



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:06 PM UTC

PDB ID : 7U39 / pdb_00007u39
Title : Structure of the apo form of Streptomyces venezuelae GlgX, the glycogen de-branching 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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

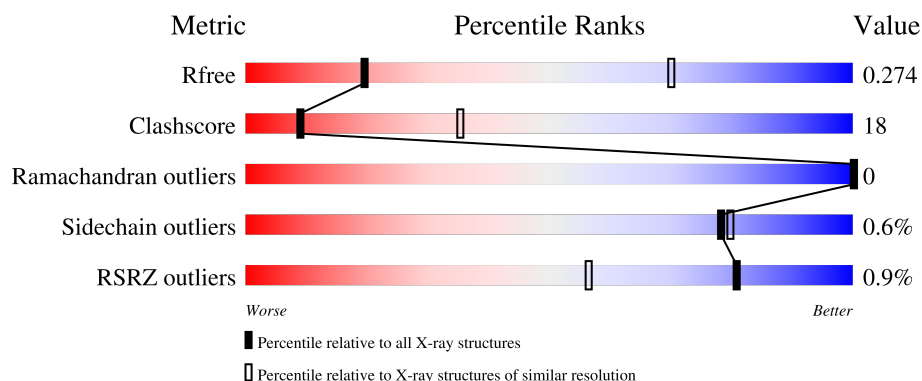
1 Overall quality at a glance

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}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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 $\leq 5\%$. 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	% 61% 38% .
1	B	709	% 59% 39% ..
1	C	709	 56% 42% ..
1	D	709	% 61% 37% .
1	E	709	% 59% 39% .

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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

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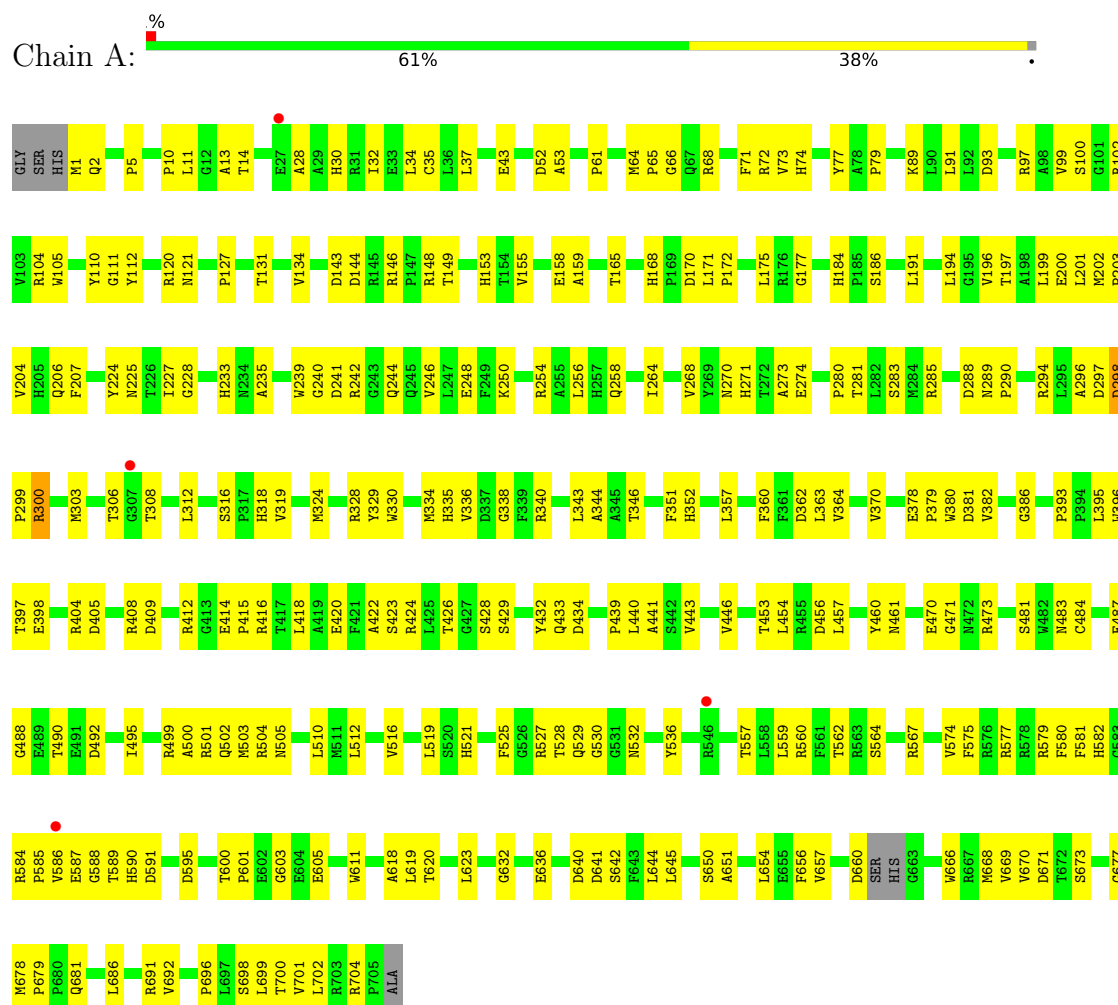
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	37	Total	O	0	0
			37	37		
2	L	34	Total	O	0	0
			34	34		

