wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:43 PM GMT

PDB ID	:	3RT1
Title	:	Maltodextarn 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

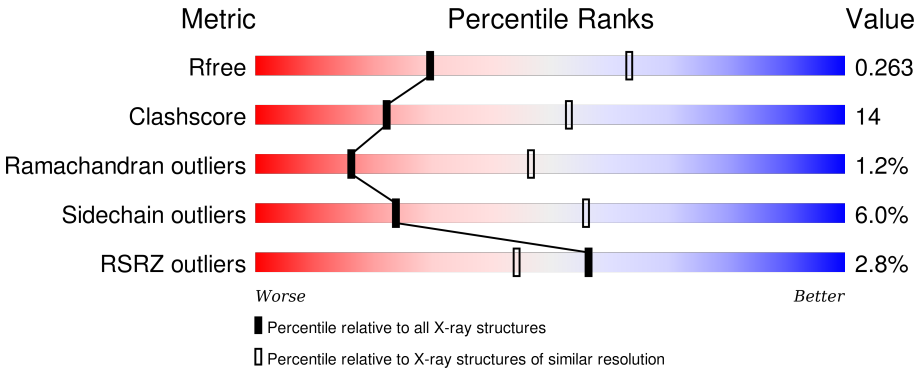
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 <=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	64% 22% • 12%
1	B	725	2% 60% 26% • 12%
1	C	725	3% 64% 23% • 11%
1	D	725	3% 57% 27% • 12%

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
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

Continued on next page...

Continued from previous page...

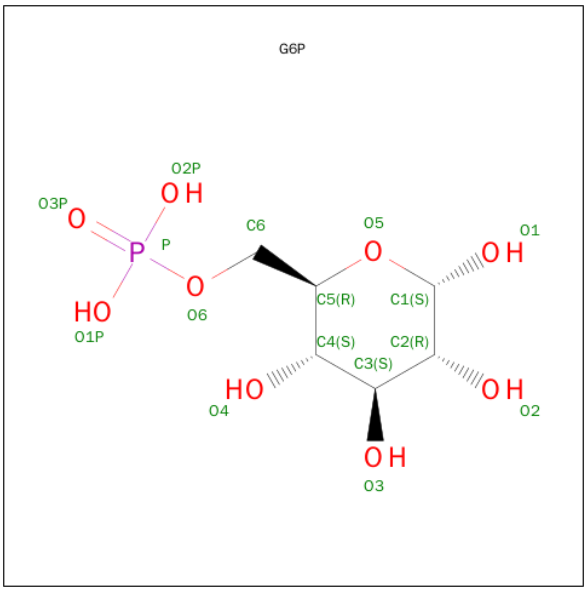
Chain	Residue	Modelled	Actual	Comment	Reference
A	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	-19	MET	-	EXPRESSION TAG	UNP P27472
B	-18	GLY	-	EXPRESSION TAG	UNP P27472
B	-17	SER	-	EXPRESSION TAG	UNP P27472
B	-16	SER	-	EXPRESSION TAG	UNP P27472
B	-15	HIS	-	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

Continued on next page...

Continued from previous page...

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: $C_6H_{13}O_9P$).



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

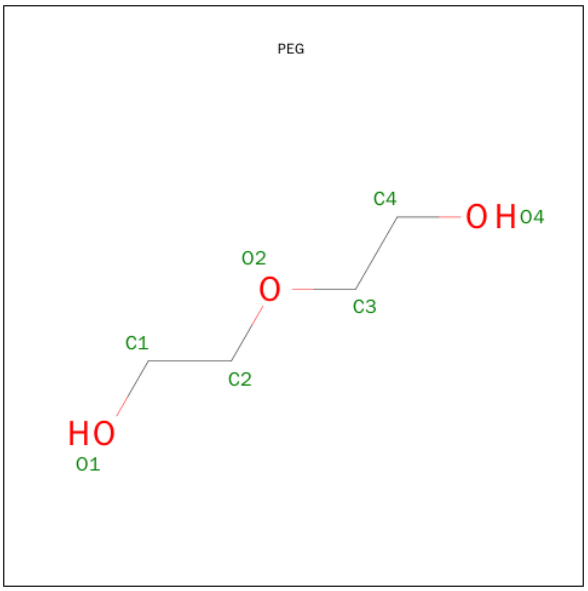
- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

