



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 08:42 pm BST

PDB ID : 3AIE
Title : Crystal Structure of glucansucrase from Streptococcus mutans
Authors : Ito, K.; Ito, S.; Shimamura, T.; Iwata, S.
Deposited on : 2010-05-12
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

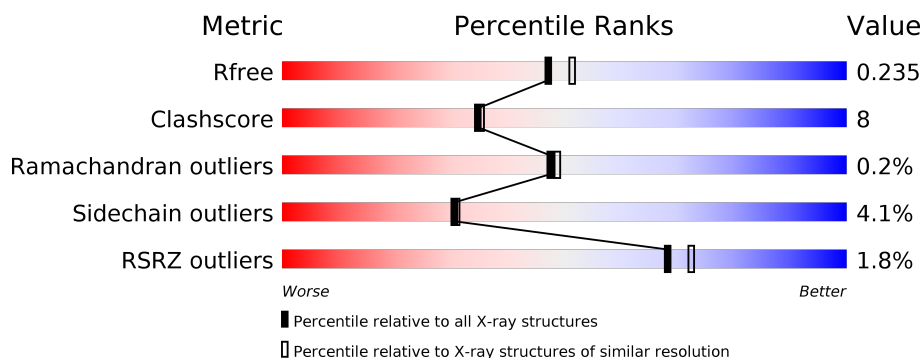
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 respectively. 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	844	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	844	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>.</div> </div> </div>
1	C	844	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	D	844	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
1	E	844	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>.</div> </div> </div>
1	F	844	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	844	<div><div><div>%</div><div><div></div><div>82%</div><div>15%</div><div></div></div><div></div></div></div>
1	H	844	<div><div><div>2%</div><div><div></div><div>81%</div><div>16%</div><div></div></div><div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 57830 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 Glucosyltransferase-SI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	B	844	Total	C	N	O	S	0	0	0
			6659	4196	1143	1304	16			
1	C	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	D	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	E	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	F	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	G	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	H	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	597	ASP	ASN	SEE REMARK 999	UNP P13470
A	600	LYS	ARG	SEE REMARK 999	UNP P13470
A	727	ILE	THR	SEE REMARK 999	UNP P13470
A	734	VAL	ALA	SEE REMARK 999	UNP P13470
B	597	ASP	ASN	SEE REMARK 999	UNP P13470
B	600	LYS	ARG	SEE REMARK 999	UNP P13470
B	727	ILE	THR	SEE REMARK 999	UNP P13470
B	734	VAL	ALA	SEE REMARK 999	UNP P13470
C	597	ASP	ASN	SEE REMARK 999	UNP P13470
C	600	LYS	ARG	SEE REMARK 999	UNP P13470
C	727	ILE	THR	SEE REMARK 999	UNP P13470
C	734	VAL	ALA	SEE REMARK 999	UNP P13470
D	597	ASP	ASN	SEE REMARK 999	UNP P13470

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Chain	Residue	Modelled	Actual	Comment	Reference
D	600	LYS	ARG	SEE REMARK 999	UNP P13470
D	727	ILE	THR	SEE REMARK 999	UNP P13470
D	734	VAL	ALA	SEE REMARK 999	UNP P13470
E	597	ASP	ASN	SEE REMARK 999	UNP P13470
E	600	LYS	ARG	SEE REMARK 999	UNP P13470
E	727	ILE	THR	SEE REMARK 999	UNP P13470
E	734	VAL	ALA	SEE REMARK 999	UNP P13470
F	597	ASP	ASN	SEE REMARK 999	UNP P13470
F	600	LYS	ARG	SEE REMARK 999	UNP P13470
F	727	ILE	THR	SEE REMARK 999	UNP P13470
F	734	VAL	ALA	SEE REMARK 999	UNP P13470
G	597	ASP	ASN	SEE REMARK 999	UNP P13470
G	600	LYS	ARG	SEE REMARK 999	UNP P13470
G	727	ILE	THR	SEE REMARK 999	UNP P13470
G	734	VAL	ALA	SEE REMARK 999	UNP P13470
H	597	ASP	ASN	SEE REMARK 999	UNP P13470
H	600	LYS	ARG	SEE REMARK 999	UNP P13470
H	727	ILE	THR	SEE REMARK 999	UNP P13470
H	734	VAL	ALA	SEE REMARK 999	UNP P13470