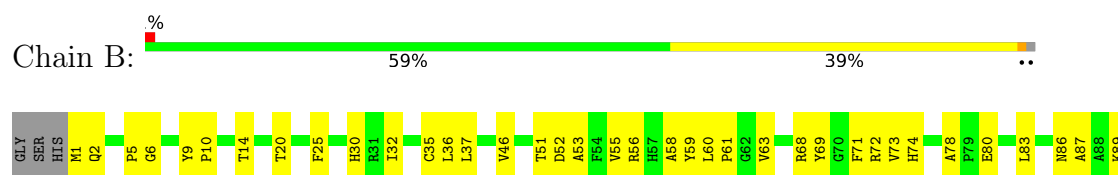
3 Residue-property plots

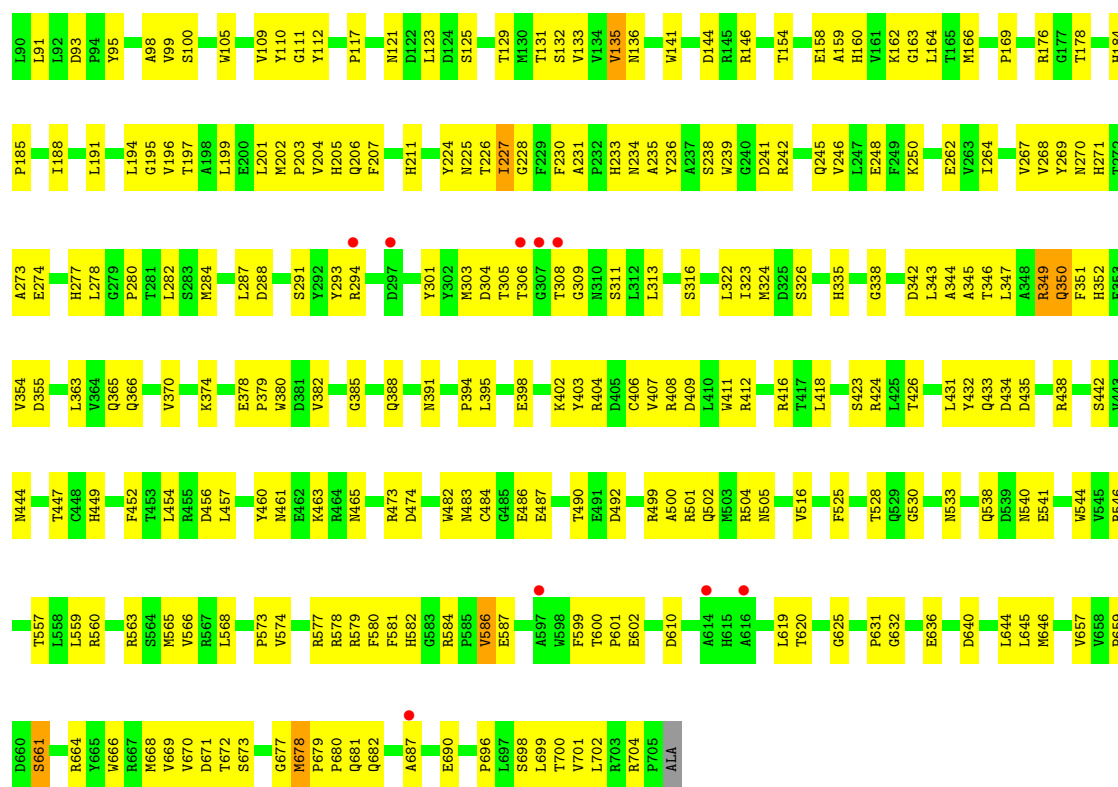
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



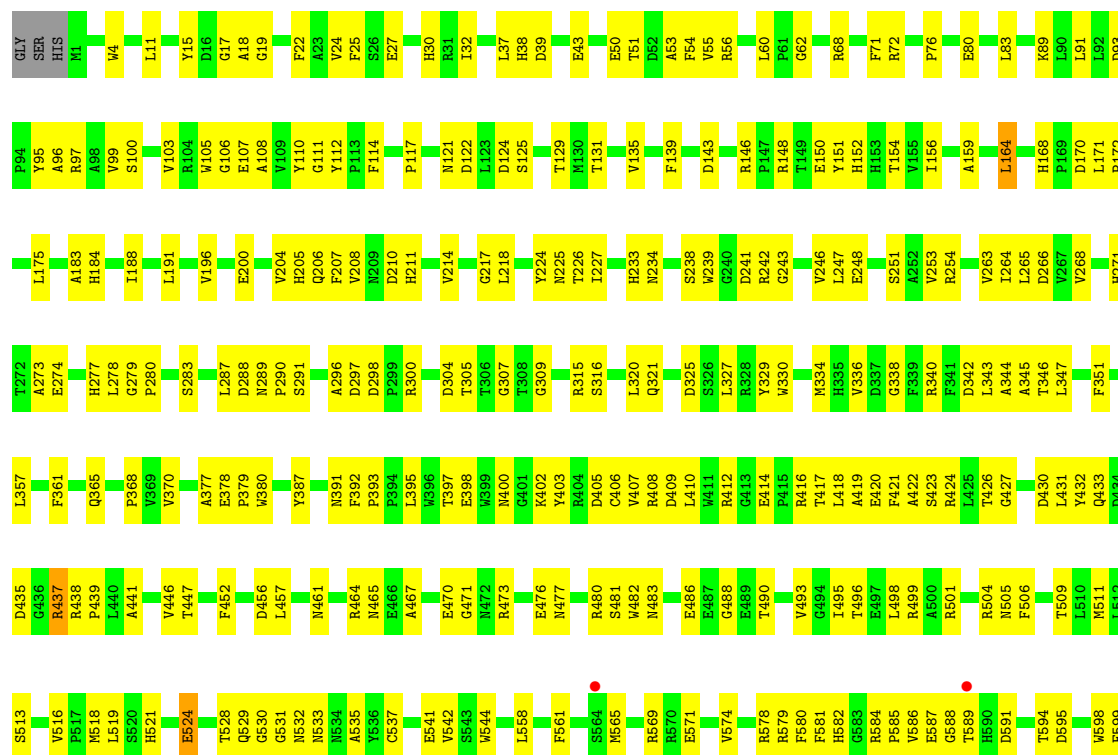
• Molecule 1: Glycogen debranching enzyme GlgX





