wwPDB X-ray Structure Validation Summary Report (i)

Feb 3, 2024 – 02:29 PM EST

PDB ID	:	1LL0
Title	:	Crystal Structure of Rabbit Muscle Glycogenin
Authors	:	Gibbons, B.J.; Roach, P.J.; Hurley, T.D.
Deposited on	:	2002-04-26
Resolution	:	3.43 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

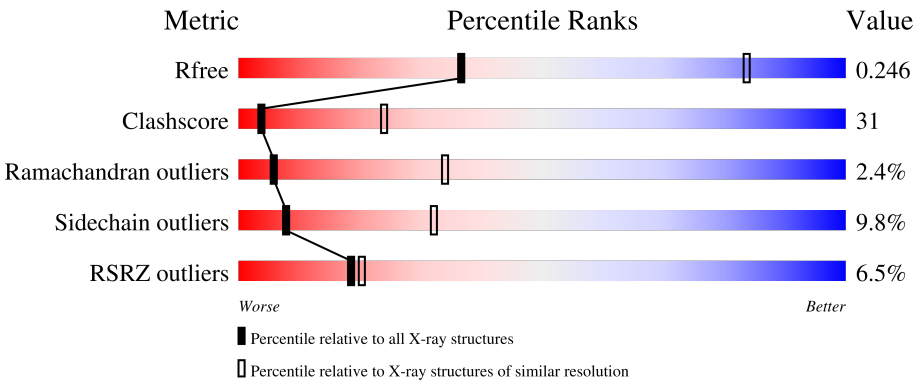
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	339	3%; 41%, 31%, 6%, 22%
1	B	339	4%; 42%, 31%, 6%, • , 21%
1	C	339	2%; 41%, 31%, 5%, 23%
1	D	339	6%; 43%, 29%, 5%, 23%
1	E	339	4%; 41%, 30%, 6%, 23%

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Mol	Chain	Length	Quality of chain
1	F	339	5% 42% 30% 5% 23%
1	G	339	4% 41% 32% 5% 23%
1	H	339	5% 41% 29% 6% 23%
1	I	339	6% 40% 33% 22%
1	J	339	11% 42% 28% 26%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 20736 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLYCOGENIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2092	1346	342	396	8	0	0	0
1	B	267	2115	1360	350	397	8	0	0	0
1	C	262	2077	1337	340	392	8	0	0	0
1	D	261	2071	1333	339	392	7	0	0	0
1	E	262	2081	1339	342	393	7	0	0	0
1	F	261	2071	1333	339	392	7	0	0	0
1	G	262	2079	1338	340	393	8	0	0	0
1	H	260	2064	1327	338	391	8	0	0	0
1	I	264	2095	1346	347	395	7	0	0	0
1	J	251	1991	1281	327	377	6	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	VAL	-	expression tag	UNP P13280
A	-6	PRO	-	expression tag	UNP P13280
A	-5	ARG	-	expression tag	UNP P13280
A	-4	GLY	-	expression tag	UNP P13280
A	-3	SER	-	expression tag	UNP P13280
A	-2	HIS	-	expression tag	UNP P13280
B	-7	VAL	-	expression tag	UNP P13280
B	-6	PRO	-	expression tag	UNP P13280
B	-5	ARG	-	expression tag	UNP P13280

