



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:51 AM GMT

PDB ID : 3NB0
Title : Glucose-6-Phosphate activated form of Yeast Glycogen Synthase
Authors : Baskaran, S.; Hurley, T.D.
Deposited on : 2010-06-02
Resolution : 2.41 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
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

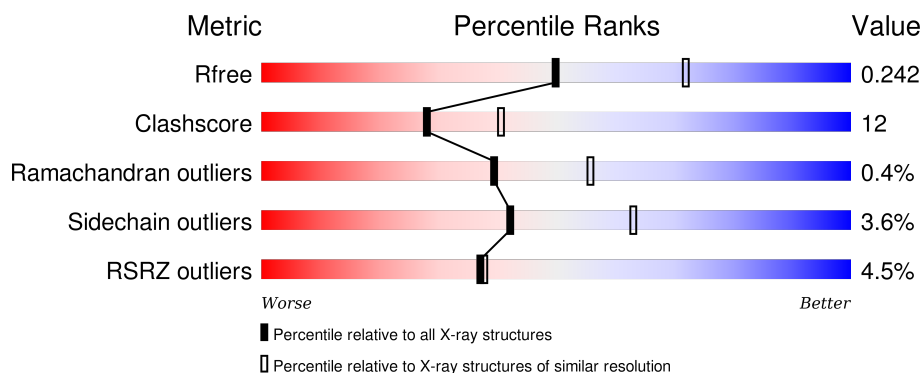
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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>2%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	725	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	725	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	725	<div> <div>6%</div> <div> <div></div> <div>60%</div> <div>26%</div> <div>•</div> <div>12%</div> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	G6P	A	902	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21392 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 [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	4	0
			5169	3302	899	949	19			
1	B	645	Total	C	N	O	S	0	3	0
			5213	3332	911	951	19			
1	C	646	Total	C	N	O	S	0	2	0
			5213	3331	910	953	19			
1	D	636	Total	C	N	O	S	0	1	0
			5135	3279	896	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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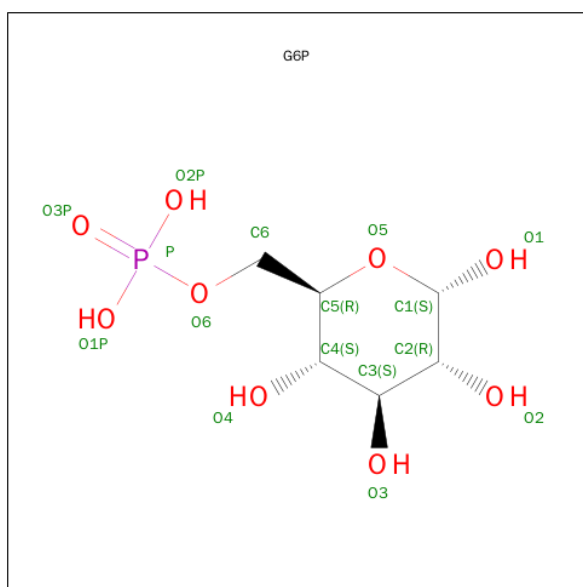
Chain	Residue	Modelled	Actual	Comment	Reference
A	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	-19	MET	-	EXPRESSION TAG	UNP P27472
B	-18	GLY	-	EXPRESSION TAG	UNP P27472
B	-17	SER	-	EXPRESSION TAG	UNP P27472
B	-16	SER	-	EXPRESSION TAG	UNP P27472
B	-15	HIS	-	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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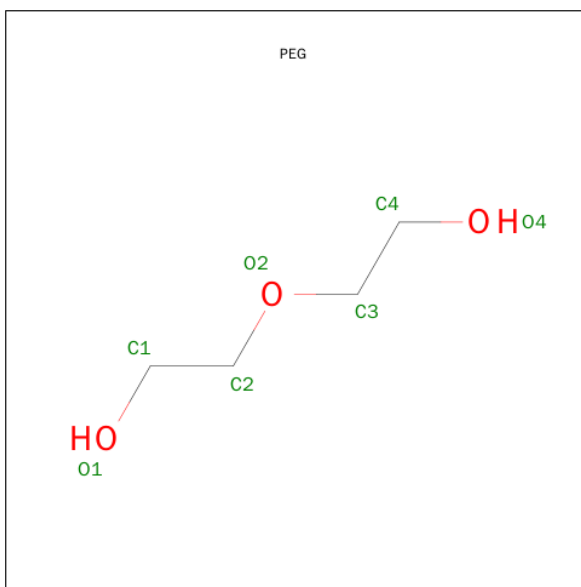
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP P27472
C	-1	SER	-	EXPRESSION TAG	UNP P27472
C	0	HIS	-	EXPRESSION TAG	UNP P27472
C	535	SER	ALA	SEE REMARK 999	UNP P27472
C	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	-19	MET	-	EXPRESSION 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 SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
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 DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

