



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:30 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

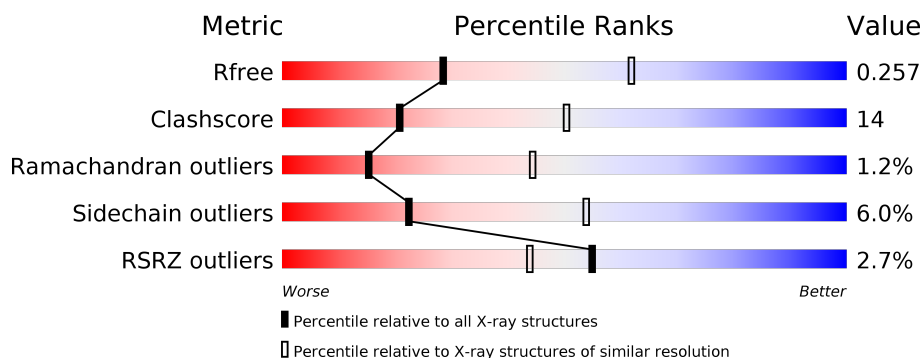
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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  $\geq 3$ , 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%;"> <span>%</span> <span>64%</span> <span>22%</span> <span>• 12%</span> </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%;"> <span>2%</span> <span>60%</span> <span>26%</span> <span>• 12%</span> </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%;"> <span>3%</span> <span>64%</span> <span>23%</span> <span>• 11%</span> </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%;"> <span>3%</span> <span>57%</span> <span>27%</span> <span>• 12%</span> </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	801	-	-	-	X
4	GLC	A	809	-	-	-	X

## 2 Entry composition

There are 7 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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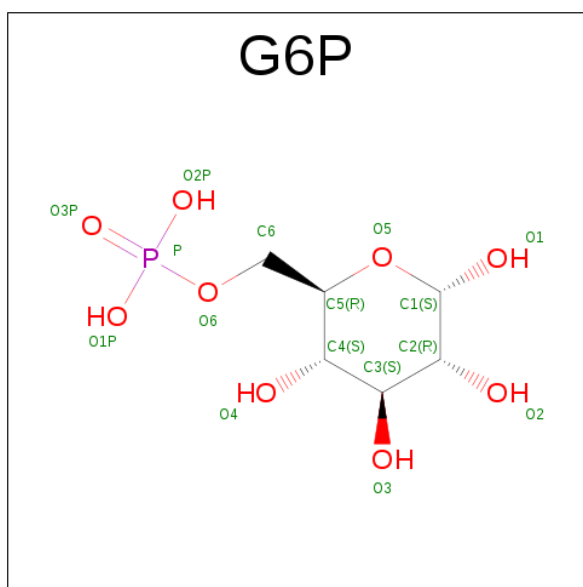
Chain	Residue	Modelled	Actual	Comment	Reference
A	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	-19	MET	-	EXPRESSION TAG	UNP P27472
B	-18	GLY	-	EXPRESSION TAG	UNP P27472
B	-17	SER	-	EXPRESSION TAG	UNP P27472
B	-16	SER	-	EXPRESSION TAG	UNP P27472
B	-15	HIS	-	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 SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



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		

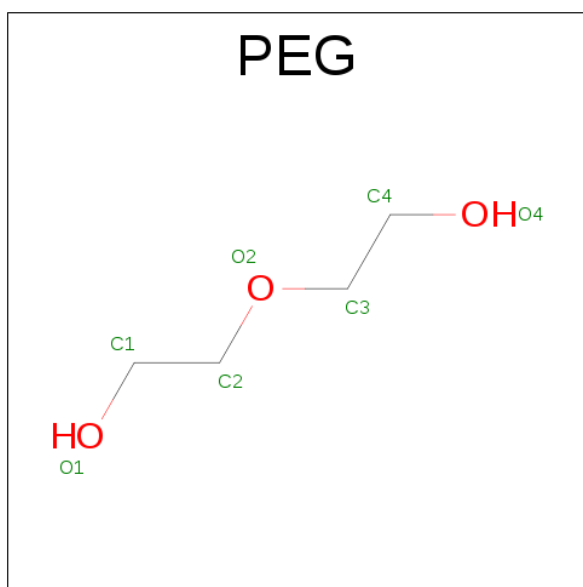
- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	8	Total	C	O	0	0
			78	42	36		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	3	Total	C	O	0	0
			23	12	11		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	4	Total	C	O	0	0
			34	18	16		

