

Protein Structure Validation Suite (PSVS)

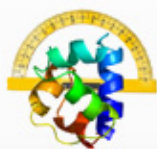


PSVS report for flSIRT1_CytoC

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PSVS report for flSIRT1_CytoC



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:

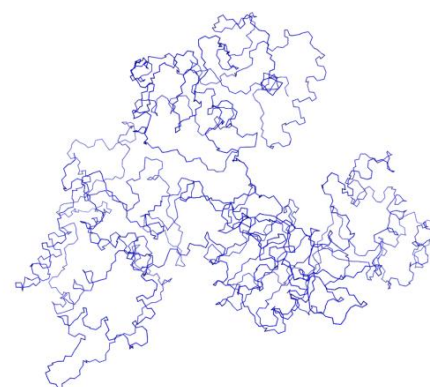
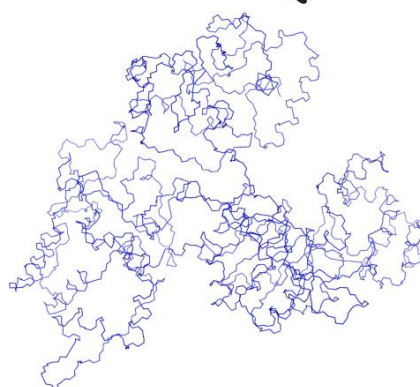
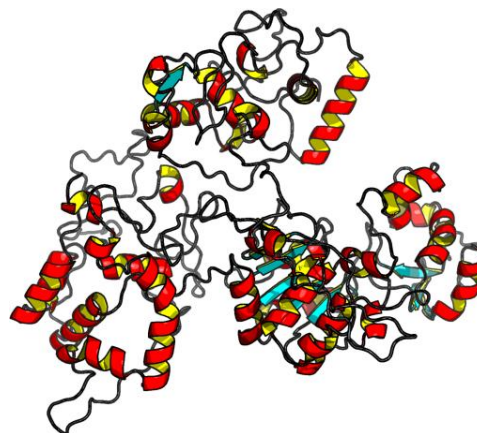
SwissProt /

TrEMBL ID:

models: 2

Oligomerization: monomer

Molecular weight: 81680



Secondary Structure Elements:

alpha helices: 3A-8A, 17A-21A, 70A-74A, 76A-86A, 89A-94A, 132A-140A, 186A-194A, 198A-205A, 217A-229A, 243A-252A, 279A-286A, 299A-304A, 307A-316A, 325A-336A, 350A-354A, 381A-388A, 420A-429A, 451A-454A, 482A-493A, 495A-500A, 551A-554A, 589A-592A, 613A-623A, 630A-638A, 668A-671A, 692A-700A, 724A-738A

beta strands: 359A-361A, 339A-344A, 256A-260A, 435A-439A, 461A-465A, 476A-479A, 522A-524A, 377A-379A, 364A-371A, 407A-411A, 601A-605A, 641A-644A

RMSD	All residues	Ordered residues ²	Selected residues ³
All backbone atoms	7.5 Å	5.6 Å	7.5 Å
All heavy atoms	7.5 Å	5.6 Å	7.5 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
89.1%	10.3%	0.4%	0.1%

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

Most favoured regions	Allowed regions	Disallowed regions	View plot	View model summary
96.7%	2.7%	0.6%		

Global quality scores

PSVS Software Environment

Program	<i>Verify3D</i>	<i>ProsaII</i> (-ve)	<i>Procheck</i> (phi-psi) ³	<i>Procheck</i> (all) ³	<i>MolProbity</i> Clashscore
-Raw score	0.40	N/A	-0.13	-0.17	26.25
Z-score ¹	-0.96	N/A	-0.20	-1.01	-2.98

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

Number of close contacts (within 2.2 Å): 0

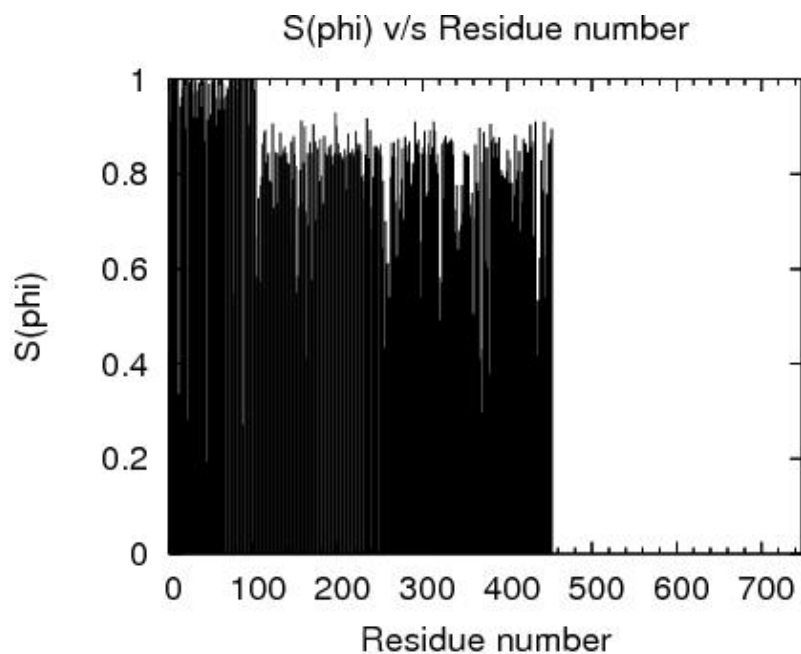
RMS deviation for bond angles: 2.4 °

RMS deviation for bond lengths: 0.012 Å

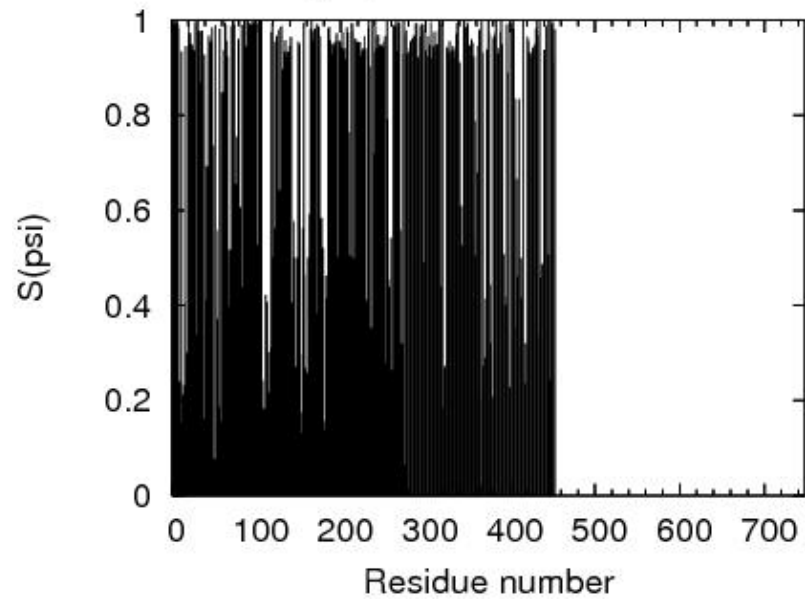
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution ≤ 1.80 Å, R-factor ≤ 0.25 and R-free ≤ 0.28; a positive value indicates a 'better' score

²Order residues: HASH(0xd7fa10)

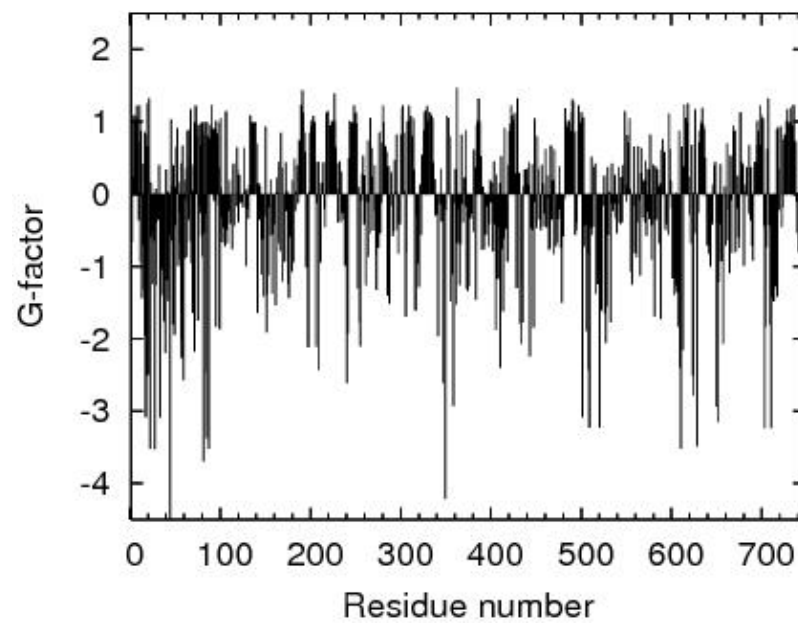
³Selected residues: all



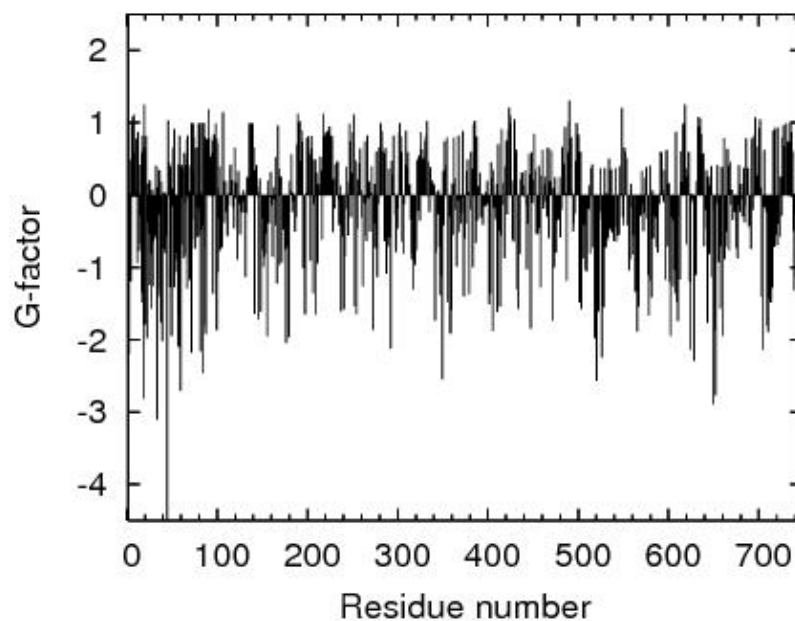
S(psi) v/s Residue number



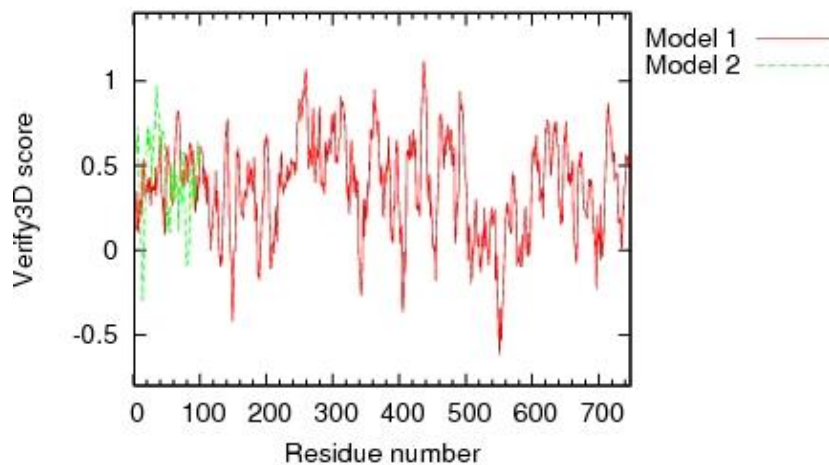
Procheck G-factor for phi-psi



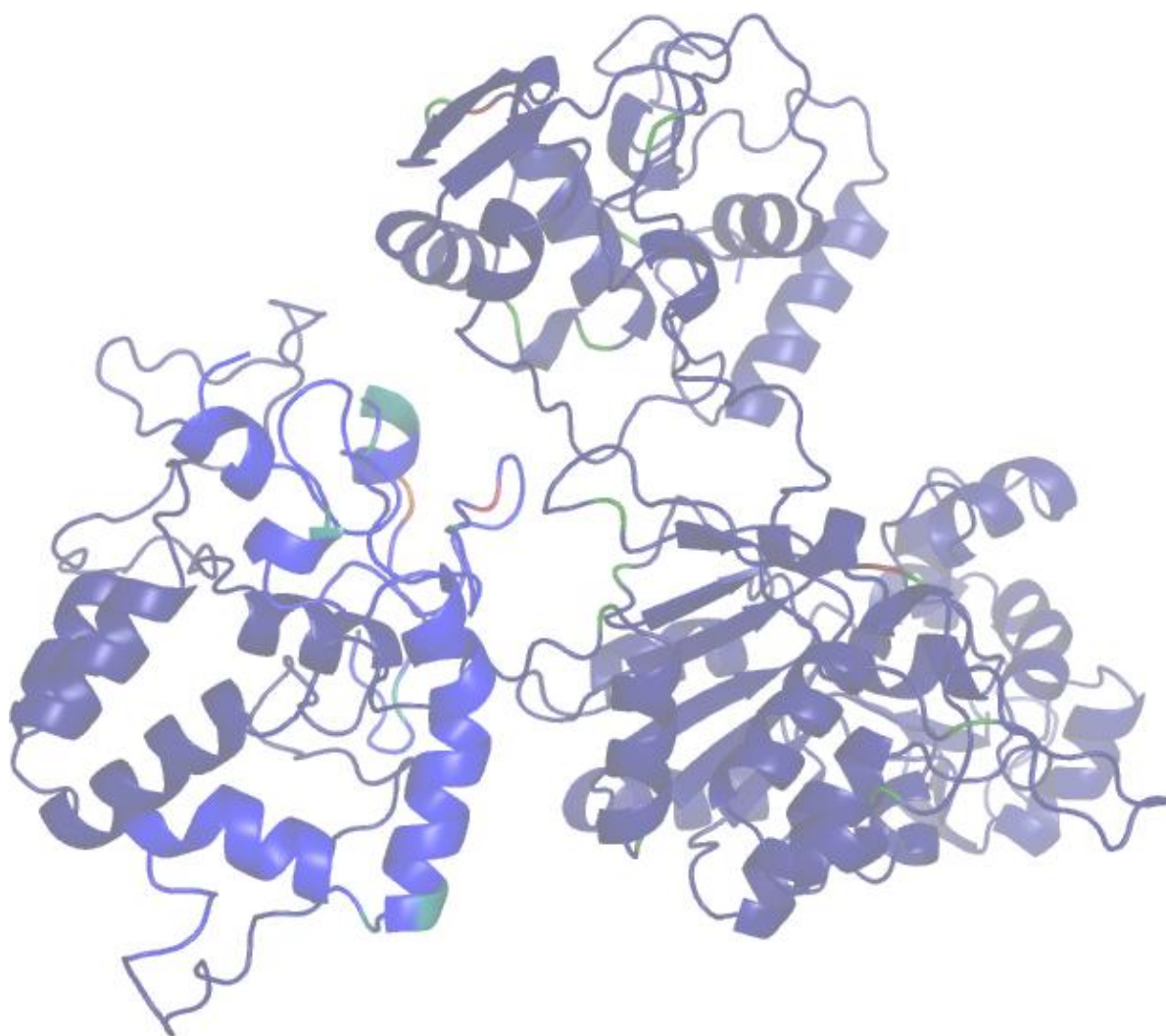
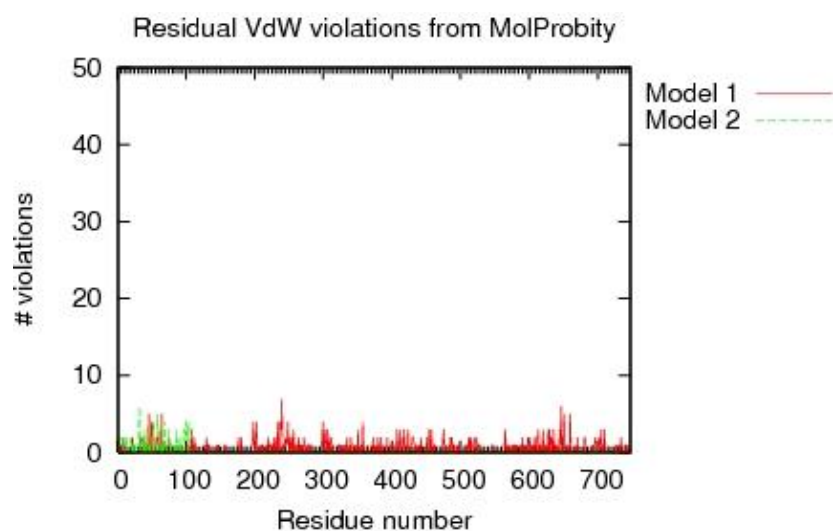
Procheck G-factor for all dihedral angles



Verify3D score over window of 7 residues



PSVS Software Environment



Residue Plot of Ramachandran analysis(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	2		
RMSD Values			
	all	ordered ^e	Selected ^f
All backbone atoms	7.5 Å	5.6 Å	7.5 Å
All heavy atoms	7.5 Å	5.6 Å	7.5 Å
Structure Quality Factors - overall statistics			
	Mean score	SD	Z-score ^g
Procheck G-factor ^e (phi / psi only)	-0.13	N/A	-0.20
Procheck G-factor ^e (all dihedral angles)	-0.17	N/A	-1.01
Verify3D	0.40	0.0424	-0.96
MolProbity clashscore	26.25	9.8217	-2.98
Ramachandran Plot Summary from Procheck ^f			
Most favoured regions	89.1%		
Additionally allowed regions	10.3%		
Generously allowed regions	0.4%		
Disallowed regions	0.1%		
Ramachandran Plot Statistics from Richardson's lab			
Most favoured regions	96.7%		
Allowed regions	2.7%		
Disallowed regions	0.6%		

^e Residues with sum of phi and psi order parameters > 1.8

Ordered residue ranges:

^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 fISIRT1_CytoC by PSVS

Output from PDBStat

S(phi)|S(psi) V/S Residue number

Text output from PDBStat of phi psi order

#	CHAIN										.GT.	SUM.GT.
#	RES	ID	DIH	S(phi)	S(psi)	S(chi1)	S(chi2)	S(chi3)	S(chi4)	S(chi5)	0.90	1.6
#	-----											
	MET	A	1		0.428							
	ALA	A	2	0.911	0.999	706.219	706.884				2	2
	ASP	A	3	0.995	0.992	0.299					3	3
	GLU	A	4	1.000	0.976	0.050	0.331	0.994			4	4
	ALA	A	5	1.000	0.998	706.392	706.094	706.457	706.418		5	5
	ALA	A	6	0.992	0.999						6	6
	LEU	A	7	0.999	0.991	0.716	0.995	705.983	706.851		7	7
	ALA	A	8	0.993	0.982	706.221	706.014	706.092	706.867		8	8
	LEU	A	9	0.998	0.094	1.000	0.990					
	GLN	A	10	0.972	0.240	0.454	0.456					
	PRO	A	11	1.000	0.152	0.778	0.192					
	GLY	A	12	0.153	0.934	705.984	706.014	706.286				
	GLY	A	13	0.336	0.013	706.283	706.149	706.008	706.125			
	SER	A	14	0.942	0.213	0.408						
	PRO	A	15	0.961	0.231	0.990						
	SER	A	16	0.982	0.407	0.921	705.963	706.721				
	ALA	A	17	0.997	0.945	706.488					17	17
	ALA	A	18	0.999	0.300	705.957	706.579					
	GLY	A	19	0.769	0.195	706.876						
	ALA	A	20	0.896	1.000	706.152						20
	ASP	A	21	0.998	0.171	0.337	0.984	706.428				
	ARG	A	22	1.000	0.972	0.977	0.956	0.691	0.374		22	22
	GLU	A	23	0.282	0.587							
	ALA	A	24	0.995	0.948						24	24
	ALA	A	25	0.992	0.924	706.252	706.017	706.045	706.263		25	25
	SER	A	26	0.988	0.936	0.876	706.865				26	26
	SER	A	27	1.000	0.936	0.136	706.161	706.896	706.068		27	27
	PRO	A	28	0.998	0.996	0.926					28	28
	ALA	A	29	0.971	0.083							
	GLY	A	30	0.183	0.338	706.877	706.473					
	GLU	A	31	0.919	0.998	0.442	0.039				31	31
	PRO	A	32	0.996	0.060	0.750	0.268					
	LEU	A	33	0.918	0.976	0.840	0.765				33	33
	ARG	A	34	0.347	0.870							
	LYS	A	35	0.975	0.131	0.540	0.443					
	ARG	A	36	0.991	0.977	0.999	0.647				36	36
	PRO	A	37	0.117	0.162							
	ARG	A	38	1.000	0.099	0.612	1.000	1.000	0.888	0.985		
	ARG	A	39	0.917	0.927	0.974	0.368	0.981	0.628		39	39
	ASP	A	40	0.941	0.412	0.347						
	GLY	A	41	0.993	0.070							
	PRO	A	42	0.870	0.693	0.973	0.506	705.956				
	GLY	A	43	0.206	0.664							
	LEU	A	44	0.997	0.967	0.277	0.988				44	44
	GLU	A	45	0.192	0.385							
	ARG	A	46	0.914	0.955	0.603	0.686				46	46

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SER	A	47	0.773	0.755	0.849				
PRO	A	48	0.989	0.984	0.893	0.414		48	48
GLY	A	49	0.279	0.736	706.875				
GLU	A	50	0.925	0.026					
PRO	A	51	1.000	0.077					
GLY	A	52	0.216	0.989	705.911	706.792			
GLY	A	53	0.993	0.558	706.341	706.354	706.896	706.068	
ALA	A	54	0.998	0.371	706.043	706.812			
ALA	A	55	0.903	0.094	706.002	706.848	706.048	705.977	
PRO	A	56	0.199	0.186					
GLU	A	57	0.960	0.981	0.752	0.410		57	57
ARG	A	58	0.995	0.057	0.987	0.593			
GLU	A	59	0.935	0.155	0.882	0.288			
VAL	A	60	0.920	0.847					60
PRO	A	61	0.959	0.293	0.862	0.934	706.035		
ALA	A	62	0.996	0.937	706.078	706.782		62	62
ALA	A	63	0.999	0.994	706.897			63	63
ALA	A	64	0.991	0.989	706.195	706.133		64	64
ARG	A	65	0.959	0.956	0.882	0.542	0.433	65	65
GLY	A	66	0.026	0.923	705.954	706.201	706.614		
CYS	A	67	0.936	0.037	0.472	706.896			
PRO	A	68	0.965	0.398	0.965	0.386			
GLY	A	69	0.983	0.516	705.978	706.869	706.700		
ALA	A	70	0.720	0.306	706.010	706.603			
ALA	A	71	0.978	0.987	706.513	706.897		71	71
ALA	A	72	1.000	0.998	705.917	705.961	706.027	705.928	72
ALA	A	73	0.998	1.000	706.169	705.954	706.113	705.952	73
ALA	A	74	0.997	0.990	705.931	706.793		74	74
LEU	A	75	0.960	0.655	0.993	1.000			
TRP	A	76	1.000	0.093	0.301	0.762			
ARG	A	77	0.548	0.755					
GLU	A	78	0.987	0.159	0.703				
ALA	A	79	0.945	0.960	706.898	706.145	706.171	706.877	79
GLU	A	80	0.995	0.510	0.984	0.998	0.968		
ALA	A	81	0.977	0.606	706.439	706.209			
GLU	A	82	0.980	0.115	0.728	0.281			
ALA	A	83	0.999	0.989	706.872			83	83
ALA	A	84	0.291	0.095					
ALA	A	85	0.998	0.438	706.421	706.094			
ALA	A	86	0.997	0.997	706.141	706.748	705.931	706.837	86
GLY	A	87	0.065	0.781	706.177	705.900	706.288	706.781	
GLY	A	88	0.271	0.944	705.992	706.100	706.119	706.896	
GLU	A	89	0.999	0.998	0.189	0.608	0.328		89
GLN	A	90	1.000	1.000	1.000	1.000	0.998		90
GLU	A	91	0.989	0.993	1.000	0.828	0.655	706.129	706.765
ALA	A	92	1.000	0.987					92
GLN	A	93	0.979	0.991	0.991	0.162			93
ALA	A	94	1.000	0.988	705.971	706.884			94
THR	A	95	0.904	0.792	0.664	706.117			
ALA	A	96	0.999	0.996					96
ALA	A	97	0.993	0.996	706.109	706.887			97
ALA	A	98	0.998	0.992	706.274	706.056			98
GLY	A	99	0.018	0.795	706.181	705.981	706.112	706.854	
GLU	A	100	0.975	0.991	0.354	0.753	0.522	706.276	100
GLY	A	101	0.962	0.527					
ASP	A	102	0.977	0.300	0.305				
ASN	A	103	0.997	0.992	0.899	0.255			103
GLY	A	104	0.584		706.818	705.990	706.220		
PRO	A	105	0.667	0.624	0.879	1.000			
GLY	A	106	0.749	0.998					
LEU	A	107	0.539	0.242	0.872	0.076			
GLN	A	108	0.573	0.173	0.861	0.747	0.468	706.882	706.826

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GLY	A	109	0.776	0.182							
PRO	A	110	0.794	0.172	0.983	0.828	706.824	706.759	706.759		
SER	A	111	0.863	0.422	0.965						
ARG	A	112	0.644	0.350	0.143	0.099	0.163	0.392	0.989		
GLU	A	113	0.887	0.407	0.053	0.075	0.958	706.882	706.832		
PRO	A	114	0.893	0.301	0.971	0.949					
PRO	A	115	0.823	0.214	0.987	0.839	706.835	706.759	706.759		
LEU	A	116	0.717	0.217	0.871	0.036					
ALA	A	117	0.840	0.311							
ASP	A	118	0.844	0.974	0.838	0.654	706.800	706.878	706.836		118
ASN	A	119	0.637	0.994	0.774	0.925					
LEU	A	120	0.785	0.501	0.017	0.961	706.835	706.759	706.759		
TYR	A	121	0.572	0.413	0.118	0.778					
ASP	A	122	0.780	0.562	0.186	0.841					
GLU	A	123	0.906	0.954	0.002	0.001	0.917	706.875	706.837	123	123
ASP	A	124	0.729	0.966	0.072	0.965					
ASP	A	125	0.586	0.547	0.699	0.726	706.831	706.759	706.759		
ASP	A	126	0.846	0.979	0.853	0.856					126
ASP	A	127	0.737	0.642	0.087	0.971					
GLU	A	128	0.738	0.609	0.049	0.095	0.948	706.887	706.824		
GLY	A	129	0.844	0.985							129
GLU	A	130	0.770	0.987	0.669	0.654	0.688	706.759	706.759		
GLU	A	131	0.836	0.343	0.190	0.509	0.980				
GLU	A	132	0.887	0.896	0.908	0.181	0.984				132
GLU	A	133	0.838	0.934	0.027	0.802	0.990	706.893	706.826		133
GLU	A	134	0.814	0.957	0.755	0.923	0.874				134
ALA	A	135	0.844	0.935	706.824	706.887	706.825	706.759	706.759		135
ALA	A	136	0.850	0.924							136
ALA	A	137	0.858	0.933							137
ALA	A	138	0.843	0.928			706.808	706.892	706.833		138
ALA	A	139	0.844	0.945							139
ILE	A	140	0.823	0.938	0.775	0.313	706.838	706.759	706.759		140
GLY	A	141	0.548	0.964							
TYR	A	142	0.821	0.406	0.043	0.821					
ARG	A	143	0.750	0.348	0.841	0.052	0.154	0.296	0.977		
ASP	A	144	0.666	0.577	0.172	0.993					
ASN	A	145	0.868	0.500	0.186	0.862	706.839	706.759	706.759		
LEU	A	146	0.707	0.167	0.869	0.038					
LEU	A	147	0.788	0.271	0.868	0.067					
PHE	A	148	0.879	0.500	0.230	0.686	706.806	706.889	706.844		
GLY	A	149	0.841	0.317							
ASP	A	150	0.816	0.954	0.837	0.996	706.829	706.759	706.759		150
GLU	A	151	0.549	0.948	0.877	0.221	0.995				
ILE	A	152	0.220	0.297	0.066	0.118					
ILE	A	153	0.585	0.174	0.889	0.018	706.812	706.895	706.844		
THR	A	154	0.730	0.131	0.942						
ASN	A	155	0.808	0.562	0.262	0.983	706.850	706.759	706.759		
GLY	A	156	0.646	0.994							
PHE	A	157	0.912	0.463	0.069	0.787					
HIS	A	158	0.739	0.268	0.022	0.743	706.809	706.897	706.844		
SER	A	159	0.823	0.086	0.887						
CYS	A	160	0.816	0.258	0.889	706.897	706.838	706.759	706.759		
GLU	A	161	0.900	0.500	0.191	0.136	0.993				
SER	A	162	0.412	0.301	0.851						
ASP	A	163	0.720	0.592	0.001	0.964	706.817	706.898	706.837		
GLU	A	164	0.843	0.981	0.906	0.067	0.114				164
GLU	A	165	0.690	0.999	0.888	0.331	0.994	706.759	706.759		
ASP	A	166	0.353	0.610	0.296	0.921					
ARG	A	167	0.866	0.955	0.874	0.002	0.002	0.082	1.000		167
ALA	A	168	0.843	0.976							168
SER	A	169	0.576	0.982	0.934						
HIS	A	170	0.573	0.300	0.092	0.752					

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ALA	A	171	0.904	0.382						
SER	A	172	0.786	0.991	0.980					
SER	A	173	0.867	0.382	0.244					
SER	A	174	0.702	0.985	0.987					
ASP	A	175	0.575	0.966	0.872	0.987				
TRP	A	176	0.853	0.195	0.754	0.574				
THR	A	177	0.653	0.584	0.998					
PRO	A	178	0.784	0.084	0.958	0.947				
ARG	A	179	0.874	0.520	0.408	0.040	0.869	0.286	1.000	
PRO	A	180	0.795	0.156	0.963	0.950				
ARG	A	181	0.736	0.137	0.859	0.005	0.009	0.079	1.000	
ILE	A	182	0.532	0.462	0.870	0.032				
GLY	A	183	0.742	0.086						
PRO	A	184	0.880	0.414	0.976	0.952				
TYR	A	185	0.843	0.981	0.813	0.618				185
THR	A	186	0.835	0.985	0.967					186
PHE	A	187	0.839	0.957	0.809	0.999				187
VAL	A	188	0.806	0.940	0.018					188
GLN	A	189	0.855	0.950	0.878	0.099	0.942			189
GLN	A	190	0.847	0.928	0.821	0.108	0.980			190
HIS	A	191	0.862	0.947	0.735	0.891				191
LEU	A	192	0.830	0.942	0.832	0.100				192
MET	A	193	0.837	0.954	0.823	0.057	0.872			193
ILE	A	194	0.819	0.926	0.836	0.075				194
GLY	A	195	0.592	0.972						
THR	A	196	0.843	0.382	0.927					
ASP	A	197	0.929	0.502	0.153	0.940				
PRO	A	198	0.900	0.956	0.973	0.951				198
ARG	A	199	0.841	0.954	0.791	0.047	0.705	0.781	0.990	199
THR	A	200	0.807	0.942	0.830					200
ILE	A	201	0.863	0.921	0.871	0.034				201
LEU	A	202	0.793	0.974	0.834	0.060				
LYS	A	203	0.844	0.927	0.468	0.200	0.149	0.916		203
ASP	A	204	0.820	0.940	0.800	0.932				204
LEU	A	205	0.835	0.917	0.801	0.041				205
LEU	A	206	0.329	0.748	0.035	0.923				
PRO	A	207	0.829	0.984	0.970	0.952				207
GLU	A	208	0.852	0.973	0.146	0.055	0.998			208
THR	A	209	0.382	0.764	0.988					
ILE	A	210	0.767	0.433	0.867	0.073				
PRO	A	211	0.838	0.504	0.973	0.953				
PRO	A	212	0.885	0.272	0.973	0.949				
PRO	A	213	0.834	0.993	0.971	0.951				213
GLU	A	214	0.843	0.976	0.912	0.033	0.523			214
LEU	A	215	0.809	0.301	0.857	0.021				
ASP	A	216	0.843	0.499	0.047	0.944				
ASP	A	217	0.852	0.960	0.833	0.997				217
MET	A	218	0.812	0.954	0.844	0.863	0.874			218
THR	A	219	0.835	0.924	0.859					219
LEU	A	220	0.843	0.954	0.863	0.084				220
TRP	A	221	0.890	0.919	0.042	0.591				221
GLN	A	222	0.800	0.953	0.865	0.080	0.696			
ILE	A	223	0.851	0.915	0.823	0.022				223
VAL	A	224	0.863	0.924	0.023					224
ILE	A	225	0.849	0.935	0.858	0.010				225
ASN	A	226	0.861	0.939	0.779	0.986				226
ILE	A	227	0.848	0.927	0.839	0.034				227
LEU	A	228	0.794	0.966	0.699	0.850				
SER	A	229	0.784	0.940	0.851					
GLU	A	230	0.747	0.412	0.894	0.173	0.997			
PRO	A	231	0.798	0.230	0.965	0.950				
PRO	A	232	0.840	0.983	0.985	0.963				232

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LYS	A	233	0.676	0.997	0.825	0.008	0.018	0.050			
ARG	A	234	0.917	0.902	0.153	0.782	0.543	0.204	1.000	234	234
LYS	A	235	0.807	0.352	0.820	0.712	0.041	0.152			
LYS	A	236	0.832	0.346	0.888	0.077	0.017	0.858			
ARG	A	237	0.740	0.999	0.975	0.847	0.015	0.112	0.996		
LYS	A	238	0.892	0.933	0.719	0.074	0.030	0.035			238
ASP	A	239	0.681	0.720	0.154	0.974					
ILE	A	240	0.730	0.985	0.775	0.085					
ASN	A	241	0.793	0.967	0.772	0.973					
THR	A	242	0.392	0.193	0.999						
ILE	A	243	0.857	0.940	0.896	0.066					243
GLU	A	244	0.844	0.968	0.925	0.786	0.975				244
ASP	A	245	0.812	0.948	0.700	0.969					245
ALA	A	246	0.858	0.946							246
VAL	A	247	0.849	0.923	0.092						247
LYS	A	248	0.846	0.947	0.204	0.795	0.135	0.777			248
LEU	A	249	0.854	0.924	0.764	0.098					249
LEU	A	250	0.861	0.943	0.812	0.141					250
GLN	A	251	0.838	0.954	0.834	0.032	0.999				251
GLU	A	252	0.643	0.966	0.961	0.862	0.469				
CYS	A	253	0.785	0.277	0.904						
LYS	A	254	0.433	1.000	0.842	0.702	0.026	0.119			
LYS	A	255	0.406	0.792	0.838	0.038	0.796	0.141			
ILE	A	256	0.701	0.440	0.906	0.054					
ILE	A	257	0.610	0.438	0.840	0.029					
VAL	A	258	0.560	0.455	0.072						
LEU	A	259	0.612	0.541	0.895	0.008					
THR	A	260	0.522	0.264	0.995						
GLY	A	261	0.539	0.197							
ALA	A	262	0.793	0.988							
GLY	A	263	0.866	0.961							263
VAL	A	264	0.836	0.987	0.843						264
SER	A	265	0.622	1.000	0.938						
VAL	A	266	0.866	0.933	0.048						266
SER	A	267	0.834	0.991	0.971						267
CYS	A	268	0.742	0.992	0.947						
GLY	A	269	0.559	0.996							
ILE	A	270	0.626	0.557	0.909	0.006					
PRO	A	271	0.874	0.319	0.982	0.958					
ASP	A	272	0.754	0.045	0.218	0.656					
PHE	A	273	0.726	0.930	0.816	0.741					
ARG	A	274	0.648	1.000	0.913	0.057	0.033	0.589	0.996		
SER	A	275	0.789	0.064	0.931						
ARG	A	276	0.853	0.969	0.907	0.041	0.061	0.170	1.000		276
ASP	A	277	0.575	0.978	0.769	0.887					
GLY	A	278	0.705	0.003							
ILE	A	279	0.878	0.928	0.851	0.027					279
TYR	A	280	0.845	0.933	0.830	0.981					280
ALA	A	281	0.859	0.941							281
ARG	A	282	0.826	0.955	0.869	0.038	0.185	0.350	1.000		282
LEU	A	283	0.806	0.956	0.868	0.057					283
ALA	A	284	0.868	0.961							284
VAL	A	285	0.718	0.917	0.019						
ASP	A	286	0.778	0.967	0.875	0.977					
PHE	A	287	0.441	0.834	0.919	0.562					
PRO	A	288	0.822	0.993	0.963	0.948					288
ASP	A	289	0.804	0.992	0.916	0.087					289
LEU	A	290	0.805	0.360	0.822	0.001					
PRO	A	291	0.910	0.922	0.967	0.949				291	291
ASP	A	292	0.209	0.090	0.607	0.822					
PRO	A	293	0.864	0.965	0.974	0.947					293
GLN	A	294	0.814	0.988	0.887	0.092	0.462				294

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ALA	A	295	0.872	0.946						295
MET	A	296	0.843	0.992	0.003	0.004	0.826			296
PHE	A	297	0.539	0.989	0.906	0.561				
ASP	A	298	0.657	0.490	0.135	0.938				
ILE	A	299	0.842	0.977	0.164	0.053				299
GLU	A	300	0.811	0.936	0.643	0.816	0.681			300
TYR	A	301	0.855	0.924	0.061	0.845				301
PHE	A	302	0.890	0.922	0.004	0.745				302
ARG	A	303	0.842	0.966	0.853	0.045	0.088	0.419	1.000	303
LYS	A	304	0.752	0.948	0.859	0.032	0.069	0.853		
ASP	A	305	0.213	0.664	0.059	1.000				
PRO	A	306	0.761	0.995	0.952	0.944				
ARG	A	307	0.864	0.920	0.927	0.187	0.070	0.566	0.998	307
PRO	A	308	0.892	0.944	0.966	0.940				308
PHE	A	309	0.840	0.914	0.013	0.841				309
PHE	A	310	0.814	0.975	0.833	0.548				310
LYS	A	311	0.855	0.919	0.903	0.133	0.057	0.111		311
PHE	A	312	0.815	0.947	0.108	0.883				312
ALA	A	313	0.910	0.928						313
LYS	A	314	0.891	0.949	0.157	0.408	0.552	0.847		314
GLU	A	315	0.822	0.976	0.906	0.956	0.882			315
ILE	A	316	0.546	0.999	0.879	0.026				
TYR	A	317	0.841	0.439	0.258	0.781				
PRO	A	318	0.801	0.137	0.963	0.946				
GLY	A	319	0.583	0.991						
GLN	A	320	0.492	1.000	0.917	0.040	0.683			
PHE	A	321	0.409	0.185	0.866	0.659				
GLN	A	322	0.572	0.267	0.779	0.852	0.880			
PRO	A	323	0.864	0.273	0.982	0.956				
SER	A	324	0.747	0.084	0.985					
LEU	A	325	0.869	0.942	0.855	0.042				325
CYS	A	326	0.875	0.916	0.778					326
HIS	A	327	0.880	0.932	0.722	0.576				327
LYS	A	328	0.835	0.955	0.852	0.196	0.022	0.219		328
PHE	A	329	0.864	0.915	0.008	0.692				329
ILE	A	330	0.842	0.934	0.900	0.082				330
ALA	A	331	0.868	0.936						331
LEU	A	332	0.838	0.945	0.829	0.042				332
SER	A	333	0.873	0.934	0.919					333
ASP	A	334	0.857	0.920	0.023	0.847				334
LYS	A	335	0.867	0.939	0.710	0.888	0.205	0.131		335
GLU	A	336	0.839	0.971	0.160	0.054	0.045			336
GLY	A	337	0.675	0.993						
LYS	A	338	0.657	0.995	0.738	0.051	0.037	0.767		
LEU	A	339	0.725	0.525	0.020	0.833				
LEU	A	340	0.776	0.911	0.026	0.881				
ARG	A	341	0.104	0.331	0.229	0.737	0.860	0.387	0.995	
ASN	A	342	0.640	0.609	0.144	0.935				
TYR	A	343	0.680	0.525	0.785	0.745				
THR	A	344	0.483	0.316	0.081					
GLN	A	345	0.692	1.000	0.896	0.069	0.628			
ASN	A	346	0.776	0.281	0.803	0.965				
ILE	A	347	0.539	0.984	0.875	0.009				
ASP	A	348	0.718	0.984	0.959	0.791				
THR	A	349	0.847	0.995	0.939					349
LEU	A	350	0.826	0.989	0.858	0.020				350
GLU	A	351	0.839	0.940	0.992	0.802	0.998			351
GLN	A	352	0.823	0.946	0.852	0.136	0.862			352
VAL	A	353	0.842	0.946	0.067					353
ALA	A	354	0.836	0.959						354
GLY	A	355	0.594	0.952						
ILE	A	356	0.710	0.541	0.889	0.021				

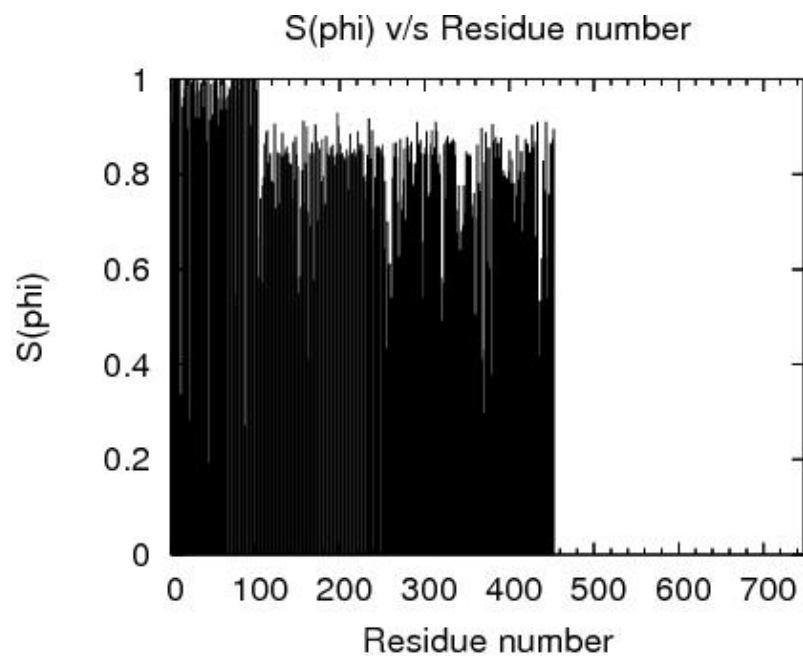
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GLN	A	357	0.735	0.923	0.894	0.041	0.531			
ARG	A	358	0.760	0.787	0.711	0.228	0.819	0.089	0.988	
ILE	A	359	0.402	0.344	0.029	0.265				
ILE	A	360	0.504	0.504	0.853	0.858				
GLN	A	361	0.709	0.679	0.732	0.029	0.960			
CYS	A	362	0.861	0.945	0.908					362
HIS	A	363	0.566	0.979	0.832	0.676				
GLY	A	364	0.782	0.205						
SER	A	365	0.088	0.021	0.968					
PHE	A	366	0.765	1.000	0.813	0.751				
ALA	A	367	0.897	0.931						367
THR	A	368	0.411	0.060	0.966					
ALA	A	369	0.297	0.273						
SER	A	370	0.430	0.290	0.923					
CYS	A	371	0.824	0.414	0.074					
LEU	A	372	0.888	0.938	0.827	0.034				372
ILE	A	373	0.783	0.872	0.960	0.124				
CYS	A	374	0.615	1.000	0.918					
LYS	A	375	0.855	0.971	0.894	0.087	0.044	0.032		375
TYR	A	376	0.856	0.443	0.003	0.793				
LYS	A	377	0.601	0.320	0.838	0.018	0.187	0.882		
VAL	A	378	0.378	0.147	0.856					
ASP	A	379	0.747	0.207	0.900	0.692				
CYS	A	380	0.905	0.963	0.911				380	380
GLU	A	381	0.869	0.967	0.870	0.831	0.960			381
ALA	A	382	0.832	0.974						382
VAL	A	383	0.524	0.999	0.878					
ARG	A	384	0.878	0.929	0.779	0.033	0.789	0.321	0.999	384
GLY	A	385	0.864	0.922						385
ASP	A	386	0.853	0.940	0.880	0.853				386
ILE	A	387	0.865	0.924	0.832	0.013				387
PHE	A	388	0.834	0.974	0.866	0.977				388
ASN	A	389	0.670	0.999	0.767	0.700				
GLN	A	390	0.877	0.949	0.862	0.054	0.970			390
VAL	A	391	0.588	0.371	0.092					
VAL	A	392	0.795	0.507	0.051					
PRO	A	393	0.807	0.400	0.996	0.976				
ARG	A	394	0.635	0.268	0.808	0.881	0.002	0.321	0.995	
CYS	A	395	0.797	0.419	0.016					
PRO	A	396	0.792	0.991	0.963	0.949				
ARG	A	397	0.758	0.890	0.003	0.018	0.035	0.091	1.000	
CYS	A	398	0.790	0.227	0.945					
PRO	A	399	0.806	0.196	0.960	0.943				
ALA	A	400	0.850	0.990						400
ASP	A	401	0.782	0.993	0.966	0.706				
GLU	A	402	0.719	0.585	0.393	0.834	0.929			
PRO	A	403	0.830	0.981	0.970	0.951				403
LEU	A	404	0.756	0.998	0.857	0.046				
ALA	A	405	0.781	0.834						
ILE	A	406	0.538	0.355	0.886	0.127				
MET	A	407	0.700	0.665	0.879	0.874	0.838			
LYS	A	408	0.754	0.460	0.154	0.221	0.859	0.225		
PRO	A	409	0.882	0.272	0.976	0.952				
GLU	A	410	0.788	0.833	0.901	0.260	0.612			
ILE	A	411	0.516	0.448	0.882	0.063				
VAL	A	412	0.806	0.499	0.014					
PHE	A	413	0.671	0.130	0.792	0.992				
PHE	A	414	0.847	0.415	0.879	0.382				
GLY	A	415	0.680	0.997						
GLU	A	416	0.633	0.321	0.098	0.070	0.997			
ASN	A	417	0.804	0.236	0.009	0.902				
LEU	A	418	0.741	0.122	0.816	0.215				

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PRO	A	419	0.873	0.318	0.972	0.949					
GLU	A	420	0.864	0.964	0.888	0.003	0.922				420
GLN	A	421	0.855	0.956	0.187	0.928	0.902				421
PHE	A	422	0.864	0.901	0.074	0.766					422
HIS	A	423	0.825	0.932	0.860	0.767					423
ARG	A	424	0.845	0.923	0.812	0.044	0.023	0.531	0.996		424
ALA	A	425	0.844	0.928							425
MET	A	426	0.857	0.940	0.157	0.832	0.616				426
LYS	A	427	0.903	0.942	0.221	0.243	0.090	0.929		427	427
TYR	A	428	0.681	0.944	0.827	0.529					
ASP	A	429	0.856	0.950	0.840	0.999					429
LYS	A	430	0.868	0.982	0.831	0.093	0.091	0.879			430
ASP	A	431	0.669	1.000	0.841	0.948					
GLU	A	432	0.543	0.968	0.692	0.810	0.734				
VAL	A	433	0.910	0.337	0.861						
ASP	A	434	0.418	1.000	0.868	0.988					
LEU	A	435	0.142	0.401	0.015	0.895					
LEU	A	436	0.533	0.458	0.041	0.838					
ILE	A	437	0.481	0.485	0.897	0.034					
VAL	A	438	0.623	0.486	0.005						
ILE	A	439	0.473	0.491	0.935	0.021					
GLY	A	440	0.828	0.937							440
SER	A	441	0.308	0.324	0.076						
SER	A	442	0.766	0.987	0.999						
LEU	A	443	0.910	0.923	0.800	0.047				443	443
LYS	A	444	0.627	1.000	0.682	0.138	0.018	0.052			
VAL	A	445	0.539	0.506	0.009						
ARG	A	446	0.758	0.242	0.862	0.004	0.043	0.051	1.000		
PRO	A	447	0.705	1.000	0.947	0.951					
VAL	A	448	0.865	0.938	0.030						448
ALA	A	449	0.864	0.991							449
LEU	A	450	0.704	0.995	0.852	0.053					
ILE	A	451	0.873	0.912	0.858	0.046					451
PRO	A	452	0.895	0.980	0.966	0.944					452

JPEG image of S(phi)~Residue_number Plot



Text report of heavy atom RMSD for entire protein

```
> Kabsch RMSD of heavy atoms in res. *[1..747],for model 1 is: 1.339 (*)
> Kabsch RMSD of heavy atoms in res. *[1..747],for model 2 is: 13.579
>
> Kabsch RMSD statistics for 2 structures:
> Mean RMSD using as refer. str. `average' for res.[1..747], is: 7.459
> Range of RMSD values to reference struct. is 1.339 to 13.579
```

Summary of heavy atom and backbone RMSDs over the whole protein and ordered residues

RMSD Values				
	all residues	ordered residues		selected residues
All backbone atoms	7.5	5.6	7.5	
All heavy atoms	7.5	5.6	7.5	

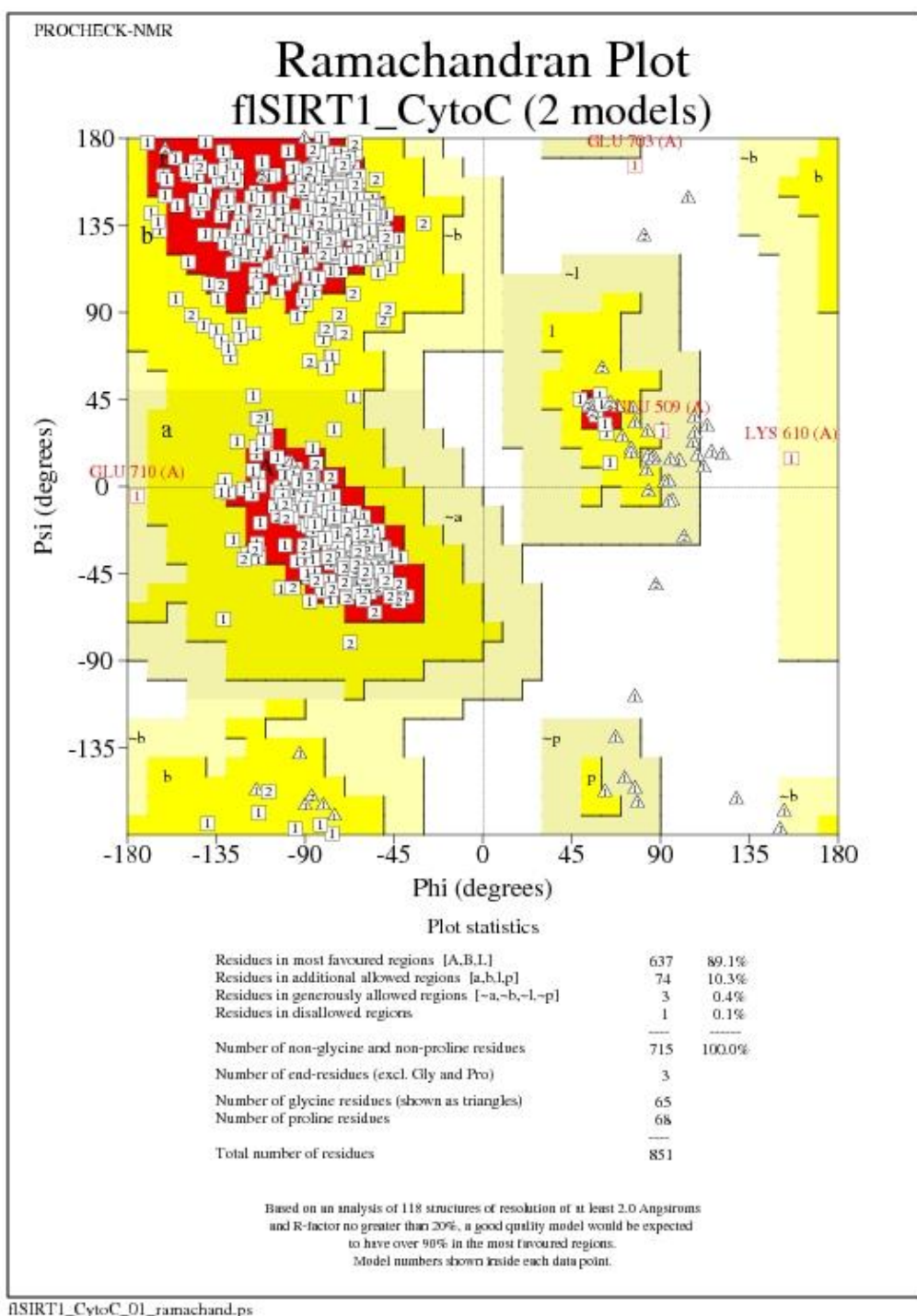
Output from PROCHECK

Ramachandran Plot for all models

Text summary of Ramachandran Plot

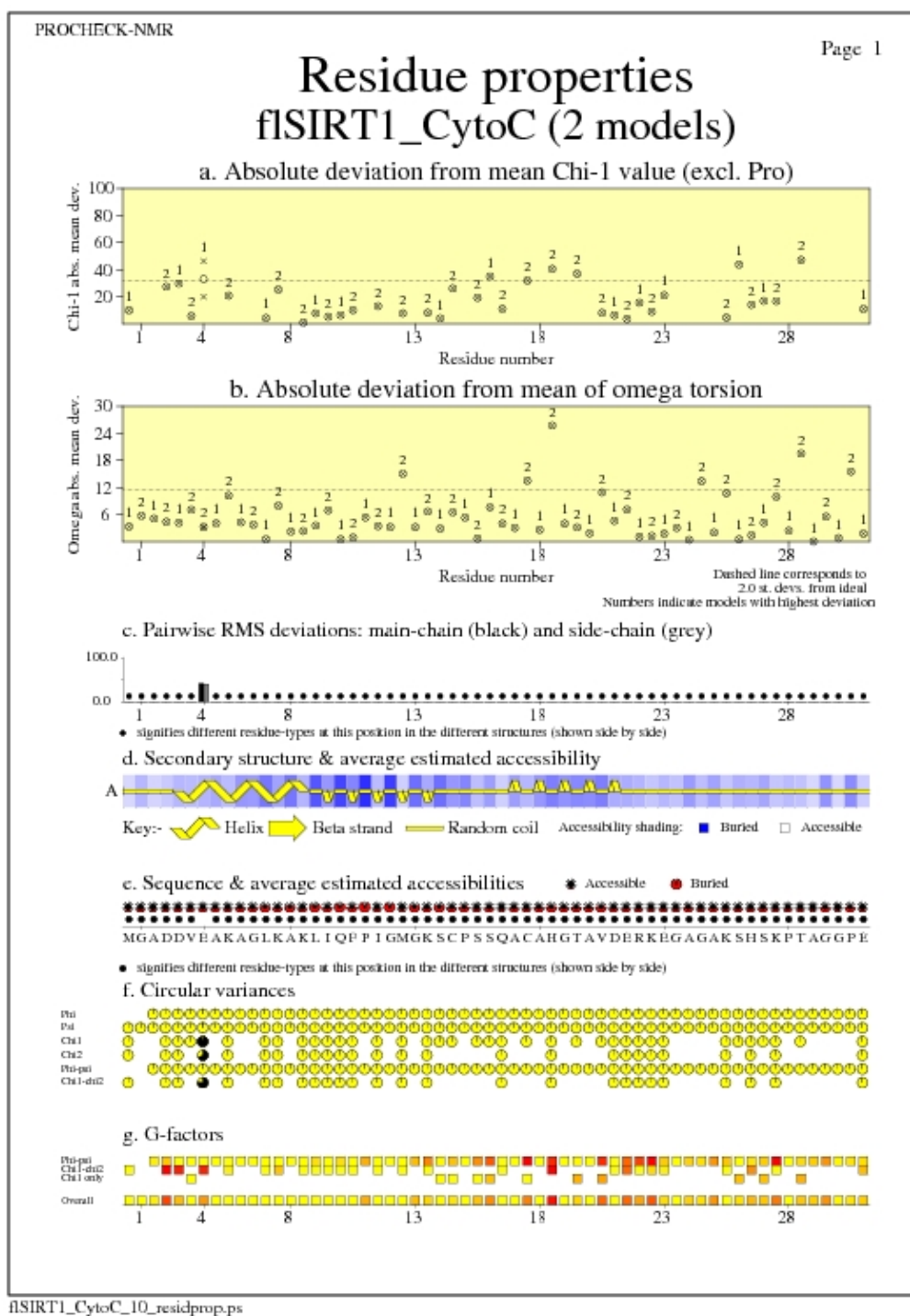
```
+-----<<< P R O C H E C K      S U M M A R Y >>>-----+
|
| flSIRT1_CytoC_002.rin    0.0                                851 residues |
|
*| Ramachandran plot:    89.1% core    10.3% allow    0.4% gener    0.1% disall |
|
+| All Ramachandrans:    18 labelled residues (out of 847)          |
*| Chi1-chi2 plots:      15 labelled residues (out of 494)          |
```

