



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 04:24 am GMT

PDB ID : 3RT1
Title : Maltodextran bound activated state form of yeast glycogen synthase isoform 2
Authors : Baskaran, S.; Hurley, T.D.
Deposited on : 2011-05-02
Resolution : 2.80 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

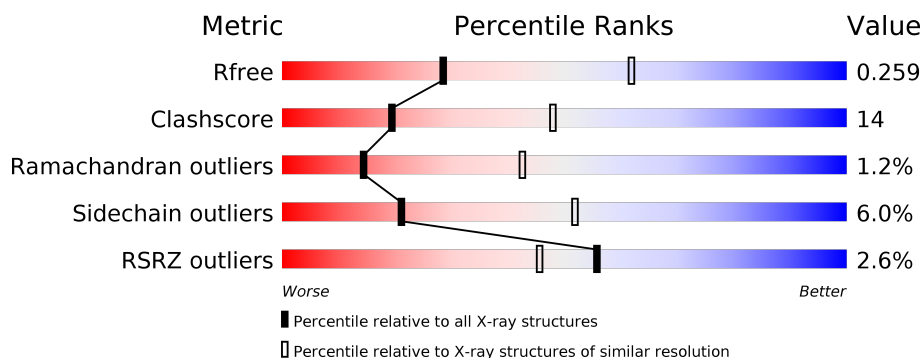
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 64%, green 22%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 64% 22% • 12% </div> </div>
1	B	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 60%, green 26%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 60% 26% • 12% </div> </div>
1	C	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 64%, green 23%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 64% 23% • 11% </div> </div>
1	D	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 57%, green 27%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 57% 27% • 12% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	A	800	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20951 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 PROTEIN (Glycogen [starch] synthase isoform 2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	B	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	C	646	Total	C	N	O	S	0	0	0
			5200	3322	907	952	19			
1	D	636	Total	C	N	O	S	0	0	0
			5128	3274	894	941	19			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P27472
A	-18	GLY	-	EXPRESSION TAG	UNP P27472
A	-17	SER	-	EXPRESSION TAG	UNP P27472
A	-16	SER	-	EXPRESSION TAG	UNP P27472
A	-15	HIS	-	EXPRESSION TAG	UNP P27472
A	-14	HIS	-	EXPRESSION TAG	UNP P27472
A	-13	HIS	-	EXPRESSION TAG	UNP P27472
A	-12	HIS	-	EXPRESSION TAG	UNP P27472
A	-11	HIS	-	EXPRESSION TAG	UNP P27472
A	-10	HIS	-	EXPRESSION TAG	UNP P27472
A	-9	SER	-	EXPRESSION TAG	UNP P27472
A	-8	SER	-	EXPRESSION TAG	UNP P27472
A	-7	GLY	-	EXPRESSION TAG	UNP P27472
A	-6	LEU	-	EXPRESSION TAG	UNP P27472
A	-5	VAL	-	EXPRESSION TAG	UNP P27472
A	-4	PRO	-	EXPRESSION TAG	UNP P27472
A	-3	ARG	-	EXPRESSION TAG	UNP P27472
A	-2	GLY	-	EXPRESSION TAG	UNP P27472
A	-1	SER	-	EXPRESSION TAG	UNP P27472
A	0	HIS	-	EXPRESSION TAG	UNP P27472
A	535	SER	ALA	SEE REMARK 999	UNP P27472