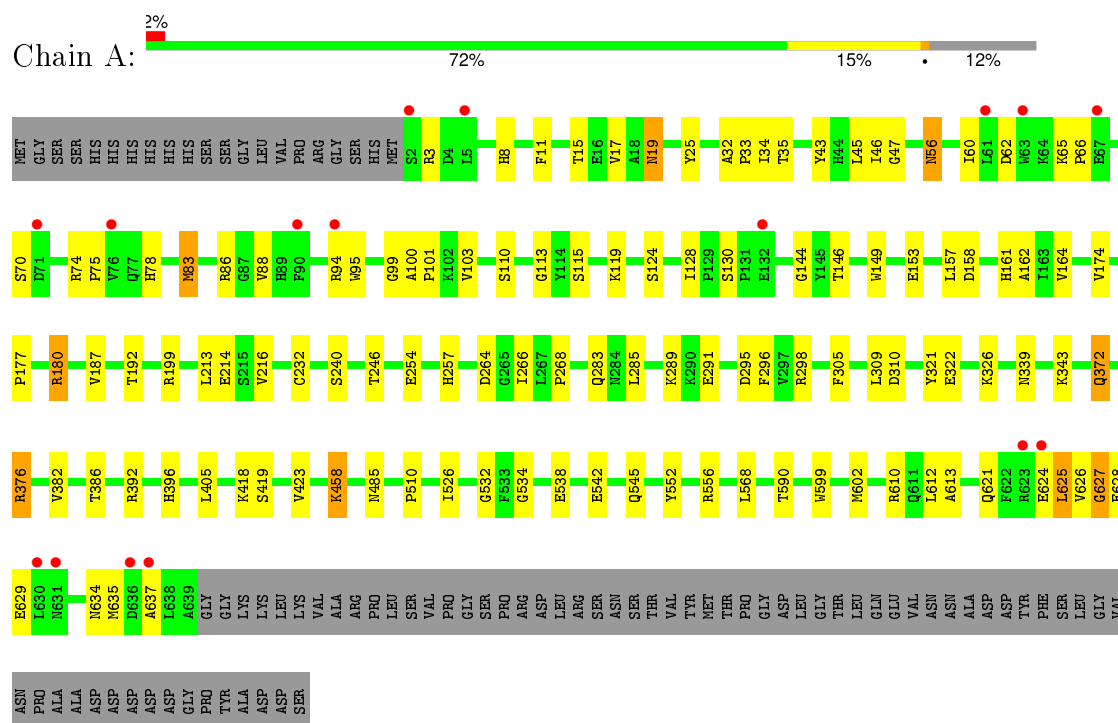
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		
4	B	127	Total	O	0	0
			127	127		
4	C	102	Total	O	0	0
			102	102		
4	D	119	Total	O	0	0
			119	119		