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

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

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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

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

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

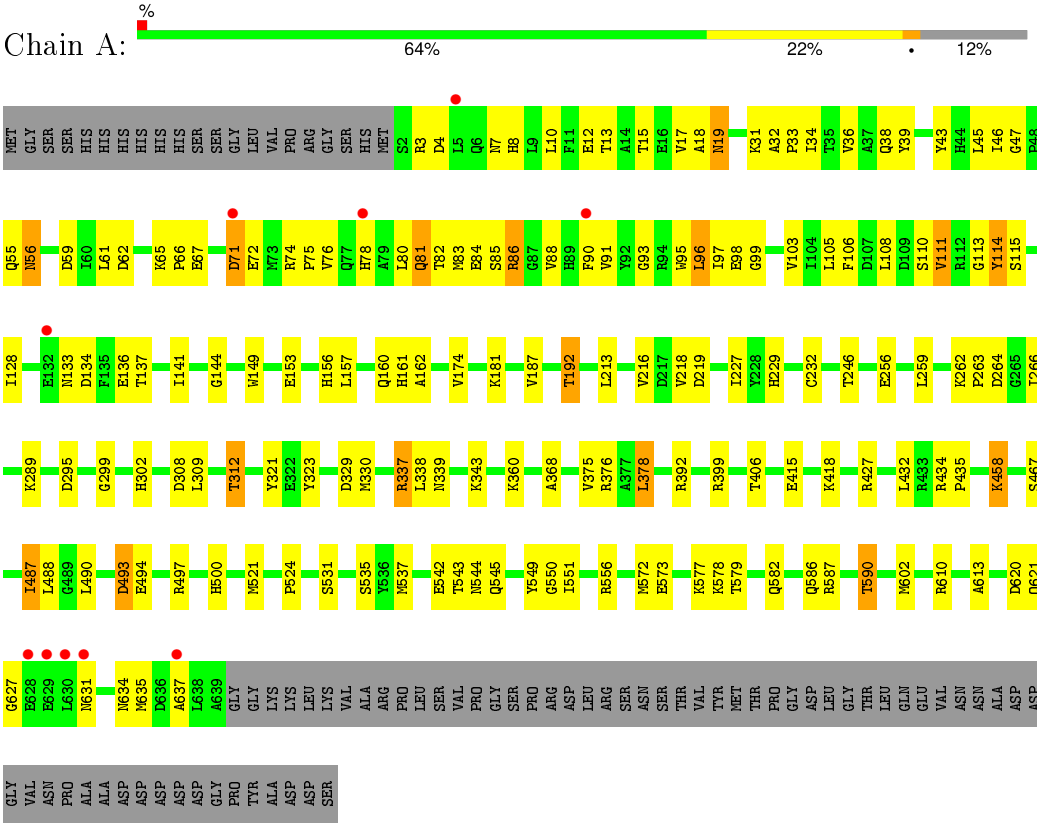
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	5	Total C O 45 24 21	0	0
7	D	5	Total C O 45 24 21	0	0

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 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.

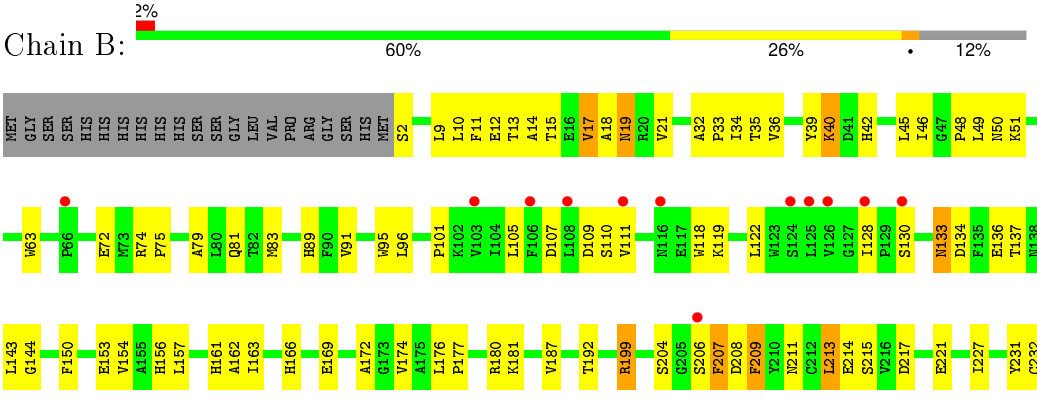
• Molecule 1: PROTEIN (Glycogen [starch] synthase isoform 2)

