



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:55 PM GMT

PDB ID : 4AYJ
Title : Molecular structure of a metal-independent bacterial glycosyltransferase that catalyzes the synthesis of histo-blood group A antigen
Authors : Thiagarajan, N.; Pham, T.T.K.; Stinson, B.; Sundriyal, A.; Tumbale, P.; Lizotte-Waniewskib, M.; Brewb, K.; Acharya, K.R.
Deposited on : 2012-06-21
Resolution : 3.00 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

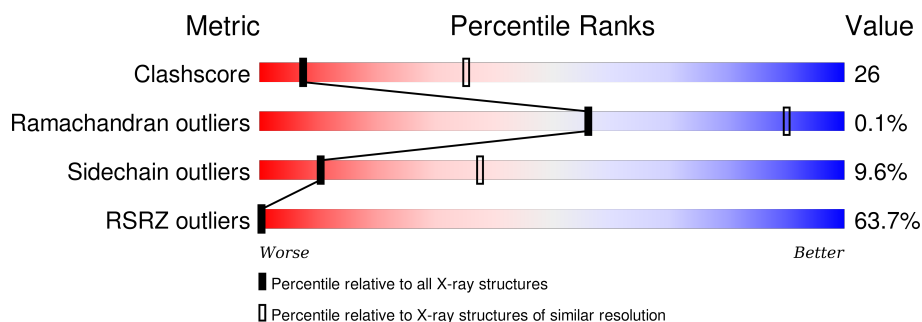
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	246	<div> <div>61%</div> <div> <div>52%</div> <div>38%</div> <div>6%</div> </div> </div>
1	B	246	<div> <div>59%</div> <div> <div>46%</div> <div>45%</div> <div>•</div> </div> </div>
1	C	246	<div> <div>61%</div> <div> <div>47%</div> <div>43%</div> <div>5%</div> </div> </div>
1	D	246	<div> <div>60%</div> <div> <div>46%</div> <div>44%</div> <div>6%</div> <div>•</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
2	BGC	A	1232	-	-	-	X
2	GAL	A	1233	-	-	-	X
2	BGC	B	1232	-	-	-	X
2	GAL	B	1233	-	-	-	X
2	FUC	B	1234	-	-	-	X
2	BGC	C	1232	-	-	X	-
2	FUC	C	1234	-	-	-	X
2	BGC	D	1232	-	-	-	X
2	GAL	D	1233	-	-	-	X
2	FUC	D	1234	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7939 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 BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	4	0	0
			1928	1262	311	348	7			
1	B	235	Total	C	N	O	S	0	0	0
			1961	1282	318	354	7			
1	C	233	Total	C	N	O	S	4	0	0
			1945	1272	315	351	7			
1	D	236	Total	C	N	O	S	0	0	0
			1973	1291	319	356	7			

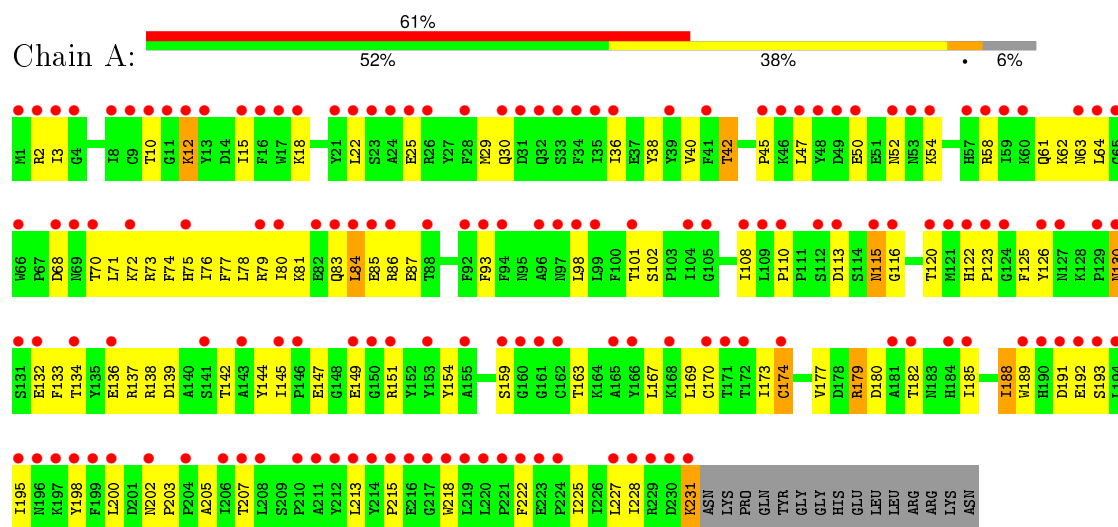
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