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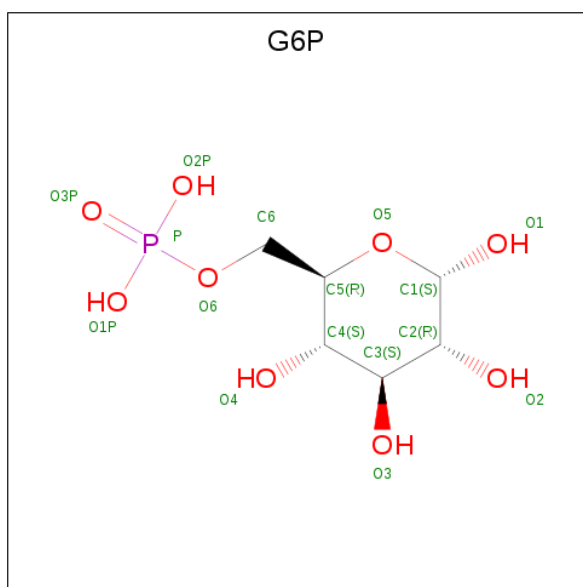
Chain	Residue	Modelled	Actual	Comment	Reference
A	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	-19	MET	-	EXPRESSION TAG	UNP P27472
B	-18	GLY	-	EXPRESSION TAG	UNP P27472
B	-17	SER	-	EXPRESSION TAG	UNP P27472
B	-16	SER	-	EXPRESSION TAG	UNP P27472
B	-15	HIS	-	EXPRESSION TAG	UNP P27472
B	-14	HIS	-	EXPRESSION TAG	UNP P27472
B	-13	HIS	-	EXPRESSION TAG	UNP P27472
B	-12	HIS	-	EXPRESSION TAG	UNP P27472
B	-11	HIS	-	EXPRESSION TAG	UNP P27472
B	-10	HIS	-	EXPRESSION TAG	UNP P27472
B	-9	SER	-	EXPRESSION TAG	UNP P27472
B	-8	SER	-	EXPRESSION TAG	UNP P27472
B	-7	GLY	-	EXPRESSION TAG	UNP P27472
B	-6	LEU	-	EXPRESSION TAG	UNP P27472
B	-5	VAL	-	EXPRESSION TAG	UNP P27472
B	-4	PRO	-	EXPRESSION TAG	UNP P27472
B	-3	ARG	-	EXPRESSION TAG	UNP P27472
B	-2	GLY	-	EXPRESSION TAG	UNP P27472
B	-1	SER	-	EXPRESSION TAG	UNP P27472
B	0	HIS	-	EXPRESSION TAG	UNP P27472
B	535	SER	ALA	SEE REMARK 999	UNP P27472
B	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	-19	MET	-	EXPRESSION TAG	UNP P27472
C	-18	GLY	-	EXPRESSION TAG	UNP P27472
C	-17	SER	-	EXPRESSION TAG	UNP P27472
C	-16	SER	-	EXPRESSION TAG	UNP P27472
C	-15	HIS	-	EXPRESSION TAG	UNP P27472
C	-14	HIS	-	EXPRESSION TAG	UNP P27472
C	-13	HIS	-	EXPRESSION TAG	UNP P27472
C	-12	HIS	-	EXPRESSION TAG	UNP P27472
C	-11	HIS	-	EXPRESSION TAG	UNP P27472
C	-10	HIS	-	EXPRESSION TAG	UNP P27472
C	-9	SER	-	EXPRESSION TAG	UNP P27472
C	-8	SER	-	EXPRESSION TAG	UNP P27472
C	-7	GLY	-	EXPRESSION TAG	UNP P27472
C	-6	LEU	-	EXPRESSION TAG	UNP P27472
C	-5	VAL	-	EXPRESSION TAG	UNP P27472
C	-4	PRO	-	EXPRESSION TAG	UNP P27472
C	-3	ARG	-	EXPRESSION TAG	UNP P27472

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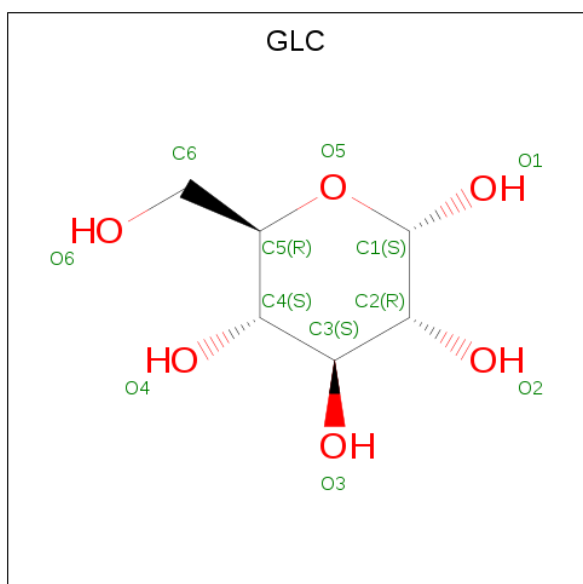
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP P27472
C	-1	SER	-	EXPRESSION TAG	UNP P27472
C	0	HIS	-	EXPRESSION TAG	UNP P27472
C	535	SER	ALA	SEE REMARK 999	UNP P27472
C	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	-19	MET	-	EXPRESSION TAG	UNP P27472
D	-18	GLY	-	EXPRESSION TAG	UNP P27472
D	-17	SER	-	EXPRESSION TAG	UNP P27472
D	-16	SER	-	EXPRESSION TAG	UNP P27472
D	-15	HIS	-	EXPRESSION TAG	UNP P27472
D	-14	HIS	-	EXPRESSION TAG	UNP P27472
D	-13	HIS	-	EXPRESSION TAG	UNP P27472
D	-12	HIS	-	EXPRESSION TAG	UNP P27472
D	-11	HIS	-	EXPRESSION TAG	UNP P27472
D	-10	HIS	-	EXPRESSION TAG	UNP P27472
D	-9	SER	-	EXPRESSION TAG	UNP P27472
D	-8	SER	-	EXPRESSION TAG	UNP P27472
D	-7	GLY	-	EXPRESSION TAG	UNP P27472
D	-6	LEU	-	EXPRESSION TAG	UNP P27472
D	-5	VAL	-	EXPRESSION TAG	UNP P27472
D	-4	PRO	-	EXPRESSION TAG	UNP P27472
D	-3	ARG	-	EXPRESSION TAG	UNP P27472
D	-2	GLY	-	EXPRESSION TAG	UNP P27472
D	-1	SER	-	EXPRESSION TAG	UNP P27472
D	0	HIS	-	EXPRESSION TAG	UNP P27472
D	535	SER	ALA	SEE REMARK 999	UNP P27472
D	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472

