



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:10 PM GMT

PDB ID : 4KQM
Title : Crystal structure of yeast glycogen synthase E169Q mutant in complex with glucose and UDP
Authors : Chikwana, V.M.; Hurley, T.D.
Deposited on : 2013-05-15
Resolution : 2.77 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

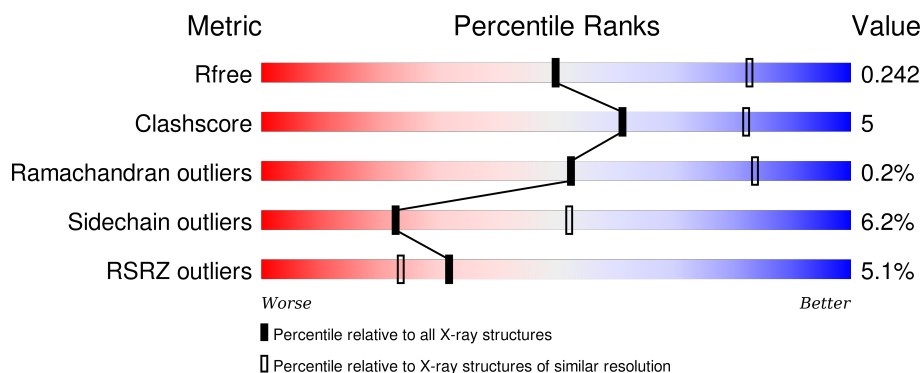
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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	724	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	724	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	724	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	724	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>15%</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
4	PEG	B	803	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20825 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 Gsy2p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5157	3292	903	943	19			
1	B	638	Total	C	N	O	S	0	1	0
			5163	3296	904	944	19			
1	C	638	Total	C	N	O	S	0	0	0
			5157	3292	903	943	19			
1	D	635	Total	C	N	O	S	0	0	0
			5132	3276	900	937	19			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1
A	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
A	-16	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
A	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
A	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
A	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
A	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
A	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
A	0	SER	-	EXPRESSION TAG	UNP E7NKU1
A	169	GLN	GLU	ENGINEERED MUTATION	UNP E7NKU1
B	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1

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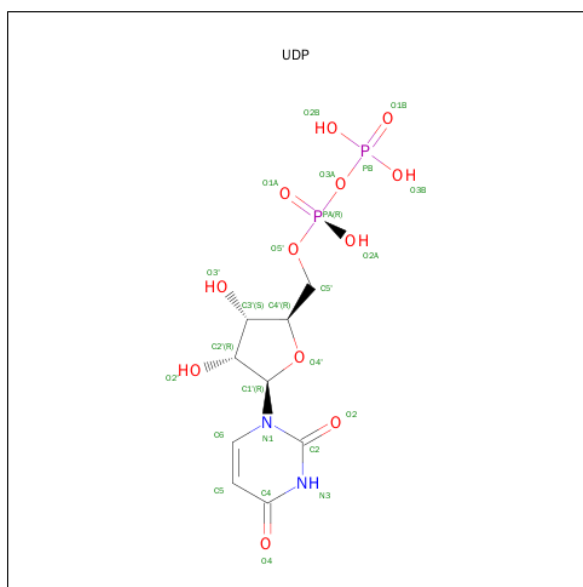
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
B	-16	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
B	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
B	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
B	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
B	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
B	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
B	0	SER	-	EXPRESSION TAG	UNP E7NKU1
B	169	GLN	GLU	ENGINEERED MUTATION	UNP E7NKU1
C	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1
C	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
C	-16	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
C	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
C	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
C	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
C	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
C	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
C	0	SER	-	EXPRESSION TAG	UNP E7NKU1
C	169	GLN	GLU	ENGINEERED MUTATION	UNP E7NKU1
D	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1
D	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
D	-16	SER	-	EXPRESSION TAG	UNP E7NKU1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
D	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
D	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
D	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
D	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
D	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
D	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
D	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
D	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
D	0	SER	-	EXPRESSION TAG	UNP E7NKU1
D	169	GLN	GLU	ENGINEERED MUTATION	UNP E7NKU1

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

-
- The chemical structure of G6P (Glucose-6-phosphate) is shown. It consists of a glucose molecule in its cyclic form (a six-membered ring) and a phosphate group. The glucose ring is labeled with carbons C1(S), C2(R), C3(S), C4(S), C5(R), and C6. The phosphate group is labeled with phosphorus (P) and oxygens O1, O2, O3, O4, O5, and O6. The structure is color-coded: carbons are grey, oxygens are red, and phosphorus is purple. Stereochemistry is indicated with wedges and dashes.