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

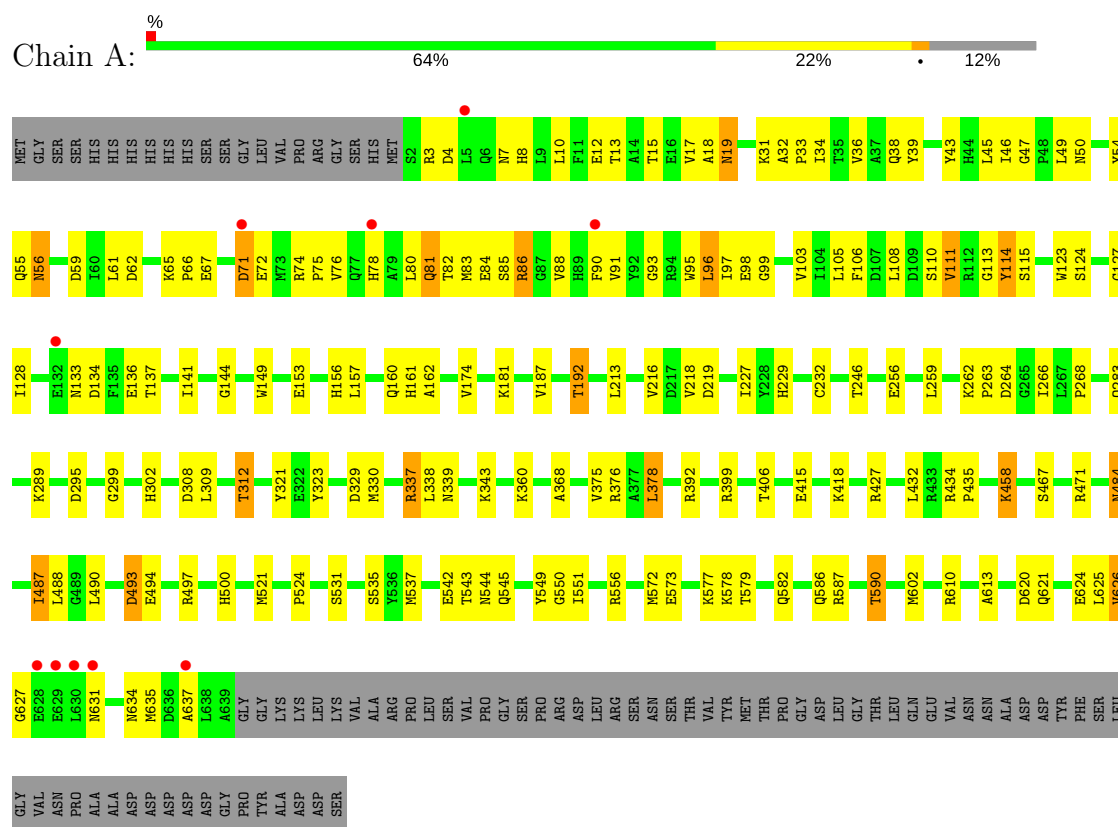
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	5	Total	C	O	0	0
			45	24	21		
7	D	5	Total	C	O	0	0
			45	24	21		



