
288	0.44
289	0.23
290	1.06
291	0.25
292	0.51
293	0.64
294	0.25
295	0.49
296	0.91
297	1.40
298	0.51
299	0.81
300	0.04
301	1.14
302	1.40
303	0.24
304	-0.10
305	0.51
306	0.64
307	-0.41
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	1.14
318	0.64
319	1.10
320	0.25
321	0.71
322	-0.03
323	0.64
324	0.17
325	-0.33
326	1.29
327	-0.61

PSVS Software Environment

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	0.29
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	1.06
351	-1.13
352	0.25
353	-0.74
354	0.49
355	1.10
356	0.81
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	0.59
371	1.29
372	1.06
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	0.49
383	1.00
384	0.71
385	1.10
386	0.34
387	0.93
388	0.71
389	0.41

PSVS Software Environment

390	0.25
391	-0.74
392	1.00
393	-0.07
394	0.24
395	1.29
396	0.44
397	0.24
398	1.29
399	0.44
400	0.14
401	0.23
402	0.28
403	0.25
404	-0.68
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	-0.46
417	0.41
418	1.06
419	0.64
420	0.28
421	0.25
422	1.40
423	0.20
424	-0.41
425	0.49
426	0.91
427	0.47
428	-0.43
429	0.34
430	0.08
431	0.51
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	0.59
443	1.06
444	0.47
445	-0.74
446	0.24
447	0.64
448	1.00
449	0.49
450	-0.68
451	0.93

PSVS Software Environment

452	0.59
453	0.34
454	0.17
455	0.93
456	0.44
457	0.20
458	0.28
459	0.66
460	0.64
461	0.10
462	0.93
463	0.77
464	0.93
465	-0.26
466	0.24
467	0.28
468	0.64
469	0.77
470	0.44
471	0.20
472	0.77
473	0.20
474	1.04
475	0.51
476	1.00
477	-1.13
478	1.06
479	0.77
480	1.10
481	0.51
482	1.29
483	0.34
484	-0.09
485	0.81
486	0.93
487	-2.61
488	-1.13
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	0.14
499	0.47
500	1.06
501	-0.35
502	-0.35
503	0.41
504	0.64
505	-0.09
506	-0.10
507	-0.68
508	0.59
509	0.28
510	-0.94
511	0.08
512	-0.46
513	0.08

PSVS Software Environment

514	0.44
515	0.44
516	0.71
517	0.08
518	0.25
519	0.08
520	-0.46
521	-0.68
522	-0.25
523	1.25
524	-0.68
525	0.59
526	-0.46
527	0.29
528	-0.07
529	0.64
530	0.55
531	0.44
532	-0.68
533	0.20
534	-0.74
535	0.34
536	0.04
537	0.23
538	0.17
539	0.34
540	0.34
541	0.25
542	0.28
543	-0.41
544	0.08
545	0.34
546	0.64
547	0.44
548	-2.63
549	0.59
550	0.34
551	-0.80
552	-0.94
553	-0.74
554	0.08
555	-0.68
556	-0.68
557	0.51
558	0.25
559	0.49
560	0.14
561	0.47
562	0.59
563	0.41
564	0.23
565	0.51
566	-0.68
567	0.51
568	-0.74
569	0.17
570	0.04
571	0.34
572	0.47
573	1.10
574	1.29
575	-0.83

PSVS Software Environment

576	0.04
577	-0.59
578	0.47
579	0.64
580	0.25
581	0.28
582	-0.74
583	0.25
584	0.08
585	0.34
586	-0.41
587	0.41
588	-0.80
589	0.28
590	0.17
591	0.93
592	0.14
593	0.28
594	0.10
595	-1.30
596	-0.46
597	0.51
598	0.44
599	0.51
600	0.77
601	0.47
602	0.51
603	-0.74
604	1.10
605	0.17
606	0.59
607	0.08
608	1.10
609	0.28
610	0.47
611	0.41
612	0.28
613	0.71
614	0.08
615	0.34
616	-0.09
617	0.49
618	1.10
619	0.08
620	-0.09
621	0.71
622	0.08
623	1.29
624	1.62
625	0.44
626	0.41
627	0.24
628	0.66
629	0.14
630	0.08
631	0.28
632	0.25
633	0.93
634	0.59
635	0.71
636	0.24
637	0.29