JPEG image for all model Ramachandran Plot

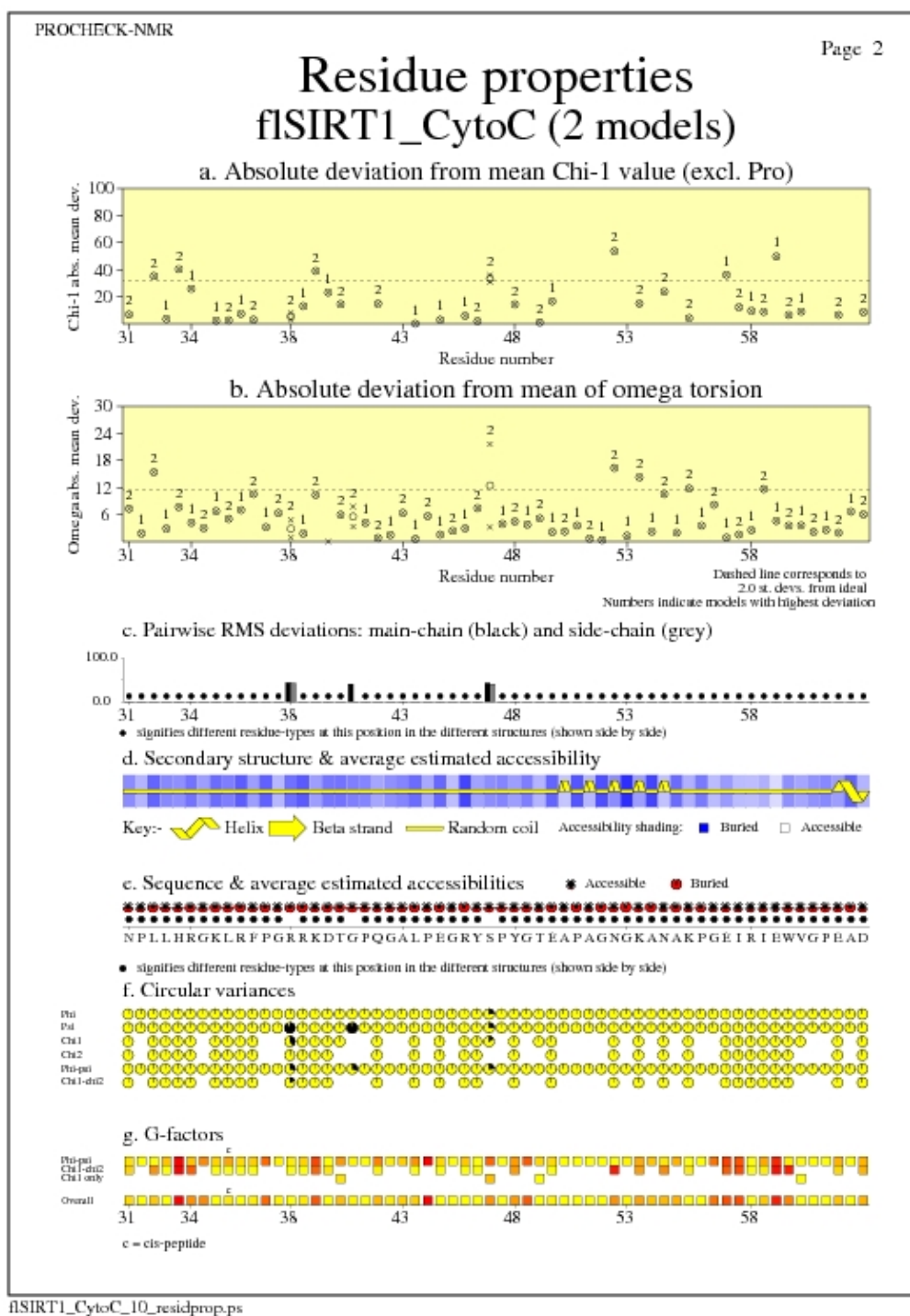


Residue Properties for all models

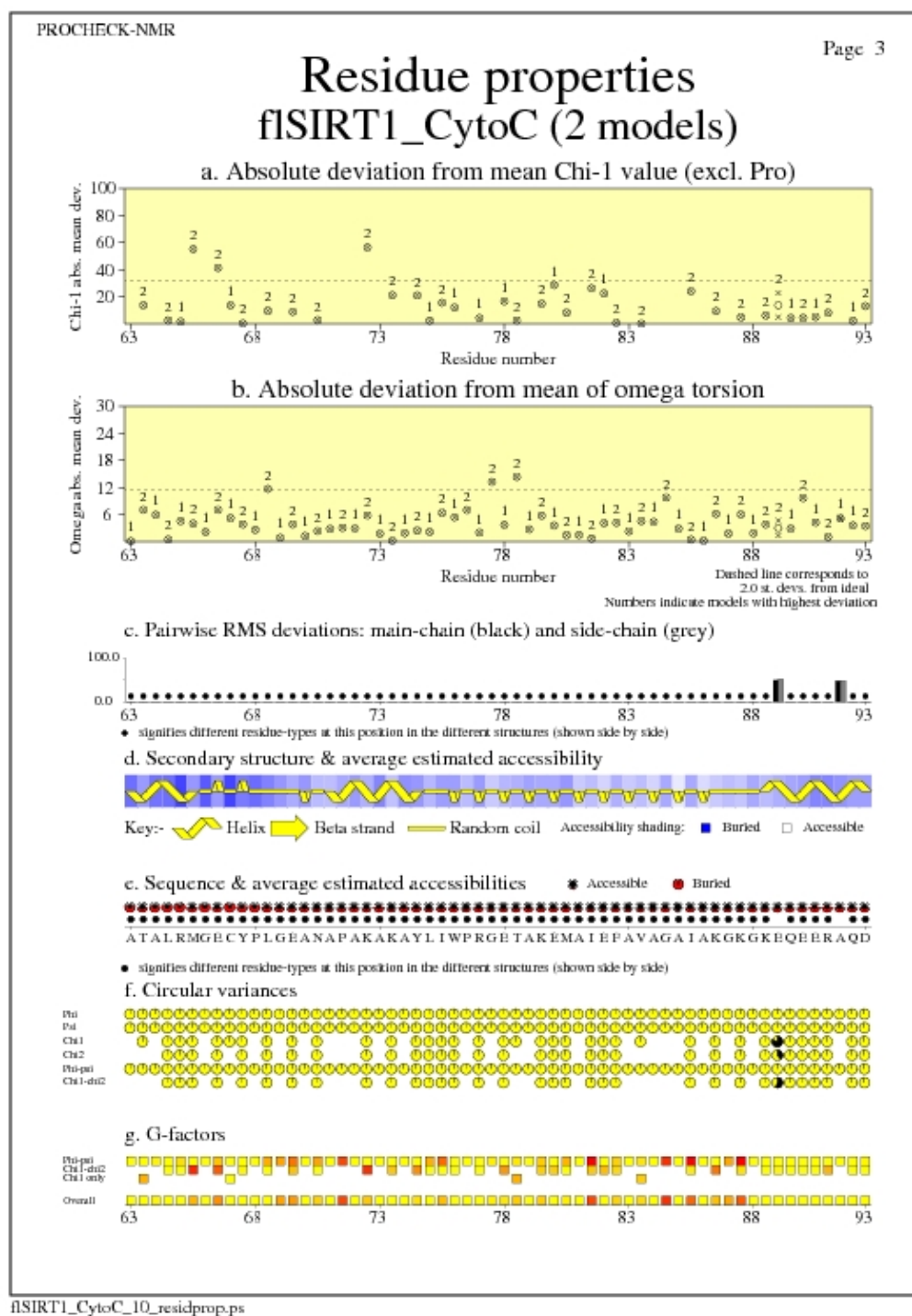
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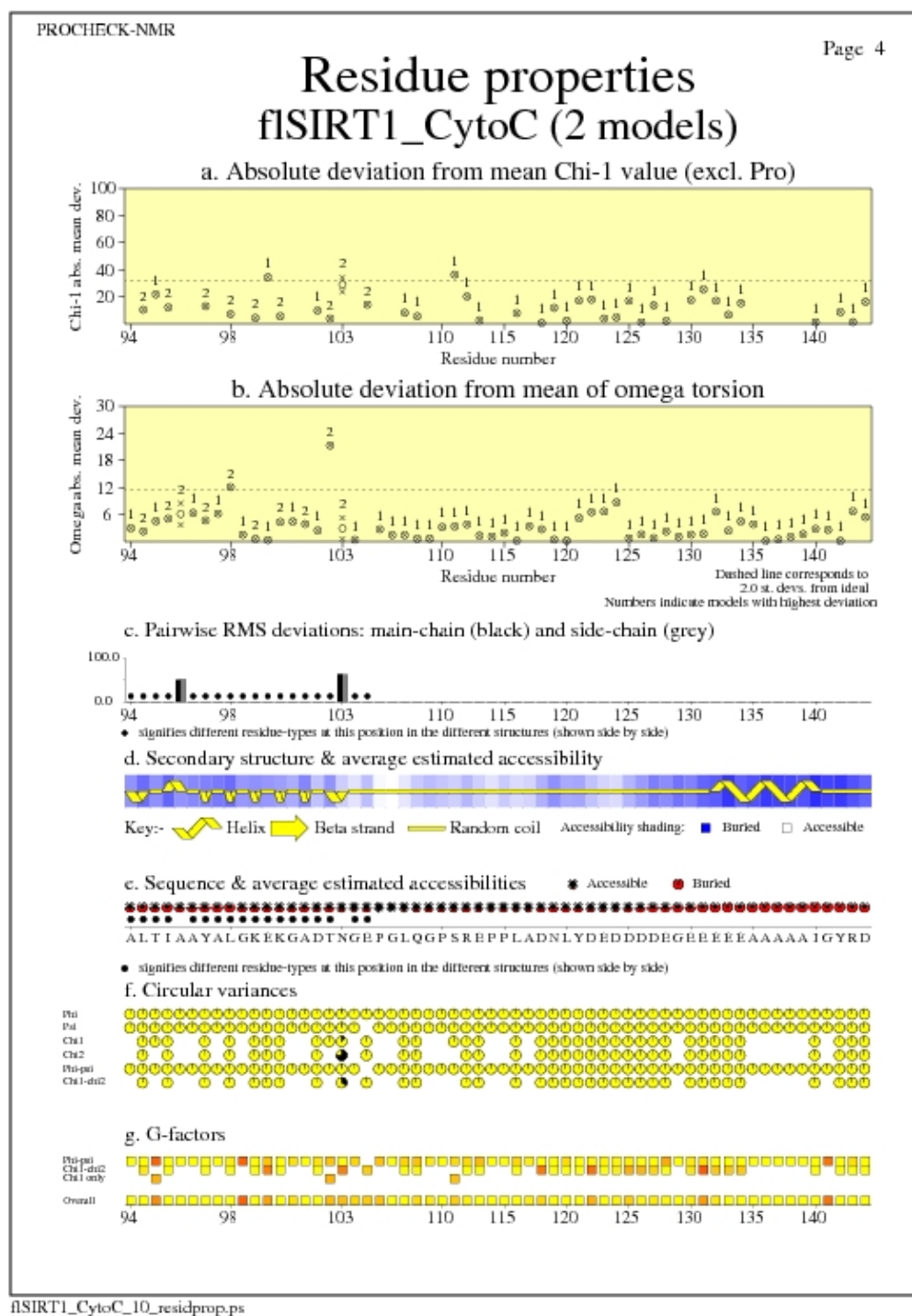
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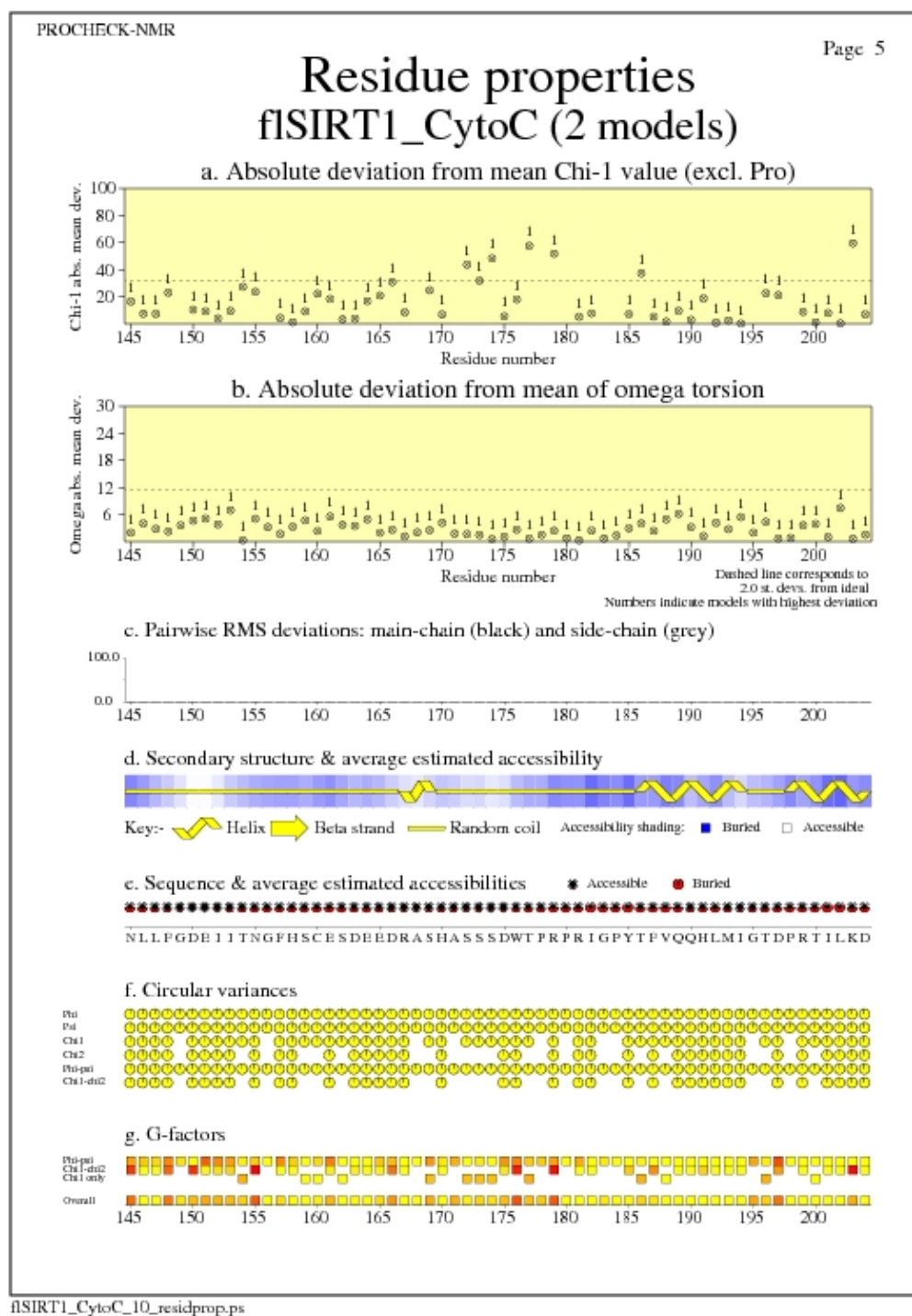
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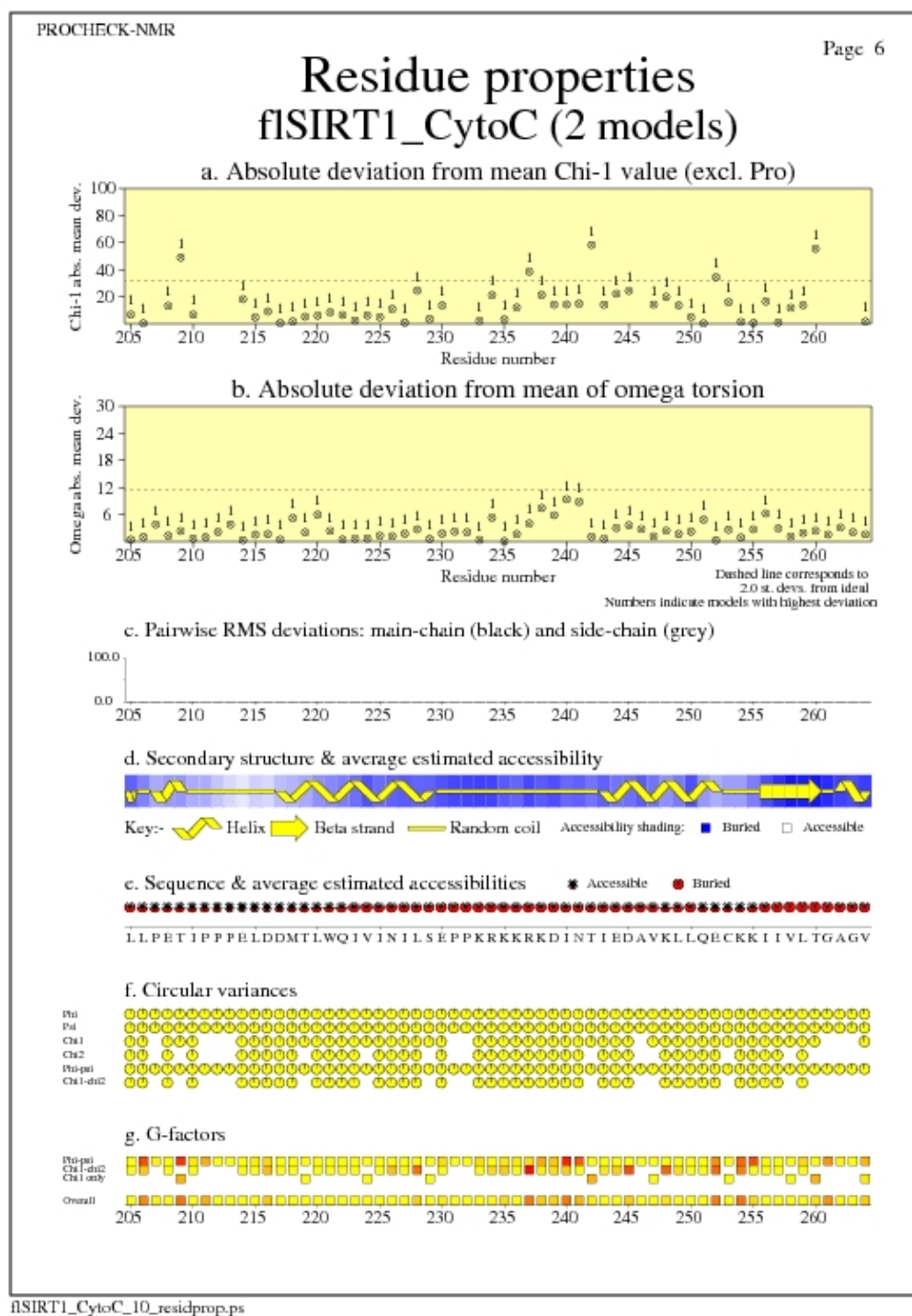
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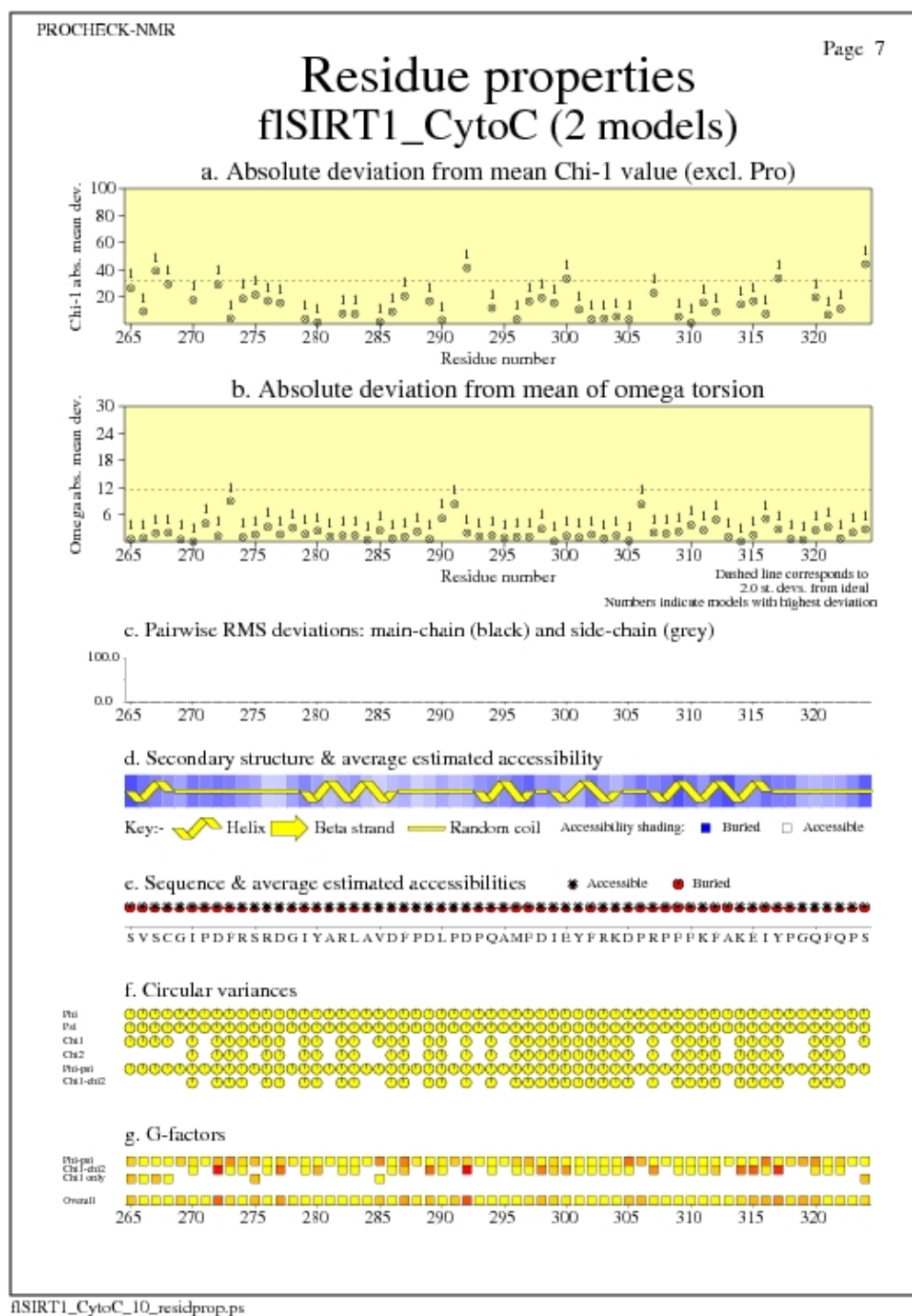
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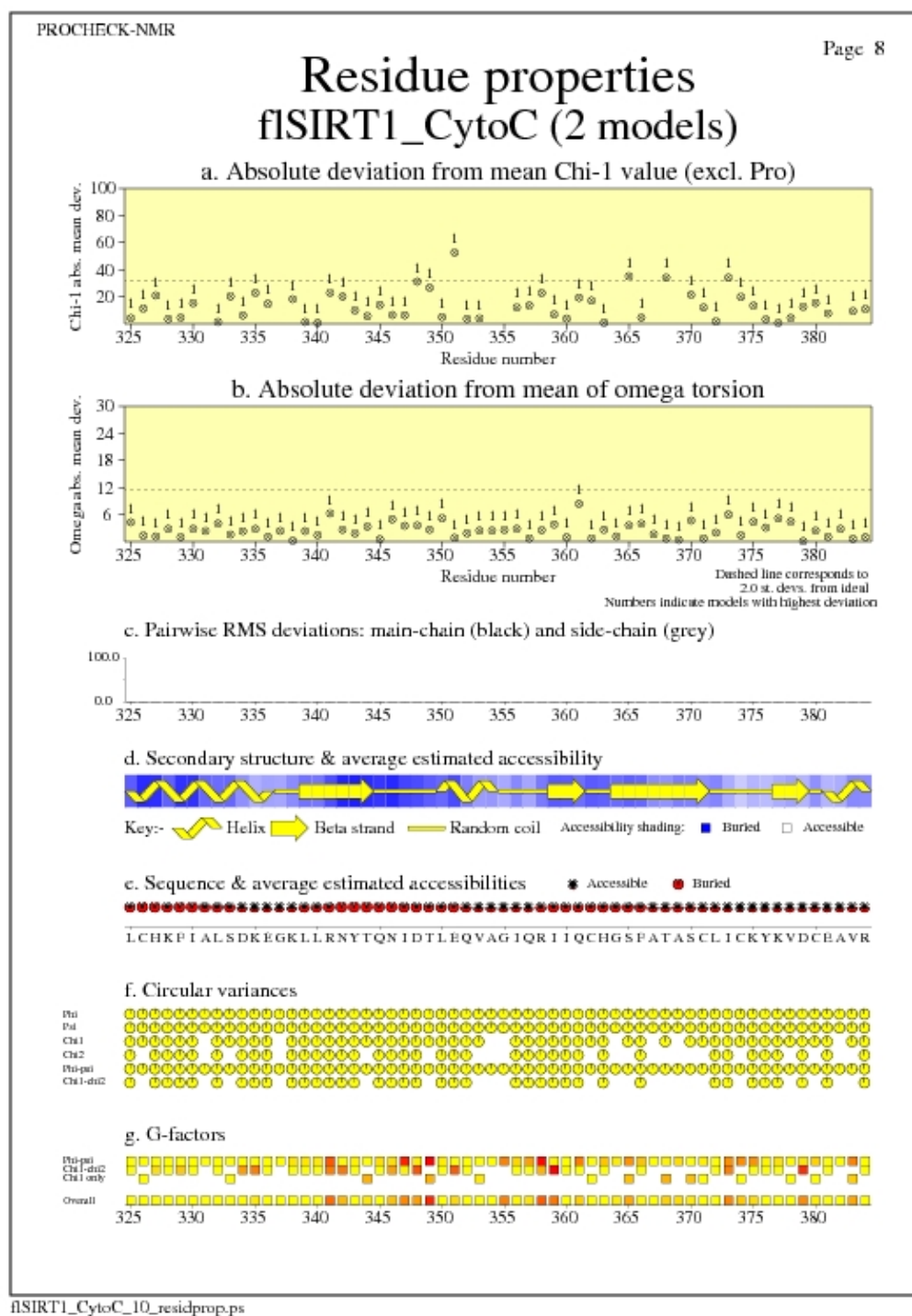
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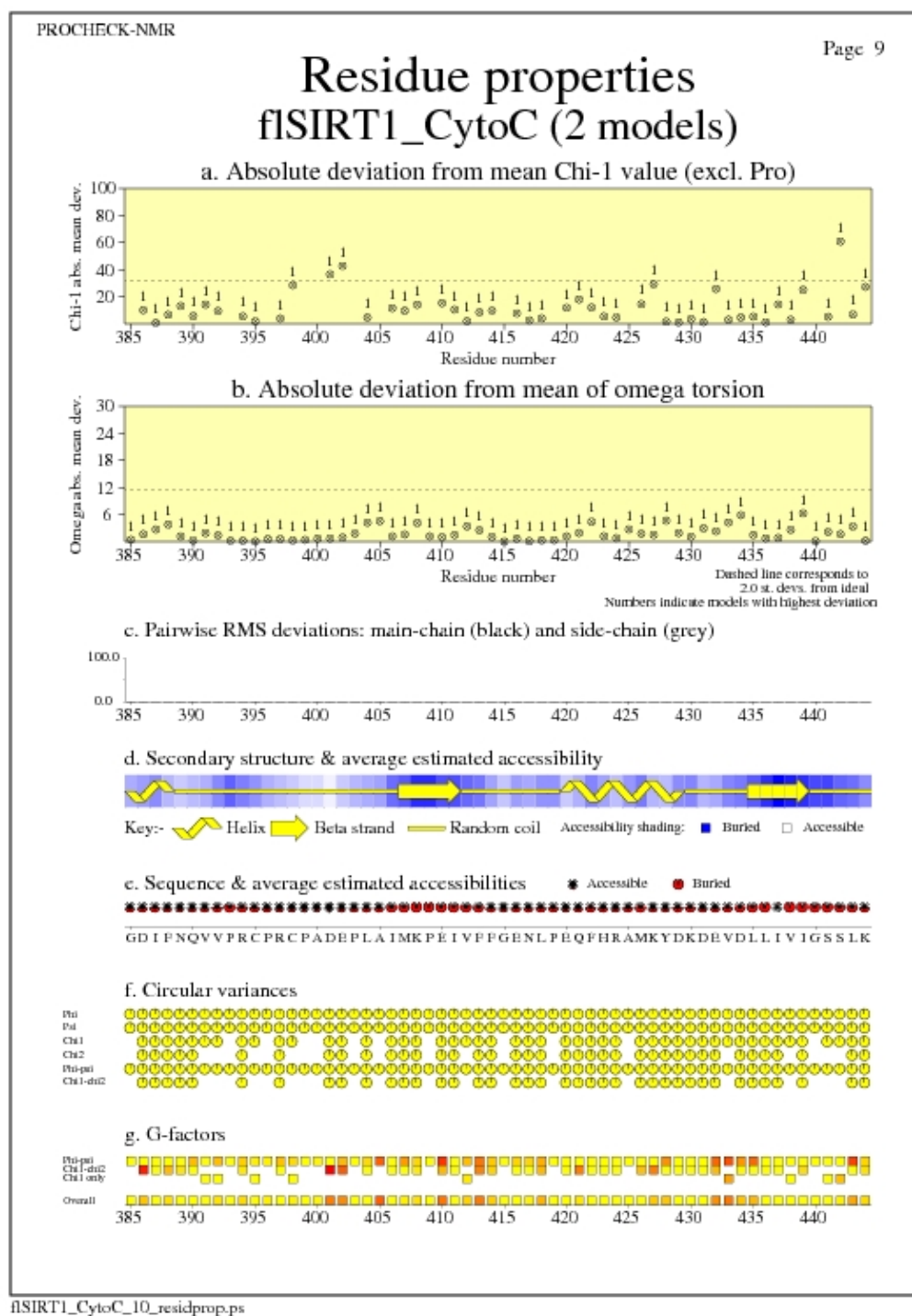
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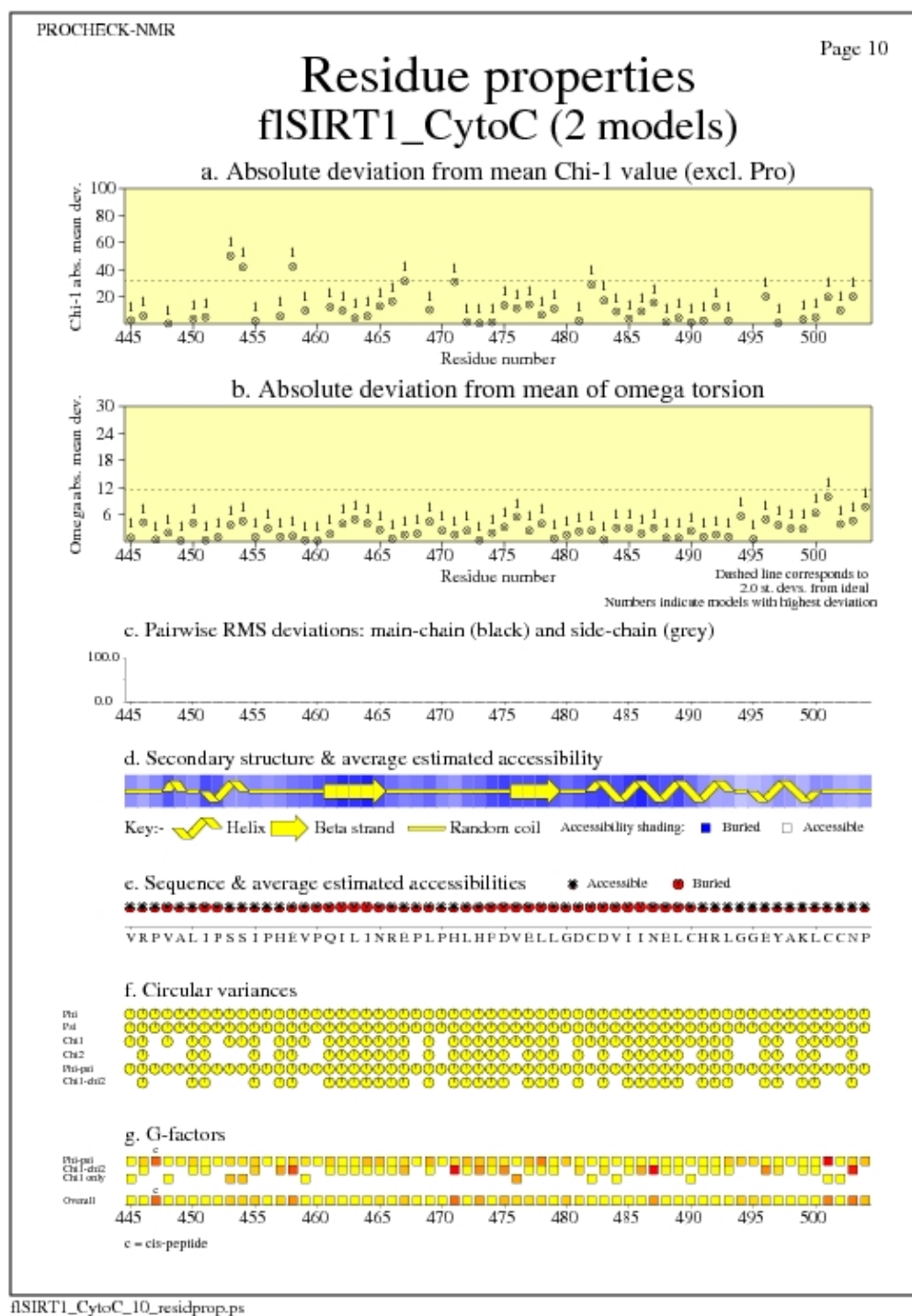
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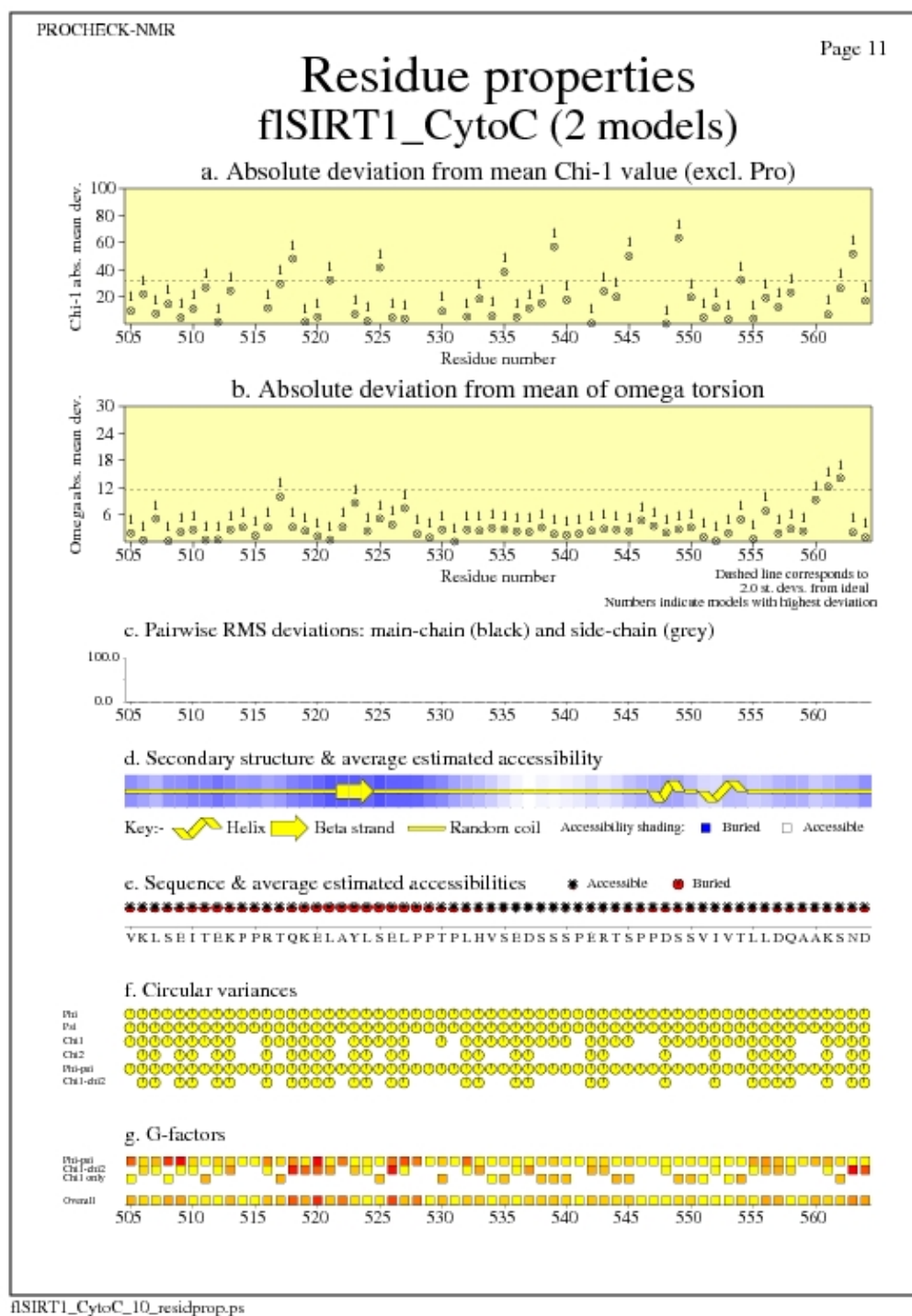
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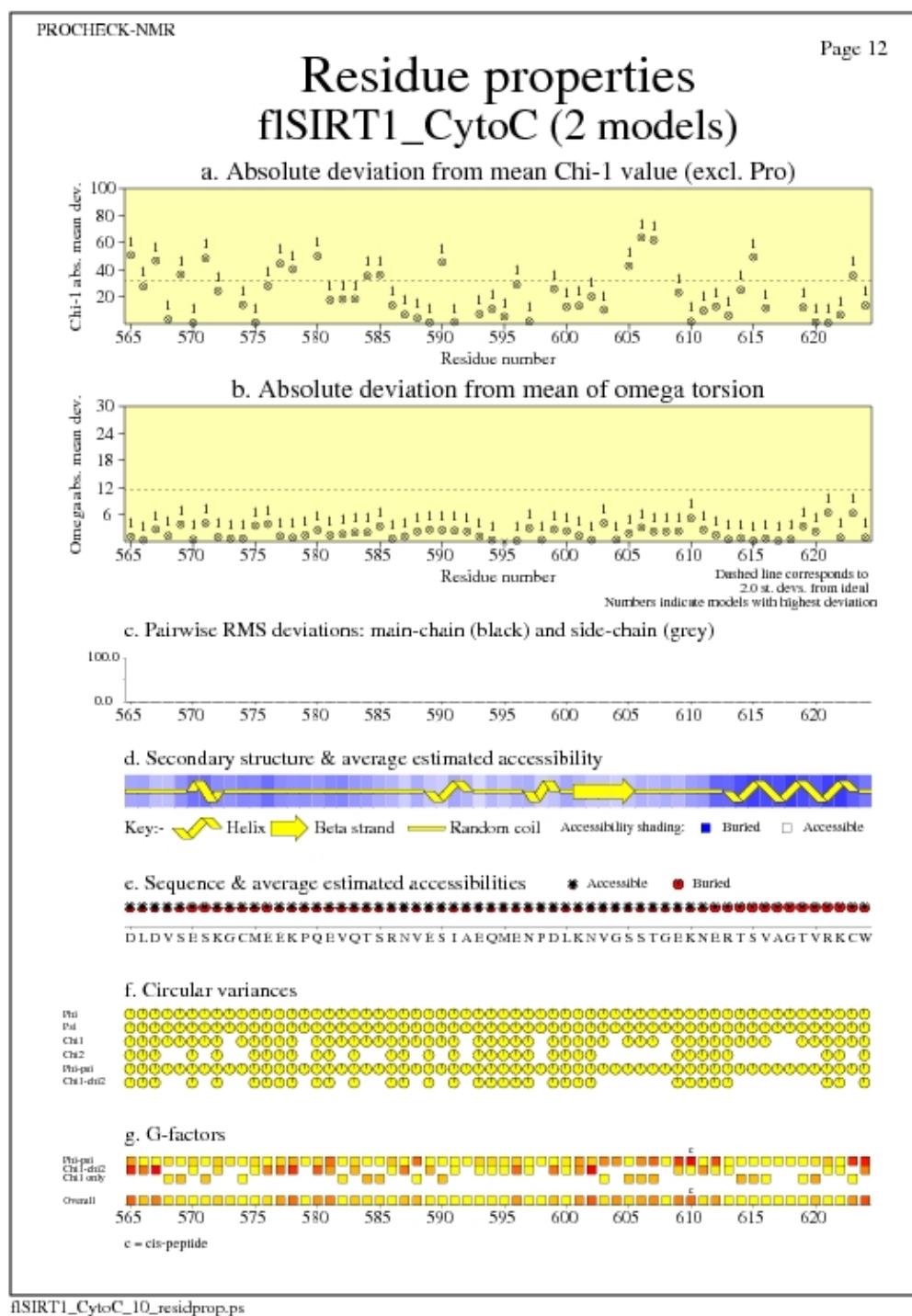
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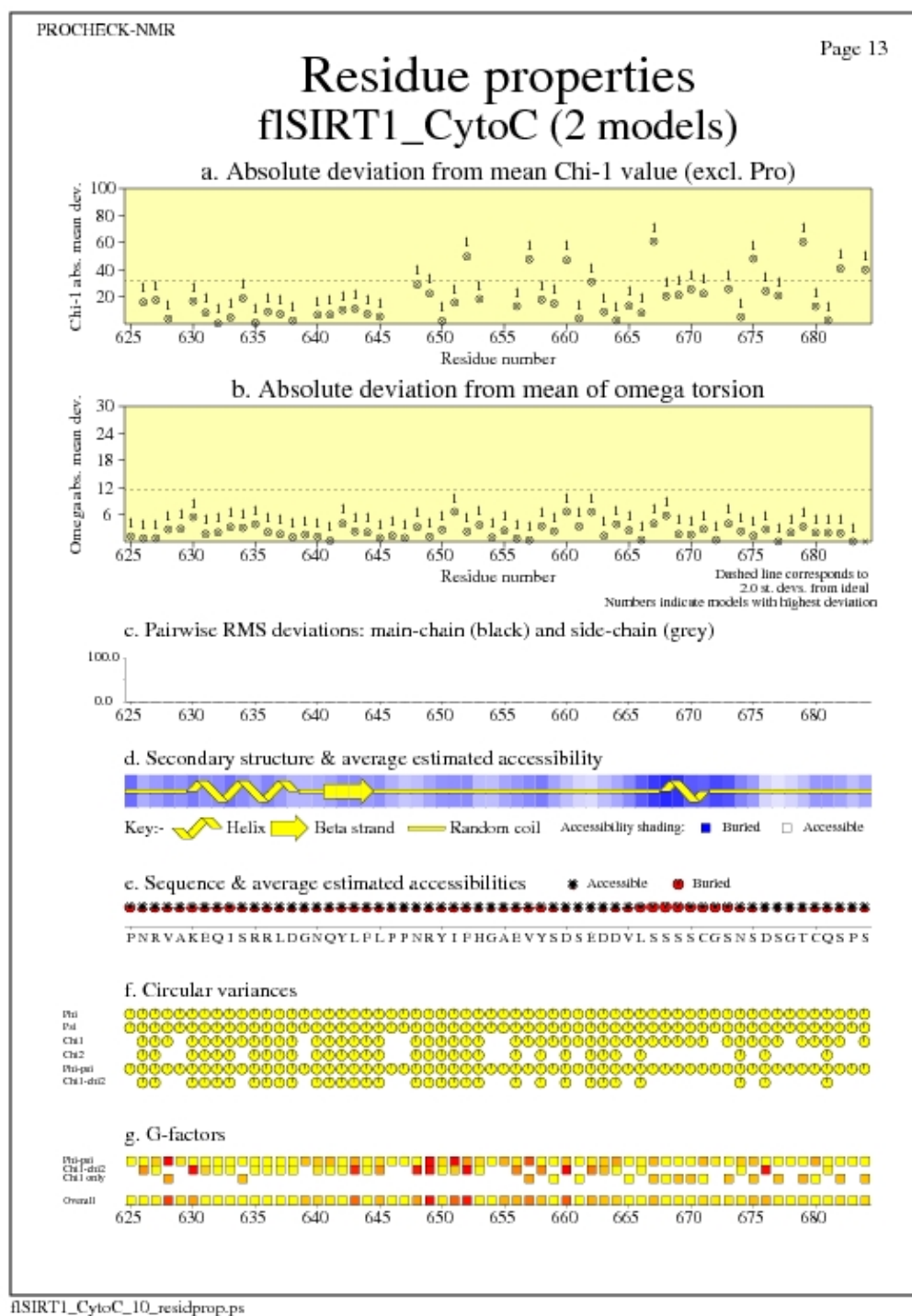
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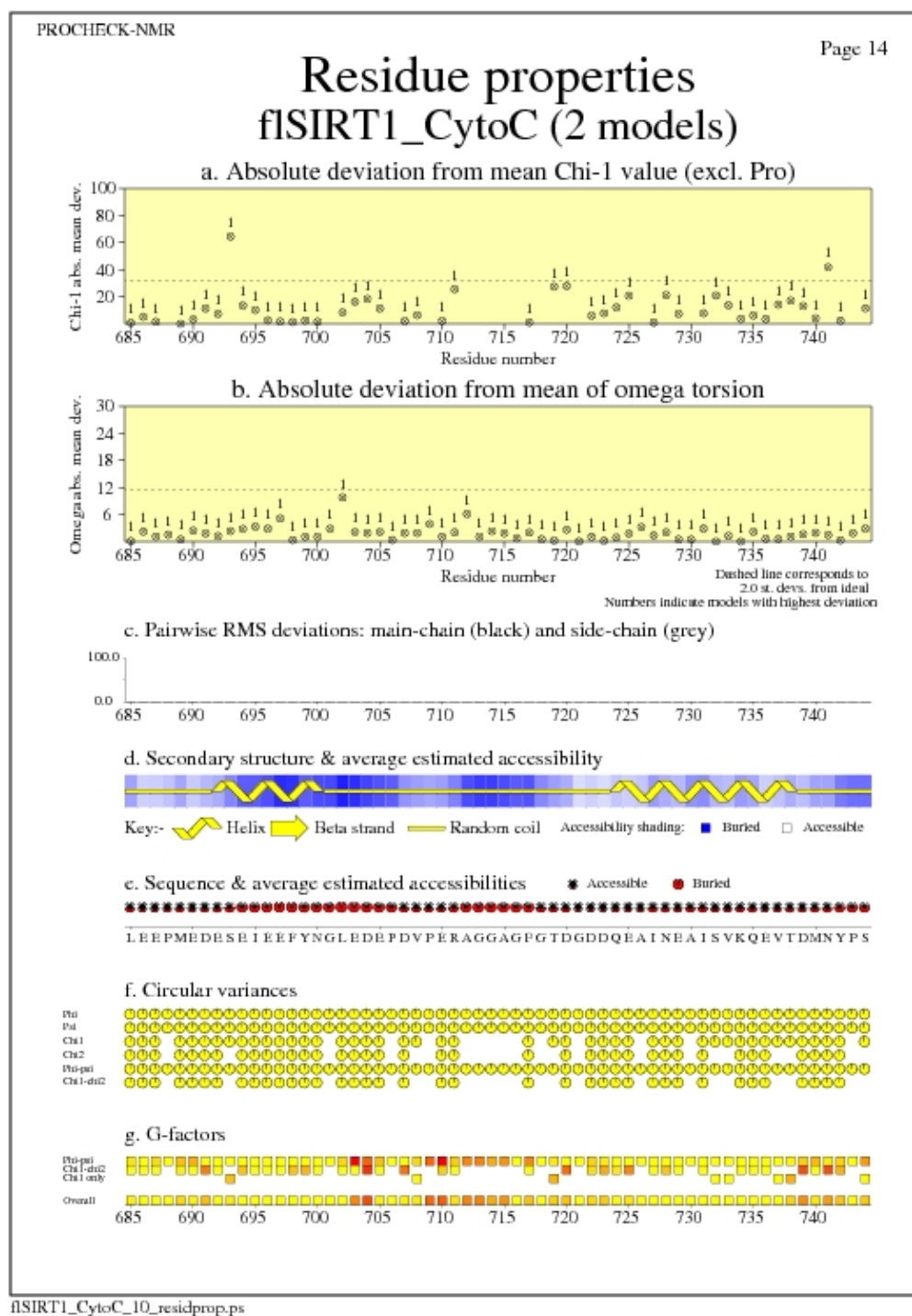
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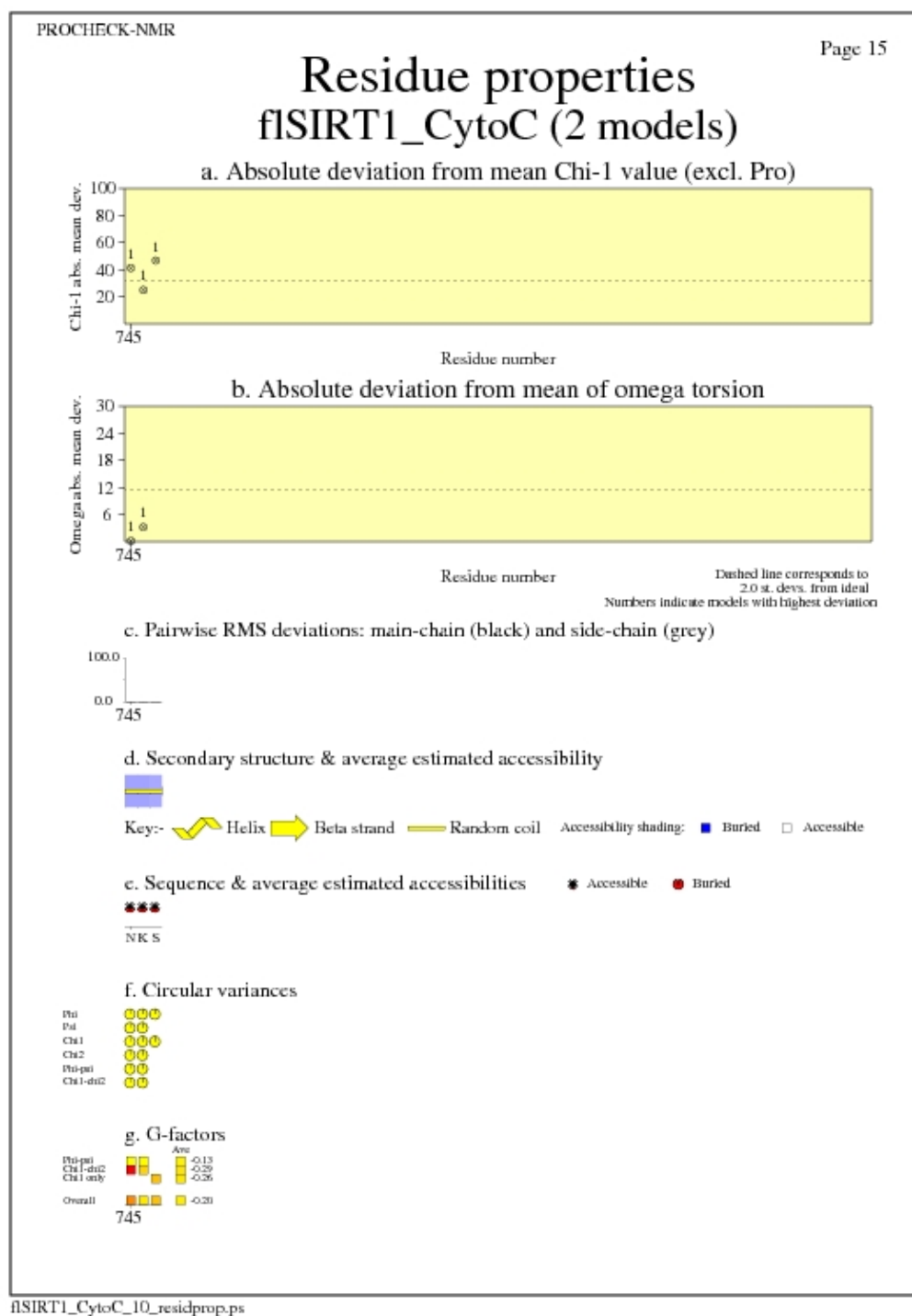
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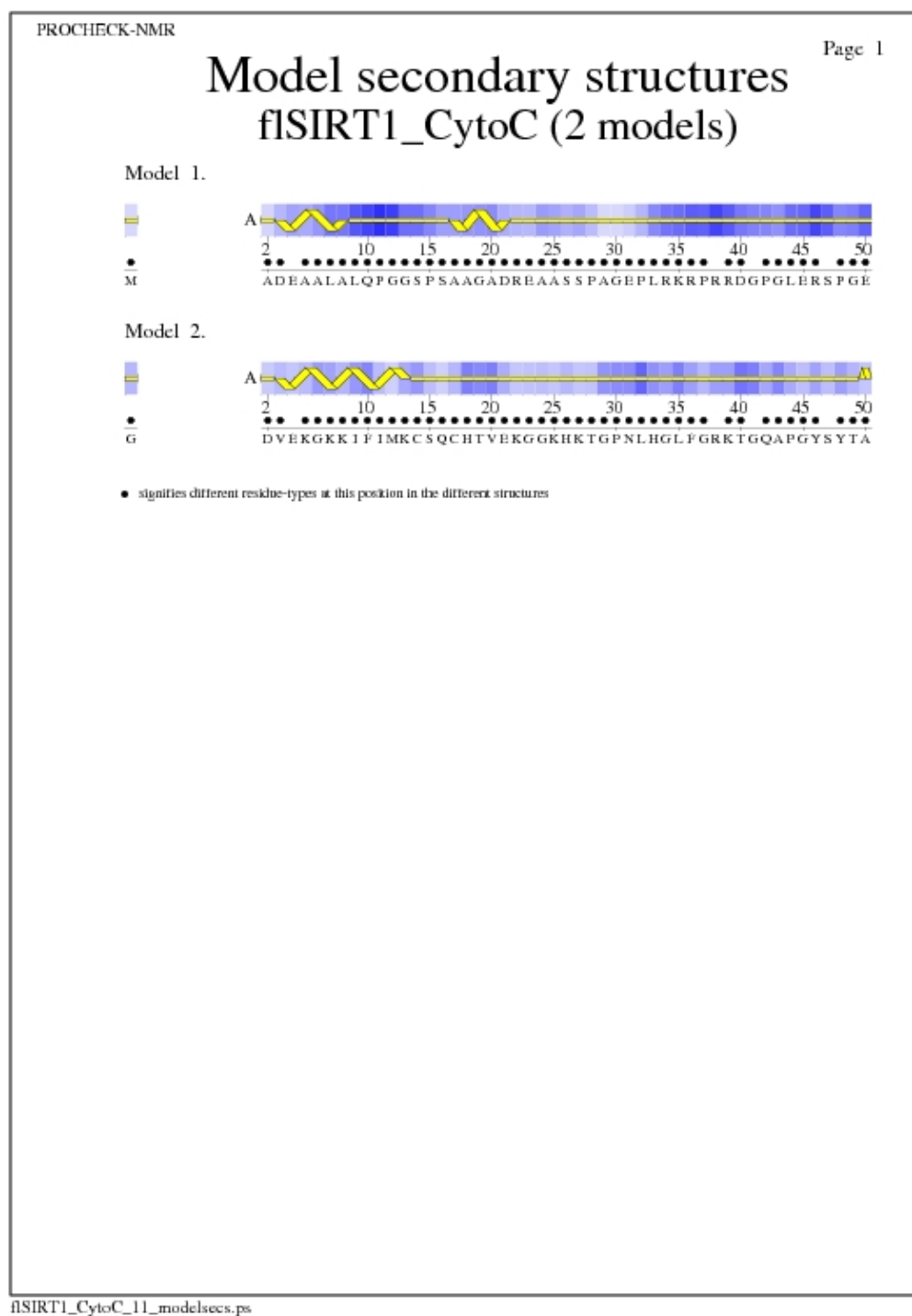


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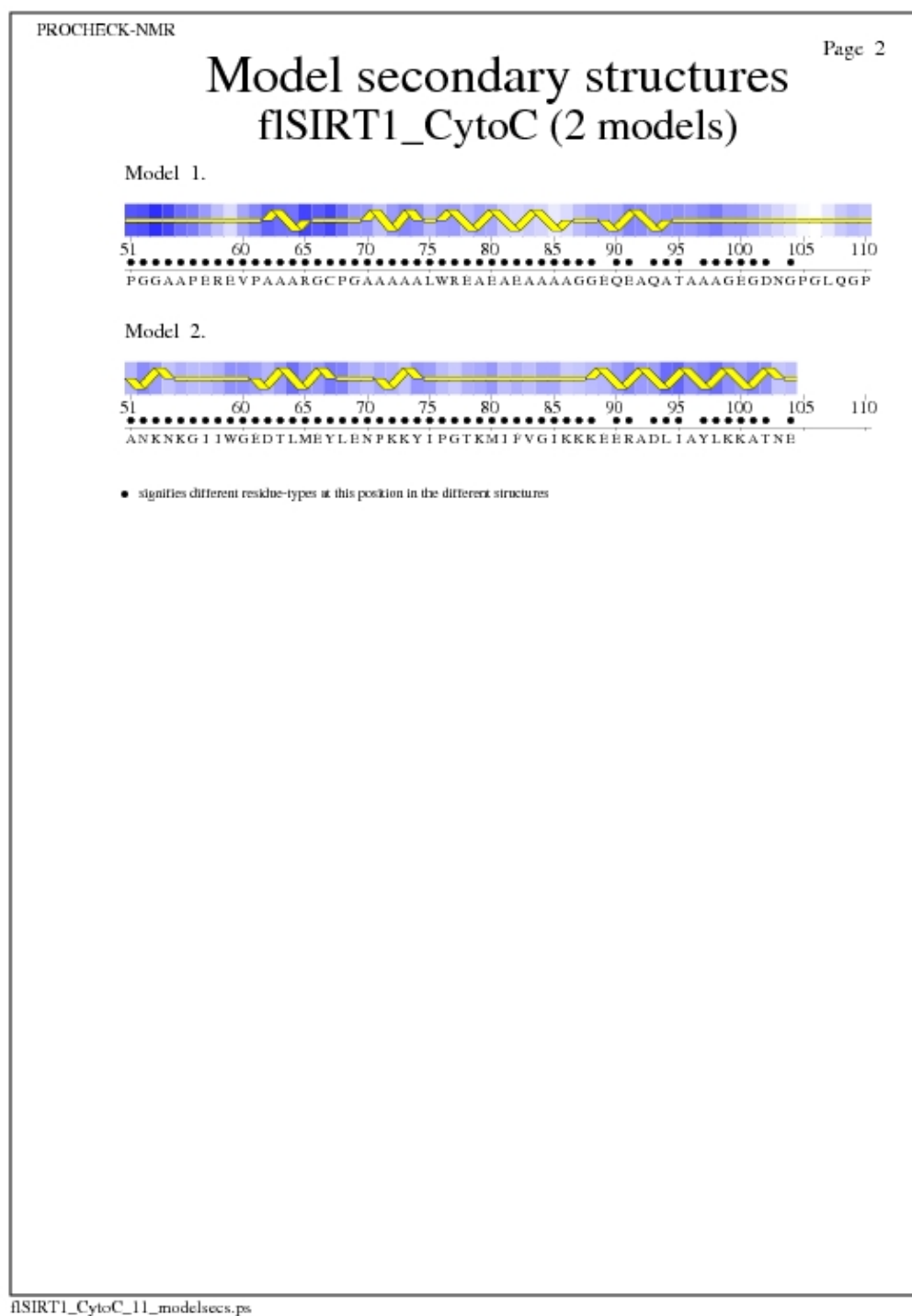