- Molecule 2 is ALPHA-D-GLUCOSE-6-PHOSPHATE (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



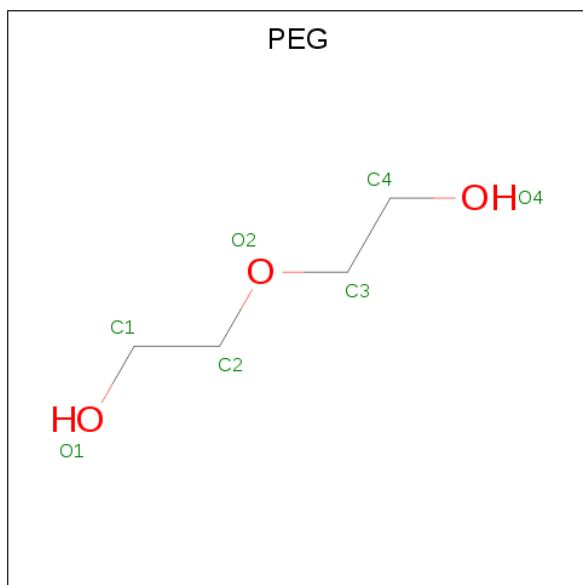
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total O 1 1	0	0
3	C	1	Total C O 11 6 5	0	0
3	C	1	Total C O 11 6 5	0	0
3	C	1	Total C O 11 6 5	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total C O 11 6 5	0	0
3	D	1	Total C O 11 6 5	0	0
3	D	1	Total C O 11 6 5	0	0
3	D	1	Total C O 11 6 5	0	0
3	D	1	Total O 1 1	0	0
3	D	1	Total C O 11 6 5	0	0
3	D	1	Total C O 11 6 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	O		0	0
			1	1			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

