wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2026 – 05:48 PM UTC

PDB ID	:	3AIB / pdb_00003aib
Title	:	Crystal Structure of Glucansucrase
Authors	:	Ito, K.; Ito, S.; Shimamura, T.; Iwata, S.
Deposited on	:	2010-05-12
Resolution	:	3.09 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

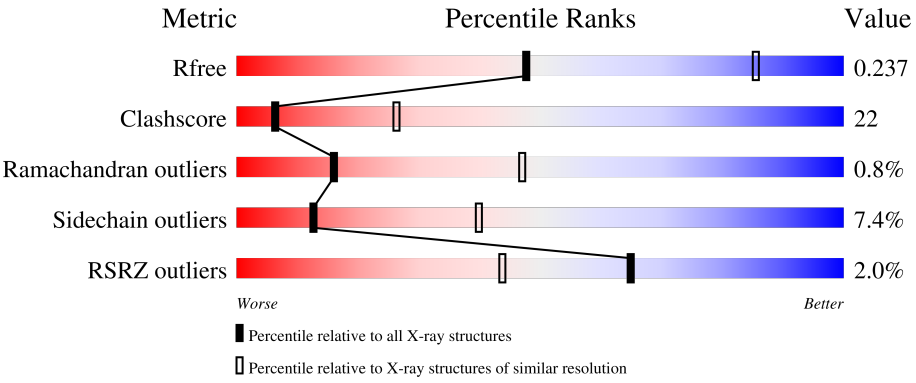
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.09 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 of 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 <=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	67% 28% 5%
1	B	844	48% 33% 7% 11%
1	C	844	70% 26%
1	D	844	65% 29% 5%
1	E	844	4% 65% 30% 5%

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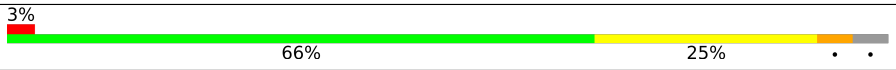
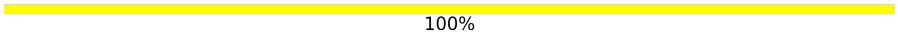
Mol	Chain	Length	Quality of chain
1	F	844	
1	G	844	
1	H	844	
2	I	2	

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	MES	A	5001	-	X	-	-
4	MES	B	5001	-	X	-	-
4	MES	D	5001	-	X	-	-
4	MES	F	5001	-	X	-	-
4	MES	G	5001	-	X	-	-
4	MES	H	5001	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 52615 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	842	Total	C	N	O	S	0	0	0
			6643	4184	1141	1302	16			
1	B	749	Total	C	N	O	S	0	0	0
			5868	3692	1008	1154	14			
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	G	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	H	808	Total	C	N	O	S	0	0	0
			6378	4022	1094	1246	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
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
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
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 an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	I	2	Total C O 23 12 11	0	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

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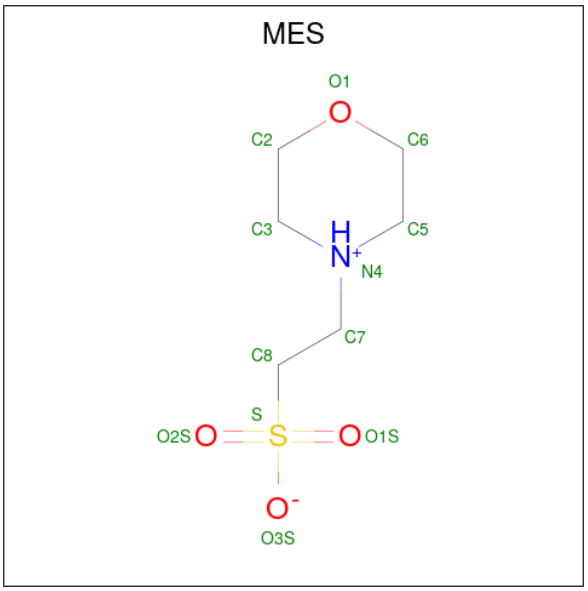
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

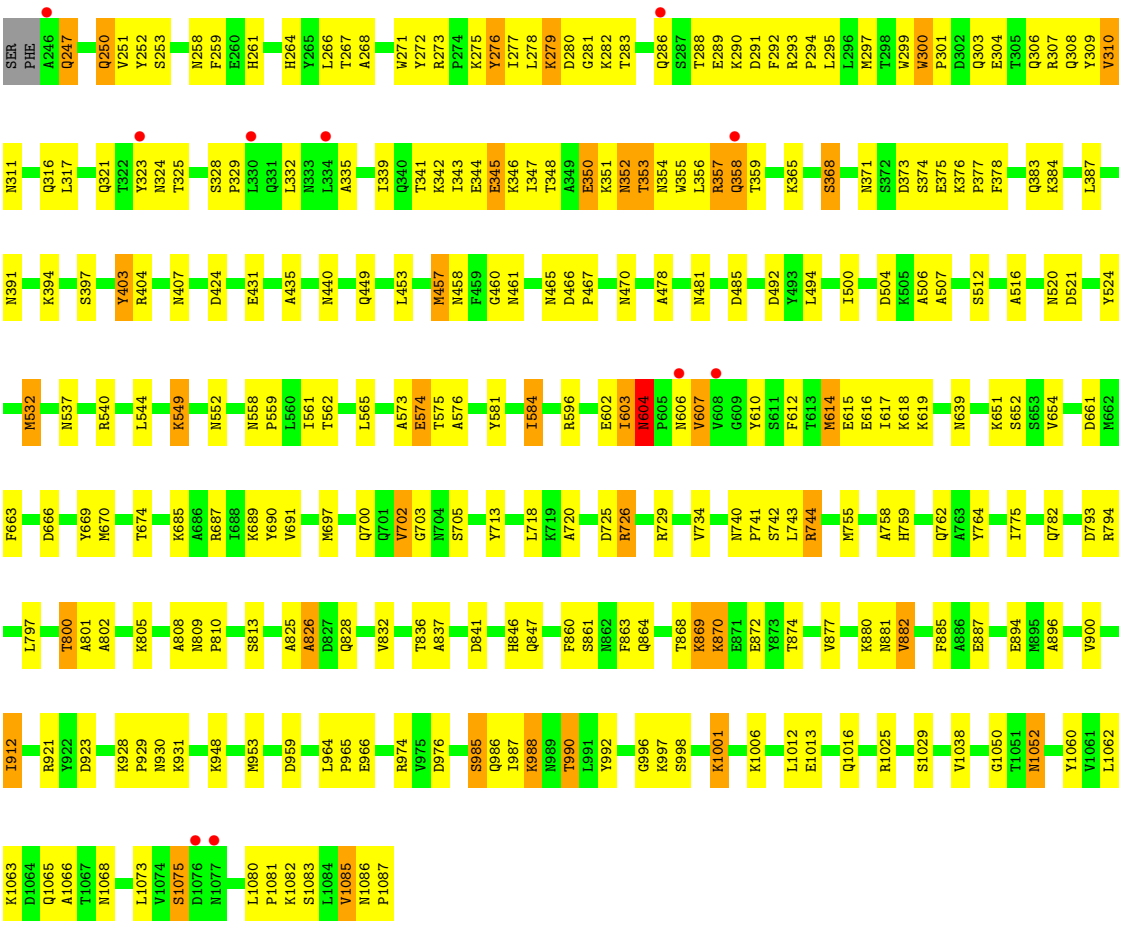
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	20	Total	O	0	0
			20	20		
5	C	59	Total	O	0	0
			59	59		
5	D	50	Total	O	0	0
			50	50		
5	G	46	Total	O	0	0
			46	46		
5	E	38	Total	O	0	0
			38	38		
5	F	23	Total	O	0	0
			23	23		
5	H	28	Total	O	0	0
			28	28		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

