wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 01:16 AM EDT

PDB ID	:	7U39
Title	:	Structure of the apo form of Streptomyces venezuelae GlgX, the glycogen debranching enzyme
Authors	:	Schumacher, M.A.
Deposited on	:	2022-02-26
Resolution	:	3.51 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:

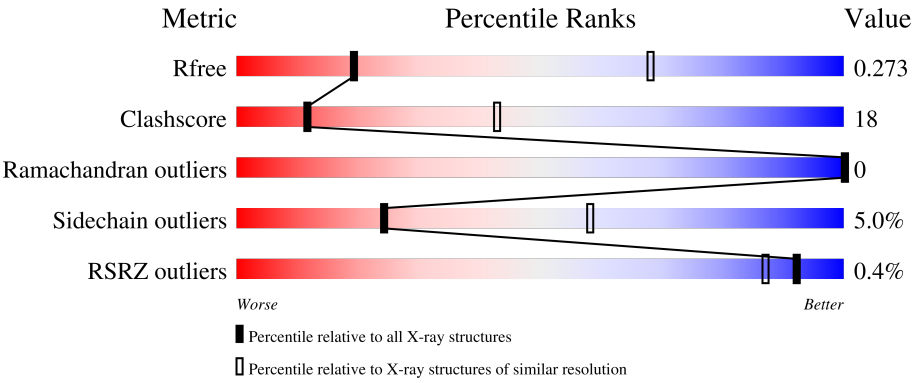
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.51 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	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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	709	60% 37%
1	B	709	% 59% 37%
1	C	709	56% 41%
1	D	709	60% 37%
1	E	709	60% 36%

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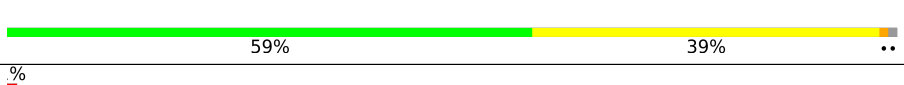
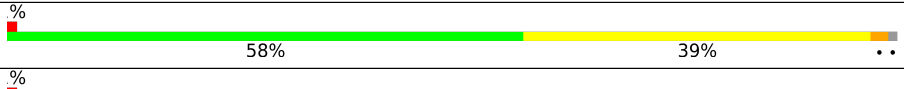
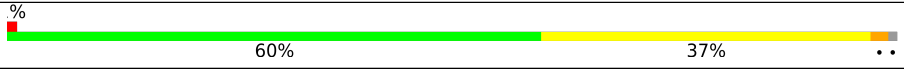
Mol	Chain	Length	Quality of chain
1	F	709	
1	G	709	
1	H	709	
1	I	709	
1	J	709	
1	K	709	
1	L	709	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 67324 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 Glycogen debranching enzyme GlgX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	703	Total	C	N	O	S	0	0	0
			5567	3499	1002	1042	24			
1	B	705	Total	C	N	O	S	0	0	0
			5595	3514	1013	1044	24			
1	C	699	Total	C	N	O	S	0	0	0
			5551	3487	1003	1037	24			
1	D	700	Total	C	N	O	S	0	0	0
			5566	3495	1007	1041	23			
1	E	700	Total	C	N	O	S	0	0	0
			5567	3497	1003	1044	23			
1	F	698	Total	C	N	O	S	0	0	0
			5549	3486	1003	1037	23			
1	G	698	Total	C	N	O	S	0	0	0
			5554	3490	1004	1037	23			
1	H	701	Total	C	N	O	S	0	0	0
			5570	3499	1009	1038	24			
1	I	701	Total	C	N	O	S	0	0	0
			5583	3506	1012	1042	23			
1	J	700	Total	C	N	O	S	0	0	0
			5557	3491	1001	1041	24			
1	K	701	Total	C	N	O	S	0	0	0
			5583	3506	1012	1042	23			
1	L	701	Total	C	N	O	S	0	0	0
			5564	3494	1004	1043	23			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A5P2ALW6
A	-1	SER	-	expression tag	UNP A0A5P2ALW6
A	0	HIS	-	expression tag	UNP A0A5P2ALW6
A	103	VAL	ILE	conflict	UNP A0A5P2ALW6
A	192	ARG	LYS	conflict	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	296	ALA	SER	conflict	UNP A0A5P2ALW6
A	297	ASP	ASN	conflict	UNP A0A5P2ALW6
A	303	MET	THR	conflict	UNP A0A5P2ALW6
A	682	GLN	GLU	conflict	UNP A0A5P2ALW6
B	-2	GLY	-	expression tag	UNP A0A5P2ALW6
B	-1	SER	-	expression tag	UNP A0A5P2ALW6
B	0	HIS	-	expression tag	UNP A0A5P2ALW6
B	103	VAL	ILE	conflict	UNP A0A5P2ALW6
B	192	ARG	LYS	conflict	UNP A0A5P2ALW6
B	296	ALA	SER	conflict	UNP A0A5P2ALW6
B	297	ASP	ASN	conflict	UNP A0A5P2ALW6
B	303	MET	THR	conflict	UNP A0A5P2ALW6
B	682	GLN	GLU	conflict	UNP A0A5P2ALW6
C	-2	GLY	-	expression tag	UNP A0A5P2ALW6
C	-1	SER	-	expression tag	UNP A0A5P2ALW6
C	0	HIS	-	expression tag	UNP A0A5P2ALW6
C	103	VAL	ILE	conflict	UNP A0A5P2ALW6
C	192	ARG	LYS	conflict	UNP A0A5P2ALW6
C	296	ALA	SER	conflict	UNP A0A5P2ALW6
C	297	ASP	ASN	conflict	UNP A0A5P2ALW6
C	303	MET	THR	conflict	UNP A0A5P2ALW6
C	682	GLN	GLU	conflict	UNP A0A5P2ALW6
D	-2	GLY	-	expression tag	UNP A0A5P2ALW6
D	-1	SER	-	expression tag	UNP A0A5P2ALW6
D	0	HIS	-	expression tag	UNP A0A5P2ALW6
D	103	VAL	ILE	conflict	UNP A0A5P2ALW6
D	192	ARG	LYS	conflict	UNP A0A5P2ALW6
D	296	ALA	SER	conflict	UNP A0A5P2ALW6
D	297	ASP	ASN	conflict	UNP A0A5P2ALW6
D	303	MET	THR	conflict	UNP A0A5P2ALW6
D	682	GLN	GLU	conflict	UNP A0A5P2ALW6
E	-2	GLY	-	expression tag	UNP A0A5P2ALW6
E	-1	SER	-	expression tag	UNP A0A5P2ALW6
E	0	HIS	-	expression tag	UNP A0A5P2ALW6
E	103	VAL	ILE	conflict	UNP A0A5P2ALW6
E	192	ARG	LYS	conflict	UNP A0A5P2ALW6
E	296	ALA	SER	conflict	UNP A0A5P2ALW6
E	297	ASP	ASN	conflict	UNP A0A5P2ALW6
E	303	MET	THR	conflict	UNP A0A5P2ALW6
E	682	GLN	GLU	conflict	UNP A0A5P2ALW6
F	-2	GLY	-	expression tag	UNP A0A5P2ALW6
F	-1	SER	-	expression tag	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP A0A5P2ALW6
F	103	VAL	ILE	conflict	UNP A0A5P2ALW6
F	192	ARG	LYS	conflict	UNP A0A5P2ALW6
F	296	ALA	SER	conflict	UNP A0A5P2ALW6
F	297	ASP	ASN	conflict	UNP A0A5P2ALW6
F	303	MET	THR	conflict	UNP A0A5P2ALW6
F	682	GLN	GLU	conflict	UNP A0A5P2ALW6
G	-2	GLY	-	expression tag	UNP A0A5P2ALW6
G	-1	SER	-	expression tag	UNP A0A5P2ALW6
G	0	HIS	-	expression tag	UNP A0A5P2ALW6
G	103	VAL	ILE	conflict	UNP A0A5P2ALW6
G	192	ARG	LYS	conflict	UNP A0A5P2ALW6
G	296	ALA	SER	conflict	UNP A0A5P2ALW6
G	297	ASP	ASN	conflict	UNP A0A5P2ALW6
G	303	MET	THR	conflict	UNP A0A5P2ALW6
G	682	GLN	GLU	conflict	UNP A0A5P2ALW6
H	-2	GLY	-	expression tag	UNP A0A5P2ALW6
H	-1	SER	-	expression tag	UNP A0A5P2ALW6
H	0	HIS	-	expression tag	UNP A0A5P2ALW6
H	103	VAL	ILE	conflict	UNP A0A5P2ALW6
H	192	ARG	LYS	conflict	UNP A0A5P2ALW6
H	296	ALA	SER	conflict	UNP A0A5P2ALW6
H	297	ASP	ASN	conflict	UNP A0A5P2ALW6
H	303	MET	THR	conflict	UNP A0A5P2ALW6
H	682	GLN	GLU	conflict	UNP A0A5P2ALW6
I	-2	GLY	-	expression tag	UNP A0A5P2ALW6
I	-1	SER	-	expression tag	UNP A0A5P2ALW6
I	0	HIS	-	expression tag	UNP A0A5P2ALW6
I	103	VAL	ILE	conflict	UNP A0A5P2ALW6
I	192	ARG	LYS	conflict	UNP A0A5P2ALW6
I	296	ALA	SER	conflict	UNP A0A5P2ALW6
I	297	ASP	ASN	conflict	UNP A0A5P2ALW6
I	303	MET	THR	conflict	UNP A0A5P2ALW6
I	682	GLN	GLU	conflict	UNP A0A5P2ALW6
J	-2	GLY	-	expression tag	UNP A0A5P2ALW6
J	-1	SER	-	expression tag	UNP A0A5P2ALW6
J	0	HIS	-	expression tag	UNP A0A5P2ALW6
J	103	VAL	ILE	conflict	UNP A0A5P2ALW6
J	192	ARG	LYS	conflict	UNP A0A5P2ALW6
J	296	ALA	SER	conflict	UNP A0A5P2ALW6
J	297	ASP	ASN	conflict	UNP A0A5P2ALW6
J	303	MET	THR	conflict	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	682	GLN	GLU	conflict	UNP A0A5P2ALW6
K	-2	GLY	-	expression tag	UNP A0A5P2ALW6
K	-1	SER	-	expression tag	UNP A0A5P2ALW6
K	0	HIS	-	expression tag	UNP A0A5P2ALW6
K	103	VAL	ILE	conflict	UNP A0A5P2ALW6
K	192	ARG	LYS	conflict	UNP A0A5P2ALW6
K	296	ALA	SER	conflict	UNP A0A5P2ALW6
K	297	ASP	ASN	conflict	UNP A0A5P2ALW6
K	303	MET	THR	conflict	UNP A0A5P2ALW6
K	682	GLN	GLU	conflict	UNP A0A5P2ALW6
L	-2	GLY	-	expression tag	UNP A0A5P2ALW6
L	-1	SER	-	expression tag	UNP A0A5P2ALW6
L	0	HIS	-	expression tag	UNP A0A5P2ALW6
L	103	VAL	ILE	conflict	UNP A0A5P2ALW6
L	192	ARG	LYS	conflict	UNP A0A5P2ALW6
L	296	ALA	SER	conflict	UNP A0A5P2ALW6
L	297	ASP	ASN	conflict	UNP A0A5P2ALW6
L	303	MET	THR	conflict	UNP A0A5P2ALW6
L	682	GLN	GLU	conflict	UNP A0A5P2ALW6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	56	Total O 56 56	0	0
2	B	56	Total O 56 56	0	0
2	C	63	Total O 63 63	0	0
2	D	43	Total O 43 43	0	0
2	E	42	Total O 42 42	0	0
2	F	43	Total O 43 43	0	0
2	G	27	Total O 27 27	0	0
2	H	41	Total O 41 41	0	0
2	I	38	Total O 38 38	0	0
2	J	38	Total O 38 38	0	0