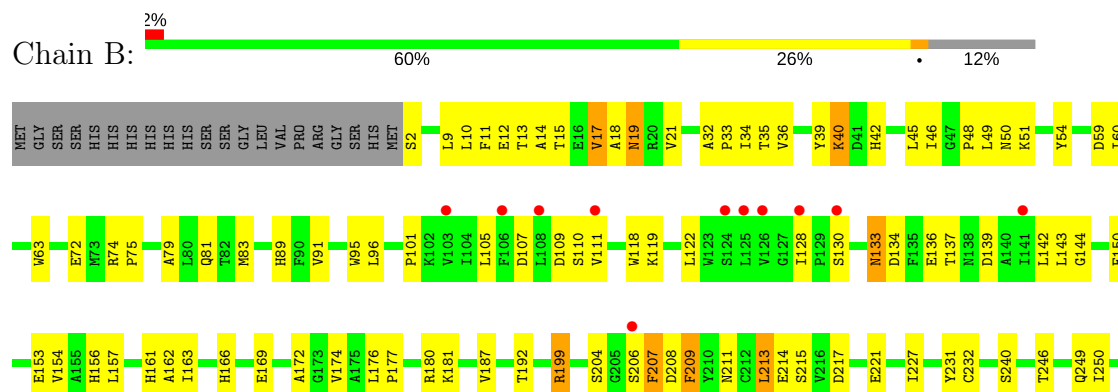
### 3 Residue-property plots [i](#)

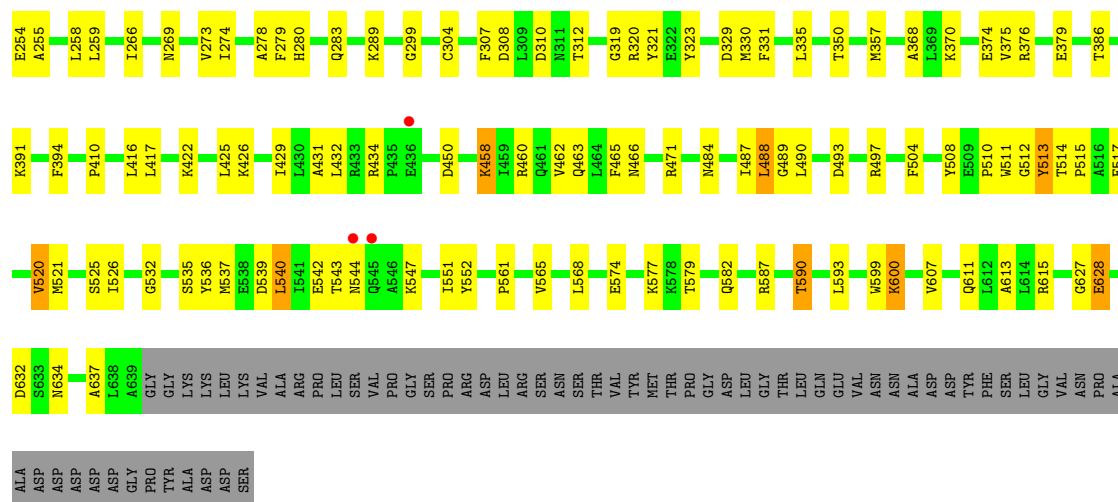
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