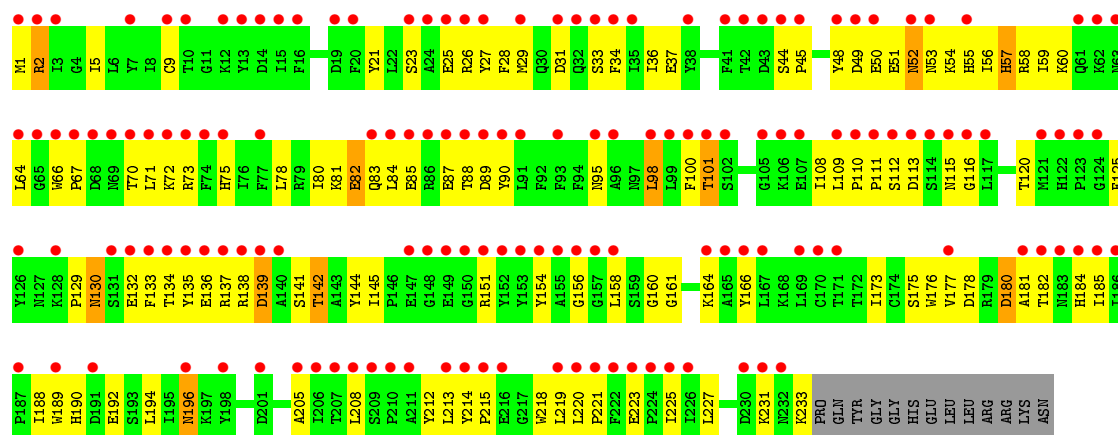
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			33	18	15		
2	B	3	Total	C	O	0	0
			33	18	15		
2	C	3	Total	C	O	0	0
			33	18	15		
2	D	3	Total	C	O	0	0
			33	18	15		

3 Residue-property plots

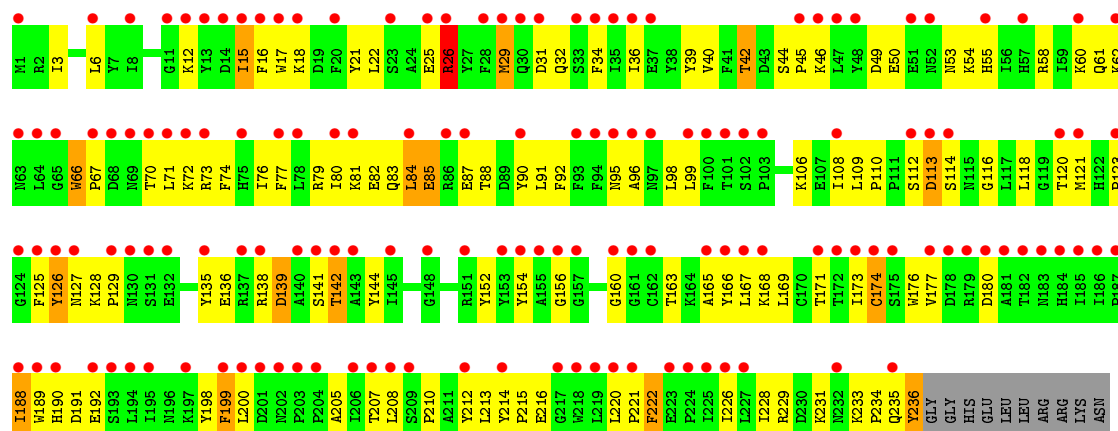
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE





• Molecule 1: BOGT - METAL-INDEPENDENT GLYCOSYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.85Å 93.87Å 75.51Å 90.00° 93.82° 90.00°	Depositor
Resolution (Å)	70.69 – 3.00 70.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.7 (70.69-3.00) 93.7 (70.69-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.36 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.181 , 0.262 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 37294 reflections	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	7939	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: BGC, GAL, FUC

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	0.50	0/1991	0.72	0/2704
1	B	0.47	0/2025	0.68	1/2750 (0.0%)
1	C	0.47	0/2008	0.65	0/2726
1	D	0.47	0/2038	0.67	1/2768 (0.0%)
All	All	0.48	0/8062	0.68	2/10948 (0.0%)

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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	26	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	220	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ASN	Peptide

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	1928	0	1869	89	0
1	B	1961	0	1903	93	1
1	C	1945	0	1888	101	0
1	D	1973	0	1911	116	1
2	A	33	0	30	9	0
2	B	33	0	30	2	0
2	C	33	0	30	7	0
2	D	33	0	30	3	0
All	All	7939	0	7691	399	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 26.