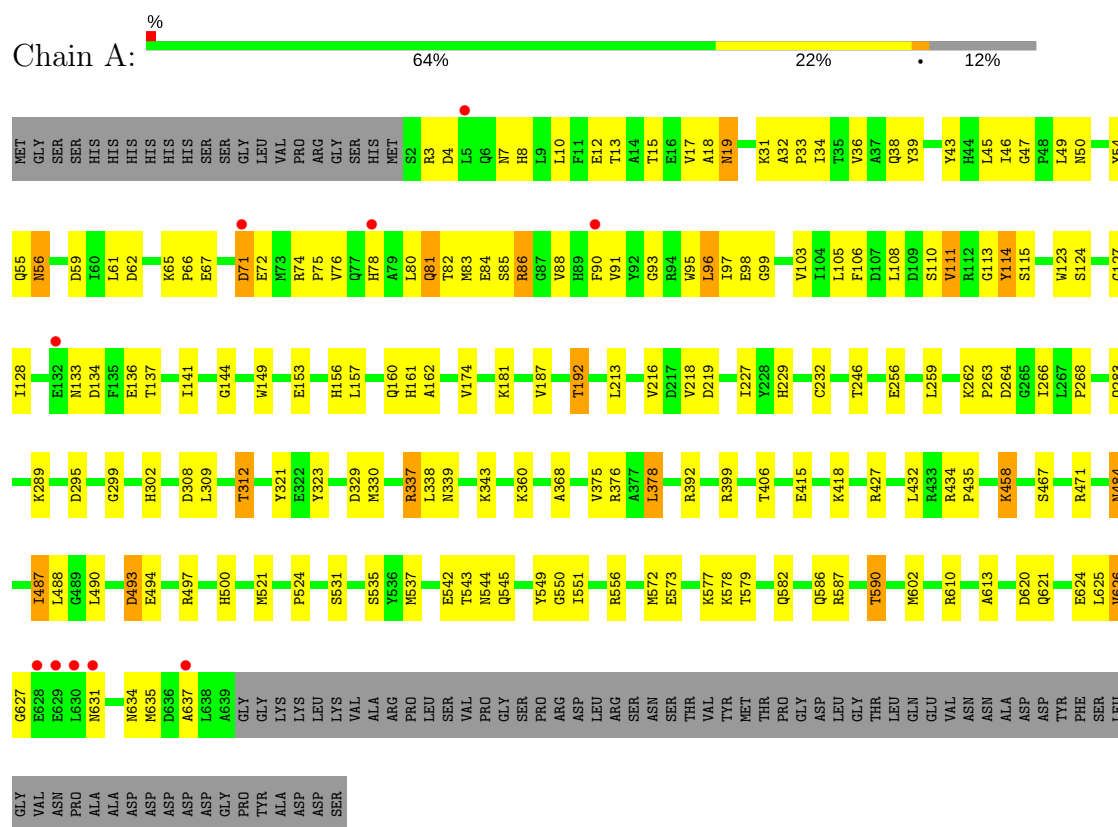


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

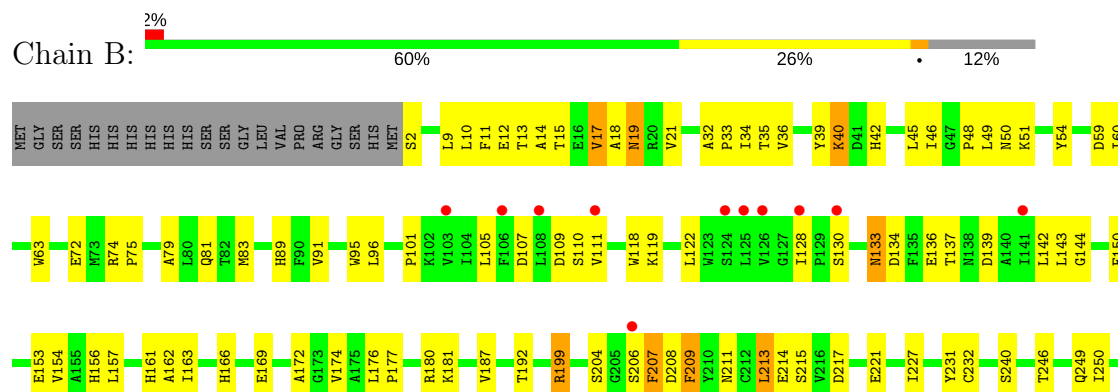
3 Residue-property plots [i](#)

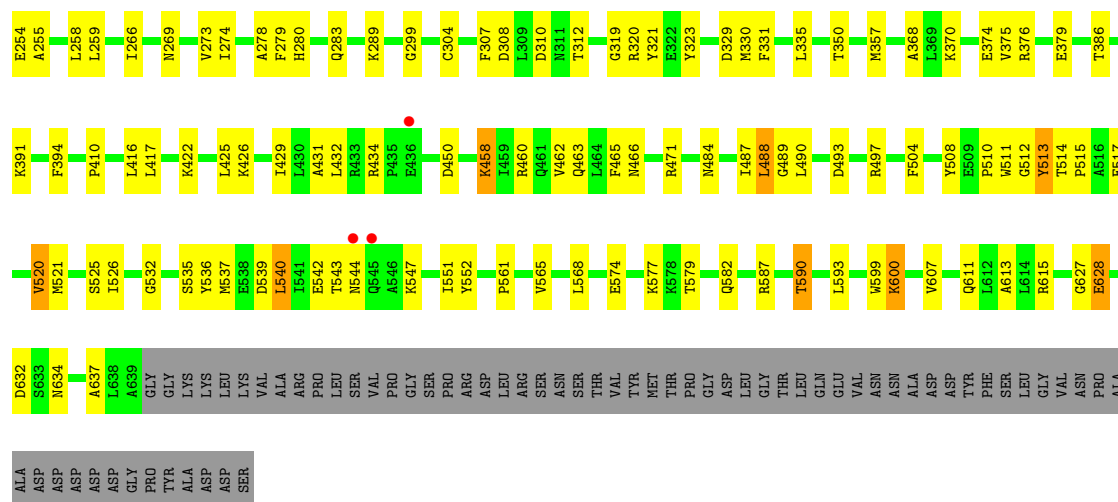
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: PROTEIN (Glycogen [starch] synthase isoform 2)