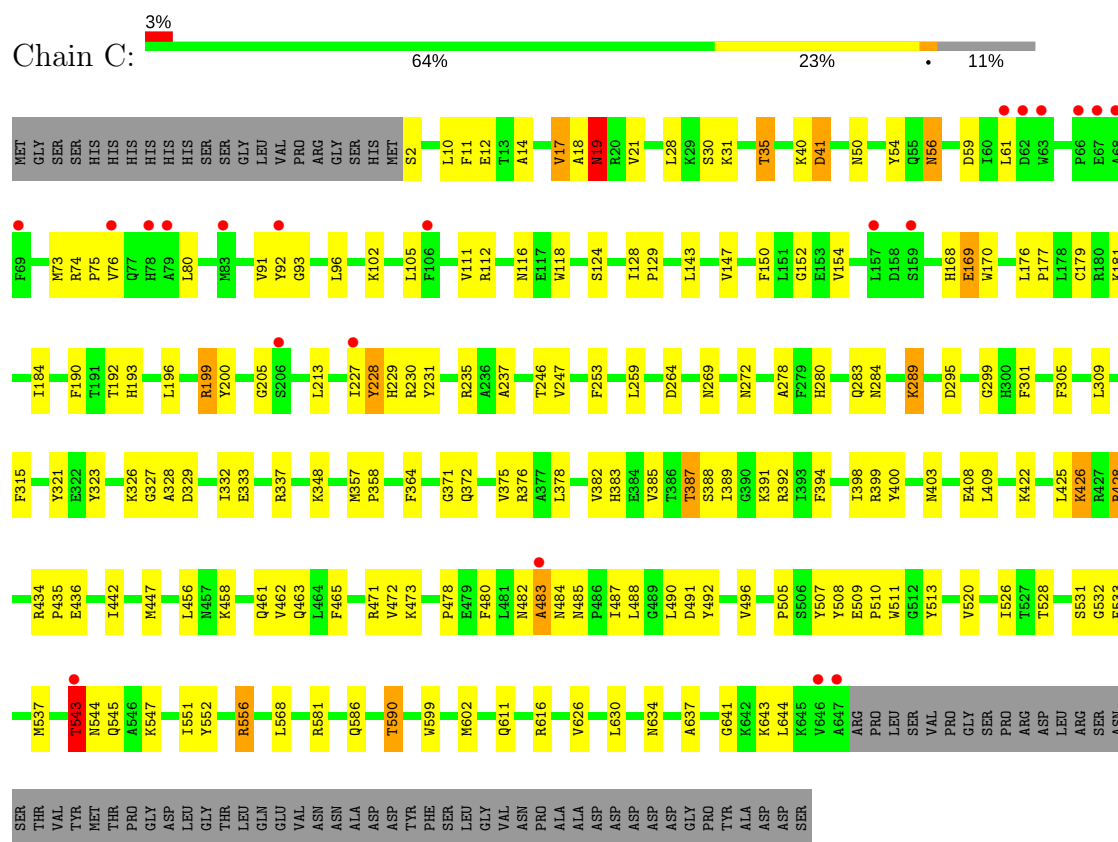


- Molecule 1: PROTEIN (Glycogen [starch] synthase isoform 2)

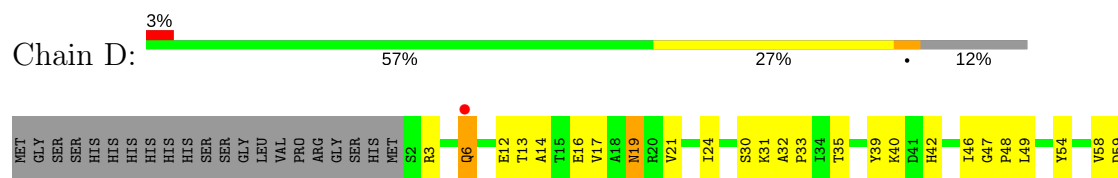




• Molecule 1: PROTEIN (Glycogen [starch] synthase isoform 2)