PSVS Software Environment

638	0.51
639	1.10
640	0.41
641	-0.03
642	1.25
643	0.29
644	-0.84
645	0.77
646	0.64
647	0.64
648	0.41
649	0.71
650	1.25
651	0.93
652	0.71
653	0.20
654	1.10
655	-0.25
656	0.28
657	1.00
658	1.25
659	0.17
660	0.51
661	0.59
662	0.04
663	0.51
664	0.23
665	-0.74
666	0.29
667	0.17
668	0.59
669	0.17
670	0.59
671	1.29
672	1.10
673	0.59
674	-0.26
675	0.17
676	0.23
677	0.34
678	1.10
679	0.08
680	-0.35
681	0.10
682	0.17
683	0.25
684	0.34
685	0.77
686	0.04
687	0.28
688	0.25
689	1.00
690	0.04
691	0.51
692	0.04
693	0.34
694	-0.46
695	-0.94
696	0.28
697	-0.46
698	1.04
699	1.14

PSVS Software Environment

```
700      -2.61
701      1.10
702      0.77
703     -0.46
704      0.51
705     -0.46
706     -0.11
707      0.51
708     -0.74
709      0.44
710      0.04
711      0.24
712      0.49
713      1.10
714      1.10
715      0.49
716      1.10
717      0.71
718      1.10
719      0.08
720      0.51
721      1.10
722      0.51
723      0.23
724     -0.03
725      0.04
726      0.14
727      0.81
728      0.51
729      0.04
730      0.14
731      0.81
732      0.17
733     -0.74
734      0.08
735      0.10
736      0.04
737     -0.74
738      0.55
739      0.23
740      0.23
741      0.41
742      1.14
743      0.64
744      0.59
745      0.41
746      0.47
747      0.17
#Reported_Model_Average 0.349
#Overall_Average_Reported      0.349
```

Output from Prosall

Prosall Score over a window of \$winsize_s residues

JPEG image for Prosall Score

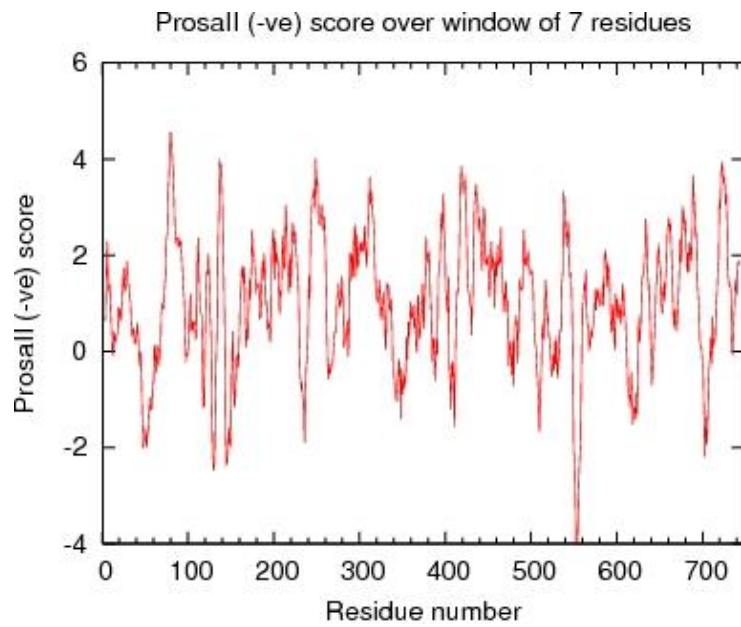


Table of Verify3D scores for ordered residues across all models

```
#verify3d
#Residue\Model  only_model
1      -0.83
2      -0.25
3       0.23
4      -0.59
5       0.14
6       0.49
7       0.77
8       0.49
9      -0.68
10     -0.87
11     -0.07
12      1.10
13      1.10
14      0.17
15      0.64
16      0.34
17      0.14
18      0.14
19      1.10
20     -0.25
21      0.23
22      0.71
23      0.28
24      0.49
25      0.14
26      0.34
27      0.59
28      0.25
29      0.49
30      1.10
31      0.28
32      0.25
33      0.29
34      0.71
35      0.08
```