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	529	Total	O	0	0
			529	529		
4	B	528	Total	O	0	0
			528	528		
4	C	593	Total	O	0	0
			593	593		
4	D	592	Total	O	0	0
			592	592		

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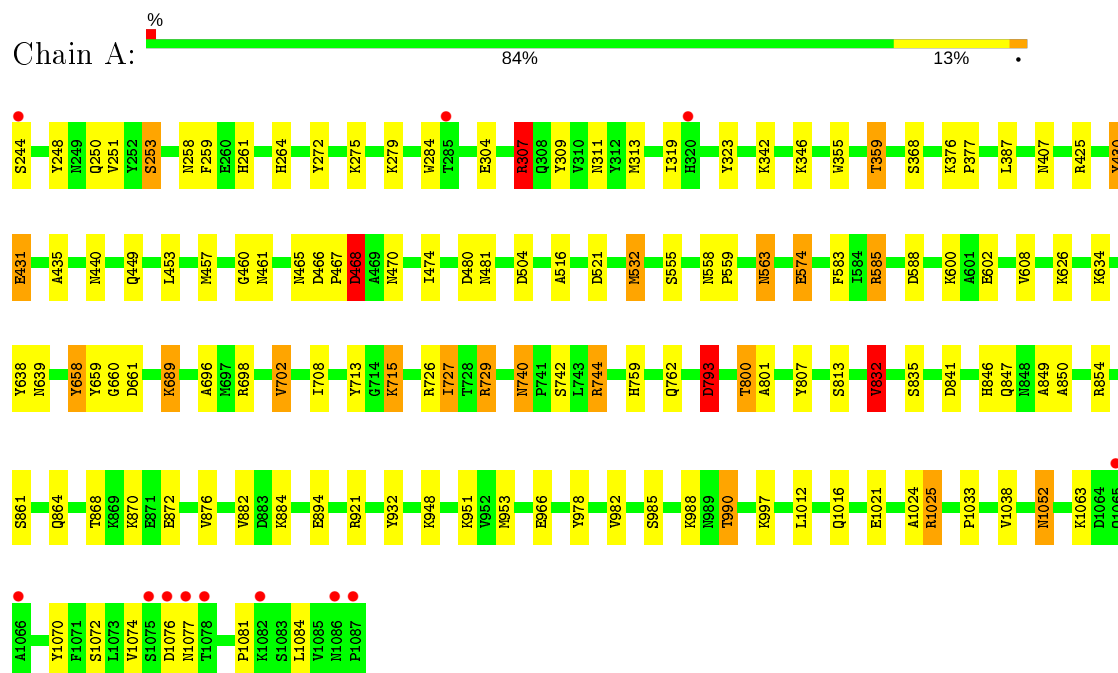
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	523	Total 523	O 523	0	0
4	F	485	Total 485	O 485	0	0
4	G	622	Total 622	O 622	0	0
4	H	575	Total 575	O 575	0	0

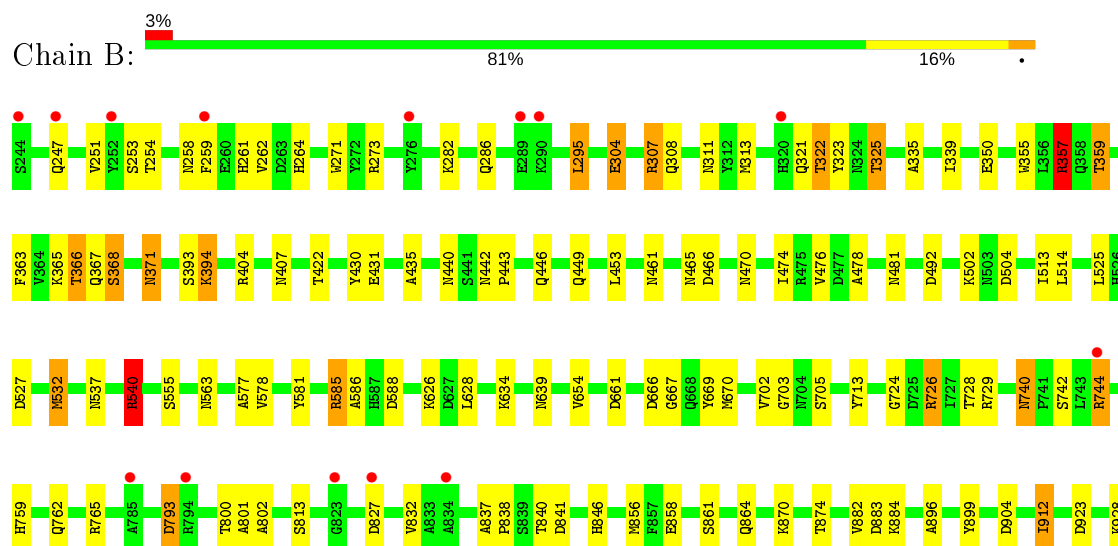
3 Residue-property plots [i](#)