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P13280
B	-3	SER	-	expression tag	UNP P13280
B	-2	HIS	-	expression tag	UNP P13280
C	-7	VAL	-	expression tag	UNP P13280
C	-6	PRO	-	expression tag	UNP P13280
C	-5	ARG	-	expression tag	UNP P13280
C	-4	GLY	-	expression tag	UNP P13280
C	-3	SER	-	expression tag	UNP P13280
C	-2	HIS	-	expression tag	UNP P13280
D	-7	VAL	-	expression tag	UNP P13280
D	-6	PRO	-	expression tag	UNP P13280
D	-5	ARG	-	expression tag	UNP P13280
D	-4	GLY	-	expression tag	UNP P13280
D	-3	SER	-	expression tag	UNP P13280
D	-2	HIS	-	expression tag	UNP P13280
E	-7	VAL	-	expression tag	UNP P13280
E	-6	PRO	-	expression tag	UNP P13280
E	-5	ARG	-	expression tag	UNP P13280
E	-4	GLY	-	expression tag	UNP P13280
E	-3	SER	-	expression tag	UNP P13280
E	-2	HIS	-	expression tag	UNP P13280
F	-7	VAL	-	expression tag	UNP P13280
F	-6	PRO	-	expression tag	UNP P13280
F	-5	ARG	-	expression tag	UNP P13280
F	-4	GLY	-	expression tag	UNP P13280
F	-3	SER	-	expression tag	UNP P13280
F	-2	HIS	-	expression tag	UNP P13280
G	-7	VAL	-	expression tag	UNP P13280
G	-6	PRO	-	expression tag	UNP P13280
G	-5	ARG	-	expression tag	UNP P13280
G	-4	GLY	-	expression tag	UNP P13280
G	-3	SER	-	expression tag	UNP P13280
G	-2	HIS	-	expression tag	UNP P13280
H	-7	VAL	-	expression tag	UNP P13280
H	-6	PRO	-	expression tag	UNP P13280
H	-5	ARG	-	expression tag	UNP P13280
H	-4	GLY	-	expression tag	UNP P13280
H	-3	SER	-	expression tag	UNP P13280
H	-2	HIS	-	expression tag	UNP P13280
I	-7	VAL	-	expression tag	UNP P13280
I	-6	PRO	-	expression tag	UNP P13280
I	-5	ARG	-	expression tag	UNP P13280

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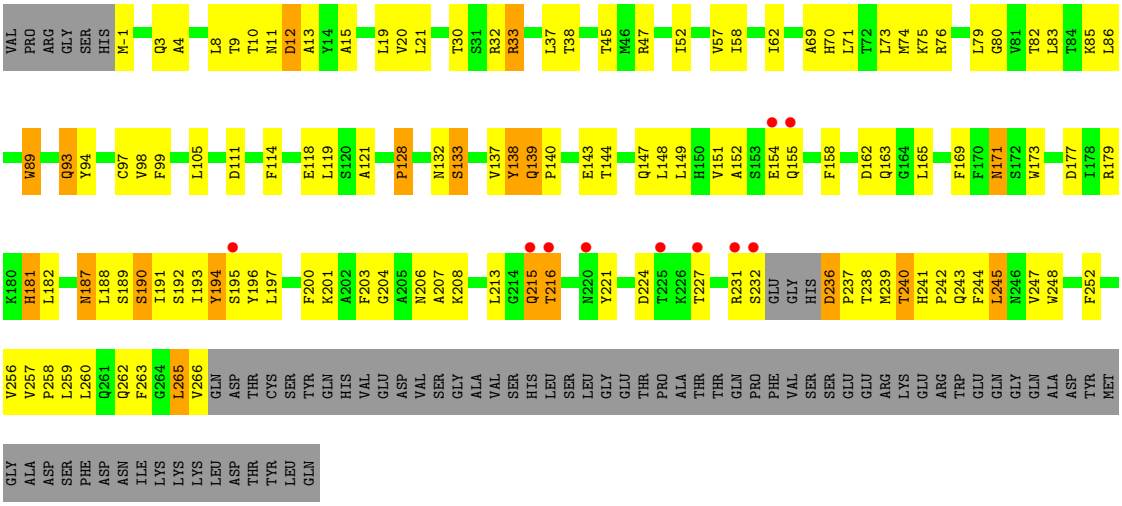
Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	GLY	-	expression tag	UNP P13280
I	-3	SER	-	expression tag	UNP P13280
I	-2	HIS	-	expression tag	UNP P13280
J	-7	VAL	-	expression tag	UNP P13280
J	-6	PRO	-	expression tag	UNP P13280
J	-5	ARG	-	expression tag	UNP P13280
J	-4	GLY	-	expression tag	UNP P13280
J	-3	SER	-	expression tag	UNP P13280
J	-2	HIS	-	expression tag	UNP P13280