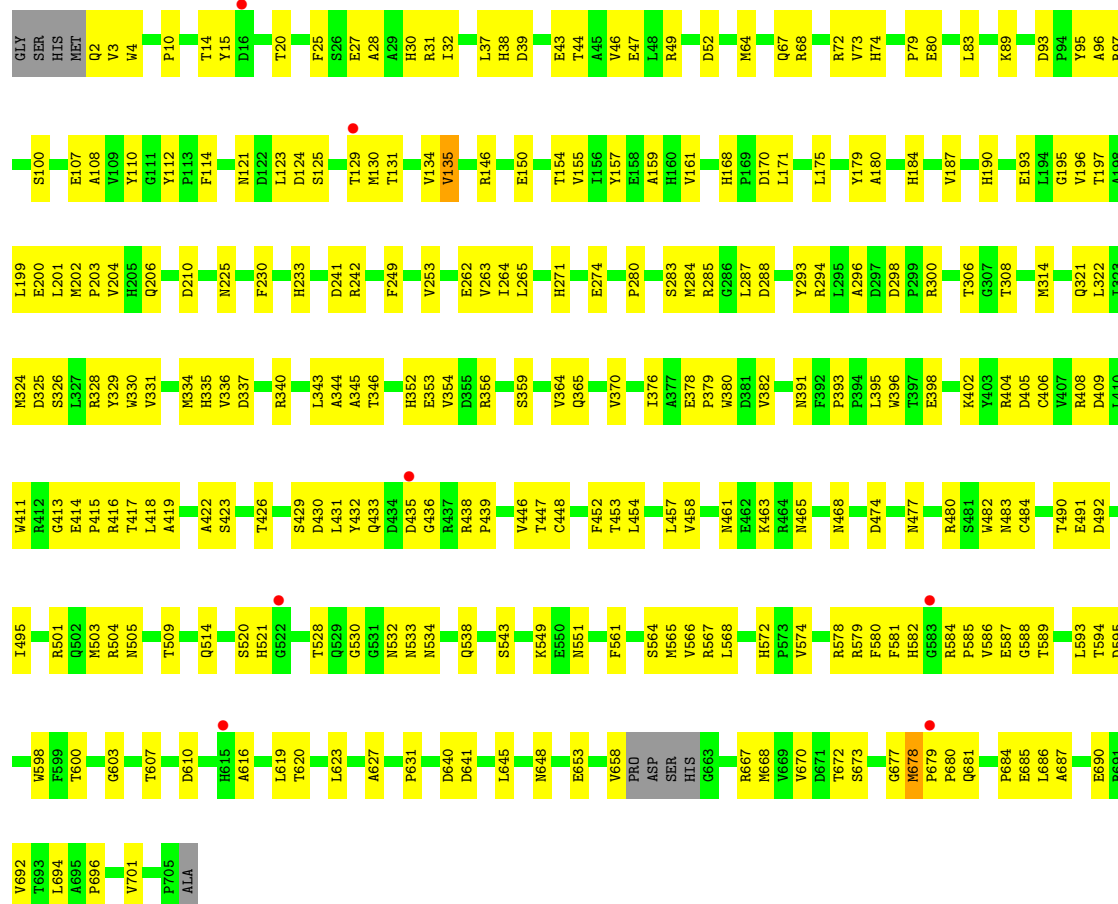
• Molecule 1: Glycogen debranching enzyme GlgX