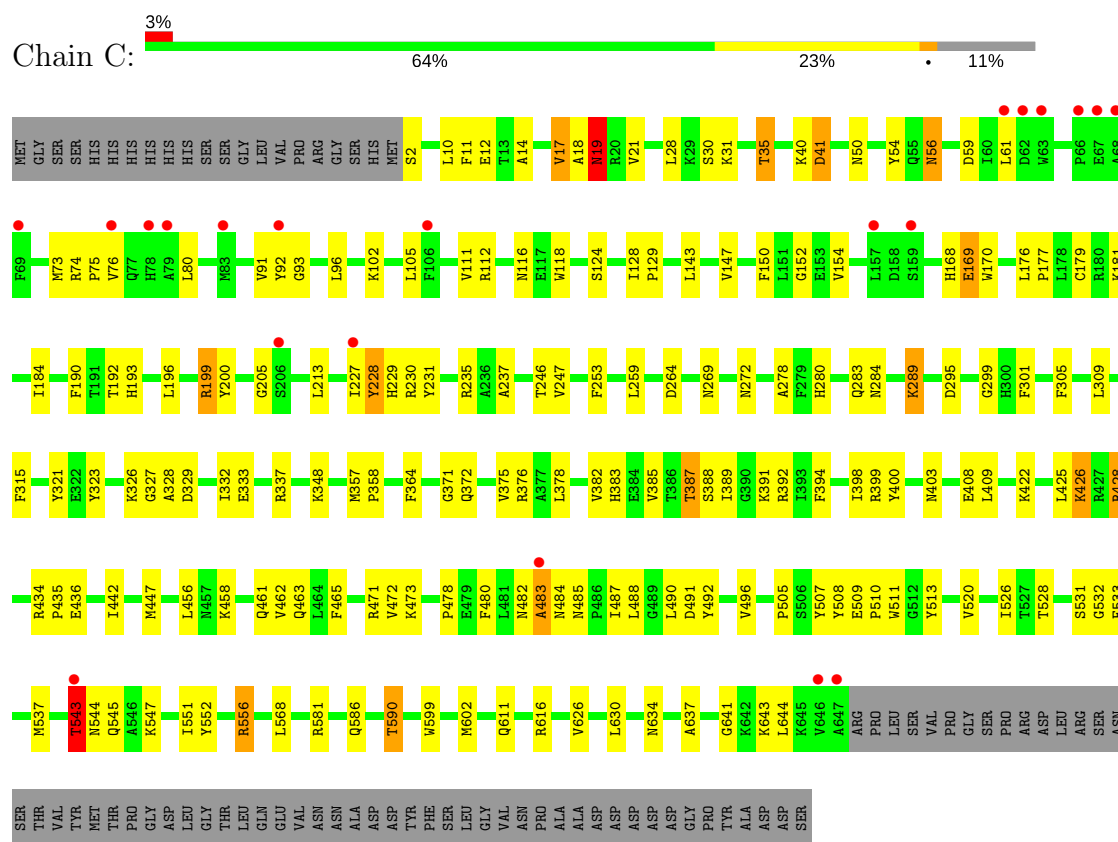


- Molecule 1: PROTEIN (Glycogen [starch] synthase isoform 2)

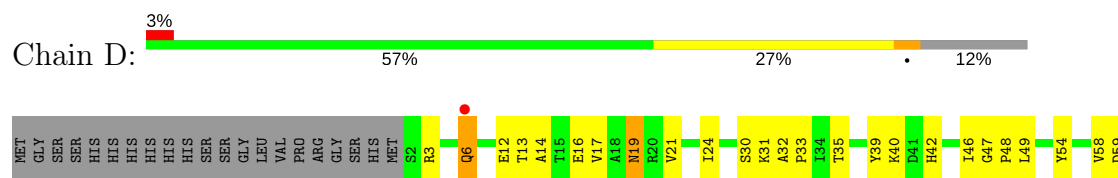




• Molecule 1: PROTEIN (Glycogen [starch] synthase isoform 2)



• Molecule 1: PROTEIN (Glycogen [starch] synthase isoform 2)