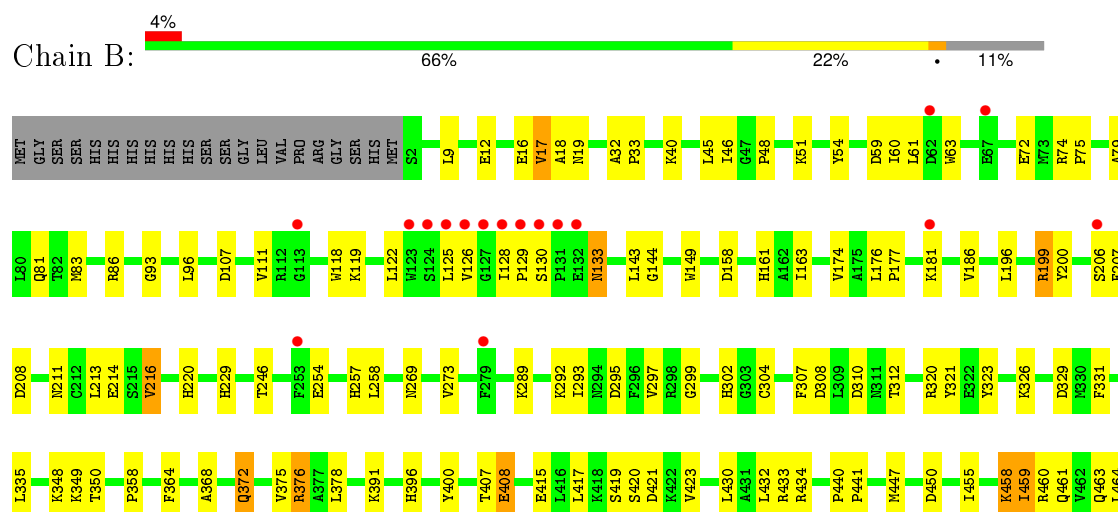
3 Residue-property plots

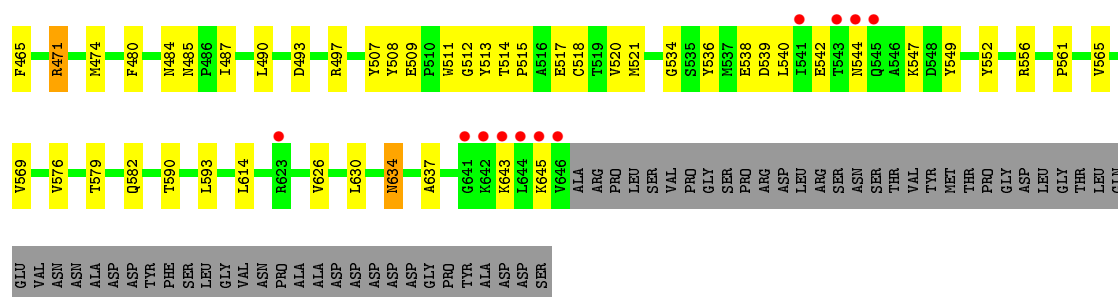
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 [starch] synthase isoform 2