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

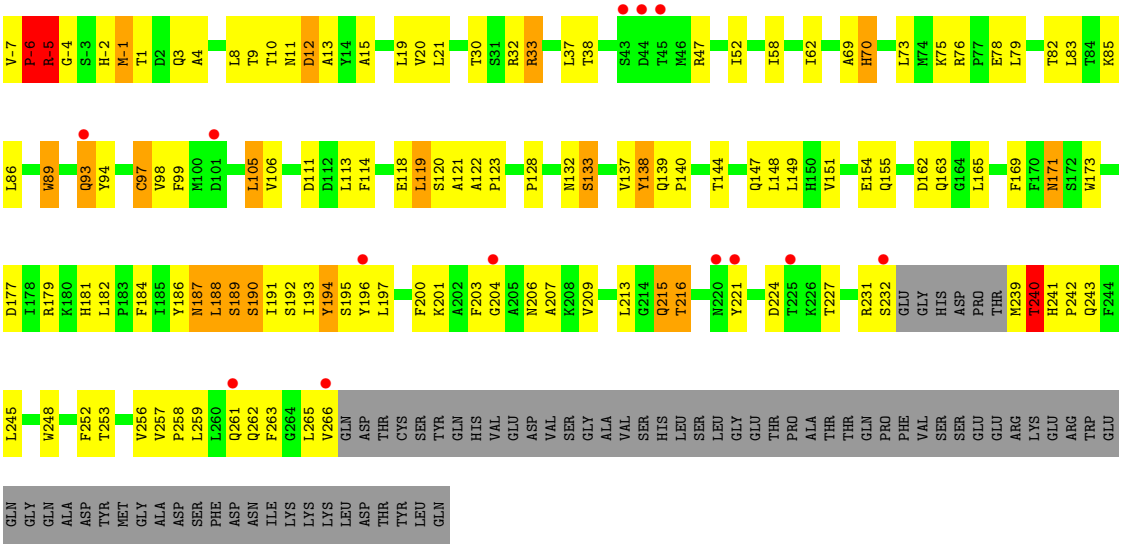
• Molecule 1: GLYCOGENIN-1

Chain A: 3% 41% 31% 6% 22%



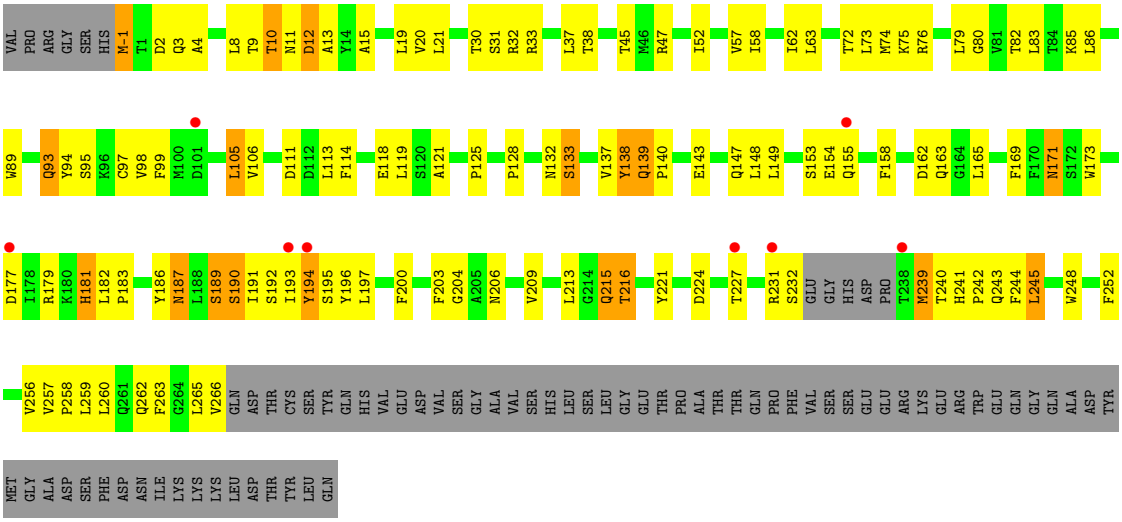
• Molecule 1: GLYCOGENIN-1