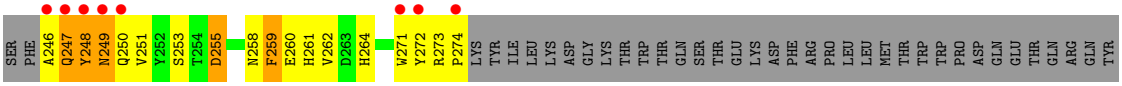
• Molecule 1: Glucosyltransferase-SI

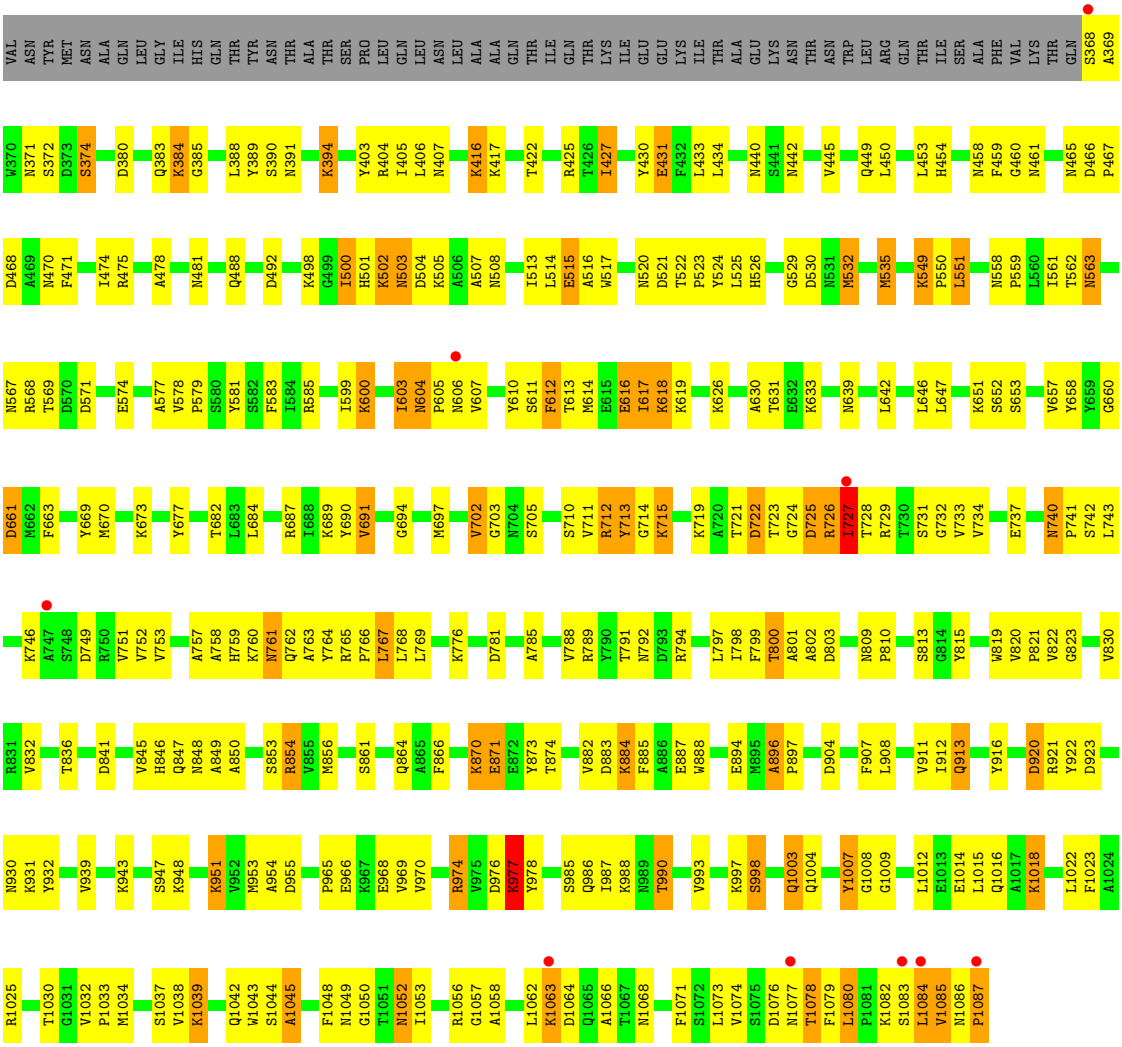
Chain A:



• Molecule 1: Glucosyltransferase-SI

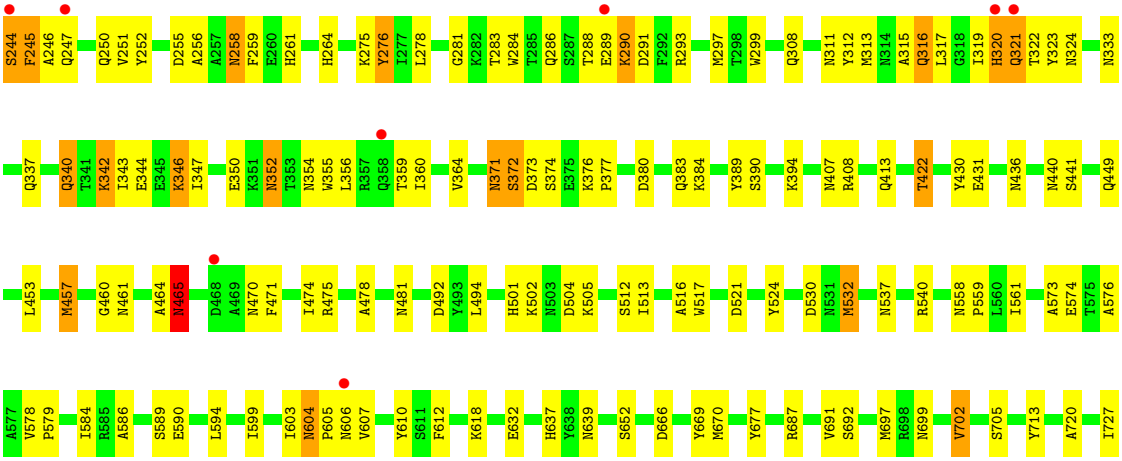
Chain B:

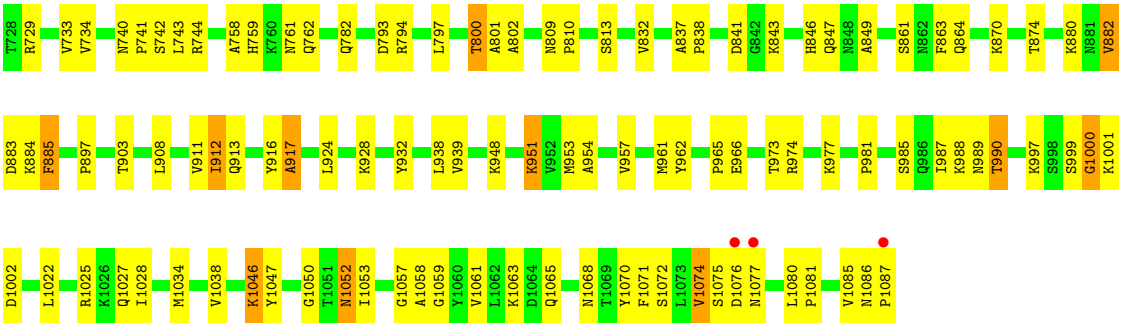




• Molecule 1: Glucosyltransferase-SI

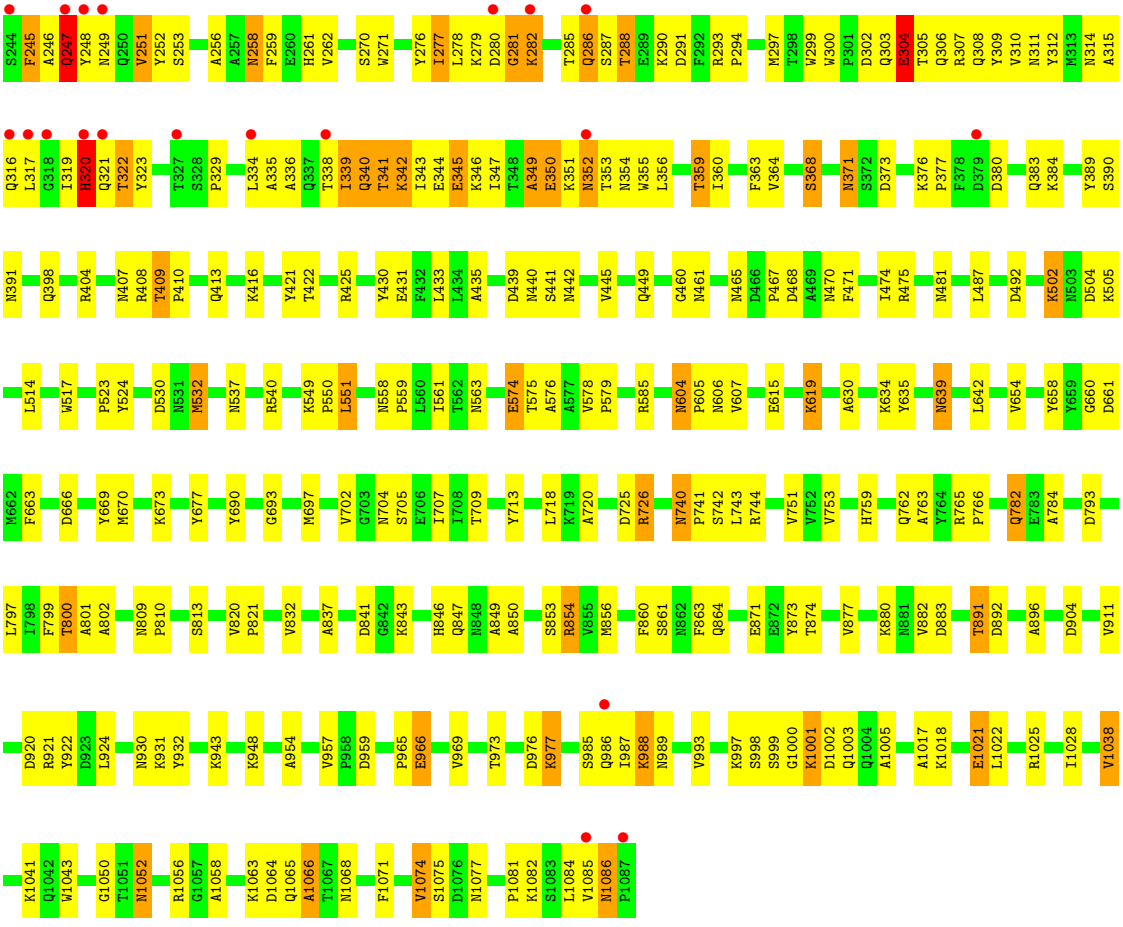
Chain C:





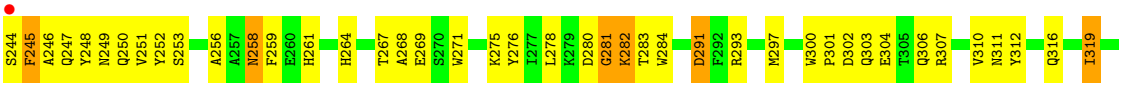
• Molecule 1: Glucosyltransferase-SI

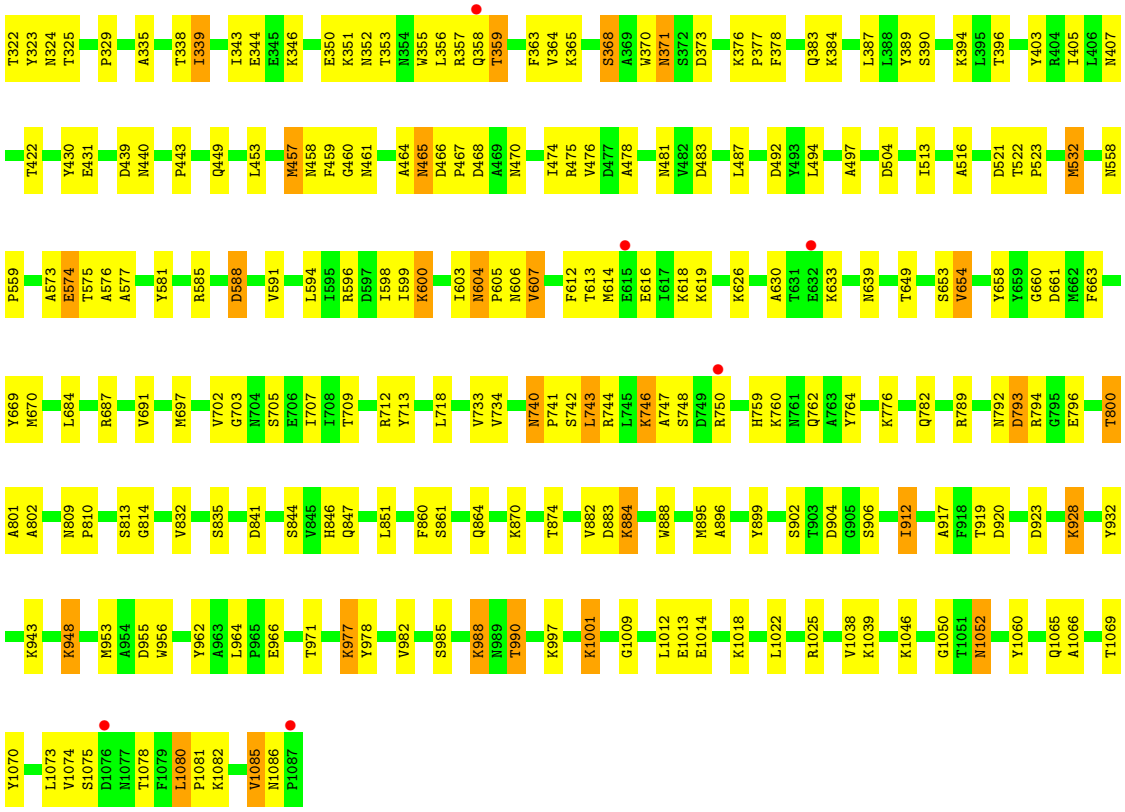
Chain D:



• Molecule 1: Glucosyltransferase-SI

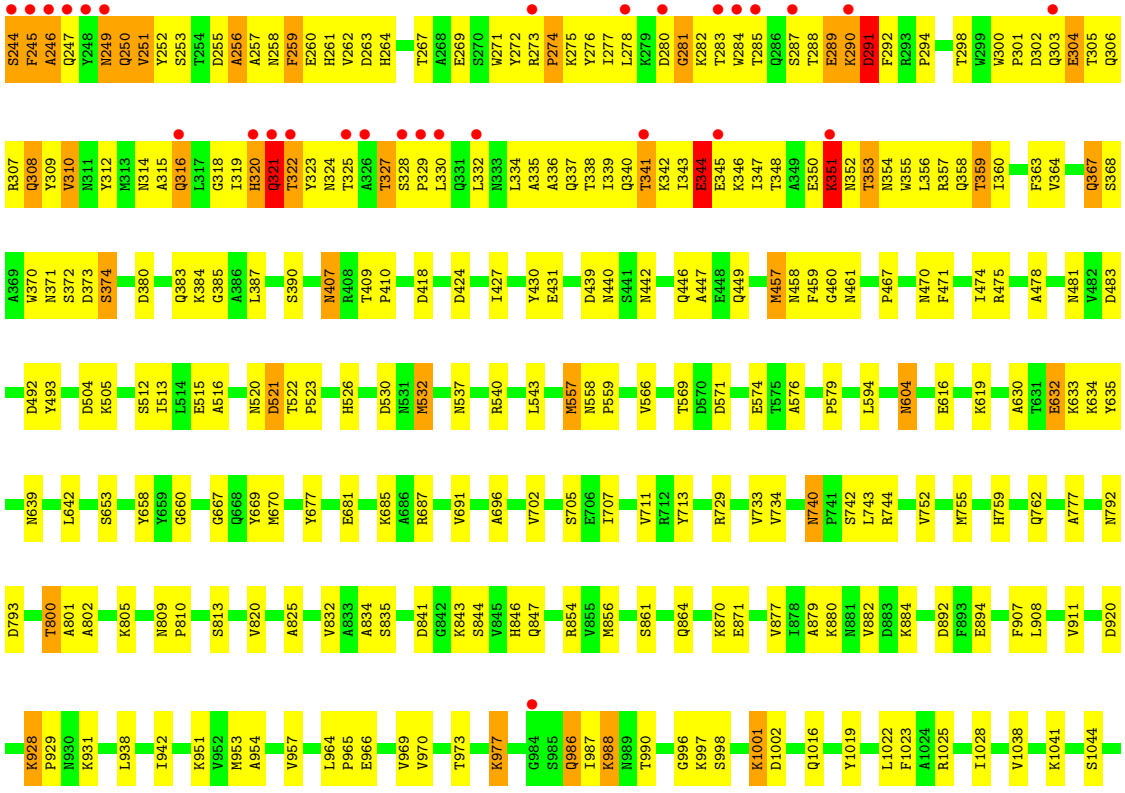
Chain G:





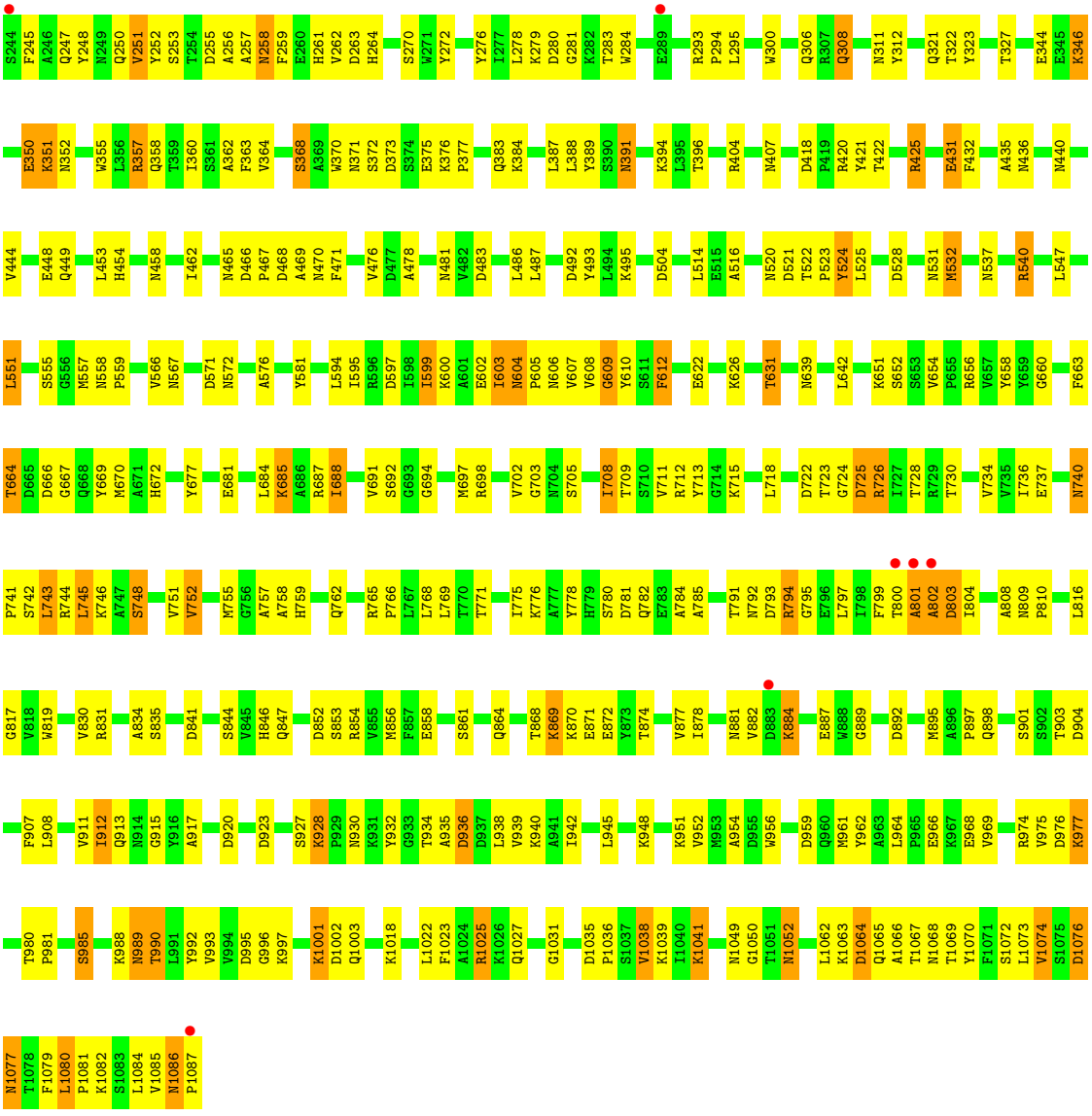
• Molecule 1: Glucosyltransferase-SI

Chain E:



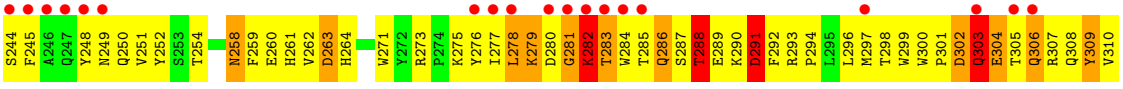
• Molecule 1: Glucosyltransferase-SI

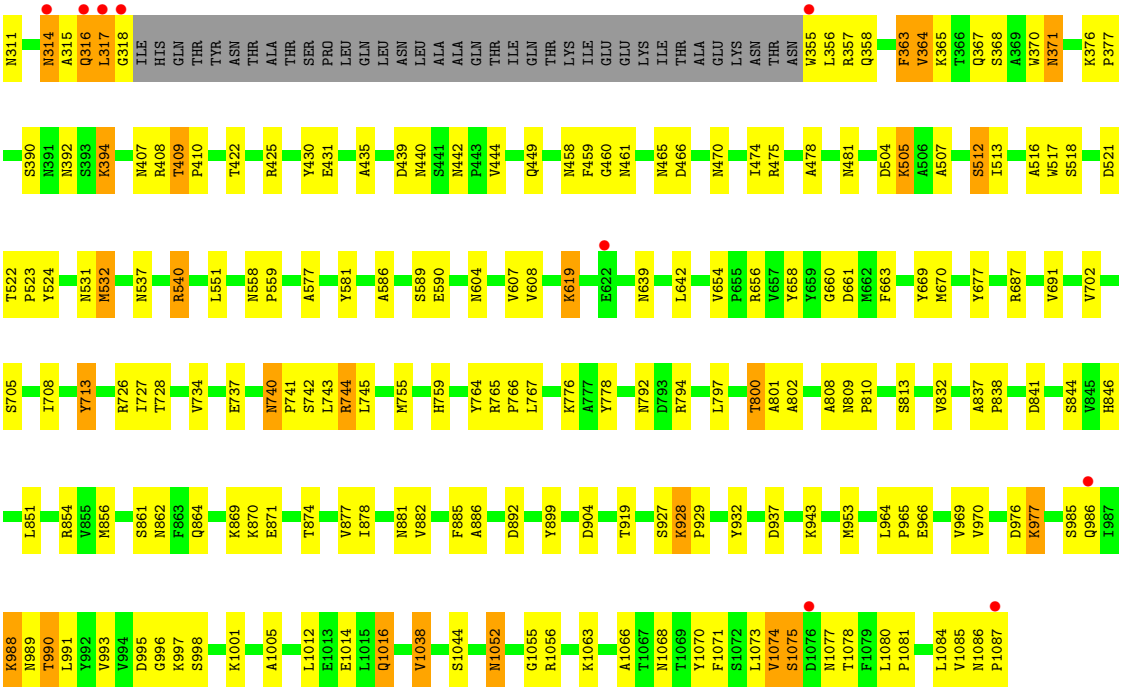
Chain F:



• Molecule 1: Glucosyltransferase-SI

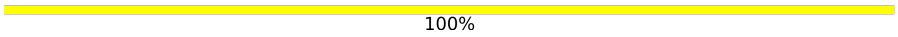
Chain H:





• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	295.42Å 213.94Å 220.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.67 – 3.09 50.67 – 3.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.67-3.09) 97.7 (50.67-3.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.211 , 0.241 0.207 , 0.237	Depositor DCC
R_{free} test set	12657 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	52615	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 32.12 % 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 9.8896e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GLC

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	1.30	17/6784 (0.3%)	1.27	19/9213 (0.2%)
1	B	1.18	7/5990 (0.1%)	1.30	40/8132 (0.5%)
1	C	1.35	18/6802 (0.3%)	1.25	26/9237 (0.3%)
1	D	1.30	11/6802 (0.2%)	1.27	38/9237 (0.4%)
1	E	1.30	14/6802 (0.2%)	1.28	36/9237 (0.4%)
1	F	1.07	5/6802 (0.1%)	1.19	27/9237 (0.3%)
1	G	1.33	12/6802 (0.2%)	1.28	28/9237 (0.3%)
1	H	1.19	7/6516 (0.1%)	1.23	27/8845 (0.3%)
All	All	1.26	91/53300 (0.2%)	1.26	241/72375 (0.3%)

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	314	ASN	CG-ND2	-10.39	1.11	1.33
1	D	340	GLN	CA-CB	10.32	1.70	1.53
1	A	507	ALA	CA-CB	-8.64	1.39	1.53
1	C	586	ALA	CA-CB	-7.37	1.42	1.53
1	B	403	TYR	N-CA	-7.34	1.41	1.46

The worst 5 of 241 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	245	PHE	N-CA-C	-13.27	97.08	113.01
1	H	289	GLU	N-CA-C	-13.27	97.13	113.18
1	H	245	PHE	N-CA-C	12.50	126.08	111.71
1	E	344	GLU	N-CA-C	11.91	124.25	111.03
1	E	320	HIS	N-CA-C	11.49	126.06	111.24

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	6643	0	6475	256	0
1	B	5868	0	5704	356	0
1	C	6660	0	6489	195	0
1	D	6660	0	6489	278	0
1	E	6660	0	6489	323	0
1	F	6660	0	6489	368	0
1	G	6660	0	6489	225	0
1	H	6378	0	6201	284	0
2	I	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	12	0	12	4	0
4	B	12	0	12	1	0
4	C	12	0	12	1	0
4	D	12	0	12	1	0
4	E	12	0	12	1	0
4	F	12	0	12	1	0
4	G	12	0	12	2	0
4	H	12	0	12	1	0
5	A	35	0	0	1	0
5	B	20	0	0	0	0
5	C	59	0	0	5	0
5	D	50	0	0	2	0
5	E	38	0	0	0	0
5	F	23	0	0	2	0
5	G	46	0	0	1	0
5	H	28	0	0	0	0
All	All	52615	0	50942	2285	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 22.

The worst 5 of 2285 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:1087:PRO:CB	1:B:1087:PRO:CG	1.77	1.54
1:E:271:TRP:CZ2	1:E:357:ARG:HD3	1.51	1.43
1:C:475:ARG:HB2	1:C:953:MET:CE	1.53	1.39
1:E:277:ILE:CD1	1:E:291:ASP:HB3	1.50	1.38
1:H:278:LEU:HD11	1:H:282:LYS:N	1.41	1.34

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	840/844 (100%)	791 (94%)	45 (5%)	4 (0%)	24	57
1	B	745/844 (88%)	693 (93%)	41 (6%)	11 (2%)	8	32
1	C	842/844 (100%)	809 (96%)	29 (3%)	4 (0%)	24	57
1	D	842/844 (100%)	789 (94%)	46 (6%)	7 (1%)	16	47
1	E	842/844 (100%)	791 (94%)	41 (5%)	10 (1%)	10	37
1	F	842/844 (100%)	783 (93%)	53 (6%)	6 (1%)	18	49
1	G	842/844 (100%)	796 (94%)	43 (5%)	3 (0%)	30	61
1	H	804/844 (95%)	743 (92%)	53 (7%)	8 (1%)	12	41
All	All	6599/6752 (98%)	6195 (94%)	351 (5%)	53 (1%)	16	47

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	713	TYR
1	B	761	ASN
1	D	351	LYS

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Mol	Chain	Res	Type
1	G	281	GLY
1	G	351	LYS

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	713/715 (100%)	668 (94%)	45 (6%)	16 45
1	B	628/715 (88%)	566 (90%)	62 (10%)	7 29
1	C	715/715 (100%)	673 (94%)	42 (6%)	18 48
1	D	715/715 (100%)	660 (92%)	55 (8%)	12 38
1	E	715/715 (100%)	658 (92%)	57 (8%)	11 37
1	F	715/715 (100%)	659 (92%)	56 (8%)	11 38
1	G	715/715 (100%)	664 (93%)	51 (7%)	13 41
1	H	683/715 (96%)	634 (93%)	49 (7%)	13 40
All	All	5599/5720 (98%)	5182 (93%)	417 (7%)	13 40

5 of 417 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	782	GLN
1	E	702	VAL
1	H	832	VAL
1	G	912	ILE
1	E	289	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 221 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	412	ASN
1	E	440	ASN
1	H	1016	GLN

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Mol	Chain	Res	Type
1	H	311	ASN
1	G	558	ASN

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)

2 monosaccharides 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	GLC	I	1	2	12,12,12	2.58	5 (41%)	17,17,17	4.48	8 (47%)
2	GLC	I	2	2	11,11,12	0.80	0	15,15,17	2.32	7 (46%)

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	GLC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	GLC	O5-C1	5.24	1.55	1.42
2	I	1	GLC	O5-C5	4.28	1.54	1.44
2	I	1	GLC	C4-C5	3.25	1.59	1.53
2	I	1	GLC	O1-C1	3.14	1.49	1.39
2	I	1	GLC	C1-C2	3.12	1.59	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1	GLC	C3-C4-C5	-12.05	88.38	110.23
2	I	1	GLC	O4-C4-C3	-9.89	87.07	110.38
2	I	1	GLC	O5-C5-C4	5.86	120.26	109.70
2	I	1	GLC	O2-C2-C3	-4.44	99.91	110.38
2	I	2	GLC	C2-C3-C4	-4.29	103.31	110.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