PSVS Software Environment

36	0.71
37	-0.11
38	0.71
39	0.71
40	0.34
41	1.10
42	0.44
43	1.10
44	0.29
45	0.28
46	-0.44
47	0.17
48	0.44
49	1.10
50	-0.46
51	0.44
52	1.10
53	1.10
54	0.49
55	-0.25
56	0.64
57	-0.59
58	0.24
59	0.28
60	0.66
61	0.44
62	0.49
63	0.14
64	0.49
65	0.71
66	1.10
67	1.29
68	0.64
69	1.10
70	0.14
71	0.14
72	0.14
73	0.49
74	0.14
75	-0.68
76	1.12
77	0.24
78	0.28
79	0.49
80	-0.46
81	0.14
82	0.28
83	0.49
84	0.14
85	0.14
86	-0.25
87	1.10
88	1.10
89	0.28
90	0.25
91	-0.46
92	-0.25
93	0.25
94	0.14
95	0.55
96	-0.25
97	0.14

PSVS Software Environment

98	0.49
99	1.10
100	-0.46
101	1.10
102	0.51
103	0.51
104	1.10
105	0.25
106	1.10
107	-0.68
108	-0.03
109	1.10
110	0.44
111	0.34
112	0.24
113	0.04
114	0.25
115	0.25
116	-0.68
117	0.14
118	0.23
119	0.51
120	-0.68
121	1.25
122	0.51
123	0.04
124	0.23
125	0.51
126	0.51
127	0.51
128	-0.46
129	1.10
130	-0.46
131	-1.13
132	-0.46
133	-0.46
134	-0.46
135	-0.25
136	0.49
137	0.49
138	0.14
139	0.49
140	0.81
141	1.10
142	1.25
143	0.71
144	0.51
145	0.51
146	-0.68
147	-1.14
148	-0.84
149	1.10
150	0.23
151	0.04
152	-1.63
153	-0.28
154	0.08
155	0.41
156	1.10
157	1.04
158	1.04
159	0.59

PSVS Software Environment

160	-0.35
161	0.28
162	0.17
163	0.34
164	0.28
165	0.28
166	0.51
167	-0.41
168	0.14
169	0.34
170	1.04
171	-0.25
172	0.34
173	0.17
174	0.34
175	0.23
176	1.12
177	0.08
178	0.44
179	0.71
180	0.44
181	0.24
182	-0.54
183	1.10
184	0.64
185	1.25
186	0.08
187	-0.84
188	1.00
189	-0.57
190	0.25
191	1.04
192	1.06
193	-0.83
194	-0.94
195	1.10
196	0.55
197	0.51
198	0.64
199	0.71
200	0.08
201	0.93
202	1.06
203	0.47
204	0.51
205	-0.33
206	0.29
207	0.64
208	-1.13
209	0.55
210	-0.94
211	-0.07
212	0.44
213	0.25
214	0.04
215	-0.33
216	0.51
217	0.51
218	-0.83
219	0.08
220	1.06
221	1.12

PSVS Software Environment

222	0.25
223	-0.28
224	1.00
225	0.81
226	-0.26
227	-0.54
228	0.77
229	0.59
230	0.28
231	0.64
232	0.59
233	0.08
234	0.71
235	0.08
236	0.47
237	0.71
238	0.47
239	0.51
240	0.93
241	0.09
242	0.08
243	0.81
244	0.28
245	0.51
246	0.49
247	0.66
248	0.47
249	1.06
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

PSVS Software Environment

284	0.14
285	-0.80
286	0.23
287	1.04
288	0.44
289	0.23
290	1.06
291	0.25
292	0.51
293	0.64
294	0.25
295	0.49
296	0.91
297	1.40
298	0.51
299	0.81
300	0.04
301	1.14
302	1.40
303	0.24
304	-0.10
305	0.51
306	0.64
307	-0.41
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	1.14
318	0.64
319	1.10
320	0.25
321	0.71
322	-0.03
323	0.64
324	0.17
325	-0.33
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	0.29
341	0.71
342	-2.61
343	0.52
344	0.08
345	0.10