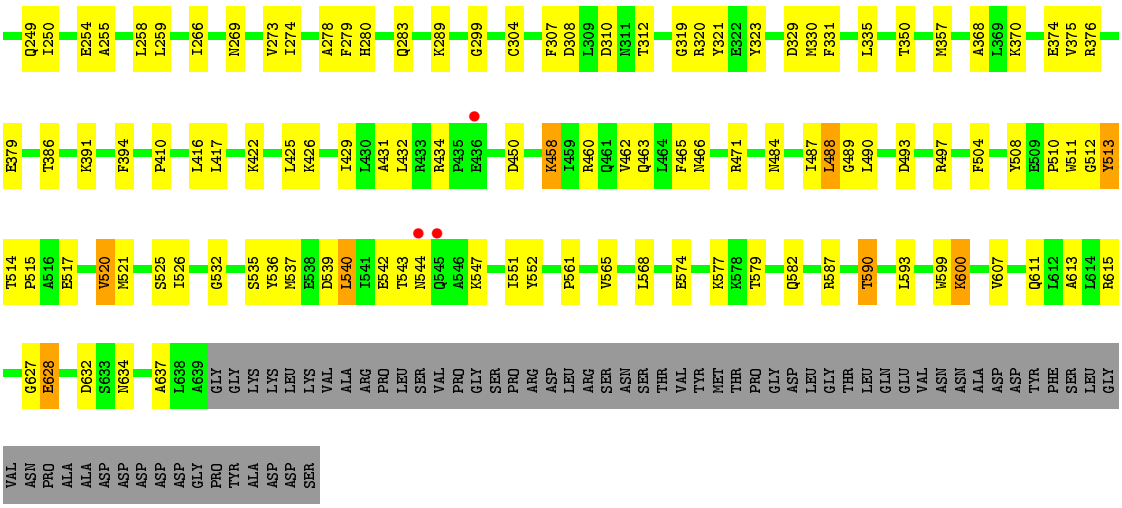
Chain A:



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

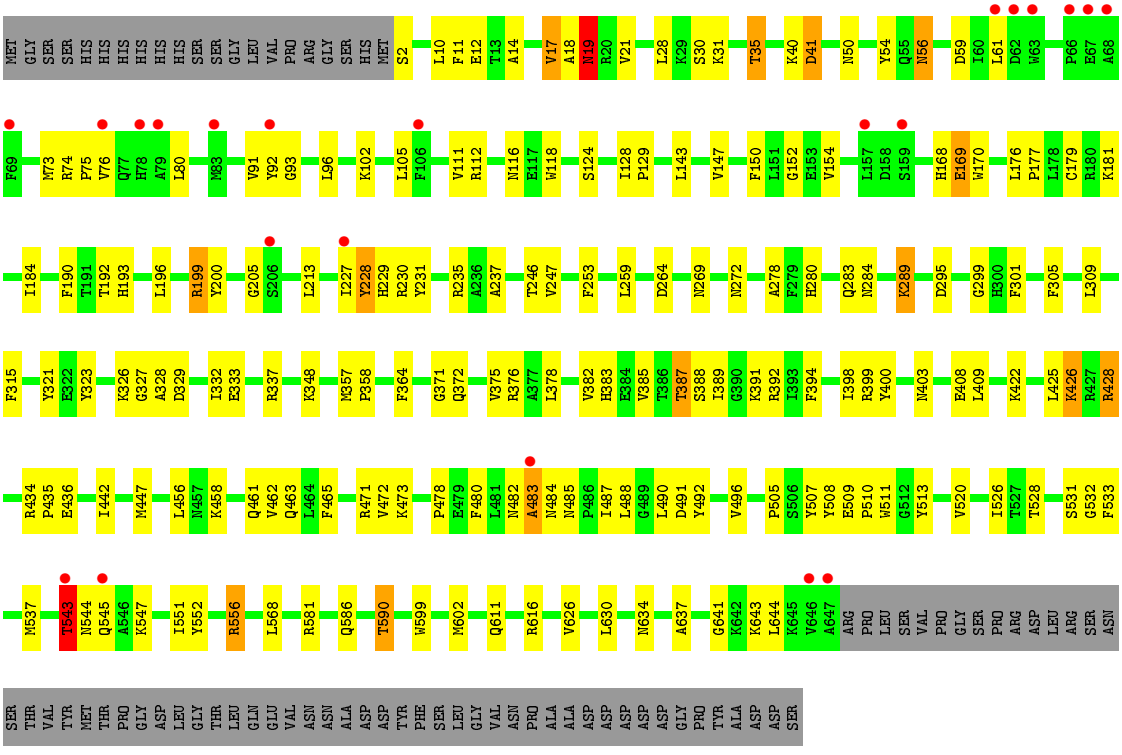
Chain B:





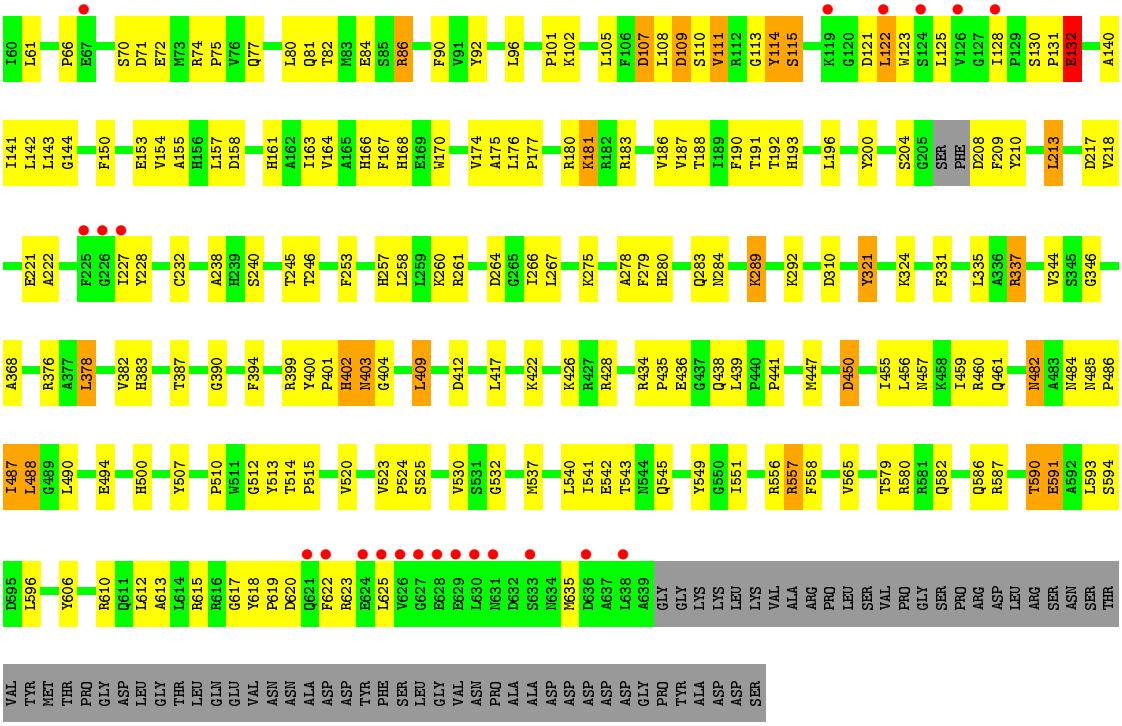
• Molecule 1: PROTEIN (Glycogen [starch] synthase isoform 2)