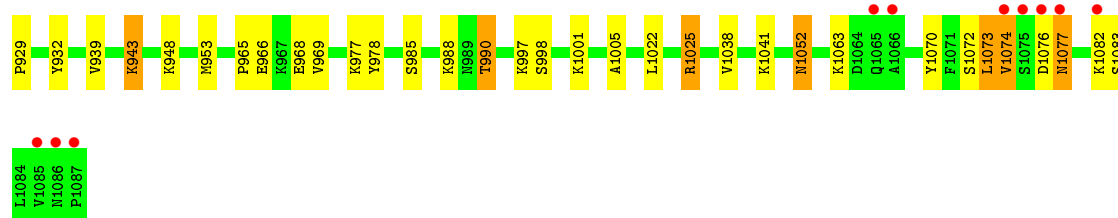
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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: Glucosyltransferase-SI

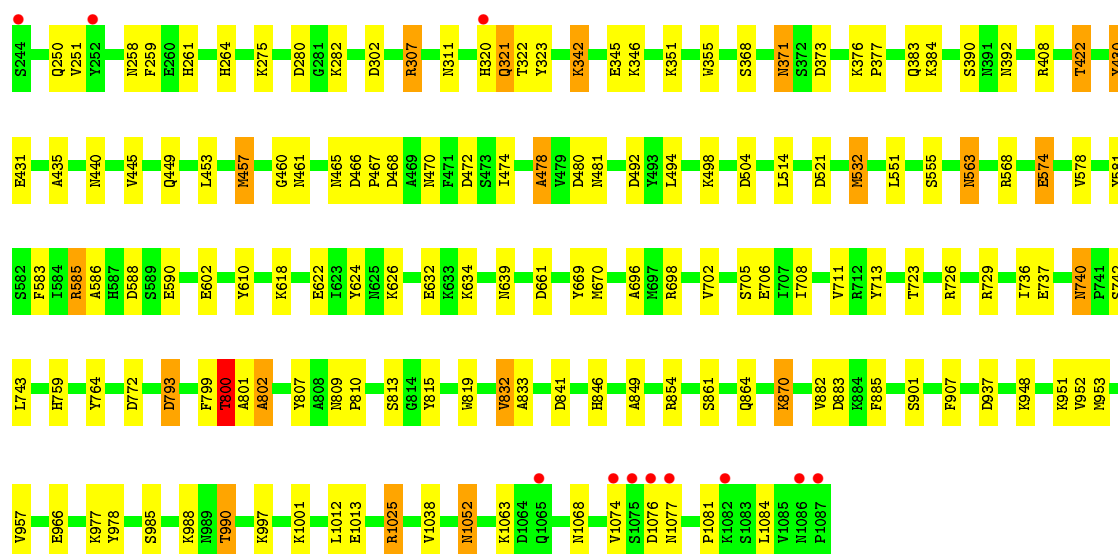
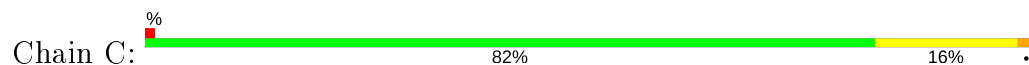