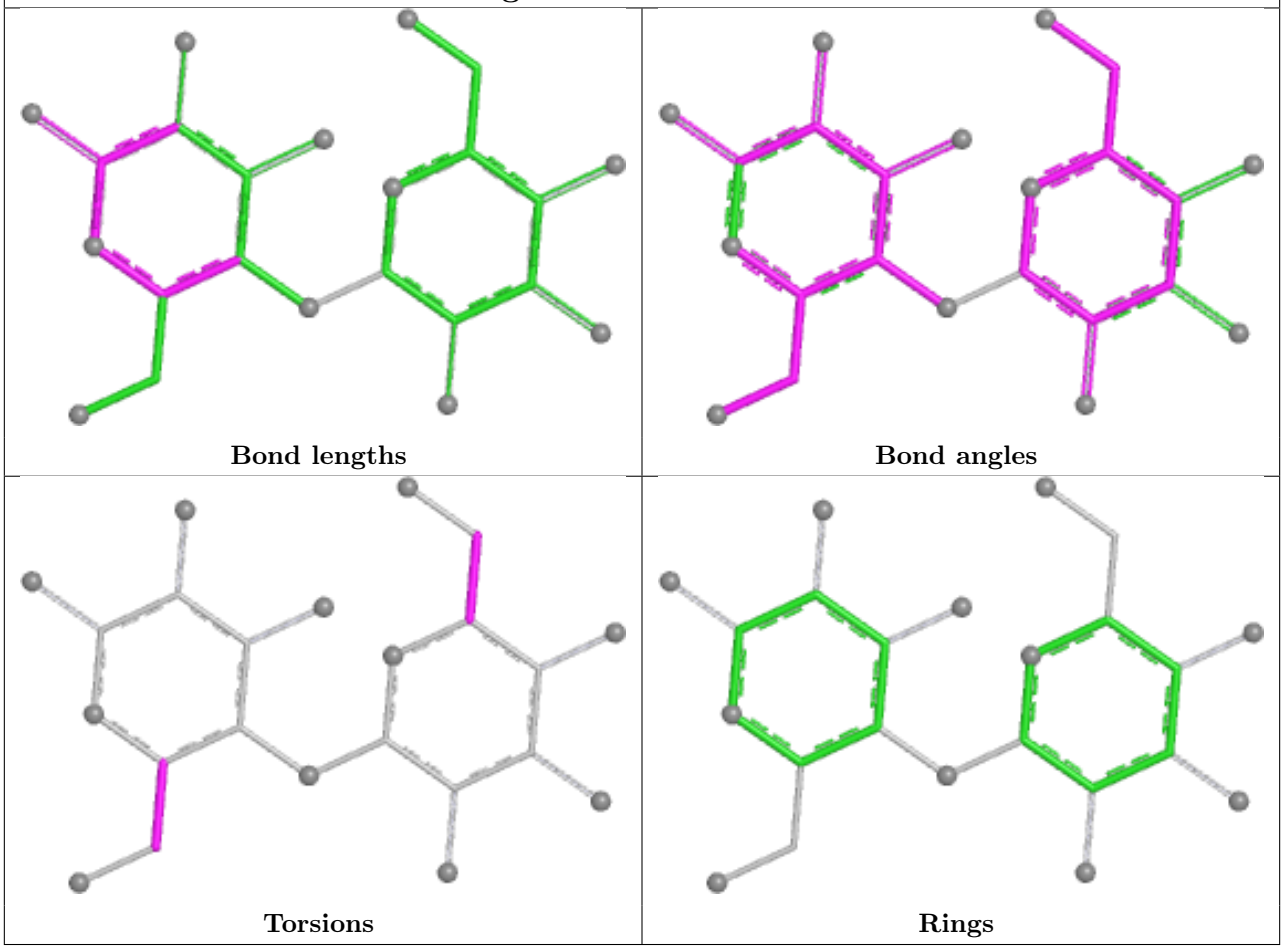
Mol	Chain	Res	Type	Atoms
2	I	1	GLC	C4-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	I	2	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain I



5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	MES	G	5001	-	12,12,12	2.63	3 (25%)	15,16,16	6.18	10 (66%)
4	MES	F	5001	-	12,12,12	3.28	4 (33%)	15,16,16	5.97	11 (73%)
4	MES	B	5001	-	12,12,12	2.26	4 (33%)	15,16,16	6.34	12 (80%)
4	MES	A	5001	-	12,12,12	3.92	7 (58%)	15,16,16	7.05	9 (60%)
4	MES	E	5001	-	12,12,12	2.87	5 (41%)	15,16,16	5.81	11 (73%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MES	D	5001	-	12,12,12	2.79	6 (50%)	15,16,16	5.53	12 (80%)
4	MES	C	5001	-	12,12,12	3.16	4 (33%)	15,16,16	5.43	7 (46%)
4	MES	H	5001	-	12,12,12	2.70	5 (41%)	15,16,16	5.63	11 (73%)

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
4	MES	G	5001	-	-	5/6/14/14	0/1/1/1
4	MES	F	5001	-	-	5/6/14/14	0/1/1/1
4	MES	B	5001	-	-	3/6/14/14	0/1/1/1
4	MES	A	5001	-	-	2/6/14/14	0/1/1/1
4	MES	E	5001	-	-	1/6/14/14	0/1/1/1
4	MES	D	5001	-	-	2/6/14/14	0/1/1/1
4	MES	C	5001	-	-	4/6/14/14	0/1/1/1
4	MES	H	5001	-	-	4/6/14/14	0/1/1/1

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5001	MES	O2S-S	8.13	1.68	1.45
4	A	5001	MES	O1S-S	8.00	1.67	1.45
4	F	5001	MES	O2S-S	7.58	1.66	1.45
4	C	5001	MES	O1S-S	6.81	1.64	1.45
4	H	5001	MES	O1S-S	6.01	1.62	1.45

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5001	MES	O1S-S-C8	-18.89	78.18	106.73
4	B	5001	MES	O2S-S-C8	-17.10	80.89	106.73
4	G	5001	MES	O1S-S-C8	-16.36	82.01	106.73
4	A	5001	MES	O2S-S-C8	-15.81	82.84	106.73
4	E	5001	MES	O1S-S-C8	-14.97	84.11	106.73

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5001	MES	C8-C7-N4-C5
4	B	5001	MES	C8-C7-N4-C5
4	B	5001	MES	N4-C7-C8-S
4	C	5001	MES	C8-C7-N4-C5
4	D	5001	MES	C8-C7-N4-C5