Model Secondary Structures from Procheck

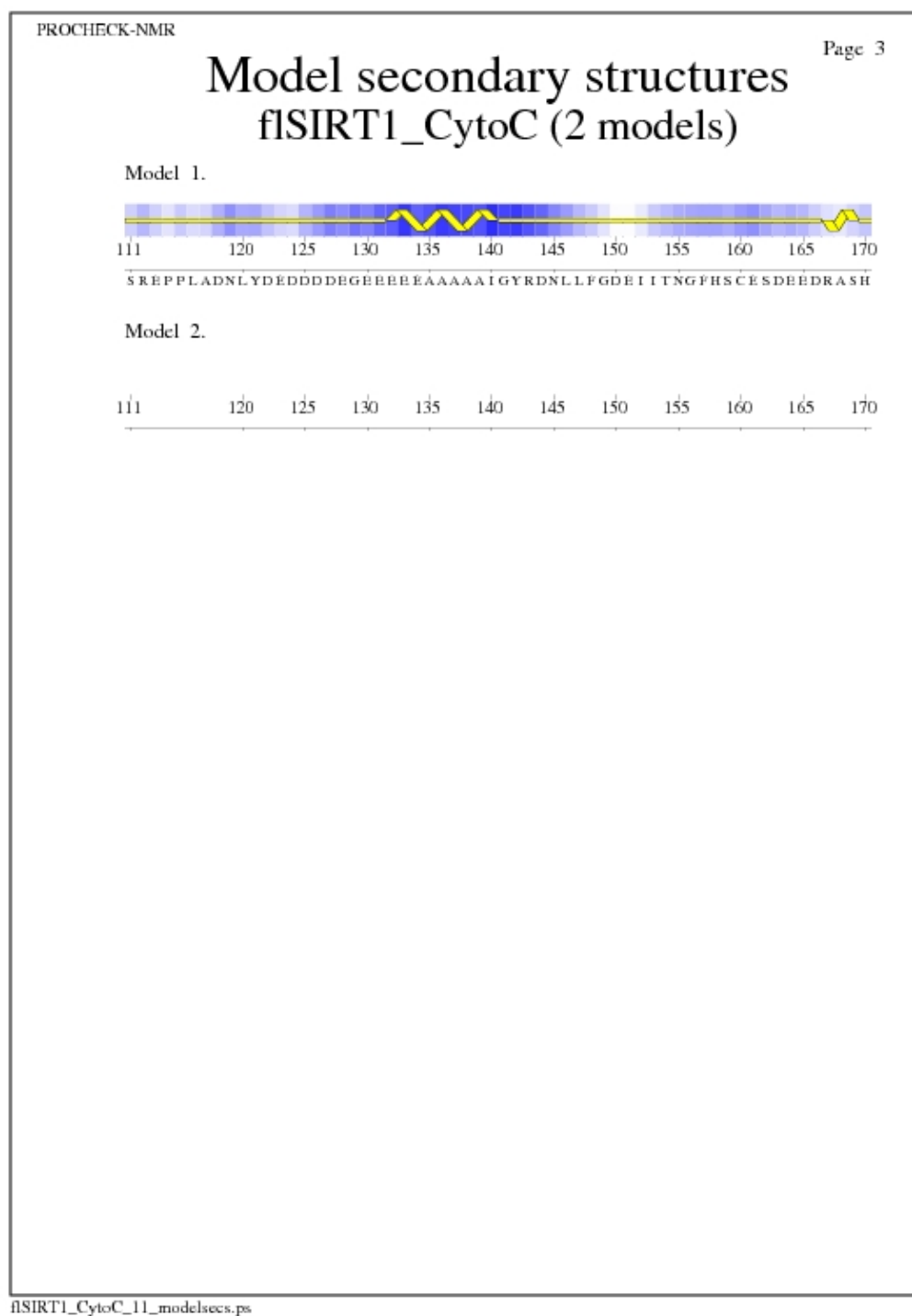
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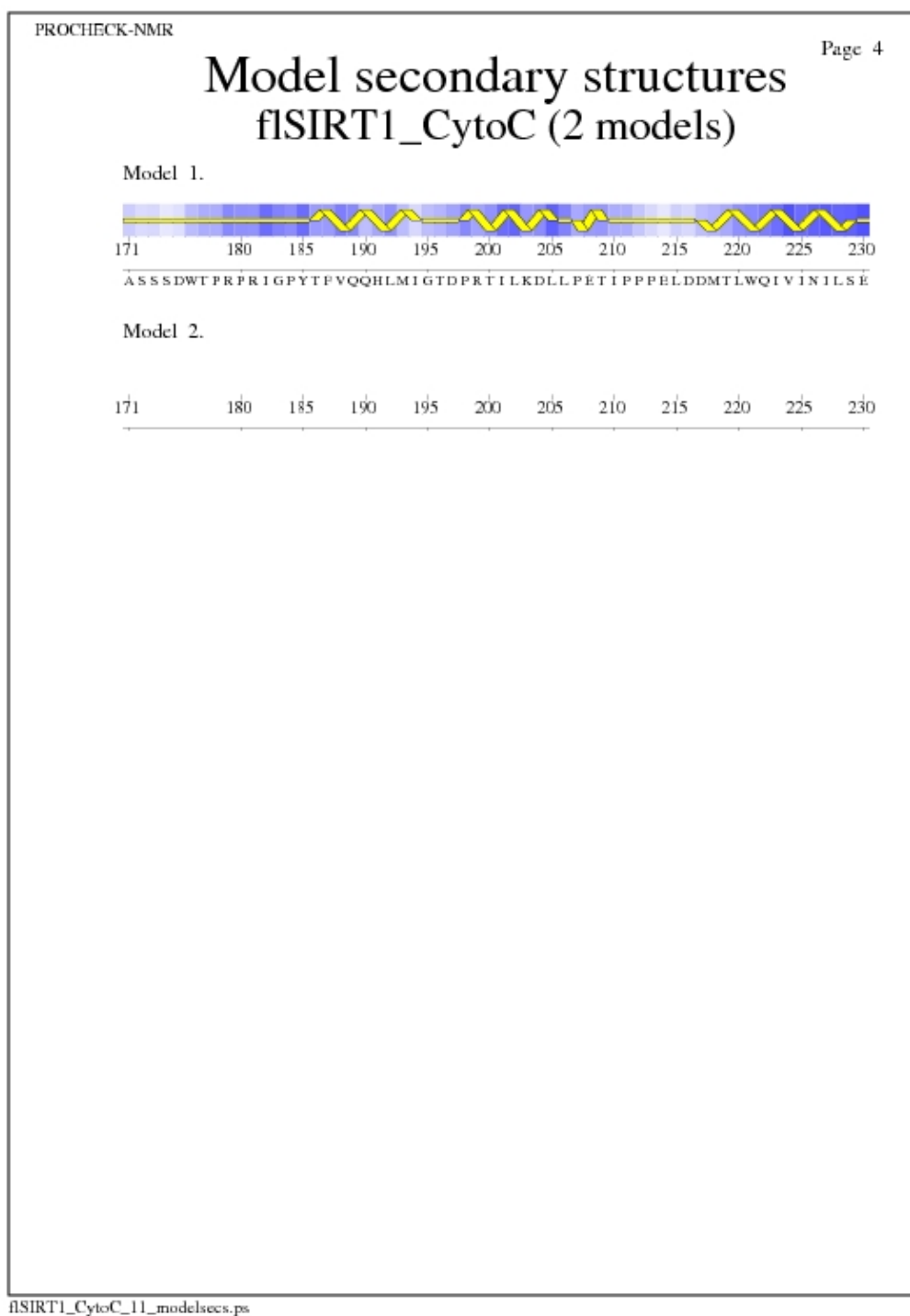
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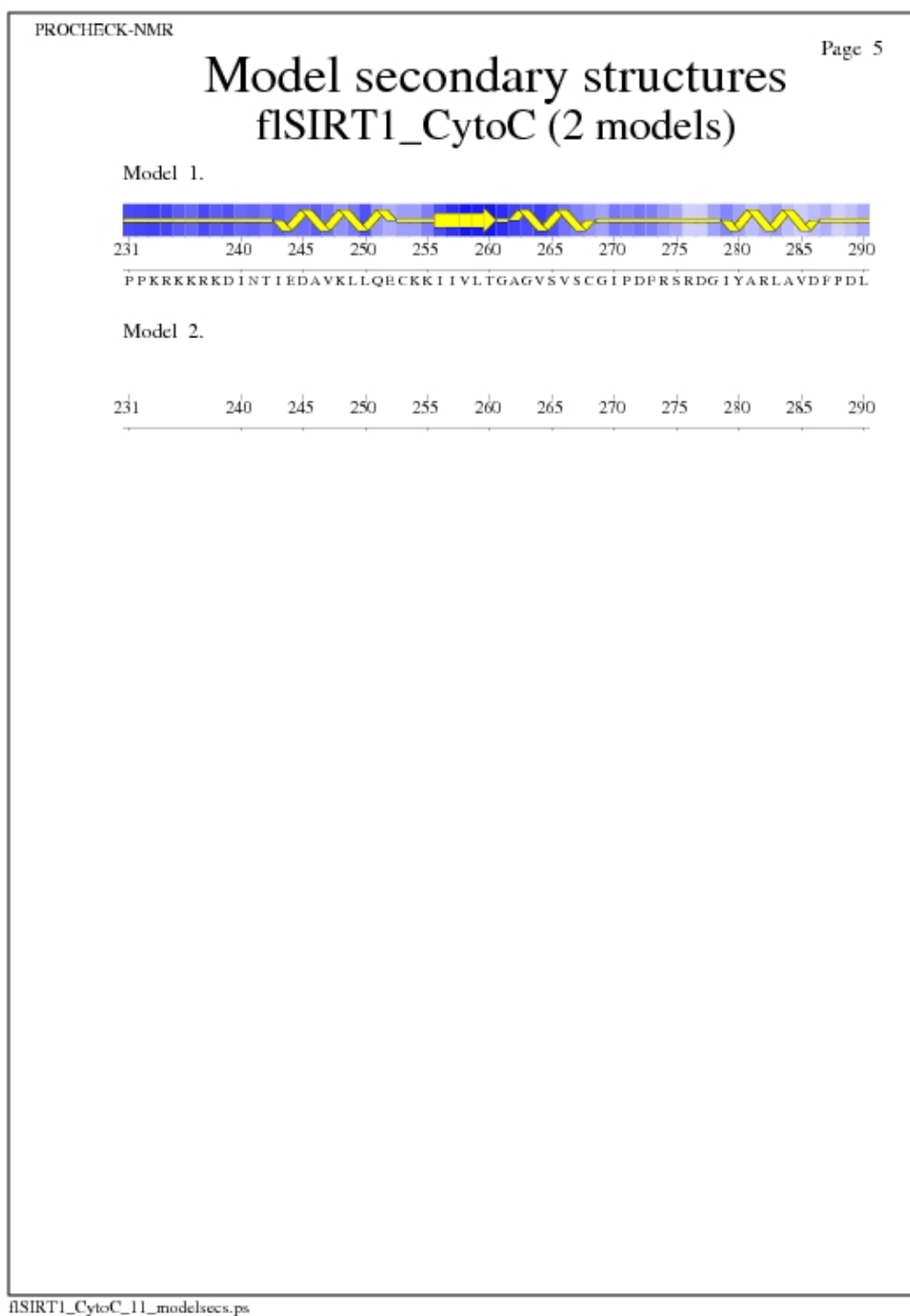
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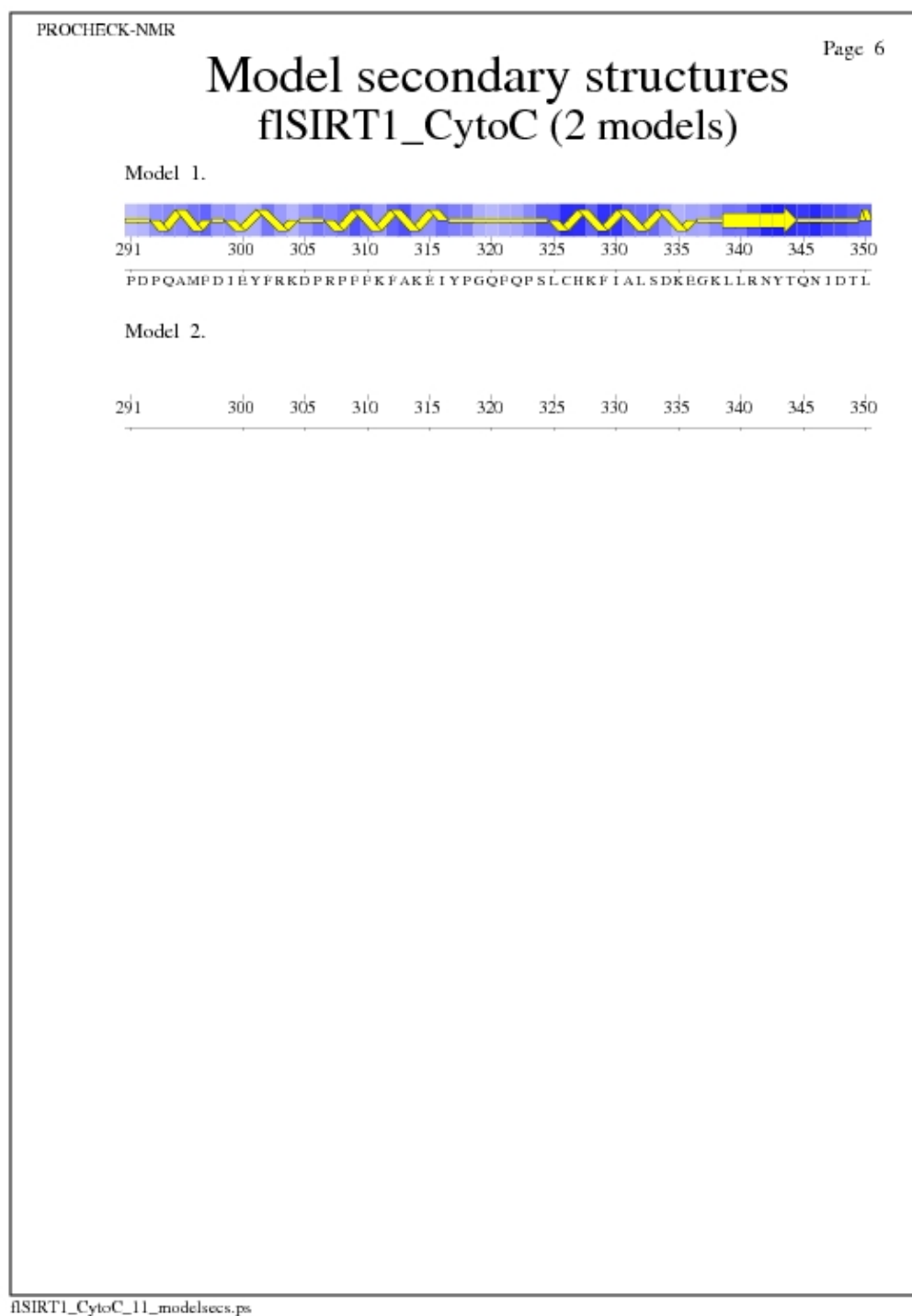
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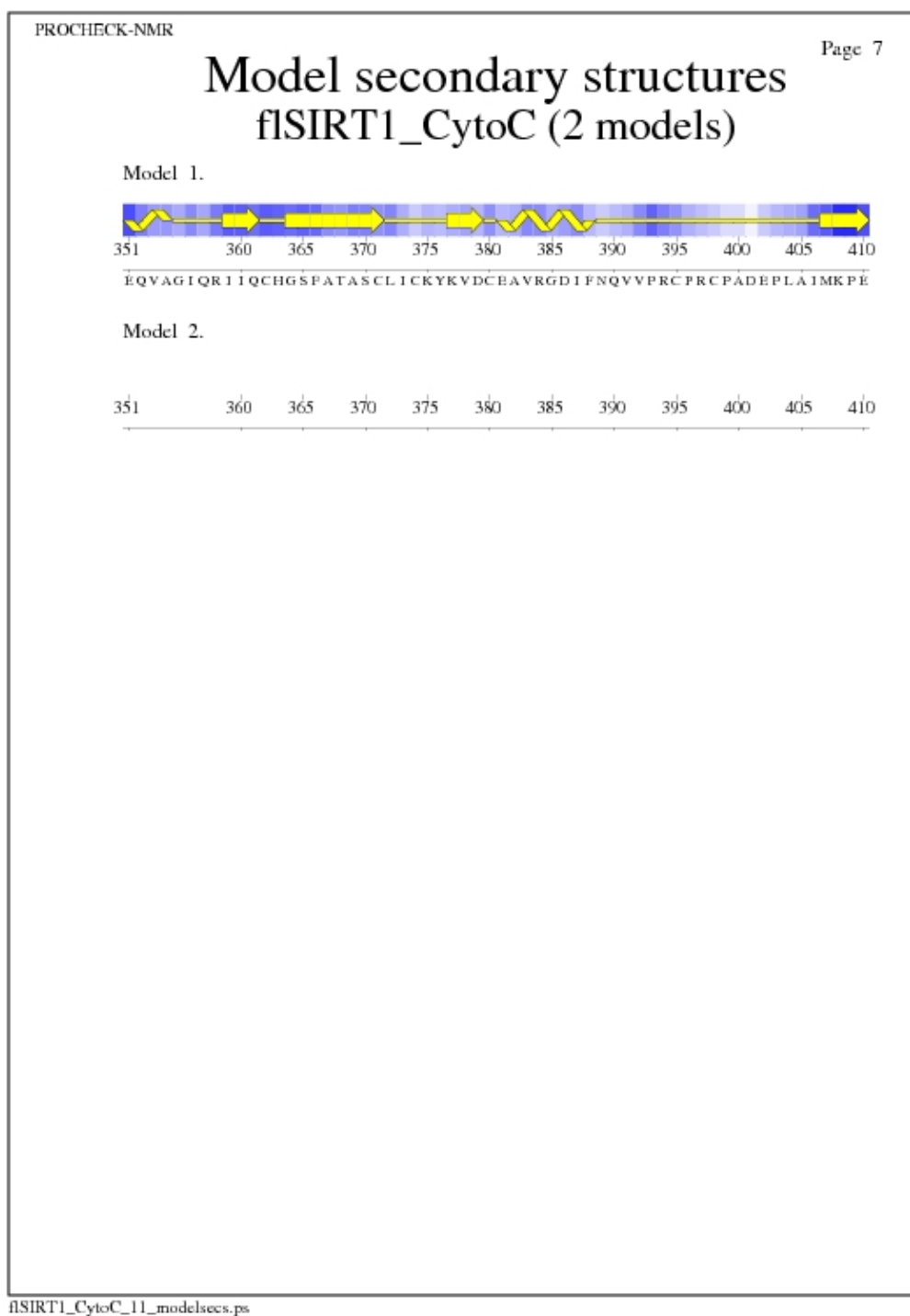
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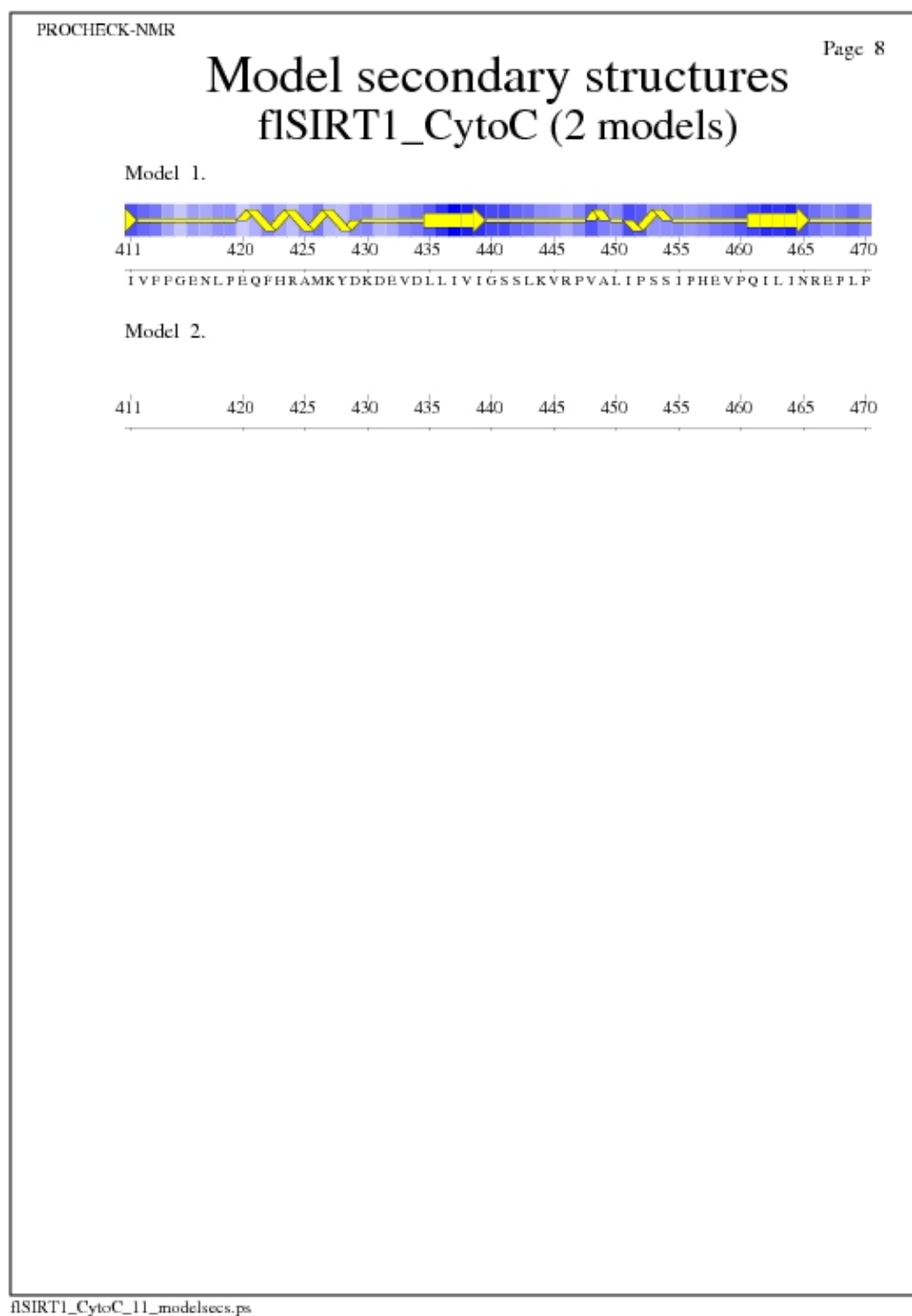
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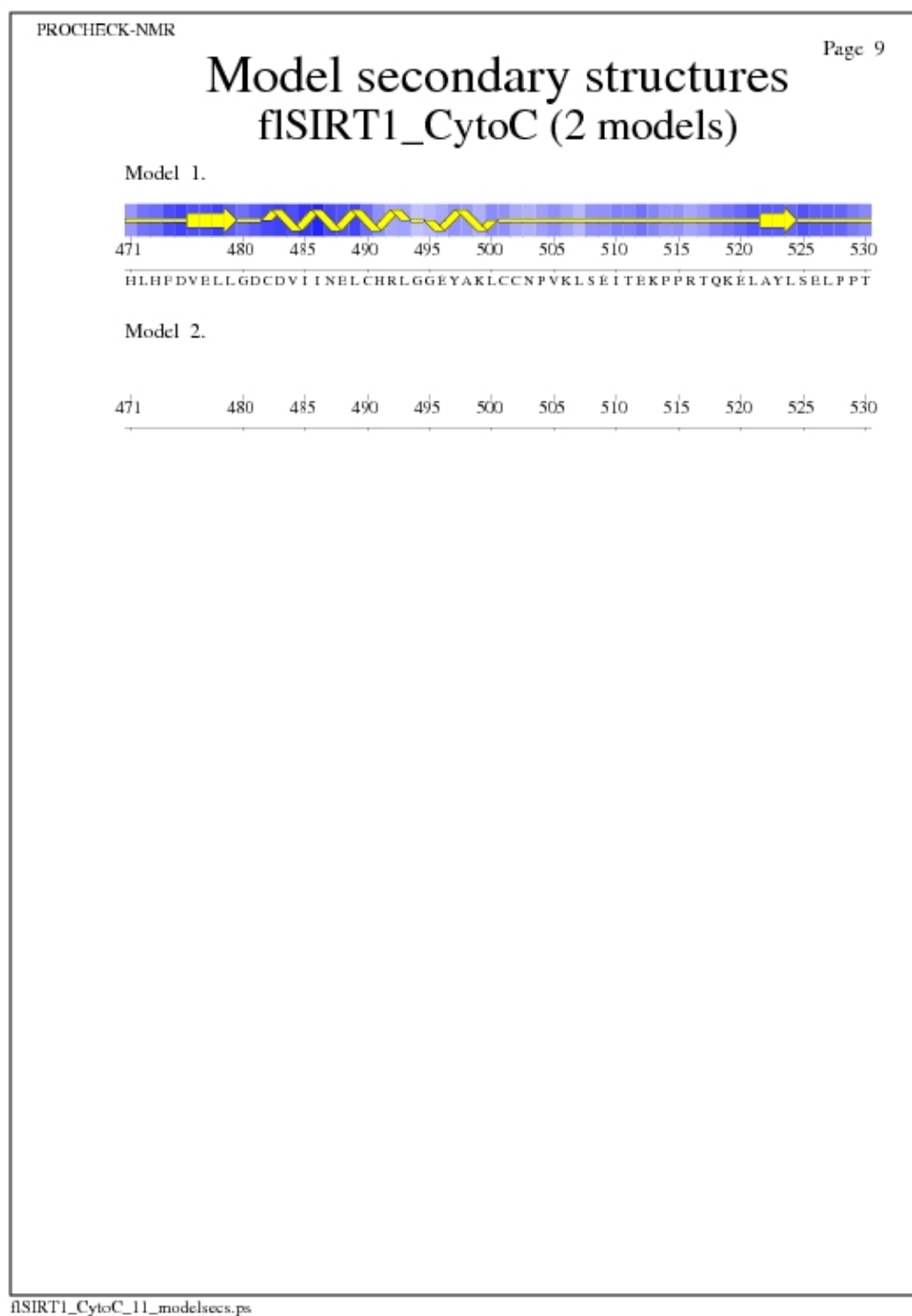
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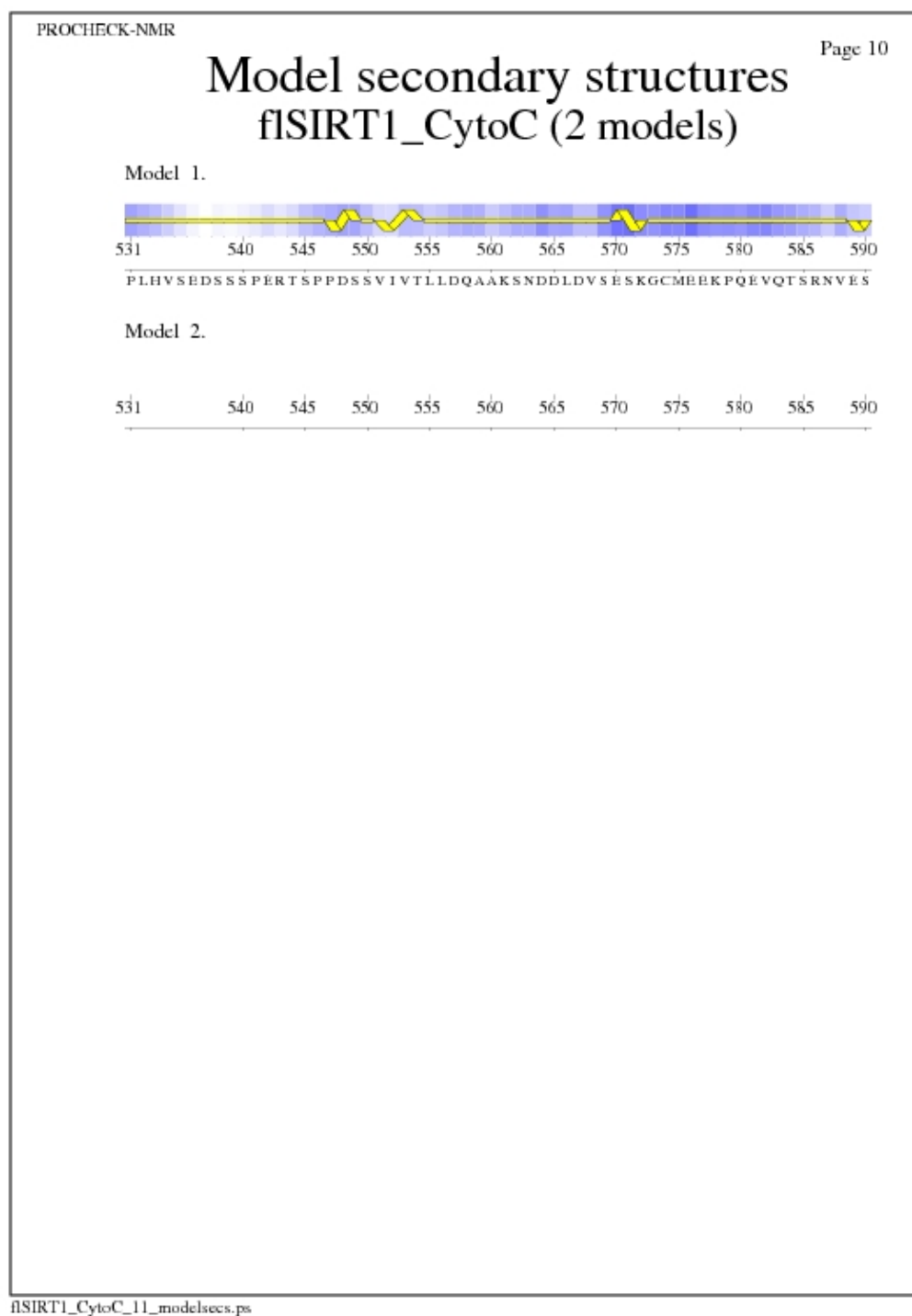
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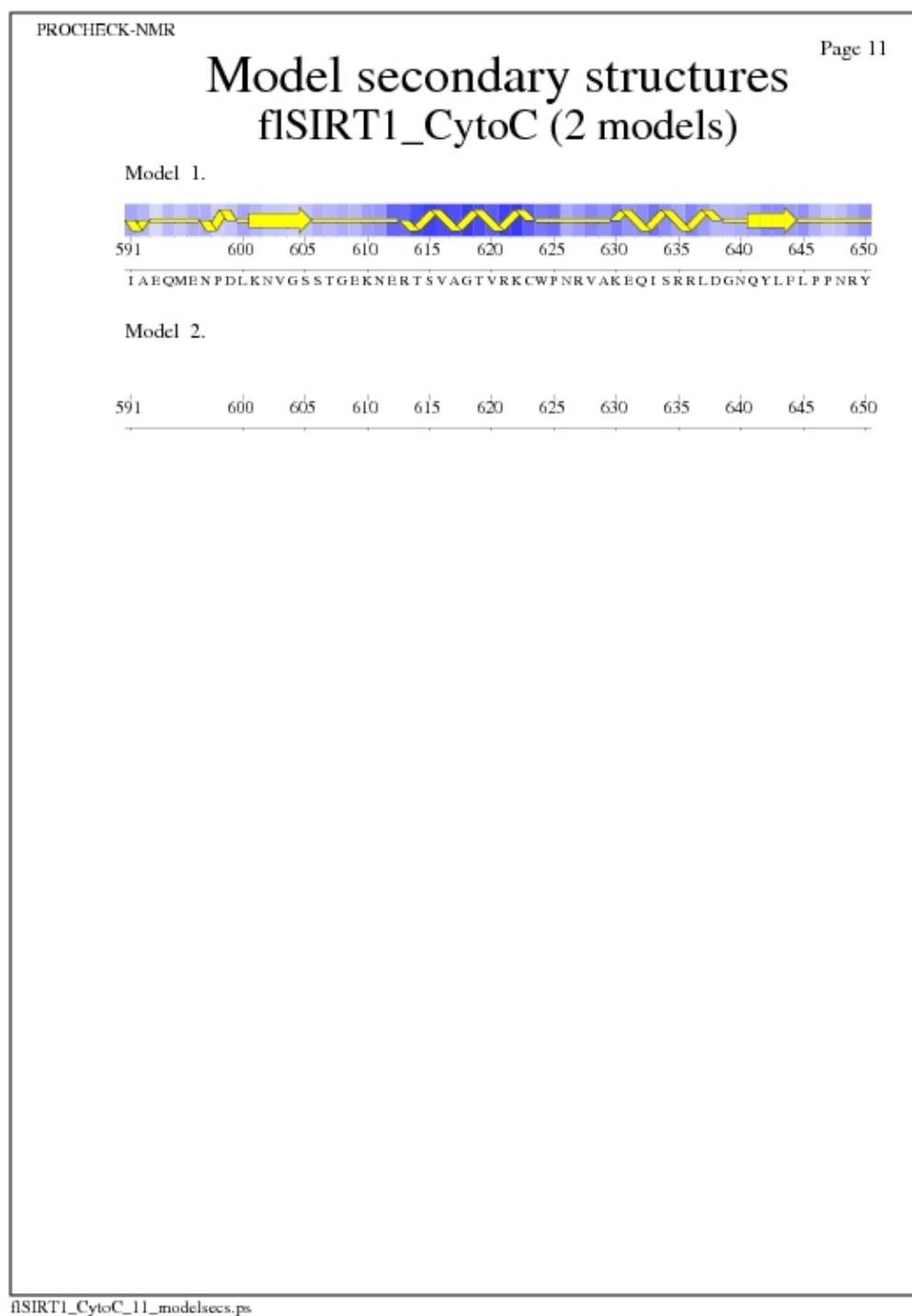
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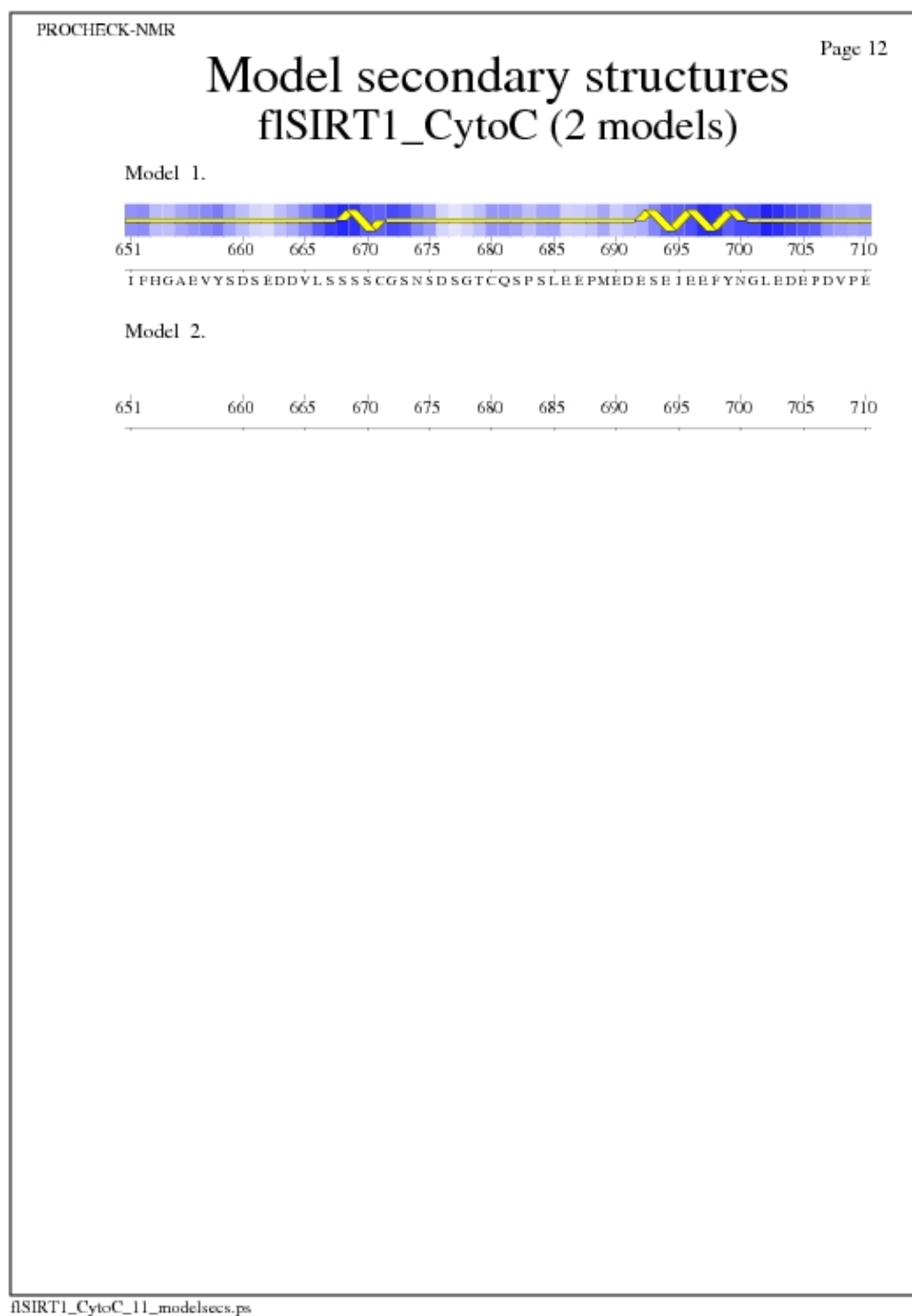
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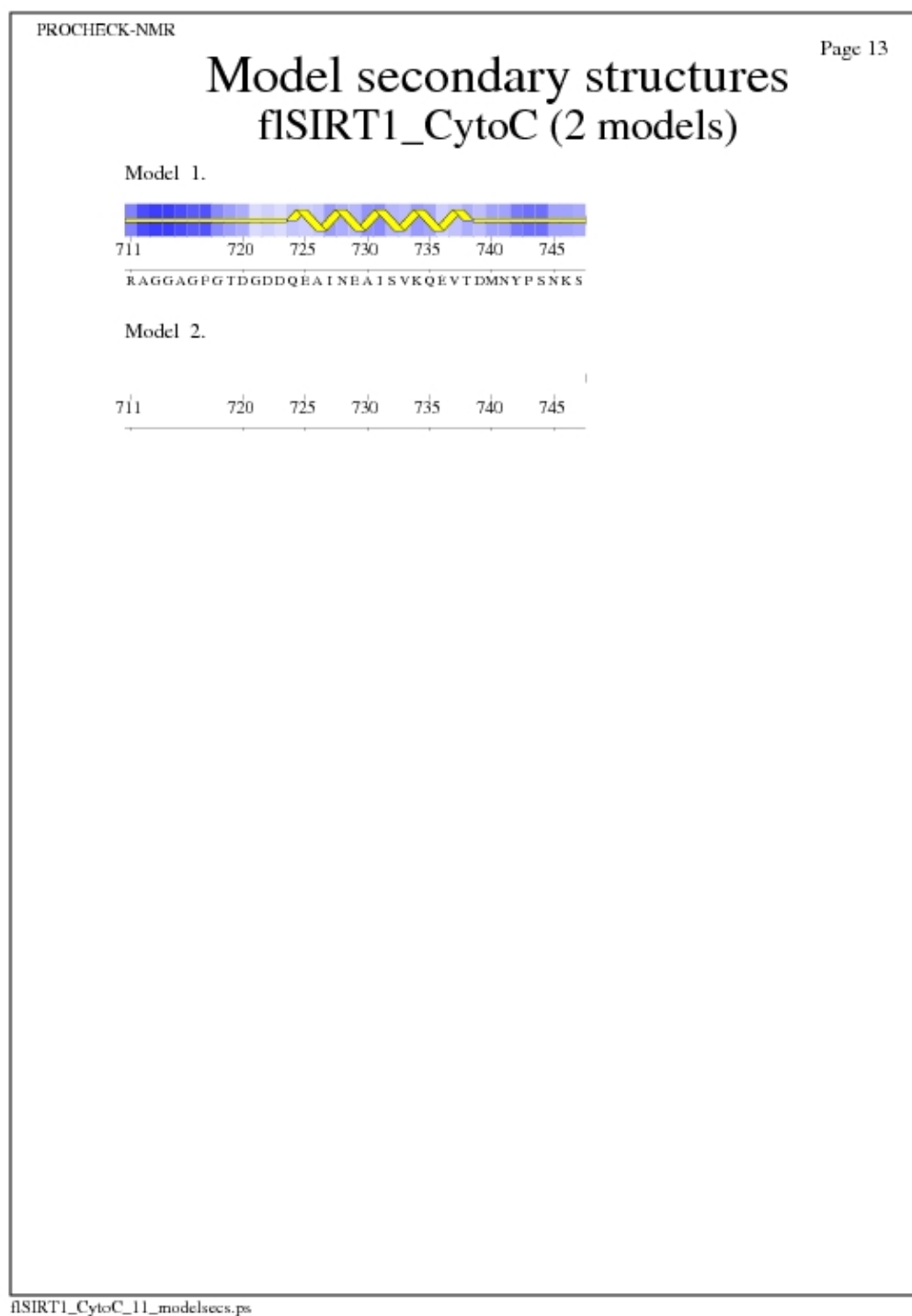
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JPEG for Model Secondary Structures - page \$num_n

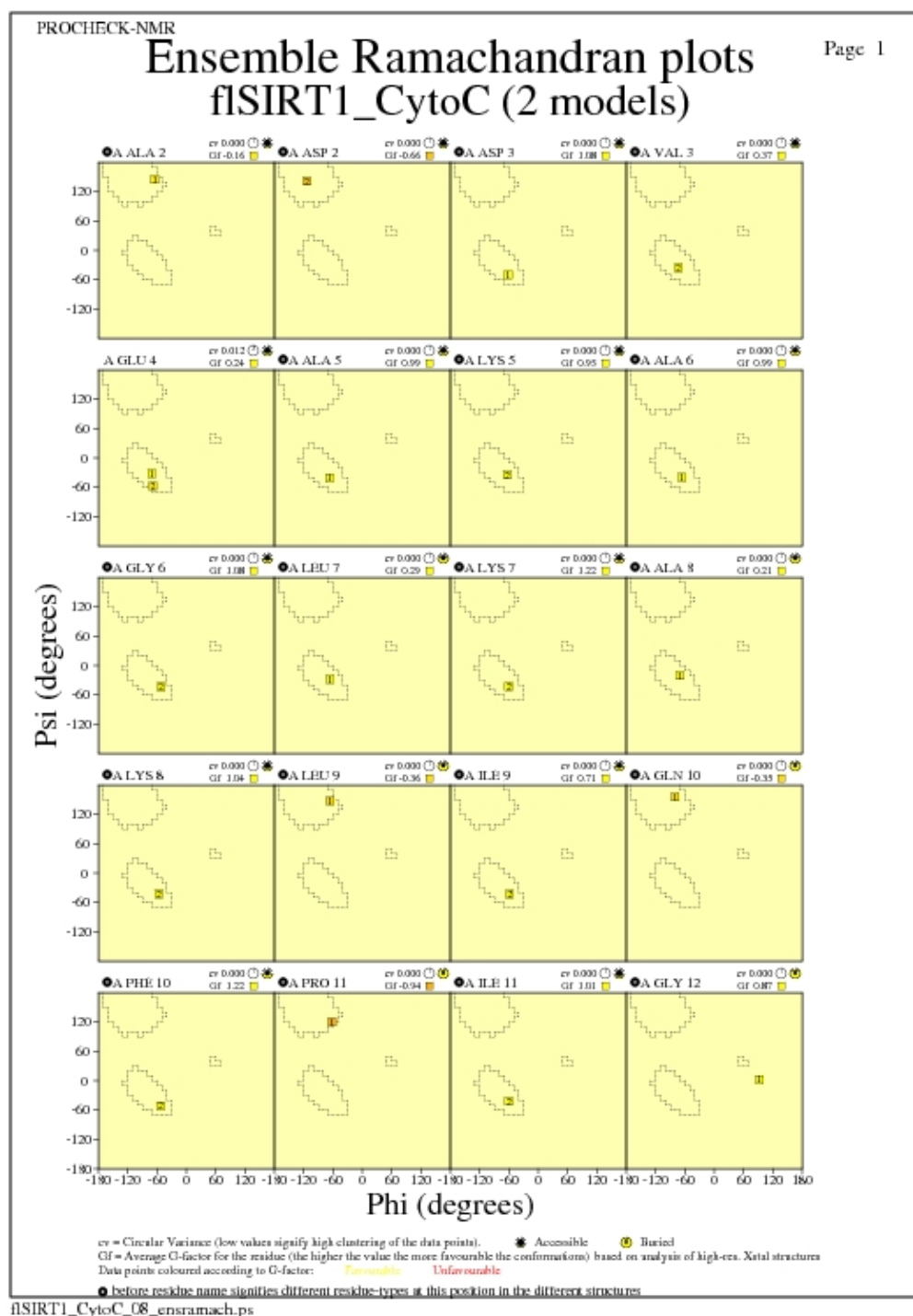


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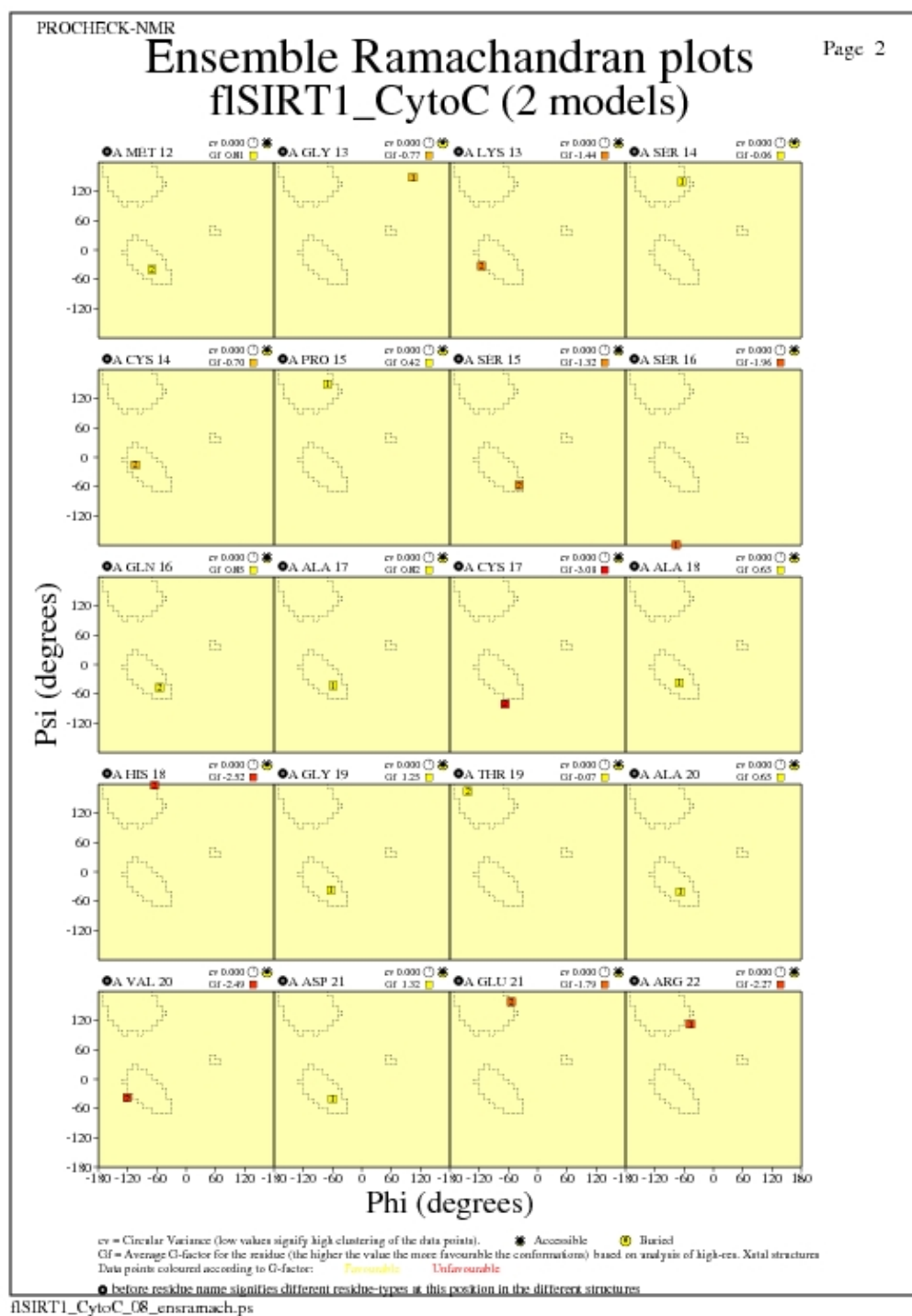