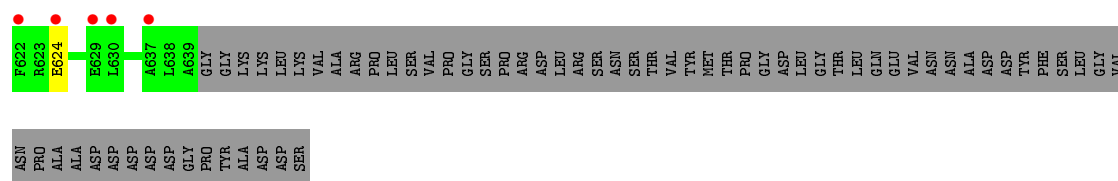
- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



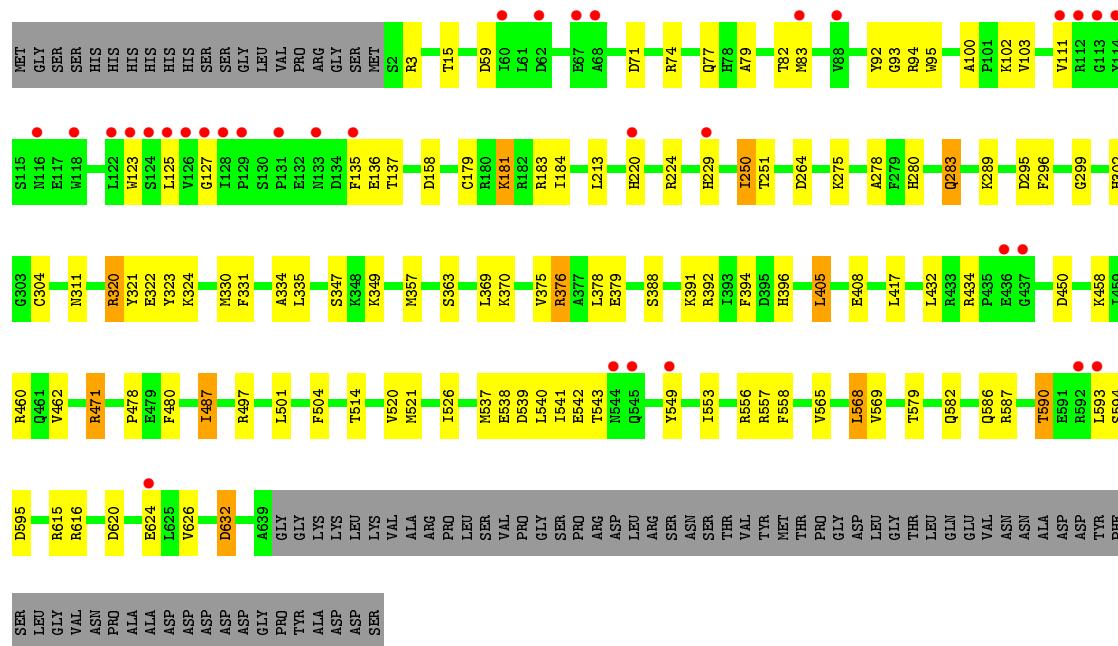
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

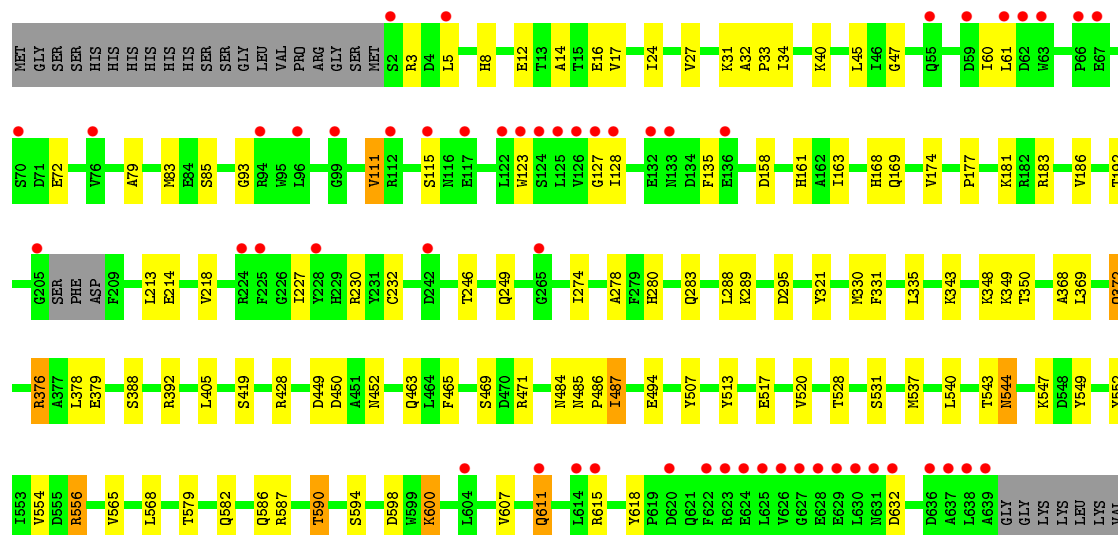
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	2	Total	C	O	0	0
			24	12	12		