• 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	
LEU	L612	H500	H383	Y228	E153	S70
THR	A613	Y507	T387	C232	V154	D71
LEU	L614	P510	G390	A238	A155	M73
GLN	R615	G512	F394	H239	H156	R74
GLU	G617	Y513	R399	S240	L157	P75
VAL	Y618	T514	Y400	T245	D158	V76
ASN	P619	P515	P401	T246	H161	Q77
ALA	D620	S525	H403	F253	A162	L80
ASP	Q621	V523	G404	H257	I163	Q81
ASP	R623	P524	L409	L258	V164	T82
TYR	F622	S525	D412	K260	A165	M83
PHE	E623	V530	L417	R261	H166	E84
SER	L625	S531	K422	D264	F167	S85
LEU	V626	G532	M537	G265	H168	R86
GLY	G627	M537	L540	I266	E169	
VAL	G628	I541	R426	L267	W170	F90
ASN	E629	E542	R427	K275	V174	V91
PRO	L630	T543	R428	A278	A175	Y92
ALA	S633	N544	R434	H280	L176	L96
ALA	N634	Q545	P435	Q283	P177	
ASP	M635	Y549	E436	N284	P101	P101
ASP	D636	G550	G437	F189	K102	K102
ASP	A637	I551	Q438	T187	L105	L105
ASP	L638	VAL	L439	T191	F106	D107
GLY	A639	ALA	P440	T192	L108	L108
PRO	GLY	ARG	P441	H193	D109	D109
TYR	GLY	PRO	H447	L196	S110	S110
LYS	LYS	ALA	V565	Y200	V111	V111
LEU	LEU	ARG	T579	K324	G113	G113
LYS	LYS	PRO	R580	F331	Y114	Y114
VAL	VAL	SER	F581	L335	S115	S115
ALA	ALA	ARG	Q582	A336	K119	K119
ARG	ARG	LEU	R586	R337	G120	G120
PRO	PRO	LEU	R587	V344	D121	D121
LEU	LEU	SER	V590	G345	W123	W123
SER	SER	ASN	E591	S346	S204	S204
ASN	ASN	THR	A592	V210	G205	G205
SER	SER	THR	L593	L213	SER	SER
THR	THR	VAL	S594	D217	PHE	PHE
VAL	VAL			V218	D208	D208
					F209	F209
					Y210	Y210
					L213	L213
					E132	E132
					A140	A140

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.211 , 0.261 0.205 , 0.257	Depositor DCC
$R_{free}$ test set	5039 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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

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	78	0	64	2	0
4	A	23	0	19	2	0
5	A	7	0	10	0	0
5	B	14	0	20	2	0
5	C	7	0	10	0	0
6	C	34	0	28	3	0
7	D	90	0	74	2	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 [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	636/725 (88%)	586 (92%)	44 (7%)	6 (1%)	20	52
1	B	636/725 (88%)	581 (91%)	48 (8%)	7 (1%)	17	47
1	C	644/725 (89%)	598 (93%)	38 (6%)	8 (1%)	15	44
1	D	632/725 (87%)	556 (88%)	67 (11%)	9 (1%)	13	39
All	All	2548/2900 (88%)	2321 (91%)	197 (8%)	30 (1%)	15	44

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%)	18	46
1	B	551/623 (88%)	518 (94%)	33 (6%)	22	54
1	C	556/623 (89%)	527 (95%)	29 (5%)	27	60
1	D	549/623 (88%)	517 (94%)	32 (6%)	23	55
All	All	2207/2492 (89%)	2075 (94%)	132 (6%)	22	54

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 ⓘ

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 ⓘ

Of 25 carbohydrates modelled in this entry, 5 are modelled with single atom - leaving 20 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	$\# Z  > 2$
3	GLC	A	801	3	11,11,12	0.83	0	13,15,17	1.30	1 (7%)
3	GLC	A	802	3	11,11,12	0.57	0	13,15,17	1.34	3 (23%)
3	GLC	A	803	3	11,11,12	0.28	0	13,15,17	1.31	2 (15%)
3	GLC	A	804	3	11,11,12	0.36	0	13,15,17	0.93	1 (7%)
3	GLC	A	805	3	11,11,12	0.55	0	13,15,17	0.81	0
3	GLC	A	806	3	11,11,12	0.86	0	13,15,17	1.22	1 (7%)
3	GLC	A	807	3	11,11,12	0.83	0	13,15,17	1.61	2 (15%)
4	GLC	A	808	4	11,11,12	0.74	0	13,15,17	0.97	1 (7%)
4	GLC	A	809	4	11,11,12	0.60	0	13,15,17	2.00	3 (23%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GLC	C	801	6	11,11,12	0.39	0	13,15,17	1.16	2 (15%)
6	GLC	C	802	6	11,11,12	0.40	0	13,15,17	0.72	0
6	GLC	C	803	6	11,11,12	0.26	0	13,15,17	0.82	0
7	GLC	D	801	7	11,11,12	0.56	0	13,15,17	0.91	0
7	GLC	D	802	7	11,11,12	0.35	0	13,15,17	1.20	1 (7%)
7	GLC	D	803	7	11,11,12	0.37	0	13,15,17	1.03	0
7	GLC	D	804	7	11,11,12	0.84	0	13,15,17	2.13	3 (23%)
7	GLC	D	806	7	11,11,12	0.68	0	13,15,17	1.78	2 (15%)
7	GLC	D	807	7	11,11,12	0.62	0	13,15,17	1.22	2 (15%)
7	GLC	D	808	7	11,11,12	0.36	0	13,15,17	1.48	1 (7%)
7	GLC	D	809	7	11,11,12	0.63	0	13,15,17	1.44	1 (7%)