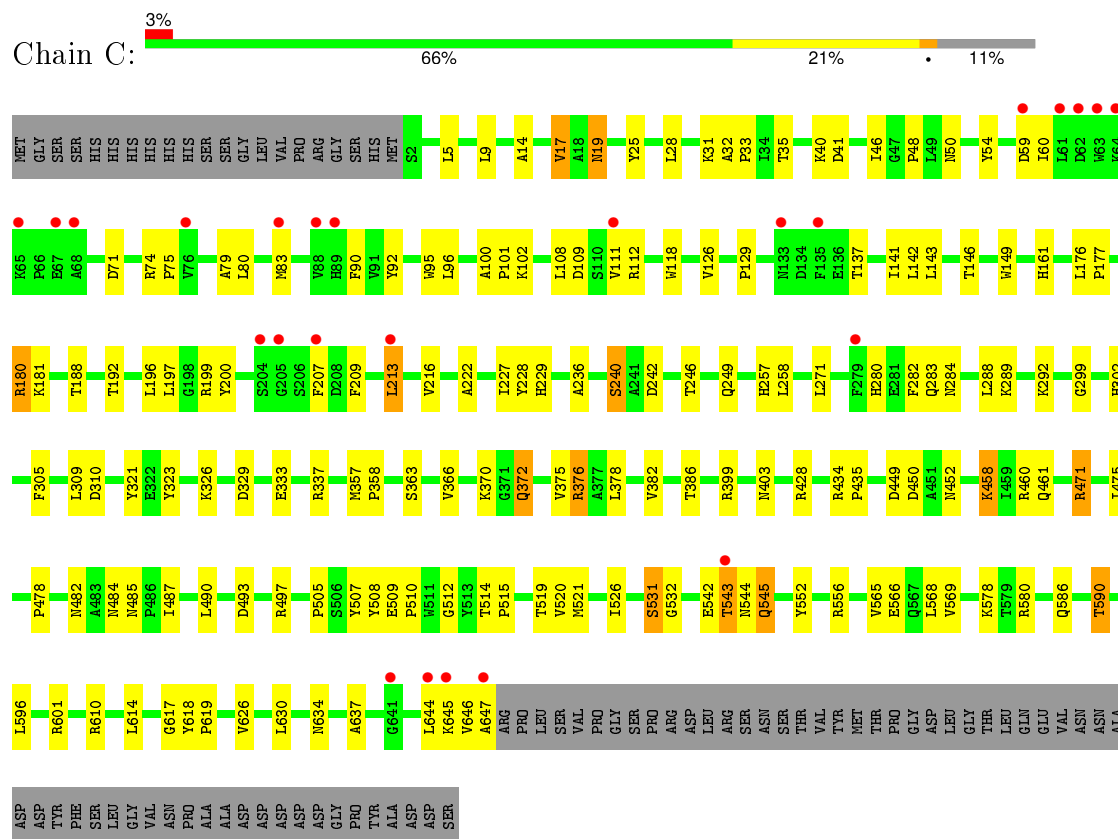


- Molecule 1: Glycogen [starch] synthase isoform 2

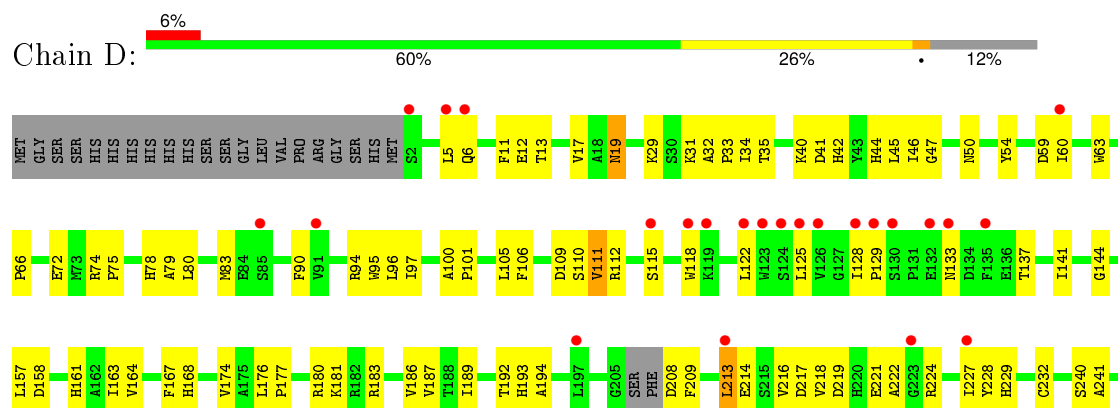




• Molecule 1: Glycogen [starch] synthase isoform 2



• Molecule 1: Glycogen [starch] synthase isoform 2



ALA	S653	D539	T387	T246
ASP	M634	L540	S368	
ASP	M635	I541	I389	F253
ASP	D636	E542		H257
ASP	A637	T543	R399	
ASP	L638	M544	Y400	K260
GLY	A639	K547	P401	
PRO	GLY	D548	H402	P268
TYR	GLY	Y549	N403	
ALA	LYS		L416	V273
ASP	LYS		L417	I274
ASP	LEU	Y552		
SER	LYS	I553	R428	Q277
	VAL			A278
	ALA	V565	L432	F279
	ARG	E566	R433	H280
	PRO		R434	
	LEU	V569	P435	Q283
	SER		E436	N284
	VAL	R581		
	PRO		P440	K289
	GLY	Q586	P441	
	SER	R587		
	PRO		K292	
	ARG	T590	D450	
	ASP	E591		F296
	LEU		L454	
	ARG	L596	I455	F301
	SER	L597	L456	H302
	ASN	D598		G303
	SER		R460	C304
	THR	V602		
	VAL	G603	S469	L309
	TYR	L604	D470	D310
	MET	E605	R471	
	THR	V606		Y321
	PRO	V607	F480	
	GLY		L481	K324
	ASP	R610	N482	
	LEU	Q611	A483	M330
	GLY	L612	N484	
	THR	A613	N485	E333
	LEU	L614	P486	
	GLN	R615	L487	R337
	GLU		L488	
	VAL	Y618	G489	K343
	ASN	P619	L490	
	ASN	D620		K349
	ALA	Q621	E494	
	ASP	F622		P358
	ASP	R623	P610	
	TYR	E624		F364
	PHE	L625	T514	T365
	SER	V626	P515	V366
	LEU	G627		
	GLY	E628	I526	K370
	VAL	E629		G371
	ASN	L630	G532	Q372
	PRO	M631		A373
	ALA	D632	E538	