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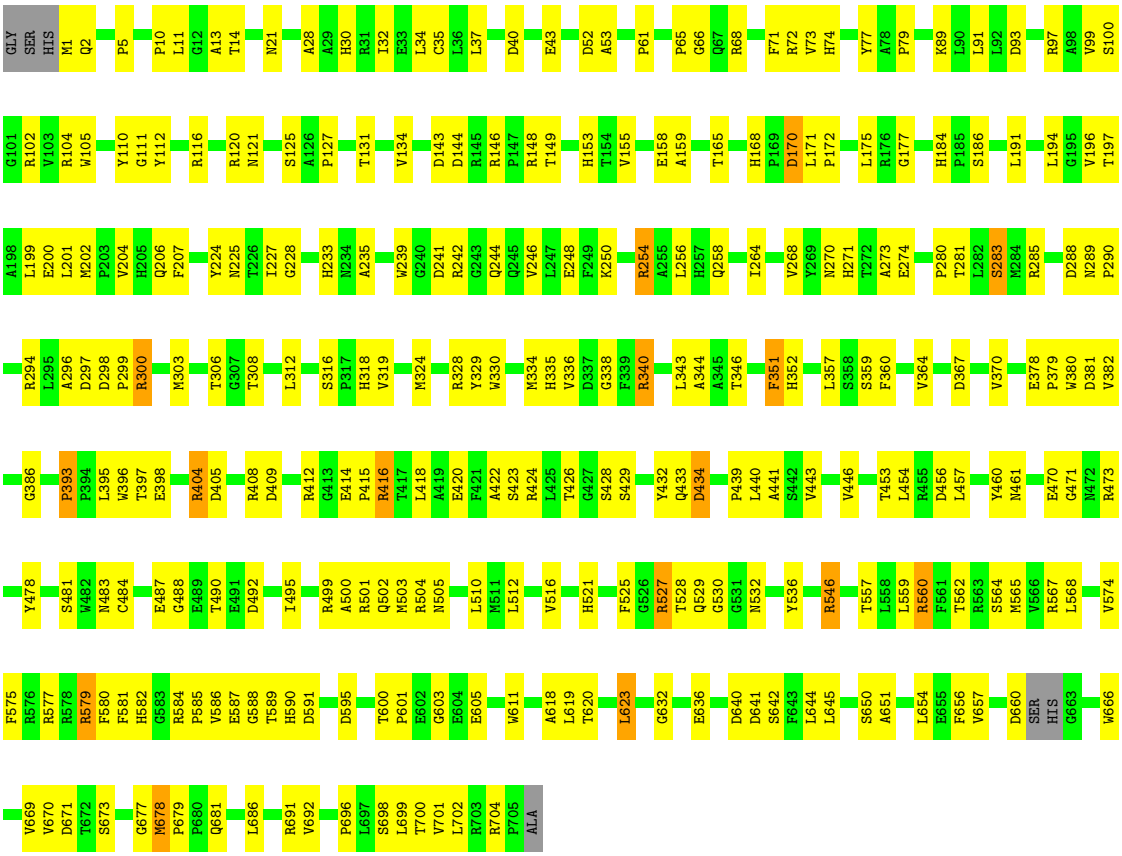
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	37	Total O 37 37	0	0
2	L	34	Total O 34 34	0	0

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.