Chain C:



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

Chain D:


I60 L61 P66 E67 S70 D71 E72 W73 R74 P75 V76 Q77 L80 Q81 T82 N83 E84 S85 R86 F90 V91 Y92 L96 P101 K102 L105 F106 D107 L108 D109 S110 V111 R112 G113 Y114 S115 K119 G120 D121 L122 W123 S124 L125 V126 G127 I128 P129 S130 P131 E132 A140
I141 L142 L143 G144 F150 E153 V154 A155 H156 L157 D158 H161 A162 I163 V164 A165 H166 F167 H168 E169 W170 V174 A175 L176 P177 R180 K181 R182 R183 V186 V187 T188 I189 F190 T191 T192 H193 L196 Y200 S204 G205 SER PHE D208 F209 Y210 L213 D217 V218
E221 A222 F225 G226 I227 Y228 C232 A238 H239 S240 T245 T246 F253 H257 L258 L259 K260 R261 D264 G265 I266 L267 K275 A278 F279 H280 Q283 N284 K289 K292 D310 Y321 K324 F331 L335 A336 R337 V344 S345 G346
A368 R376 A377 L378 V382 H383 T387 G390 F394 R399 Y400 P401 H402 N403 G404 L409 D412 L417 K422 K426 R427 R428 R434 P435 E436 G437 Q438 L439 P440 P441 M447 D450 I455 L456 N457 K458 I459 R460 Q461 N482 A483 N484 N485 P486
I487 L488 G489 L490 E494 H500 Y507 P510 W511 G512 Y513 T514 P515 V520 V523 P524 S525 V530 S531 G532 M537 L540 I541 E542 T543 N544 Q545 Y549 G550 I551 R556 R557 F558 V565 T579 R580 R581 Q582 Q586 R587 T590 E591 A592 L593 S594
D595 L596 Y606 R610 Q611 L612 A613 L614 R615 R616 G617 Y618 P619 D620 Q621 F622 R623 E624 L625 V626 G627 E628 E629 L630 N631 D632 S633 N634 M635 D636 A637 L638 A639 GLY GLY LYS LYS LEU LYS VAL ALA ARG PRO LEU SER VAL PRO GLY SER PRO ARG ASP LEU ARG SER ASN SER THR
VAL TYR MET THR PRO GLY ASP LEU GLY THR LEU GLN GLU VAL ASN ASN ALA ASP ASP TYR PHE SER LEU GLY VAL ASN PRO ALA ALA ASP ASP ASP ASP GLY PRO TYR ALA ASP ASP SER

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.12 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.211 , 0.261 0.215 , 0.263	Depositor DCC
R_{free} test set	5042 reflections (5.26%)	DCC
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
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 101270 reflections (0.001%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

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%)	21	55
1	B	636/725 (88%)	581 (91%)	48 (8%)	7 (1%)	17	50
1	C	644/725 (89%)	598 (93%)	38 (6%)	8 (1%)	16	47
1	D	632/725 (87%)	556 (88%)	67 (11%)	9 (1%)	14	42
All	All	2548/2900 (88%)	2321 (91%)	197 (8%)	30 (1%)	16	47

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	551/623 (88%)	513 (93%)	38 (7%)	19	48
1	B	551/623 (88%)	518 (94%)	33 (6%)	24	56
1	C	556/623 (89%)	527 (95%)	29 (5%)	29	62
1	D	549/623 (88%)	517 (94%)	32 (6%)	25	57
All	All	2207/2492 (89%)	2075 (94%)	132 (6%)	24	56

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)

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	0.81	0	14,15,17	1.27	1 (7%)
3	GLC	A	802	3	11,11,12	0.55	0	14,15,17	1.36	3 (21%)
3	GLC	A	803	3	11,11,12	0.28	0	14,15,17	1.33	2 (14%)
3	GLC	A	804	3	11,11,12	0.35	0	14,15,17	0.96	1 (7%)
3	GLC	A	805	3	11,11,12	0.53	0	14,15,17	0.83	0
3	GLC	A	806	3	11,11,12	0.83	0	14,15,17	1.25	1 (7%)
3	GLC	A	807	3	11,11,12	0.82	0	14,15,17	1.71	2 (14%)
4	GLC	A	808	4	11,11,12	0.72	0	14,15,17	0.99	1 (7%)
4	GLC	A	809	4	11,11,12	0.58	0	14,15,17	2.02	4 (28%)