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	192.74Å 206.98Å 205.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.23 – 2.41 46.23 – 2.41	Depositor EDS
% Data completeness (in resolution range)	93.6 (46.23-2.41) 99.1 (46.23-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.211 , 0.242 0.214 , 0.242	Depositor DCC
R_{free} test set	7893 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.4	EDS
Estimated twinning fraction	0.006 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 157071 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21392	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.26	0/5307	0.43	0/7191
1	B	0.26	0/5349	0.42	0/7246
1	C	0.25	0/5345	0.41	0/7239
1	D	0.25	0/5262	0.41	0/7129
All	All	0.25	0/21263	0.42	0/28805

There are no bond length outliers.

There are no bond angle outliers.

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	5169	0	5079	78	0
1	B	5213	0	5136	123	0
1	C	5213	0	5139	122	0
1	D	5135	0	5046	161	0
2	A	32	0	20	1	0
2	B	32	0	20	2	0
2	C	16	0	10	2	0
2	D	16	0	10	3	0
3	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	30	2	0
3	C	7	0	10	0	0
3	D	7	0	10	0	0
4	A	176	0	0	4	0
4	B	127	0	0	5	0
4	C	102	0	0	7	0
4	D	119	0	0	9	0
All	All	21392	0	20520	482	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 12.

The worst 5 of 482 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:D:482:ASN:HD22	1:D:484:ASN:H	1.01	0.97
1:C:180:ARG:HG3	1:C:180:ARG:HH11	1.27	0.96
1:C:283:GLN:HG2	1:D:280:HIS:CE1	2.07	0.90
1:C:399:ARG:HD3	1:C:403:ASN:HD22	1.40	0.86
1:C:280:HIS:CE1	1:D:283:GLN:HG2	2.12	0.85

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	640/725 (88%)	606 (95%)	32 (5%)	2 (0%)	46 63
1	B	646/725 (89%)	622 (96%)	22 (3%)	2 (0%)	46 63
1	C	646/725 (89%)	618 (96%)	25 (4%)	3 (0%)	34 48
1	D	633/725 (87%)	597 (94%)	32 (5%)	4 (1%)	30 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2565/2900 (88%)	2443 (95%)	111 (4%)	11 (0%)	39 56

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	625	LEU
1	B	17	VAL
1	B	643	LYS
1	C	543	THR
1	D	111	VAL

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	555/623 (89%)	538 (97%)	17 (3%)	47 69
1	B	558/623 (90%)	533 (96%)	25 (4%)	34 52
1	C	558/623 (90%)	538 (96%)	20 (4%)	42 63
1	D	550/623 (88%)	530 (96%)	20 (4%)	42 63
All	All	2221/2492 (89%)	2139 (96%)	82 (4%)	42 62