TYR	D595	L487	A368	E221	I141	I60
MET	L596	L488	R376	A222	L142	L61
THR	Y606	G489	A377	F225	L143	P66
PRO	R610	L490	L378	G226	G144	E67
GLY	G611	E494	Y382	I227	F150	
ASP	L612	H500	H383	Y228	E153	S70
LEU	A613	Y507	T387	C232	V154	D71
THR	L614	P510	G390	A238	A155	M73
LEU	R615	G512	F394	H239	H156	R74
GLN	R616	Y513	R399	S240	L157	P75
GLU	G617	T514	Y400	T245	D158	V76
VAL	Y618	P515	P401	T246	H161	Q77
ASN	D620	V520	H402	F253	A162	L80
ASN	F621	V523	M403	H257	I163	Q81
ASP	R622	P524	G404	L258	V164	T82
ASP	R623	S525	L409	L259	A165	M83
TYR	E624	V530	D412	K260	H166	E84
PHE	L625	S531	L417	R261	F167	S85
SER	V626	G532	K422	D264	H168	R86
LEU	G627	M537	R426	I266	E169	
GLY	G627	I541	R427	L267	W170	F90
VAL	E628	E542	N544	K275	V174	V91
VAL	E629	T543	R428	A278	A175	Y92
ASN	E629	N545	P435	H280	L176	L96
PRO	L630	Q545	E436	Q283	P177	P101
ALA	S633	Y549	G437	N284	R180	K102
ALA	N634	G550	Q438	F190	K181	L105
ASP	M635	I551	L439	T191	R182	F106
ASP	D636	VAL	P440	T192	R183	D107
ASP	A637	ALA	P441	H193	V186	L108
ASP	L638	ARG	R556	L196	D109	S110
GLY	A639	PRO	F557	Y200	V187	V111
PRO	GLY	LEU	F558	S204	T188	G113
TYR	LYS	VAL		G205	F189	Y114
LYS	LYS	ALA	H447	SER	T191	S115
LEU	LYS	ARG	D450	PHE	T192	
LYS	LYS	PRO	V565	D208	H193	K119
VAL	VAL	GLY	T579	F209	L196	G120
ALA	VAL	SER	R580	Y210	Y200	D121
ASP	PRO	GLY	F581	L213	S204	W122
ASP	ARG	SER	Q582	G345	G205	W123
ASP	ASP	PRO	R586	V344	SER	S124
LEU	LEU	ARG	R587	S345	PHE	L125
LEU	ARG	ASP	Q587	G346	D208	G127
SER	SER	LEU	T590	V344	F209	I128
ASN	ASN	ARG	M482	V344	Y210	P129
SER	ASN	ASN	E483	S345	L213	S130
THR	SER	THR	N484	G346	D217	P131
VAL	VAL	P496	N485		V218	E132
			S594			A140

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	193.44Å 205.33Å 206.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.80 48.58 – 2.79	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.58-2.80) 99.7 (48.58-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.211 , 0.261 0.210 , 0.259	Depositor DCC
R_{free} test set	5059 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20951	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, G6P, PEG

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	0.39	0/5270	0.52	0/7141
1	B	0.35	0/5270	0.49	0/7141
1	C	0.35	1/5325 (0.0%)	0.49	1/7212 (0.0%)
1	D	0.38	0/5251	0.51	1/7114 (0.0%)
All	All	0.37	1/21116 (0.0%)	0.51	2/28608 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	434	ARG	C-N	-5.21	1.24	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	TYR	CB-CA-C	-5.88	98.64	110.40
1	C	435	PRO	O-C-N	5.20	131.02	122.70

There are no chirality outliers.

There are no planarity outliers.

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	5145	0	5054	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5145	0	5054	133	0
1	C	5200	0	5124	148	0
1	D	5128	0	5039	180	0
2	A	16	0	11	1	0
2	B	32	0	22	1	0
2	C	16	0	11	1	0
2	D	16	0	11	2	0
3	A	101	0	83	4	0
3	C	34	0	28	3	0
3	D	90	0	74	2	0
4	A	7	0	10	0	0
4	B	14	0	20	2	0
4	C	7	0	10	0	0
All	All	20951	0	20551	573	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 14.

The worst 5 of 573 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:C:399:ARG:HD3	1:C:403:ASN:HD22	1.20	1.07
1:D:579:THR:H	1:D:582:GLN:HE21	1.17	0.93
1:B:48:PRO:HG3	1:B:143:LEU:HD22	1.53	0.90
1:A:110:SER:O	1:A:111:VAL:HG13	1.78	0.84
1:B:19:ASN:OD1	1:B:21:VAL:HG23	1.79	0.83

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	636/725 (88%)	586 (92%)	44 (7%)	6 (1%)	19	50
1	B	636/725 (88%)	581 (91%)	48 (8%)	7 (1%)	16	45
1	C	644/725 (89%)	598 (93%)	38 (6%)	8 (1%)	14	42
1	D	632/725 (87%)	556 (88%)	67 (11%)	9 (1%)	12	38
All	All	2548/2900 (88%)	2321 (91%)	197 (8%)	30 (1%)	14	42

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	SER
1	C	483	ALA
1	C	543	THR
1	D	132	GLU
1	D	204	SER

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	551/623 (88%)	513 (93%)	38 (7%)	17	44
1	B	551/623 (88%)	518 (94%)	33 (6%)	21	52
1	C	556/623 (89%)	527 (95%)	29 (5%)	25	58
1	D	549/623 (88%)	517 (94%)	32 (6%)	22	53
All	All	2207/2492 (89%)	2075 (94%)	132 (6%)	21	52