Chain B: 4% 42% 31% 6% • 21%



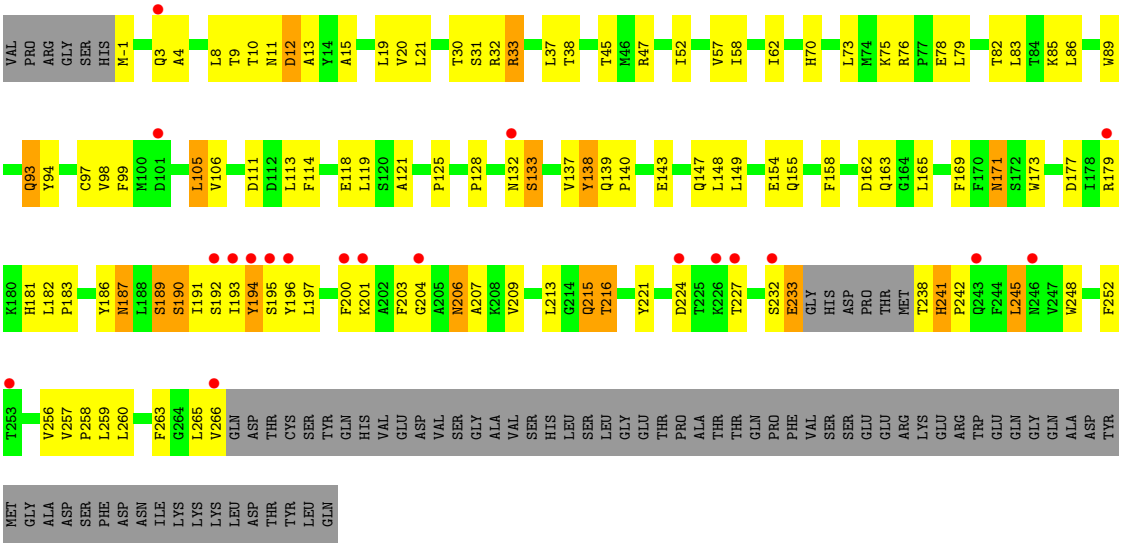
- Molecule 1: GLYCOGENIN-1

Chain C:



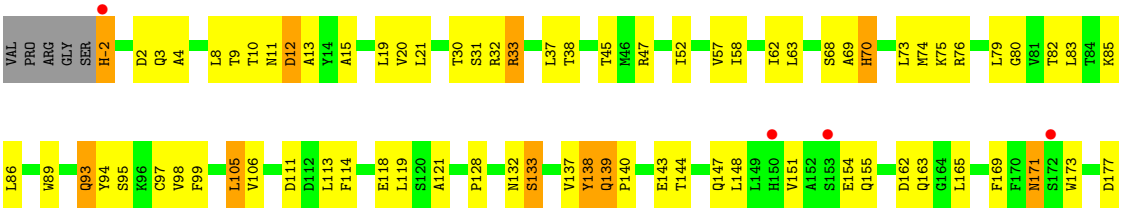
- Molecule 1: GLYCOGENIN-1

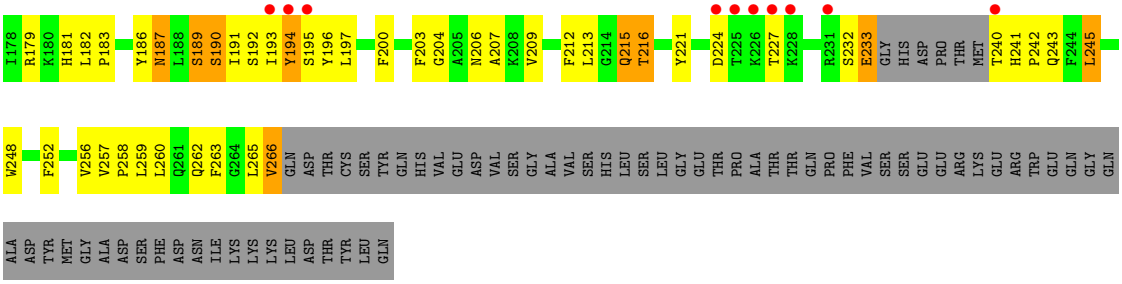
Chain D:



- Molecule 1: GLYCOGENIN-1

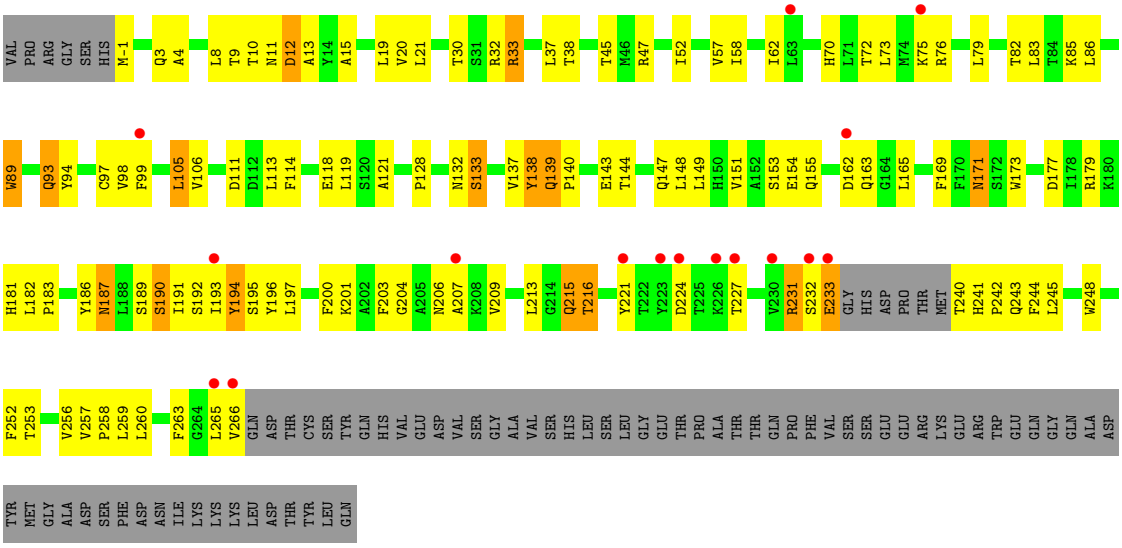
Chain E:





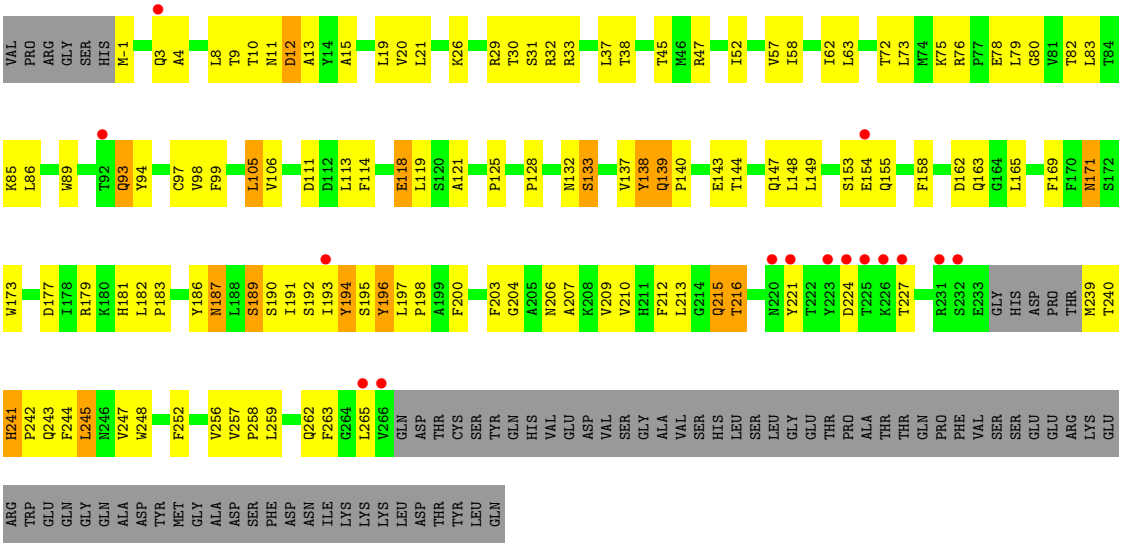
- Molecule 1: GLYCOGENIN-1

Chain F:



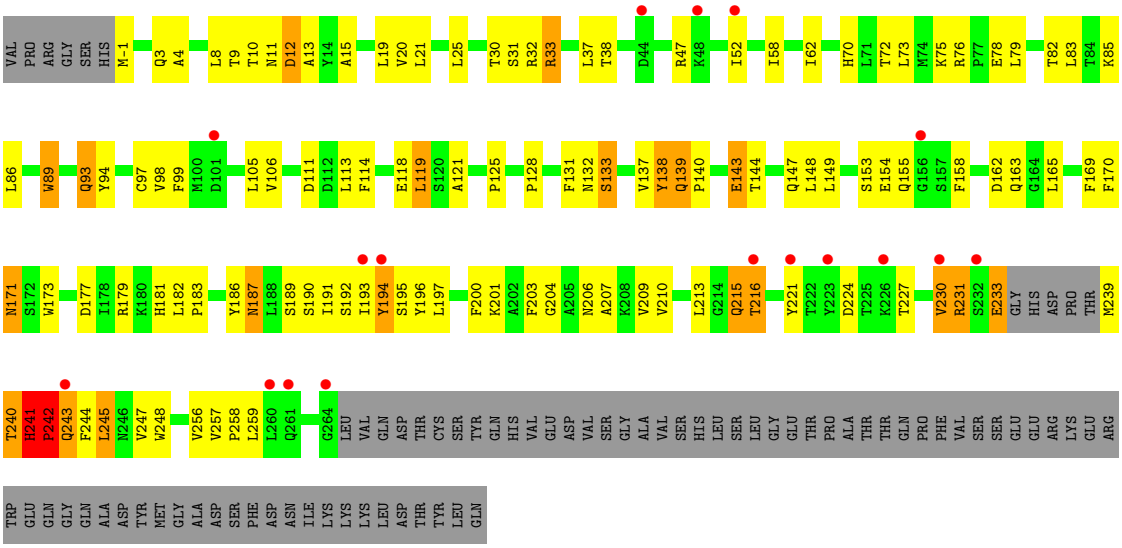
- Molecule 1: GLYCOGENIN-1

Chain G:



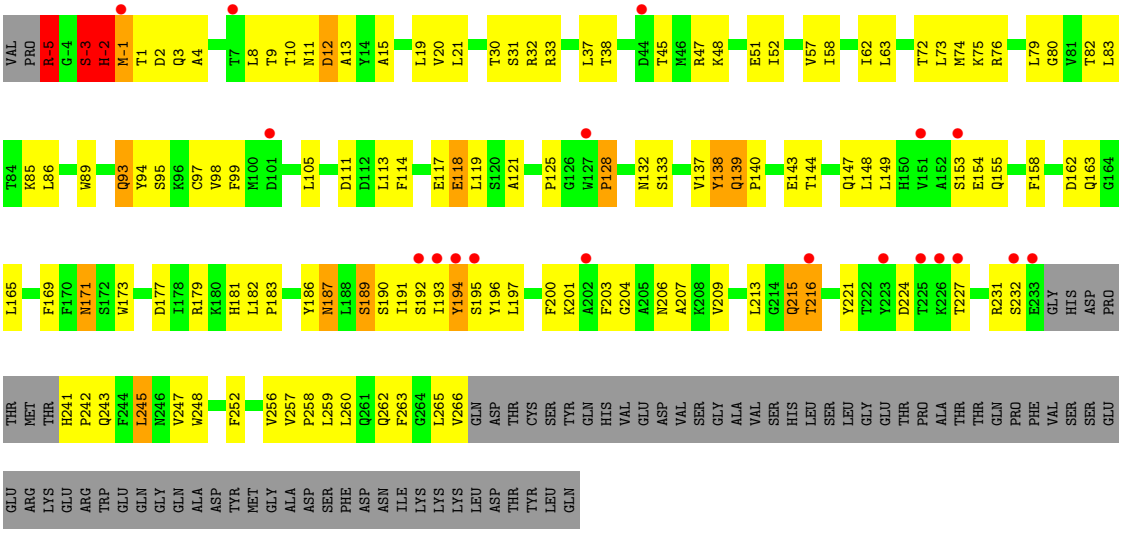
- Molecule 1: GLYCOGENIN-1

Chain H:



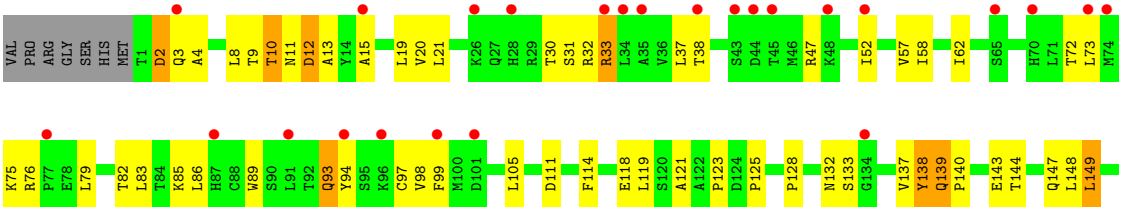
- Molecule 1: GLYCOGENIN-1

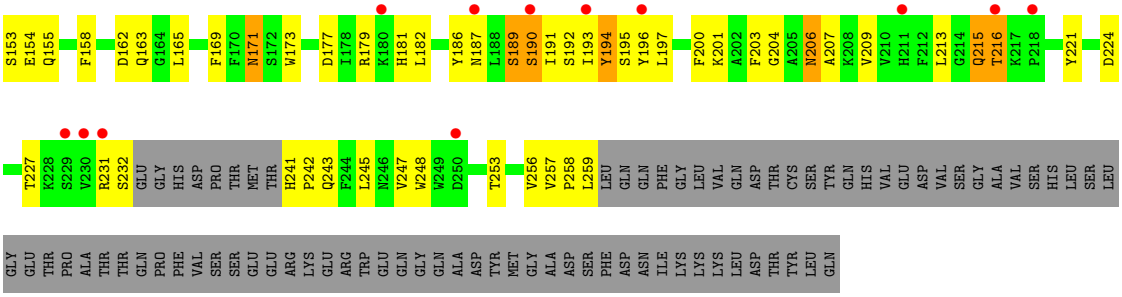
Chain I:



- Molecule 1: GLYCOGENIN-1

Chain J:




S153
E154
Q155
F158
D162
Q163
G164
L165
F169
F170
N171
S172
W173
D177
I178
R179
K180
H181
L182
Y186
N187
L188
S189
S190
I191
S192
I193
Y194
S195
Y196
L197
F200
K201
A202
F203
G204
A205
N206
A207
K208
V209
V210
H211
F212
L213
G214
Q215
T216
K217
P218
Y221
D224
T227
K228
S229
V230
R231
S232
GLU
GLY
HIS
ASP
PRO
THR
MET
THR
H241
P242
Q243
F244
L245
N246
V247
W248
W249
D250
T253
V256
V257
P258
L259
LEU
GLN
GLN
PHE
GLY
LEU
VAL
GLN
ASP
THR
CYS
SER
TYR
GLN
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GLU
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GLU
ARG
TRP
GLU
GLN
GLY
GLN
ALA
ASP
TYR
MET
GLY
ALA
ASP
SER
PHE
ASP
ASN
ILE
LYS
LYS
LYS
LEU
ASP
THR
TYR
LEU
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.46Å 139.46Å 416.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.43 29.87 – 3.43	Depositor EDS
% Data completeness (in resolution range)	95.8 (25.00-3.43) 95.8 (29.87-3.43)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.44 (at 3.47Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.287 0.245 , 0.246	Depositor DCC
R_{free} test set	2837 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	90.2	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 80.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	20736	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.55	1/2146 (0.0%)	0.75	4/2927 (0.1%)
1	B	0.64	4/2170 (0.2%)	0.78	6/2958 (0.2%)
1	C	0.52	0/2130	0.70	2/2904 (0.1%)
1	D	0.54	0/2123	0.74	4/2893 (0.1%)
1	E	0.50	0/2135	0.71	3/2911 (0.1%)
1	F	0.52	0/2124	0.73	2/2896 (0.1%)
1	G	0.49	0/2132	0.71	2/2906 (0.1%)
1	H	0.62	2/2117 (0.1%)	0.80	8/2885 (0.3%)
1	I	0.55	2/2149 (0.1%)	0.76	5/2928 (0.2%)
1	J	0.50	0/2043	0.71	3/2787 (0.1%)
All	All	0.55	9/21269 (0.0%)	0.74	39/28995 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	7

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	LEU	N-CA	10.90	1.68	1.46
1	H	241	HIS	C-N	8.55	1.50	1.34
1	A	188	LEU	N-CA	8.08	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	241	HIS	CA-C	6.87	1.70	1.52
1	B	120	SER	N-CA	5.77	1.57	1.46

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	187	ASN	O-C-N	-14.53	99.45	122.70
1	A	208	LYS	N-CA-CB	11.37	131.07	110.60
1	D	187	ASN	O-C-N	-11.09	104.95	122.70
1	H	187	ASN	O-C-N	-11.06	105.00	122.70
1	G	187	ASN	O-C-N	-11.02	105.07	122.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	187	ASN	Mainchain
1	D	187	ASN	Mainchain
1	E	187	ASN	Mainchain
1	F	187	ASN	Mainchain
1	G	187	ASN	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2092	0	2048	155	0
1	B	2115	0	2074	157	0
1	C	2077	0	2037	144	0
1	D	2071	0	2026	109	0
1	E	2081	0	2034	127	0
1	F	2071	0	2026	119	0
1	G	2079	0	2036	137	0
1	H	2064	0	2016	122	0
1	I	2095	0	2048	140	0
1	J	1991	0	1946	100	0
All	All	20736	0	20291	1274	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