PSVS Software Environment

346	0.51
347	0.81
348	0.34
349	0.08
350	1.06
351	-1.13
352	0.25
353	-0.74
354	0.49
355	1.10
356	0.81
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	0.59
371	1.29
372	1.06
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	0.49
383	1.00
384	0.71
385	1.10
386	0.34
387	0.93
388	0.71
389	0.41
390	0.25
391	-0.74
392	1.00
393	-0.07
394	0.24
395	1.29
396	0.44
397	0.24
398	1.29
399	0.44
400	0.14
401	0.23
402	0.28
403	0.25
404	-0.68
405	0.49
406	0.81
407	0.91

PSVS Software Environment

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	-0.46
417	0.41
418	1.06
419	0.64
420	0.28
421	0.25
422	1.40
423	0.20
424	-0.41
425	0.49
426	0.91
427	0.47
428	-0.43
429	0.34
430	0.08
431	0.51
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	0.59
443	1.06
444	0.47
445	-0.74
446	0.24
447	0.64
448	1.00
449	0.49
450	-0.68
451	0.93
452	0.59
453	0.34
454	0.17
455	0.93
456	0.44
457	0.20
458	0.28
459	0.66
460	0.64
461	0.10
462	0.93
463	0.77
464	0.93
465	-0.26
466	0.24
467	0.28
468	0.64
469	0.77

PSVS Software Environment

470	0.44
471	0.20
472	0.77
473	0.20
474	1.04
475	0.51
476	1.00
477	-1.13
478	1.06
479	0.77
480	1.10
481	0.51
482	1.29
483	0.34
484	-0.09
485	0.81
486	0.93
487	-2.61
488	-1.13
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	0.14
499	0.47
500	1.06
501	-0.35
502	-0.35
503	0.41
504	0.64
505	-0.09
506	-0.10
507	-0.68
508	0.59
509	0.28
510	-0.94
511	0.08
512	-0.46
513	0.08
514	0.44
515	0.44
516	0.71
517	0.08
518	0.25
519	0.08
520	-0.46
521	-0.68
522	-0.25
523	1.25
524	-0.68
525	0.59
526	-0.46
527	0.29
528	-0.07
529	0.64
530	0.55
531	0.44

PSVS Software Environment

532	-0.68
533	0.20
534	-0.74
535	0.34
536	0.04
537	0.23
538	0.17
539	0.34
540	0.34
541	0.25
542	0.28
543	-0.41
544	0.08
545	0.34
546	0.64
547	0.44
548	-2.63
549	0.59
550	0.34
551	-0.80
552	-0.94
553	-0.74
554	0.08
555	-0.68
556	-0.68
557	0.51
558	0.25
559	0.49
560	0.14
561	0.47
562	0.59
563	0.41
564	0.23
565	0.51
566	-0.68
567	0.51
568	-0.74
569	0.17
570	0.04
571	0.34
572	0.47
573	1.10
574	1.29
575	-0.83
576	0.04
577	-0.59
578	0.47
579	0.64
580	0.25
581	0.28
582	-0.74
583	0.25
584	0.08
585	0.34
586	-0.41
587	0.41
588	-0.80
589	0.28
590	0.17
591	0.93
592	0.14
593	0.28

PSVS Software Environment

594	0.10
595	-1.30
596	-0.46
597	0.51
598	0.44
599	0.51
600	0.77
601	0.47
602	0.51
603	-0.74
604	1.10
605	0.17
606	0.59
607	0.08
608	1.10
609	0.28
610	0.47
611	0.41
612	0.28
613	0.71
614	0.08
615	0.34
616	-0.09
617	0.49
618	1.10
619	0.08
620	-0.09
621	0.71
622	0.08
623	1.29
624	1.62
625	0.44
626	0.41
627	0.24
628	0.66
629	0.14
630	0.08
631	0.28
632	0.25
633	0.93
634	0.59
635	0.71
636	0.24
637	0.29
638	0.51
639	1.10
640	0.41
641	-0.03
642	1.25
643	0.29
644	-0.84
645	0.77
646	0.64
647	0.64
648	0.41
649	0.71
650	1.25
651	0.93
652	0.71
653	0.20
654	1.10
655	-0.25