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	488	LEU
1	C	35	THR
1	D	450	ASP
1	B	520	VAL
1	B	593	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	81	GLN
1	C	277	GLN
1	D	403	ASN
1	C	168	HIS
1	C	249	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 5 are modelled with single atom - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PEG	A	1009	-	6,6,6	0.52	0	5,5,5	0.23	0
3	GLC	A	801	3	11,11,12	0.80	0	15,15,17	1.30	1 (6%)
3	GLC	A	802	3	11,11,12	0.54	0	15,15,17	1.25	3 (20%)
3	GLC	A	803	3	11,11,12	0.28	0	15,15,17	1.26	2 (13%)
3	GLC	A	804	3	11,11,12	0.35	0	15,15,17	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	A	805	3	11,11,12	0.53	0	15,15,17	0.78	0
3	GLC	A	806	3	11,11,12	0.83	0	15,15,17	1.17	1 (6%)
3	GLC	A	807	3	11,11,12	0.83	0	15,15,17	1.65	3 (20%)
3	GLC	A	808	3	11,11,12	0.71	0	15,15,17	0.94	1 (6%)
3	GLC	A	809	3	11,11,12	0.60	0	15,15,17	1.97	4 (26%)
2	G6P	A	901	-	16,16,16	0.50	0	24,24,24	0.89	0
4	PEG	B	1001	-	6,6,6	0.53	0	5,5,5	0.19	0
4	PEG	B	706	-	6,6,6	0.54	0	5,5,5	0.18	0
2	G6P	B	901	-	16,16,16	0.53	0	24,24,24	1.07	1 (4%)
2	G6P	B	902	-	16,16,16	0.67	0	24,24,24	1.55	3 (12%)
4	PEG	C	1004	-	6,6,6	0.55	0	5,5,5	0.15	0
3	GLC	C	801	3	11,11,12	0.38	0	15,15,17	1.10	2 (13%)
3	GLC	C	802	3	11,11,12	0.39	0	15,15,17	0.88	0
3	GLC	C	803	3	11,11,12	0.26	0	15,15,17	0.89	0
2	G6P	C	901	-	16,16,16	0.52	0	24,24,24	0.86	0
3	GLC	D	801	3	11,11,12	0.54	0	15,15,17	0.99	1 (6%)
3	GLC	D	802	3	11,11,12	0.35	0	15,15,17	1.24	1 (6%)
3	GLC	D	803	3	11,11,12	0.36	0	15,15,17	1.01	0
3	GLC	D	804	3	11,11,12	0.84	0	15,15,17	2.03	3 (20%)
3	GLC	D	806	3	11,11,12	0.66	0	15,15,17	1.77	3 (20%)
3	GLC	D	807	3	11,11,12	0.60	0	15,15,17	1.24	2 (13%)
3	GLC	D	808	3	11,11,12	0.35	0	15,15,17	1.47	1 (6%)
3	GLC	D	809	3	11,11,12	0.63	0	15,15,17	1.48	2 (13%)
2	G6P	D	901	-	16,16,16	0.43	0	24,24,24	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	1009	-	-	0/4/4/4	0/0/0/0
3	GLC	A	801	3	-	0/2/19/22	0/1/1/1
3	GLC	A	802	3	-	0/2/19/22	0/1/1/1
3	GLC	A	803	3	-	0/2/19/22	0/1/1/1
3	GLC	A	804	3	-	0/2/19/22	0/1/1/1
3	GLC	A	805	3	-	0/2/19/22	0/1/1/1
3	GLC	A	806	3	-	0/2/19/22	0/1/1/1
3	GLC	A	807	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	A	808	3	-	0/2/19/22	0/1/1/1
3	GLC	A	809	3	-	0/2/19/22	0/1/1/1
2	G6P	A	901	-	-	0/6/26/26	0/1/1/1
4	PEG	B	1001	-	-	0/4/4/4	0/0/0/0
4	PEG	B	706	-	-	0/4/4/4	0/0/0/0
2	G6P	B	901	-	-	0/6/26/26	0/1/1/1
2	G6P	B	902	-	-	0/6/26/26	0/1/1/1
4	PEG	C	1004	-	-	0/4/4/4	0/0/0/0
3	GLC	C	801	3	-	0/2/19/22	0/1/1/1
3	GLC	C	802	3	-	0/2/19/22	0/1/1/1
3	GLC	C	803	3	-	0/2/19/22	0/1/1/1
2	G6P	C	901	-	-	0/6/26/26	0/1/1/1
3	GLC	D	801	3	-	0/2/19/22	0/1/1/1
3	GLC	D	802	3	-	0/2/19/22	0/1/1/1
3	GLC	D	803	3	-	0/2/19/22	0/1/1/1
3	GLC	D	804	3	-	0/2/19/22	0/1/1/1
3	GLC	D	806	3	-	0/2/19/22	0/1/1/1
3	GLC	D	807	3	-	0/2/19/22	0/1/1/1
3	GLC	D	808	3	-	0/2/19/22	0/1/1/1
3	GLC	D	809	3	-	0/2/19/22	0/1/1/1
2	G6P	D	901	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	G6P	C3-C4-C5	-3.55	103.90	110.24
2	B	902	G6P	C4-C3-C2	-3.14	105.33	110.83
3	A	803	GLC	C2-C3-C4	-2.59	106.37	110.87
3	D	804	GLC	C2-C3-C4	-2.36	106.77	110.87
3	A	802	GLC	O5-C1-C2	-2.11	107.49	110.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	GLC	2	0
3	A	808	GLC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	809	GLC	1	0
2	A	901	G6P	1	0
4	B	1001	PEG	2	0
2	B	901	G6P	1	0
3	C	801	GLC	1	0
3	C	802	GLC	1	0
3	C	803	GLC	2	0
2	C	901	G6P	1	0
3	D	802	GLC	1	0
3	D	803	GLC	1	0
2	D	901	G6P	2	0