• Molecule 1: Glucosyltransferase-SI

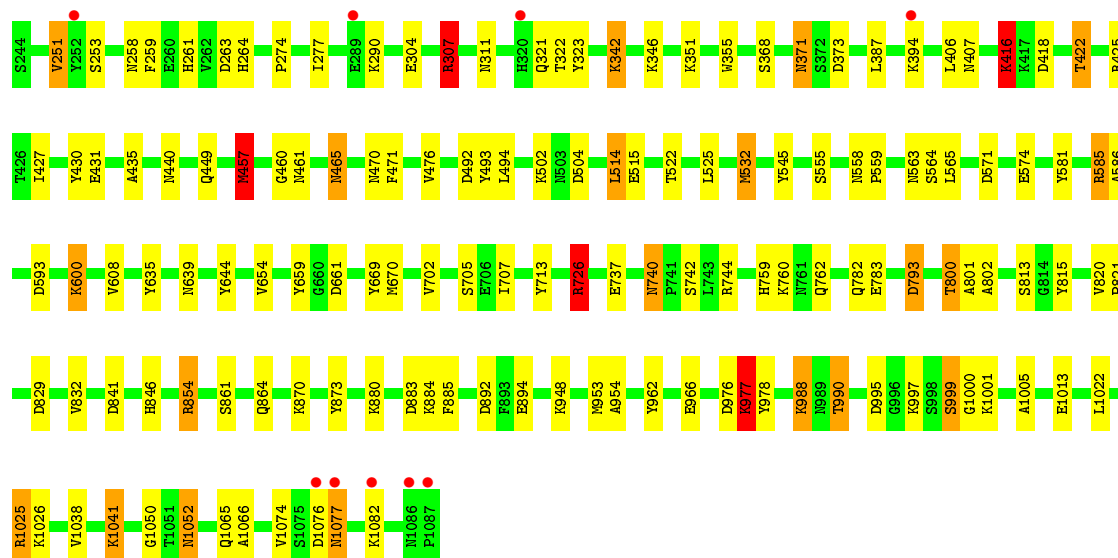
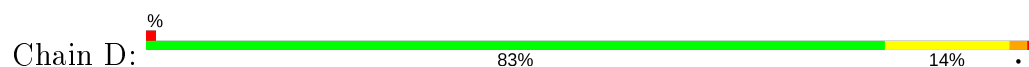