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	0.38	0	14,15,17	1.19	2 (14%)
6	GLC	C	802	6	11,11,12	0.39	0	14,15,17	0.82	0
6	GLC	C	803	6	11,11,12	0.26	0	14,15,17	0.89	1 (7%)
7	GLC	D	801	7	11,11,12	0.55	0	14,15,17	0.99	0
7	GLC	D	802	7	11,11,12	0.34	0	14,15,17	1.27	1 (7%)
7	GLC	D	803	7	11,11,12	0.36	0	14,15,17	1.02	0
7	GLC	D	804	7	11,11,12	0.82	0	14,15,17	2.19	3 (21%)
7	GLC	D	806	7	11,11,12	0.67	0	14,15,17	1.87	2 (14%)
7	GLC	D	807	7	11,11,12	0.60	0	14,15,17	1.27	2 (14%)
7	GLC	D	808	7	11,11,12	0.35	0	14,15,17	1.51	1 (7%)
7	GLC	D	809	7	11,11,12	0.62	0	14,15,17	1.53	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 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	GLC	C2-C3-C4	-2.75	106.37	111.04
7	D	804	GLC	C2-C3-C4	-2.52	106.77	111.04
4	A	809	GLC	O4-C4-C3	-2.09	105.63	110.34
3	A	802	GLC	O5-C1-C2	-2.08	107.49	110.86
4	A	809	GLC	C3-C4-C5	2.01	113.71	110.20

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 (i)

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	0.52	0	5,5,5	0.25	0
2	G6P	A	901	-	16,16,16	0.55	0	23,24,24	0.95	1 (4%)
5	PEG	B	1001	-	6,6,6	0.53	0	5,5,5	0.21	0
5	PEG	B	706	-	6,6,6	0.54	0	5,5,5	0.21	0
2	G6P	B	901	-	16,16,16	0.55	0	23,24,24	1.16	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	G6P	B	902	-	16,16,16	0.68	0	23,24,24	1.56	3 (13%)
5	PEG	C	1004	-	6,6,6	0.55	0	5,5,5	0.14	0
2	G6P	C	901	-	16,16,16	0.53	0	23,24,24	0.94	1 (4%)
2	G6P	D	901	-	16,16,16	0.45	0	23,24,24	1.00	1 (4%)

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 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	902	G6P	C3-C4-C5	-3.61	103.90	110.20
2	B	902	G6P	C4-C3-C2	-2.93	105.33	110.79
2	B	901	G6P	C1-C2-C3	-2.65	106.48	110.43
2	A	901	G6P	C1-C2-C3	-2.31	107.00	110.43
2	D	901	G6P	O6-P-O3P	-2.25	101.42	107.14

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	G6P	1	0
2	D	901	G6P	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	638/725 (88%)	-0.00	10 (1%)	74	66	27, 58, 110, 124	0
1	B	638/725 (88%)	0.09	16 (2%)	61	48	38, 65, 110, 123	0
1	C	646/725 (89%)	0.16	22 (3%)	49	36	42, 70, 111, 126	0
1	D	636/725 (87%)	0.16	23 (3%)	46	34	32, 76, 127, 136	0
All	All	2558/2900 (88%)	0.10	71 (2%)	56	44	27, 66, 118, 136	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	627	GLY	6.3
1	D	624	GLU	5.1
1	D	625	LEU	4.1
1	D	630	LEU	4.1
1	C	62	ASP	3.8

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

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

6.3 Carbohydrates

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^{th} 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(Å^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^{th} 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(Å^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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	PEG	C	1004	7/7	0.94	0.16	-2.06	48,51,58,60	0
5	PEG	B	1001	7/7	0.90	0.14	-2.13	50,52,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.