PSVS Software Environment

656	0.28
657	1.00
658	1.25
659	0.17
660	0.51
661	0.59
662	0.04
663	0.51
664	0.23
665	-0.74
666	0.29
667	0.17
668	0.59
669	0.17
670	0.59
671	1.29
672	1.10
673	0.59
674	-0.26
675	0.17
676	0.23
677	0.34
678	1.10
679	0.08
680	-0.35
681	0.10
682	0.17
683	0.25
684	0.34
685	0.77
686	0.04
687	0.28
688	0.25
689	1.00
690	0.04
691	0.51
692	0.04
693	0.34
694	-0.46
695	-0.94
696	0.28
697	-0.46
698	1.04
699	1.14
700	-2.61
701	1.10
702	0.77
703	-0.46
704	0.51
705	-0.46
706	-0.11
707	0.51
708	-0.74
709	0.44
710	0.04
711	0.24
712	0.49
713	1.10
714	1.10
715	0.49
716	1.10
717	0.71

PSVS Software Environment

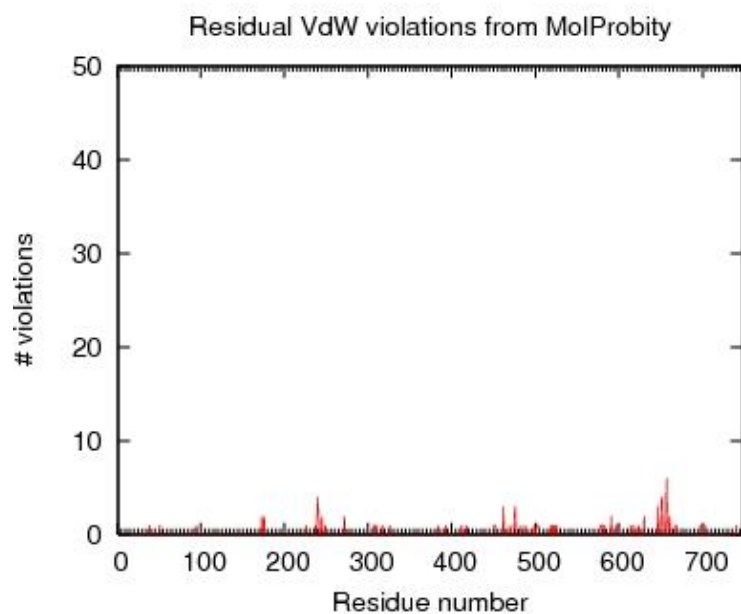
718	1.10
719	0.08
720	0.51
721	1.10
722	0.51
723	0.23
724	-0.03
725	0.04
726	0.14
727	0.81
728	0.51
729	0.04
730	0.14
731	0.81
732	0.17
733	-0.74
734	0.08
735	0.10
736	0.04
737	-0.74
738	0.55
739	0.23
740	0.23
741	0.41
742	1.14
743	0.64
744	0.59
745	0.41
746	0.47
747	0.17