Ramachandran Plots for each residue

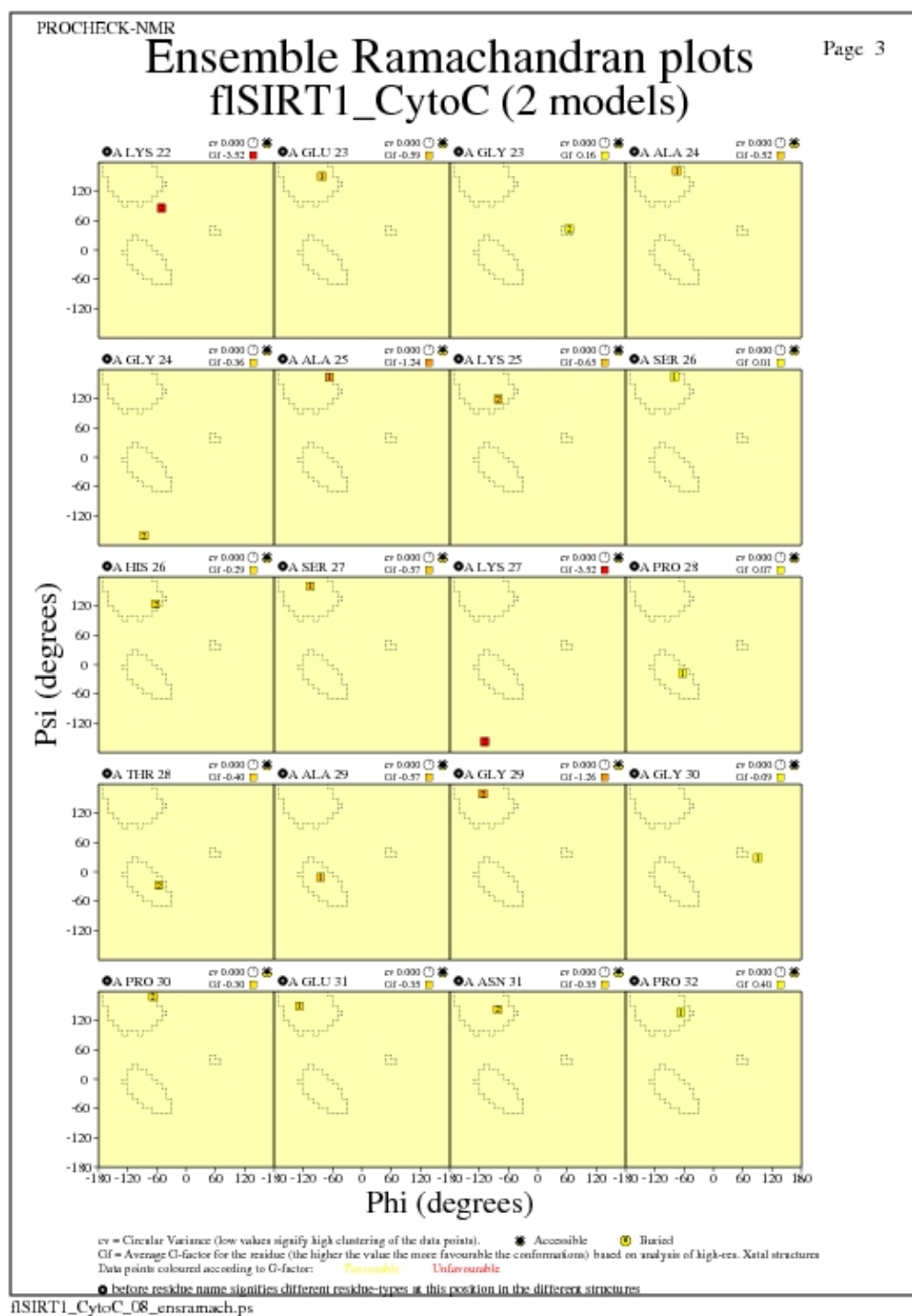
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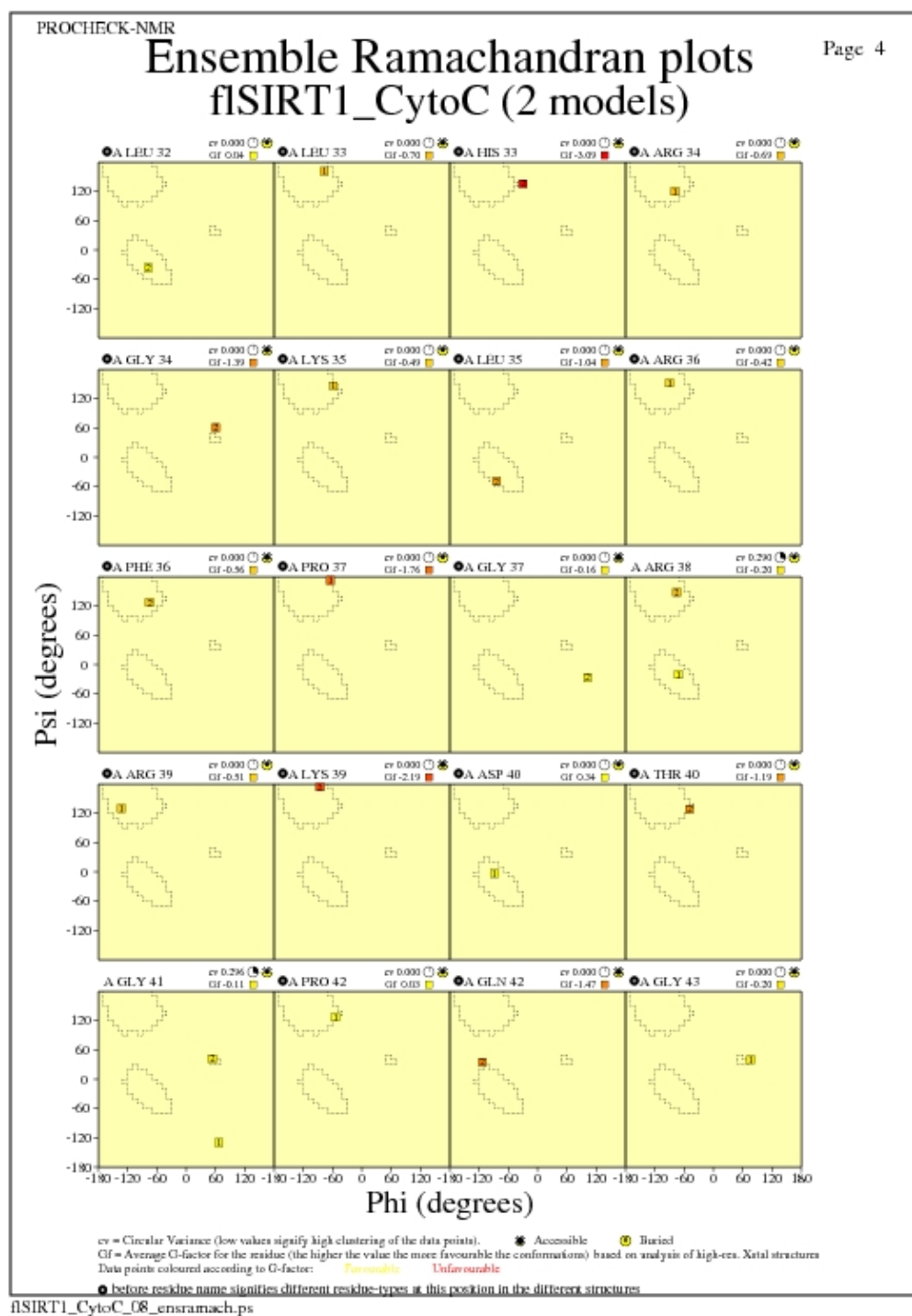
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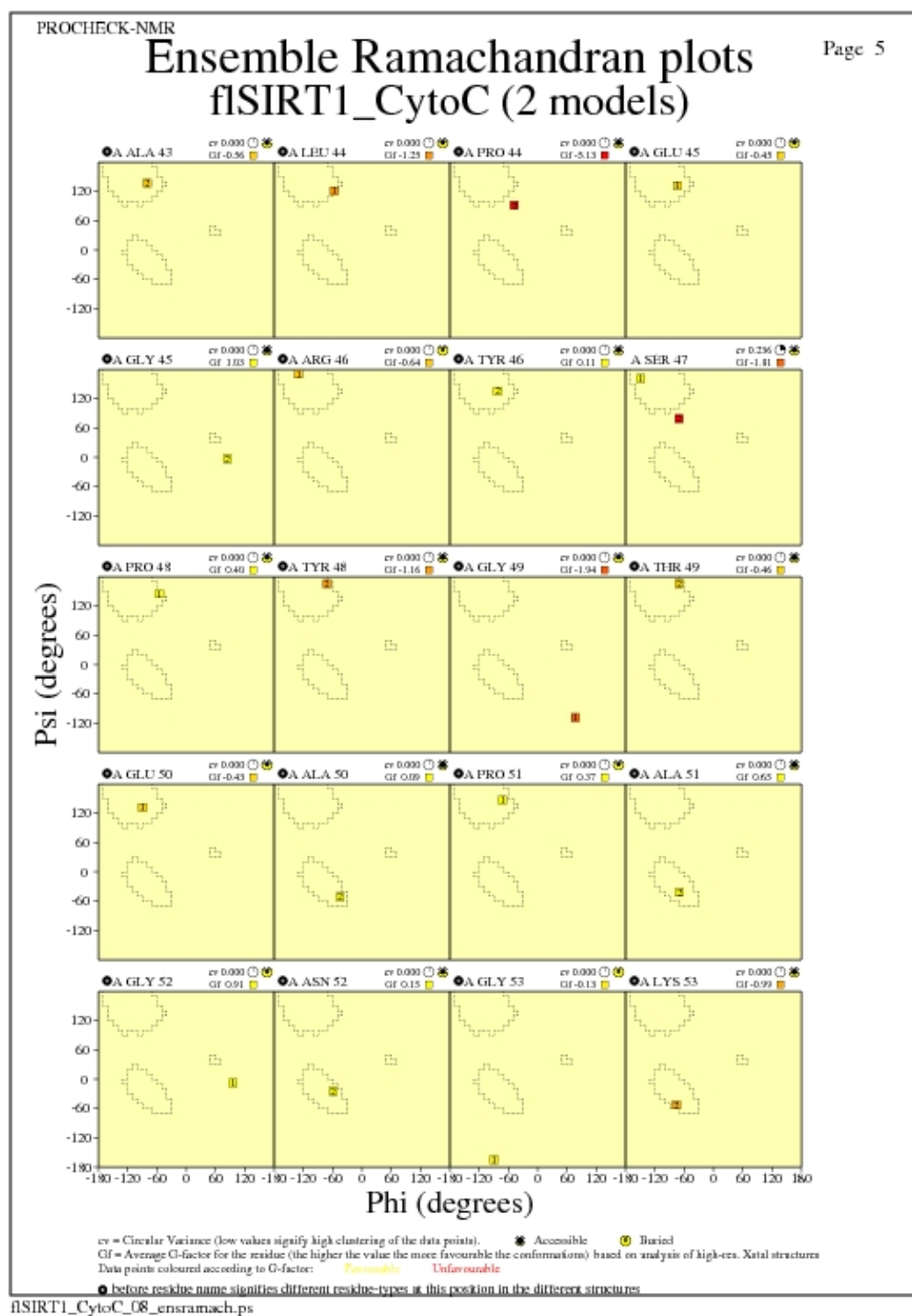
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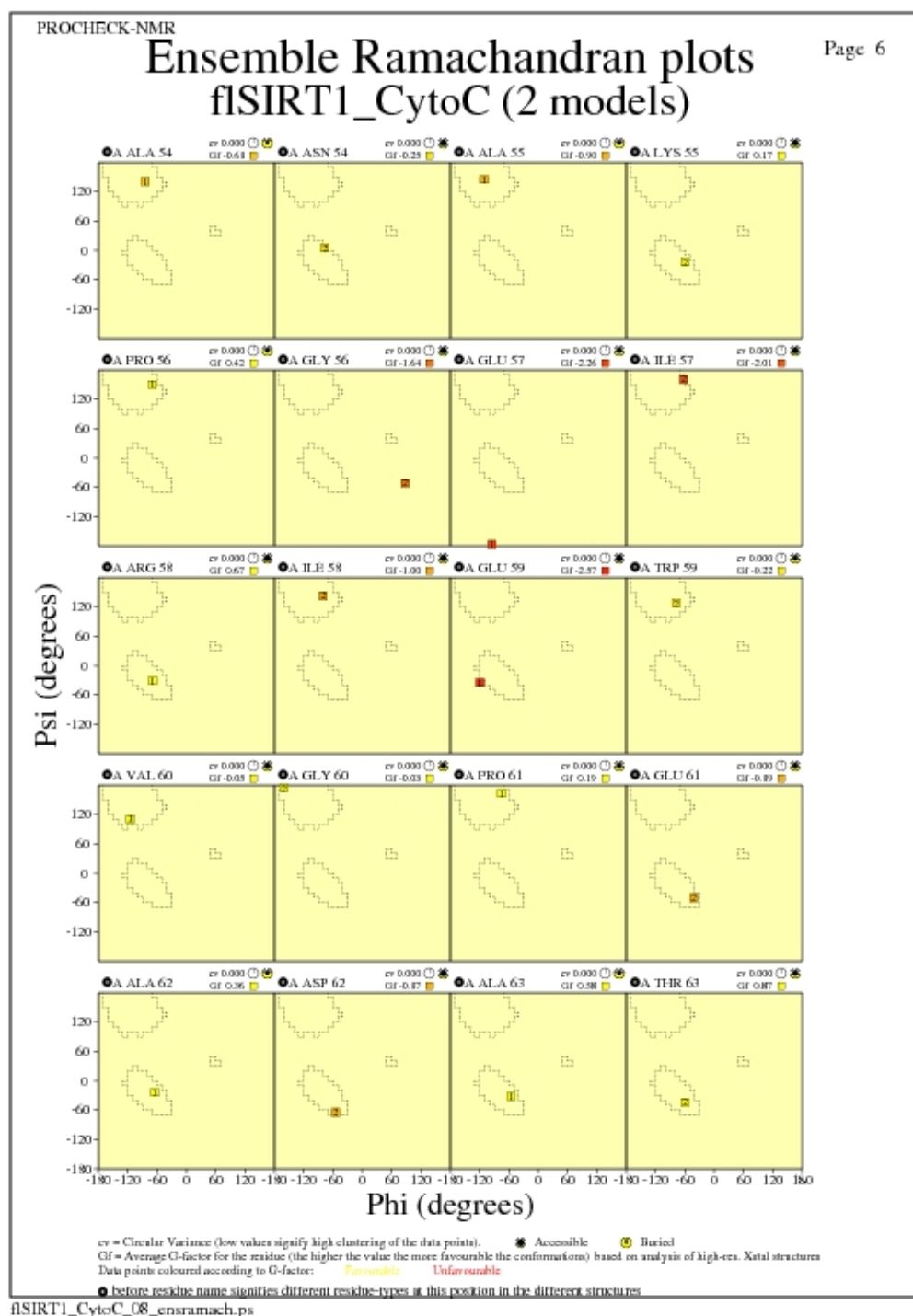
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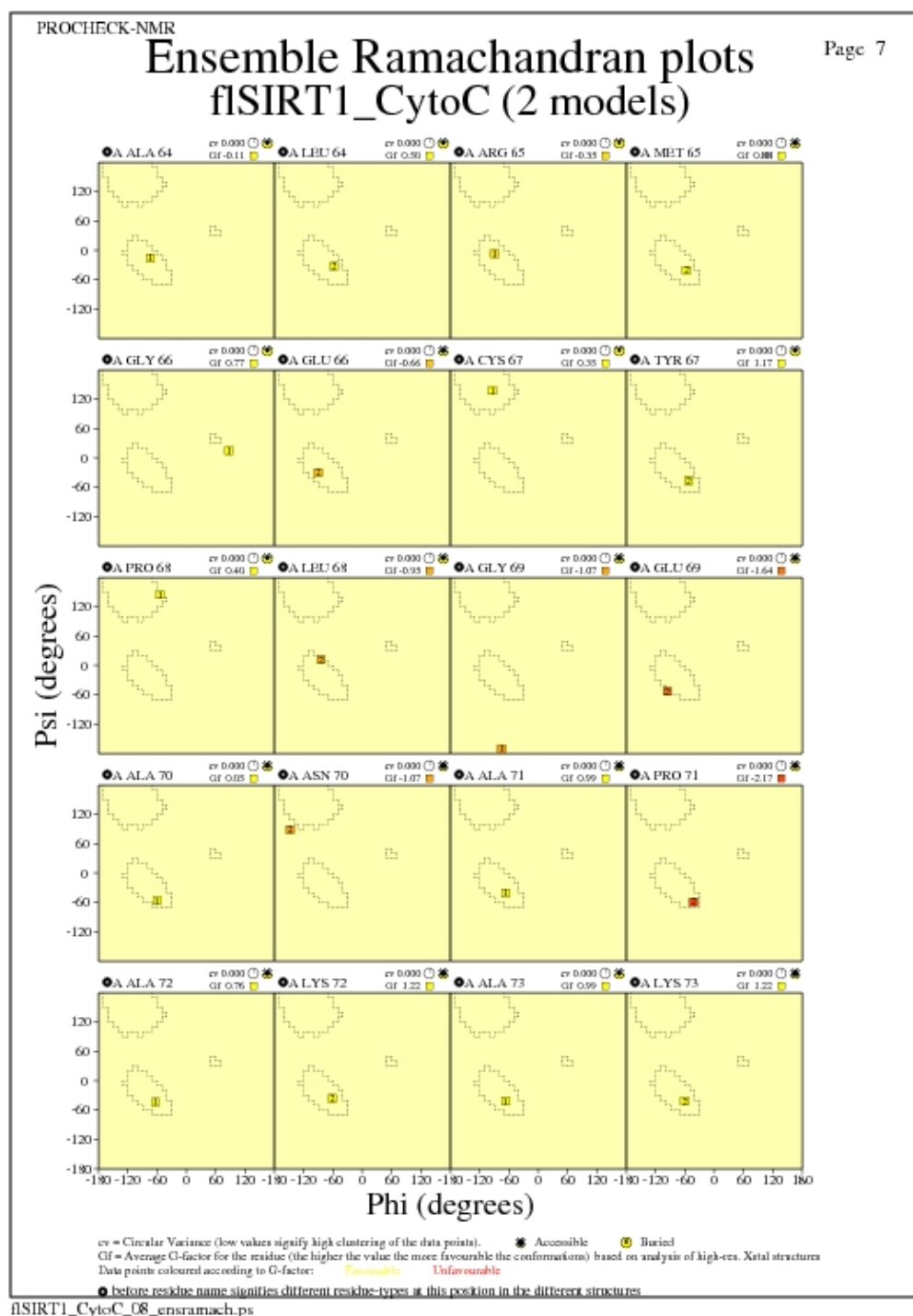
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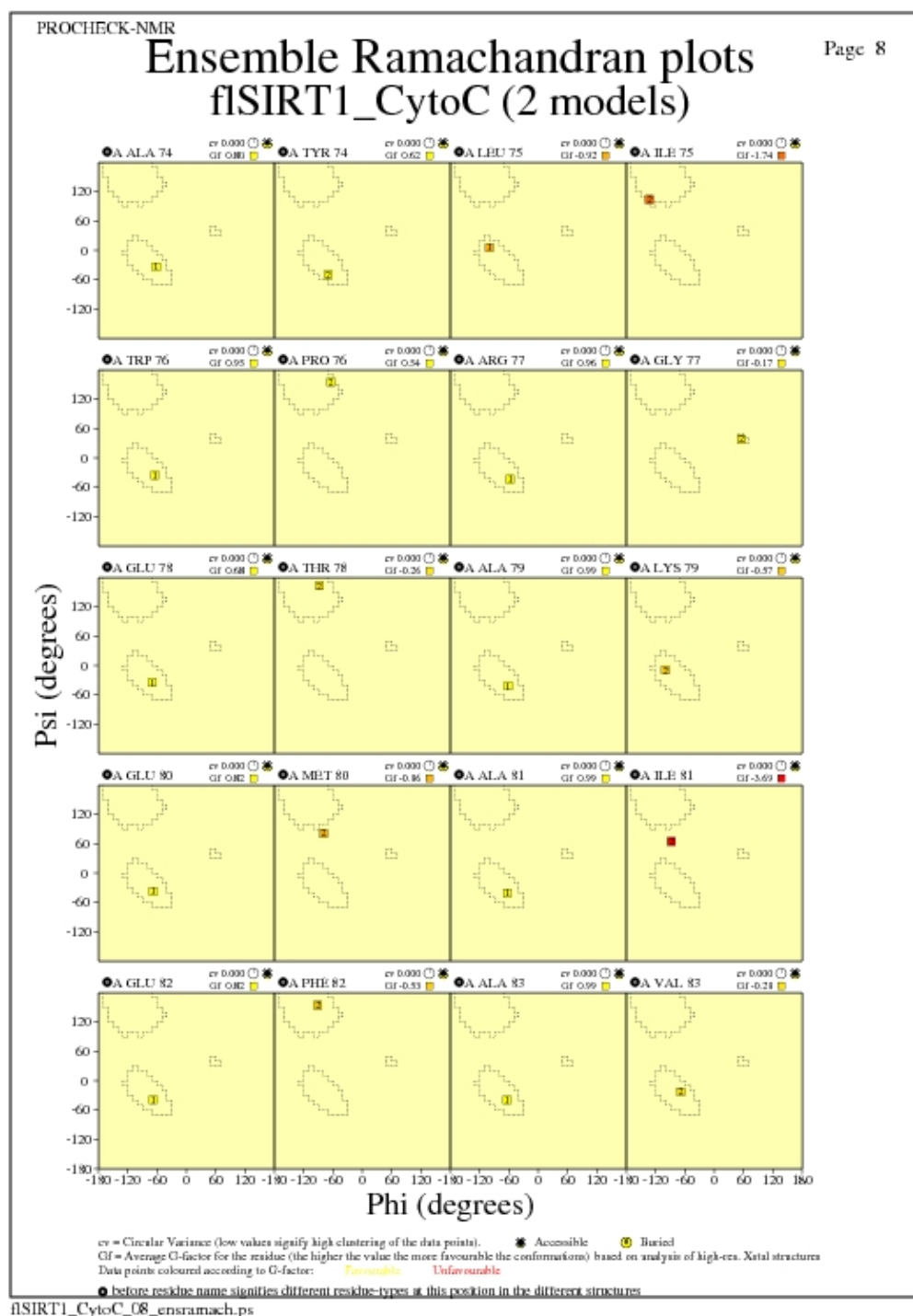
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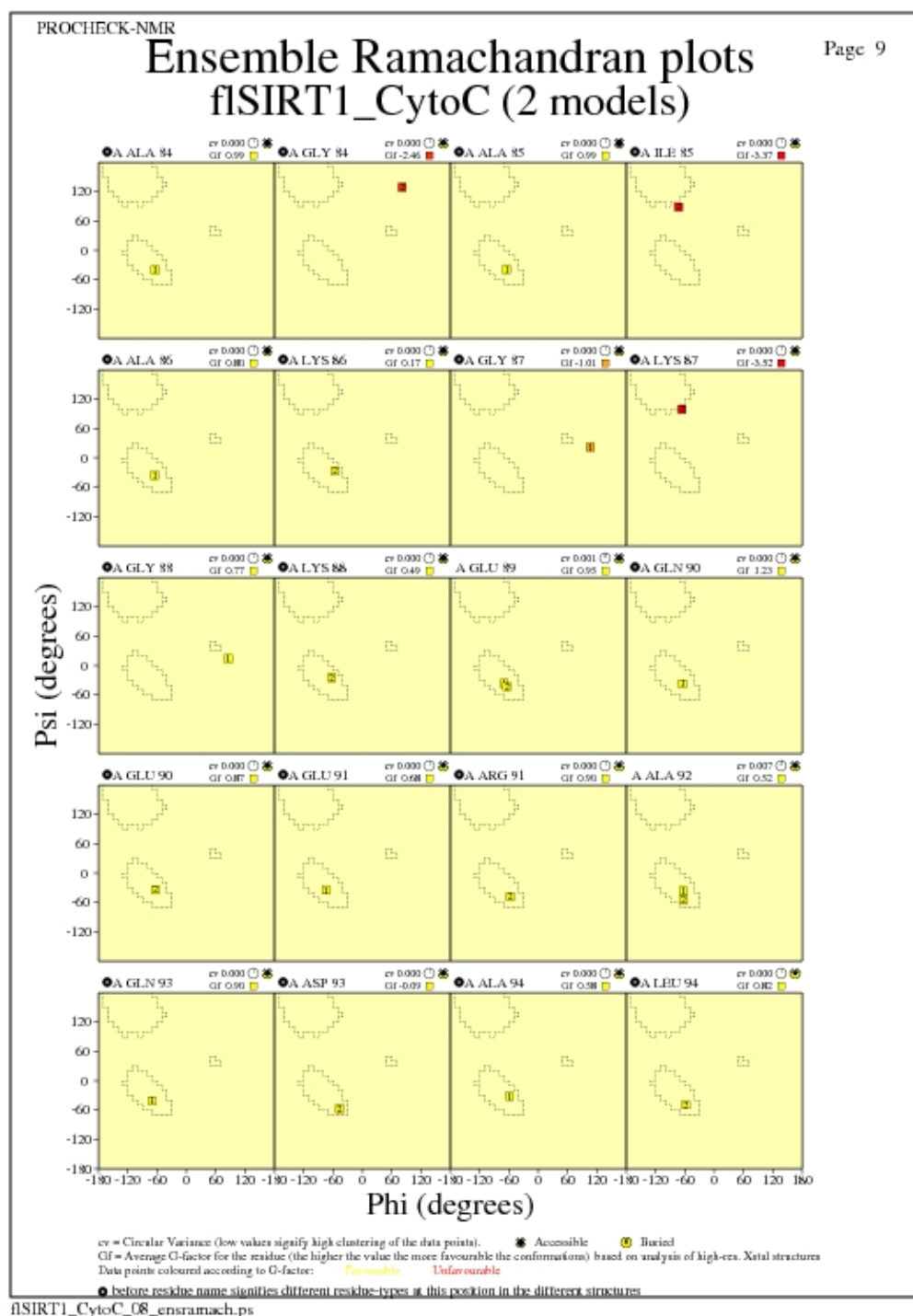
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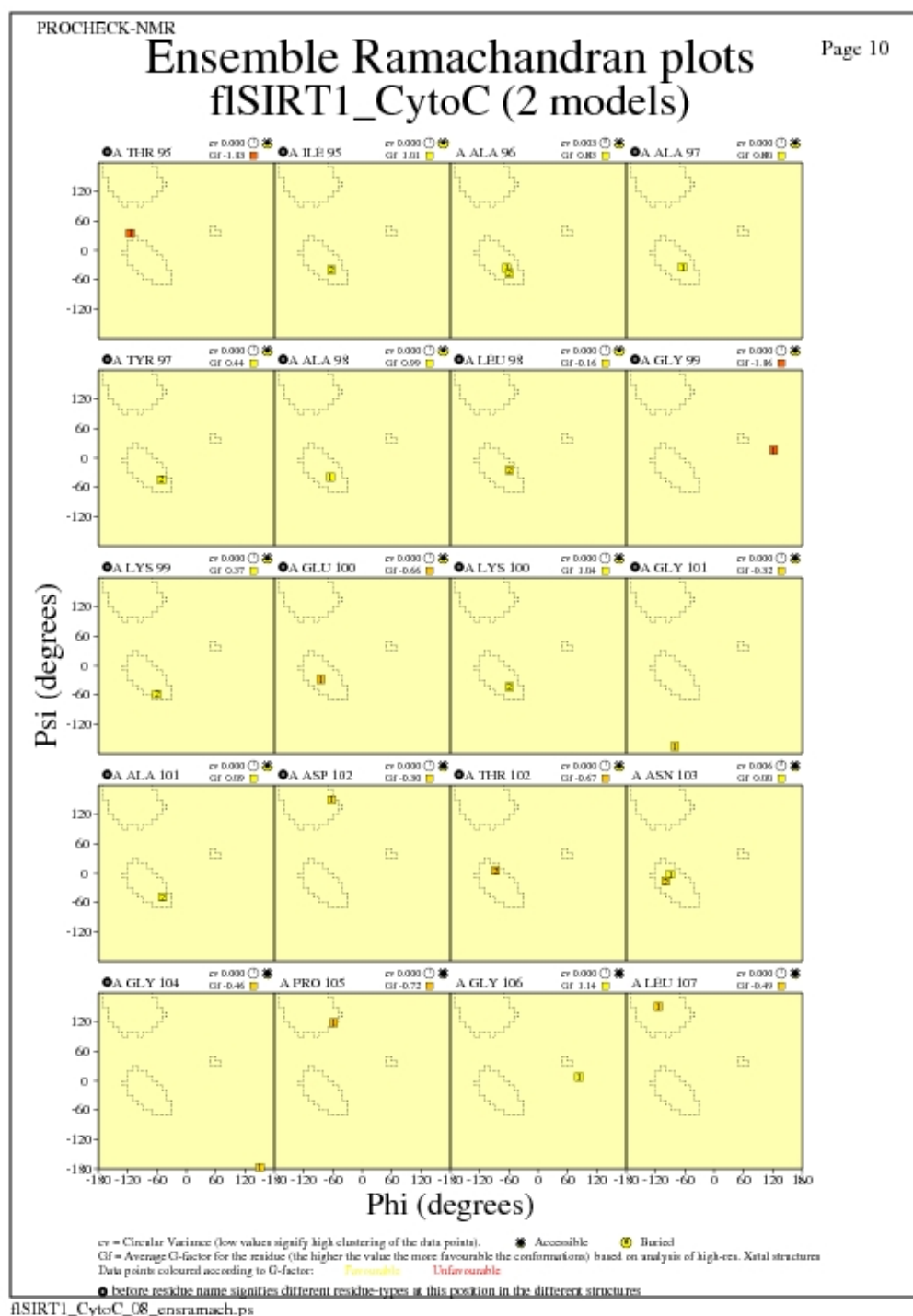
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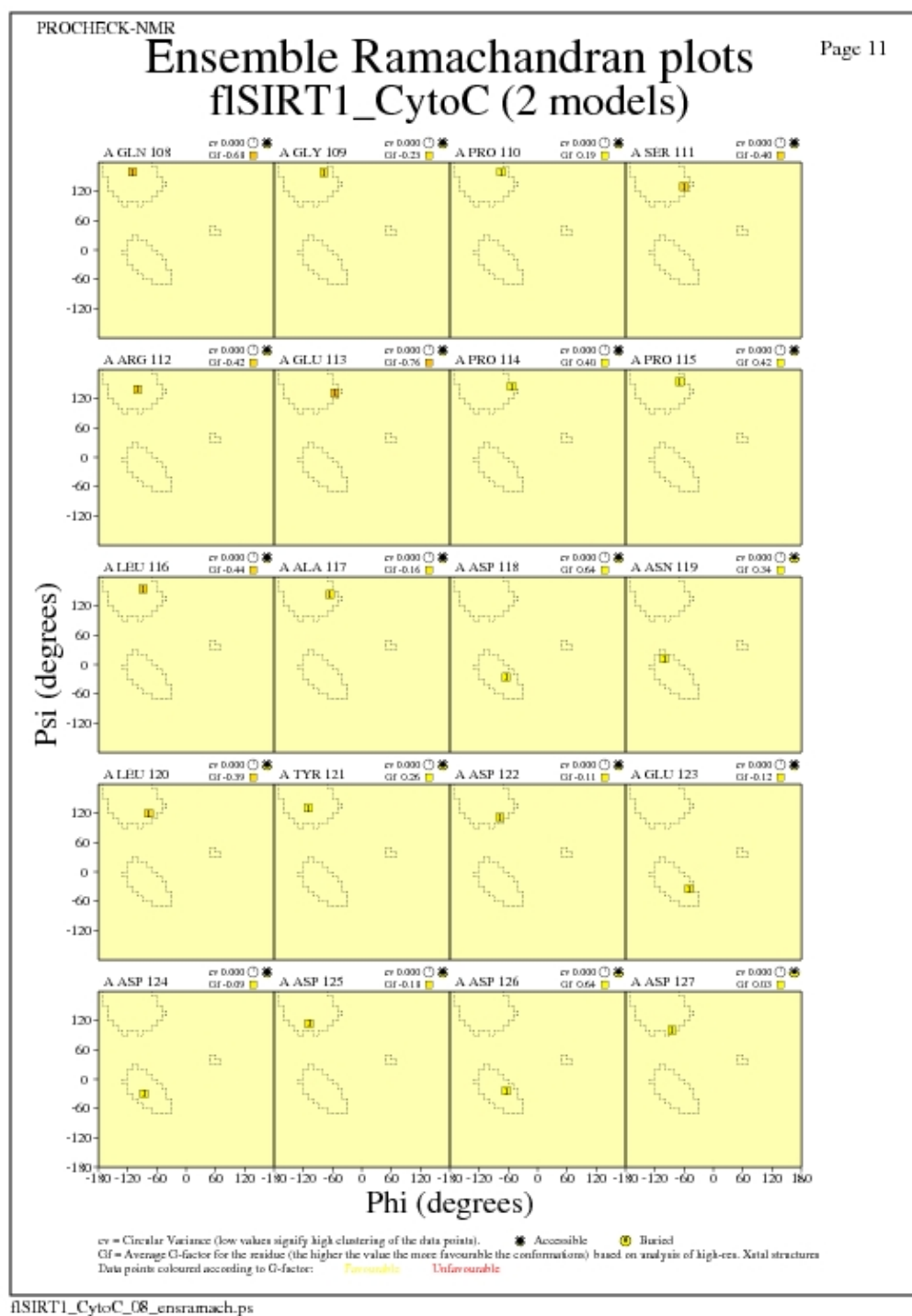
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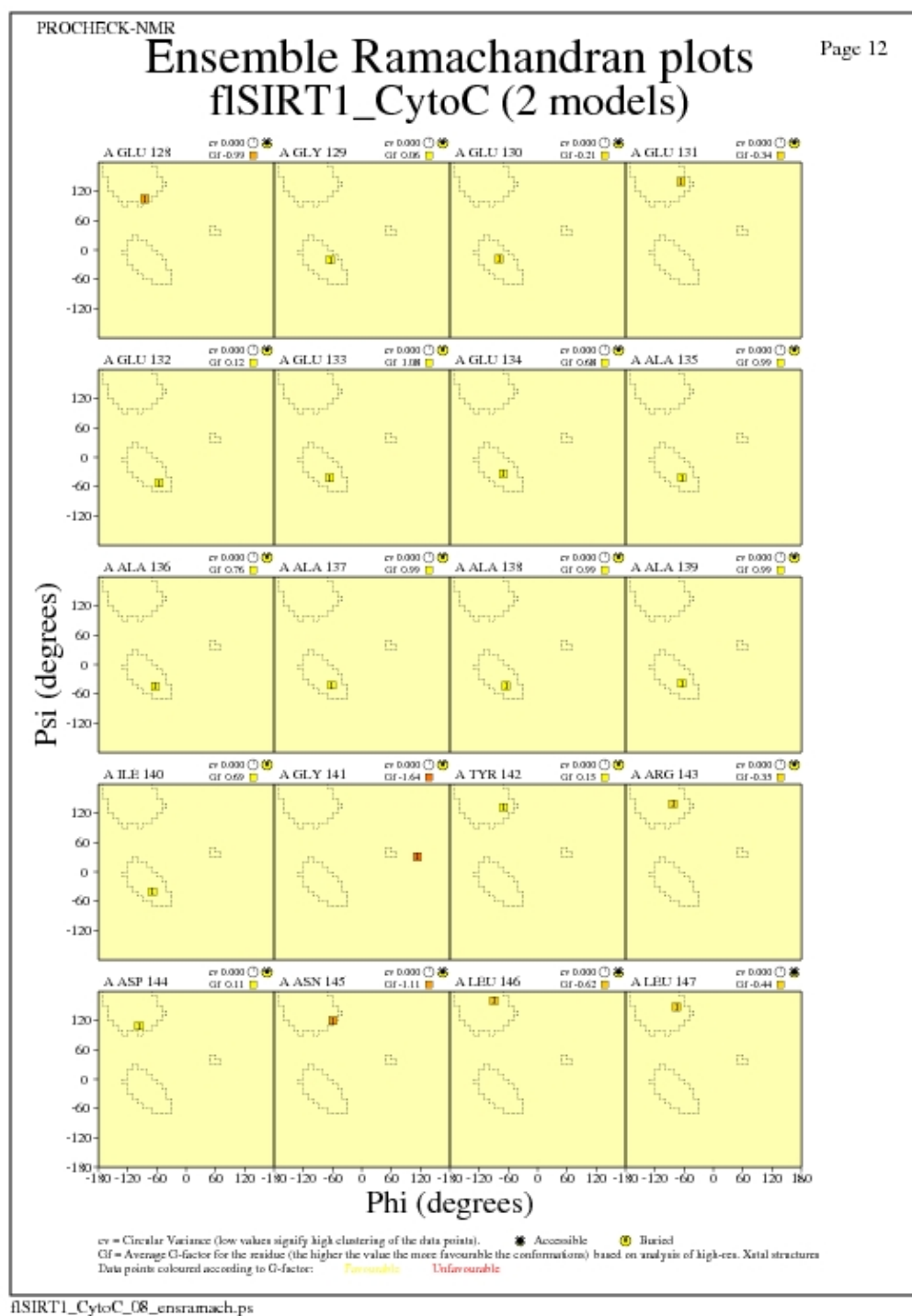
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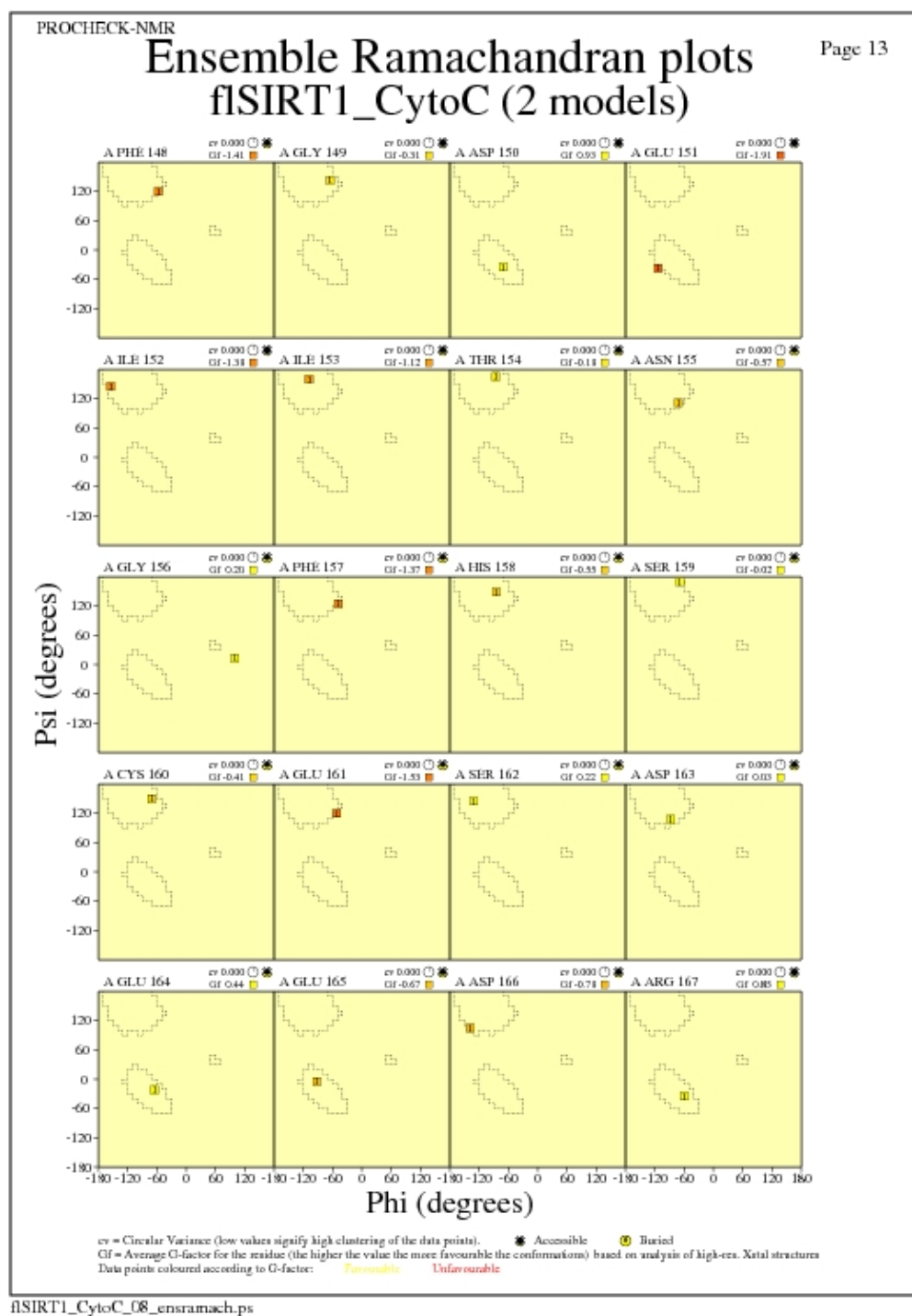
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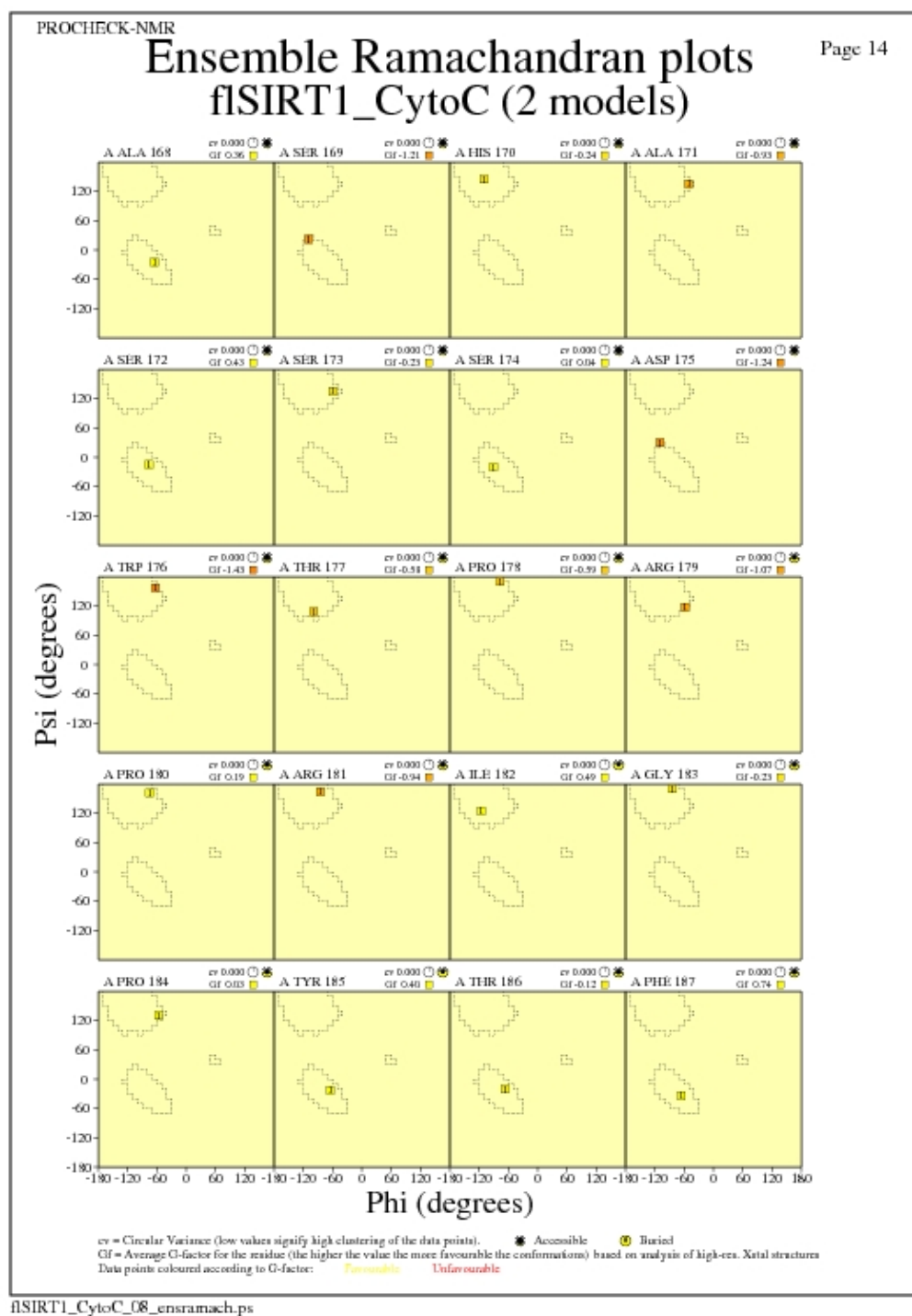
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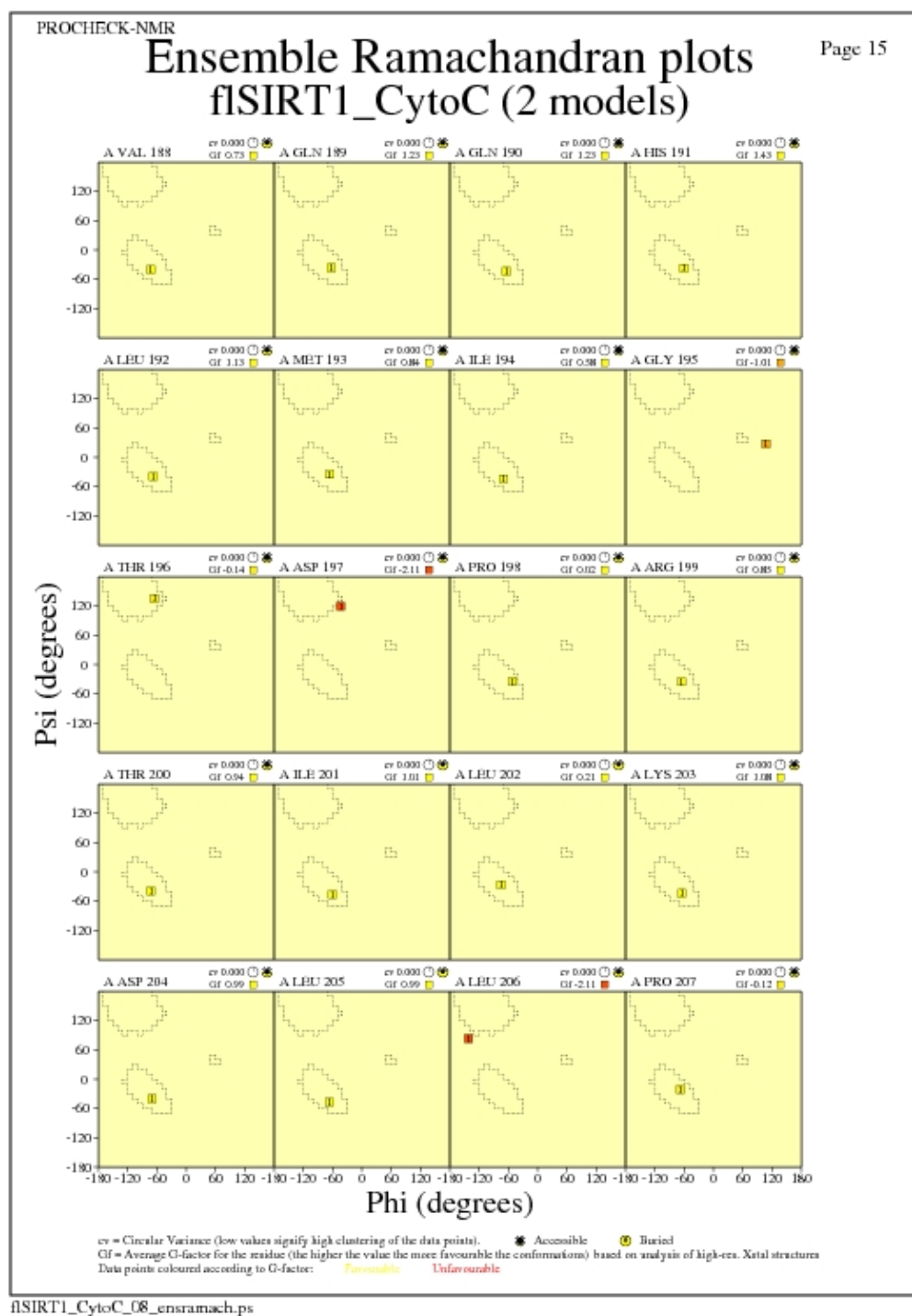
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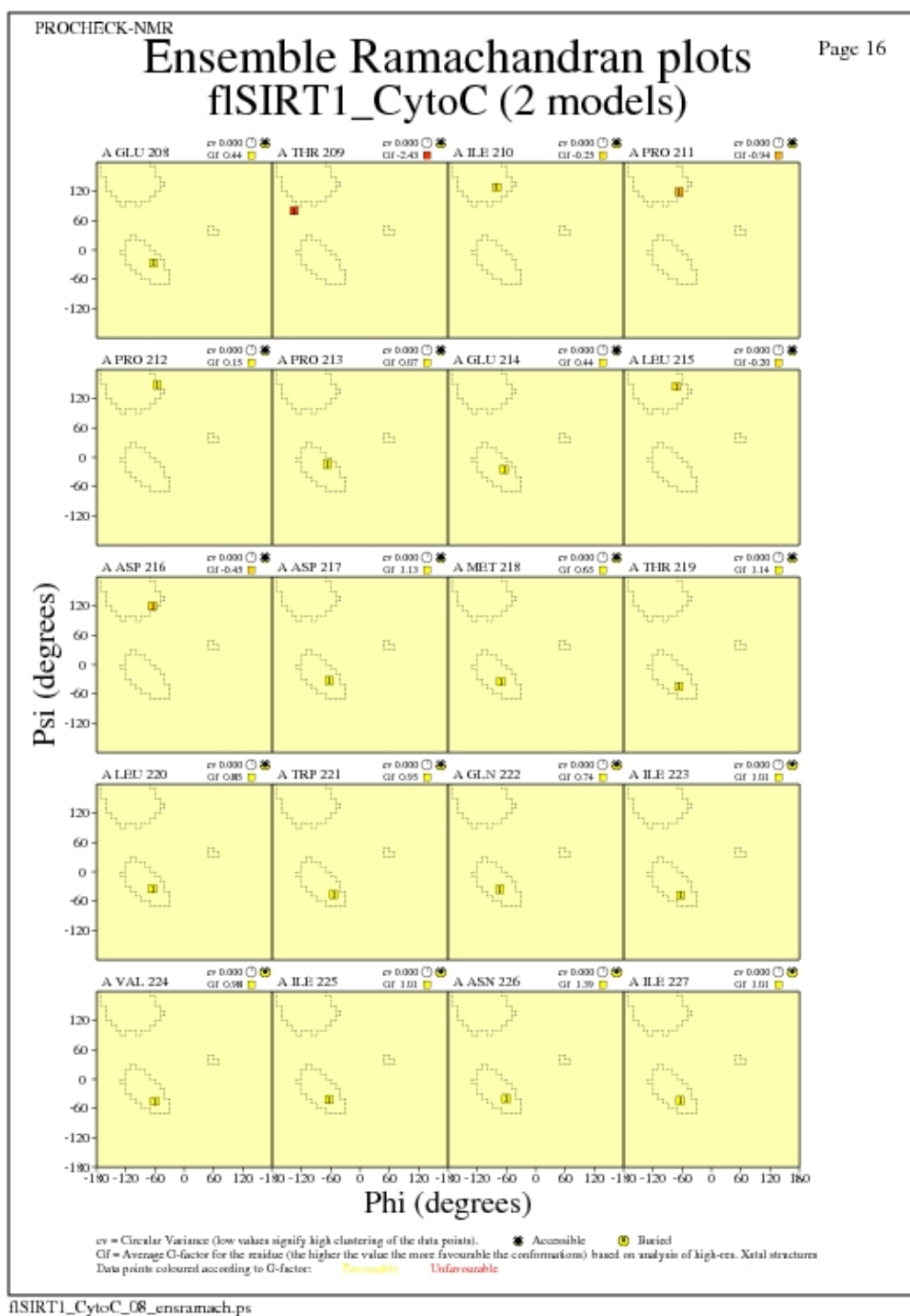
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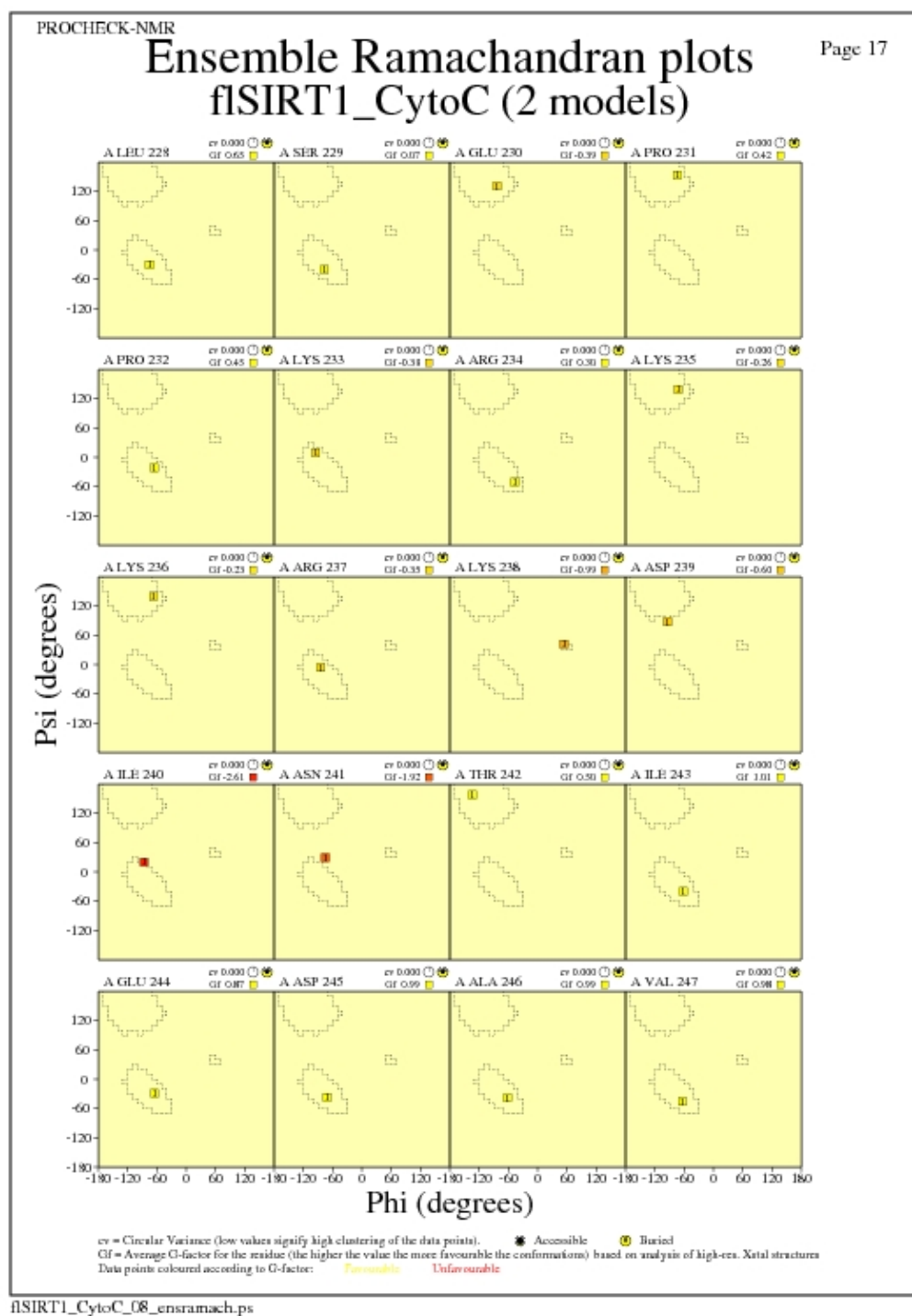
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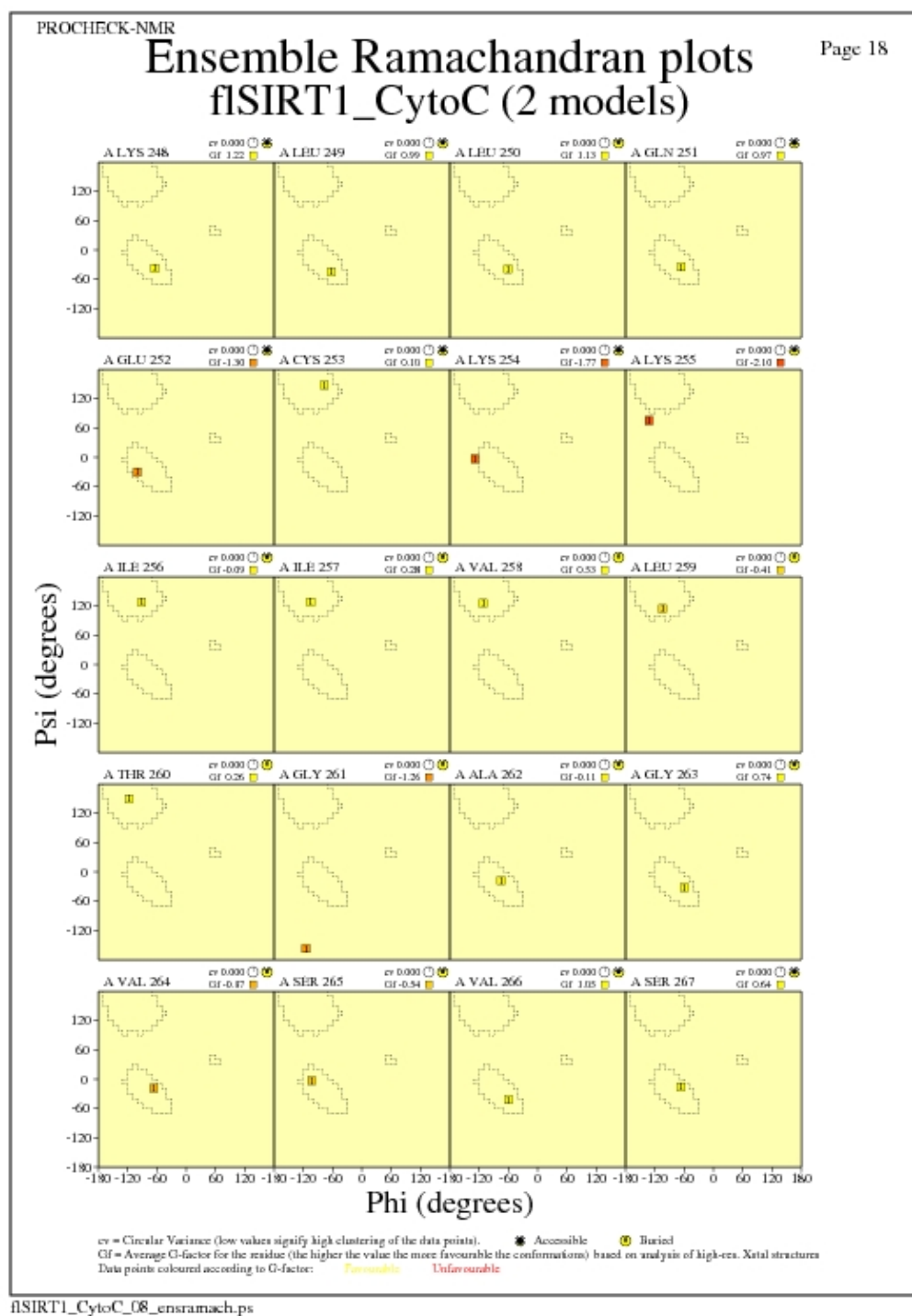
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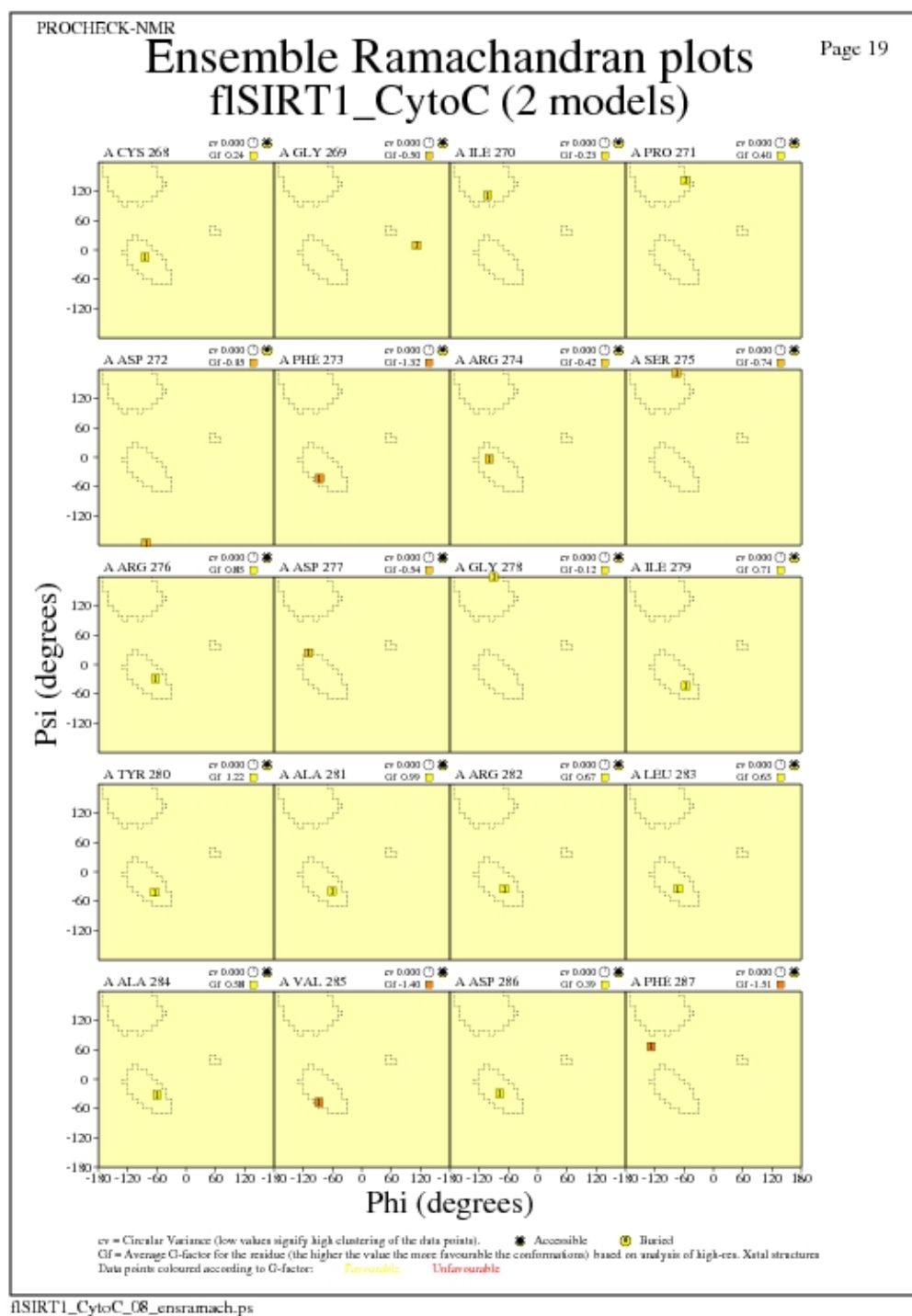
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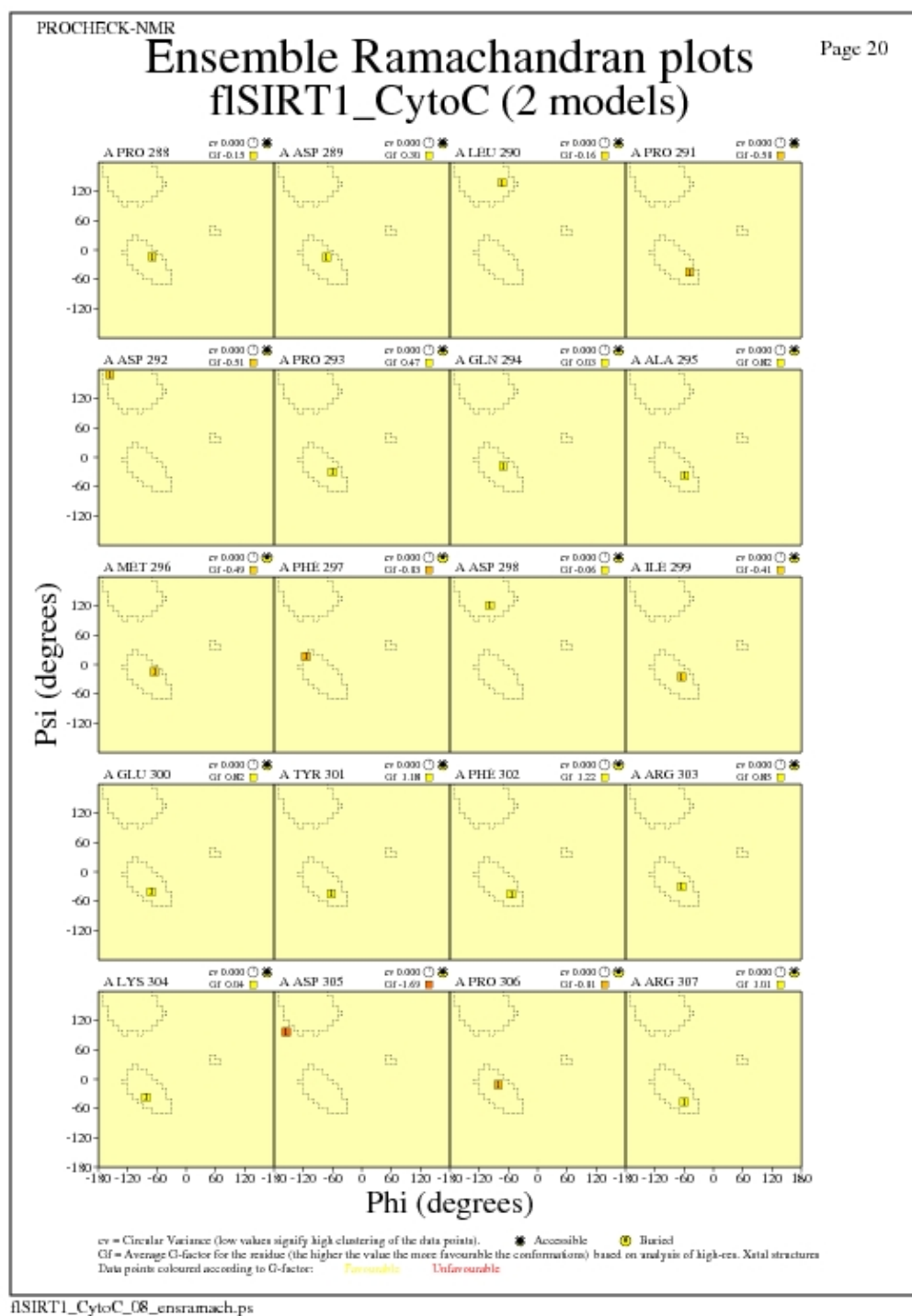
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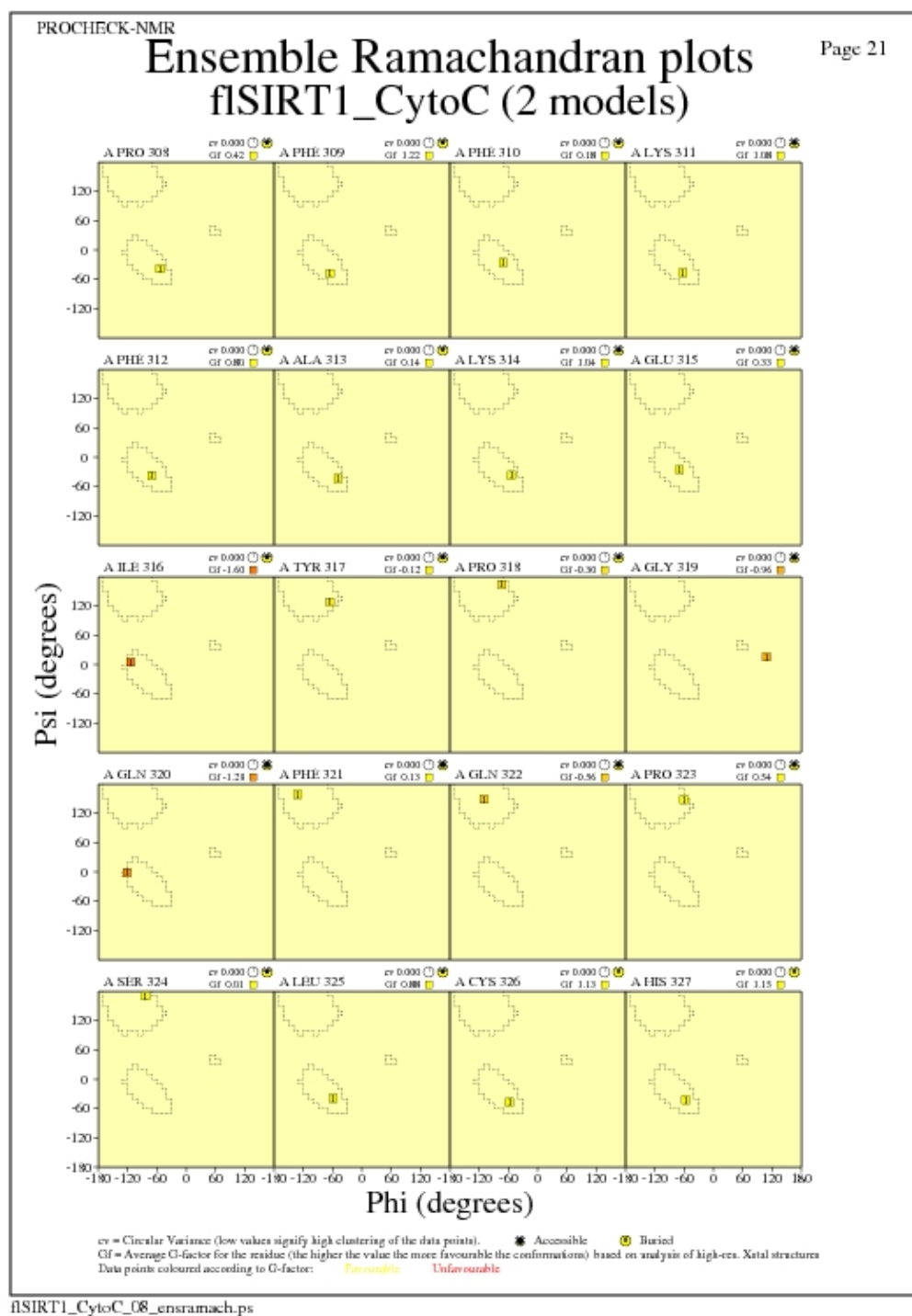
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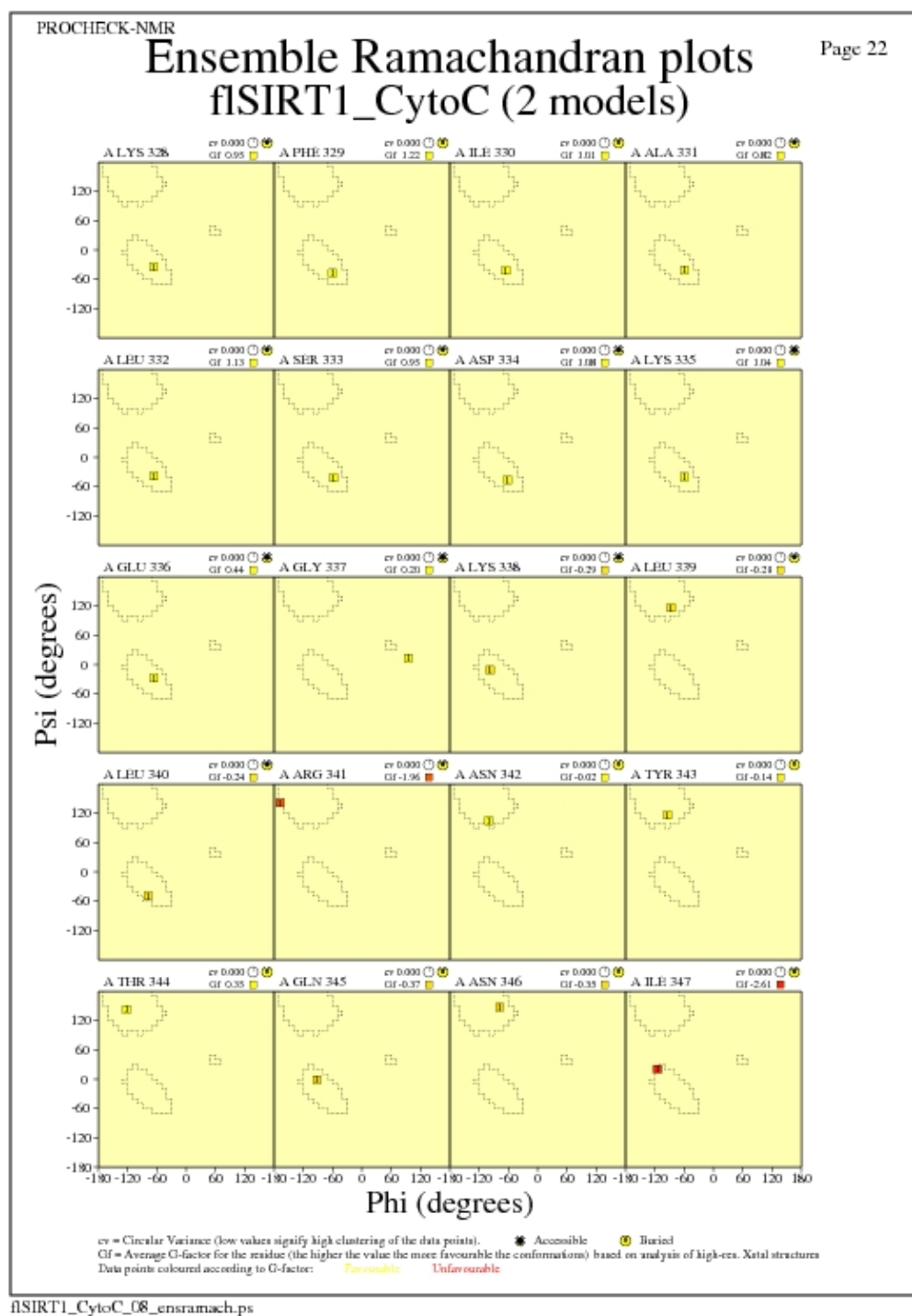