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	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
4	GLC	A	808	4	-	0/2/19/22	0/1/1/1
4	GLC	A	809	4	-	0/2/19/22	0/1/1/1
6	GLC	C	801	6	-	0/2/19/22	0/1/1/1
6	GLC	C	802	6	-	0/2/19/22	0/1/1/1
6	GLC	C	803	6	-	0/2/19/22	0/1/1/1
7	GLC	D	801	7	-	0/2/19/22	0/1/1/1
7	GLC	D	802	7	-	0/2/19/22	0/1/1/1
7	GLC	D	803	7	-	0/2/19/22	0/1/1/1
7	GLC	D	804	7	-	0/2/19/22	0/1/1/1
7	GLC	D	806	7	-	0/2/19/22	0/1/1/1
7	GLC	D	807	7	-	0/2/19/22	0/1/1/1
7	GLC	D	808	7	-	0/2/19/22	0/1/1/1
7	GLC	D	809	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	GLC	C2-C3-C4	-2.58	106.37	110.88
7	D	804	GLC	C2-C3-C4	-2.35	106.77	110.88
4	A	809	GLC	O4-C4-C3	-2.17	105.63	110.36
3	A	802	GLC	O5-C1-C2	-2.11	107.49	110.79
3	A	804	GLC	C1-O5-C5	2.15	115.13	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	GLC	2	0
4	A	808	GLC	2	0
4	A	809	GLC	1	0
6	C	801	GLC	1	0
6	C	802	GLC	1	0
6	C	803	GLC	2	0
7	D	802	GLC	1	0
7	D	803	GLC	1	0