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	5001	MES	2	0
4	F	5001	MES	1	0
4	B	5001	MES	1	0
4	A	5001	MES	4	0
4	E	5001	MES	1	0
4	D	5001	MES	1	0
4	C	5001	MES	1	0
4	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, 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	842/844 (99%)	-0.33	10 (1%)	76	58	23, 36, 90, 112	0
1	B	749/844 (88%)	-0.04	17 (2%)	61	39	30, 51, 98, 148	0
1	C	844/844 (100%)	-0.46	11 (1%)	75	56	25, 35, 61, 71	0
1	D	844/844 (100%)	-0.28	20 (2%)	59	38	25, 36, 89, 110	0
1	E	844/844 (100%)	-0.23	30 (3%)	46	26	22, 36, 111, 136	0
1	F	844/844 (100%)	-0.11	7 (0%)	82	65	39, 55, 78, 91	0
1	G	844/844 (100%)	-0.39	7 (0%)	82	65	24, 36, 72, 85	0
1	H	808/844 (95%)	-0.27	28 (3%)	47	27	25, 43, 101, 144	0
All	All	6619/6752 (98%)	-0.27	130 (1%)	65	44	22, 40, 88, 148	0

The worst 5 of 130 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	303	GLN	5.5
1	H	318	GLY	5.4
1	B	246	ALA	5.0
1	H	249	ASN	4.8
1	H	282	LYS	4.8

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

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

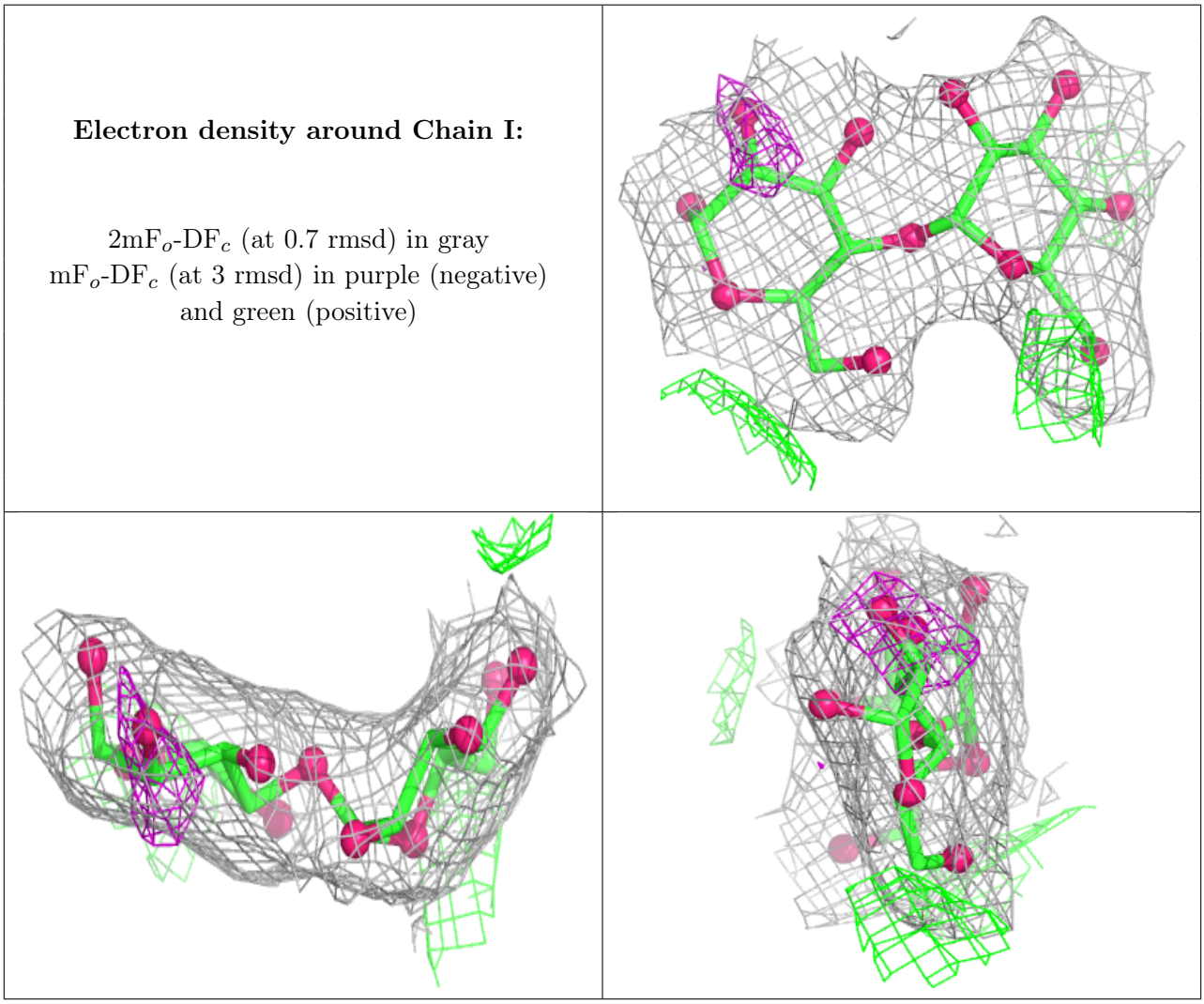
6.3 Carbohydrates

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, 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	B-factors(Å^2)	Q<0.9
2	GLC	I	2	11/12	0.91	0.11	30,32,34,35	0
2	GLC	I	1	12/12	0.92	0.09	31,36,39,40	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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, 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	B-factors(Å^2)	Q<0.9
4	MES	A	5001	12/12	0.77	0.23	31,33,33,34	0
4	MES	D	5001	12/12	0.81	0.23	32,34,36,36	0
4	MES	E	5001	12/12	0.81	0.23	32,35,37,37	0
4	MES	C	5001	12/12	0.82	0.23	30,31,32,33	0
4	MES	G	5001	12/12	0.85	0.21	29,31,32,33	0
4	MES	H	5001	12/12	0.86	0.20	30,32,34,35	0
4	MES	F	5001	12/12	0.87	0.20	38,38,39,39	0
4	MES	B	5001	12/12	0.89	0.20	39,41,43,44	0
3	CA	B	4001	1/1	0.94	0.05	32,32,32,32	0
3	CA	C	4001	1/1	0.95	0.05	29,29,29,29	0
3	CA	H	4001	1/1	0.96	0.05	32,32,32,32	0
3	CA	G	4001	1/1	0.96	0.05	28,28,28,28	0
3	CA	E	4001	1/1	0.96	0.07	32,32,32,32	0
3	CA	A	4001	1/1	0.97	0.06	29,29,29,29	0
3	CA	D	4001	1/1	0.97	0.04	30,30,30,30	0
3	CA	F	4001	1/1	0.97	0.06	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.