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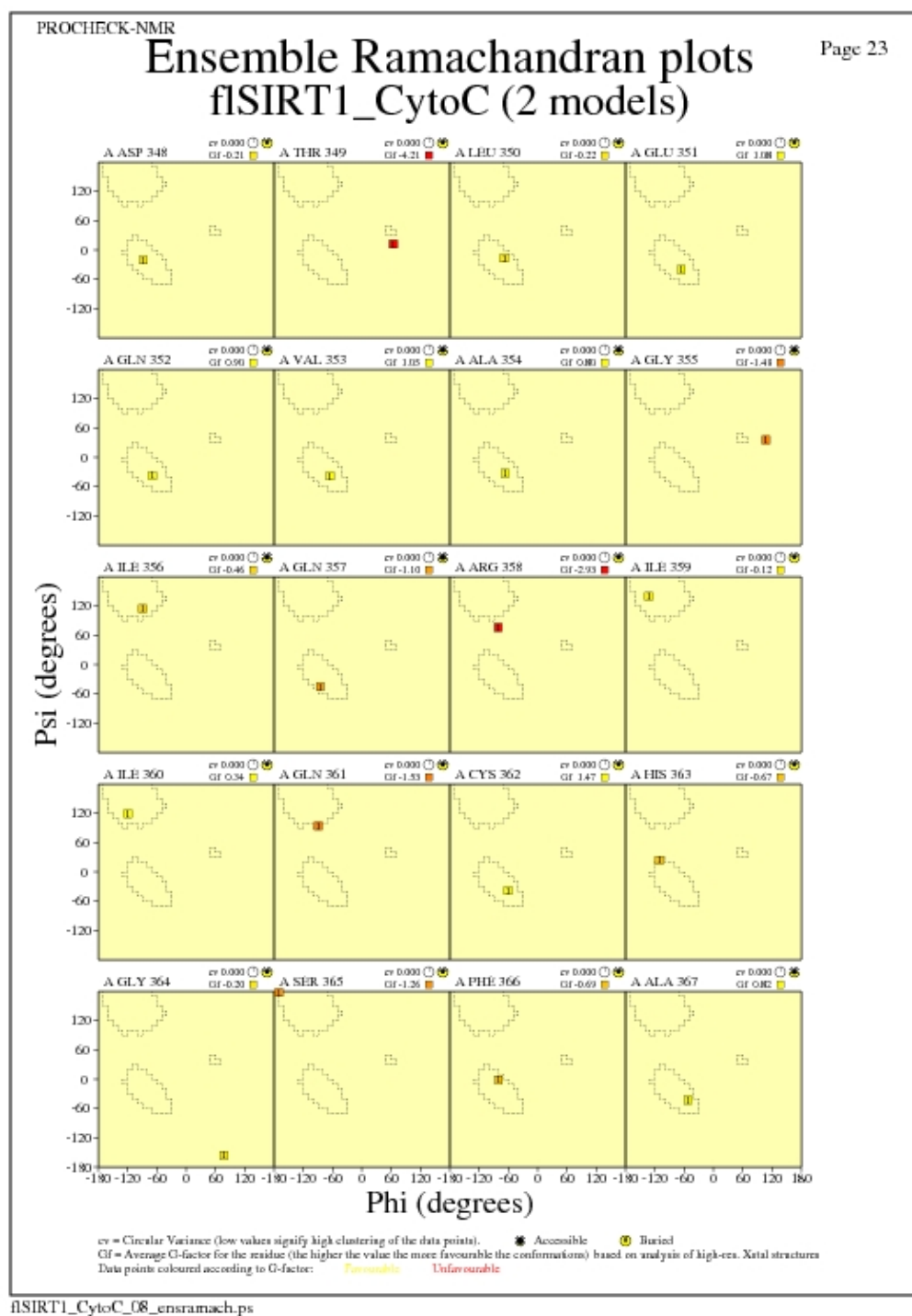
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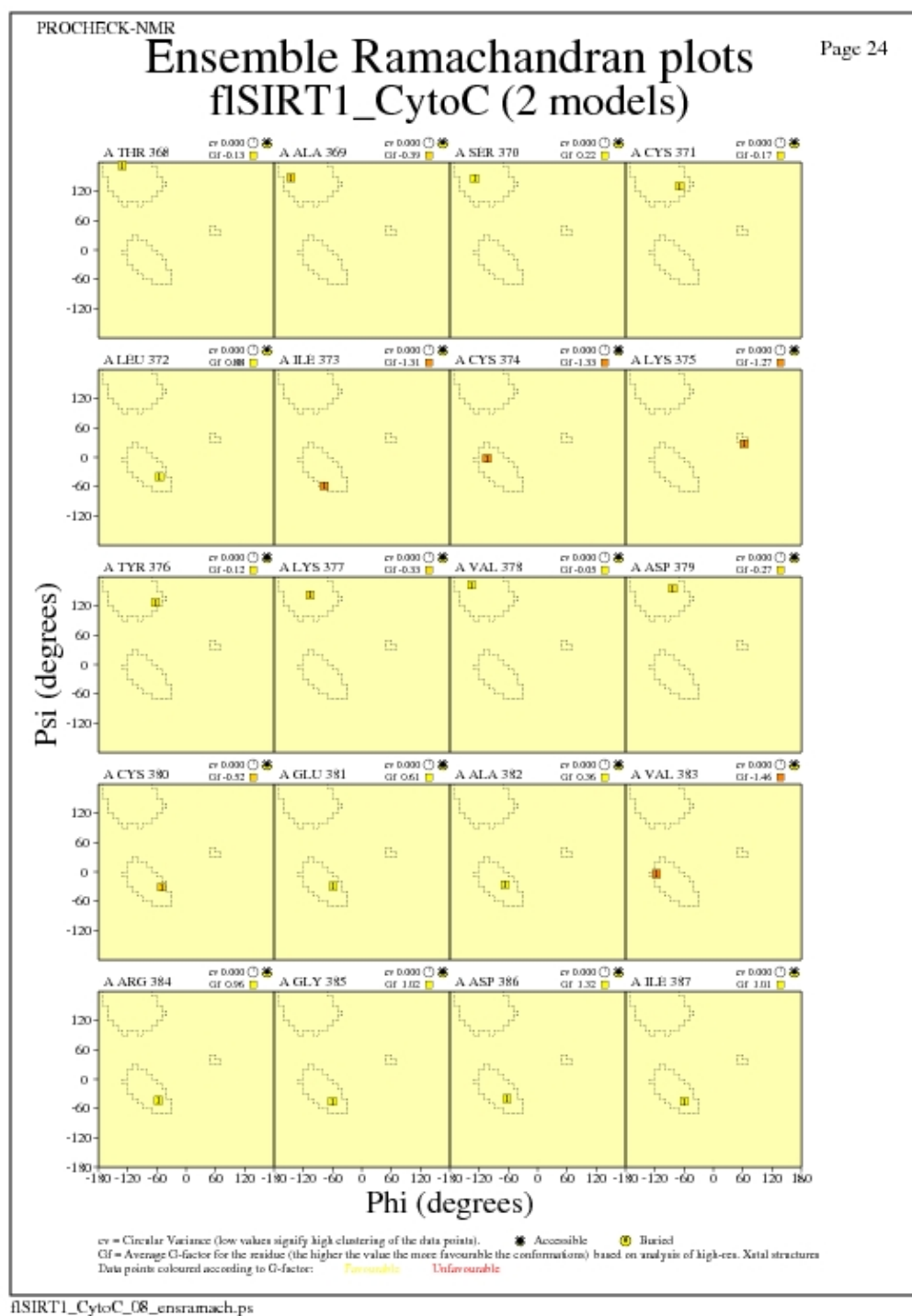
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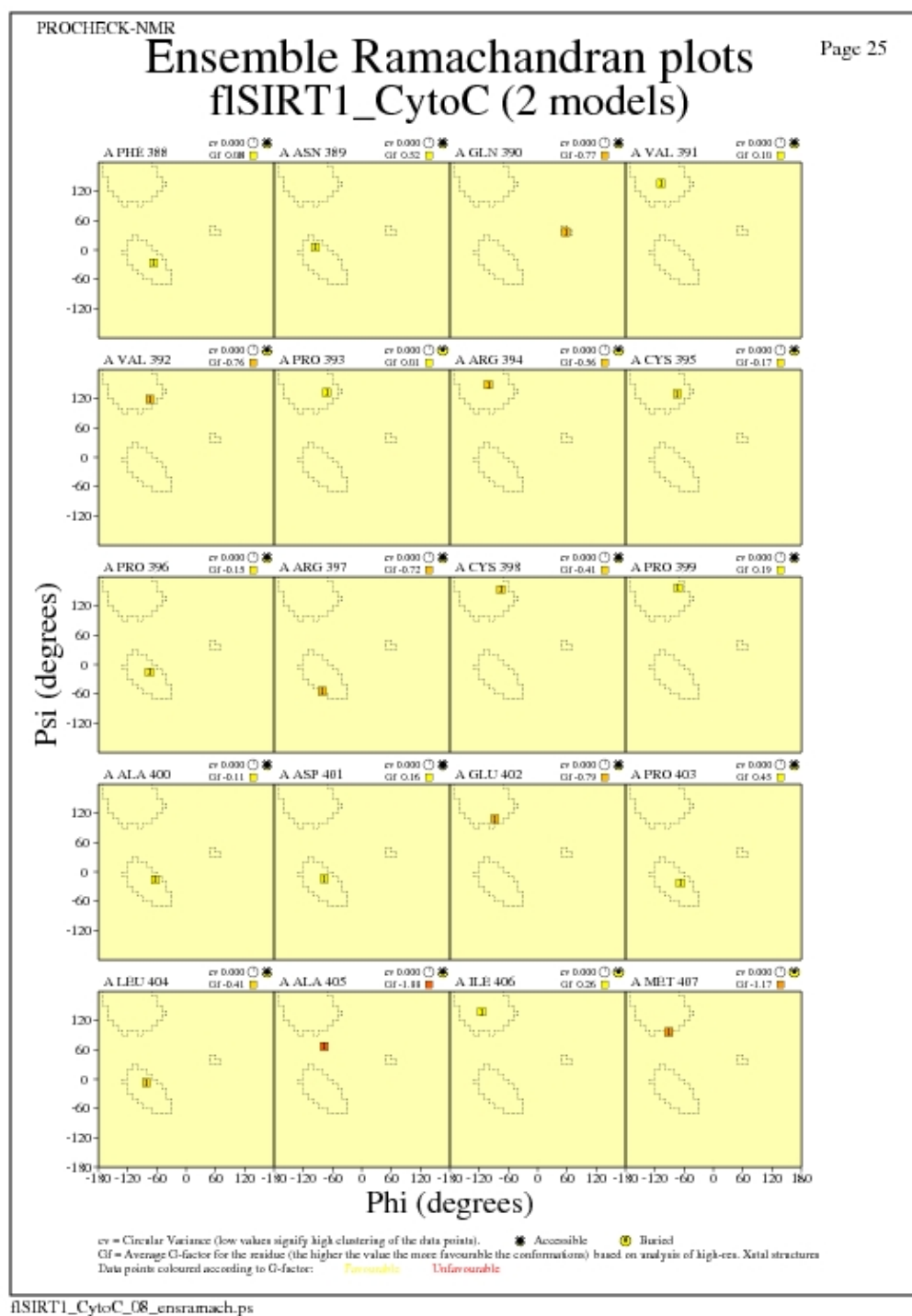
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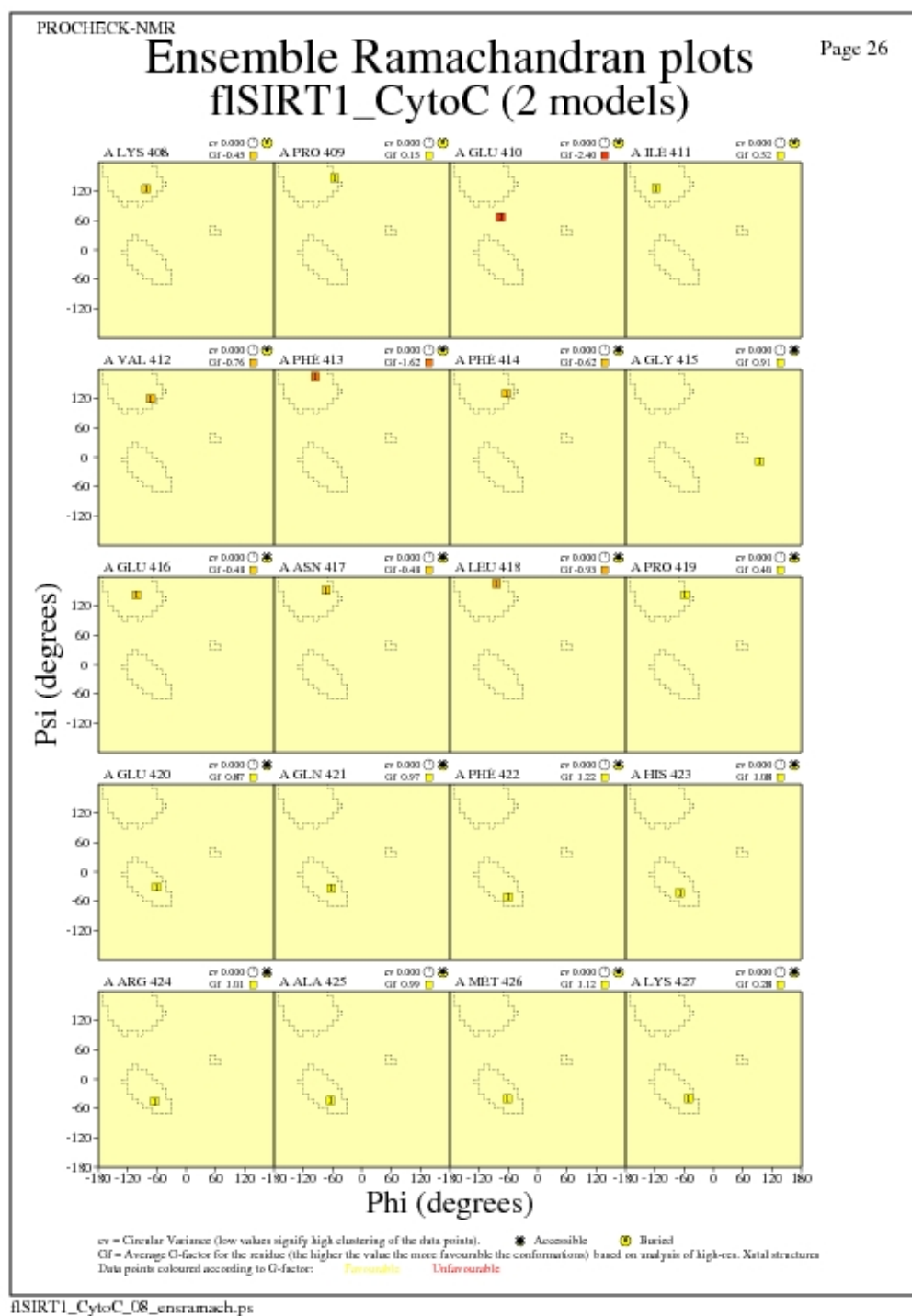
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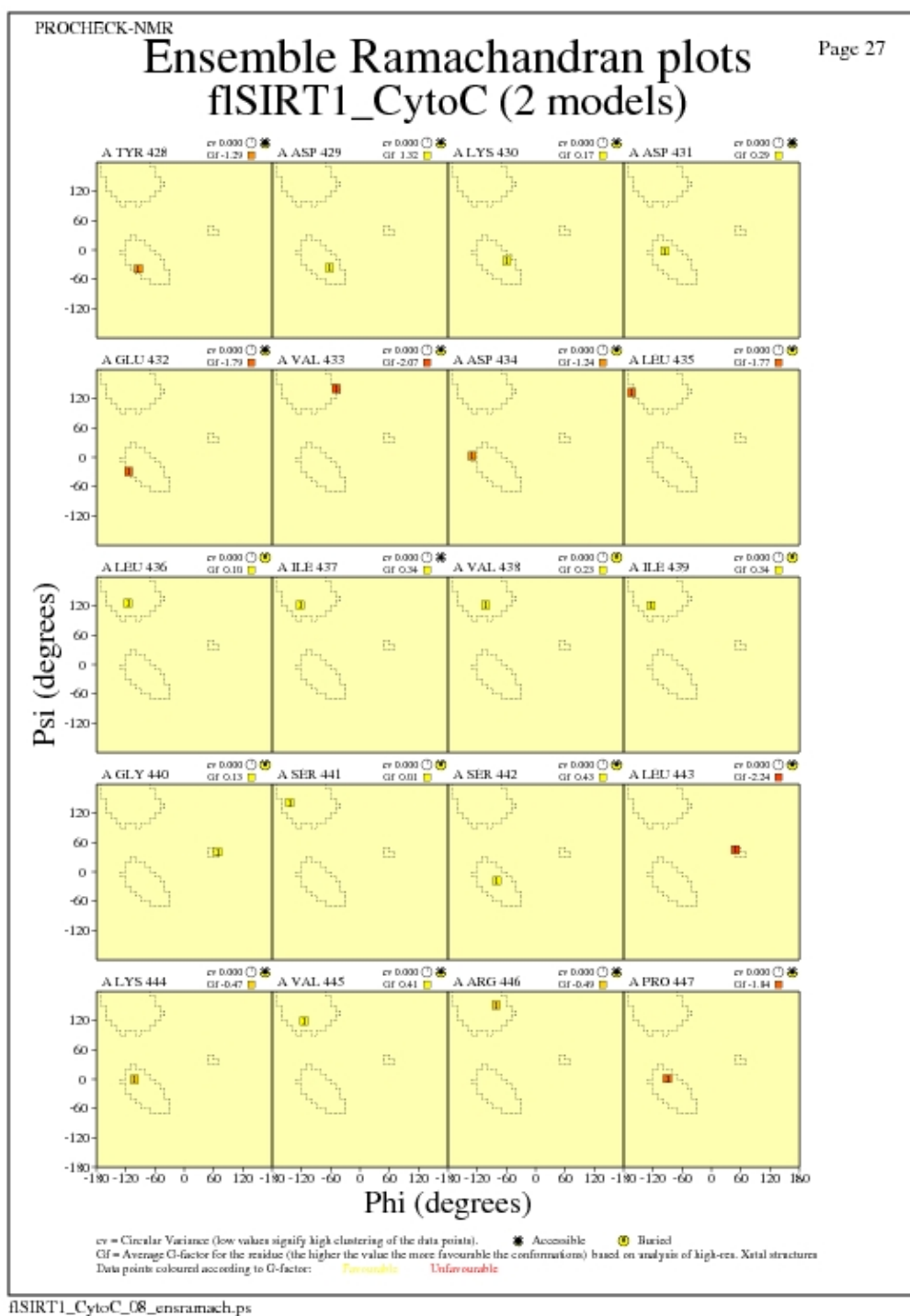
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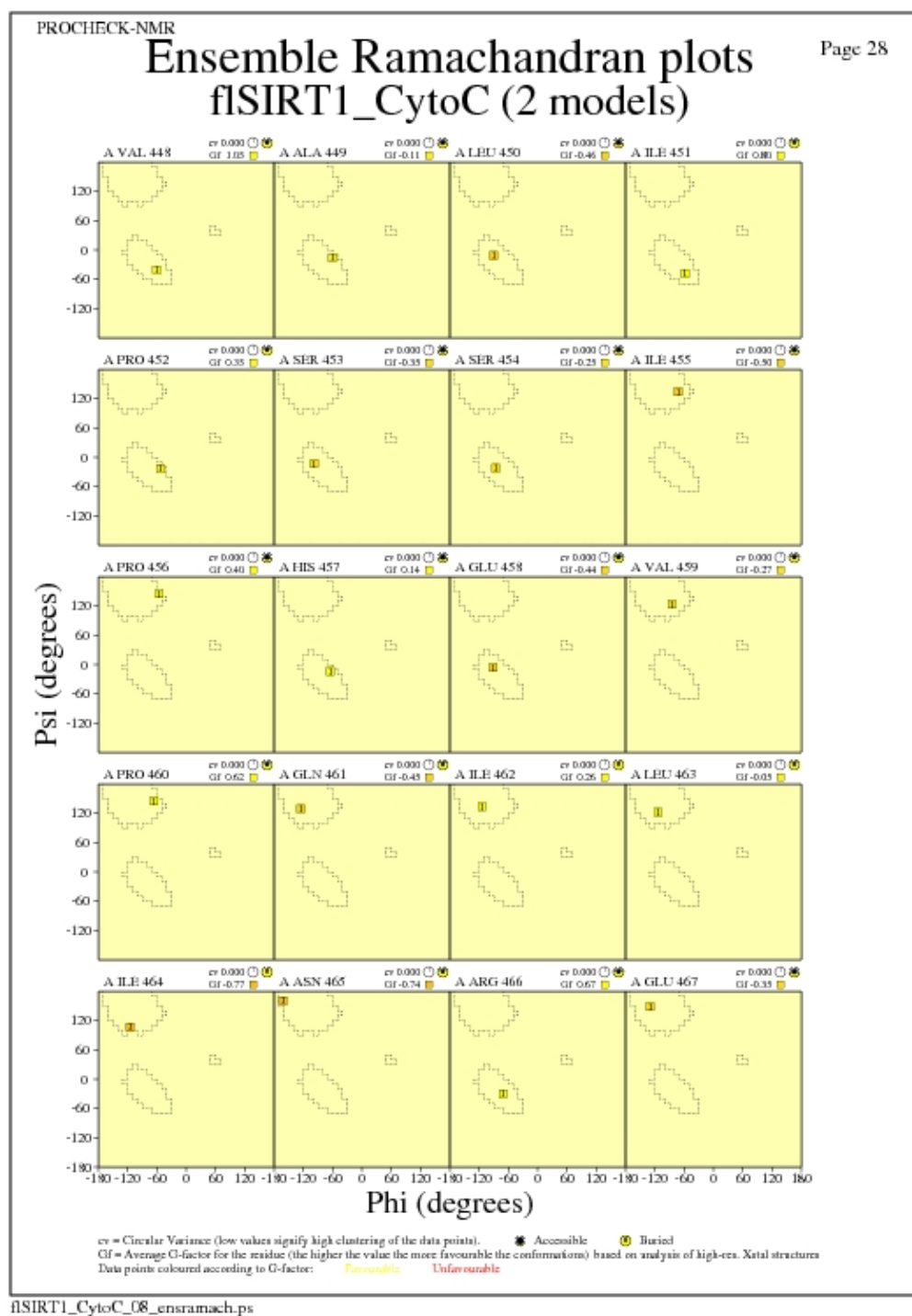
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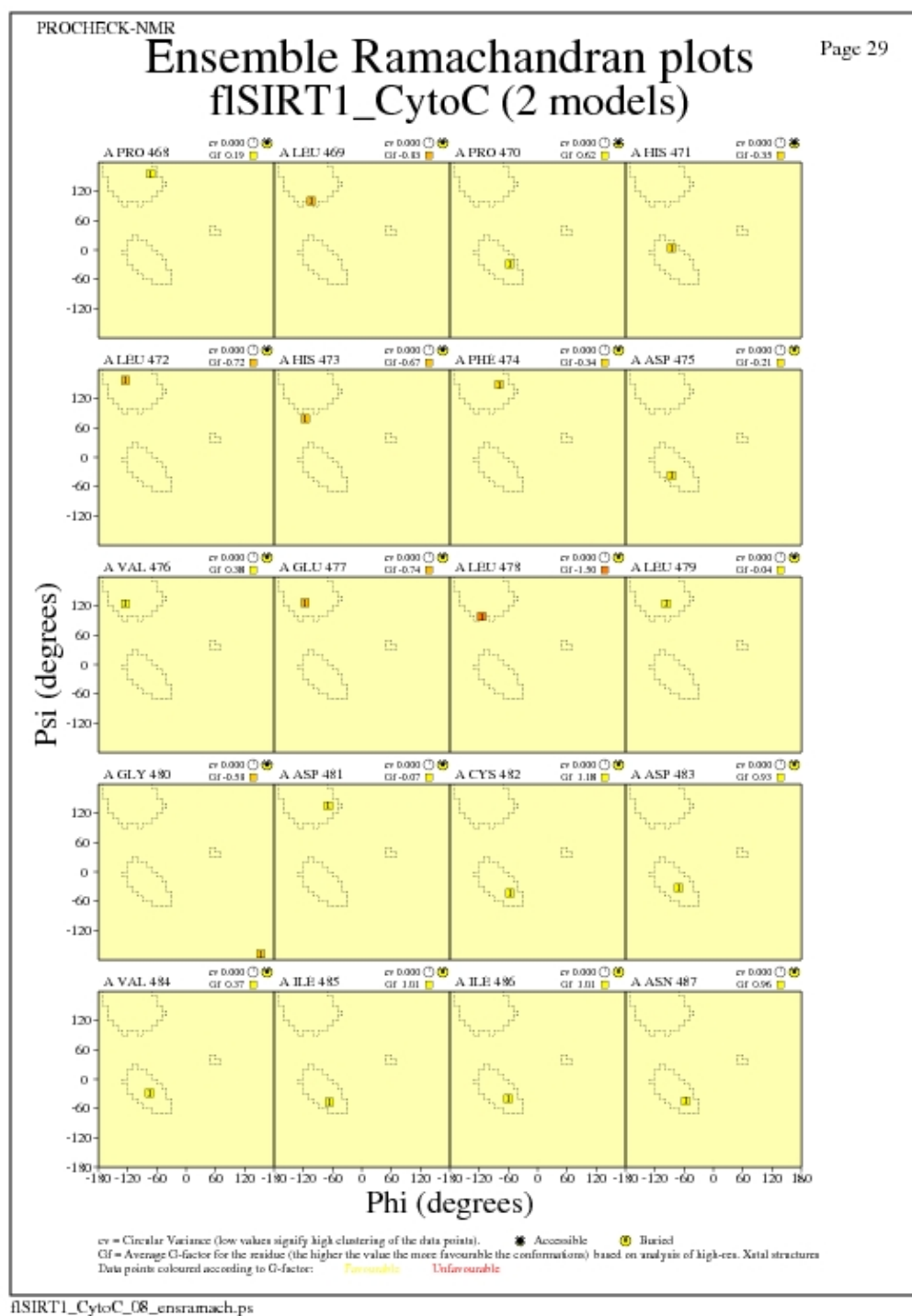
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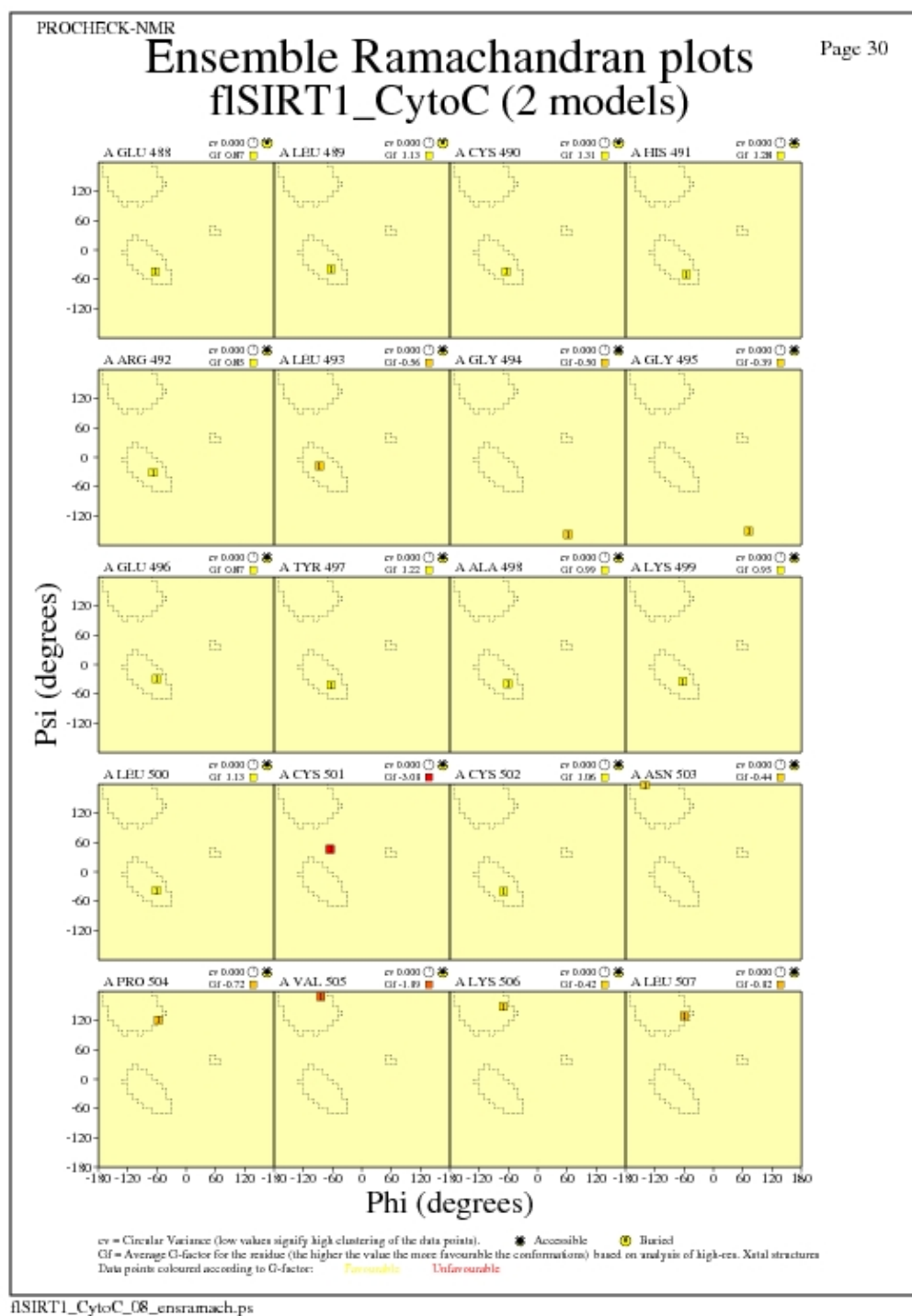
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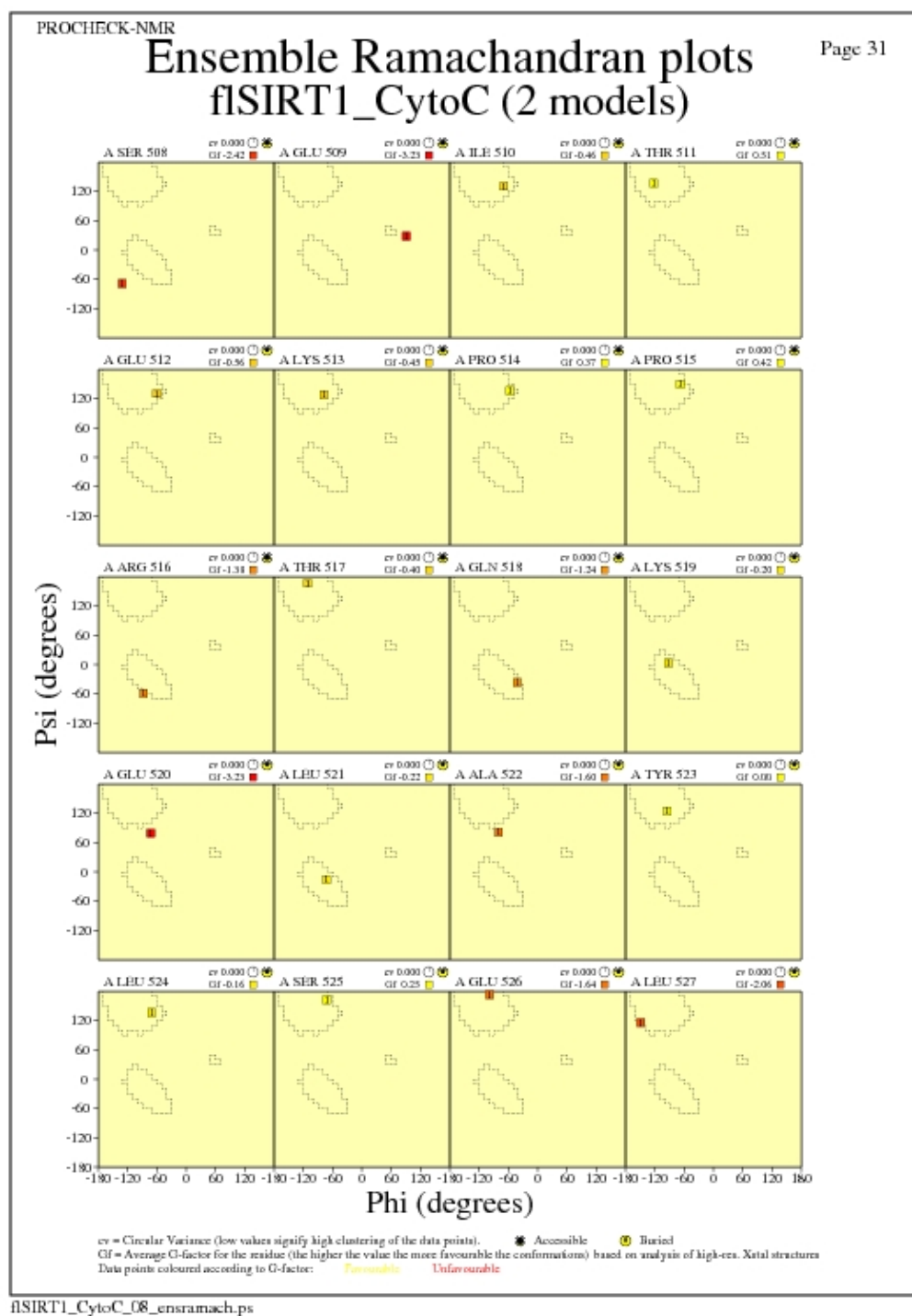
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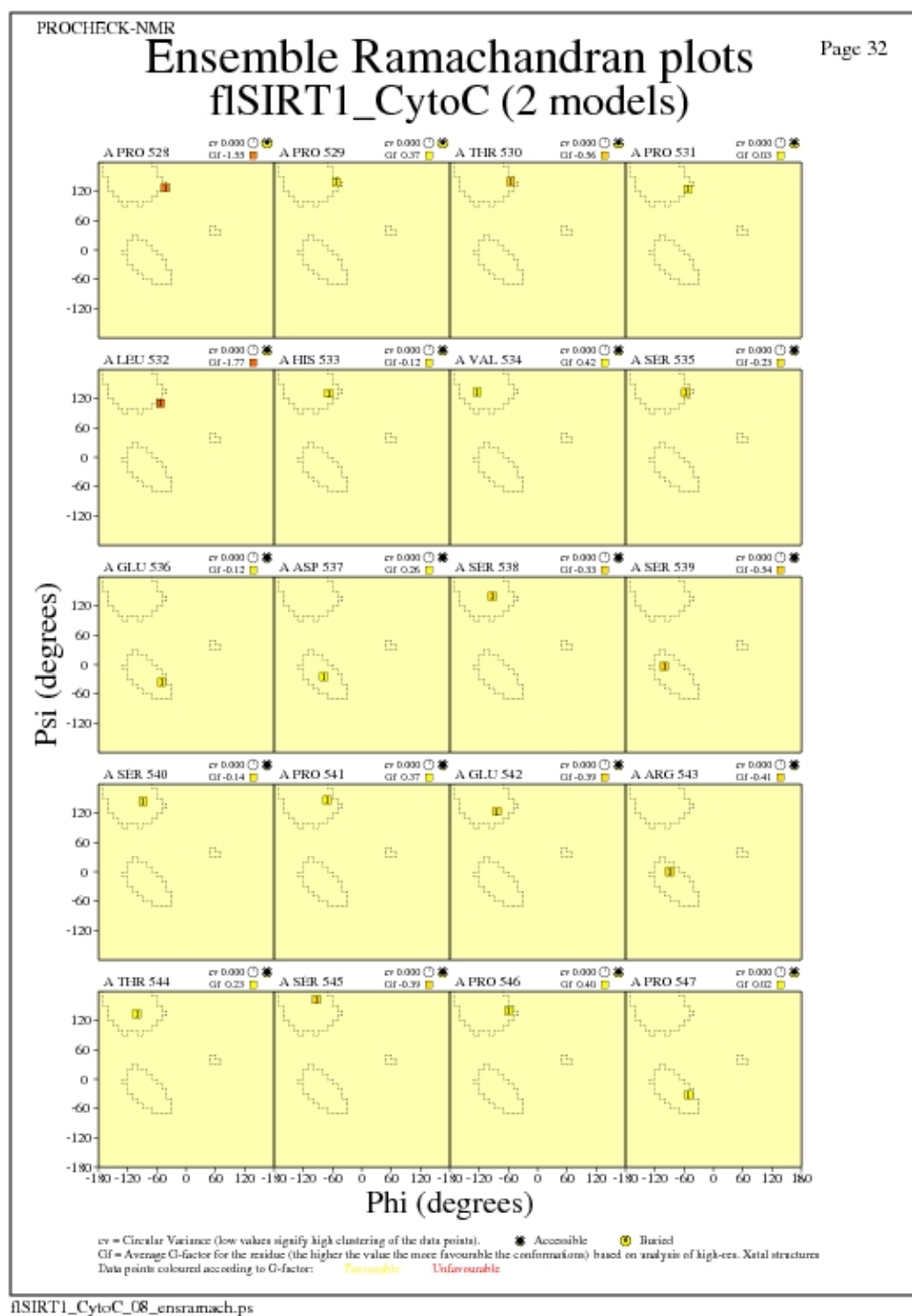
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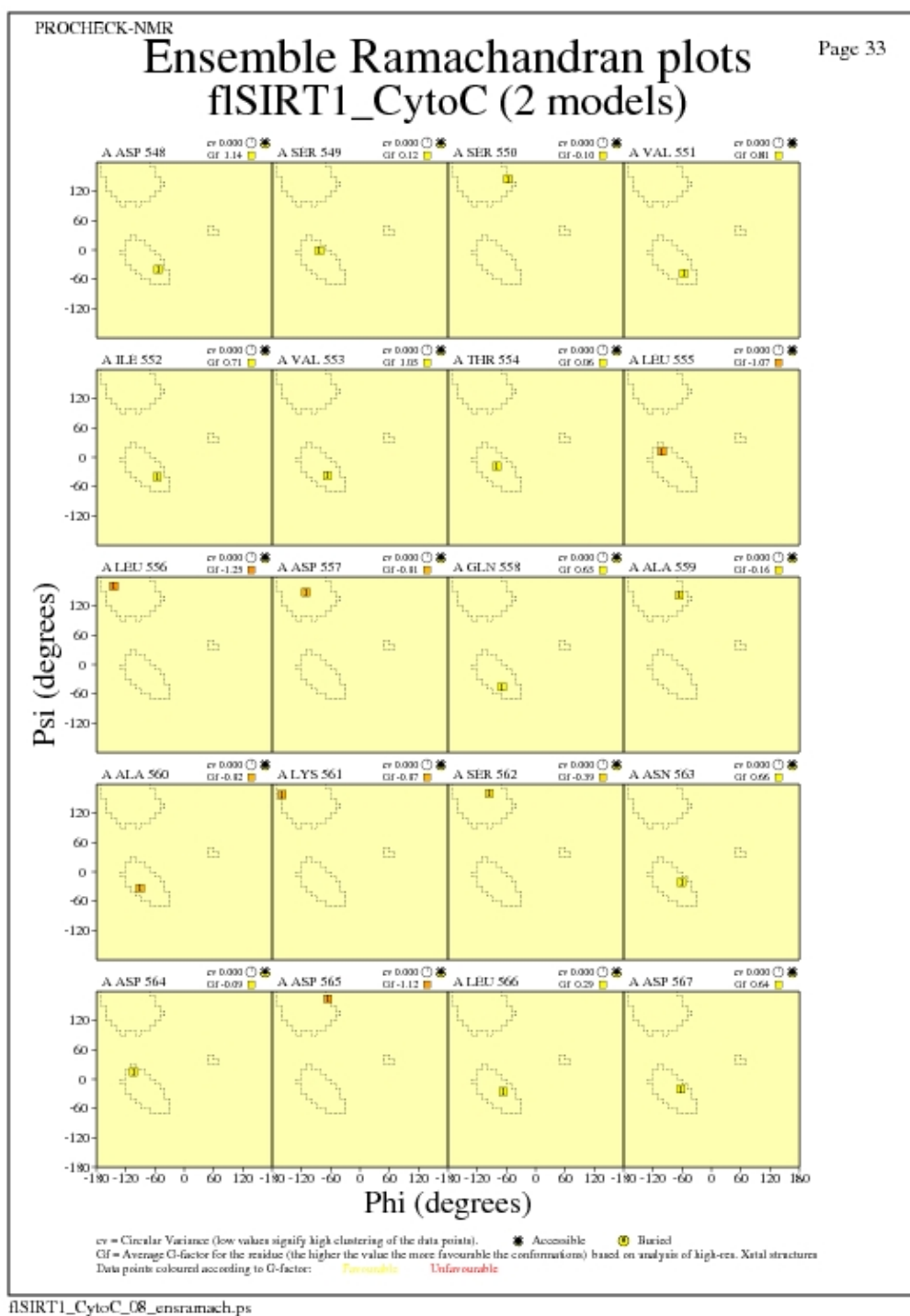
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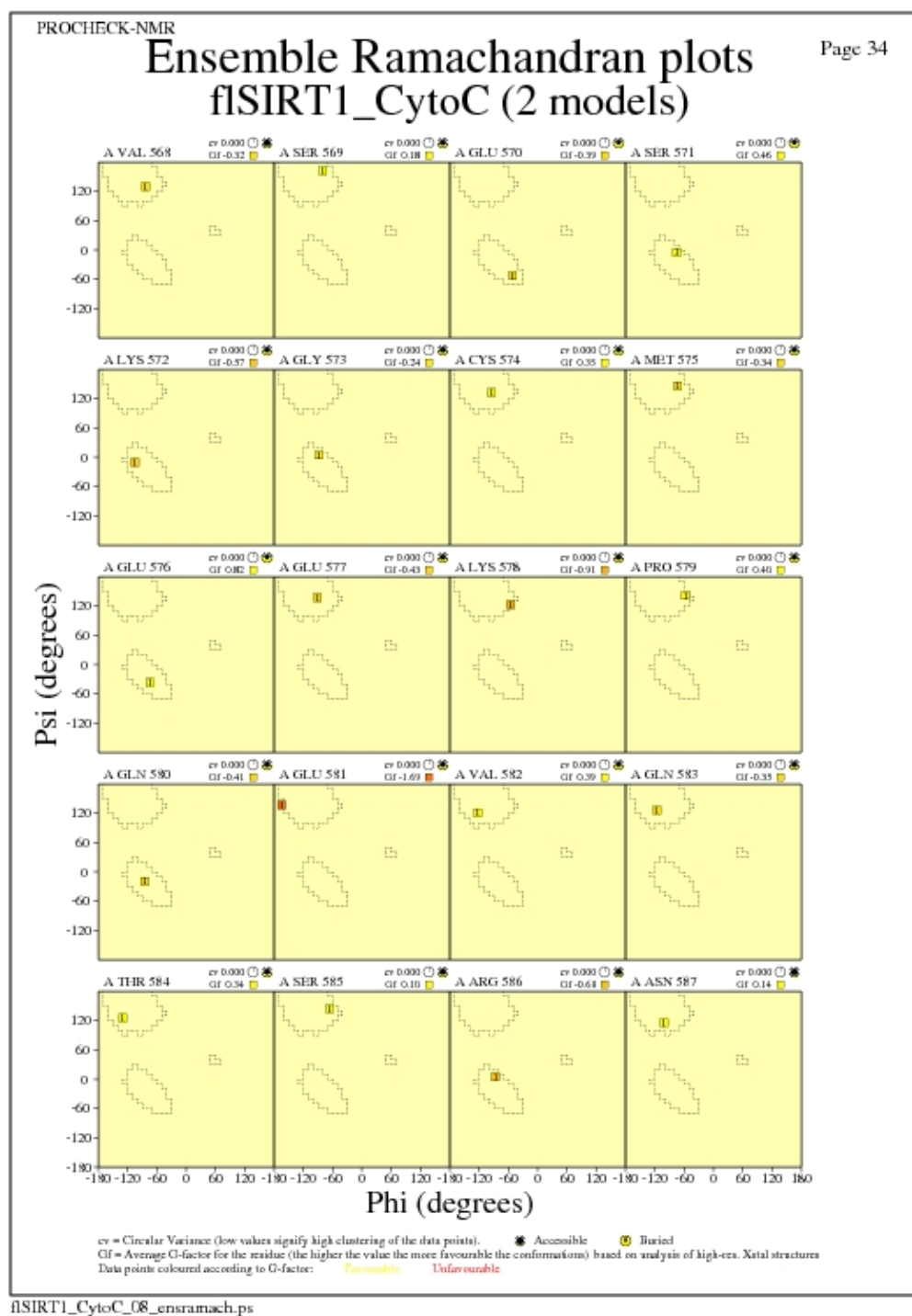
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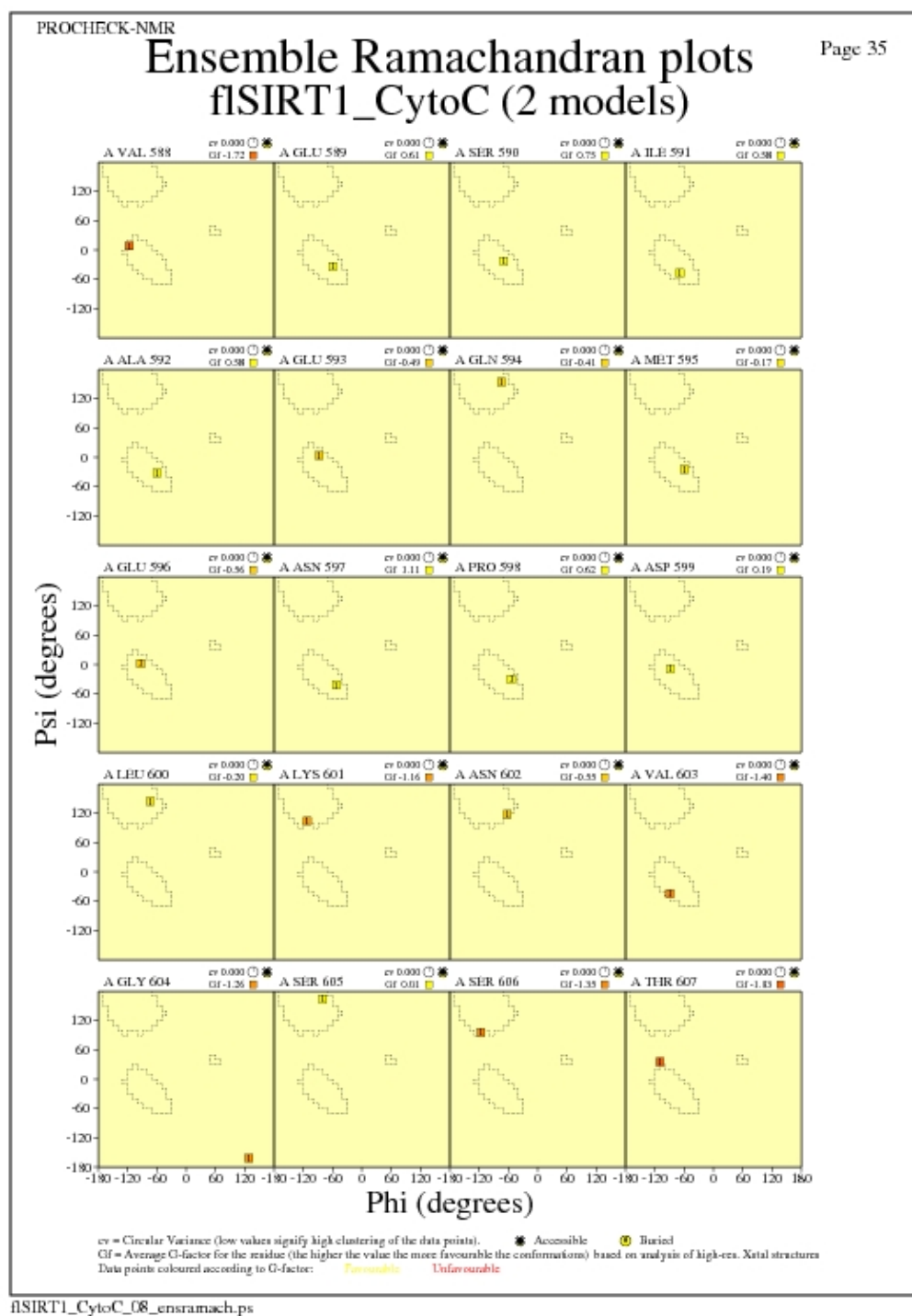
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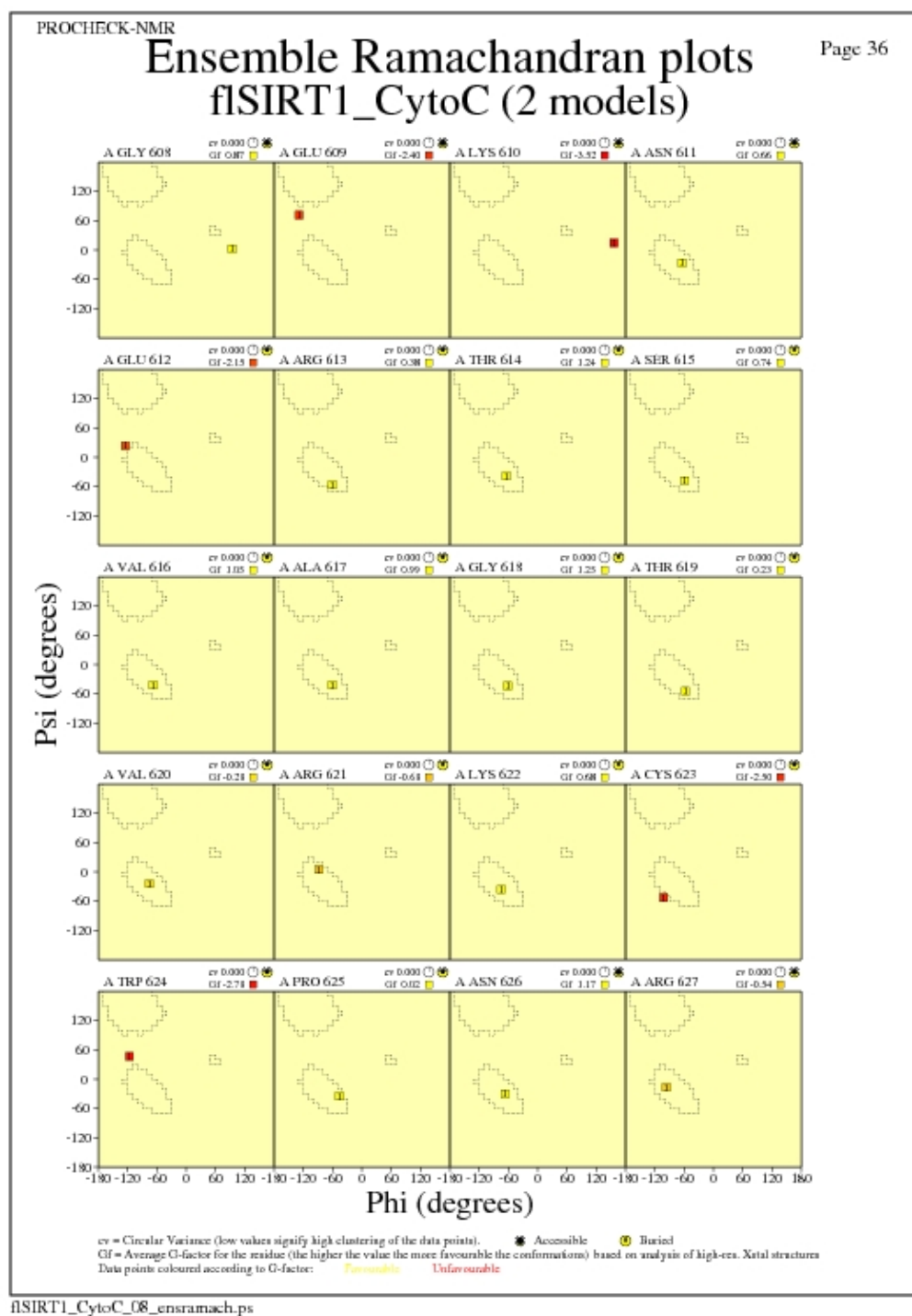
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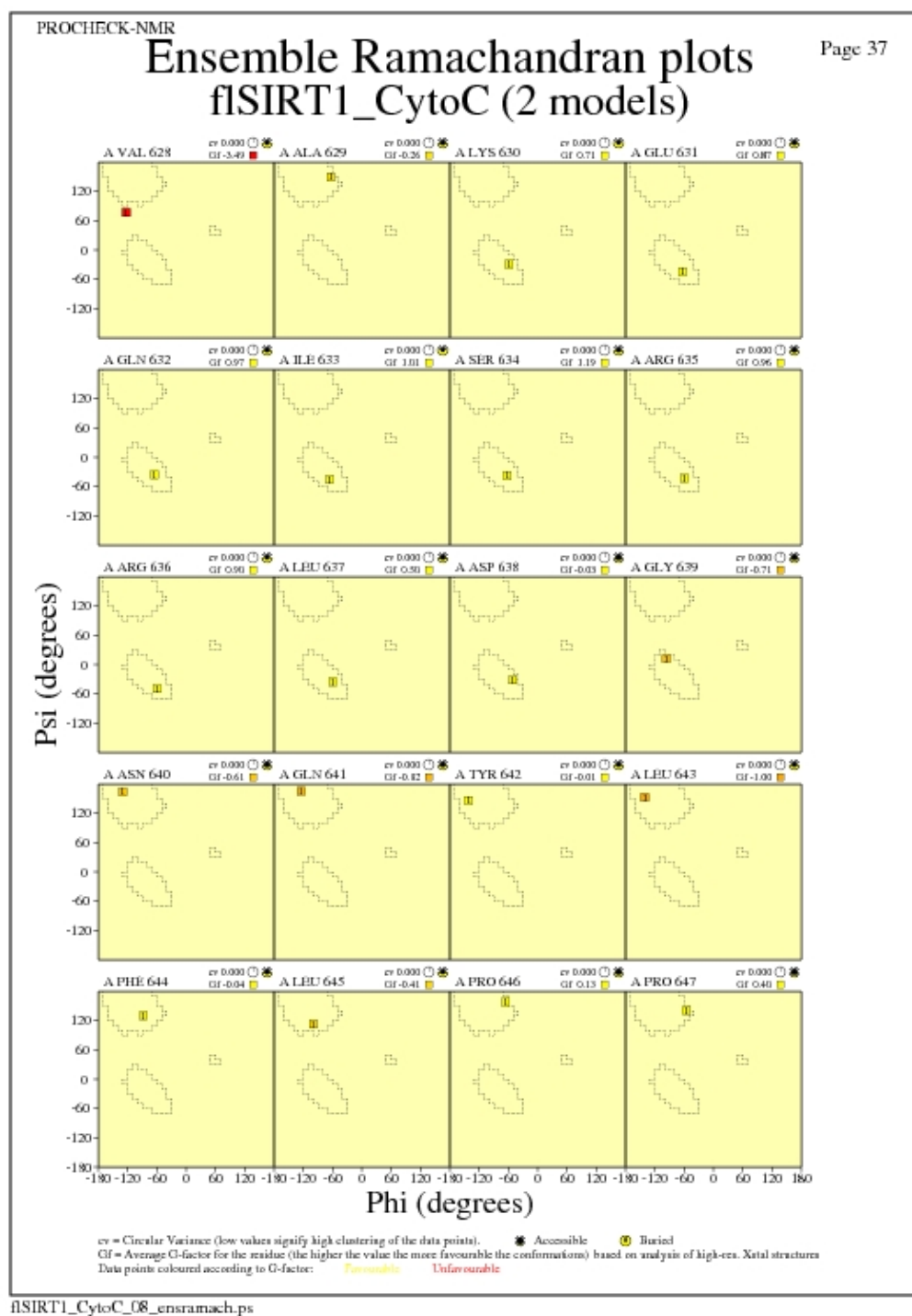
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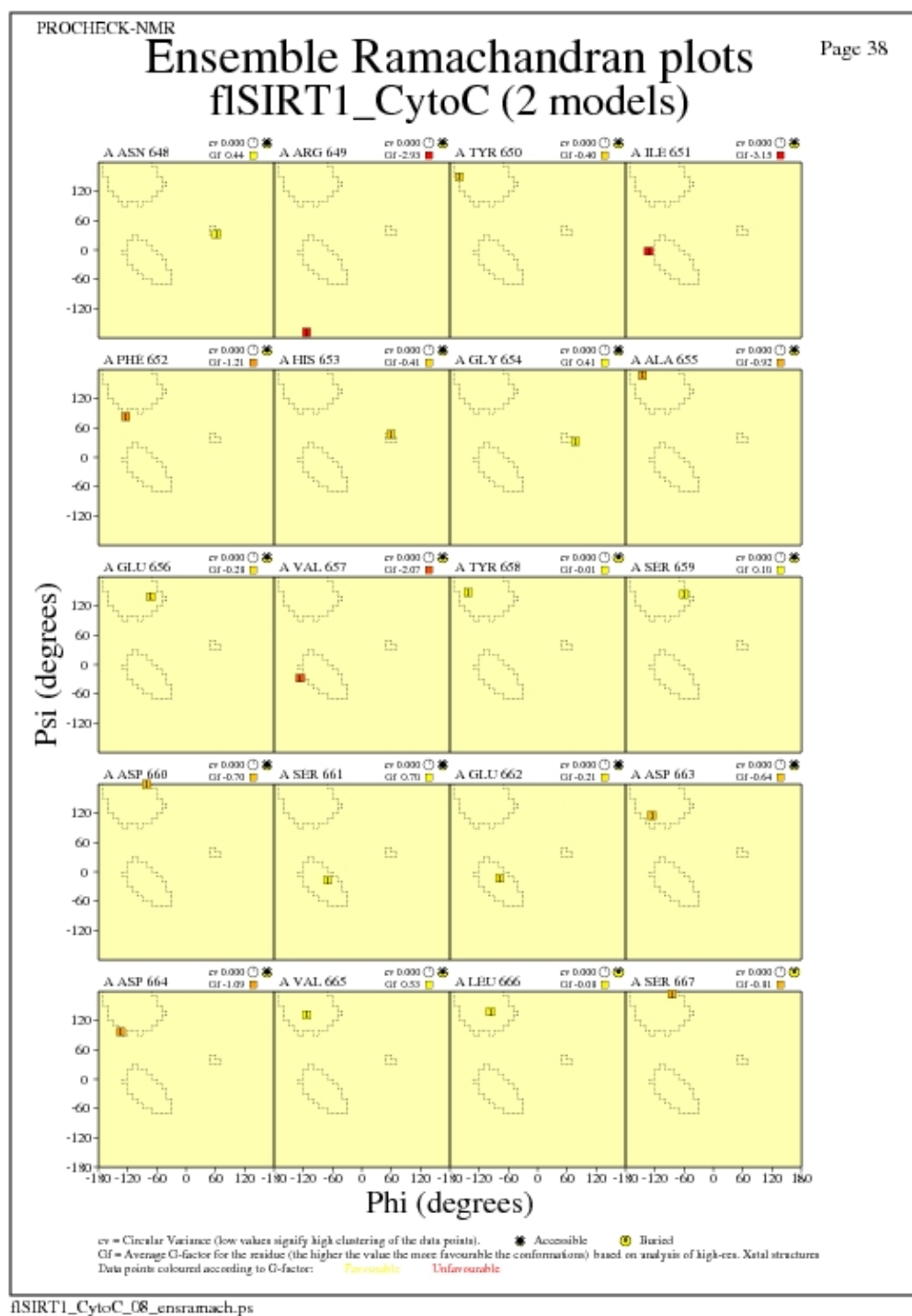
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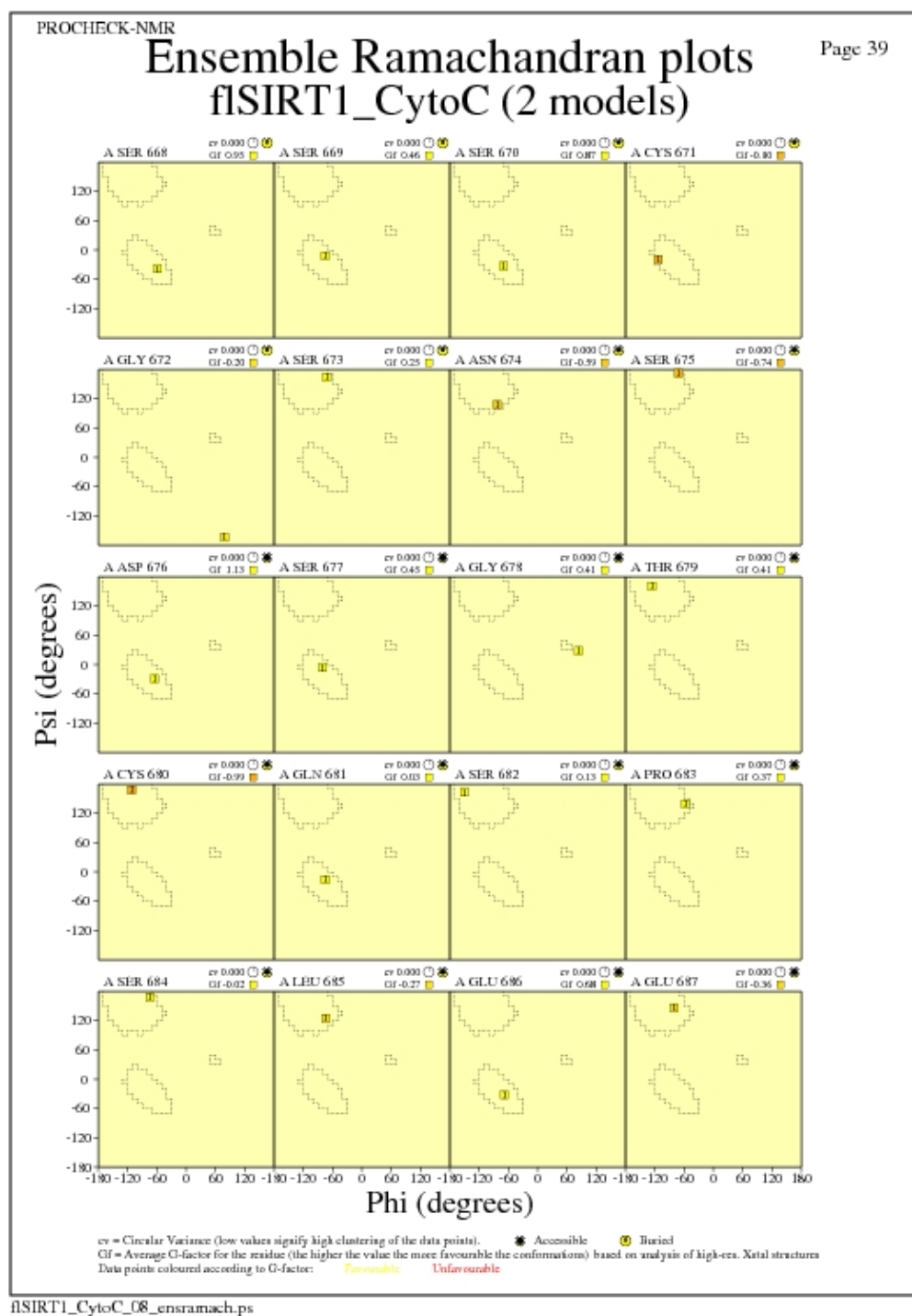
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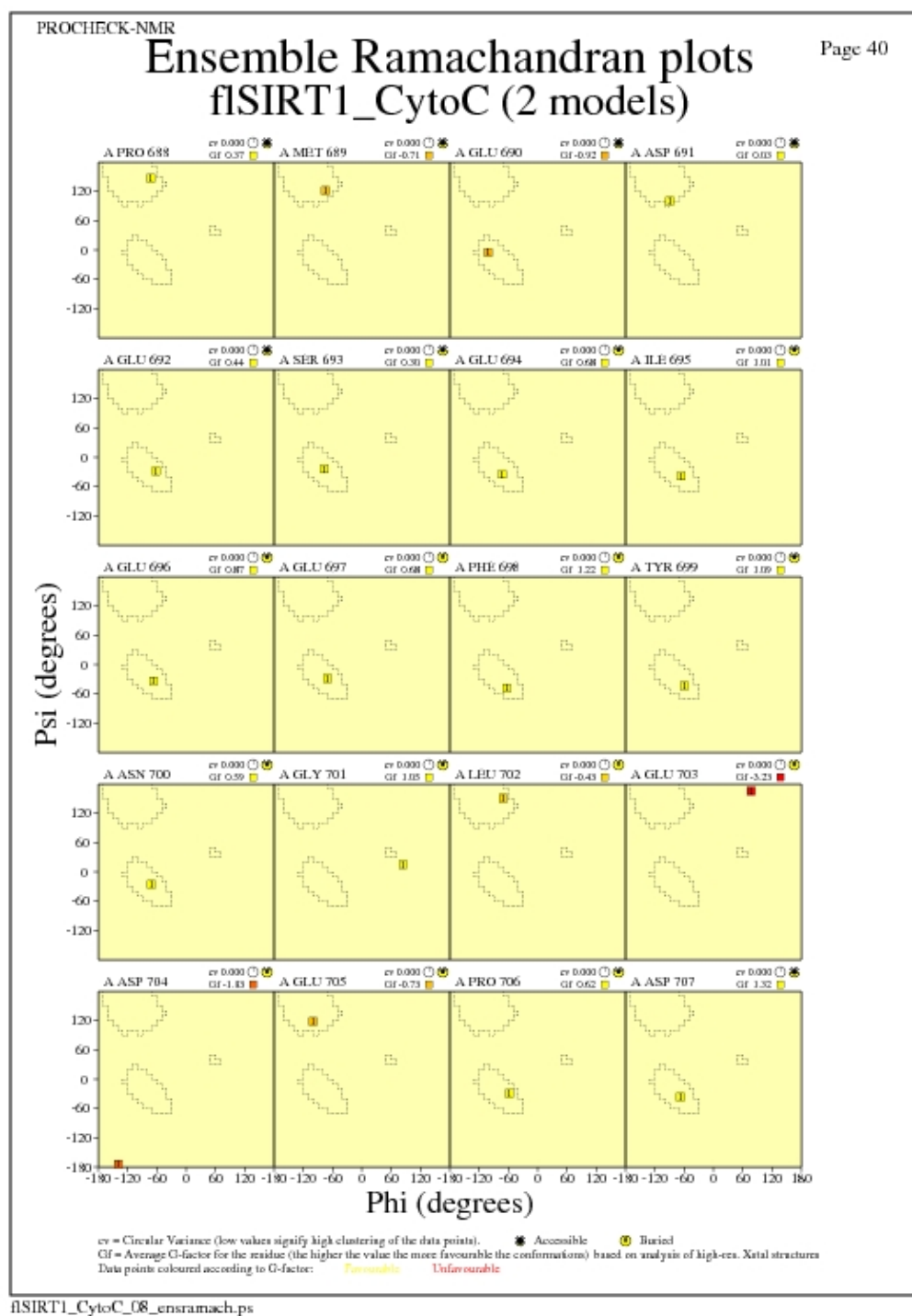
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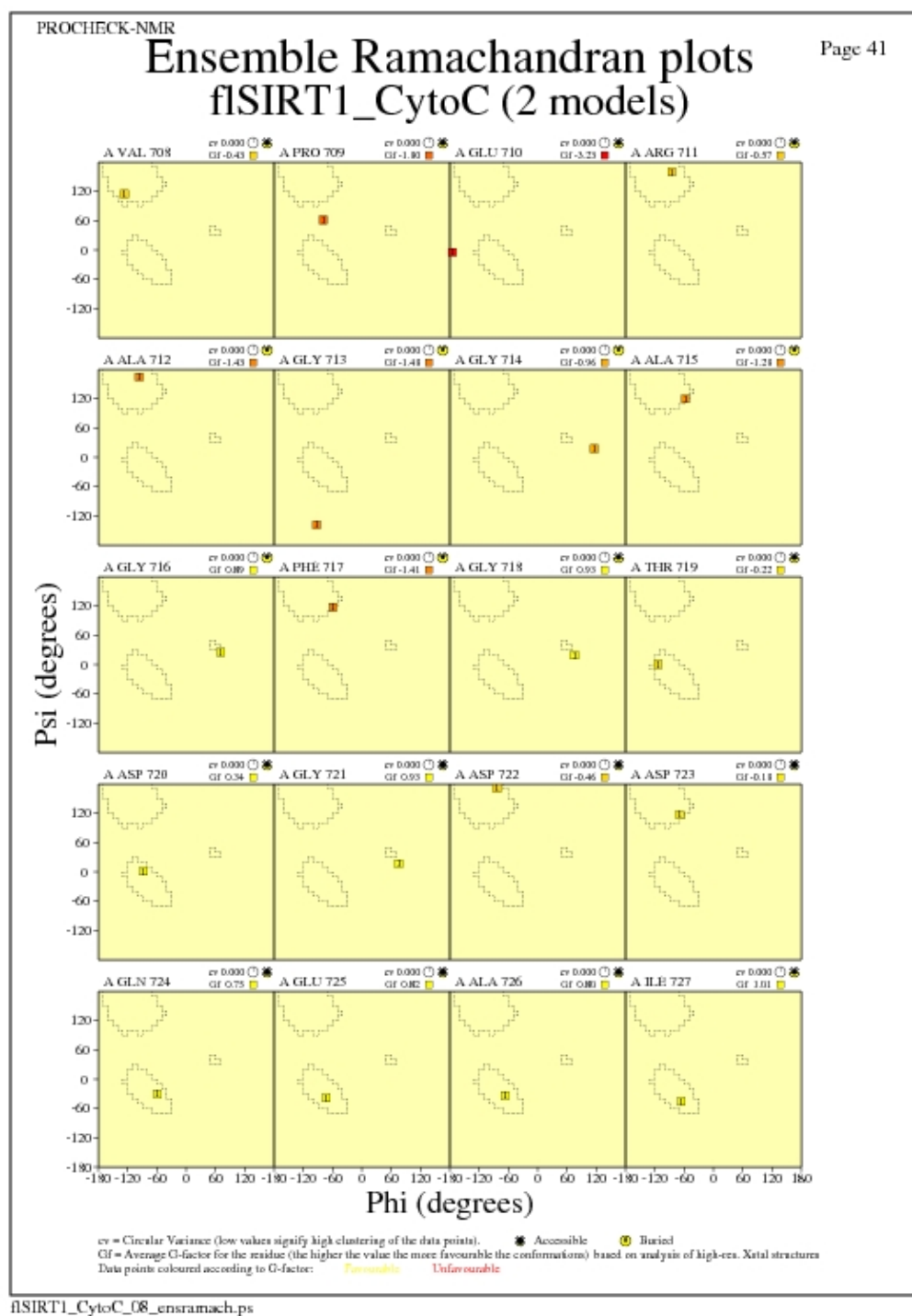
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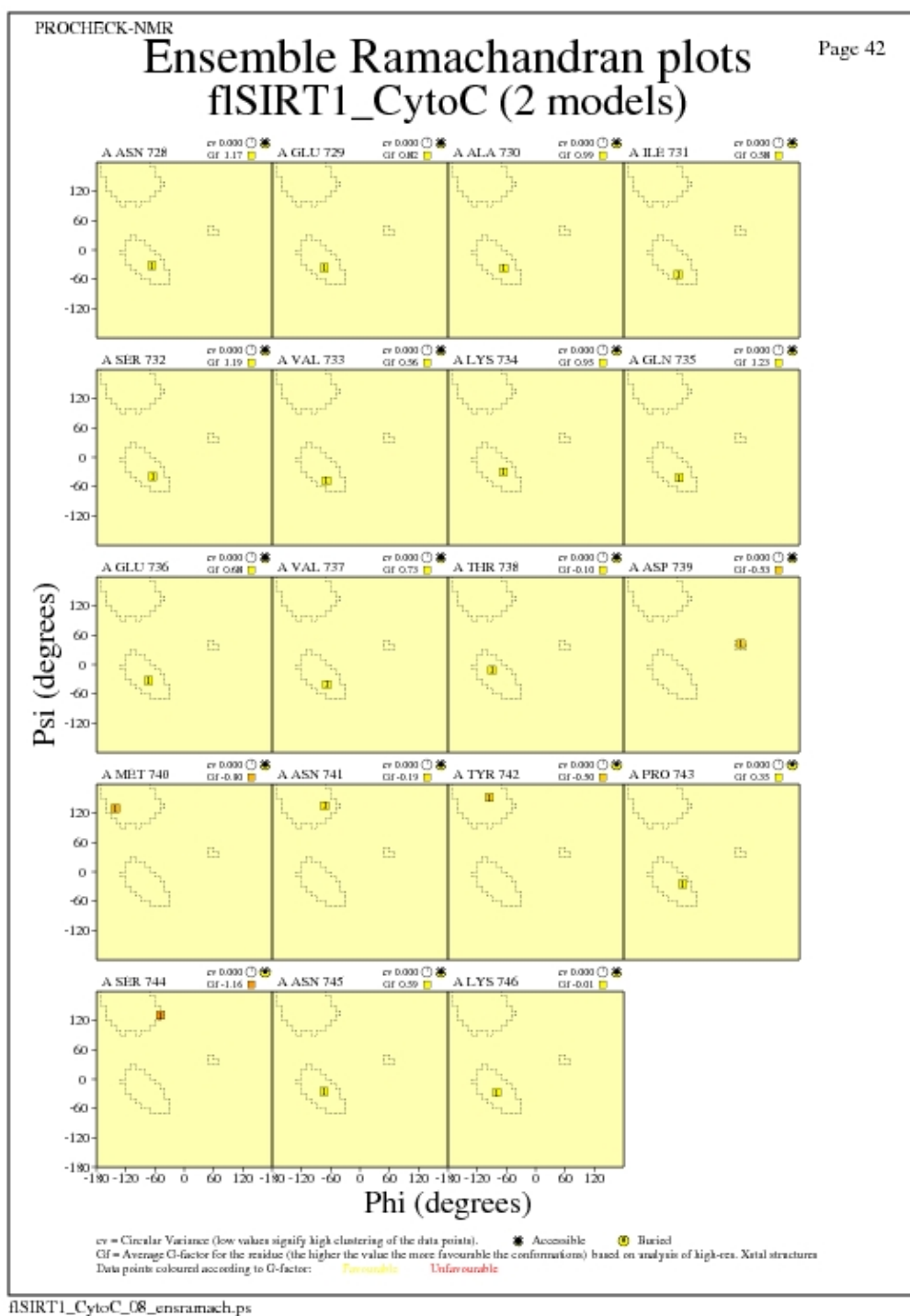
JPEG for residue Ramachandran Plots - page \$num_n