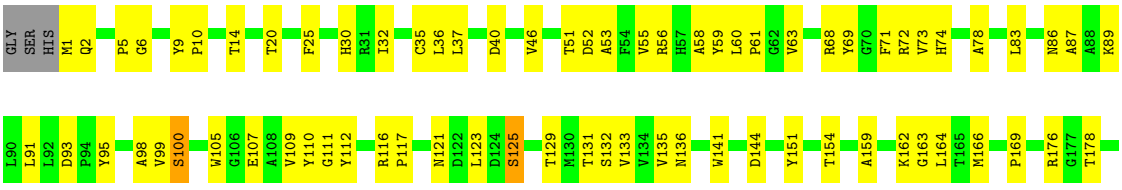
• Molecule 1: Glycogen debranching enzyme GlgX

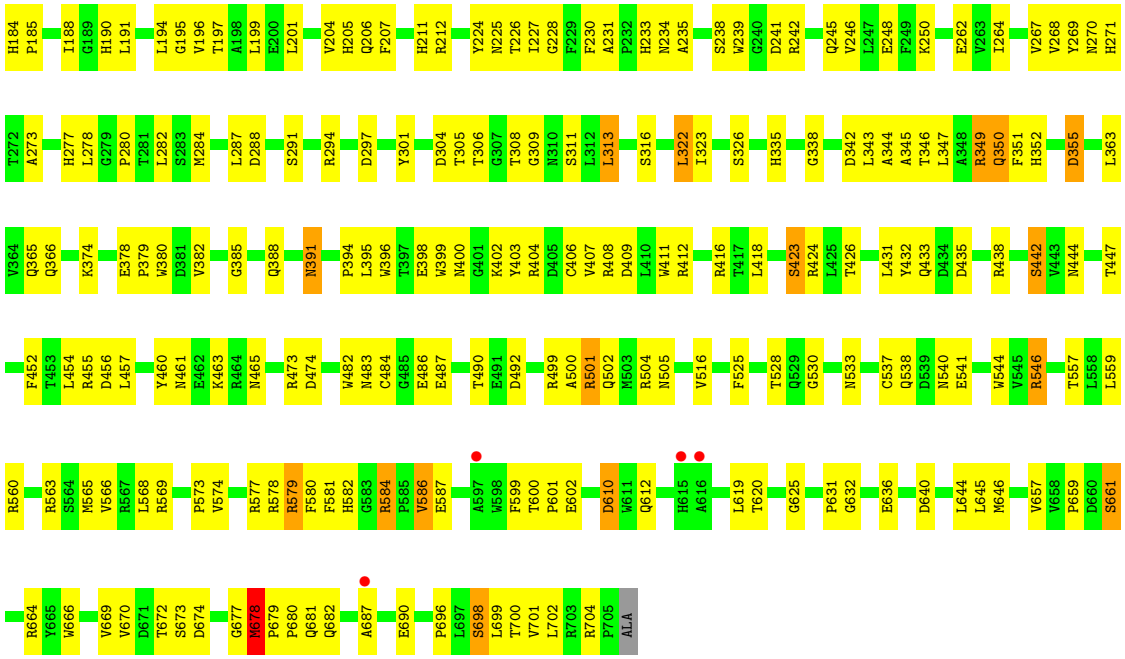
Chain A:



• Molecule 1: Glycogen debranching enzyme GlgX

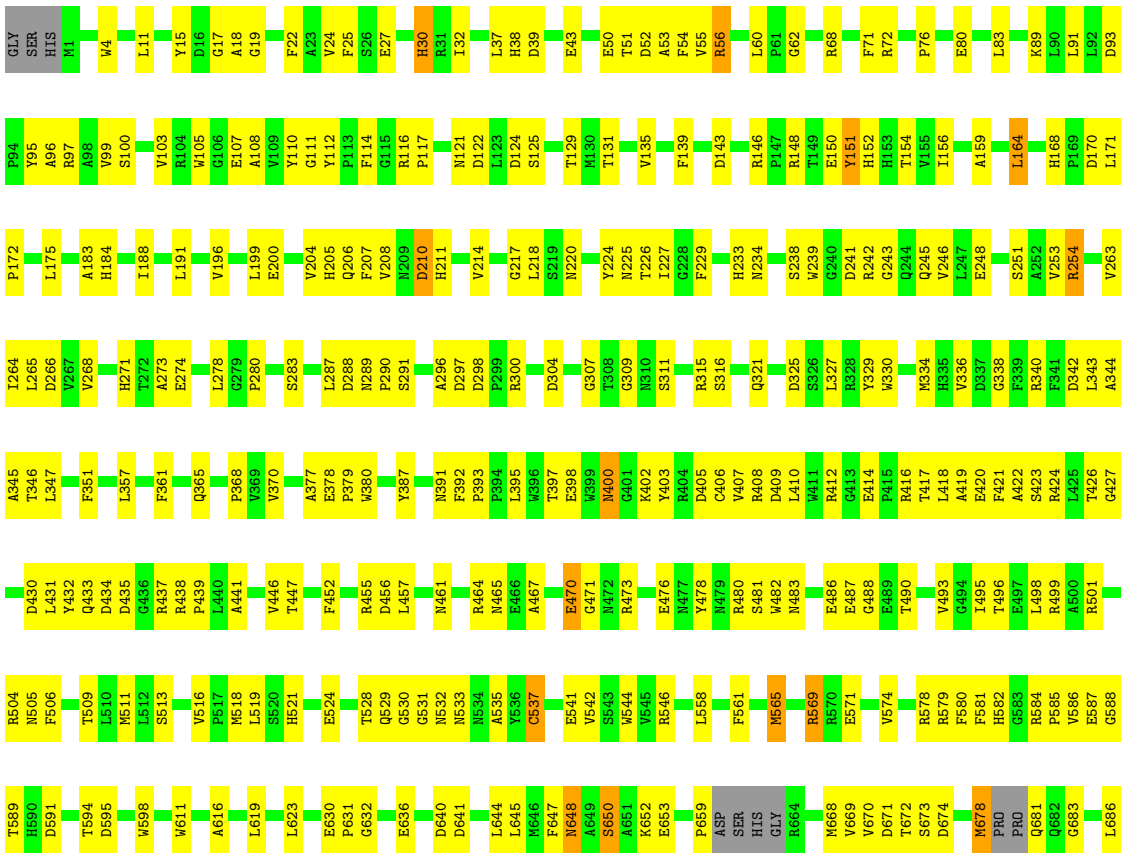
Chain B:

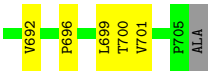




• Molecule 1: Glycogen debranching enzyme GlgX

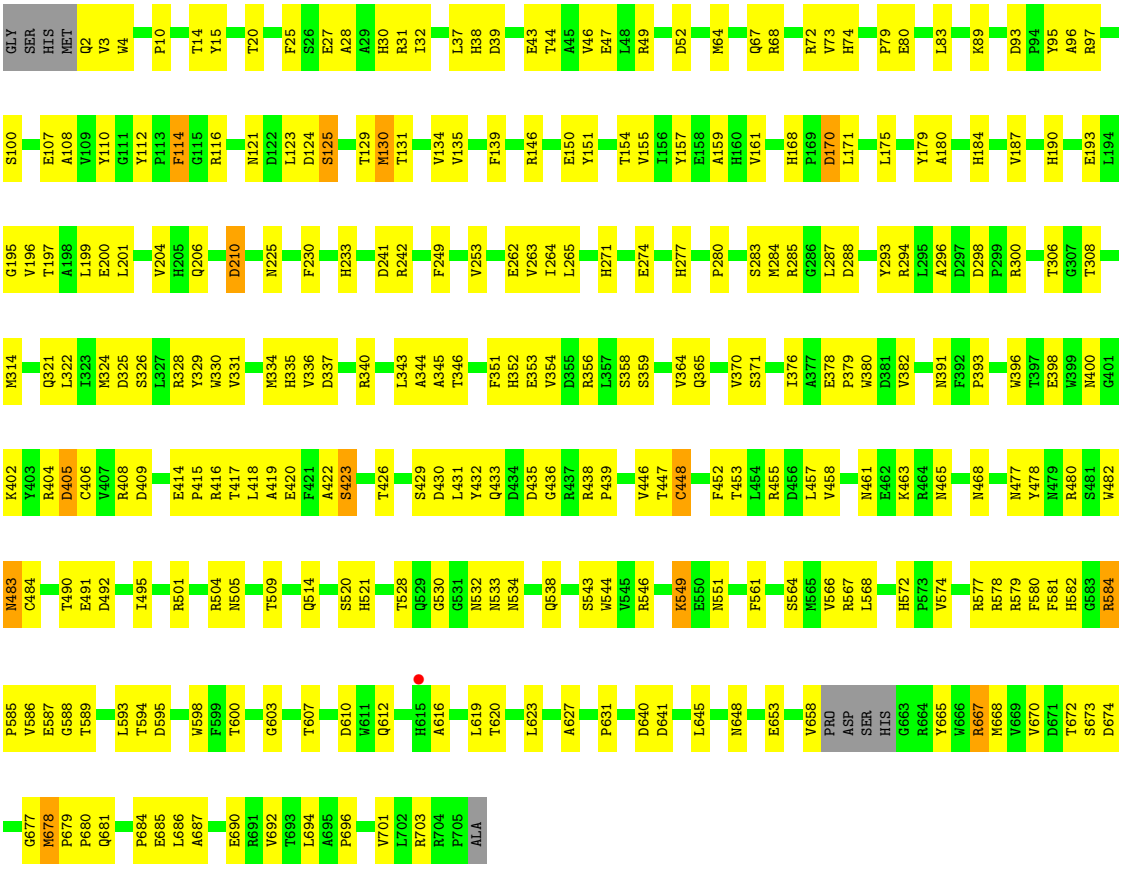
Chain C:





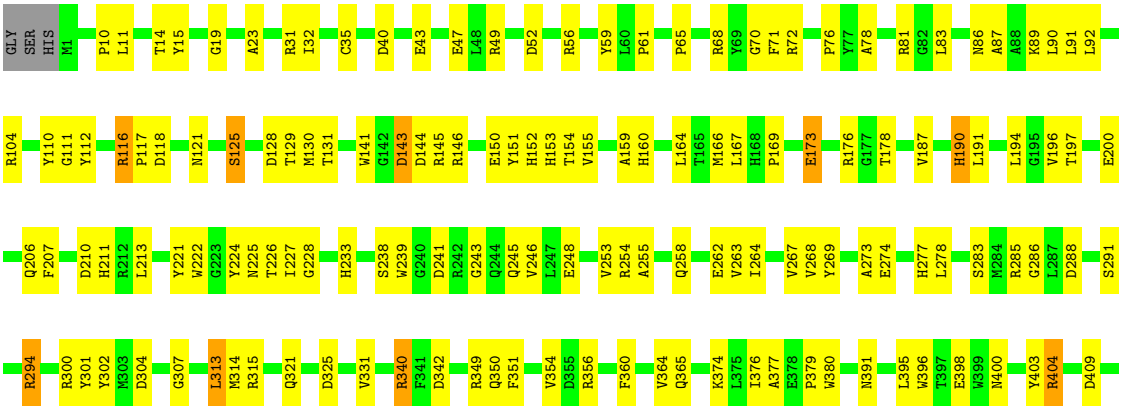
• Molecule 1: Glycogen debranching enzyme GlgX

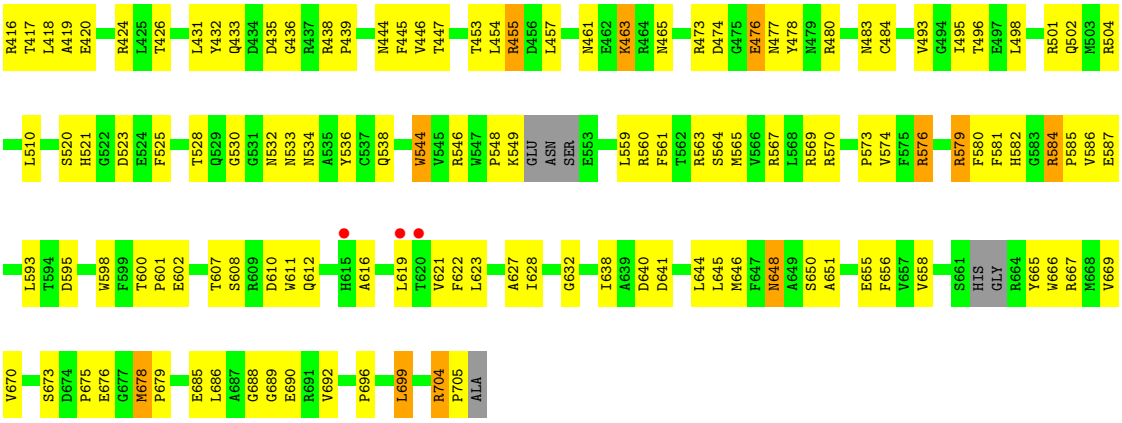
Chain D:



• Molecule 1: Glycogen debranching enzyme GlgX

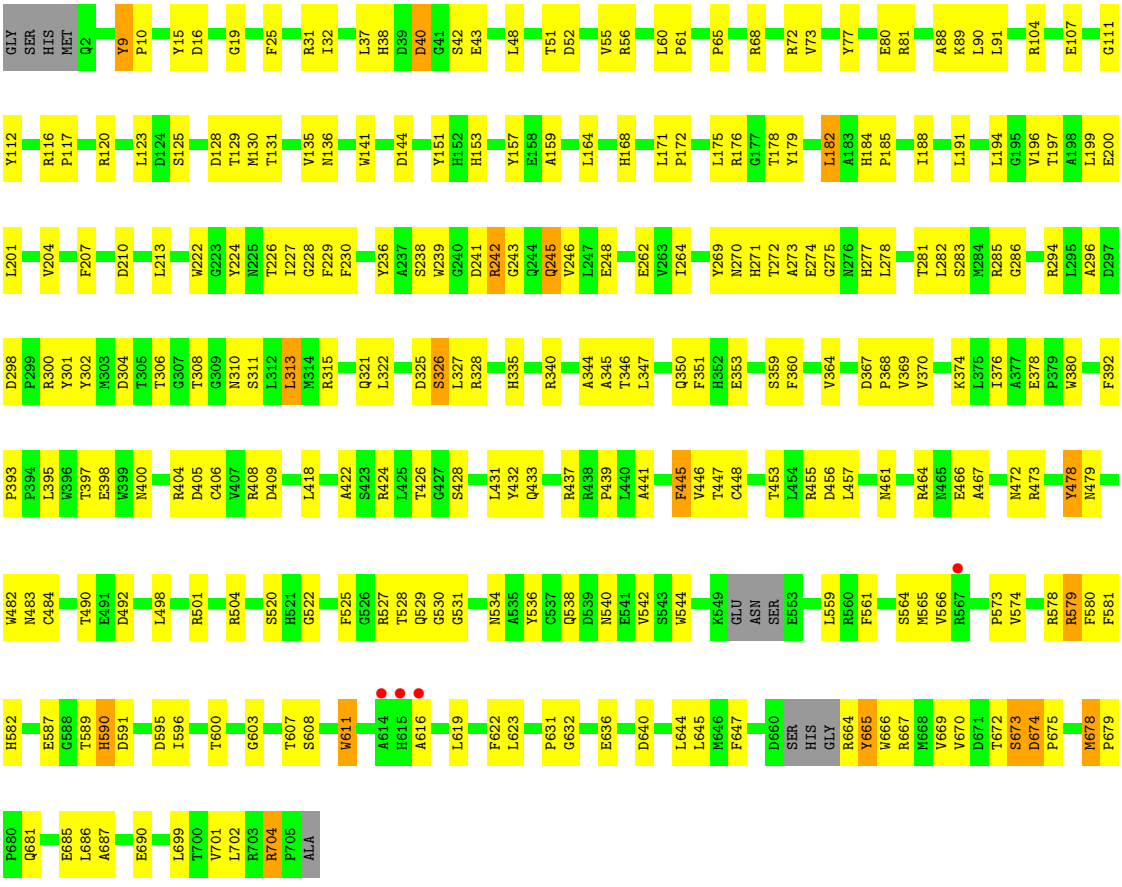
Chain E:





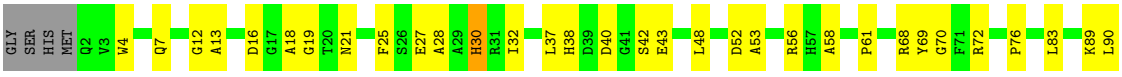
• Molecule 1: Glycogen debranching enzyme GlgX

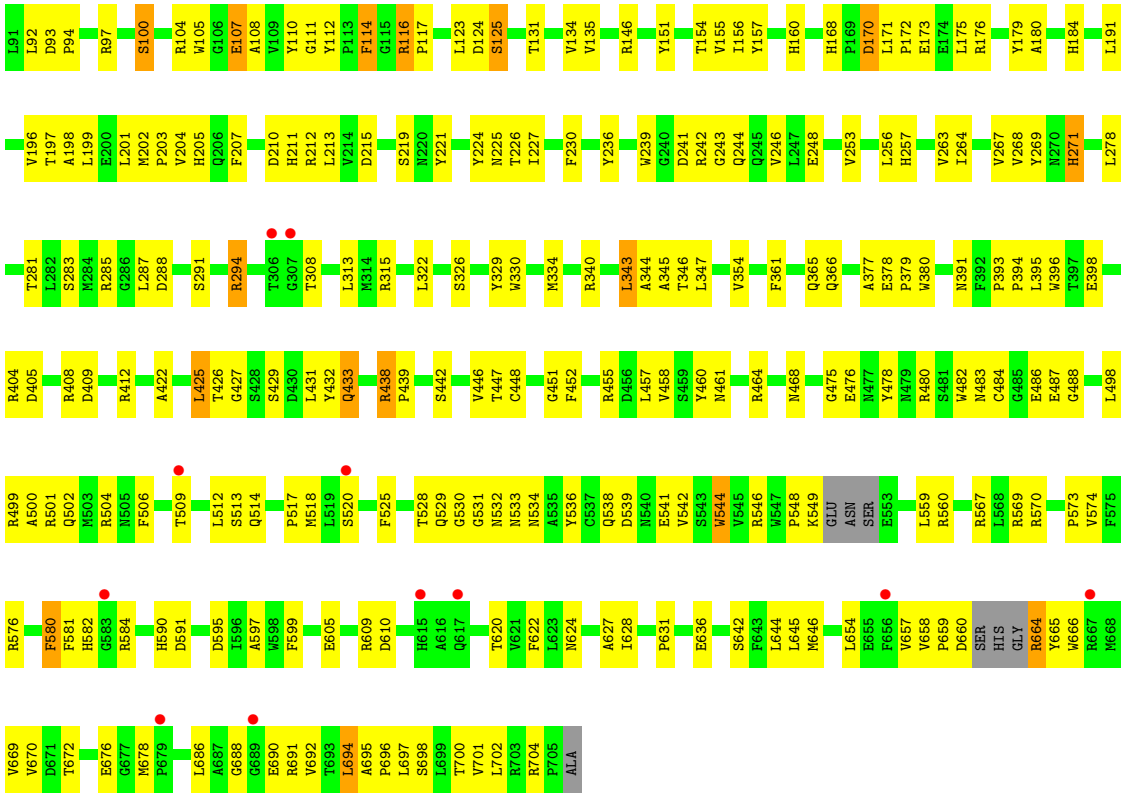
Chain F:



• Molecule 1: Glycogen debranching enzyme GlgX

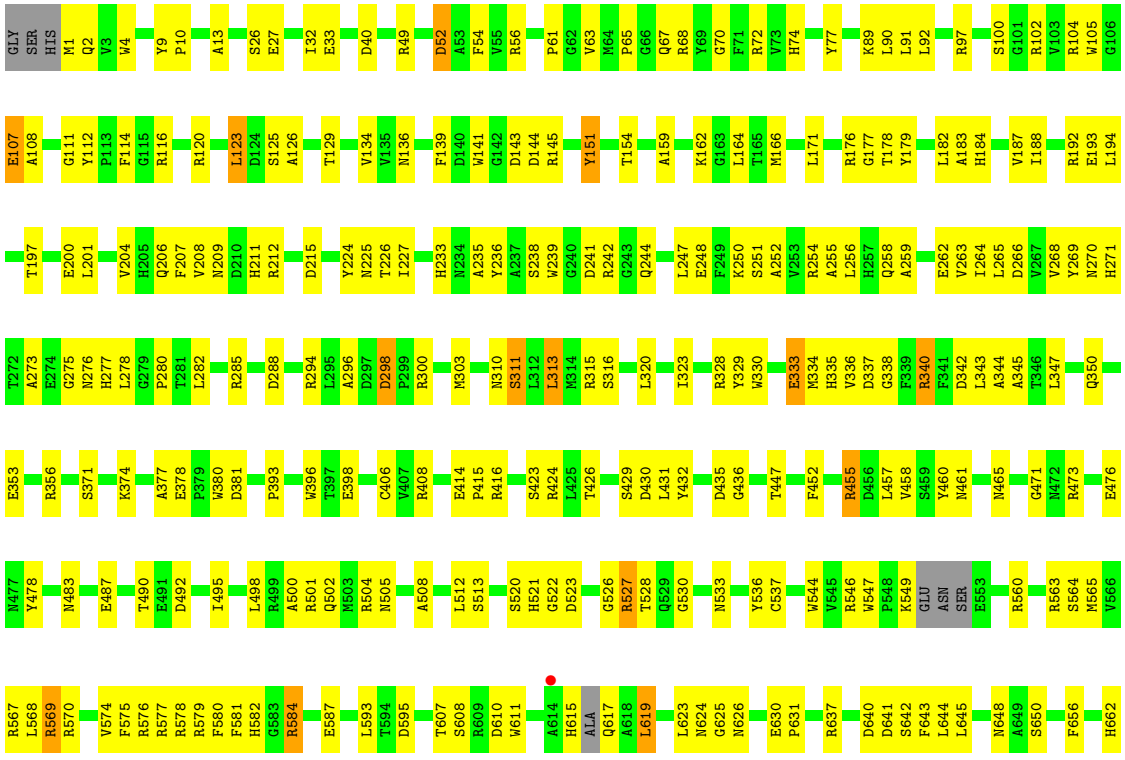
Chain G:

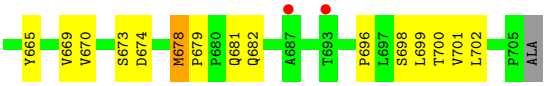




• Molecule 1: Glycogen debranching enzyme GlgX

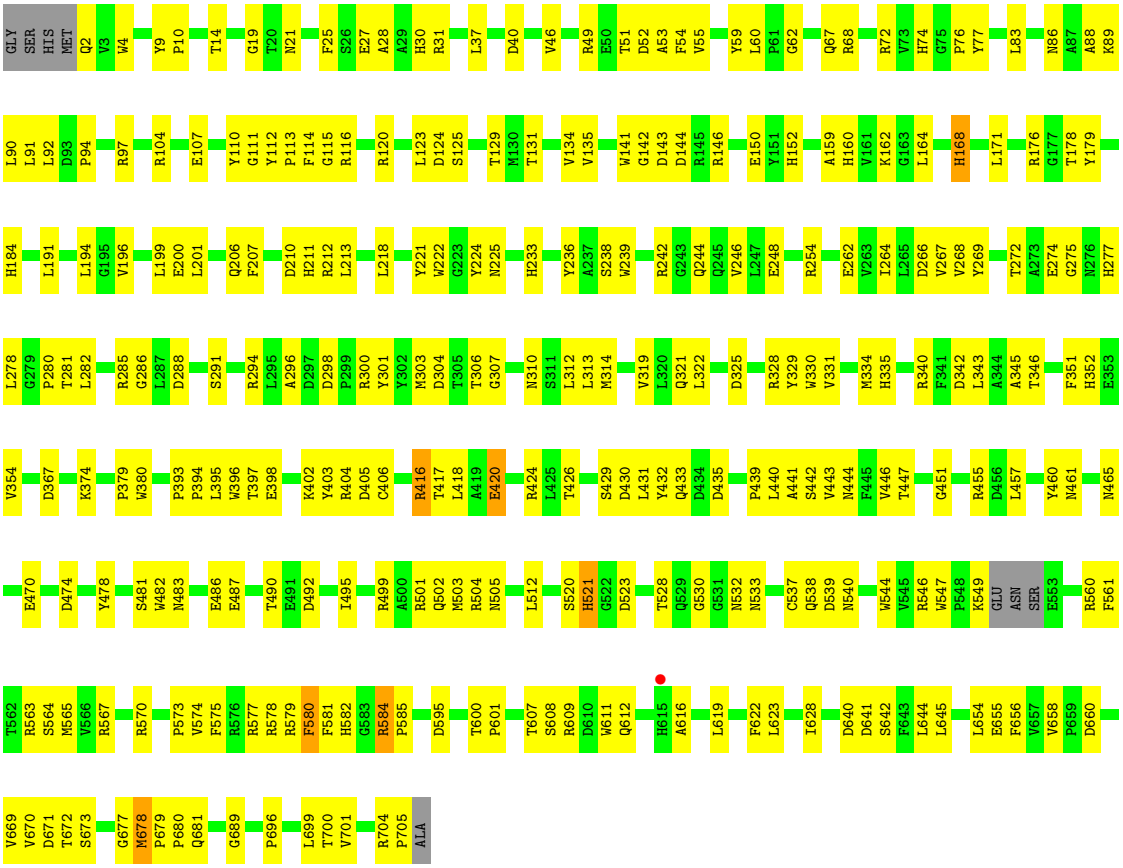
Chain H:





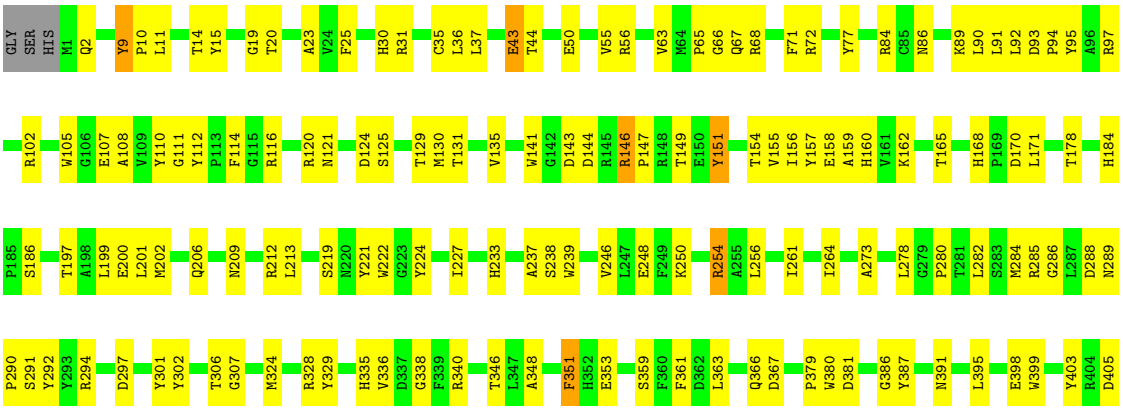
• Molecule 1: Glycogen debranching enzyme GlgX

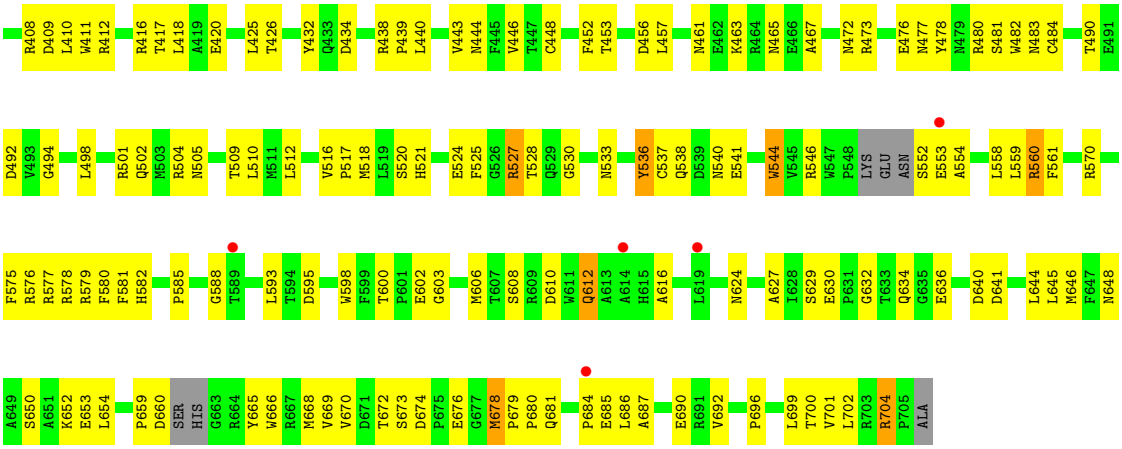
Chain I:



• Molecule 1: Glycogen debranching enzyme GlgX

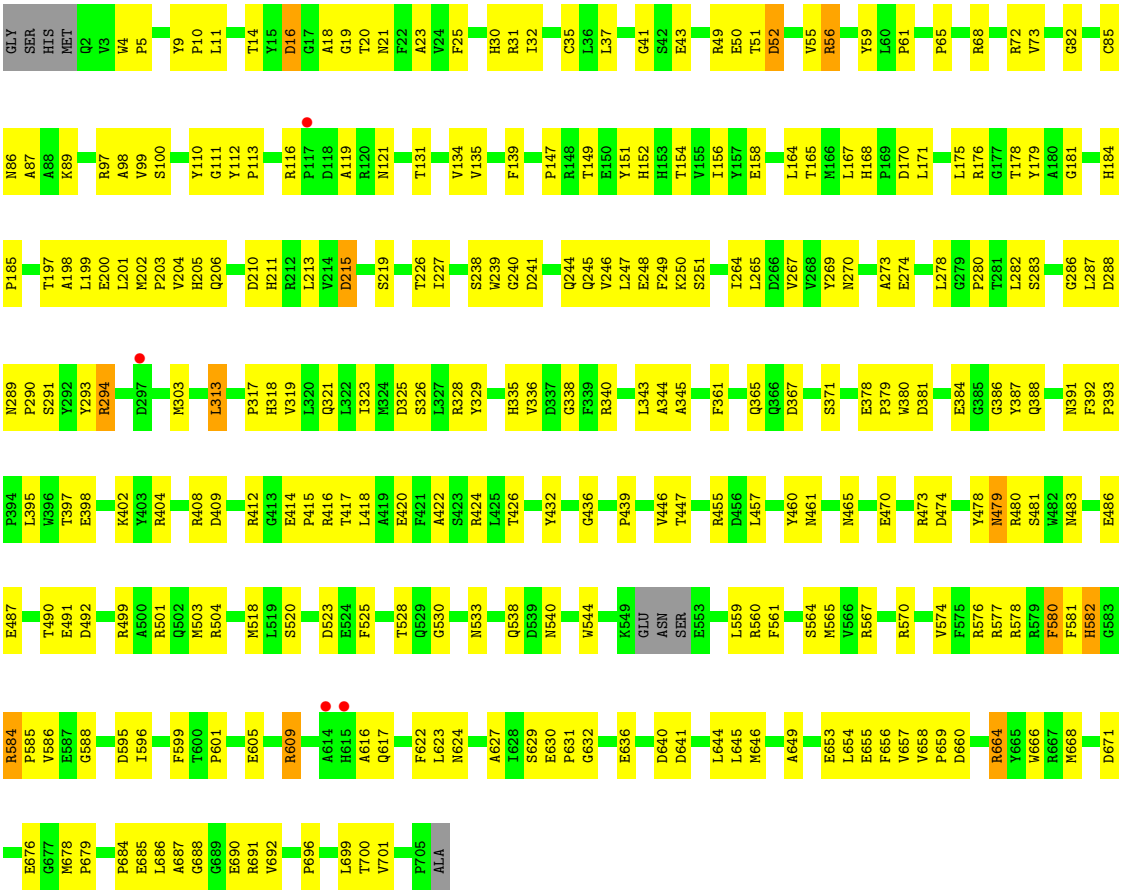
Chain J:





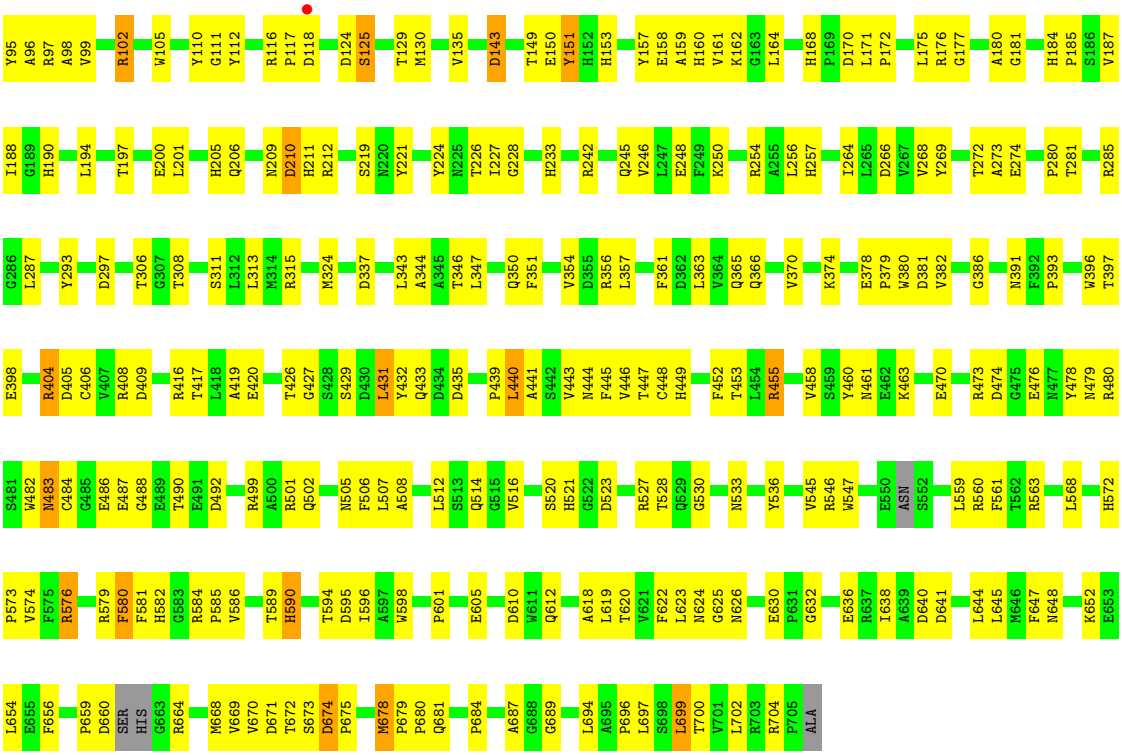
• Molecule 1: Glycogen debranching enzyme GlgX

Chain K:



• Molecule 1: Glycogen debranching enzyme GlgX

Chain L:


Y95 A96 R97 A98 V99 R102 W105 Y110 G111 Y112 R116 P117 D118 D124 S125 T129 M130 V135 D143 T149 E150 Y151 H152 H153 Y157 E158 A159 H160 V161 K162 G163 L164 H168 P169 D170 L171 P172 L175 R176 G177 A180 G181 H184 P185 S186 V187
I188 G189 H190 L194 T197 E200 L201 H205 Q206 N209 D210 H211 R212 S219 N220 Y221 Y224 N225 T226 I227 G228 H233 R242 Q245 V246 L247 E248 F249 K250 R254 A255 L256 H257 I264 L265 D266 V267 V268 Y269 T272 A273 E274 P280 T281 R285
G286 L287 Y293 D297 T306 G307 T308 S311 L312 L313 M314 R315 M324 D337 L343 A344 A345 T346 L347 Q350 F351 V354 D355 R356 L357 F361 D362 L363 V364 Q365 Q366 V370 K374 E378 P379 W380 D381 V382 G386 N391 F392 P393 W396 T397
E398 R404 D405 C406 V407 R408 D409 R416 T417 L418 A419 E420 T426 G427 S428 S429 D430 L431 Y432 Q433 D434 D435 P439 L440 A441 S442 V443 N444 F445 V446 T447 C448 H449 F452 T453 L454 R455 V458 S459 Y460 N461 E462 K463 E470 R473 D474 G475 E476 N477 Y478 N479 R480
S481 W482 N483 C484 G485 E486 E487 G488 E489 T490 E491 D492 R499 A500 R501 Q502 N505 F506 L507 A508 L512 S513 Q514 G515 V516 S520 H521 G522 D523 R527 T528 Q529 G530 N533 Y536 V545 R546 W547 E550 ASN S552 L559 R560 F561 T562 R563 L568 H572
P573 V574 F575 R576 R579 F580 F581 H582 G583 R584 P585 V586 T589 H590 T594 D595 I596 A597 W598 P601 E605 D610 W611 Q612 A618 L619 T620 V621 F622 L623 N624 G625 N626 E630 P631 G632 E636 R637 I638 A639 D640 D641 L644 L645 M646 F647 N648 K652 E653
L654 E655 F656 P659 D660 SER HIS G663 R664 M668 V669 V670 D671 T672 S673 D674 P675 M678 P679 P680 Q681 P684 A687 G688 G689 L694 A695 P696 L697 S698 L699 T700 V701 L702 R703 R704 P705 ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	181.50Å 204.86Å 195.72Å 90.00° 90.43° 90.00°	Depositor
Resolution (Å)	67.92 – 3.51 67.92 – 3.66	Depositor EDS
% Data completeness (in resolution range)	83.5 (67.92-3.51) 83.5 (67.92-3.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.211 , 0.276 0.209 , 0.273	Depositor DCC
R_{free} test set	1920 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.912	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 20.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.037 for -h,-l,-k 0.035 for -h,l,k 0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	67324	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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