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	638/725 (88%)	-0.01	10 (1%) 72 65	27, 58, 110, 124	0
1	B	638/725 (88%)	0.08	14 (2%) 62 52	38, 65, 110, 123	0
1	C	646/725 (89%)	0.15	21 (3%) 46 36	42, 70, 111, 126	0
1	D	636/725 (87%)	0.15	22 (3%) 44 33	32, 76, 127, 136	0
All	All	2558/2900 (88%)	0.09	67 (2%) 56 45	27, 66, 118, 136	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	627	GLY	6.1
1	D	624	GLU	5.0
1	D	630	LEU	4.0
1	D	625	LEU	4.0
1	C	62	ASP	3.7

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLC	A	800	1/12	0.57	0.47	76,76,76,76	0
3	GLC	C	801	11/12	0.69	0.23	111,113,115,116	0
3	GLC	D	810	1/12	0.73	0.27	78,78,78,78	0
3	GLC	D	806	11/12	0.82	0.36	84,94,99,99	0
3	GLC	A	807	11/12	0.83	0.23	70,80,85,86	0
3	GLC	D	805	1/12	0.83	0.18	52,52,52,52	0
3	GLC	A	801	11/12	0.84	0.32	61,70,74,76	0
3	GLC	A	809	11/12	0.85	0.25	60,62,69,69	0
3	GLC	A	810	1/12	0.85	0.28	64,64,64,64	0
3	GLC	C	803	11/12	0.86	0.18	103,106,109,110	0
3	GLC	A	808	11/12	0.87	0.32	66,71,75,75	0
3	GLC	D	801	11/12	0.89	0.31	78,85,87,87	0
4	PEG	B	706	7/7	0.89	0.21	51,56,63,63	0
3	GLC	D	809	11/12	0.90	0.18	66,71,75,77	0
2	G6P	B	902	16/16	0.90	0.19	78,83,88,89	0
4	PEG	B	1001	7/7	0.90	0.14	50,52,55,55	0
3	GLC	D	807	11/12	0.91	0.23	65,71,75,80	0
3	GLC	C	802	11/12	0.91	0.23	108,110,113,113	0
3	GLC	D	804	11/12	0.91	0.19	46,56,60,63	0
3	GLC	A	806	11/12	0.92	0.23	76,82,87,88	0
3	GLC	A	805	11/12	0.92	0.21	68,77,83,86	0
3	GLC	A	802	11/12	0.92	0.18	54,61,66,67	0
4	PEG	A	1009	7/7	0.93	0.18	58,60,62,62	0
3	GLC	D	802	11/12	0.93	0.16	58,63,69,75	0
4	PEG	C	1004	7/7	0.94	0.16	48,51,58,60	0
3	GLC	D	808	11/12	0.94	0.20	57,60,65,69	0
3	GLC	A	804	11/12	0.94	0.16	64,65,71,75	0
3	GLC	C	804	1/12	0.96	0.18	105,105,105,105	0
3	GLC	A	803	11/12	0.96	0.15	53,60,63,66	0
3	GLC	D	803	11/12	0.97	0.12	49,53,56,56	0
2	G6P	C	901	16/16	0.97	0.19	46,50,52,52	0
2	G6P	B	901	16/16	0.98	0.17	42,45,48,50	0
2	G6P	D	901	16/16	0.99	0.15	35,37,40,41	0
2	G6P	A	901	16/16	0.99	0.18	34,36,41,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.