Chain C: 56% 42%

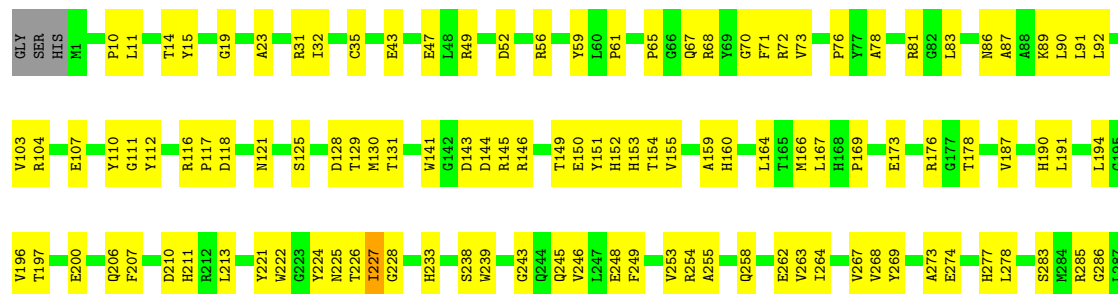


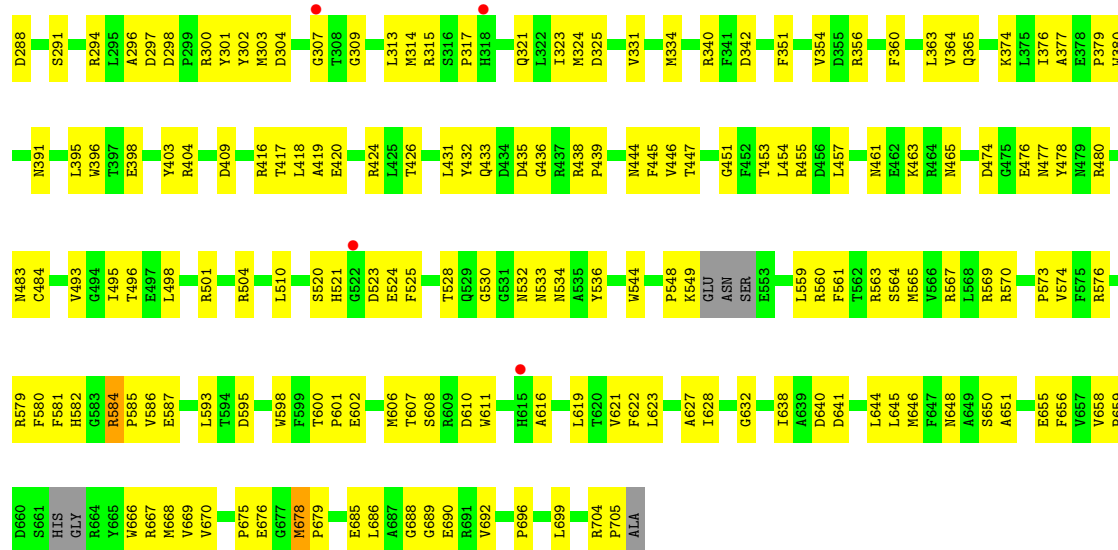


• Molecule 1: Glycogen debranching enzyme GlgX

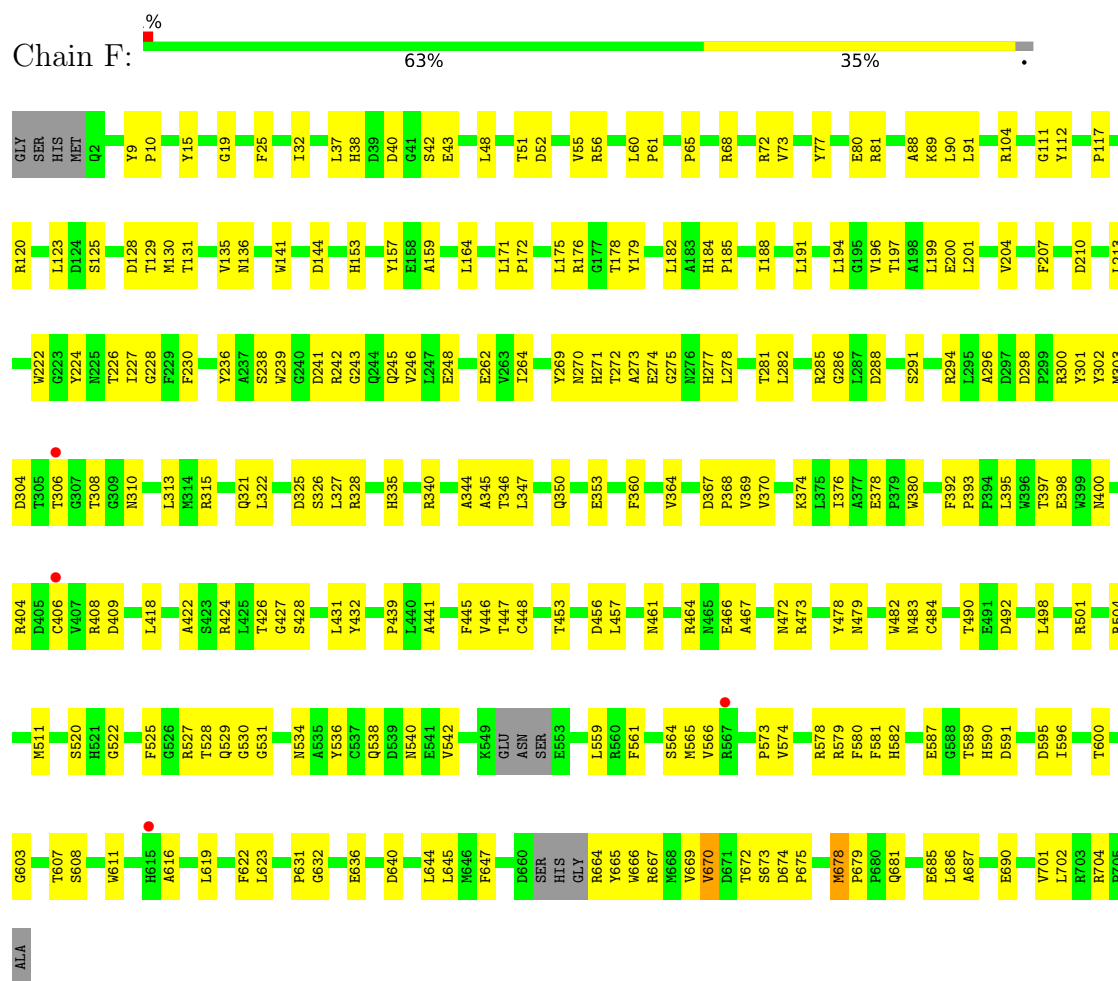


• Molecule 1: Glycogen debranching enzyme GlgX