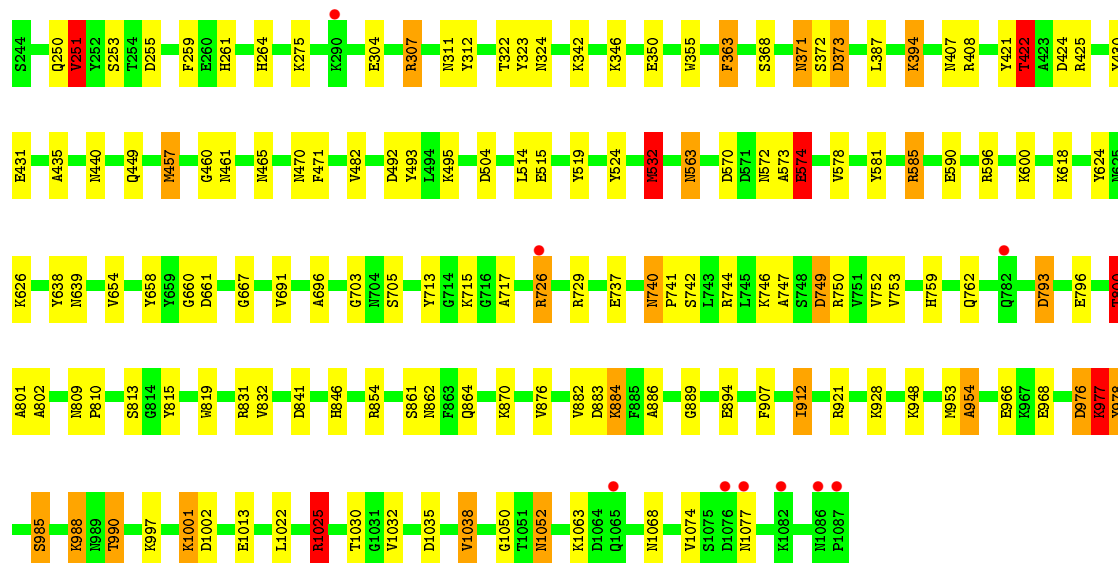
• Molecule 1: Glucosyltransferase-SI



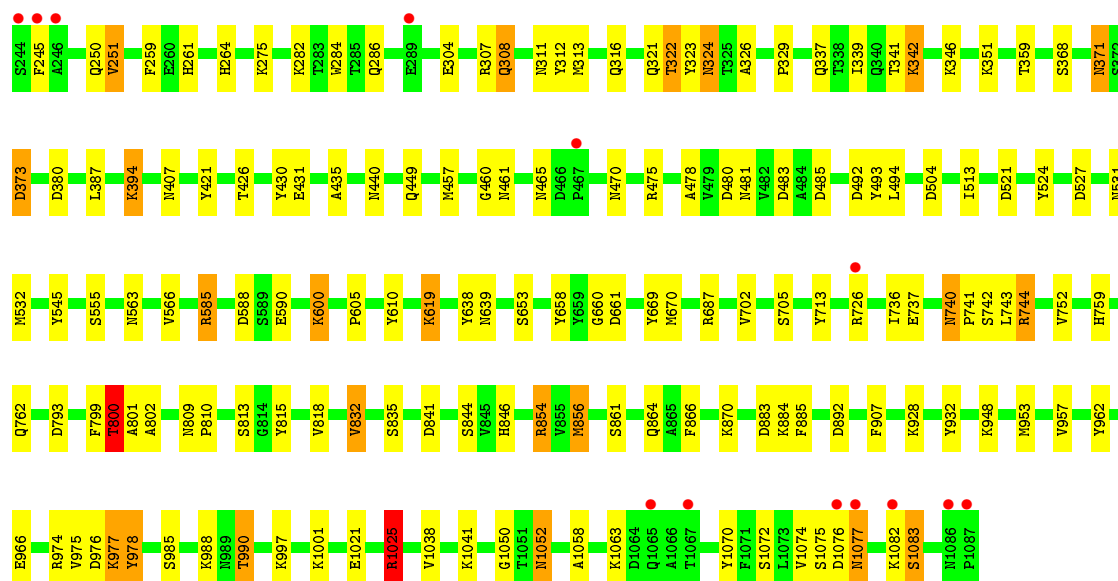
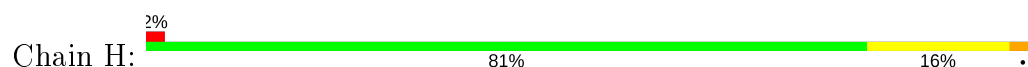
• Molecule 1: Glucosyltransferase-SI



• Molecule 1: Glucosyltransferase-SI



• Molecule 1: Glucosyltransferase-SI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	293.88Å 215.42Å 218.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.10) 99.6 (50.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.203 , 0.236 0.208 , 0.235	Depositor DCC
R_{free} test set	39655 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	57830	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6894e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: CA, MES

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	1.34	30/6802 (0.4%)	1.20	30/9237 (0.3%)
1	B	1.19	11/6801 (0.2%)	1.15	30/9237 (0.3%)
1	C	1.32	39/6802 (0.6%)	1.17	31/9237 (0.3%)
1	D	1.31	27/6802 (0.4%)	1.22	31/9237 (0.3%)
1	E	1.37	37/6802 (0.5%)	1.23	34/9237 (0.4%)
1	F	1.13	10/6802 (0.1%)	1.12	30/9237 (0.3%)
1	G	1.42	47/6802 (0.7%)	1.30	36/9237 (0.4%)
1	H	1.28	26/6802 (0.4%)	1.18	29/9237 (0.3%)
All	All	1.30	227/54415 (0.4%)	1.20	251/73896 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	1	0

The worst 5 of 227 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1083	SER	CB-OG	12.42	1.58	1.42
1	E	574	GLU	CB-CG	-10.80	1.31	1.52
1	C	574	GLU	CB-CG	-10.38	1.32	1.52
1	G	421	TYR	CD2-CE2	9.85	1.54	1.39
1	H	371	ASN	CB-CG	-9.70	1.28	1.51

The worst 5 of 251 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	854	ARG	NE-CZ-NH2	-35.02	102.79	120.30
1	A	854	ARG	NE-CZ-NH2	-33.32	103.64	120.30
1	D	854	ARG	NE-CZ-NH2	-33.26	103.67	120.30
1	E	854	ARG	NE-CZ-NH2	-32.09	104.26	120.30
1	B	540	ARG	NE-CZ-NH2	-31.61	104.50	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	800	THR	CB