#Reported_Model_Average 0.349
#Overall_Average_Reported 0.349

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
```

PSVS Software Environment

36.000	0
37.000	0
38.000	0
39.000	1
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	1
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	0
73.000	0
74.000	0
75.000	0
76.000	0
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	1
96.000	0
97.000	0

PSVS Software Environment

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
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138.000 0
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141.000 0
142.000 0
143.000 0
144.000 0
145.000 0
146.000 0
147.000 0
148.000 0
149.000 0
150.000 0
151.000 0
152.000 0
153.000 0
154.000 0
155.000 0
156.000 0
157.000 0
158.000 0
159.000 0

PSVS Software Environment

160.000 0
161.000 0
162.000 0
163.000 0
164.000 0
165.000 0
166.000 0
167.000 0
168.000 0
169.000 0
170.000 0
171.000 0
172.000 0
173.000 2
174.000 0
175.000 0
176.000 2
177.000 0
178.000 0
179.000 0
180.000 0
181.000 0
182.000 0
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184.000 0
185.000 0
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212.000 0
213.000 0
214.000 0
215.000 0
216.000 0
217.000 0
218.000 0
219.000 0
220.000 0
221.000 0

PSVS Software Environment

222.000	0
223.000	0
224.000	0
225.000	0
226.000	1
227.000	0
228.000	0
229.000	0
230.000	0
231.000	0
232.000	0
233.000	0
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235.000	0
236.000	0
237.000	1
238.000	0
239.000	2
240.000	4
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243.000	0
244.000	0
245.000	2
246.000	0
247.000	0
248.000	0
249.000	1
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251.000	0
252.000	0
253.000	0
254.000	0
255.000	0
256.000	0
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261.000	0
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263.000	0
264.000	0
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269.000	0
270.000	0
271.000	0
272.000	2
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274.000	0
275.000	0
276.000	0
277.000	0
278.000	0
279.000	0
280.000	0
281.000	0
282.000	0
283.000	0

PSVS Software Environment

284.000	0
285.000	0
286.000	0
287.000	0
288.000	0
289.000	0
290.000	0
291.000	0
292.000	0
293.000	0
294.000	0
295.000	0
296.000	0
297.000	0
298.000	0
299.000	0
300.000	0
301.000	0
302.000	0
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304.000	0
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306.000	0
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334.000	0
335.000	0
336.000	0
337.000	0
338.000	0
339.000	0
340.000	0
341.000	0
342.000	0
343.000	0
344.000	0
345.000	0

PSVS Software Environment

346.000 0
347.000 0
348.000 0
349.000 0
350.000 0
351.000 0
352.000 0
353.000 0
354.000 0
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400.000 0
401.000 0
402.000 0
403.000 0
404.000 0
405.000 0
406.000 0
407.000 0

PSVS Software Environment

408.000 0
409.000 0
410.000 0
411.000 0
412.000 1
413.000 0
414.000 0
415.000 0
416.000 0
417.000 0
418.000 1
419.000 0
420.000 0
421.000 0
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459.000 0
460.000 0
461.000 0
462.000 3
463.000 0
464.000 0
465.000 0
466.000 0
467.000 0
468.000 0
469.000 0

PSVS Software Environment

470.000	1
471.000	0
472.000	0
473.000	0
474.000	0
475.000	2
476.000	3
477.000	0
478.000	0
479.000	0
480.000	0
481.000	0
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521.000	1
522.000	0
523.000	1
524.000	0
525.000	0
526.000	1
527.000	0
528.000	0
529.000	0
530.000	0
531.000	0

PSVS Software Environment

532.000 0
533.000 0
534.000 0
535.000 0
536.000 0
537.000 0
538.000 0
539.000 0
540.000 0
541.000 0
542.000 0
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575.000 0
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582.000 0
583.000 1
584.000 0
585.000 0
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587.000 0
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589.000 0
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591.000 2
592.000 0
593.000 0

PSVS Software Environment

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596.000 0
597.000 1
598.000 1
599.000 0
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619.000 0
620.000 0
621.000 0
622.000 0
623.000 0
624.000 1
625.000 0
626.000 0
627.000 0
628.000 0
629.000 0
630.000 2
631.000 0
632.000 0
633.000 0
634.000 0
635.000 0
636.000 0
637.000 0
638.000 0
639.000 0
640.000 0
641.000 0
642.000 0
643.000 0
644.000 0
645.000 0
646.000 0
647.000 3
648.000 0
649.000 0
650.000 0
651.000 4
652.000 4
653.000 0
654.000 0
655.000 0

PSVS Software Environment

656.000 0
657.000 6
658.000 2
659.000 0
660.000 1
661.000 2
662.000 0
663.000 0
664.000 0
665.000 0
666.000 0
667.000 0
668.000 1
669.000 1
670.000 0
671.000 0
672.000 0
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708.000 0
709.000 0
710.000 0
711.000 0
712.000 0
713.000 0
714.000 0
715.000 0
716.000 0
717.000 0

PSVS Software Environment

```

718.000 0
719.000 0
720.000 0
721.000 0
722.000 0
723.000 0
724.000 0
725.000 0
726.000 0
727.000 0
728.000 0
729.000 0
730.000 0
731.000 0
732.000 0
733.000 0
734.000 0
735.000 0
736.000 0
737.000 0
738.000 0
739.000 0
740.000 1
741.000 0
742.000 0
743.000 0
744.000 0
745.000 0
746.000 0
747.000 0
#Reported_Model_Average 0.123
#Overall_Average_Reported 0.123

```

List of bad contacts calculated by MAGE

/farm/software/bin/probe

```

: 5731: 657 VAL CG2 : 652 PHE CE1 : -1.587: 5
: 5731: 657 VAL CG2 : 652 PHE CZ : -1.276: 5
: 5731: 657 VAL CB : 652 PHE CE1 : -1.076: 5
: 5731: 652 PHE CD1 : 657 VAL CB : -0.908: 5
: 5731: 657 VAL CG2 : 658 TYR CE1 : -0.426: 5
: 5731: 657 VAL CG1 : 658 TYR CD1 : -0.419: 5