JPEG for residue Ramachandran Plots - page \$num_n



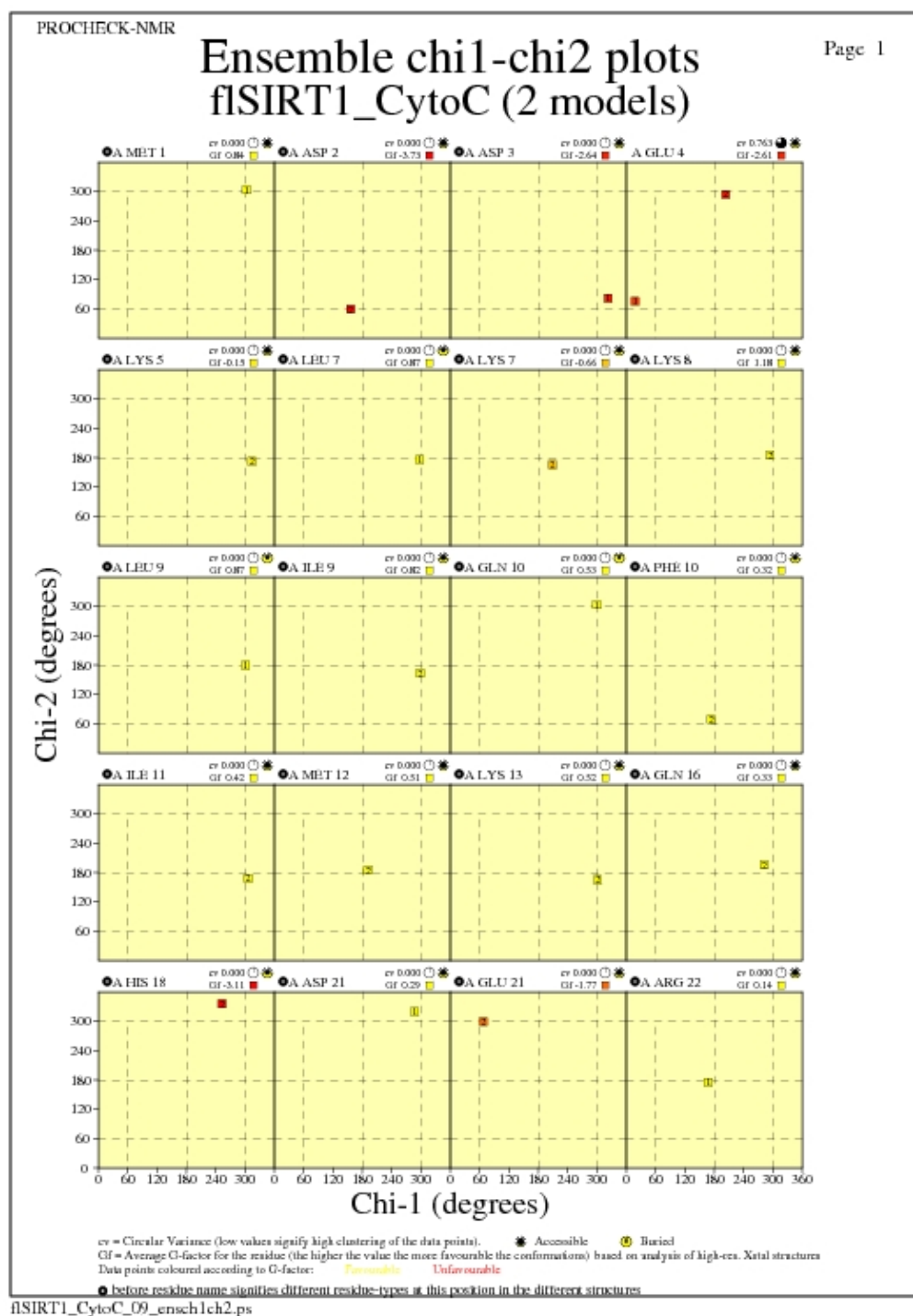
JPEG for residue Ramachandran Plots - page \$num_n



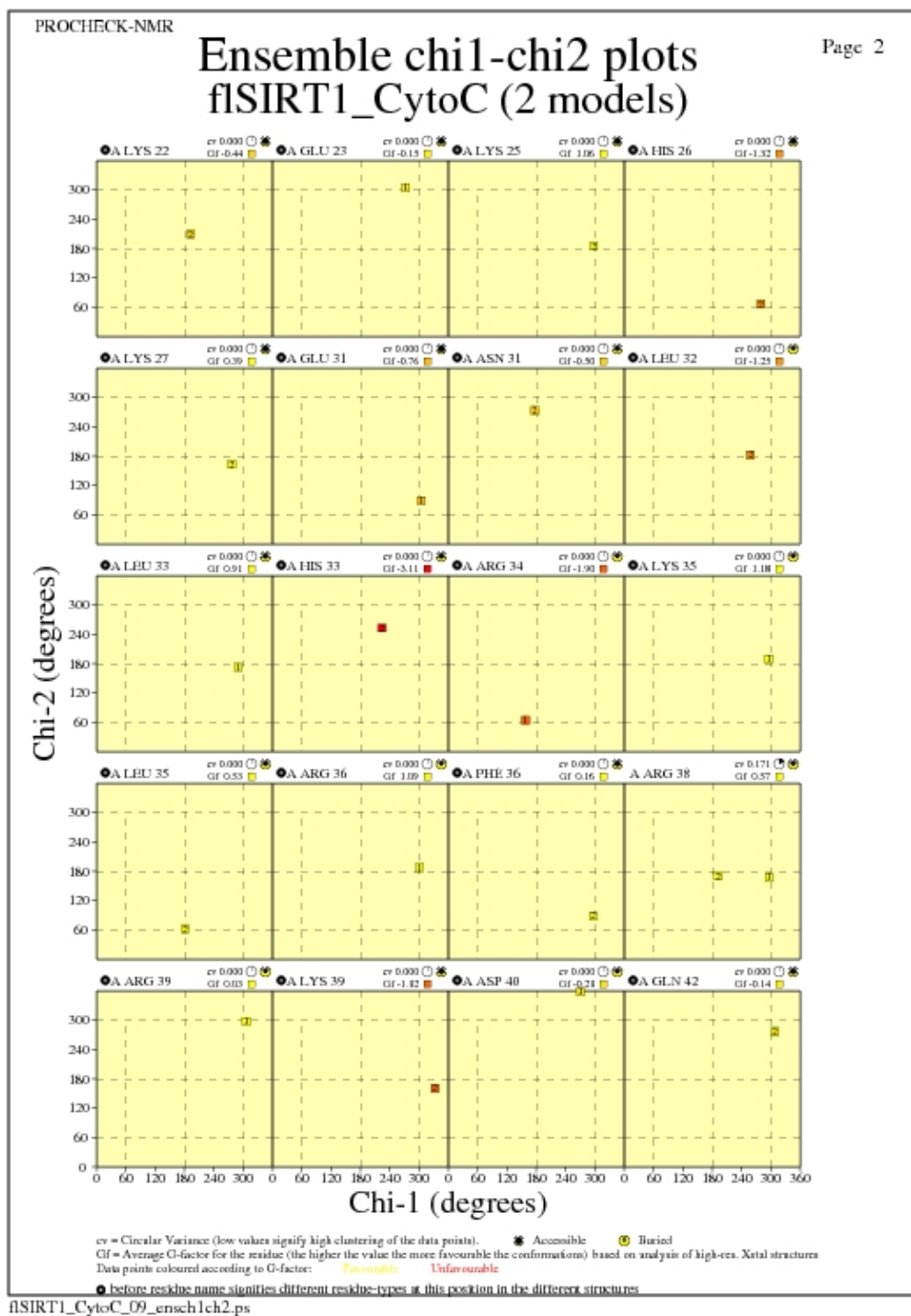
Ramachandran analysis for each residue from Molprobit

Chi1-Chi2 Plots for each residue

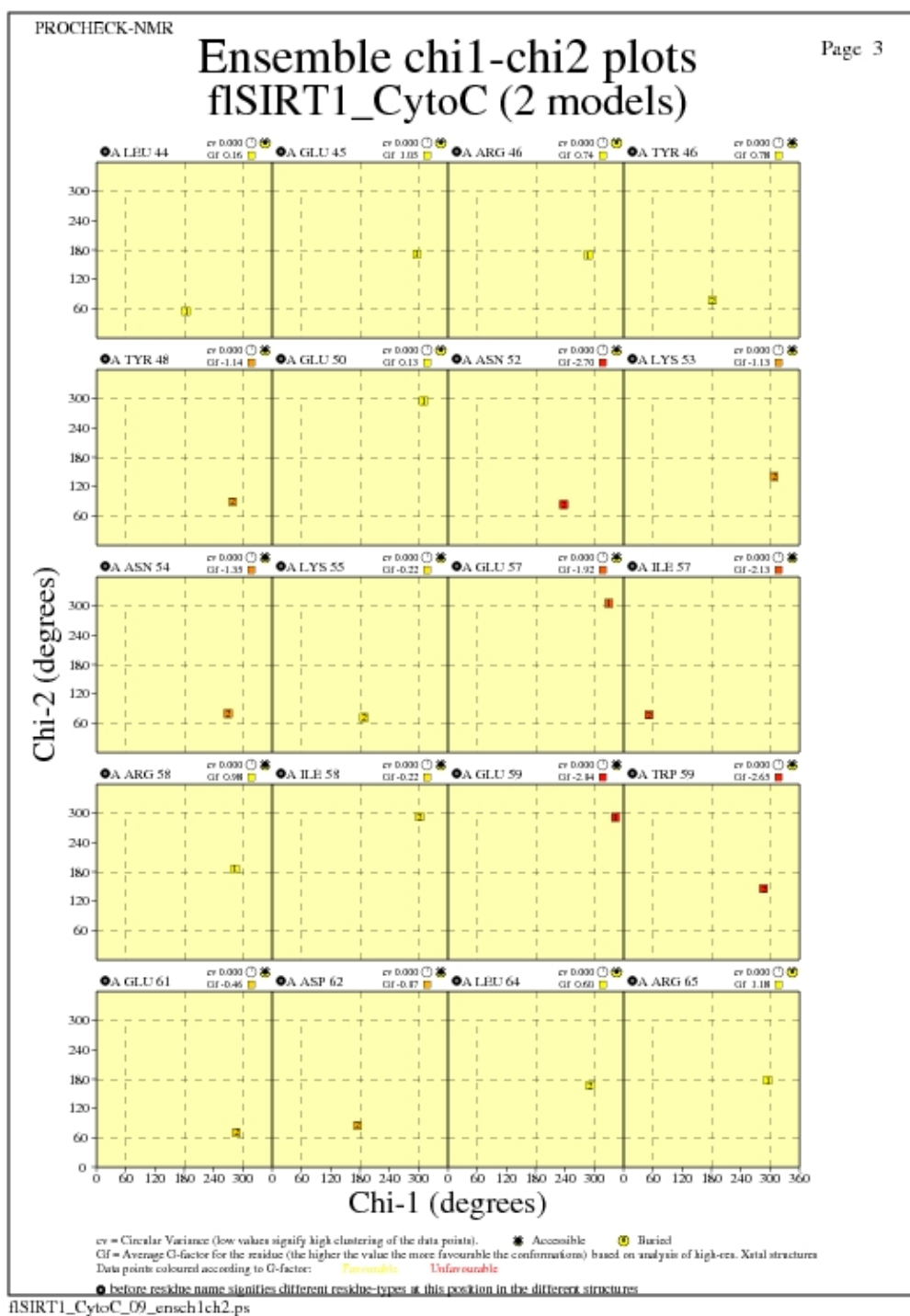
JPEG for residue Chi1-Chi2 Plots - page \$num_n



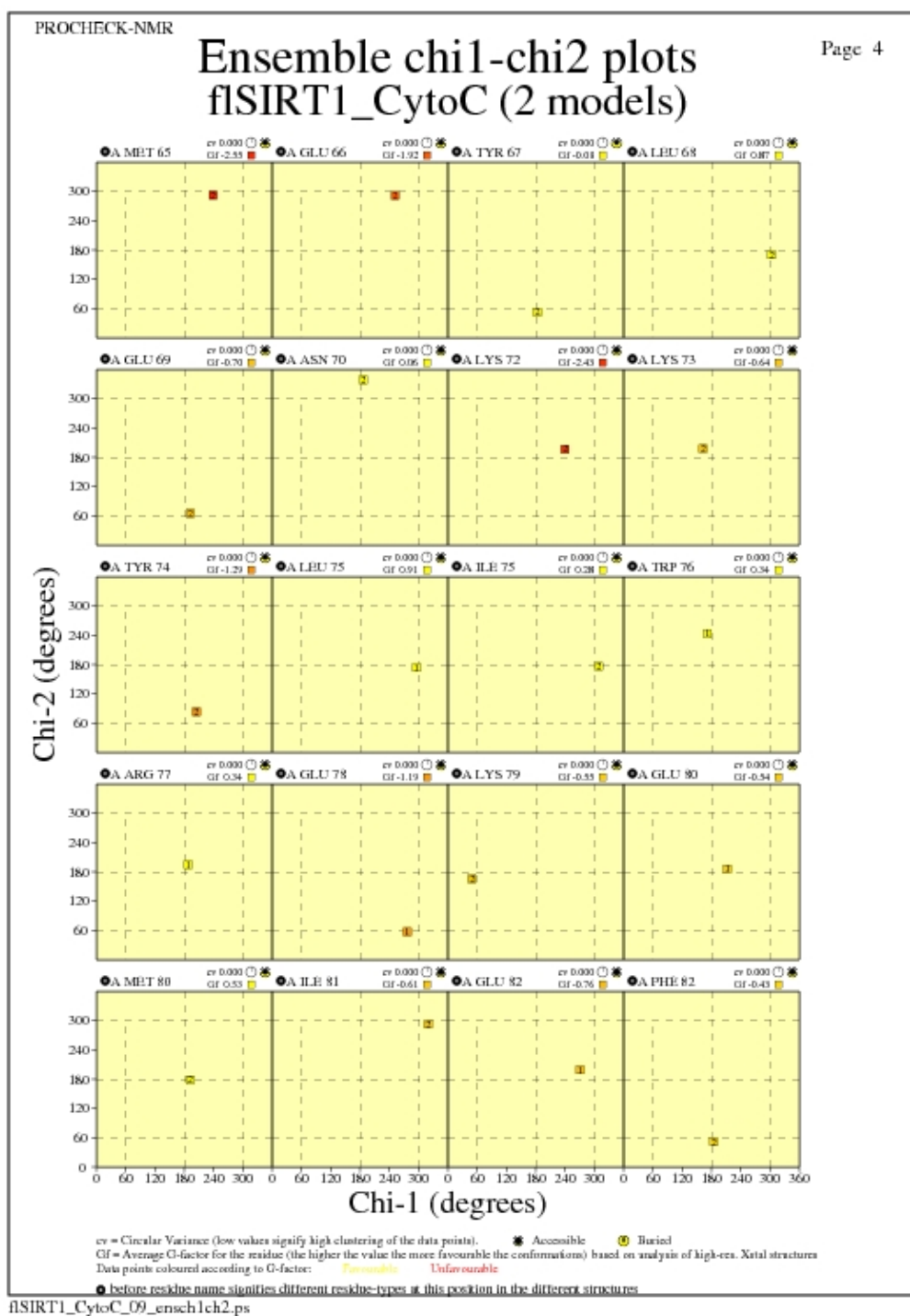
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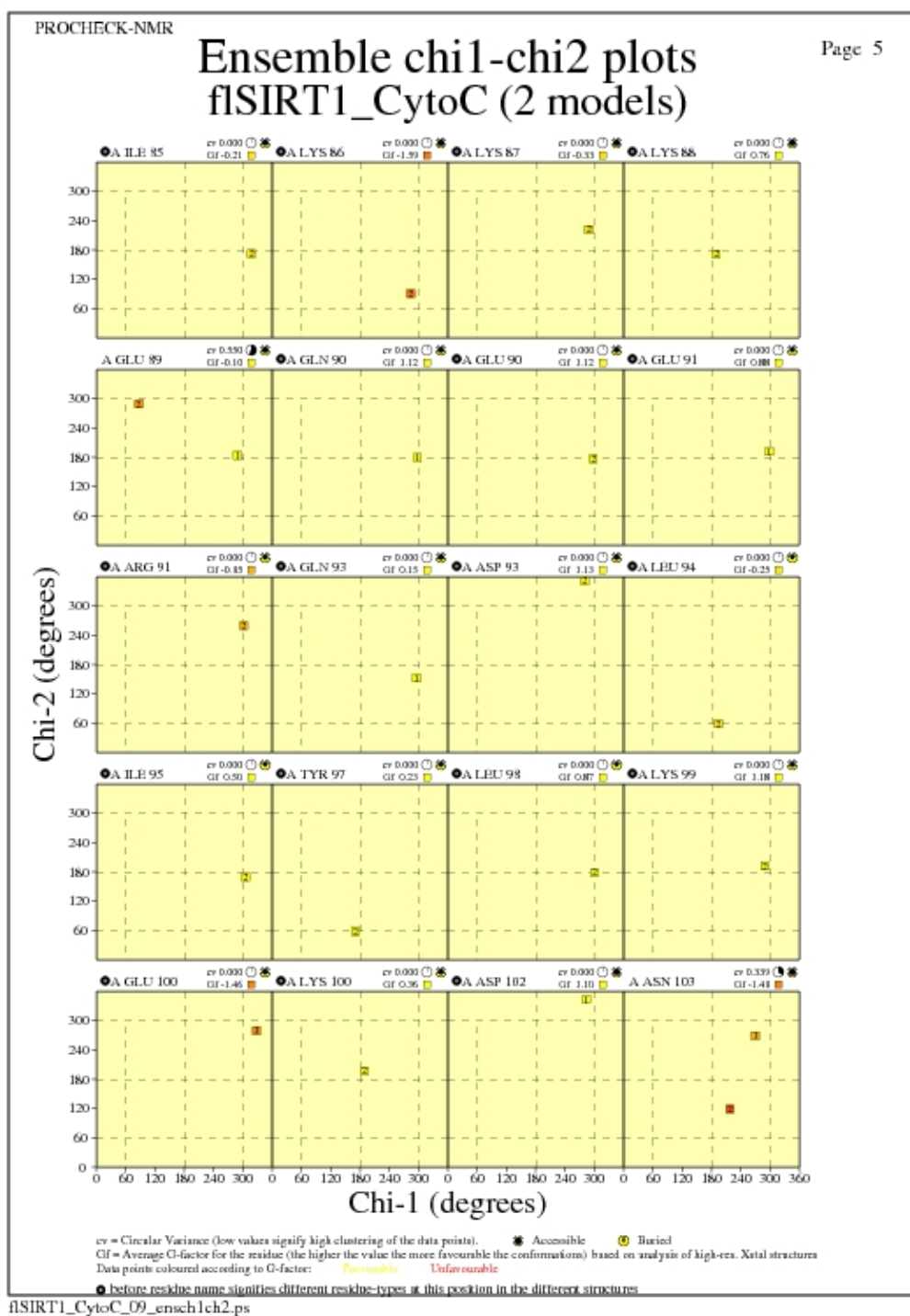
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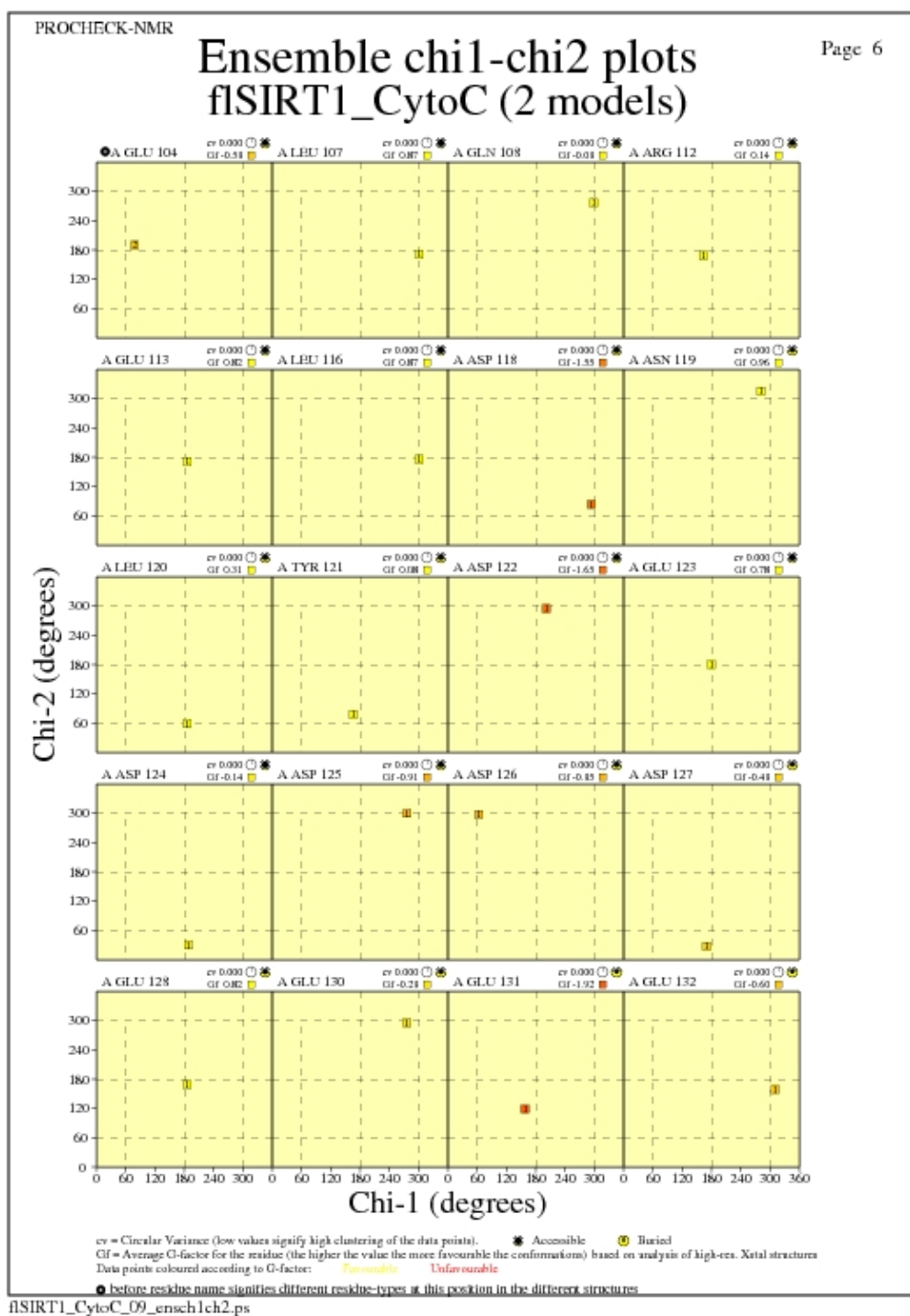
JPEG for residue Chi1-Chi2 Plots - page \$num_n



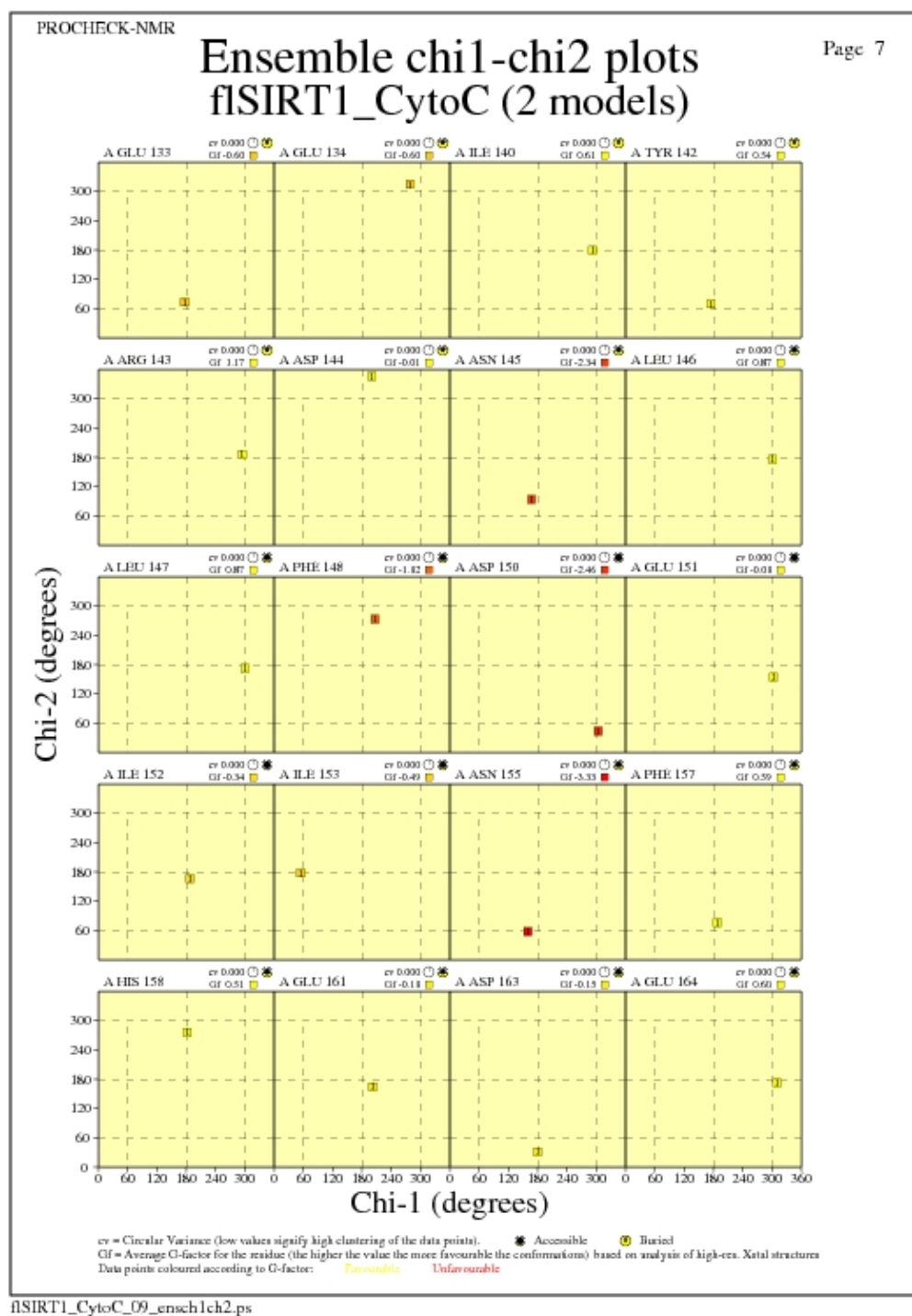
JPEG for residue Chi1-Chi2 Plots - page \$num_n



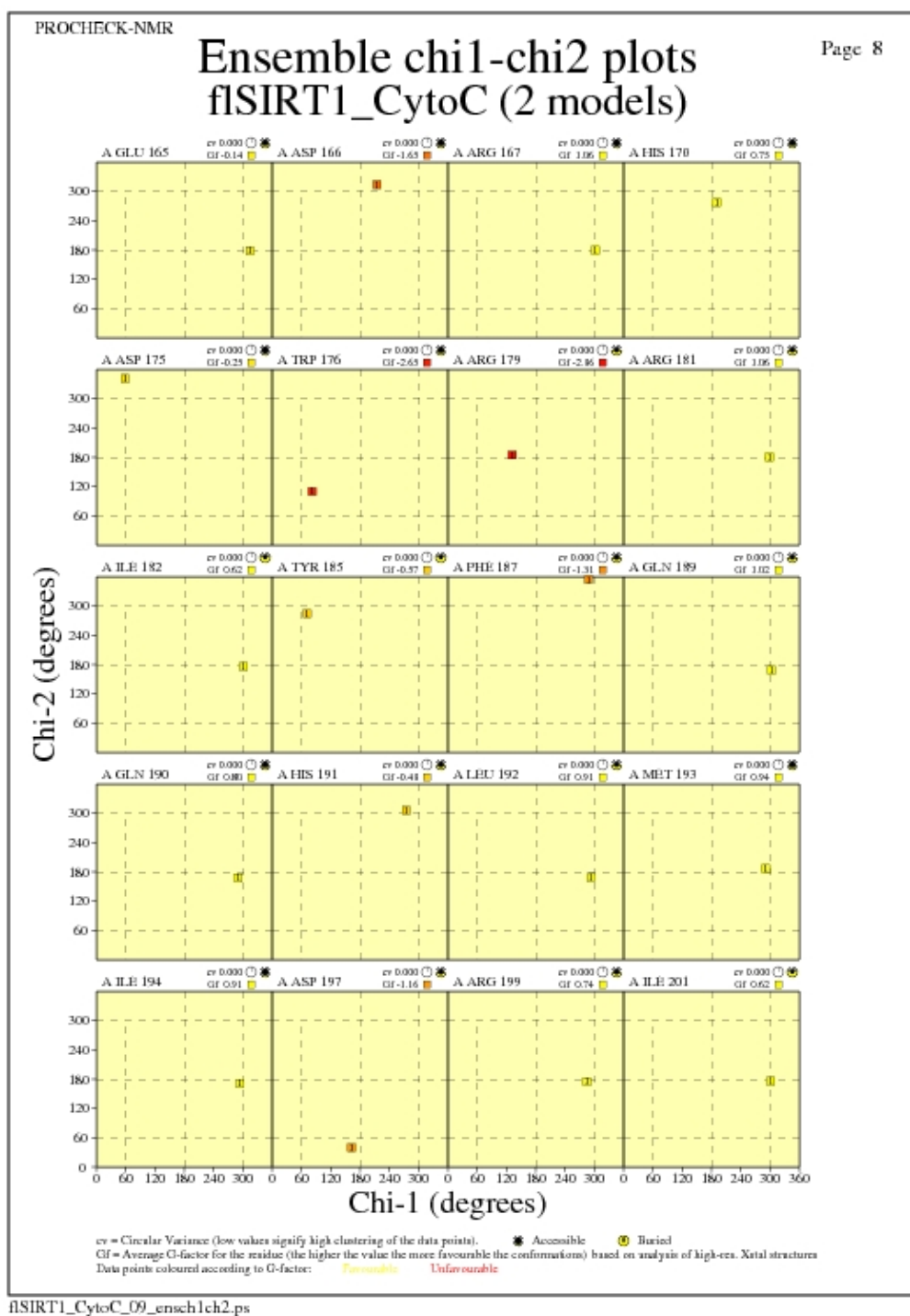
JPEG for residue Chi1-Chi2 Plots - page \$num_n



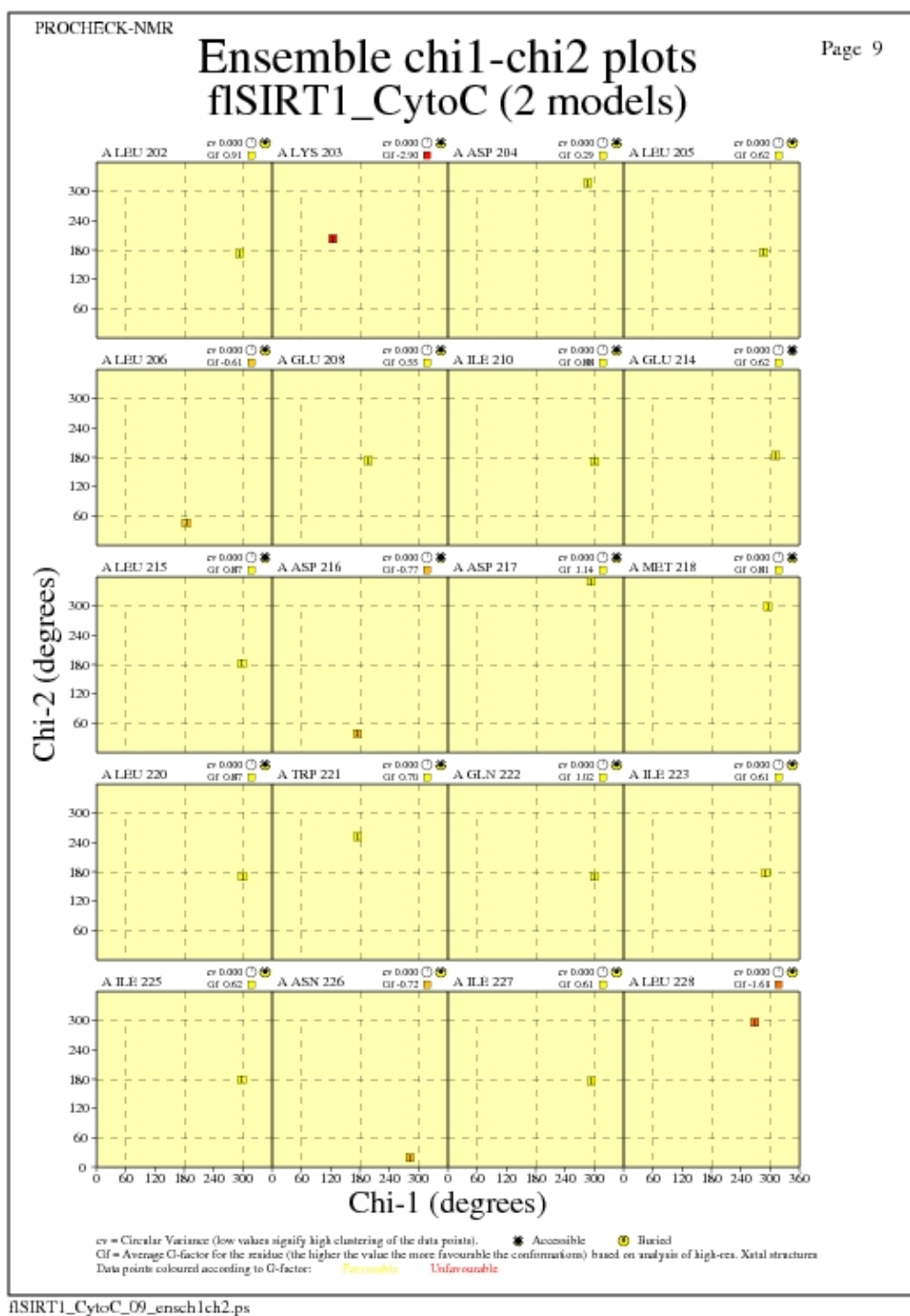
JPEG for residue Chi1-Chi2 Plots - page \$num_n



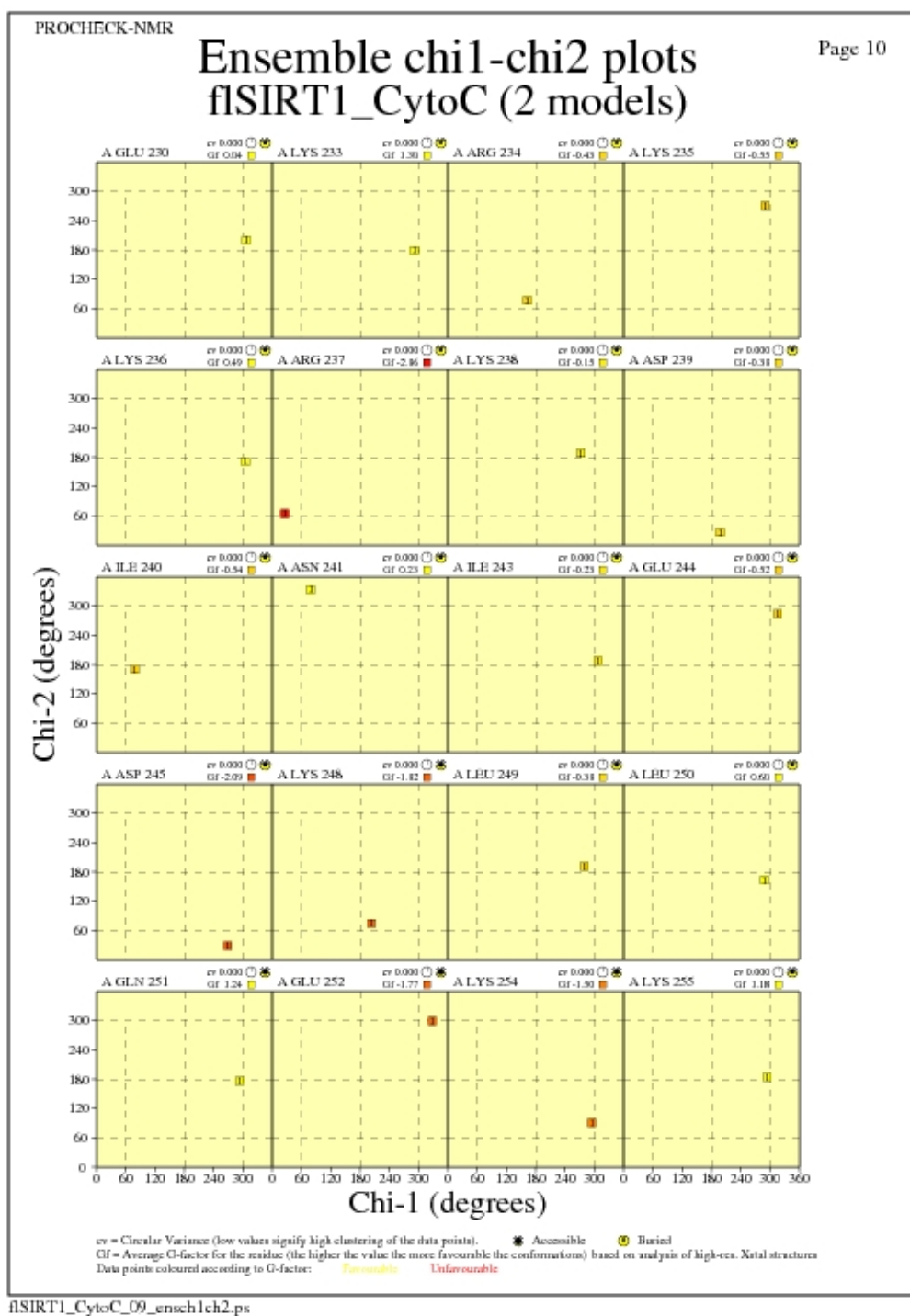
JPEG for residue Chi1-Chi2 Plots - page \$num_n



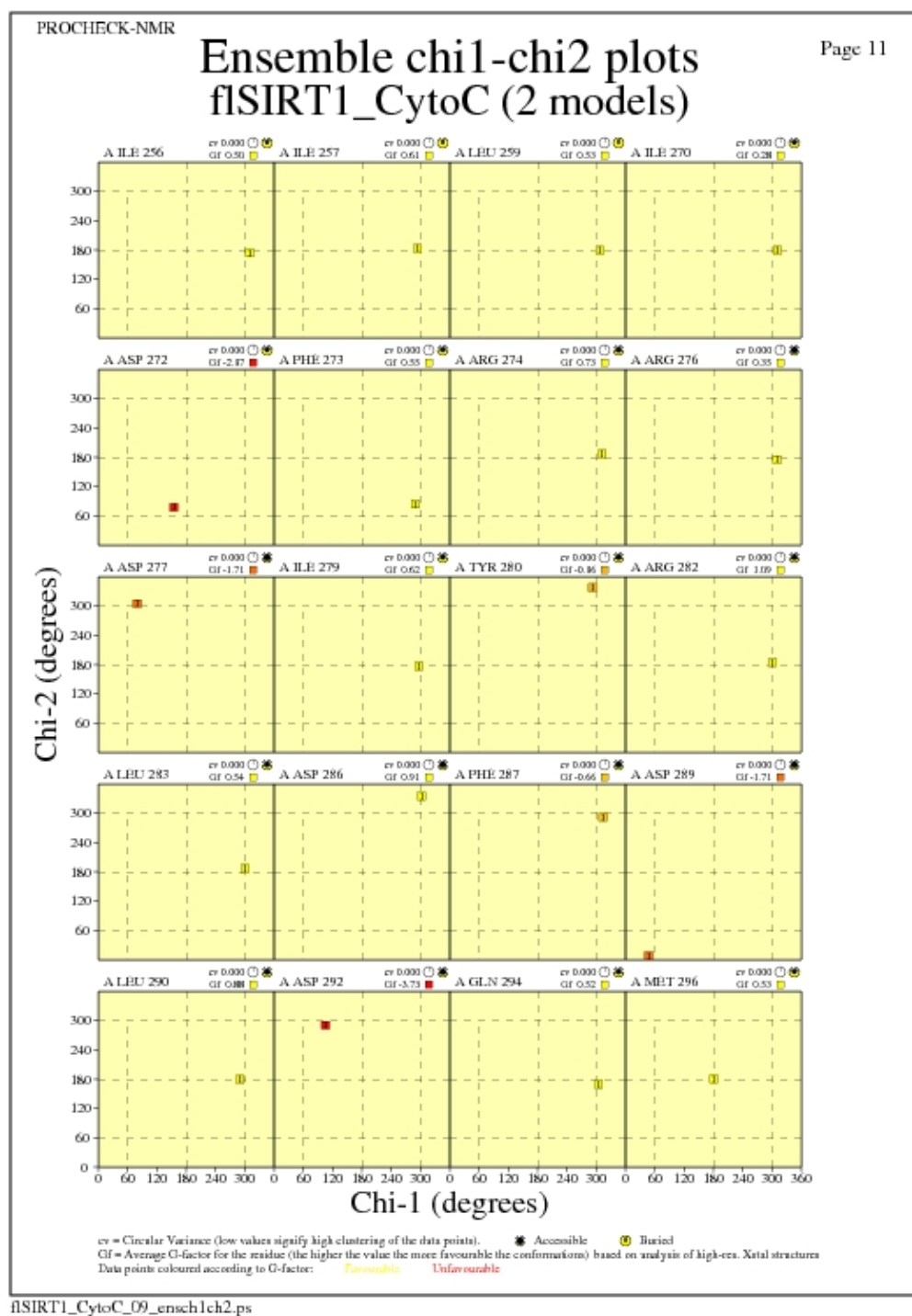
JPEG for residue Chi1-Chi2 Plots - page \$num_n