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	6660	0	6489	79	0
1	B	6659	0	6489	117	0
1	C	6660	0	6487	98	0
1	D	6660	0	6489	107	0
1	E	6660	0	6489	110	0
1	F	6660	0	6489	139	0
1	G	6660	0	6489	110	0
1	H	6660	0	6489	117	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	12	0	0
3	B	12	0	12	2	0
3	C	12	0	12	0	0
3	D	12	0	12	1	0
3	E	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	12	0	12	0	0
3	G	12	0	12	0	0
3	H	12	0	12	1	0
4	A	529	0	0	8	0
4	B	528	0	0	13	0
4	C	593	0	0	10	0
4	D	592	0	0	15	0
4	E	523	0	0	2	0
4	F	485	0	0	10	0
4	G	622	0	0	13	0
4	H	575	0	0	5	0
All	All	57830	0	52006	878	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 8.

The worst 5 of 878 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:H:475:ARG:HB2	1:H:953:MET:CE	1.39	1.52
1:G:394:LYS:CD	1:G:394:LYS:H	1.44	1.27
1:E:277:ILE:CD1	1:E:291:ASP:HB3	1.69	1.20
1:H:475:ARG:CB	1:H:953:MET:HE2	1.69	1.20
1:A:250:GLN:NE2	1:A:275:LYS:HE3	1.56	1.18

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	842/844 (100%)	816 (97%)	25 (3%)	1 (0%)	51 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	842/844 (100%)	812 (96%)	29 (3%)	1 (0%)	51	54
1	C	842/844 (100%)	817 (97%)	24 (3%)	1 (0%)	51	54
1	D	842/844 (100%)	815 (97%)	25 (3%)	2 (0%)	47	49
1	E	842/844 (100%)	815 (97%)	25 (3%)	2 (0%)	47	49
1	F	842/844 (100%)	818 (97%)	24 (3%)	0	100	100
1	G	842/844 (100%)	817 (97%)	23 (3%)	2 (0%)	47	49
1	H	842/844 (100%)	817 (97%)	23 (3%)	2 (0%)	47	49
All	All	6736/6752 (100%)	6527 (97%)	198 (3%)	11 (0%)	47	49

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1077	ASN
1	D	1077	ASN
1	E	1077	ASN
1	C	793	ASP
1	G	747	ALA

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	715/715 (100%)	689 (96%)	26 (4%)	35	36
1	B	715/715 (100%)	673 (94%)	42 (6%)	19	17
1	C	715/715 (100%)	690 (96%)	25 (4%)	36	38
1	D	715/715 (100%)	686 (96%)	29 (4%)	30	31
1	E	715/715 (100%)	687 (96%)	28 (4%)	32	33
1	F	715/715 (100%)	686 (96%)	29 (4%)	30	31
1	G	715/715 (100%)	688 (96%)	27 (4%)	33	34
1	H	715/715 (100%)	685 (96%)	30 (4%)	30	30
All	All	5720/5720 (100%)	5484 (96%)	236 (4%)	30	31

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	600	LYS
1	E	619	LYS
1	H	619	LYS
1	D	726	ARG
1	D	1025	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 171 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	759	HIS
1	E	531	ASN
1	H	470	ASN
1	D	846	HIS
1	E	250	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	MES	D	5001	-	12,12,12	1.80	2 (16%)	14,16,16	7.21	9 (64%)
3	MES	B	5001	-	12,12,12	1.80	1 (8%)	14,16,16	6.64	11 (78%)
3	MES	H	5001	-	12,12,12	2.32	1 (8%)	14,16,16	7.79	10 (71%)
3	MES	E	5001	-	12,12,12	1.29	1 (8%)	14,16,16	5.01	11 (78%)
3	MES	C	5001	-	12,12,12	2.31	1 (8%)	14,16,16	7.77	10 (71%)
3	MES	A	5001	-	12,12,12	2.47	3 (25%)	14,16,16	6.09	9 (64%)
3	MES	G	5001	-	12,12,12	2.16	1 (8%)	14,16,16	5.14	8 (57%)
3	MES	F	5001	-	12,12,12	2.53	1 (8%)	14,16,16	2.78	6 (42%)