: 5731: 591 ILE CG2 : 651 ILE CD1 : -1.302: 0
: 5731: 651 ILE CG1 : 591 ILE CG2 : -1.019: 0
: 5731: 651 ILE O : 651 ILE CG1 : -0.445: 0

: 5731: 173 SER O : 176 TRP CE3 : -1.153: 5
: 5731: 173 SER O : 176 TRP CZ3 : -0.592: 5

: 5731: 579 PRO O : 624 TRP CZ2 : -1.145: 0

: 5731: 241 ASN CB : 521 LEU CD2 : -1.051: 5
: 5731: 523 TYR CE1 : 241 ASN O : -0.769: 5

: 5731: 647 PRO CA : 660 ASP CB : -0.949: 5
: 5731: 647 PRO CG : 661 SER OG : -0.946: 5
: 5731: 647 PRO CD : 661 SER CB : -0.513: 5

: 5731: 462 ILE CG1 : 476 VAL CG1 : -0.843: 0
: 5731: 476 VAL CG1 : 462 ILE CB : -0.464: 0

```

VdW violations from MAGE

PSVS Software Environment

```
: 5731: 476 VAL CG1 : 462 ILE CA : -0.455: 0
: 5731: 502 CYS SG : 499 LYS O : -0.823: 0
: 5731: 504 PRO CD : 503 ASN CB : -0.749: 0
: 5731: 240 ILE CG2 : 249 LEU CD1 : -0.727: 5
: 5731: 245 ASP OD2 : 239 ASP O : -0.630: 5
: 5731: 475 ASP CB : 240 ILE CD1 : -0.604: 5
: 5731: 51 PRO CG : 239 ASP OD2 : -0.517: 5
: 5731: 475 ASP CB : 240 ILE CG1 : -0.514: 5
: 5731: 245 ASP CB : 240 ILE CA : -0.419: 5