• Molecule 1: Gsy2p



• Molecule 1: Gsy2p



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	SER	LEU	GLY	VAL	ASN	PRO	ALA	ALA	ASP	ASP	ASP	ASP	GLY	PRO	TYR	ALA	ASP	ASP	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	192.71Å 204.44Å 206.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 2.77 48.41 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.41-2.77) 98.7 (48.41-2.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.201 , 0.241 0.201 , 0.242	Depositor DCC
R_{free} test set	5073 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.8	EDS
Estimated twinning fraction	0.005 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 102101 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20825	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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: GLC, UDP, BGC, PEG, G6P

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	0.42	0/5282	0.59	0/7155
1	B	0.51	0/5291	0.67	0/7167
1	C	0.44	0/5282	0.61	0/7155
1	D	0.45	0/5255	0.59	0/7117
All	All	0.46	0/21110	0.62	0/28594

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	5157	0	5072	60	0
1	B	5163	0	5080	57	0
1	C	5157	0	5072	64	0
1	D	5132	0	5053	54	1
2	A	25	0	11	0	0
2	B	25	0	11	1	0
2	C	25	0	11	3	0
2	D	25	0	11	0	0
3	A	16	0	11	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	11	1	0
3	C	16	0	11	0	0
3	D	16	0	11	0	0
4	A	7	0	10	1	0
4	B	7	0	10	1	0
4	C	7	0	10	2	0
4	D	7	0	10	1	0
5	C	24	0	12	0	0
All	All	20825	0	20417	226	1

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 5.

The worst 5 of 226 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:B:283:GLN:HG2	1:C:280:HIS:CE1	2.00	0.96
1:A:280:HIS:CE1	1:D:283:GLN:HG2	2.07	0.88
1:B:280:HIS:CE1	1:C:283:GLN:HG2	2.10	0.86
1:A:379:GLU:HG2	4:B:803:PEG:H41	1.65	0.78
1:B:349:LYS:HE2	1:B:576:VAL:O	1.85	0.77

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:SER:OG	1:D:85:SER:OG[2_555]	1.92	0.28

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	636/724 (88%)	610 (96%)	24 (4%)	2 (0%)	46	78
1	B	637/724 (88%)	620 (97%)	16 (2%)	1 (0%)	52	84
1	C	636/724 (88%)	611 (96%)	25 (4%)	0	100	100
1	D	631/724 (87%)	600 (95%)	29 (5%)	2 (0%)	46	78
All	All	2540/2896 (88%)	2441 (96%)	94 (4%)	5 (0%)	52	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	GLY
1	D	111	VAL
1	D	544	ASN
1	A	111	VAL
1	B	512	GLY

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	553/624 (89%)	523 (95%)	30 (5%)	27	59
1	B	554/624 (89%)	519 (94%)	35 (6%)	22	51
1	C	553/624 (89%)	516 (93%)	37 (7%)	20	47
1	D	550/624 (88%)	514 (94%)	36 (6%)	21	49
All	All	2210/2496 (88%)	2072 (94%)	138 (6%)	23	52

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	556	ARG
1	C	283	GLN
1	D	450	ASP
1	B	590	THR
1	C	181	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	6	GLN
1	C	89	HIS
1	D	249	GLN
1	B	89	HIS
1	B	582	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 ⓘ