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	MES	D	5001	-	-	4/6/14/14	0/1/1/1
3	MES	B	5001	-	-	1/6/14/14	0/1/1/1
3	MES	H	5001	-	-	1/6/14/14	0/1/1/1
3	MES	E	5001	-	-	1/6/14/14	0/1/1/1
3	MES	C	5001	-	-	2/6/14/14	0/1/1/1
3	MES	A	5001	-	-	2/6/14/14	0/1/1/1
3	MES	G	5001	-	-	1/6/14/14	0/1/1/1
3	MES	F	5001	-	-	1/6/14/14	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5001	MES	C8-S	-7.99	1.66	1.77
3	H	5001	MES	C8-S	-7.69	1.66	1.77
3	C	5001	MES	C8-S	-7.66	1.66	1.77
3	A	5001	MES	C8-S	-7.44	1.66	1.77
3	G	5001	MES	C8-S	-7.15	1.67	1.77

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5001	MES	O2S-S-C8	-20.61	82.10	106.92
3	C	5001	MES	O2S-S-C8	-17.31	86.07	106.92
3	H	5001	MES	O1S-S-C8	-17.28	86.11	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5001	MES	O1S-S-C8	-17.28	86.11	106.92
3	H	5001	MES	O2S-S-C8	-17.27	86.12	106.92

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5001	MES	C8-C7-N4-C5
3	D	5001	MES	C8-C7-N4-C5
3	D	5001	MES	C7-C8-S-O1S
3	D	5001	MES	C7-C8-S-O2S
3	H	5001	MES	C8-C7-N4-C5

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5001	MES	1	0
3	B	5001	MES	2	0
3	H	5001	MES	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 ⓘ

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, 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	844/844 (100%)	-0.22	12 (1%) 75 78	19, 30, 49, 66	0
1	B	844/844 (100%)	-0.09	24 (2%) 53 59	27, 37, 52, 70	0
1	C	844/844 (100%)	-0.25	11 (1%) 77 80	22, 30, 45, 61	0
1	D	844/844 (100%)	-0.28	9 (1%) 80 84	21, 30, 47, 64	0
1	E	844/844 (100%)	-0.22	20 (2%) 59 64	19, 29, 53, 70	0
1	F	844/844 (100%)	-0.04	24 (2%) 53 59	26, 38, 54, 65	0
1	G	844/844 (100%)	-0.23	9 (1%) 80 84	19, 28, 45, 62	0
1	H	844/844 (100%)	-0.24	13 (1%) 73 77	21, 30, 44, 61	0
All	All	6752/6752 (100%)	-0.20	122 (1%) 68 72	19, 32, 50, 70	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1087	PRO	5.5
1	B	1087	PRO	5.1
1	A	1087	PRO	5.0
1	B	1076	ASP	5.0
1	B	1077	ASN	4.8

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 ⓘ

There are no carbohydrates in this entry.

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MES	F	5001	12/12	0.89	0.14	2,16,32,98	0
3	MES	H	5001	12/12	0.92	0.17	5,22,93,99	0
3	MES	C	5001	12/12	0.94	0.23	2,2,7,10	0
3	MES	B	5001	12/12	0.94	0.17	6,13,15,16	0
2	CA	B	4001	1/1	0.95	0.04	19,19,19,19	0
3	MES	D	5001	12/12	0.97	0.15	2,6,13,14	0
3	MES	A	5001	12/12	0.97	0.10	22,22,62,81	0
3	MES	G	5001	12/12	0.98	0.09	4,8,15,21	0
2	CA	D	4001	1/1	0.98	0.06	18,18,18,18	0
2	CA	F	4001	1/1	0.99	0.03	16,16,16,16	0
2	CA	E	4001	1/1	0.99	0.07	18,18,18,18	0
3	MES	E	5001	12/12	0.99	0.08	19,24,27,28	0
2	CA	H	4001	1/1	0.99	0.10	18,18,18,18	0
2	CA	A	4001	1/1	1.00	0.08	17,17,17,17	0
2	CA	G	4001	1/1	1.00	0.10	16,16,16,16	0
2	CA	C	4001	1/1	1.00	0.05	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.