5.1 Standard geometry

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	0.30	0/5720	0.58	4/7785 (0.1%)
1	B	0.30	0/5750	0.56	5/7825 (0.1%)
1	C	0.31	0/5700	0.54	0/7752
1	D	0.30	0/5718	0.55	1/7779 (0.0%)
1	E	0.31	0/5719	0.56	0/7781
1	F	0.30	0/5701	0.54	2/7757 (0.0%)
1	G	0.30	0/5706	0.53	0/7763
1	H	0.31	0/5723	0.54	0/7785
1	I	0.29	0/5737	0.54	0/7805
1	J	0.31	0/5709	0.56	2/7768 (0.0%)
1	K	0.30	0/5737	0.56	0/7805
1	L	0.30	0/5715	0.54	3/7776 (0.0%)
All	All	0.30	0/68635	0.55	17/93381 (0.0%)

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	B	0	3
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	L	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	298	ASP	N-CA-C	-8.64	87.67	111.00
1	J	673	SER	C-N-CA	-7.04	104.10	121.70
1	A	298	ASP	CB-CA-C	6.68	123.76	110.40
1	A	546	ARG	C-N-CA	-6.09	106.48	121.70
1	B	673	SER	C-N-CA	-6.05	106.57	121.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	586	VAL	Peptide
1	B	661	SER	Peptide
1	B	678	MET	Peptide
1	D	678	MET	Peptide
1	E	678	MET	Peptide

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	5567	0	5245	200	0
1	B	5595	0	5282	204	0
1	C	5551	0	5244	228	0
1	D	5566	0	5256	179	0
1	E	5567	0	5253	194	0
1	F	5549	0	5234	173	0
1	G	5554	0	5246	186	0
1	H	5570	0	5254	178	0
1	I	5583	0	5274	192	0
1	J	5557	0	5240	199	0
1	K	5583	0	5274	192	0
1	L	5564	0	5244	201	0
2	A	56	0	0	1	0
2	B	56	0	0	0	0
2	C	63	0	0	0	0
2	D	43	0	0	1	0
2	E	42	0	0	2	0
2	F	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	27	0	0	0	0
2	H	41	0	0	1	0
2	I	38	0	0	4	0
2	J	38	0	0	1	0
2	K	37	0	0	0	0
2	L	34	0	0	2	0
All	All	67324	0	63046	2278	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 18.

The worst 5 of 2278 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:H:102:ARG:HH12	1:H:208:VAL:HA	1.32	0.94
1:B:294:ARG:HH22	1:B:305:THR:HG23	1.32	0.94
1:C:493:VAL:HA	1:C:496:THR:HB	1.54	0.90
1:J:391:ASN:HD21	1:K:317:PRO:HG3	1.36	0.90
1:B:501:ARG:NH2	1:B:696:PRO:O	2.05	0.89

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	699/709 (99%)	620 (89%)	79 (11%)	0	100	100
1	B	703/709 (99%)	636 (90%)	67 (10%)	0	100	100
1	C	693/709 (98%)	614 (89%)	79 (11%)	0	100	100
1	D	696/709 (98%)	604 (87%)	92 (13%)	0	100	100
1	E	694/709 (98%)	628 (90%)	66 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	692/709 (98%)	617 (89%)	75 (11%)	0	100	100
1	G	692/709 (98%)	612 (88%)	80 (12%)	0	100	100
1	H	695/709 (98%)	623 (90%)	72 (10%)	0	100	100
1	I	697/709 (98%)	622 (89%)	75 (11%)	0	100	100
1	J	694/709 (98%)	622 (90%)	72 (10%)	0	100	100
1	K	697/709 (98%)	619 (89%)	78 (11%)	0	100	100
1	L	695/709 (98%)	617 (89%)	78 (11%)	0	100	100
All	All	8347/8508 (98%)	7434 (89%)	913 (11%)	0	100	100

There are no Ramachandran outliers to report.

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	576/590 (98%)	551 (96%)	25 (4%)	29	62
1	B	580/590 (98%)	549 (95%)	31 (5%)	22	56
1	C	575/590 (98%)	546 (95%)	29 (5%)	24	58
1	D	578/590 (98%)	548 (95%)	30 (5%)	23	57
1	E	579/590 (98%)	548 (95%)	31 (5%)	22	56
1	F	576/590 (98%)	544 (94%)	32 (6%)	21	55
1	G	577/590 (98%)	544 (94%)	33 (6%)	20	54
1	H	577/590 (98%)	544 (94%)	33 (6%)	20	54
1	I	580/590 (98%)	557 (96%)	23 (4%)	31	64
1	J	577/590 (98%)	548 (95%)	29 (5%)	24	58
1	K	580/590 (98%)	554 (96%)	26 (4%)	27	62
1	L	577/590 (98%)	549 (95%)	28 (5%)	25	59
All	All	6932/7080 (98%)	6582 (95%)	350 (5%)	24	58

5 of 350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	455	ARG
1	J	527	ARG
1	H	584	ARG
1	I	455	ARG
1	K	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	483	ASN
1	L	365	GLN
1	C	391	ASN
1	C	365	GLN
1	L	391	ASN

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)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	703/709 (99%)	-0.31	0 100 100	26, 44, 73, 95	0
1	B	705/709 (99%)	-0.34	4 (0%) 89 81	27, 41, 69, 102	0
1	C	699/709 (98%)	-0.45	0 100 100	25, 41, 70, 93	0
1	D	700/709 (98%)	-0.44	1 (0%) 95 93	28, 45, 73, 112	0
1	E	700/709 (98%)	-0.34	3 (0%) 92 87	27, 46, 72, 106	0
1	F	698/709 (98%)	-0.35	4 (0%) 89 81	26, 43, 72, 98	0
1	G	698/709 (98%)	-0.08	11 (1%) 72 59	30, 56, 87, 113	0
1	H	701/709 (98%)	-0.35	3 (0%) 92 87	30, 43, 73, 96	0
1	I	701/709 (98%)	-0.39	1 (0%) 95 93	29, 45, 75, 96	0
1	J	700/709 (98%)	-0.34	5 (0%) 87 79	27, 44, 74, 103	0
1	K	701/709 (98%)	-0.30	4 (0%) 89 81	31, 49, 79, 122	0
1	L	701/709 (98%)	-0.32	1 (0%) 95 93	34, 50, 78, 102	0
All	All	8407/8508 (98%)	-0.33	37 (0%) 92 87	25, 45, 76, 122	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	615	HIS	4.4
1	F	615	HIS	3.9
1	G	306	THR	3.6
1	K	615	HIS	3.6
1	D	615	HIS	3.5

6.2 Non-standard residues in protein, DNA, RNA chains

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.