: 5731: 740 MET SD : 578 LYS CD : -0.716: 0
: 5731: 326 CYS SG : 483 ASP OD1 : -0.657: 0
: 5731: 583 GLN CB : 519 LYS CE : -0.613: 0
: 5731: 614 THR CG2 : 669 SER O : -0.564: 0
: 5731: 526 GLU CG : 488 GLU OE2 : -0.537: 0
: 5731: 630 LYS C : 630 LYS CD : -0.529: 0
: 5731: 452 PRO CD : 451 ILE N : -0.515: 0
: 5731: 598 PRO CD : 597 ASN N : -0.513: 0
: 5731: 317 TYR OH : 384 ARG CD : -0.513: 0
: 5731: 470 PRO O : 580 GLN CG : -0.500: 0
: 5731: 703 GLU CG : 618 GLY O : -0.493: 0
: 5731: 310 PHE CE2 : 393 PRO CD : -0.484: 0
: 5731: 272 ASP OD1 : 272 ASP C : -0.473: 0
: 5731: 95 THR CG2 : 226 ASN OD1 : -0.461: 5
: 5731: 308 PRO CD : 307 ARG N : -0.452: 0
: 5731: 668 SER CB : 698 PHE CE1 : -0.448: 0
: 5731: 39 ARG NH2 : 237 ARG O : -0.428: 10
: 5731: 412 VAL CG1 : 418 LEU CD2 : -0.402: 0
#sum2 ::8.03 clashscore : 8.03 clashscore B
```

Output from PDB validation software

Summary from PDB validation

Jan. 29, 14:10:50 2017

Greetings,

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

PSVS Software Environment

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
	CG2	ILE	651	-	CG1	VAL	657	(1, 5, 5, 5)	Dist = 1.65
	CE1	PHE	652	-	CG2	VAL	657	(1, 5, 5, 5)	Dist = 1.84
	O	SER	173	-	CE3	TRP	176	(1, 5, 5, 5)	Dist = 1.98
	O	PRO	579	-	CZ2	TRP	624	(1, 5, 5, 5)	Dist = 1.99
	O	ASP	239	-	OD2	ASP	245	(1, 5, 5, 5)	Dist = 2.15
	CG2	ILE	591	-	CD1	ILE	651	(1, 5, 5, 5)	Dist = 2.19

=> 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

PSVS Software Environment

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
0.147	PRO		42	CG	-	CD	1.650	1.503
0.124	PRO		48	CG	-	CD	1.627	1.503
0.127	PRO		68	CG	-	CD	1.630	1.503
0.123	PRO		105	CG	-	CD	1.626	1.503
0.120	PRO		110	CG	-	CD	1.623	1.503
0.130	PRO		114	CG	-	CD	1.633	1.503
0.138	PRO		178	CG	-	CD	1.641	1.503
0.122	PRO		180	CG	-	CD	1.625	1.503
0.135	PRO		184	CG	-	CD	1.638	1.503
0.174	PRO		198	CG	-	CD	1.677	1.503
0.118	PRO		212	CG	-	CD	1.621	1.503
0.106	PRO		231	CG	-	CD	1.609	1.503
0.119	PRO		271	CG	-	CD	1.622	1.503
0.205	PRO		291	CG	-	CD	1.708	1.503
0.137	PRO		293	CG	-	CD	1.640	1.503
0.125	PRO		306	CG	-	CD	1.628	1.503
0.176	PRO		308	CG	-	CD	1.679	1.503
0.118	PRO		318	CG	-	CD	1.621	1.503
0.105	PRO		399	CG	-	CD	1.608	1.503
0.115	PRO		409	CG	-	CD	1.618	1.503
0.117	PRO		419	CG	-	CD	1.620	1.503
0.207	PRO		447	CG	-	CD	1.710	1.503
0.142	PRO		452	CG	-	CD	1.645	1.503
0.123	PRO		456	CG	-	CD	1.626	1.503
0.104	PRO		468	CG	-	CD	1.607	1.503
0.143	PRO		470	CG	-	CD	1.646	1.503
0.134	PRO		504	CG	-	CD	1.637	1.503
0.129	PRO		514	CG	-	CD	1.632	1.503
0.204	PRO		528	CG	-	CD	1.707	1.503
0.141	PRO		529	CG	-	CD	1.644	1.503
0.152	PRO		531	CG	-	CD	1.655	1.503
0.171	PRO		547	CG	-	CD	1.674	1.503
0.122	PRO		579	CG	-	CD	1.625	1.503
0.158	PRO		598	CG	-	CD	1.661	1.503
0.195	PRO		625	CG	-	CD	1.698	1.503
0.126	PRO		683	CG	-	CD	1.629	1.503
0.144	PRO		706	CG	-	CD	1.647	1.503
0.195	PRO		709	CG	-	CD	1.698	1.503
0.125	PRO		743	CG	-	CD	1.628	1.503

*** Covalent Angle Values:

The RMS deviation for covalent angles relative to the standard dictionary is 1.6 degrees.

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

Deviation	Residue Name	Chain ID	Sequence Number	AT1	-	AT2	-	AT3	Bond Angle	Dictionary Value
9.6	ARG		274	N	-	CA	-	C	120.8	111.2
-9.9	PRO		291	CB	-	CG	-	CD	96.2	106.1

PSVS Software Environment

-10.0	PRO	447	CB	-	CG	-	CD	96.1	106.1
-10.1	VAL	505	N	-	CA	-	C	101.1	111.2
-22.8	LEU	527	C	-	N	-	CA	98.9	121.7
-9.9	PRO	528	CB	-	CG	-	CD	96.2	106.1
15.3	LYS	610	C	-	N	-	CA	137.0	121.7
10.8	TRP	624	N	-	CA	-	C	122.0	111.2
-10.9	PRO	709	O	-	C	-	N	112.1	123.0
-45.1	GLY	713	CA	-	C	-	O	75.7	120.8
33.0	GLY	713	CA	-	C	-	N	149.4	116.4
-40.5	GLY	713	O	-	C	-	N	82.5	123.0

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	198	CG	2HG	
	PRO	291	CG	2HG	
	PRO	308	CG	2HG	
	PRO	528	CG	2HG	
	PRO	547	CG	2HG	
	PRO	625	CG	2HG	

OTHER IMPORTANT ISSUES

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

fl-SIRT1.pdb: Missing KEYWDS records

fl-SIRT1.pdb: Missing TITLE record