2 carbohydrates 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	GLC	C	801	-	12,12,12	0.50	0	17,17,17	0.88	0
5	BGC	C	802	-	12,12,12	0.46	0	17,17,17	0.84	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	GLC	C	801	-	-	0/2/22/22	0/1/1/1
5	BGC	C	802	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
2	UDP	A	801	-	18,26,26	0.81	0	26,40,40	1.55	2 (7%)
3	G6P	A	802	-	16,16,16	0.52	0	23,24,24	0.92	2 (8%)
4	PEG	A	803	-	6,6,6	0.48	0	5,5,5	0.30	0
2	UDP	B	801	-	18,26,26	0.66	0	26,40,40	1.59	3 (11%)
3	G6P	B	802	-	16,16,16	0.49	0	23,24,24	0.77	0
4	PEG	B	803	-	6,6,6	0.44	0	5,5,5	0.43	0
2	UDP	C	803	-	18,26,26	0.86	1 (5%)	26,40,40	1.60	2 (7%)
3	G6P	C	804	-	16,16,16	0.57	0	23,24,24	0.90	2 (8%)
4	PEG	C	805	-	6,6,6	0.39	0	5,5,5	0.41	0
2	UDP	D	801	-	18,26,26	0.77	0	26,40,40	1.70	2 (7%)
3	G6P	D	802	-	16,16,16	0.51	0	23,24,24	1.04	1 (4%)
4	PEG	D	803	-	6,6,6	0.42	0	5,5,5	0.38	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
2	UDP	A	801	-	-	0/12/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G6P	A	802	-	-	0/6/26/26	0/1/1/1
4	PEG	A	803	-	-	0/4/4/4	0/0/0/0
2	UDP	B	801	-	-	0/12/32/32	0/2/2/2
3	G6P	B	802	-	-	0/6/26/26	0/1/1/1
4	PEG	B	803	-	-	0/4/4/4	0/0/0/0
2	UDP	C	803	-	-	0/12/32/32	0/2/2/2
3	G6P	C	804	-	-	0/6/26/26	0/1/1/1
4	PEG	C	805	-	-	0/4/4/4	0/0/0/0
2	UDP	D	801	-	-	0/12/32/32	0/2/2/2
3	G6P	D	802	-	-	0/6/26/26	0/1/1/1
4	PEG	D	803	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	803	UDP	O4'-C1'	2.38	1.44	1.41

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	UDP	PA-O3A-PB	-3.06	122.40	132.67
2	D	801	UDP	PA-O3A-PB	-3.03	122.51	132.67
2	B	801	UDP	PA-O3A-PB	-2.63	123.86	132.67
3	D	802	G6P	O3-C3-C4	-2.12	105.56	110.34
3	A	802	G6P	O2P-P-O6	-2.10	100.53	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	G6P	3	0
4	A	803	PEG	1	0
2	B	801	UDP	1	0
3	B	802	G6P	1	0
4	B	803	PEG	1	0
2	C	803	UDP	3	0
4	C	805	PEG	2	0
4	D	803	PEG	1	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	638/724 (88%)	0.29	28 (4%)	38 30	41, 61, 110, 139	0
1	B	638/724 (88%)	0.07	15 (2%)	62 55	33, 53, 106, 139	0
1	C	638/724 (88%)	0.25	33 (5%)	31 23	40, 59, 111, 142	1 (0%)
1	D	635/724 (87%)	0.42	53 (8%)	14 8	35, 72, 137, 165	0
All	All	2549/2896 (88%)	0.26	129 (5%)	32 23	33, 59, 123, 165	1 (0%)

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	630	LEU	7.3
1	D	637	ALA	6.6
1	D	626	VAL	6.2
1	D	627	GLY	5.6
1	D	122	LEU	5.5

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, 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
5	BGC	C	802	12/12	0.98	0.16	-0.25	53,57,59,60	12
5	GLC	C	801	12/12	0.98	0.15	-0.86	46,49,51,53	12

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
4	PEG	B	803	7/7	0.91	0.26	2.73	68,69,76,76	0
4	PEG	D	803	7/7	0.92	0.21	1.76	55,65,75,78	0
2	UDP	C	803	25/25	0.97	0.19	0.26	39,51,55,59	0
3	G6P	B	802	16/16	0.98	0.17	0.01	36,41,45,47	0
4	PEG	A	803	7/7	0.86	0.18	-0.03	73,77,85,85	0
3	G6P	A	802	16/16	0.99	0.17	-0.39	42,48,52,52	0
3	G6P	D	802	16/16	0.99	0.16	-0.54	35,40,44,46	0
3	G6P	C	804	16/16	0.98	0.15	-1.05	43,47,49,52	0
2	UDP	B	801	25/25	0.97	0.15	-1.28	46,57,85,89	0
2	UDP	A	801	25/25	0.97	0.14	-1.40	47,59,72,73	0
2	UDP	D	801	25/25	0.98	0.12	-1.84	48,58,70,71	0
4	PEG	C	805	7/7	0.94	0.13	-1.91	62,69,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.