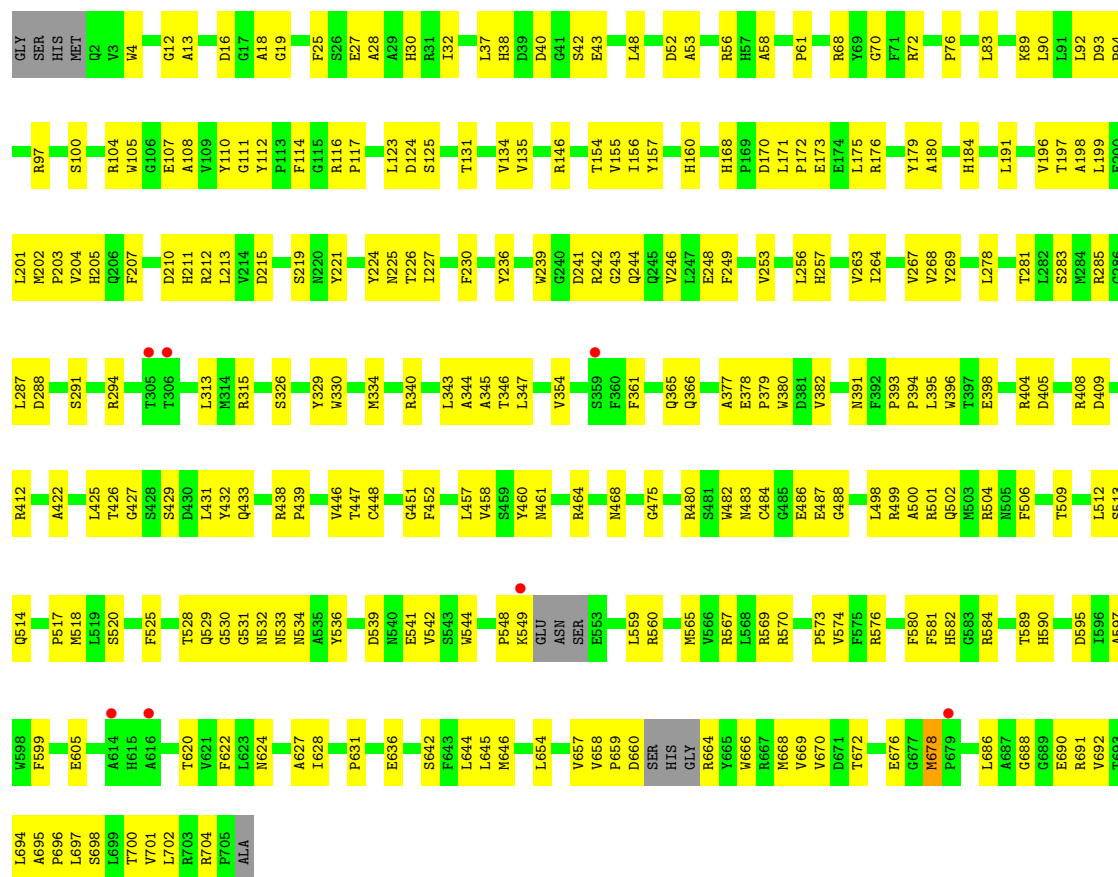


• Molecule 1: Glycogen debranching enzyme GlgX

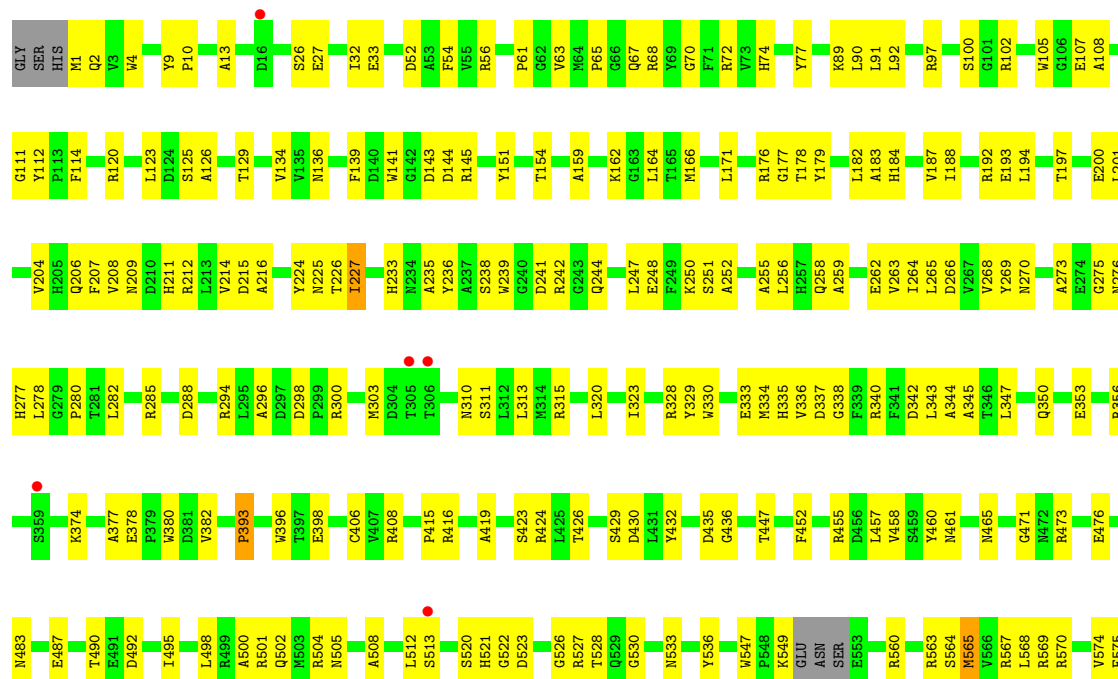


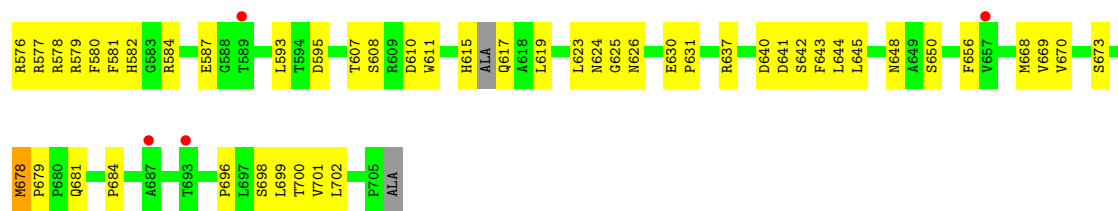
• Molecule 1: Glycogen debranching enzyme GlgX