## 5.6 Ligand geometry

9 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	$\# Z  > 2$
5	PEG	A	1009	-	6,6,6	0.53	0	5,5,5	0.24	0
2	G6P	A	901	-	16,16,16	0.51	0	24,24,24	0.95	1 (4%)
5	PEG	B	1001	-	6,6,6	0.54	0	5,5,5	0.19	0
5	PEG	B	706	-	6,6,6	0.55	0	5,5,5	0.18	0
2	G6P	B	901	-	16,16,16	0.53	0	24,24,24	1.10	2 (8%)
2	G6P	B	902	-	16,16,16	0.69	0	24,24,24	1.56	3 (12%)
5	PEG	C	1004	-	6,6,6	0.56	0	5,5,5	0.14	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	0.52	0	24,24,24	0.87	0
2	G6P	D	901	-	16,16,16	0.43	0	24,24,24	0.94	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
5	PEG	A	1009	-	-	0/4/4/4	0/0/0/0
2	G6P	A	901	-	-	0/6/26/26	0/1/1/1
5	PEG	B	1001	-	-	0/4/4/4	0/0/0/0
5	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
5	PEG	C	1004	-	-	0/4/4/4	0/0/0/0
2	G6P	C	901	-	-	0/6/26/26	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 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	G6P	C3-C4-C5	-3.59	103.90	110.22
2	B	902	G6P	C4-C3-C2	-3.12	105.33	110.84
2	B	901	G6P	C1-C2-C3	-2.31	106.48	110.65
2	A	901	G6P	C1-C2-C3	-2.02	107.00	110.65
2	B	901	G6P	O5-C5-C6	2.44	111.50	106.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	G6P	1	0
5	B	1001	PEG	2	0
2	B	901	G6P	1	0
2	C	901	G6P	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, 95<sup>th</sup> 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 <sup>2</sup> )	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%) 47 36	42, 70, 111, 126	0
1	D	636/725 (87%)	0.15	23 (3%) 43 32	32, 76, 127, 136	0
All	All	2558/2900 (88%)	0.09	68 (2%) 55 44	27, 66, 118, 136	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	627	GLY	6.2
1	D	624	GLU	5.0
1	D	625	LEU	4.0
1	D	630	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](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	GLC	A	801	11/12	0.84	0.32	6.80	61,70,74,76	0
4	GLC	A	809	11/12	0.85	0.25	3.05	60,62,69,69	0
6	GLC	C	802	11/12	0.91	0.23	0.12	108,110,113,113	0
7	GLC	D	804	11/12	0.91	0.20	0.09	46,56,60,63	0
3	GLC	A	802	11/12	0.92	0.18	-0.04	54,61,66,67	0
7	GLC	D	802	11/12	0.93	0.16	-0.04	58,63,69,75	0
6	GLC	C	801	11/12	0.70	0.23	-0.11	111,113,115,116	0
3	GLC	A	804	11/12	0.94	0.16	-0.84	64,65,71,75	0
3	GLC	A	803	11/12	0.96	0.15	-1.40	53,60,63,66	0
7	GLC	D	803	11/12	0.98	0.12	-1.64	49,53,56,56	0
7	GLC	D	809	11/12	0.90	0.18	-	66,71,75,77	0
7	GLC	D	807	11/12	0.91	0.23	-	65,71,75,80	0
7	GLC	D	808	11/12	0.94	0.20	-	57,60,65,69	0
3	GLC	A	800	1/12	0.57	0.47	-	76,76,76,76	0
7	GLC	D	806	11/12	0.82	0.36	-	84,94,99,99	0
3	GLC	A	805	11/12	0.92	0.21	-	68,77,83,86	0
7	GLC	D	805	1/12	0.82	0.18	-	52,52,52,52	0
7	GLC	D	801	11/12	0.89	0.31	-	78,85,87,87	0
7	GLC	D	810	1/12	0.73	0.27	-	78,78,78,78	0
4	GLC	A	808	11/12	0.86	0.32	-	66,71,75,75	0
3	GLC	A	807	11/12	0.83	0.23	-	70,80,85,86	0
3	GLC	A	806	11/12	0.92	0.23	-	76,82,87,88	0
4	GLC	A	810	1/12	0.85	0.28	-	64,64,64,64	0
6	GLC	C	804	1/12	0.96	0.18	-	105,105,105,105	0
6	GLC	C	803	11/12	0.86	0.18	-	103,106,109,110	0

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	G6P	B	902	16/16	0.90	0.19	0.59	78,83,88,89	0
5	PEG	B	706	7/7	0.89	0.21	0.48	51,56,63,63	0
2	G6P	C	901	16/16	0.97	0.19	0.46	46,50,52,52	0
2	G6P	A	901	16/16	0.99	0.18	0.22	34,36,41,43	0
5	PEG	A	1009	7/7	0.93	0.18	-0.66	58,60,62,62	0
2	G6P	B	901	16/16	0.98	0.17	-0.66	42,45,48,50	0
2	G6P	D	901	16/16	0.99	0.15	-1.11	35,37,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEG	C	1004	7/7	0.94	0.16	-2.04	48,51,58,60	0
5	PEG	B	1001	7/7	0.90	0.15	-2.09	50,52,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.