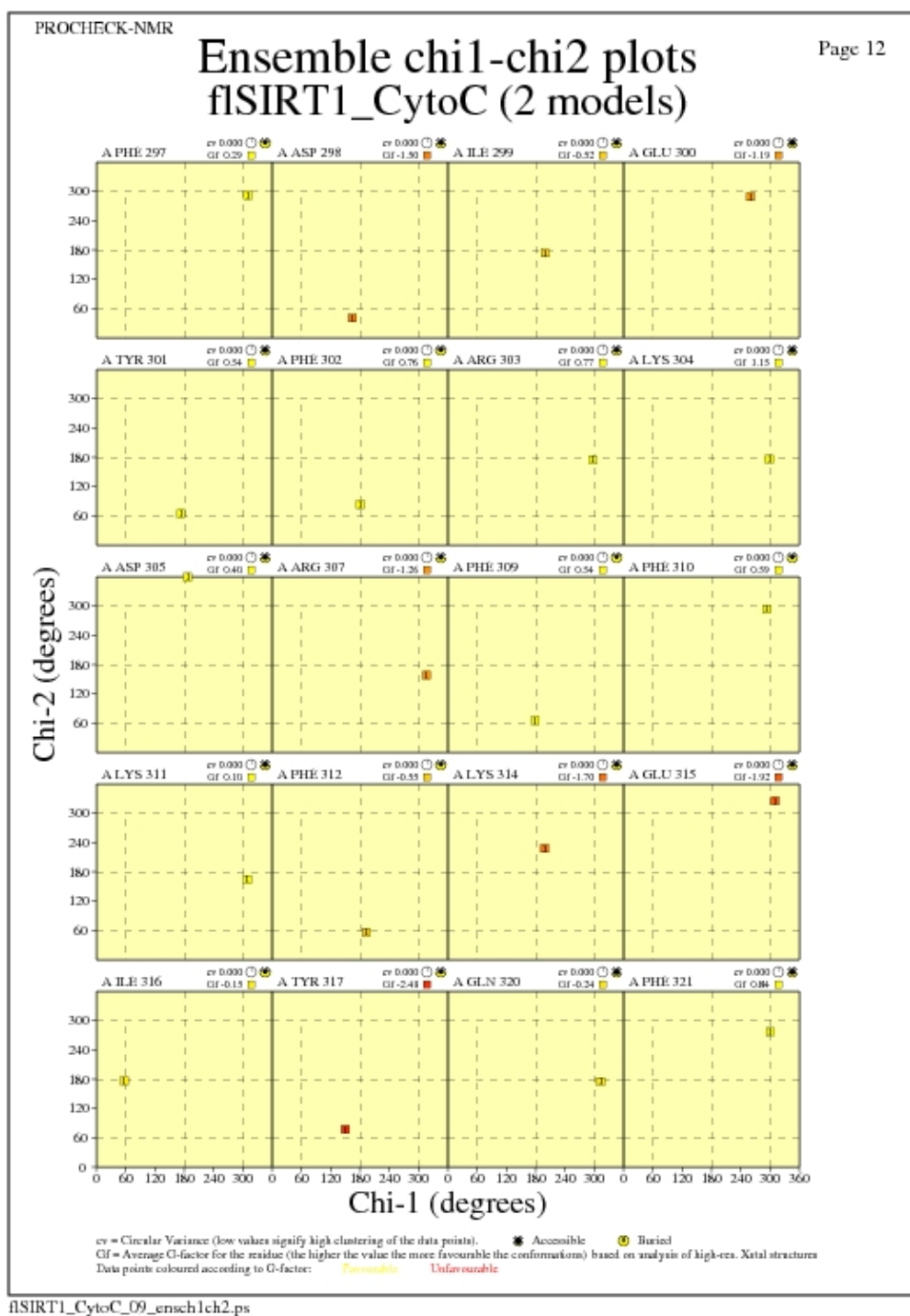
JPEG for residue Chi1-Chi2 Plots - page \$num_n



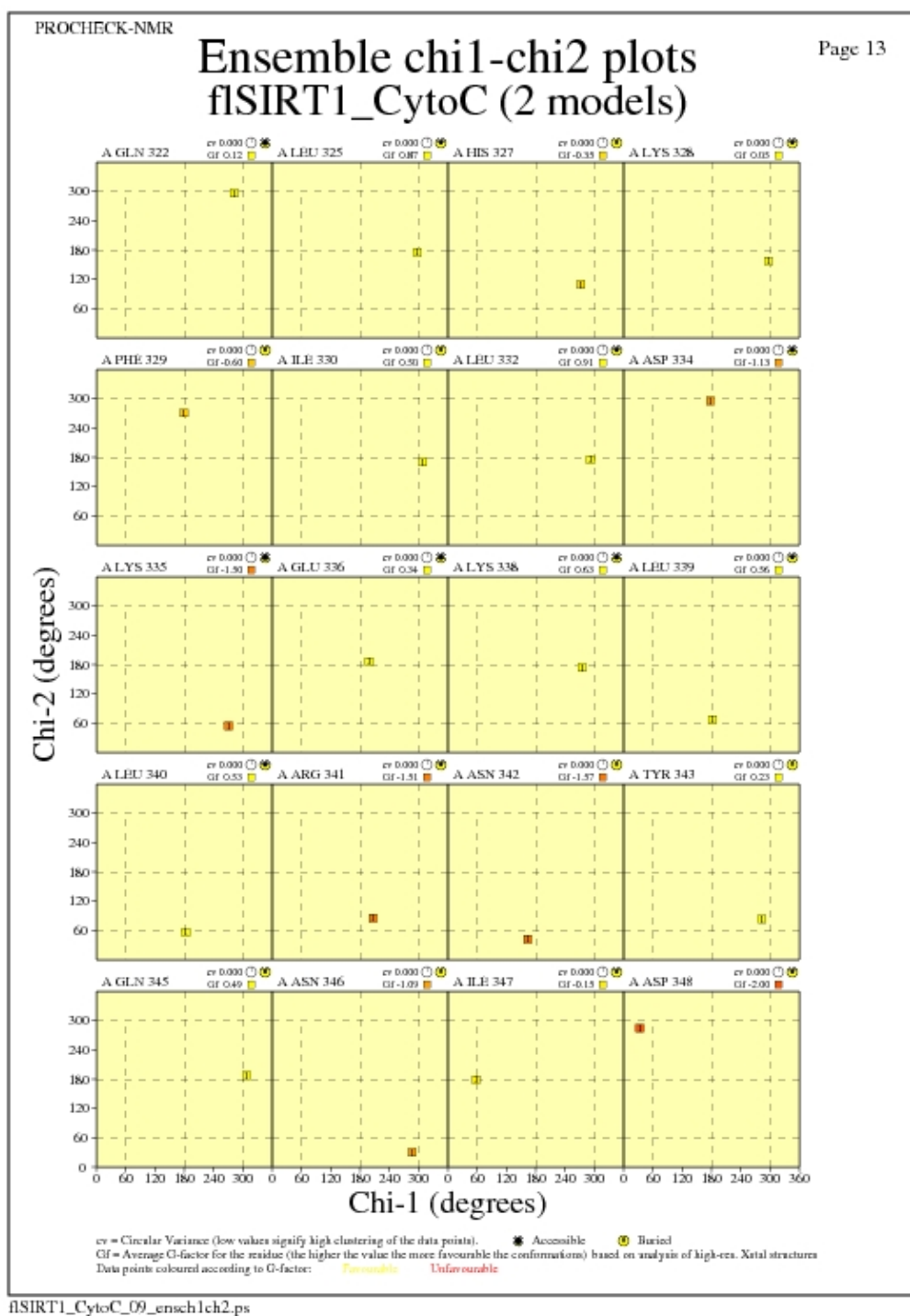
JPEG for residue Chi1-Chi2 Plots - page \$num_n



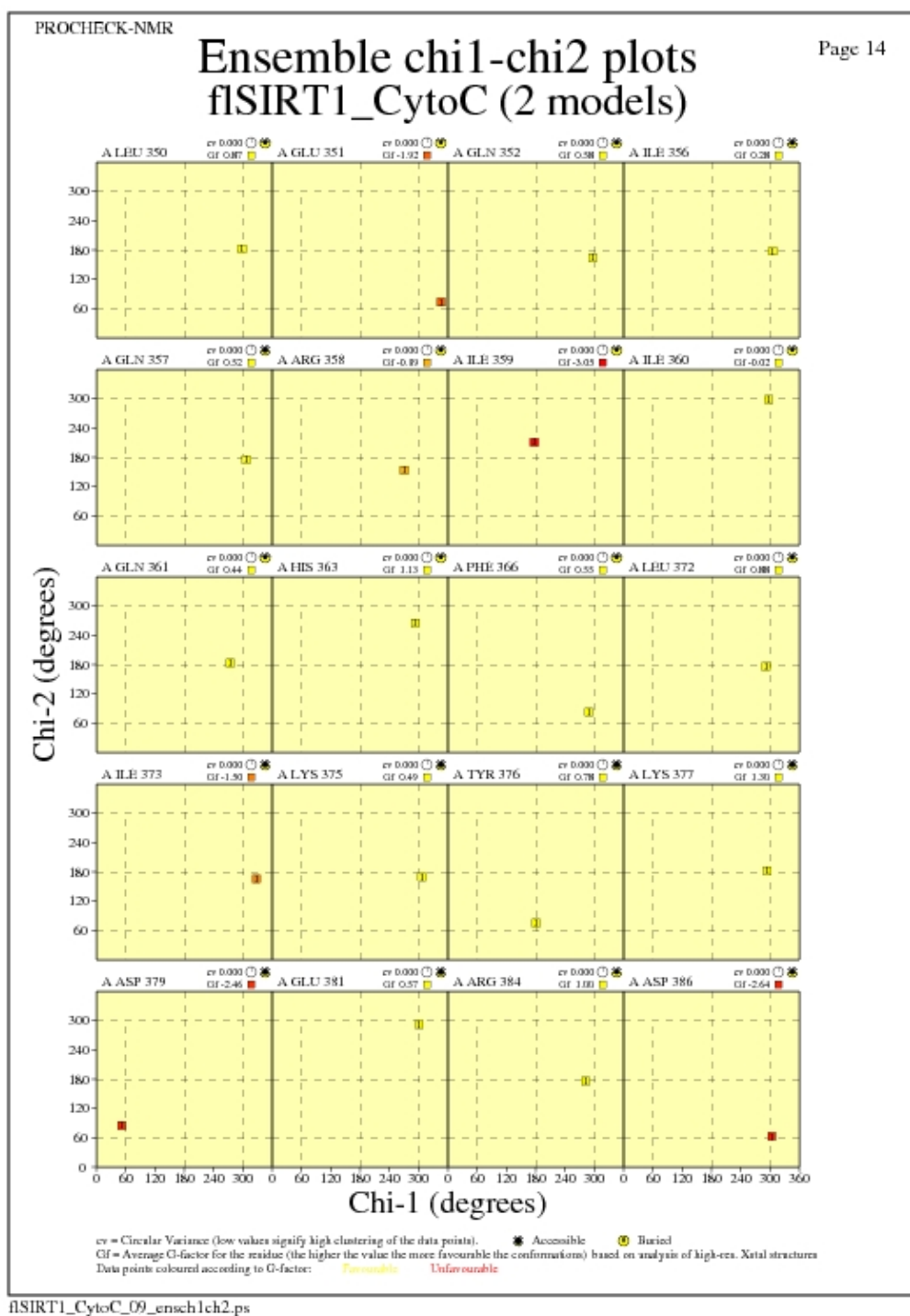
JPEG for residue Chi1-Chi2 Plots - page \$num_n



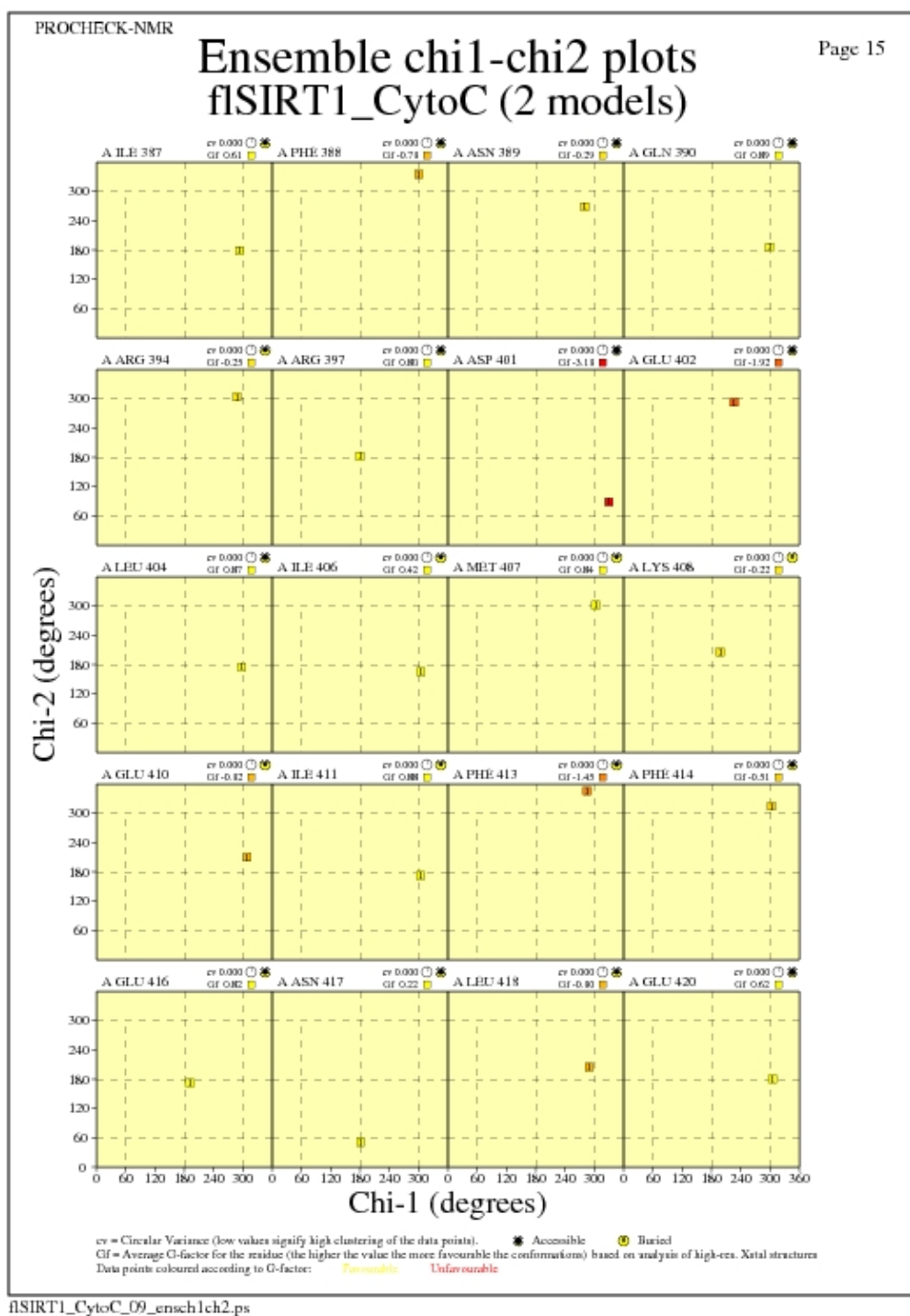
JPEG for residue Chi1-Chi2 Plots - page \$num_n



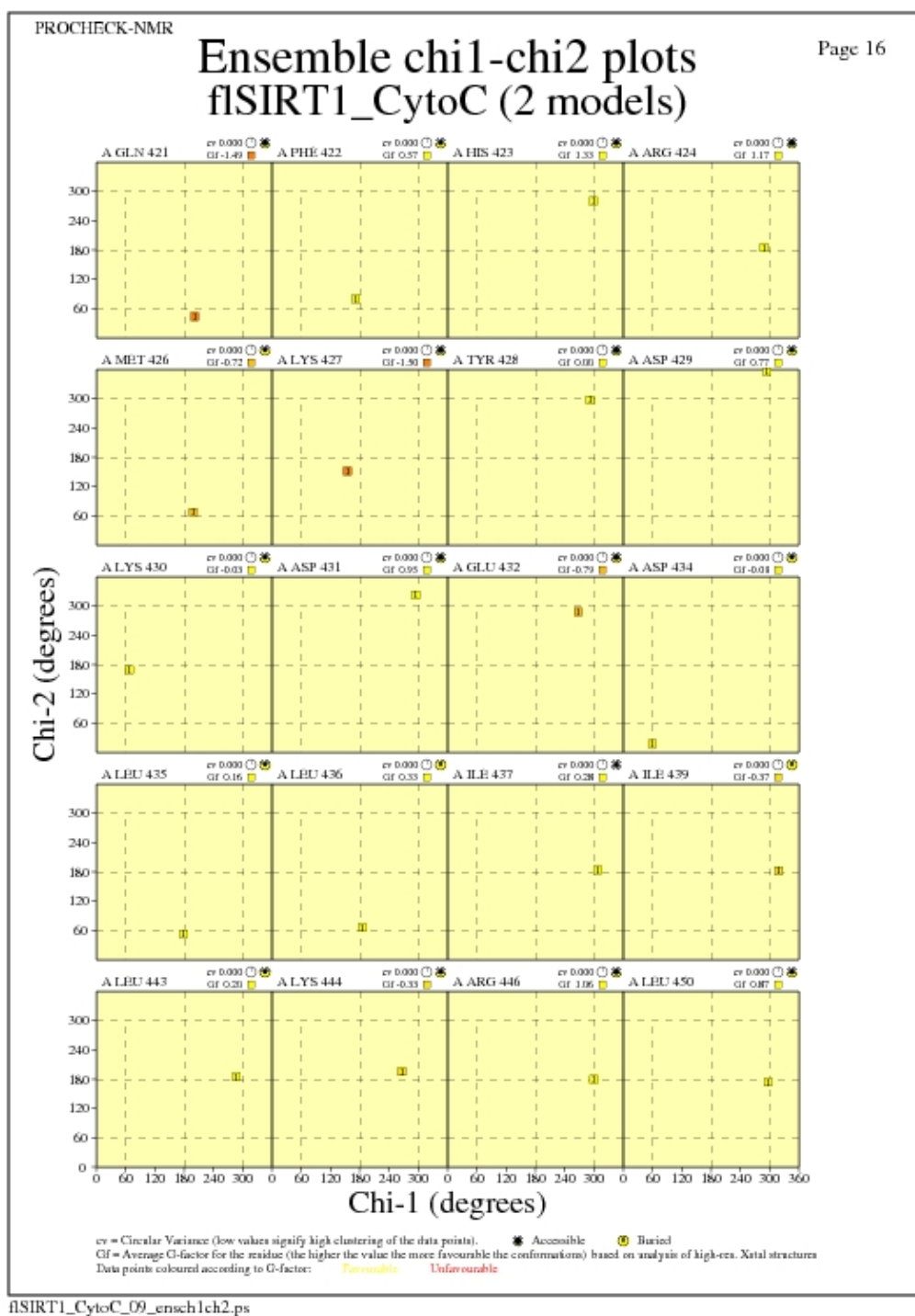
JPEG for residue Chi1-Chi2 Plots - page \$num_n



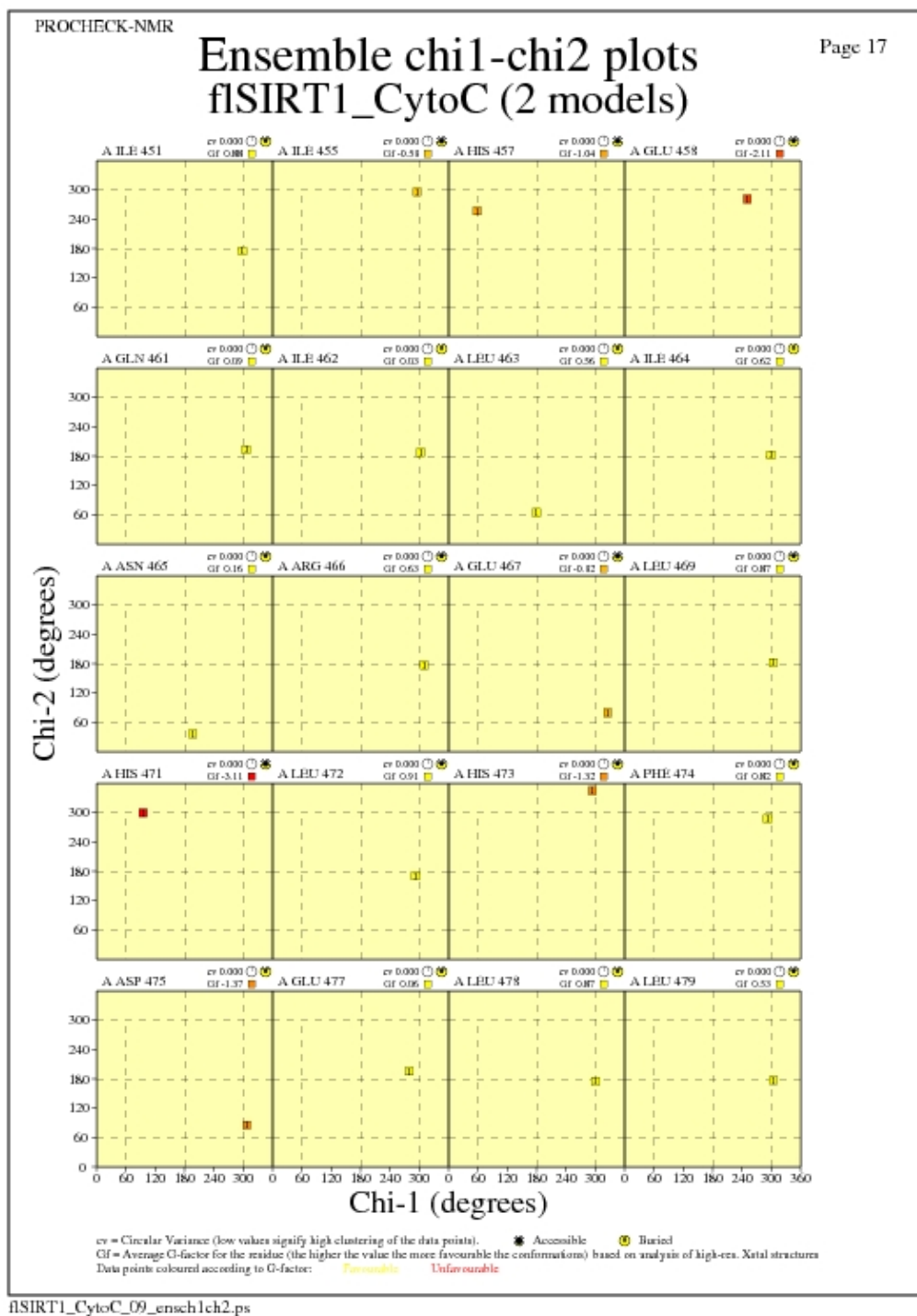
JPEG for residue Chi1-Chi2 Plots - page \$num_n



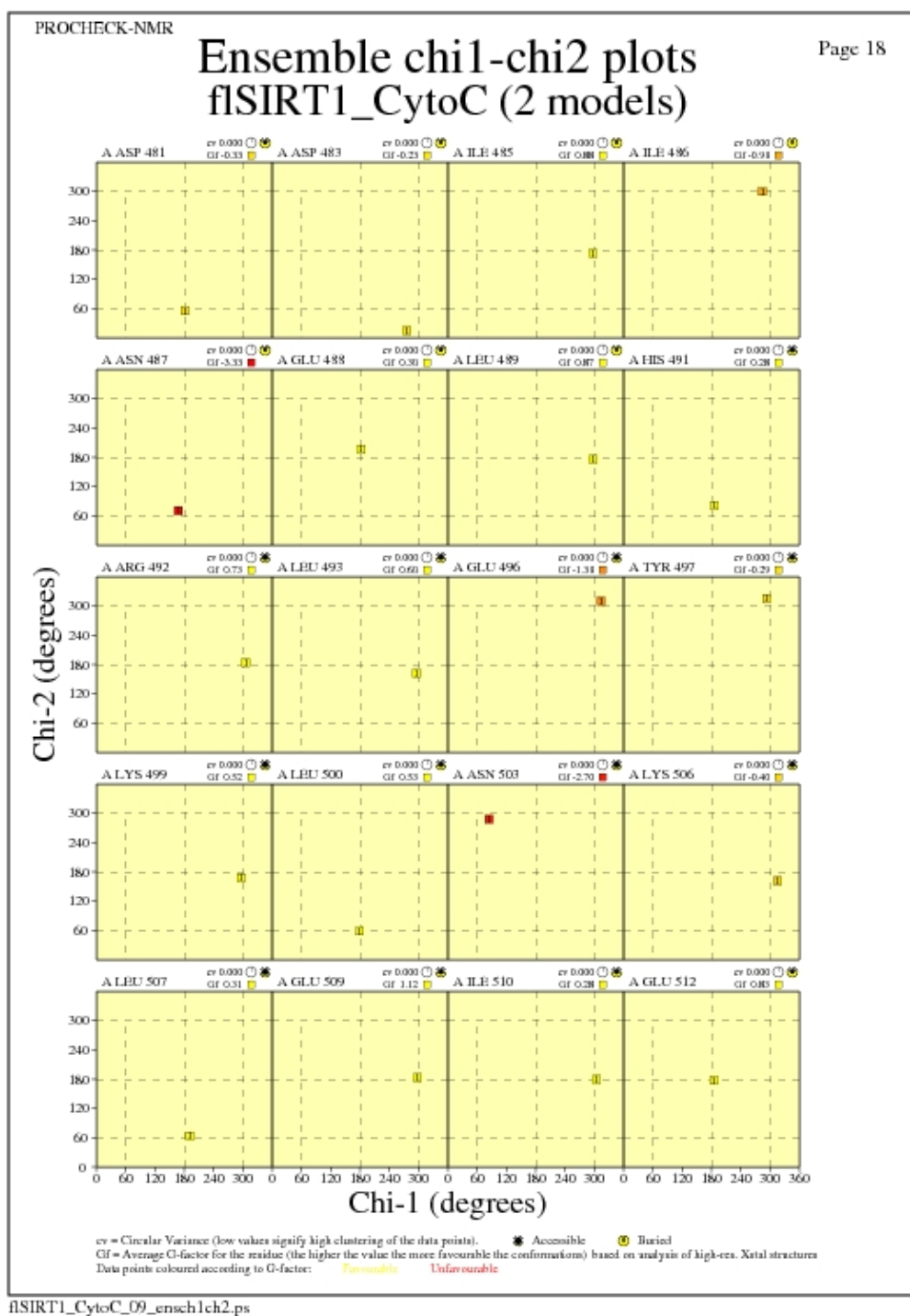
JPEG for residue Chi1-Chi2 Plots - page \$num_n



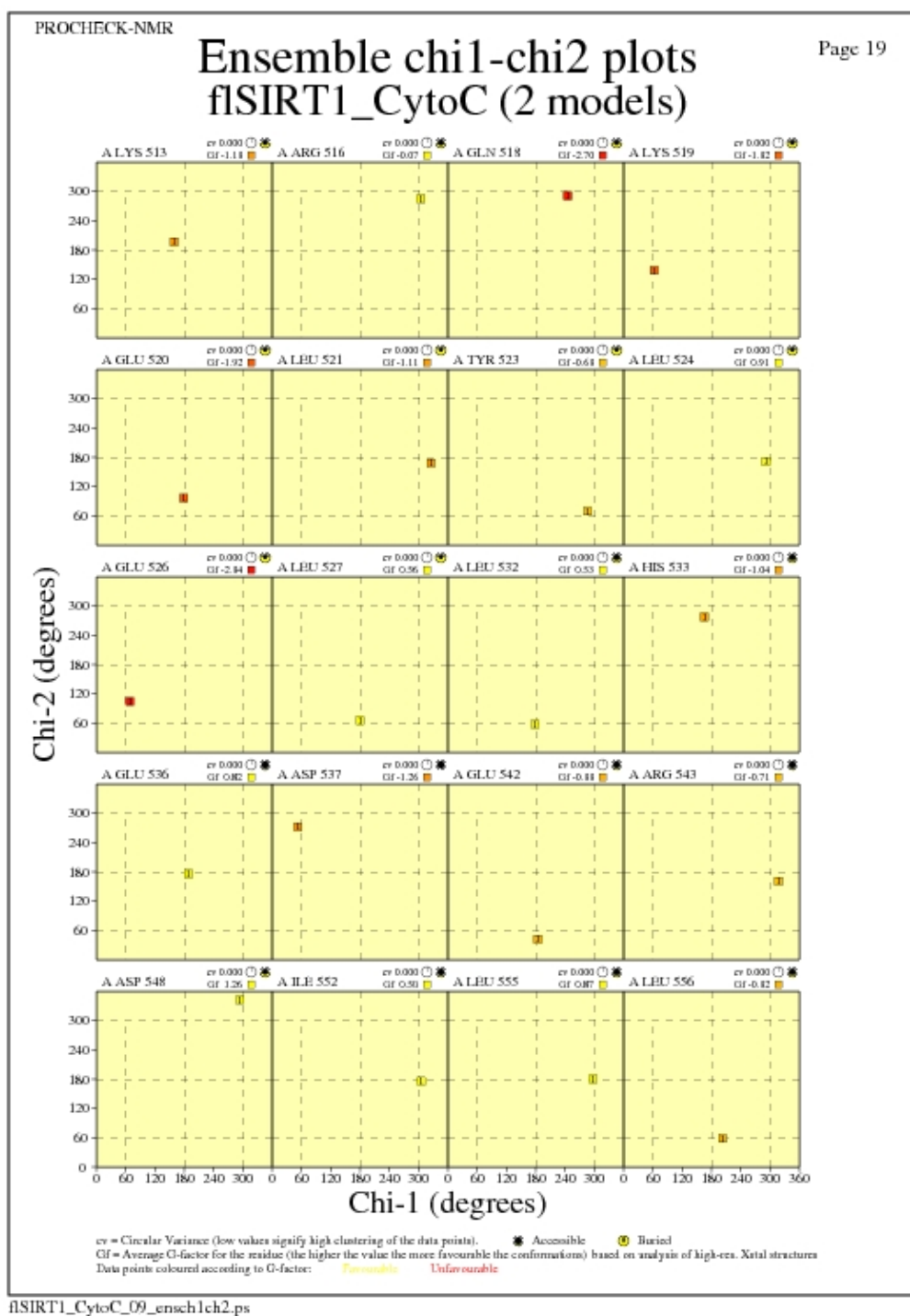
JPEG for residue Chi1-Chi2 Plots - page \$num_n



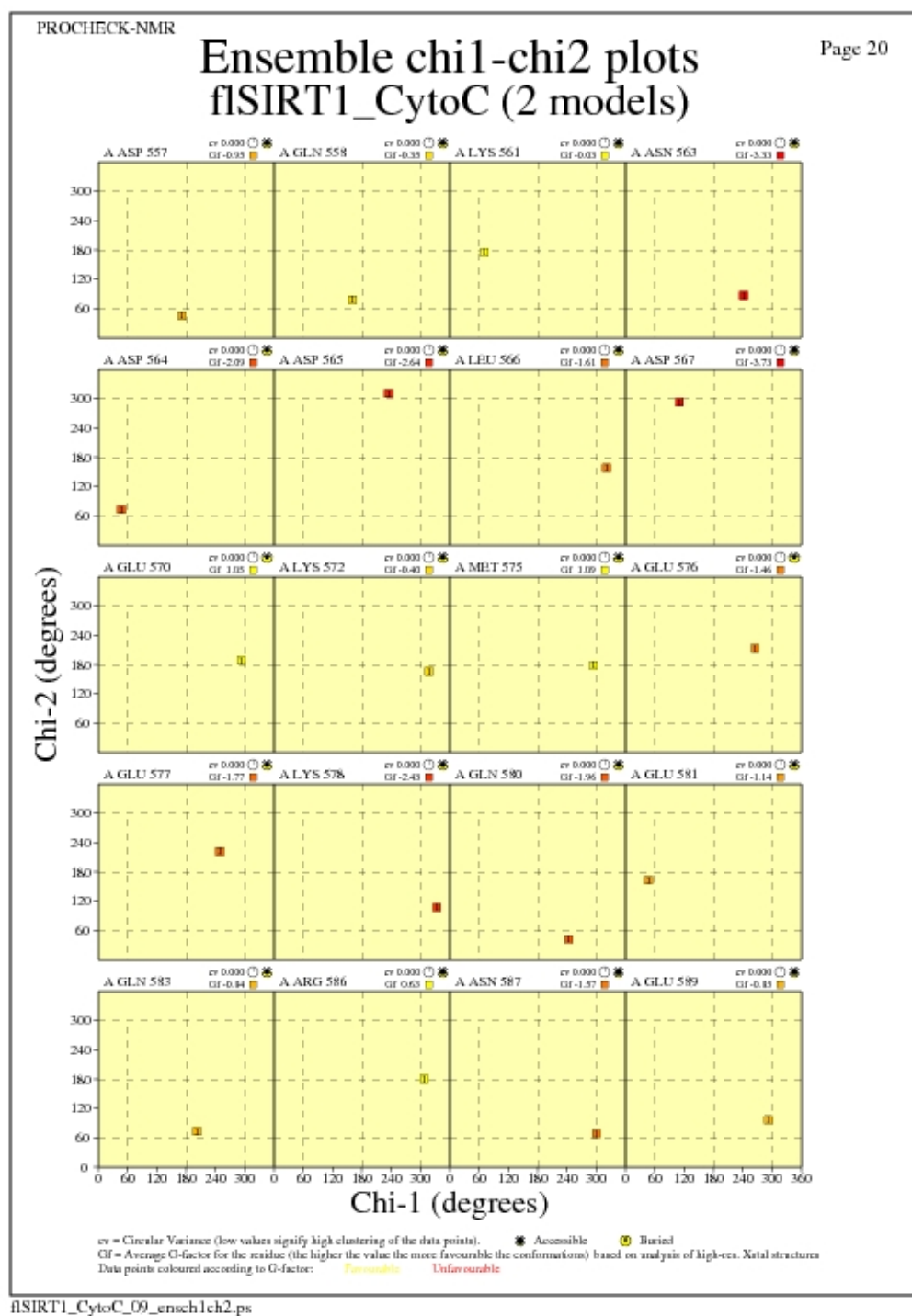
JPEG for residue Chi1-Chi2 Plots - page \$num_n



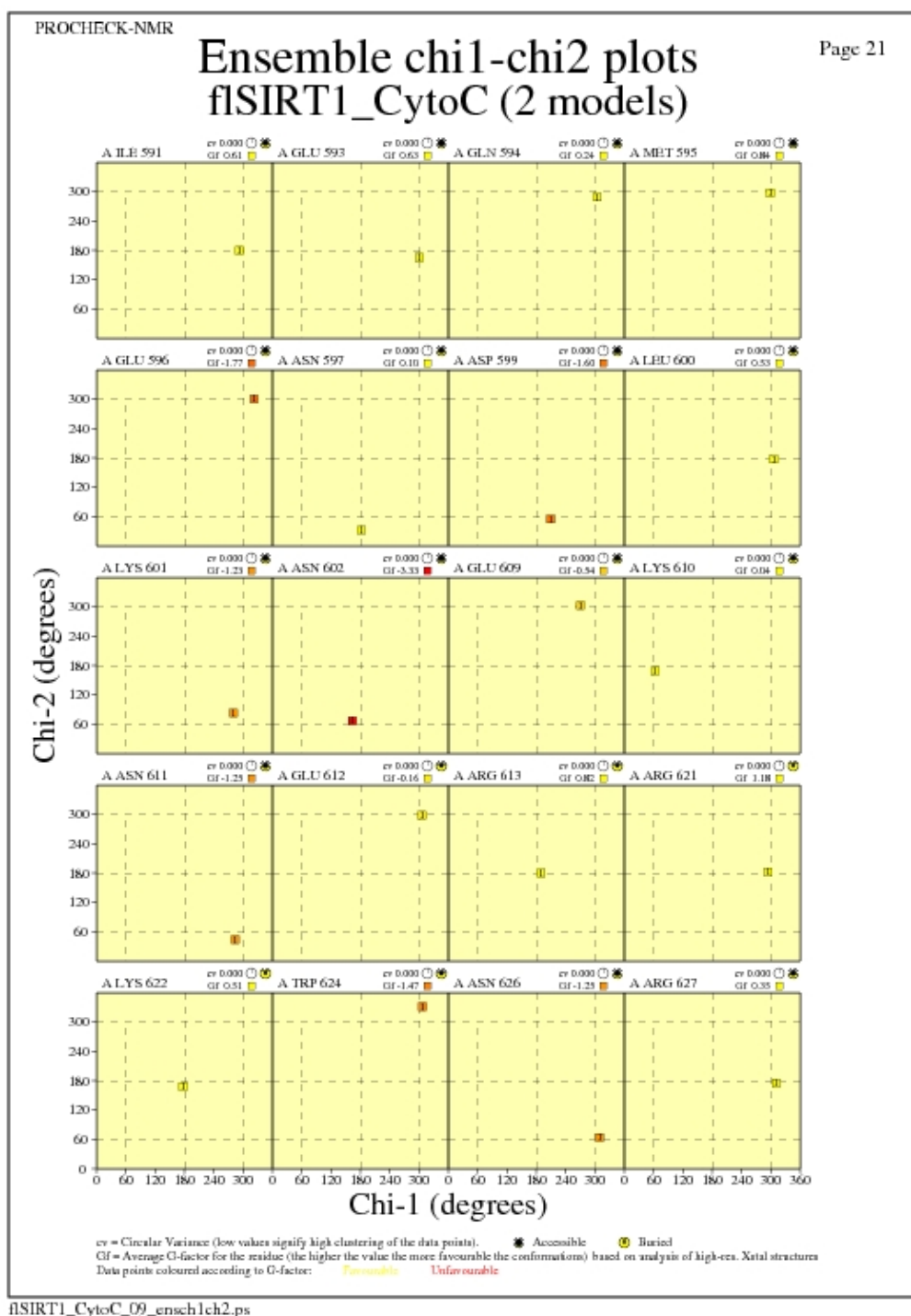
JPEG for residue Chi1-Chi2 Plots - page \$num_n



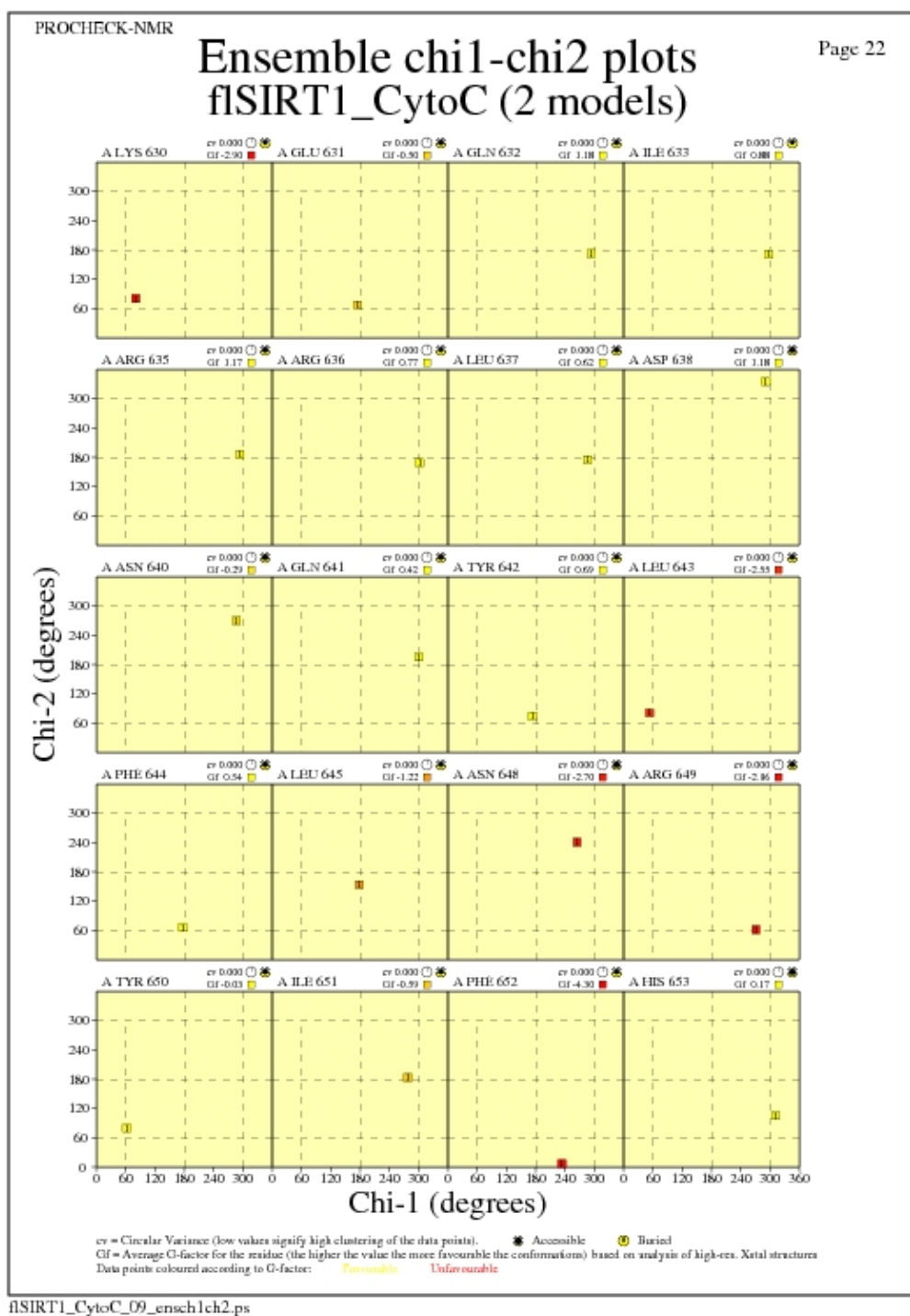
JPEG for residue Chi1-Chi2 Plots - page \$num_n



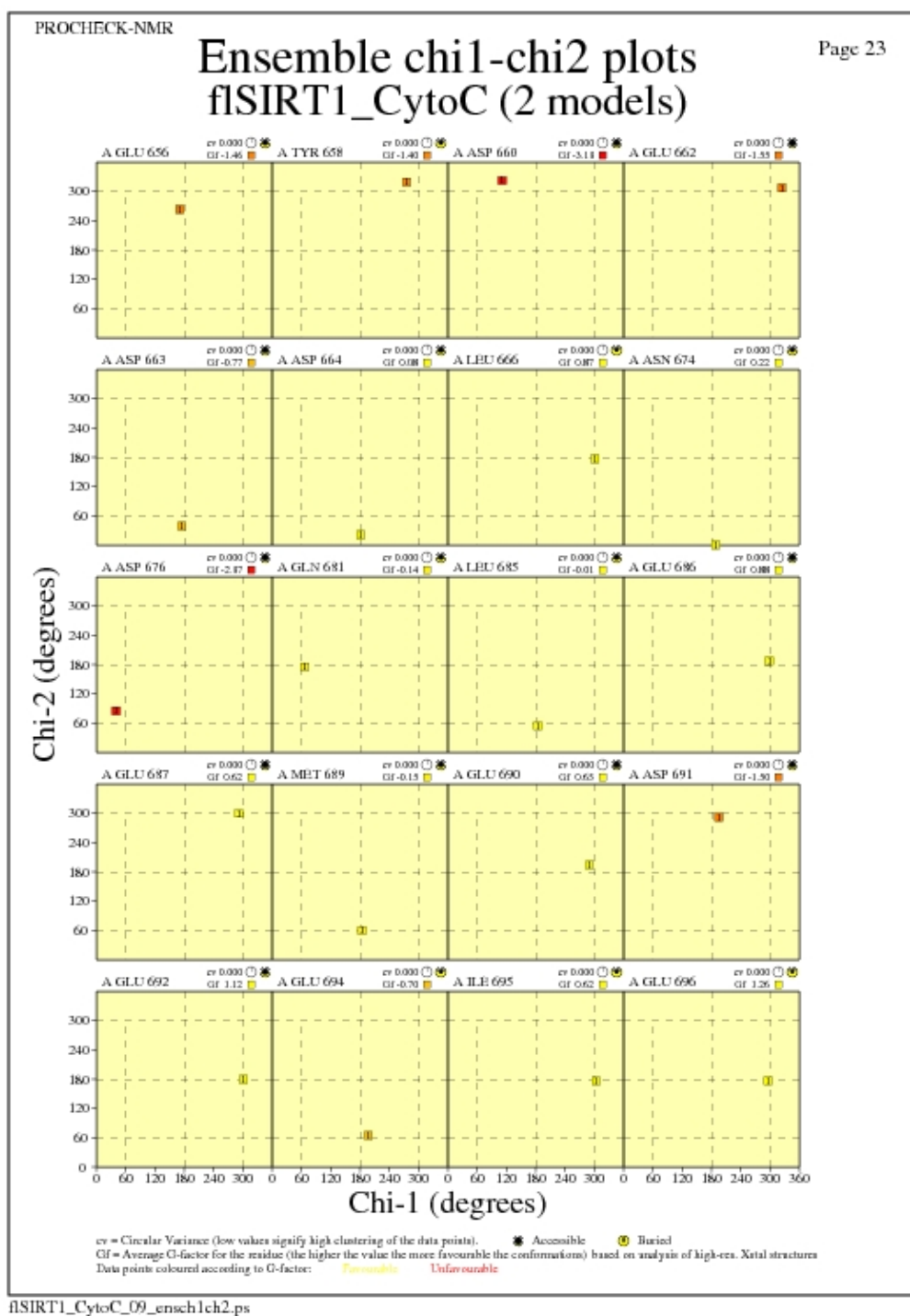
JPEG for residue Chi1-Chi2 Plots - page \$num_n



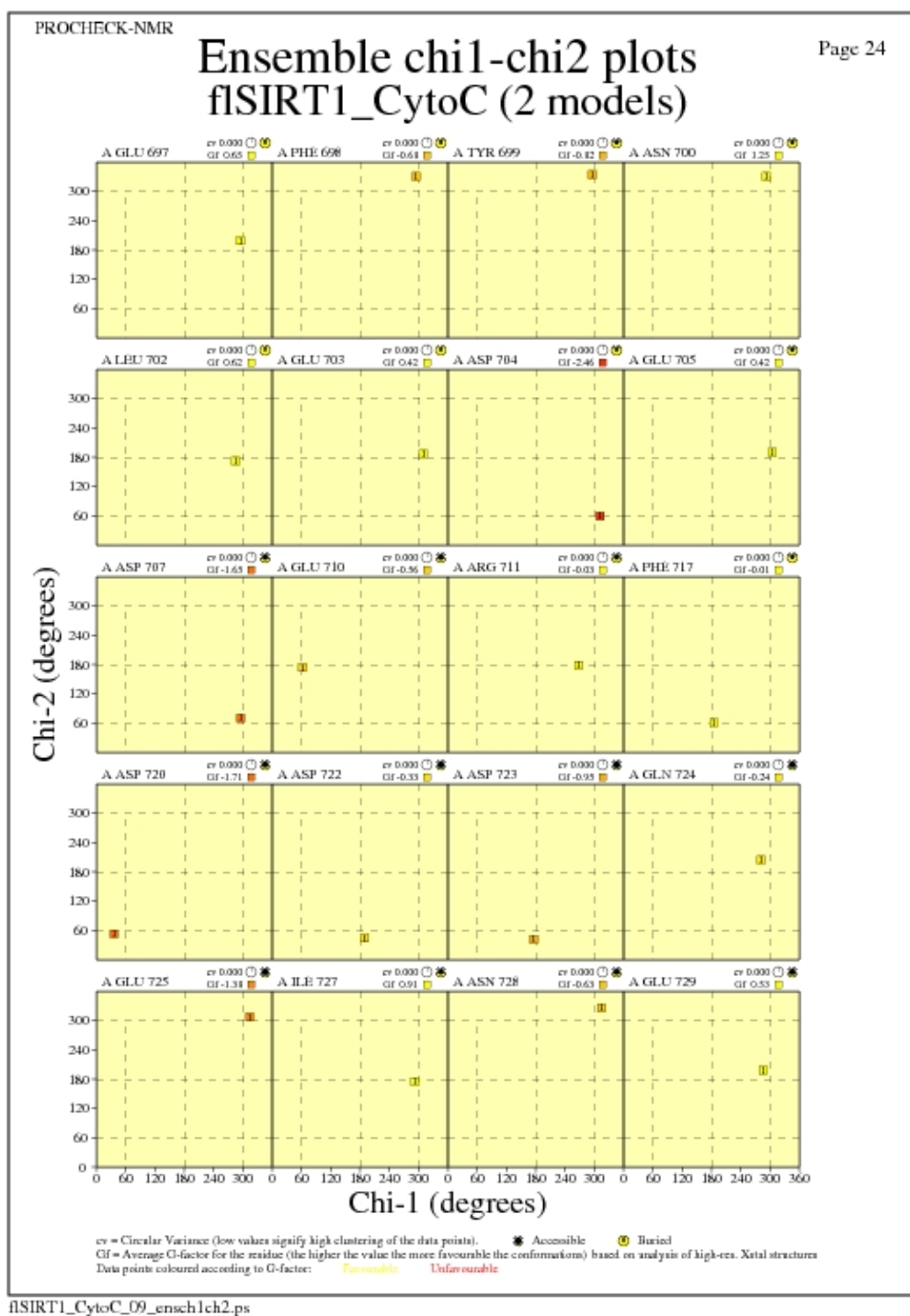
JPEG for residue Chi1-Chi2 Plots - page \$num_n



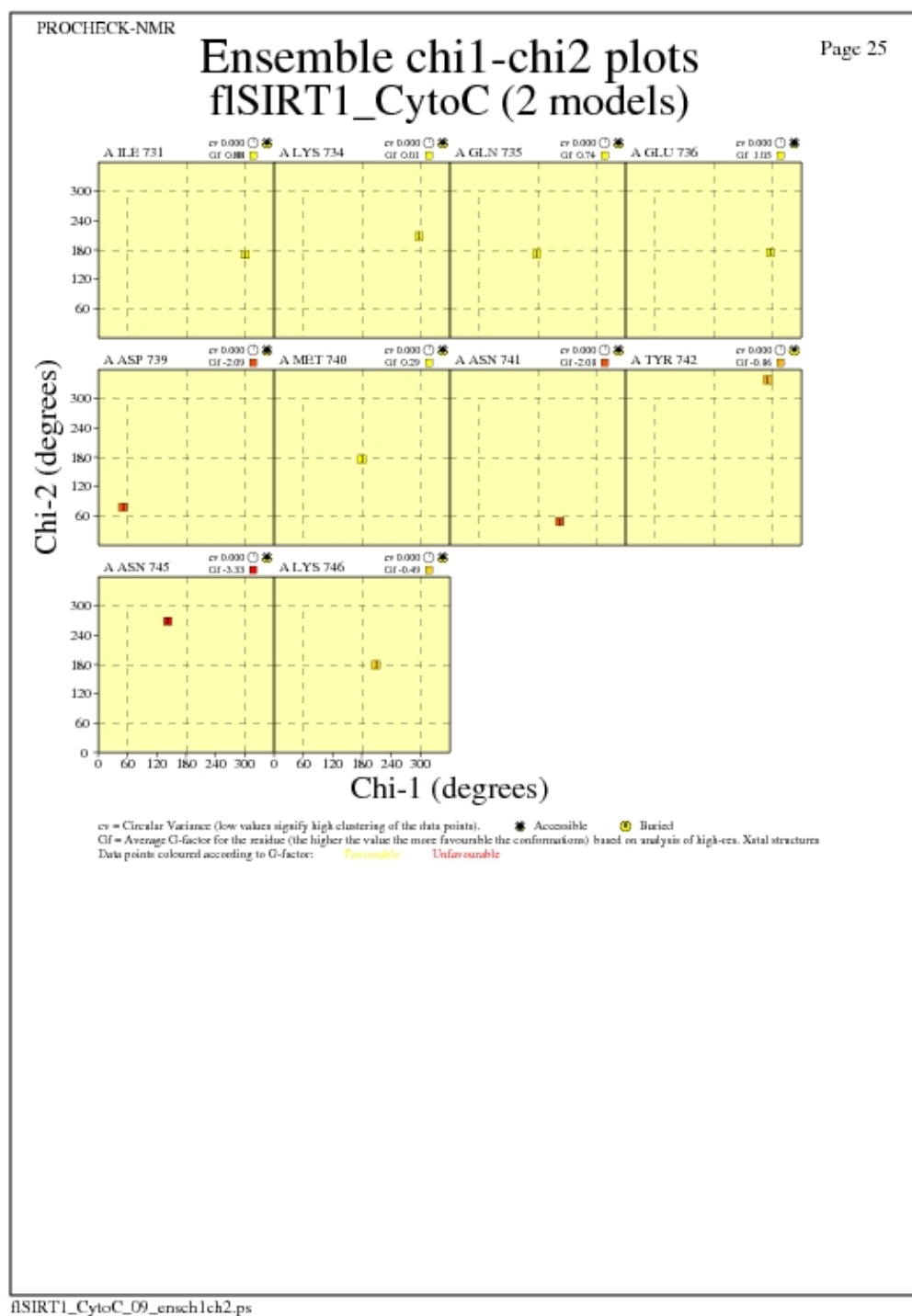
JPEG for residue Chi1-Chi2 Plots - page \$num_n



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



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

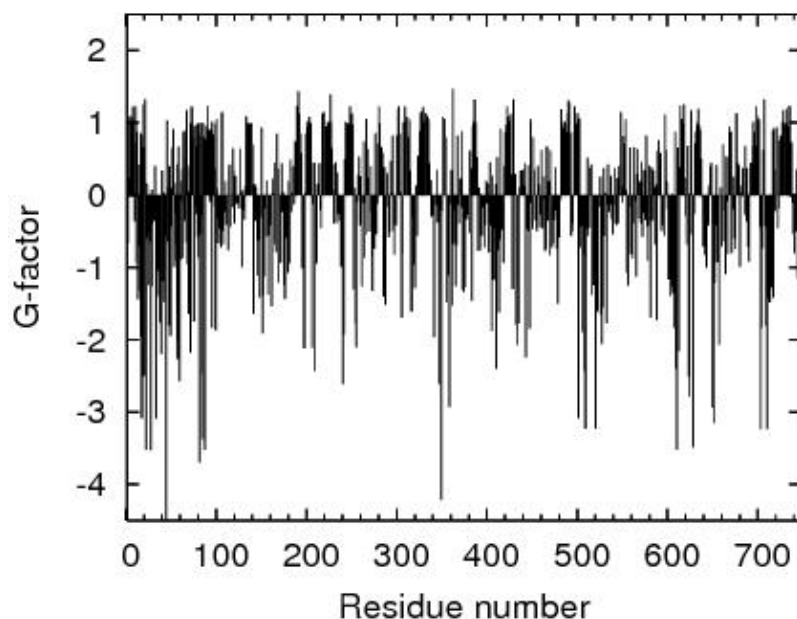


Table of Procheck G-factors for phi-psi for ordered residues

No ordered residues found for phipsi_gfactor.

Procheck G-factors for all dihedral angles for each residue

JPEG image for residue all dihedral G-factors

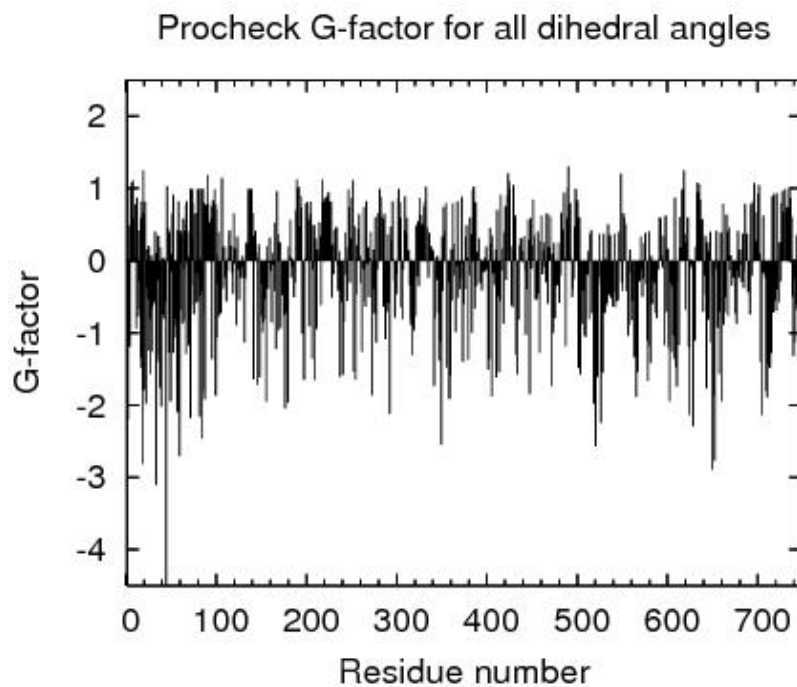


Table of Procheck G-factors for all dihedrals for ordered residues

No ordered residues found for alldih_gfactor.

Output from Verify3D

Verify3D Score over a window of \$wsize_s residues

JPEG image for Verify3D Score

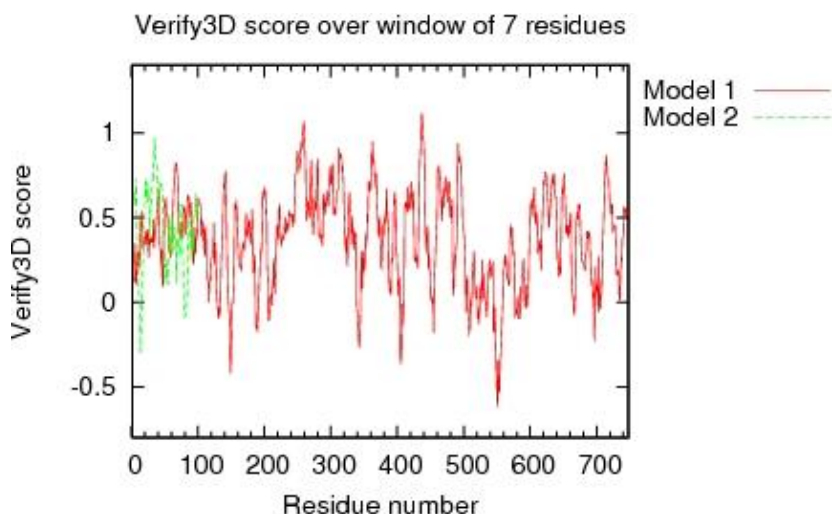


Table of Verify3D scores for ordered residues across all models

No ordered residues found for verify3d.

Output from Prosall

Prosall Score over a window of \$wsize_s residues

JPEG image for Prosall Score

Table of Verify3D scores for ordered residues across all models

No ordered residues found for verify3d.

Output from MolProbity

VdW violations from MAGE

JPEG image for MAGE VdW violation

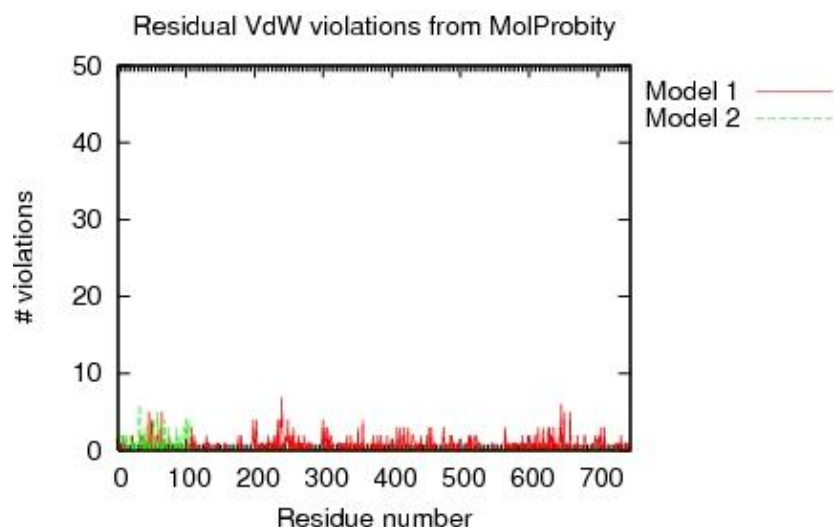


Table of MAGE VdW violations for ordered residues across all models

No ordered residues found for mage_clash.