The worst 5 of 1274 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LEU:N	1:B:188:LEU:CA	1.68	1.52
1:A:193:ILE:CB	1:A:240:THR:HG21	1.55	1.37
1:B:200:PHE:CE2	1:B:240:THR:HB	1.58	1.36
1:A:193:ILE:HB	1:A:240:THR:CG2	1.57	1.32
1:C:200:PHE:CE2	1:C:240:THR:HB	1.66	1.30

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/339 (77%)	223 (86%)	31 (12%)	6 (2%)	6	35
1	B	263/339 (78%)	223 (85%)	31 (12%)	9 (3%)	3	27
1	C	258/339 (76%)	220 (85%)	33 (13%)	5 (2%)	8	38
1	D	256/339 (76%)	219 (86%)	31 (12%)	6 (2%)	6	35
1	E	258/339 (76%)	224 (87%)	28 (11%)	6 (2%)	6	35
1	F	257/339 (76%)	221 (86%)	29 (11%)	7 (3%)	5	32
1	G	258/339 (76%)	225 (87%)	28 (11%)	5 (2%)	8	38
1	H	256/339 (76%)	221 (86%)	26 (10%)	9 (4%)	3	26
1	I	260/339 (77%)	226 (87%)	30 (12%)	4 (2%)	10	43
1	J	247/339 (73%)	213 (86%)	30 (12%)	4 (2%)	9	42
All	All	2573/3390 (76%)	2215 (86%)	297 (12%)	61 (2%)	6	34

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	240	THR
1	H	241	HIS
1	A	128	PRO
1	A	190	SER
1	A	215	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/299 (78%)	211 (90%)	23 (10%)	8	32
1	B	236/299 (79%)	214 (91%)	22 (9%)	9	34
1	C	232/299 (78%)	209 (90%)	23 (10%)	8	32
1	D	231/299 (77%)	207 (90%)	24 (10%)	7	30
1	E	232/299 (78%)	209 (90%)	23 (10%)	8	32
1	F	231/299 (77%)	210 (91%)	21 (9%)	9	35
1	G	232/299 (78%)	210 (90%)	22 (10%)	8	33
1	H	230/299 (77%)	206 (90%)	24 (10%)	7	30
1	I	233/299 (78%)	211 (91%)	22 (9%)	8	34
1	J	222/299 (74%)	200 (90%)	22 (10%)	8	32
All	All	2313/2990 (77%)	2087 (90%)	226 (10%)	8	32

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	-1	MET
1	J	196	TYR
1	G	119	LEU
1	J	189	SER
1	I	196	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	109	ASN
1	H	163	GLN
1	G	146	ASN
1	H	93	GLN
1	I	93	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	238:THR	C	241:HIS	N	5.99

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	264/339 (77%)	0.13	10 (3%)	40	39	12, 58, 138, 194	0
1	B	267/339 (78%)	0.17	13 (4%)	29	30	16, 49, 129, 200	0
1	C	262/339 (77%)	0.02	8 (3%)	49	48	18, 49, 119, 189	0
1	D	261/339 (76%)	0.24	20 (7%)	13	16	25, 61, 143, 200	0
1	E	262/339 (77%)	0.14	14 (5%)	26	27	23, 56, 122, 200	0
1	F	261/339 (76%)	0.32	16 (6%)	21	23	27, 73, 151, 189	0
1	G	262/339 (77%)	0.25	15 (5%)	23	24	21, 56, 130, 199	0
1	H	260/339 (76%)	0.35	17 (6%)	18	20	30, 75, 154, 200	0
1	I	264/339 (77%)	0.17	19 (7%)	15	18	19, 59, 134, 187	0
1	J	251/339 (74%)	0.73	37 (14%)	2	3	48, 99, 160, 200	0
All	All	2614/3390 (77%)	0.25	169 (6%)	18	20	12, 63, 145, 200	0

The worst 5 of 169 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	SER	6.7
1	J	52	ILE	5.6
1	D	227	THR	5.2
1	H	193	ILE	5.2
1	A	216	THR	5.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.