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	539	ASP
1	C	213	LEU
1	D	387	THR
1	B	590	THR
1	B	645	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	249	GLN
1	C	403	ASN
1	D	302	HIS
1	C	284	ASN
1	C	477	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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	$\# Z > 2$
3	PEG	A	1001	-	6,6,6	0.61	0	5,5,5	0.41	0
2	G6P	A	901	-	16,16,16	0.92	1 (6%)	23,24,24	1.45	4 (17%)
2	G6P	A	902	-	16,16,16	0.91	1 (6%)	23,24,24	1.42	5 (21%)
3	PEG	B	1001	-	6,6,6	0.55	0	5,5,5	0.46	0
3	PEG	B	1002	-	6,6,6	0.57	0	5,5,5	0.47	0
3	PEG	B	706	-	6,6,6	0.61	0	5,5,5	0.47	0
2	G6P	B	901	-	16,16,16	0.90	1 (6%)	23,24,24	1.39	3 (13%)
2	G6P	B	902	-	16,16,16	0.90	0	23,24,24	1.97	6 (26%)
3	PEG	C	1001	-	6,6,6	0.61	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G6P	C	901	-	16,16,16	0.87	1 (6%)	23,24,24	1.48	4 (17%)
3	PEG	D	1002	-	6,6,6	0.63	0	5,5,5	0.48	0
2	G6P	D	901	-	16,16,16	0.87	0	23,24,24	1.37	3 (13%)

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
3	PEG	A	1001	-	-	0/4/4/4	0/0/0/0
2	G6P	A	901	-	-	0/6/26/26	0/1/1/1
2	G6P	A	902	-	-	0/6/26/26	0/1/1/1
3	PEG	B	1001	-	-	0/4/4/4	0/0/0/0
3	PEG	B	1002	-	-	0/4/4/4	0/0/0/0
3	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
3	PEG	C	1001	-	-	0/4/4/4	0/0/0/0
2	G6P	C	901	-	-	0/6/26/26	0/1/1/1
3	PEG	D	1002	-	-	0/4/4/4	0/0/0/0
2	G6P	D	901	-	-	0/6/26/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	G6P	P-O2P	-2.10	1.47	1.54
2	C	901	G6P	P-O2P	-2.09	1.47	1.54
2	A	901	G6P	P-O2P	-2.07	1.47	1.54
2	A	902	G6P	P-O2P	-2.05	1.47	1.54

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	G6P	C4-C3-C2	-4.85	101.74	110.79
2	B	902	G6P	O5-C5-C4	-3.99	102.19	109.68
2	A	901	G6P	C4-C3-C2	-3.41	104.42	110.79
2	C	901	G6P	C4-C3-C2	-3.14	104.94	110.79
2	B	901	G6P	C4-C3-C2	-2.84	105.50	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	G6P	1	0
3	B	1001	PEG	2	0
2	B	902	G6P	2	0
2	C	901	G6P	2	0
2	D	901	G6P	3	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%)	0.23	16 (2%) 61 60	25, 49, 89, 101	0
1	B	645/725 (88%)	0.11	28 (4%) 39 40	33, 50, 83, 96	0
1	C	646/725 (89%)	0.21	25 (3%) 43 44	36, 53, 87, 101	0
1	D	636/725 (87%)	0.35	47 (7%) 17 17	28, 61, 103, 114	0
All	All	2565/2900 (88%)	0.22	116 (4%) 37 38	25, 52, 95, 114	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	630	LEU	8.3
1	D	627	GLY	7.4
1	D	622	PHE	6.5
1	D	126	VAL	6.2
1	B	644	LEU	6.2

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	G6P	A	902	16/16	0.92	0.21	2.06	46,52,58,60	16
2	G6P	A	901	16/16	0.99	0.18	1.54	30,35,38,40	0
3	PEG	D	1002	7/7	0.86	0.15	1.52	47,50,55,58	0
2	G6P	C	901	16/16	0.99	0.16	0.22	39,42,43,44	0
2	G6P	D	901	16/16	0.99	0.14	0.14	32,34,36,38	0
3	PEG	A	1001	7/7	0.85	0.16	-0.47	49,50,54,56	0
2	G6P	B	902	16/16	0.93	0.15	-0.54	51,54,56,60	0
2	G6P	B	901	16/16	0.99	0.13	-0.77	35,38,42,42	0
3	PEG	B	1001	7/7	0.87	0.13	-0.79	42,44,46,50	0
3	PEG	C	1001	7/7	0.90	0.12	-1.43	43,45,49,50	0
3	PEG	B	706	7/7	0.93	0.11	-2.11	43,46,48,49	0
3	PEG	B	1002	7/7	0.81	0.29	-	60,61,65,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.