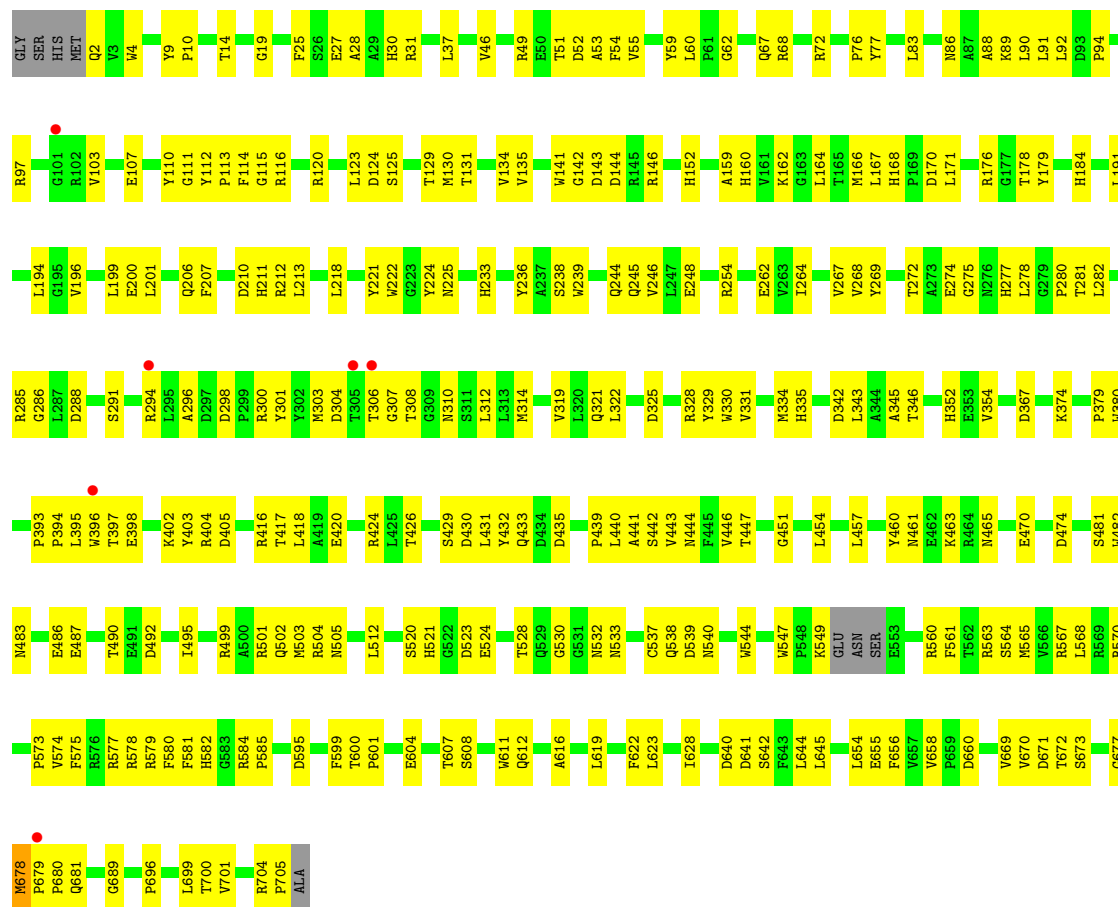


• Molecule 1: Glycogen debranching enzyme GlgX

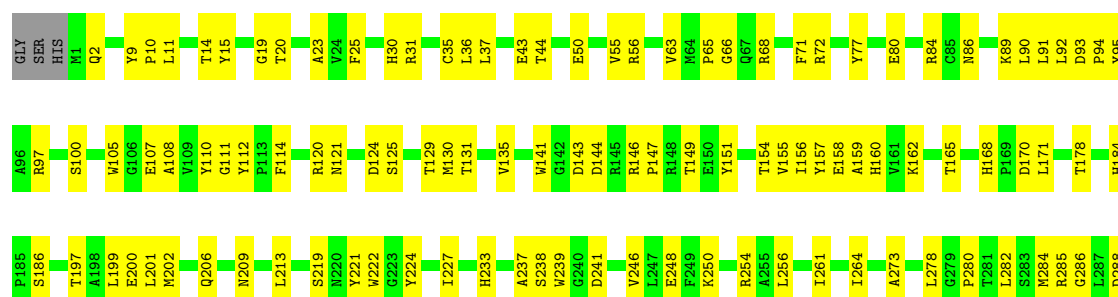


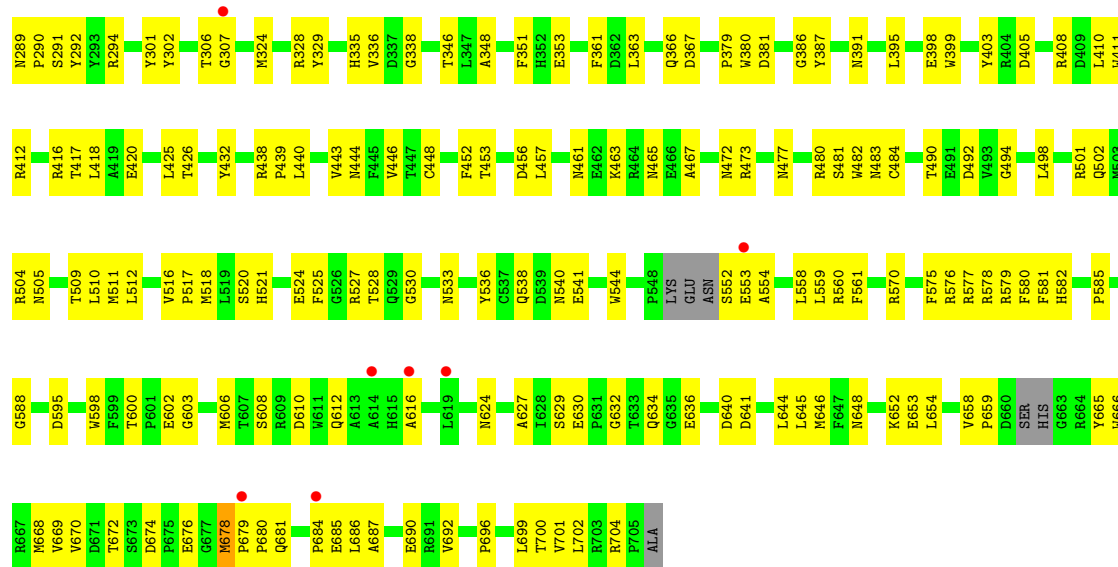


● Molecule 1: Glycogen debranching enzyme GlgX

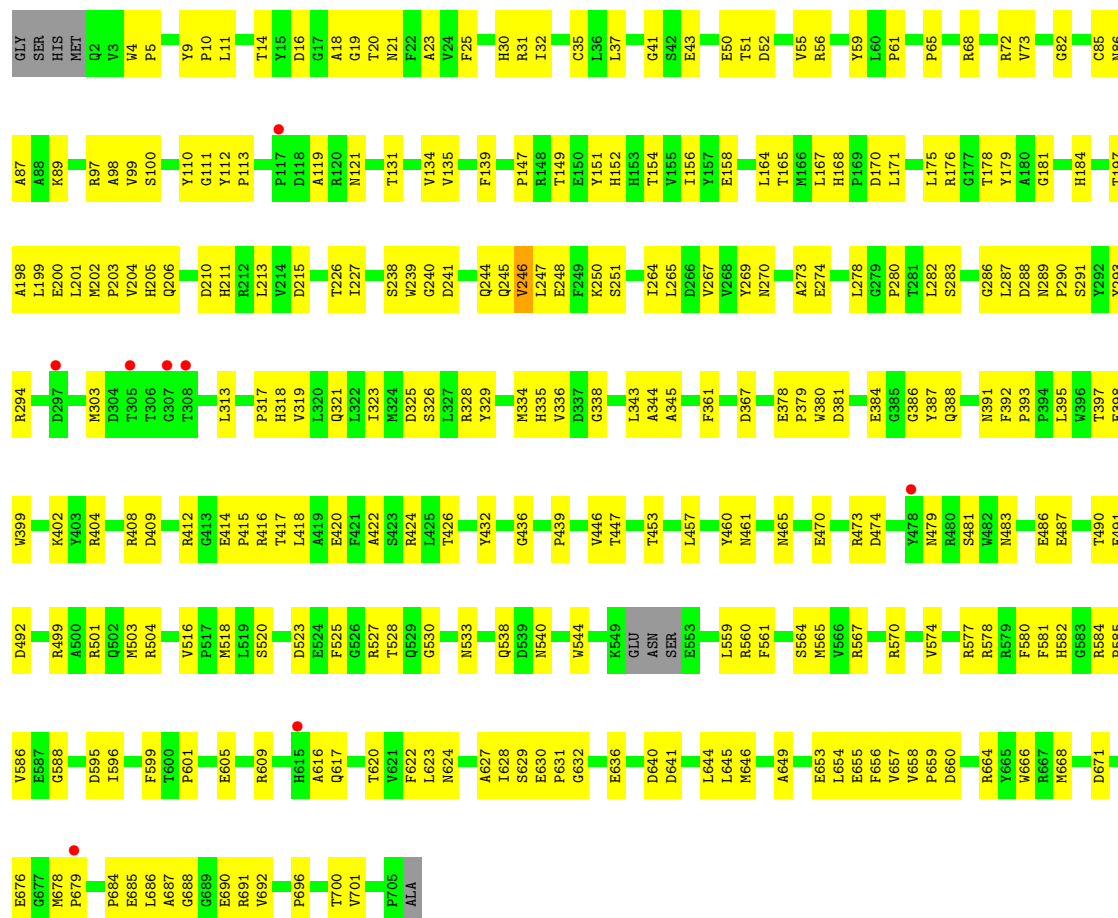


● Molecule 1: Glycogen debranching enzyme GlgX

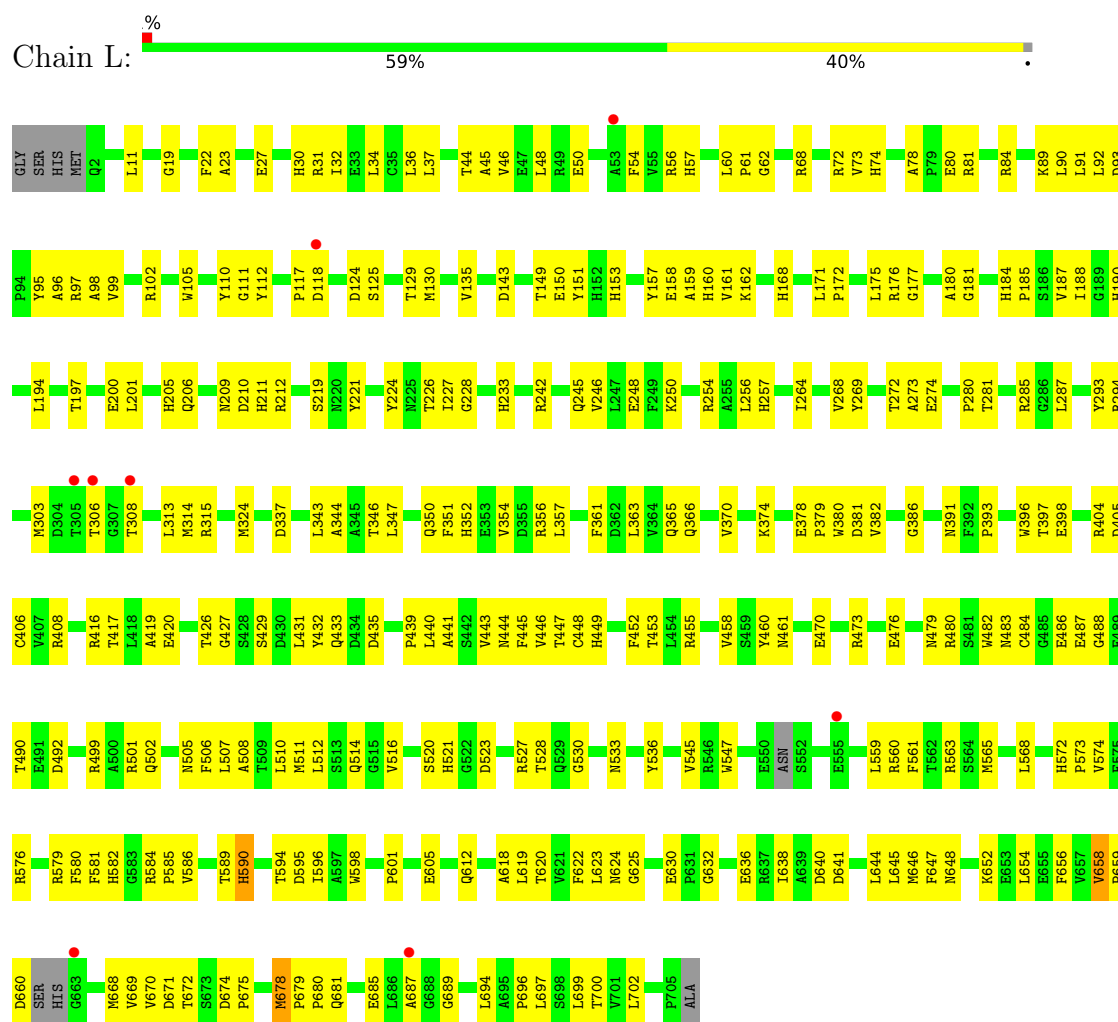




• Molecule 1: Glycogen debranching enzyme GlgX



• Molecule 1: Glycogen debranching enzyme GlgX



4 Data and refinement statistics

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 – 3.51	Depositor EDS
% Data completeness (in resolution range)	83.5 (67.92-3.51) 83.4 (67.92-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.211 , 0.276 0.211 , 0.274	Depositor DCC
R_{free} test set	2014 reflections (1.23%)	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)	0.29 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.25	1/5720 (0.0%)	0.57	6/7785 (0.1%)
1	B	0.24	1/5750 (0.0%)	0.56	6/7825 (0.1%)
1	C	0.22	0/5700	0.52	2/7752 (0.0%)
1	D	0.22	0/5718	0.53	1/7779 (0.0%)
1	E	0.22	0/5719	0.54	4/7781 (0.1%)
1	F	0.22	0/5701	0.50	0/7757
1	G	0.21	0/5706	0.49	0/7763
1	H	0.23	0/5723	0.51	2/7785 (0.0%)
1	I	0.20	0/5737	0.50	0/7805
1	J	0.23	1/5709 (0.0%)	0.50	0/7768
1	K	0.25	1/5737 (0.0%)	0.53	0/7805
1	L	0.26	2/5715 (0.0%)	0.51	1/7776 (0.0%)
All	All	0.23	6/68635 (0.0%)	0.52	22/93381 (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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	350	GLN	CA-C	7.75	1.63	1.52