List of bad contacts calculated by MAGE for model \$num_n

/farm/software/bin/probe

: 11242:A 647 PRO HA	:A 660 ASP 1HB	: -0.952:	0
: 11242:A 647 PRO HA	:A 660 ASP CB	: -0.949:	0
: 11242:A 660 ASP CA	:A 647 PRO HA	: -0.552:	0
: 11242:A 661 SER CB	:A 647 PRO 2HD	: -0.523:	0
: 11242:A 661 SER OG	:A 647 PRO 2HD	: -0.454:	0
: 11242:A 648 ASN H	:A 660 ASP 1HB	: -0.453:	0
: 11242:A 660 ASP 1HB	:A 647 PRO CA	: -0.434:	0
: 11242:A 614 THR HA	:A 706 PRO 1HG	: -0.931:	0
: 11242:A 706 PRO 1HG	:A 614 THR CA	: -0.678:	0
: 11242:A 706 PRO CG	:A 614 THR HA	: -0.644:	0
: 11242:A 565 ASP HA	:A 516 ARG NH2	: -0.847:	0
: 11242:A 565 ASP HA	:A 516 ARG 2HH2	: -0.488:	0
: 11242:A 245 ASP 2HB	:A 240 ILE HA	: -0.792:	0
: 11242:A 249 LEU 1HD1	:A 240 ILE 1HG2	: -0.673:	0
: 11242:A 476 VAL HB	:A 240 ILE 2HG1	: -0.643:	0
: 11242:A 240 ILE HA	:A 245 ASP CB	: -0.630:	0
: 11242:A 435 LEU 3HD1	:A 249 LEU 3HD1	: -0.551:	0
: 11242:A 462 ILE 1HG1	:A 476 VAL 2HG1	: -0.531:	0
: 11242:A 242 THR H	:A 240 ILE C	: -0.493:	0
: 11242:A 475 ASP 1HB	:A 240 ILE 1HD1	: -0.475:	0
: 11242:A 476 VAL 1HG1	:A 246 ALA 2HB	: -0.459:	0
: 11242:A 249 LEU 3HD2	:A 249 LEU HA	: -0.417:	0
: 11242:A 475 ASP 1HB	:A 240 ILE CD1	: -0.401:	0
: 11242:A 412 VAL 1HG1	:A 418 LEU 3HD2	: -0.758:	0
: 11242:A 412 VAL 1HG1	:A 418 LEU CD2	: -0.477:	0
: 11242:A 418 LEU 1HB	:A 423 HIS NE2	: -0.448:	0
: 11242:A 412 VAL 1HG2	:A 419 PRO 2HD	: -0.432:	0
: 11242:A 512 GLU 1HB	:A 526 GLU 2HB	: -0.742:	0

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: 11242:A 569 SER H	:A 572 LYS 1HD	: -0.713:	0
: 11242:A 203 LYS 2HD	:A 200 THR HA	: -0.689:	0
: 11242:A 217 ASP CG	:A 199 ARG 1HH2	: -0.634:	0
: 11242:A 199 ARG NH1	:A 199 ARG 1HB	: -0.496:	0
: 11242:A 203 LYS NZ	:A 204 ASP OD2	: -0.464:	0
: 11242:A 199 ARG O	:A 203 LYS 2HB	: -0.450:	0
: 11242:A 204 ASP CG	:A 203 LYS NZ	: -0.439:	0
: 11242:A 280 TYR HE2	:A 274 ARG CZ	: -0.663:	0
: 11242:A 234 ARG 2HD	:A 76 TRP HZ2	: -0.661:	0
: 11242:A 234 ARG 1HH2	:A 230 GLU CD	: -0.564:	0
: 11242:A 91 GLU CD	:A 234 ARG 2HH2	: -0.544:	0
: 11242:A 234 ARG 2HD	:A 76 TRP CZ2	: -0.419:	0
: 11242:A 57 GLU CD	:A 65 ARG 2HH2	: -0.647:	0
: 11242:A 65 ARG 1HH2	:A 9 LEU 1HB	: -0.588:	0
: 11242:A 60 VAL O	:A 57 GLU 1HG	: -0.519:	0
: 11242:A 9 LEU 1HB	:A 65 ARG NH2	: -0.433:	0
: 11242:A 65 ARG 1HH1	:A 65 ARG 1HD	: -0.420:	0
: 11242:A 61 PRO 2HD	:A 60 VAL HA	: -0.408:	0
: 11242:A 283 LEU HG	:A 279 ILE O	: -0.640:	0
: 11242:A 50 GLU 1HG	:A 73 ALA 1HB	: -0.635:	0
: 11242:A 237 ARG 2HD	:A 239 ASP CB	: -0.608:	0
: 11242:A 237 ARG 1HG	:A 51 PRO 1HD	: -0.524:	0
: 11242:A 51 PRO 1HG	:A 239 ASP OD2	: -0.507:	0
: 11242:A 46 ARG 2HH2	:A 239 ASP CG	: -0.497:	0
: 11242:A 46 ARG 2HD	:A 518 GLN OE1	: -0.462:	0
: 11242:A 51 PRO 2HB	:A 46 ARG 1HG	: -0.445:	0
: 11242:A 51 PRO 2HD	:A 50 GLU HA	: -0.428:	0
: 11242:A 237 ARG 1HH2	:A 50 GLU CD	: -0.419:	0
: 11242:A 50 GLU CD	:A 237 ARG HE	: -0.418:	0
: 11242:A 46 ARG 1HH1	:A 46 ARG 2HD	: -0.414:	0
: 11242:A 695 ILE HA	:A 698 PHE CD2	: -0.625:	0
: 11242:A 591 ILE 3HG2	:A 651 ILE 3HG2	: -0.614:	0
: 11242:A 588 VAL O	:A 591 ILE HB	: -0.509:	0
: 11242:A 645 LEU 2HD1	:A 651 ILE 2HD1	: -0.500:	0
: 11242:A 651 ILE HA	:A 594 GLN 2HG	: -0.475:	0
: 11242:A 645 LEU 3HD2	:A 646 PRO O	: -0.469:	0
: 11242:A 658 TYR O	:A 645 LEU 2HD2	: -0.451:	0
: 11242:A 651 ILE 3HD1	:A 651 ILE 1HG2	: -0.448:	0
: 11242:A 356 ILE 2HD1	:A 351 GLU 2HB	: -0.613:	0
: 11242:A 351 GLU CD	:A 351 GLU H	: -0.494:	0
: 11242:A 380 CYS 2HB	:A 366 PHE O	: -0.595:	0
: 11242:A 380 CYS O	:A 384 ARG 2HG	: -0.488:	0
: 11242:A 381 GLU CD	:A 384 ARG 1HH1	: -0.449:	0
: 11242:A 548 ASP HA	:A 509 GLU 1HG	: -0.591:	0
: 11242:A 408 LYS 2HE	:A 409 PRO O	: -0.587:	0
: 11242:A 416 GLU OE2	:A 408 LYS NZ	: -0.445:	0
: 11242:A 416 GLU OE1	:A 408 LYS NZ	: -0.427:	0
: 11242:A 527 LEU 3HD1	:A 484 VAL HB	: -0.574:	0

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: 11242:A 252 GLU 1HG	:A 248 LYS O	: -0.570:	0
: 11242:A 248 LYS NZ	:A 252 GLU CD	: -0.473:	0
: 11242:A 45 GLU CD	:A 36 ARG 2HH1	: -0.556:	0
: 11242:A 133 GLU 1HG	:A 36 ARG 1HB	: -0.556:	0
: 11242:A 300 GLU CD	:A 304 LYS 3HZ	: -0.554:	0
: 11242:A 40 ASP HA	:A 22 ARG NE	: -0.554:	0
: 11242:A 300 GLU CD	:A 304 LYS NZ	: -0.492:	0
: 11242:A 40 ASP HA	:A 22 ARG HE	: -0.444:	0
: 11242:A 300 GLU HA	:A 300 GLU OE2	: -0.404:	0
: 11242:A 671 CYS O	:A 681 GLN 1HG	: -0.553:	0
: 11242:A 682 SER OG	:A 681 GLN 2HG	: -0.547:	0
: 11242:A 682 SER OG	:A 671 CYS HA	: -0.503:	0
: 11242:A 708 VAL 2HG1	:A 710 GLU 1HG	: -0.552:	0
: 11242:A 515 PRO HA	:A 520 GLU 1HG	: -0.551:	0
: 11242:A 479 LEU 1HB	:A 524 LEU 3HD2	: -0.486:	0
: 11242:A 524 LEU H	:A 513 LYS 2HB	: -0.482:	0
: 11242:A 513 LYS NZ	:A 520 GLU OE2	: -0.443:	0
: 11242:A 341 ARG 1HH1	:A 358 ARG 1HG	: -0.546:	0
: 11242:A 358 ARG 1HG	:A 341 ARG NH1	: -0.475:	0
: 11242:A 334 ASP O	:A 358 ARG NH2	: -0.457:	0
: 11242:A 358 ARG 1HD	:A 339 LEU O	: -0.415:	0
: 11242:A 335 LYS 2HD	:A 331 ALA O	: -0.545:	0
: 11242:A 335 LYS NZ	:A 355 GLY O	: -0.510:	0
: 11242:A 633 ILE 3HD1	:A 617 ALA HA	: -0.541:	0
: 11242:A 455 ILE 2HD1	:A 433 VAL 1HG1	: -0.541:	0
: 11242:A 633 ILE 2HD1	:A 630 LYS HA	: -0.530:	0
: 11242:A 454 SER OG	:A 451 ILE HA	: -0.487:	0
: 11242:A 630 LYS C	:A 630 LYS 1HD	: -0.438:	0
: 11242:A 455 ILE 1HG1	:A 451 ILE O	: -0.415:	0
: 11242:A 456 PRO 2HD	:A 455 ILE HA	: -0.404:	0
: 11242:A 697 GLU OE1	:A 622 LYS 2HG	: -0.540:	0
: 11242:A 693 SER O	:A 697 GLU 2HG	: -0.429:	0
: 11242:A 496 GLU HA	:A 499 LYS 1HD	: -0.537:	0
: 11242:A 58 ARG 1HH2	:A 589 GLU CD	: -0.535:	0
: 11242:A 34 ARG 2HH1	:A 134 GLU CD	: -0.533:	0
: 11242:A 127 ASP HA	:A 34 ARG 2HB	: -0.516:	0
: 11242:A 510 ILE 2HG1	:A 508 SER 1HB	: -0.521:	0
: 11242:A 576 GLU CD	:A 734 LYS 1HZ	: -0.521:	0
: 11242:A 696 GLU OE1	:A 734 LYS NZ	: -0.417:	0

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: 11242:A 232 PRO 1HG :A 67 CYS SG : -0.514: 0
: 11242:A 704 ASP CG :A 621 ARG HE : -0.514: 0
: 11242:A 628 VAL 2HG2 :A 624 TRP O : -0.499: 0
: 11242:A 636 ARG 1HH2 :A 632 GLN 2HB : -0.491: 0
: 11242:A 632 GLN O :A 636 ARG 2HG : -0.488: 0
: 11242:A 621 ARG NH2 :A 625 PRO 2HB : -0.479: 0
: 11242:A 621 ARG 1HG :A 628 VAL 3HG2 : -0.464: 0
: 11242:A 232 PRO 2HD :A 231 PRO HA : -0.455: 0
: 11242:A 636 ARG CZ :A 628 VAL 2HG1 : -0.428: 0
: 11242:A 259 LEU 2HD1 :A 438 VAL 2HG2 : -0.504: 0
: 11242:A 308 PRO HA :A 311 LYS CD : -0.503: 0
: 11242:A 301 TYR OH :A 308 PRO 1HG : -0.491: 0
: 11242:A 311 LYS 2HG :A 307 ARG O : -0.485: 0
: 11242:A 307 ARG 1HH1 :A 307 ARG 1HD : -0.457: 0
: 11242:A 492 ARG 1HD :A 247 VAL 1HG2 : -0.496: 0
: 11242:A 108 GLN 2HE2 :A 108 GLN HA : -0.495: 0
: 11242:A 108 GLN HA :A 102 ASP OD1 : -0.414: 0
: 11242:A 432 GLU CD :A 255 LYS 3HZ : -0.489: 0
: 11242:A 255 LYS NZ :A 432 GLU OE2 : -0.418: 0
: 11242:A 703 GLU 2HB :A 618 GLY 1HA : -0.483: 0
: 11242:A 669 SER 1HB :A 703 GLU 2HB : -0.409: 0
: 11242:A 731 ILE 2HG1 :A 727 ILE O : -0.481: 0
: 11242:A 566 LEU H :A 566 LEU HG : -0.481: 0
: 11242:A 652 PHE 2HB :A 566 LEU 2HB : -0.415: 0
: 11242:A 132 GLU CD :A 38 ARG HE : -0.479: 0
: 11242:A 1 MET 2HB :A 59 GLU 2HG : -0.477: 0
: 11242:A 1 MET CB :A 59 GLU 2HG : -0.445: 0
: 11242:A 4 GLU CD :A 181 ARG 1HH1 : -0.476: 0
: 11242:A 8 ALA 2HB :A 181 ARG HA : -0.445: 0
: 11242:A 599 ASP O :A 601 LYS 1HD : -0.475: 0
: 11242:A 599 ASP CG :A 601 LYS NZ : -0.402: 0
: 11242:A 7 LEU HG :A 3 ASP O : -0.474: 0
: 11242:A 431 ASP OD1 :A 430 LYS NZ : -0.473: 0
: 11242:A 430 LYS 1HZ :A 431 ASP CG : -0.469: 0
: 11242:A 243 ILE 1HG2 :A 488 GLU OE2 : -0.472: 0
: 11242:A 528 PRO 1HG :A 488 GLU HA : -0.464: 0
: 11242:A 224 VAL 3HG2 :A 220 LEU O : -0.471: 0
: 11242:A 223 ILE 2HD1 :A 220 LEU 3HD2 : -0.417: 0
: 11242:A 607 THR HA :A 638 ASP OD1 : -0.470: 0
: 11242:A 486 ILE 2HG1 :A 326 CYS SG : -0.470: 0

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: 11242:A 486 ILE 3HD1	:A 489 LEU 2HD1	:	-0.429:	0
: 11242:A 303 ARG 1HH1	:A 303 ARG 1HD	:	-0.469:	0
: 11242:A 208 GLU 1HG	:A 146 LEU 2HD1	:	-0.469:	0
: 11242:A 303 ARG 2HG	:A 299 ILE O	:	-0.432:	0
: 11242:A 413 PHE 1HB	:A 299 ILE HB	:	-0.409:	0
: 11242:A 597 ASN HA	:A 600 LEU HG	:	-0.465:	0
: 11242:A 78 GLU CD	:A 77 ARG 1HH2	:	-0.465:	0
: 11242:A 610 LYS 2HB	:A 609 GLU HA	:	-0.465:	0
: 11242:A 609 GLU OE1	:A 610 LYS NZ	:	-0.434:	0
: 11242:A 410 GLU OE2	:A 377 LYS NZ	:	-0.462:	0
: 11242:A 490 CYS SG	:A 329 PHE HD1	:	-0.461:	0
: 11242:A 198 PRO 2HG	:A 221 TRP HE3	:	-0.461:	0
: 11242:A 198 PRO 2HD	:A 197 ASP HA	:	-0.401:	0
: 11242:A 429 ASP 2HB	:A 257 ILE 1HD1	:	-0.460:	0
: 11242:A 257 ILE 3HD1	:A 257 ILE 1HG2	:	-0.401:	0
: 11242:A 265 SER HA	:A 268 CYS SG	:	-0.454:	0
: 11242:A 114 PRO 2HD	:A 113 GLU HA	:	-0.454:	0
: 11242:A 655 ALA O	:A 650 TYR 1HB	:	-0.454:	0
: 11242:A 265 SER 1HB	:A 270 ILE 2HD1	:	-0.401:	0
: 11242:A 581 GLU OE2	:A 519 LYS NZ	:	-0.448:	0
: 11242:A 260 THR 2HG2	:A 264 VAL 1HG1	:	-0.448:	0
: 11242:A 740 MET O	:A 735 GLN 2HG	:	-0.447:	0
: 11242:A 273 PHE N	:A 272 ASP CG	:	-0.445:	0
: 11242:A 272 ASP OD2	:A 262 ALA 3HB	:	-0.408:	0
: 11242:A 253 CYS 2HB	:A 434 ASP OD1	:	-0.443:	0
: 11242:A 228 LEU 3HD1	:A 228 LEU HA	:	-0.440:	0
: 11242:A 711 ARG 1HH1	:A 705 GLU CD	:	-0.439:	0
: 11242:A 711 ARG 1HH1	:A 711 ARG 2HD	:	-0.401:	0
: 11242:A 420 GLU CD	:A 424 ARG 2HH2	:	-0.435:	0
: 11242:A 424 ARG 1HD	:A 424 ARG 1HH1	:	-0.411:	0
: 11242:A 95 THR 2HG2	:A 225 ILE 2HG2	:	-0.434:	0
: 11242:A 212 PRO 2HD	:A 211 PRO HA	:	-0.432:	0
: 11242:A 583 GLN OE1	:A 43 GLY 1HA	:	-0.432:	0
: 11242:A 394 ARG HA	:A 394 ARG 2HD	:	-0.428:	0
: 11242:A 282 ARG 2HG	:A 278 GLY O	:	-0.428:	0

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: 11242:A 443 LEU HA :A 443 LEU 3HD2 : -0.427: 0
: 11242:A 48 PRO 2HD :A 47 SER HA : -0.427: 0
: 11242:A 238 LYS NZ :A 458 GLU O : -0.426: 0
: 11242:A 238 LYS NZ :A 458 GLU CD : -0.416: 0
: 11242:A 238 LYS 2HZ :A 458 GLU CD : -0.412: 0
: 11242:A 314 LYS 2HG :A 388 PHE HD1 : -0.425: 0
: 11242:A 261 GLY 2HA :A 441 SER 2HB : -0.425: 0
: 11242:A 547 PRO 2HD :A 546 PRO HA : -0.424: 0
: 11242:A 742 TYR HA :A 743 PRO 2HD : -0.422: 0
: 11242:A 348 ASP OD1 :A 346 ASN 2HB : -0.421: 0
: 11242:A 37 PRO 2HB :A 24 ALA HA : -0.419: 0
: 11242:A 157 PHE CZ :A 148 PHE HA : -0.419: 0
: 11242:A 130 GLU OE2 :A 130 GLU HA : -0.418: 0
: 11242:A 103 ASN 1HD2 :A 110 PRO 2HD : -0.417: 0
: 11242:A 579 PRO 2HD :A 578 LYS HA : -0.417: 0
: 11242:A 360 ILE N :A 359 ILE 1HG1 : -0.416: 0
: 11242:A 373 ILE 3HD1 :A 373 ILE 1HG2 : -0.414: 0
: 11242:A 178 PRO 1HD :A 177 THR HA : -0.413: 0
: 11242:A 158 HIS HA :A 177 THR HB : -0.402: 0
: 11242:A 323 PRO 2HD :A 322 GLN HA : -0.410: 0
: 11242:A 399 PRO 1HB :A 401 ASP OD2 : -0.409: 0
: 11242:A 372 LEU 1HD1 :A 302 PHE HE2 : -0.408: 0
: 11242:A 403 PRO 1HD :A 402 GLU HA : -0.408: 0
: 11242:A 35 LYS 2HD :A 23 GLU HA : -0.406: 0
: 11242:A 112 ARG 1HH1 :A 112 ARG 1HD : -0.405: 0
: 11242:A 463 LEU 2HB :A 477 GLU 1HG : -0.404: 0
: 11242:A 605 SER HA :A 641 GLN HA : -0.403: 0
#sum2 ::19.30 clashscore : 19.30 clashscore B

```

List of bad contacts calculated by MAGE for model \$num_n

/farm/software/bin/probe

```

: 1657:A 70 ASN 2HB :A 73 LYS 2HD : -0.730: 0
: 1657:A 101 ALA HA :A 104 GLU 1HG : -0.682: 0
: 1657:A 3 VAL 3HG1 :A 97 TYR HD1 : -0.644: 0

```

VdW violations from MAGE

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: 1657:A 94 LEU O	:A 98 LEU HG	: -0.629:	0
: 1657:A 7 LYS 2HG	:A 97 TYR CZ	: -0.467:	0
: 1657:A 104 GLU CD	:A 100 LYS NZ	: -0.459:	0
: 1657:A 98 LEU HA	:A 101 ALA 3HB	: -0.426:	0
: 1657:A 100 LYS 2HZ	:A 104 GLU CD	: -0.417:	0
: 1657:A 101 ALA 2HB	:A 97 TYR CZ	: -0.417:	0
: 1657:A 104 GLU 1HG	:A 101 ALA CA	: -0.417:	0
: 1657:A 9 ILE 3HG2	:A 13 LYS 1HD	: -0.657:	0
: 1657:A 13 LYS NZ	:A 90 GLU CD	: -0.479:	0
: 1657:A 6 GLY 1HA	:A 9 ILE 2HD1	: -0.457:	0
: 1657:A 32 LEU 2HB	:A 102 THR 2HG2	: -0.644:	0
: 1657:A 20 VAL HA	:A 32 LEU 1HB	: -0.584:	0
: 1657:A 102 THR 1HG2	:A 35 LEU 1HB	: -0.538:	0
: 1657:A 32 LEU 2HD1	:A 20 VAL 2HG1	: -0.516:	0
: 1657:A 34 GLY N	:A 102 THR HB	: -0.477:	0
: 1657:A 32 LEU 2HB	:A 102 THR CG2	: -0.460:	0
: 1657:A 32 LEU 3HD2	:A 32 LEU HA	: -0.433:	0
: 1657:A 27 LYS 2HD	:A 19 THR 3HG2	: -0.627:	0
: 1657:A 40 THR 1HG2	:A 55 LYS 2HB	: -0.586:	0
: 1657:A 59 TRP CZ2	:A 40 THR 2HG2	: -0.565:	0
: 1657:A 52 ASN O	:A 40 THR HB	: -0.510:	0
: 1657:A 52 ASN 2HB	:A 48 TYR 2HB	: -0.508:	0
: 1657:A 59 TRP HA	:A 59 TRP HE3	: -0.493:	0
: 1657:A 59 TRP HA	:A 59 TRP CE3	: -0.483:	0
: 1657:A 52 ASN HA	:A 75 ILE 1HG2	: -0.443:	0
: 1657:A 74 TYR HD2	:A 75 ILE 2HG1	: -0.420:	0
: 1657:A 76 PRO 1HD	:A 75 ILE HA	: -0.418:	0
: 1657:A 89 GLU OE2	:A 87 LYS 2HB	: -0.582:	0
: 1657:A 87 LYS 2HB	:A 87 LYS 2HZ	: -0.510:	0
: 1657:A 91 ARG NH2	:A 69 GLU 1HB	: -0.532:	0
: 1657:A 84 GLY 2HA	:A 69 GLU O	: -0.480:	0
: 1657:A 86 LYS NZ	:A 69 GLU O	: -0.423:	0
: 1657:A 91 ARG 2HH1	:A 69 GLU CD	: -0.416:	0
: 1657:A 10 PHE HE1	:A 18 HIS 2HB	: -0.508:	0
: 1657:A 53 LYS 1HB	:A 53 LYS NZ	: -0.493:	0
: 1657:A 41 GLY 2HA	:A 53 LYS HA	: -0.428:	0
: 1657:A 54 ASN OD1	:A 53 LYS NZ	: -0.408:	0
: 1657:A 95 ILE 1HG2	:A 61 GLU HA	: -0.489:	0
: 1657:A 99 LYS NZ	:A 61 GLU OE1	: -0.438:	0
: 1657:A 61 GLU CD	:A 99 LYS NZ	: -0.418:	0
: 1657:A 60 GLY 1HA	:A 36 PHE HD2	: -0.447:	0
: 1657:A 60 GLY 1HA	:A 36 PHE CD2	: -0.438:	0
: 1657:A 4 GLU OE2	:A 8 LYS NZ	: -0.441:	0
: 1657:A 4 GLU OE1	:A 8 LYS NZ	: -0.438:	0
: 1657:A 26 HIS HD2	:A 46 TYR 1HB	: -0.436:	0
: 1657:A 21 GLU OE2	:A 24 GLY 2HA	: -0.436:	0
: 1657:A 38 ARG 2HD	:A 38 ARG 1HH1	: -0.430:	0

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```
: 1657:A 44 PRO 2HD :A 43 ALA HA : -0.430: 0
: 1657:A 79 LYS 1HG :A 49 THR 3HG2 : -0.428: 0
: 1657:A 33 HIS CD2 :A 22 LYS HA : -0.427: 0
: 1657:A 2 ASP 2HB :A 5 LYS NZ : -0.411: 0
: 1657:A 67 TYR 2HB :A 64 LEU HA : -0.404: 0
#sum2 ::33.19 clashscore : 33.19 clashscore B
```

Output from PDB validation software

Summary from PDB validation

Aug. 26, 21:35:31 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.

none

=> 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

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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 0.012 Angstroms

All covalent bonds lie within a 6.0*RMSD range about the standard dictionary values.

*** Covalent Angle Values:

The RMS deviation for covalent angles relative to the standard dictionary is 2.4 degrees.

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

Deviation	Residue Name	Chain ID	Sequence Number	Model	AT1	-	AT2	-	AT3	Bond Angle	Dictionary Value
-17.4	THR	A	260	1	N	-	CA	-	CB	94.1	111.5
16.5	LYS	A	311	1	CA	-	CB	-	CG	130.6	114.1
-22.8	LEU	A	527	1	C	-	N	-	CA	98.9	121.7
15.3	LYS	A	610	1	C	-	N	-	CA	137.0	121.7
14.6	ASP	A	660	1	CB	-	CA	-	C	124.7	110.1
-21.8	ASP	A	660	1	N	-	CA	-	CB	88.7	110.5
-45.1	GLY	A	713	1	CA	-	C	-	O	75.7	120.8
33.0	GLY	A	713	1	CA	-	C	-	N	149.4	116.4
-40.5	GLY	A	713	1	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.

OTHER IMPORTANT ISSUES

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

PSVS Software Environment

appropriate.

==> The following residues are missing:

(Note: The SEQ number starts from 1 for each chain according to SEQRES sequence record.)

RES MOD#C SEQ

```
MET( 2 A -17 )
ALA( 2 A -16 )
ASP( 2 A -15 )
GLU( 2 A -14 )
ALA( 2 A -13 )
ALA( 2 A -12 )
LEU( 2 A -11 )
ALA( 2 A -10 )
LEU( 2 A -9 )
GLN( 2 A -8 )
PRO( 2 A -7 )
GLY( 2 A -6 )
GLY( 2 A -5 )
SER( 2 A -4 )
PRO( 2 A -3 )
SER( 2 A -2 )
ALA( 2 A -1 )
ALA( 2 A 0 )
ALA( 2 A 1 )
ALA( 2 A -6 )
ALA( 2 A -5 )
SER( 2 A -4 )
SER( 2 A -3 )
PRO( 2 A -2 )
ALA( 2 A -1 )
GLY( 2 A 0 )
GLU( 2 A 1 )
PRO( 2 A 2 )
LEU( 2 A 3 )
ARG( 2 A 4 )
ARG( 2 A -87 )
PRO( 2 A -86 )
ARG( 2 A -85 )
ARG( 2 A -84 )
ASP( 2 A -83 )
GLY( 2 A -82 )
PRO( 2 A -81 )
GLY( 2 A -80 )
LEU( 2 A -79 )
GLU( 2 A -78 )
ARG( 2 A -77 )
SER( 2 A -76 )
PRO( 2 A -75 )
GLY( 2 A -74 )
GLU( 2 A -73 )
PRO( 2 A -72 )
GLY( 2 A -71 )
GLY( 2 A -70 )
ALA( 2 A -69 )
ALA( 2 A -68 )
PRO( 2 A -67 )
GLU( 2 A -66 )
ARG( 2 A -65 )
```

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```
GLU( 2 A -64 )
VAL( 2 A -63 )
PRO( 2 A -62 )
ALA( 2 A -61 )
ALA( 2 A -60 )
ALA( 2 A -59 )
ARG( 2 A -58 )
GLY( 2 A -57 )
CYS( 2 A -56 )
PRO( 2 A -55 )
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ALA( 2 A -53 )
ALA( 2 A -52 )
ALA( 2 A -51 )
ALA( 2 A -50 )
ALA( 2 A -49 )
LEU( 2 A -48 )
TRP( 2 A -47 )
ARG( 2 A -46 )
GLU( 2 A -45 )
ALA( 2 A -44 )
GLU( 2 A -43 )
ALA( 2 A -42 )
GLU( 2 A -41 )
ALA( 2 A -40 )
ALA( 2 A -39 )
ALA( 2 A -38 )
ALA( 2 A -37 )
GLY( 2 A -36 )
GLY( 2 A -35 )
GLU( 2 A -34 )
GLN( 2 A -33 )
GLU( 2 A -32 )
ALA( 2 A -31 )
GLN( 2 A -30 )
ALA( 2 A -29 )
THR( 2 A -28 )
ALA( 2 A -27 )
ALA( 2 A -26 )
ALA( 2 A -25 )
GLY( 2 A -24 )
GLU( 2 A -23 )
GLY( 2 A -22 )
ASP( 2 A -21 )
ASN( 2 A -20 )
GLY( 2 A -19 )
PRO( 2 A -18 )
GLY( 2 A -17 )
LEU( 2 A -16 )
GLN( 2 A -15 )
GLY( 2 A -14 )
PRO( 2 A -13 )
SER( 2 A -12 )
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GLU( 2 A -10 )
PRO( 2 A -9 )
PRO( 2 A -8 )
LEU( 2 A -7 )
ALA( 2 A -6 )
ASP( 2 A -5 )
ASN( 2 A -4 )
LEU( 2 A -3 )
```

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```
TYR( 2 A -2 )
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GLU( 2 A 0 )
ASP( 2 A 1 )
ASP( 2 A 2 )
ASP( 2 A 3 )
ASP( 2 A 4 )
GLU( 2 A 5 )
GLU( 2 A -1 )
GLU( 2 A 0 )
GLU( 2 A 1 )
GLU( 2 A 2 )
GLU( 2 A 3 )
ALA( 2 A 4 )
ALA( 2 A 5 )
ALA( 2 A 6 )
GLY( 2 A 3 )
TYR( 2 A 4 )
ARG( 2 A 5 )
ASP( 2 A 6 )
ASN( 2 A 7 )
LEU( 2 A 8 )
LEU( 2 A 9 )
GLY( 2 A 8 )
ASP( 2 A 9 )
GLU( 2 A 10 )
ILE( 2 A 7 )
THR( 2 A 8 )
ASN( 2 A 9 )
GLY( 2 A 10 )
PHE( 2 A 11 )
GLU( 2 A 3 )
SER( 2 A 4 )
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GLU( 2 A 6 )
GLU( 2 A 7 )
ASP( 2 A 8 )
ARG( 2 A 9 )
ALA( 2 A 10 )
SER( 2 A 11 )
HIS( 2 A 12 )
ALA( 2 A 13 )
SER( 2 A 14 )
SER( 2 A 1 )
ASP( 2 A 2 )
TRP( 2 A 3 )
THR( 2 A 4 )
PRO( 2 A 5 )
ARG( 2 A 6 )
PRO( 2 A 7 )
ARG( 2 A 8 )
ILE( 2 A 9 )
GLY( 2 A 10 )
PRO( 2 A 11 )
TYR( 2 A 12 )
THR( 2 A 13 )
PHE( 2 A 14 )
VAL( 2 A 15 )
LEU( 2 A -8 )
MET( 2 A -7 )
ILE( 2 A -6 )
GLY( 2 A -5 )
```

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```
THR( 2 A -4 )
ASP( 2 A -3 )
PRO( 2 A -2 )
ARG( 2 A -1 )
THR( 2 A 0 )
ILE( 2 A 1 )
LEU( 2 A 2 )
LYS( 2 A 3 )
ASP( 2 A 4 )
LEU( 2 A 5 )
LEU( 2 A 6 )
PRO( 2 A 7 )
GLU( 2 A 8 )
THR( 2 A 9 )
ILE( 2 A 10 )
PRO( 2 A 11 )
PRO( 2 A 12 )
PRO( 2 A 13 )
GLU( 2 A 14 )
LEU( 2 A 15 )
ASP( 2 A 16 )
ASP( 2 A 17 )
MET( 2 A 18 )
LEU( 2 A 16 )
TRP( 2 A 17 )
GLN( 2 A 18 )
ILE( 2 A 19 )
ILE( 2 A 16 )
ASN( 2 A 17 )
ILE( 2 A 18 )
LEU( 2 A 19 )
SER( 2 A 20 )
PRO( 2 A 20 )
PRO( 2 A 21 )
ASP( 2 A 7 )
ILE( 2 A 8 )
ASN( 2 A 9 )
THR( 2 A 10 )
ILE( 2 A 11 )
GLU( 2 A 12 )
ASP( 2 A 13 )
ALA( 2 A 14 )
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GLU( 2 A 20 )
CYS( 2 A 21 )
LYS( 2 A 22 )
LYS( 2 A 23 )
ILE( 2 A 24 )
ILE( 2 A 25 )
VAL( 2 A 26 )
LEU( 2 A 27 )
ALA( 2 A 4 )
GLY( 2 A 5 )
VAL( 2 A 6 )
SER( 2 A 7 )
VAL( 2 A 8 )
SER( 2 A 9 )
CYS( 2 A 10 )
```


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SER( 2 A 17 )
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ASP( 2 A 13 )
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PRO( 2 A 23 )
PHE( 2 A 24 )
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PHE( 2 A 27 )
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LYS( 2 A 29 )
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GLN( 2 A 30 )
PHE( 2 A 31 )
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CYS( 2 A 33 )
HIS( 2 A 34 )
LYS( 2 A 35 )
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ALA( 2 A 31 )
LEU( 2 A 32 )
SER( 2 A 33 )
ASP( 2 A 34 )
LYS( 2 A 35 )
GLU( 2 A 36 )
LYS( 2 A 35 )
```

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```
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LEU( 2 A 37 )
ASN( 2 A 33 )
TYR( 2 A 34 )
THR( 2 A 35 )
GLN( 2 A 36 )
ASN( 2 A 37 )
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GLU( 2 A 37 )
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PRO( 2 A 46 )
GLU( 2 A 47 )
ILE( 2 A 48 )
VAL( 2 A 49 )
PHE( 2 A 50 )
PHE( 2 A 51 )
GLY( 2 A 52 )
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LEU(2 A 43)
PRO(2 A 44)
GLU(2 A 45)
GLN(2 A 46)
PHE(2 A 47)
HIS(2 A 48)
ARG(2 A 49)
ALA(2 A 50)
MET(2 A 51)
LYS(2 A 52)
TYR(2 A 53)
ASP(2 A 54)
ASP(2 A 47)
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VAL(2 A 49)
ASP(2 A 50)
LEU(2 A 51)
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SER(2 A 37)
LEU(2 A 38)
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LEU(2 A 45)
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PRO(2 A 47)
SER(2 A 48)
SER(2 A 49)
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PRO(2 A 51)
HIS(2 A 52)
GLU(2 A 53)
VAL(2 A 54)
PRO(2 A 55)
GLN(2 A 56)
LEU(2 A 57)
PRO(2 A 47)
LEU(2 A 48)
PRO(2 A 49)
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LEU(2 A 51)
HIS(2 A 52)
PHE(2 A 53)
ASP(2 A 54)
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LEU(2 A 57)
LEU(2 A 58)
GLY(2 A 59)
ASP(2 A 60)
CYS(2 A 61)
VAL(2 A 55)
ILE(2 A 56)
ILE(2 A 57)

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GLU(2 A 59)
LEU(2 A 60)
CYS(2 A 61)
HIS(2 A 62)
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ALA(2 A 66)
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CYS(2 A 68)
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GLU(2 A 68)
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GLU(2 A 71)
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GLN(2 A 72)
GLU(2 A 71)
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GLU(2 A 43)
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GLU(2 A 49)
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SER(2 A 56)
SER(2 A 57)
VAL(2 A 58)
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VAL(2 A 60)
THR(2 A 61)
LEU(2 A 62)
LEU(2 A 63)
ASP(2 A 64)
GLN(2 A 65)
ALA(2 A 66)
ALA(2 A 67)
LYS(2 A 68)
SER(2 A 69)
ASN(2 A 70)
ASP(2 A 71)

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```
ASP ( 2 A 72 )
LEU ( 2 A 73 )
ASP ( 2 A 74 )
VAL ( 2 A 75 )
SER ( 2 A 76 )
GLU ( 2 A 77 )
SER ( 2 A 78 )
GLY ( 2 A 78 )
CYS ( 2 A 79 )
GLU ( 2 A 66 )
GLU ( 2 A 67 )
LYS ( 2 A 68 )
PRO ( 2 A 69 )
GLN ( 2 A 70 )
GLU ( 2 A 71 )
VAL ( 2 A 72 )
GLN ( 2 A 73 )
THR ( 2 A 74 )
SER ( 2 A 75 )
ARG ( 2 A 76 )
ASN ( 2 A 77 )
VAL ( 2 A 78 )
GLU ( 2 A 79 )
SER ( 2 A 80 )
ALA ( 2 A 72 )
GLU ( 2 A 73 )
GLN ( 2 A 74 )
MET ( 2 A 75 )
GLU ( 2 A 76 )
ASN ( 2 A 77 )
PRO ( 2 A 78 )
ASP ( 2 A 79 )
LEU ( 2 A 80 )
LYS ( 2 A 81 )
SER ( 2 A 81 )
SER ( 2 A 82 )
THR ( 2 A 83 )
GLY ( 2 A 84 )
ASN ( 2 A 76 )
GLU ( 2 A 77 )
ARG ( 2 A 78 )
THR ( 2 A 79 )
SER ( 2 A 80 )
VAL ( 2 A 81 )
ALA ( 2 A 82 )
GLY ( 2 A 83 )
THR ( 2 A 84 )
VAL ( 2 A 85 )
ARG ( 2 A 86 )
CYS ( 2 A 81 )
TRP ( 2 A 82 )
PRO ( 2 A 83 )
ASN ( 2 A 84 )
ARG ( 2 A 85 )
VAL ( 2 A 86 )
ALA ( 2 A 87 )
GLN ( 2 A 87 )
ILE ( 2 A 88 )
SER ( 2 A 89 )
GLY ( 2 A 88 )
ASN ( 2 A 89 )
GLN ( 2 A 90 )
```

PSVS Software Environment

```
TYR( 2 A 91 )
LEU( 2 A 92 )
PHE( 2 A 93 )
PRO( 2 A 90 )
PRO( 2 A 91 )
ASN( 2 A 92 )
ARG( 2 A 93 )
TYR( 2 A 94 )
PHE( 2 A 93 )
HIS( 2 A 94 )
GLY( 2 A 95 )
GLU( 2 A 54 )
VAL( 2 A 55 )
TYR( 2 A 56 )
SER( 2 A 57 )
ASP( 2 A 58 )
SER( 2 A 59 )
GLU( 2 A 60 )
ASP( 2 A 61 )
ASP( 2 A 62 )
VAL( 2 A 63 )
LEU( 2 A 64 )
SER( 2 A 65 )
SER( 2 A 66 )
SER( 2 A 67 )
SER( 2 A 68 )
CYS( 2 A 69 )
GLY( 2 A 70 )
SER( 2 A 71 )
ASN( 2 A 72 )
SER( 2 A 73 )
ASP( 2 A 74 )
SER( 2 A 75 )
GLY( 2 A 76 )
THR( 2 A 77 )
CYS( 2 A 78 )
GLN( 2 A 79 )
SER( 2 A 80 )
PRO( 2 A 81 )
SER( 2 A 82 )
LEU( 2 A 83 )
GLU( 2 A 84 )
GLU( 2 A 85 )
PRO( 2 A 86 )
MET( 2 A 87 )
GLU( 2 A 88 )
ASP( 2 A 89 )
GLU( 2 A 90 )
SER( 2 A 91 )
GLU( 2 A 92 )
ILE( 2 A 93 )
GLU( 2 A 94 )
GLU( 2 A 95 )
PHE( 2 A 96 )
ASN( 2 A 96 )
GLY( 2 A 97 )
GLU( 2 A 89 )
ASP( 2 A 90 )
GLU( 2 A 91 )
PRO( 2 A 92 )
ASP( 2 A 93 )
VAL( 2 A 94 )
```

PSVS Software Environment

```

PRO(  2 A  95 )
GLU(  2 A  96 )
ARG(  2 A  97 )
ALA(  2 A  98 )
GLY(  2 A  99 )
PHE(  2 A 100 )
GLY(  2 A 101 )
ASP(  2 A  95 )
GLY(  2 A  96 )
ASP(  2 A  97 )
ASP(  2 A  98 )
GLN(  2 A  99 )
GLU(  2 A 100 )
ALA(  2 A 101 )
ILE(  2 A 102 )
ALA(  2 A 105 )
ILE(  2 A 106 )
SER(  2 A 107 )
VAL(  2 A 108 )
LYS(  2 A 109 )
GLN(  2 A 110 )
GLU(  2 A 111 )
VAL(  2 A 112 )
THR(  2 A 113 )
ASP(  2 A 114 )
MET(  2 A 115 )
ASN(  2 A 116 )
TYR(  2 A 117 )
PRO(  2 A 118 )
SER(  2 A 119 )
ASN(  2 A 120 )
LYS(  2 A 121 )
SER(  2 A 122 )

```

```

MISMATCH: ChainID=A ResNum=3  (ARG  VAL)
MISMATCH: ChainID=A ResNum=7  (ALA  LYS)
MISMATCH: ChainID=A ResNum=8  (ALA  LYS)
MISMATCH: ChainID=A ResNum=12 (HIS  MET)
MISMATCH: ChainID=A ResNum=13 (SER  LYS)
MISMATCH: ChainID=A ResNum=17 (GLN  CYS)
MISMATCH: ChainID=A ResNum=23 (ARG  GLY)
MISMATCH: ChainID=A ResNum=24 (LYS  GLY)
MISMATCH: ChainID=A ResNum=26 (ARG  HIS)
MISMATCH: ChainID=A ResNum=31 (ASP  ASN)
MISMATCH: ChainID=A ResNum=33 (PRO  HIS)
MISMATCH: ChainID=A ResNum=39 (ASP  LYS)
MISMATCH: ChainID=A ResNum=43 (CYS  ALA)
MISMATCH: ChainID=A ResNum=44 (HIS  PRO)
MISMATCH: ChainID=A ResNum=46 (...  TYR)
MISMATCH: ChainID=A ResNum=48 (ALA  TYR)
MISMATCH: ChainID=A ResNum=59 (ASN  TRP)
MISMATCH: ChainID=A ResNum=60 (ARG  GLY)
MISMATCH: ChainID=A ResNum=63 (ARG  THR)
MISMATCH: ChainID=A ResNum=65 (GLY  MET)
MISMATCH: ChainID=A ResNum=69 (CYS  GLU)
MISMATCH: ChainID=A ResNum=75 (LEU  ILE)
MISMATCH: ChainID=A ResNum=77 (PRO  GLY)
MISMATCH: ChainID=A ResNum=82 (ASN  PHE)
MISMATCH: ChainID=A ResNum=85 (GLU  ILE)
MISMATCH: ChainID=A ResNum=90 (ARG  GLU)
MISMATCH: ChainID=A ResNum=92 (LEU  ALA)

```

PSVS Software Environment

MISMATCH: ChainID=A ResNum=99 (GLY LYS)
MISMATCH: ChainID=A ResNum=100 (GLY LYS)
SEQUENCE WARNING: Residue (A GLY 1) and Residue (A ASP 2) are linked together
SEQUENCE WARNING: Residue (A GLU 4) and Residue (A LYS 5) are linked together
SEQUENCE WARNING: Residue (A LYS 5) and Residue (A GLY 6) are linked together
SEQUENCE WARNING: Residue (A GLY 6) and Residue (A LYS 7) are linked together
SEQUENCE WARNING: Residue (A ILE 9) and Residue (A PHE 10) are linked together
SEQUENCE WARNING: Residue (A PHE 10) and Residue (A ILE 11) are linked together
SEQUENCE WARNING: Residue (A ILE 11) and Residue (A MET 12) are linked together
SEQUENCE WARNING: Residue (A CYS 14) and Residue (A SER 15) are linked together
SEQUENCE WARNING: Residue (A SER 15) and Residue (A GLN 16) are linked together
SEQUENCE WARNING: Residue (A HIS 18) and Residue (A THR 19) are linked together
SEQUENCE WARNING: Residue (A THR 19) and Residue (A VAL 20) are linked together
SEQUENCE WARNING: Residue (A VAL 20) and Residue (A GLU 21) are linked together
SEQUENCE WARNING: Residue (A GLU 21) and Residue (A LYS 22) are linked together
SEQUENCE WARNING: Residue (A LYS 27) and Residue (A THR 28) are linked together
SEQUENCE WARNING: Residue (A GLY 29) and Residue (A PRO 30) are linked together
SEQUENCE WARNING: Residue (A LEU 32) and Residue (A HIS 33) are linked together
SEQUENCE WARNING: Residue (A GLY 34) and Residue (A LEU 35) are linked together
SEQUENCE WARNING: Residue (A LEU 35) and Residue (A PHE 36) are linked together
SEQUENCE WARNING: Residue (A PHE 36) and Residue (A GLY 37) are linked together
SEQUENCE WARNING: Residue (A GLY 37) and Residue (A ARG 38) are linked together
SEQUENCE WARNING: Residue (A ARG 38) and Residue (A LYS 39) are linked together
SEQUENCE WARNING: Residue (A THR 40) and Residue (A GLY 41) are linked together
SEQUENCE WARNING: Residue (A GLY 41) and Residue (A GLN 42) are linked together
SEQUENCE WARNING: Residue (A SER 47) and Residue (A TYR 48) are linked together
SEQUENCE WARNING: Residue (A ALA 50) and Residue (A ALA 51) are linked together
SEQUENCE WARNING: Residue (A ALA 51) and Residue (A ASN 52) are linked together
SEQUENCE WARNING: Residue (A ASN 52) and Residue (A LYS 53) are linked together
SEQUENCE WARNING: Residue (A LYS 53) and Residue (A ASN 54) are linked together
SEQUENCE WARNING: Residue (A ASN 54) and Residue (A LYS 55) are linked together
SEQUENCE WARNING: Residue (A LYS 55) and Residue (A GLY 56) are linked together
SEQUENCE WARNING: Residue (A GLY 56) and Residue (A ILE 57) are linked together
SEQUENCE WARNING: Residue (A ILE 57) and Residue (A ILE 58) are linked together
SEQUENCE WARNING: Residue (A GLU 61) and Residue (A ASP 62) are linked together
SEQUENCE WARNING: Residue (A ASP 62) and Residue (A THR 63) are linked together
SEQUENCE WARNING: Residue (A LEU 64) and Residue (A MET 65) are linked together
SEQUENCE WARNING: Residue (A TYR 67) and Residue (A LEU 68) are linked together
SEQUENCE WARNING: Residue (A LEU 68) and Residue (A GLU 69) are linked together
SEQUENCE WARNING: Residue (A PRO 71) and Residue (A LYS 72) are linked together
SEQUENCE WARNING: Residue (A LYS 72) and Residue (A LYS 73) are linked together
SEQUENCE WARNING: Residue (A LYS 73) and Residue (A TYR 74) are linked together
SEQUENCE WARNING: Residue (A TYR 74) and Residue (A ILE 75) are linked together
SEQUENCE WARNING: Residue (A THR 78) and Residue (A LYS 79) are linked together
SEQUENCE WARNING: Residue (A LYS 79) and Residue (A MET 80) are linked together
SEQUENCE WARNING: Residue (A MET 80) and Residue (A ILE 81) are linked together
SEQUENCE WARNING: Residue (A ILE 81) and Residue (A PHE 82) are linked together
SEQUENCE WARNING: Residue (A GLY 84) and Residue (A ILE 85) are linked together
SEQUENCE WARNING: Residue (A LYS 86) and Residue (A LYS 87) are linked together
SEQUENCE WARNING: Residue (A LYS 87) and Residue (A LYS 88) are linked together
SEQUENCE WARNING: Residue (A GLU 89) and Residue (A GLU 90) are linked together
SEQUENCE WARNING: Residue (A ASP 93) and Residue (A LEU 94) are linked together
SEQUENCE WARNING: Residue (A LEU 94) and Residue (A ILE 95) are linked together
SEQUENCE WARNING: Residue (A ILE 95) and Residue (A ALA 96) are linked together
SEQUENCE WARNING: Residue (A ALA 96) and Residue (A TYR 97) are linked together
SEQUENCE WARNING: Residue (A TYR 97) and Residue (A LEU 98) are linked together
SEQUENCE WARNING: Residue (A LEU 98) and Residue (A LYS 99) are linked together
SEQUENCE WARNING: Residue (A ALA 101) and Residue (A THR 102) are linked together
SEQUENCE WARNING: Residue (A THR 102) and Residue (A ASN 103) are linked together

There were mismatches between the deposited sequence and sequence in coordinates involving alanines and/or glycines. The residue

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names have been changed to match the deposited sequence and/or the sequence database unless engineered mutation were specified in the deposition. The missing side chain atoms are listed in remark 470.

PDB Chain_ID: A

```

1
SEQRES: MET ALA ASP GLU ALA ALA LEU ALA LEU GLN PRO GLY GLY SER PRO
COORDS: ... ..

```

```

16
SEQRES: SER ALA ALA GLY ALA ASP ARG GLU ALA ALA SER SER PRO ALA GLY
COORDS: ... ..
          1
          4
          ^^^

```

```

31
SEQRES: GLU PRO LEU ARG LYS ARG PRO ARG ARG ASP GLY PRO GLY LEU GLU
COORDS: ... ..
          5

```

```

46
SEQRES: ARG SER PRO GLY GLU PRO GLY GLY ALA ALA PRO GLU ARG GLU VAL
COORDS: ... ..

```

```

61
SEQRES: PRO ALA ALA ALA ARG GLY CYS PRO GLY ALA ALA ALA ALA ALA LEU
COORDS: ... ..

```

```

76
SEQRES: TRP ARG GLU ALA GLU ALA GLU ALA ALA ALA ALA GLY GLY GLU GLN
COORDS: ... ..

```

```

91
SEQRES: GLU ALA GLN ALA THR ALA ALA ALA GLY GLU GLY ASP ASN GLY PRO
COORDS: ... ..

```

```

106
SEQRES: GLY LEU GLN GLY PRO SER ARG GLU PRO PRO LEU ALA ASP ASN LEU
COORDS: ... ..

```

```

121
SEQRES: TYR ASP GLU ASP ASP ASP ASP GLU GLY GLU GLU GLU GLU GLU ALA
COORDS: ... ..
          6

```

```

136
SEQRES: ALA ALA ALA ALA ILE GLY TYR ARG ASP ASN LEU LEU PHE GLY ASP
COORDS: ... ..
          7
          10
          ^^^ ^^^

```

```

151
SEQRES: GLU ILE ILE THR ASN GLY PHE HIS SER CYS GLU SER ASP GLU GLU

```

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```

COORDS: ... ILE ... .. met lys CYS ... ..
          11                               14
          ^^^ ^^^

166                                           180
SEQRES: ASP ARG ALA SER HIS ALA SER SER SER ASP TRP THR PRO ARG PRO
COORDS: ... .. SER ... ..
          15

181                                           195
SEQRES: ARG ILE GLY PRO TYR THR PHE VAL GLN GLN HIS LEU MET ILE GLY
COORDS: ... .. GLN cys HIS ... ..
          16           18
          ^^^

196                                           210
SEQRES: THR ASP PRO ARG THR ILE LEU LYS ASP LEU LEU PRO GLU THR ILE
COORDS: ... ..

211                                           225
SEQRES: PRO PRO PRO GLU LEU ASP ASP MET THR LEU TRP GLN ILE VAL ILE
COORDS: ... .. THR ... .. VAL ...
          19           20

226                                           240
SEQRES: ASN ILE LEU SER GLU PRO PRO LYS ARG LYS LYS ARG LYS ASP ILE
COORDS: ... .. GLU ... .. LYS gly gly LYS his LYS ... ..
          21                               27
          ^^^ ^^^ ^^^

241                                           255
SEQRES: ASN THR ILE GLU ASP ALA VAL LYS LEU LEU GLN GLU CYS LYS LYS
COORDS: ... ..

256                                           270
SEQRES: ILE ILE VAL LEU THR GLY ALA GLY VAL SER VAL SER CYS GLY ILE
COORDS: ... .. THR GLY ... ..
          28           29

271                                           285
SEQRES: PRO ASP PHE ARG SER ARG ASP GLY ILE TYR ALA ARG LEU ALA VAL
COORDS: ... ..

286                                           300
SEQRES: ASP PHE PRO ASP LEU PRO ASP PRO GLN ALA MET PHE ASP ILE GLU
COORDS: ... .. PRO asn LEU ... ..
          30           32
          ^^^

301                                           315
SEQRES: TYR PHE ARG LYS ASP PRO ARG PRO PHE PHE LYS PHE ALA LYS GLU
COORDS: ... ..

316                                           330
SEQRES: ILE TYR PRO GLY GLN PHE GLN PRO SER LEU CYS HIS LYS PHE ILE
COORDS: ... .. his GLY ... .. LEU ... .. PHE ...
          33                               36
          ^^^

```

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```

331                                     345
SEQRES: ALA LEU SER ASP LYS GLU GLY LYS LEU LEU ARG ASN TYR THR GLN
COORDS: ... .. GLY ... .. ARG ... ..
              37              38

346                                     360
SEQRES: ASN ILE ASP THR LEU GLU GLN VAL ALA GLY ILE GLN ARG ILE ILE
COORDS: ... .. lys THR ... .. GLY ... ..
              39              41
              ^^^

361                                     374
SEQRES: GLN CYS HIS GLY ... SER PHE ALA THR ALA SER CYS LEU ILE CYS
COORDS: GLN ala pro GLY tyr SER ... tyr THR ALA ... ..
              42              50
              ^^^ ^^^ ^^^ ^^^

375                                     389
SEQRES: LYS TYR LYS VAL ASP CYS GLU ALA VAL ARG GLY ASP ILE PHE ASN
COORDS: ... .. ALA ... .. ASN
              51              52

390                                     404
SEQRES: GLN VAL VAL PRO ARG CYS PRO ARG CYS PRO ALA ASP GLU PRO LEU
COORDS: ... ..

405                                     419
SEQRES: ALA ILE MET LYS PRO GLU ILE VAL PHE PHE GLY GLU ASN LEU PRO
COORDS: ... .. LYS ... .. ASN ... ..
              53              54

420                                     434
SEQRES: GLU GLN PHE HIS ARG ALA MET LYS TYR ASP LYS ASP GLU VAL ASP
COORDS: ... .. LYS ... ..
              55

435                                     449
SEQRES: LEU LEU ILE VAL ILE GLY SER SER LEU LYS VAL ARG PRO VAL ALA
COORDS: ... .. GLY ... ..
              56

450                                     464
SEQRES: LEU ILE PRO SER SER ILE PRO HIS GLU VAL PRO GLN ILE LEU ILE
COORDS: ... .. ILE ... ..
              57              58

465                                     479
SEQRES: ASN ARG GLU PRO LEU PRO HIS LEU HIS PHE ASP VAL GLU LEU LEU
COORDS: trp gly GLU ... ..
              59              61
              ^^^ ^^^

480                                     494
SEQRES: GLY ASP CYS ASP VAL ILE ILE ASN GLU LEU CYS HIS ARG LEU GLY
COORDS: ... .. ASP ... .. thr LEU ...
              62              64
              ^^^

495                                     509
SEQRES: GLY GLU TYR ALA LYS LEU CYS CYS ASN PRO VAL LYS LEU SER GLU

```

PSVS Software Environment

```

COORDS: met  GLU  TYR  ...  ...  LEU  ...  glu  ASN  PRO  ...  ...  ...  ...  ...
          65                                     71
          ^^^                               ^^^

510                                           524
SEQRES: ILE  THR  GLU  LYS  PRO  PRO  ARG  THR  GLN  LYS  GLU  LEU  ALA  TYR  LEU
COORDS: ...  ...  ...  LYS  ...  ...  ...  ...  ...  LYS  ...  ...  ...  TYR  ...
          72                                           74

525                                           539
SEQRES: SER  GLU  LEU  PRO  PRO  THR  PRO  LEU  HIS  VAL  SER  GLU  ASP  SER  SER
COORDS: ...  ...  ile  PRO  gly  THR  ...  ...  ...  ...  ...  ...  ...  ...  ...
          75                                     78
          ^^^       ^^^

540                                           554
SEQRES: SER  PRO  GLU  ARG  THR  SER  PRO  PRO  ASP  SER  SER  VAL  ILE  VAL  THR
COORDS: ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...

555                                           569
SEQRES: LEU  LEU  ASP  GLN  ALA  ALA  LYS  SER  ASN  ASP  ASP  LEU  ASP  VAL  SER
COORDS: ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...

570                                           584
SEQRES: GLU  SER  LYS  GLY  CYS  MET  GLU  GLU  LYS  PRO  GLN  GLU  VAL  GLN  THR
COORDS: ...  ...  LYS  ...  ...  MET  ...  ...  ...  ...  ...  ...  ...  ...  ...
          79                                     80

585                                           599
SEQRES: SER  ARG  ASN  VAL  GLU  SER  ILE  ALA  GLU  GLN  MET  GLU  ASN  PRO  ASP
COORDS: ...  ...  ...  ...  ...  ...  ILE  ...  ...  ...  ...  ...  ...  ...  ...
          81

600                                           614
SEQRES: LEU  LYS  ASN  VAL  GLY  SER  SER  THR  GLY  GLU  LYS  ASN  GLU  ARG  THR
COORDS: ...  ...  phe  VAL  GLY  ...  ...  ...  ...  ile  LYS  ...  ...  ...  ...
          82                                     86
          ^^^                               ^^^

615                                           629
SEQRES: SER  VAL  ALA  GLY  THR  VAL  ARG  LYS  CYS  TRP  PRO  ASN  ARG  VAL  ALA
COORDS: ...  ...  ...  ...  ...  ...  LYS  ...  ...  ...  ...  ...  ...  ...  ...
          87

630                                           644
SEQRES: LYS  GLU  GLN  ILE  SER  ARG  ARG  LEU  ASP  GLY  ASN  GLN  TYR  LEU  PHE
COORDS: LYS  GLU  ...  ...  ...  glu  ARG  ala  ASP  ...  ...  ...  ...  ...  ...
          88                                     93
          ^^^       ^^^

645                                           659
SEQRES: LEU  PRO  PRO  ASN  ARG  TYR  ILE  PHE  HIS  GLY  ALA  GLU  VAL  TYR  SER
COORDS: LEU  ...  ...  ...  ...  ...  ILE  ...  ...  ...  ALA  ...  ...  ...  ...
          94                                     96

660                                           674
SEQRES: ASP  SER  GLU  ASP  ASP  VAL  LEU  SER  SER  SER  SER  CYS  GLY  SER  ASN
COORDS: ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...  ...

```

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```

675
SEQRES: SER ASP SER GLY THR CYS GLN SER PRO SER LEU GLU GLU PRO MET
COORDS: ... ..

```

```

690
SEQRES: GLU ASP GLU SER GLU ILE GLU GLU PHE TYR ASN GLY LEU GLU ASP
COORDS: ... .. TYR ... .. LEU ... ..
97 98

```

```

705
SEQRES: GLU PRO ASP VAL PRO GLU ARG ALA GLY GLY ALA GLY PHE GLY THR
COORDS: ... .. lys lys ALA ... .. THR
99 102
^^^ ^^

```

```

720
SEQRES: ASP GLY ASP ASP GLN GLU ALA ILE ASN GLU ALA ILE SER VAL LYS
COORDS: ... .. ASN GLU ... ..
103 104

```

```

735
SEQRES: GLN GLU VAL THR ASP MET ASN TYR PRO SER ASN LYS SER
COORDS: ... ..
747

```

f1SIRT1_CytoC.pdb: Missing KEYWDS records

f1SIRT1_CytoC.pdb: Missing TITLE record