1	L	658	VAL	CA-C	-7.47	1.47	1.53
1	K	516	VAL	N-CA	6.03	1.50	1.46
1	A	299	PRO	C-O	-5.48	1.16	1.24
1	L	658	VAL	N-CA	5.27	1.50	1.46

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	PHE	N-CA-C	11.45	125.11	111.82
1	B	350	GLN	N-CA-C	11.07	124.67	111.82
1	A	298	ASP	CB-CA-C	10.22	123.76	110.16
1	A	298	ASP	CA-C-N	8.56	130.54	119.84
1	A	298	ASP	C-N-CA	8.56	130.54	119.84

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	206	0
1	B	5595	0	5282	217	0
1	C	5551	0	5244	231	0
1	D	5566	0	5256	186	0
1	E	5567	0	5253	211	0
1	F	5549	0	5234	182	0
1	G	5554	0	5246	192	0
1	H	5570	0	5254	182	0
1	I	5583	0	5274	207	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	5557	0	5240	207	0
1	K	5583	0	5274	204	0
1	L	5564	0	5244	211	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
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	2385	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 2385 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
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 ⓘ

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%)	572 (99%)	4 (1%)	76	78
1	B	580/590 (98%)	576 (99%)	4 (1%)	76	78
1	C	575/590 (98%)	565 (98%)	10 (2%)	53	70
1	D	578/590 (98%)	577 (100%)	1 (0%)	87	85
1	E	579/590 (98%)	574 (99%)	5 (1%)	70	76
1	F	576/590 (98%)	575 (100%)	1 (0%)	87	85
1	G	577/590 (98%)	573 (99%)	4 (1%)	76	78
1	H	577/590 (98%)	574 (100%)	3 (0%)	81	81
1	I	580/590 (98%)	578 (100%)	2 (0%)	86	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	577/590 (98%)	577 (100%)	0	100	100
1	K	580/590 (98%)	577 (100%)	3 (0%)	81	81
1	L	577/590 (98%)	575 (100%)	2 (0%)	86	83
All	All	6932/7080 (98%)	6893 (99%)	39 (1%)	78	80

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	589	THR
1	K	270	ASN
1	H	227	ILE
1	I	367	ASP
1	L	118	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	534	ASN
1	I	206	GLN
1	L	350	GLN
1	F	225	ASN
1	G	533	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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 [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	703/709 (99%)	-0.03	4 (0%) 85 64	26, 44, 73, 95	0
1	B	705/709 (99%)	0.03	9 (1%) 75 48	27, 41, 69, 102	0
1	C	699/709 (98%)	-0.01	2 (0%) 90 75	25, 41, 70, 93	0
1	D	700/709 (98%)	0.02	7 (1%) 79 54	28, 45, 73, 112	0
1	E	700/709 (98%)	0.02	4 (0%) 85 64	27, 46, 72, 106	0
1	F	698/709 (98%)	0.05	4 (0%) 85 64	26, 43, 72, 98	0
1	G	698/709 (98%)	0.18	7 (1%) 79 54	30, 56, 87, 113	0
1	H	701/709 (98%)	0.11	9 (1%) 75 48	30, 43, 73, 96	0
1	I	701/709 (98%)	0.05	6 (0%) 81 56	29, 45, 75, 96	0
1	J	700/709 (98%)	0.01	7 (1%) 79 54	27, 44, 74, 103	0
1	K	701/709 (98%)	0.10	8 (1%) 78 52	31, 49, 79, 122	0
1	L	701/709 (98%)	0.12	8 (1%) 78 52	34, 50, 78, 102	0
All	All	8407/8508 (98%)	0.05	75 (0%) 81 56	25, 45, 76, 122	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	GLY	5.6
1	J	684	PRO	4.5
1	B	616	ALA	4.4
1	L	663	GLY	4.1
1	G	306	THR	3.9

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 oligosaccharides 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.