The worst 5 of 399 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)
2:C:1232:BGC:O5	1:D:128:LYS:NZ	1.79	1.15
1:C:2:ARG:NH1	1:C:89:ASP:H	1.50	1.08
1:C:2:ARG:O	1:C:2:ARG:NH1	1.93	1.02
1:A:134:THR:HG21	1:A:189:TRP:HE1	1.28	0.98
1:B:229:ARG:HD3	1:C:223:GLU:OE2	1.64	0.97

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:B:12:LYS:NZ	1:D:200:LEU:O[2_645]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	229/246 (93%)	225 (98%)	4 (2%)	0	100	100
1	B	233/246 (95%)	221 (95%)	11 (5%)	1 (0%)	39	80
1	C	231/246 (94%)	219 (95%)	12 (5%)	0	100	100
1	D	234/246 (95%)	223 (95%)	11 (5%)	0	100	100
All	All	927/984 (94%)	888 (96%)	38 (4%)	1 (0%)	56	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	PRO

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	208/221 (94%)	191 (92%)	17 (8%)	14	46
1	B	212/221 (96%)	190 (90%)	22 (10%)	9	32
1	C	210/221 (95%)	189 (90%)	21 (10%)	9	34
1	D	213/221 (96%)	192 (90%)	21 (10%)	10	35
All	All	843/884 (95%)	762 (90%)	81 (10%)	10	38

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	188	ILE
1	C	98	LEU
1	D	174	CYS
1	B	219	LEU
1	C	52	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	130	ASN
1	D	190	HIS
1	C	196	ASN
1	B	75	HIS
1	C	75	HIS

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 ⓘ

12 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	$\# Z > 2$
2	BGC	A	1232	2	12,12,12	1.37	2 (16%)	17,17,17	1.59	3 (17%)
2	GAL	A	1233	2	11,11,12	1.99	1 (9%)	14,15,17	1.66	4 (28%)
2	FUC	A	1234	2	10,10,11	1.90	3 (30%)	14,14,16	2.40	5 (35%)
2	BGC	B	1232	2	12,12,12	1.33	2 (16%)	17,17,17	1.55	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	B	1233	2	11,11,12	1.92	1 (9%)	14,15,17	1.93	3 (21%)
2	FUC	B	1234	2	10,10,11	2.17	4 (40%)	14,14,16	2.52	3 (21%)
2	BGC	C	1232	2	12,12,12	1.15	2 (16%)	17,17,17	2.19	5 (29%)
2	GAL	C	1233	2	11,11,12	1.91	1 (9%)	14,15,17	1.87	5 (35%)
2	FUC	C	1234	2	10,10,11	1.95	4 (40%)	14,14,16	2.74	5 (35%)
2	BGC	D	1232	2	12,12,12	1.55	2 (16%)	17,17,17	1.04	2 (11%)
2	GAL	D	1233	2	11,11,12	2.35	1 (9%)	14,15,17	2.16	3 (21%)
2	FUC	D	1234	2	10,10,11	2.30	4 (40%)	14,14,16	2.47	2 (14%)

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	BGC	A	1232	2	-	0/2/22/22	0/1/1/1
2	GAL	A	1233	2	-	0/2/19/22	0/1/1/1
2	FUC	A	1234	2	-	0/0/17/20	0/1/1/1
2	BGC	B	1232	2	-	0/2/22/22	0/1/1/1
2	GAL	B	1233	2	-	0/2/19/22	0/1/1/1
2	FUC	B	1234	2	-	0/0/17/20	0/1/1/1
2	BGC	C	1232	2	-	0/2/22/22	0/1/1/1
2	GAL	C	1233	2	-	0/2/19/22	0/1/1/1
2	FUC	C	1234	2	-	0/0/17/20	0/1/1/1
2	BGC	D	1232	2	-	0/2/22/22	0/1/1/1
2	GAL	D	1233	2	-	0/2/19/22	0/1/1/1
2	FUC	D	1234	2	-	0/0/17/20	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1232	BGC	O4-C4	2.18	1.48	1.43
2	C	1234	FUC	C4-C3	2.27	1.58	1.52
2	D	1234	FUC	C4-C3	2.47	1.58	1.52
2	B	1232	BGC	O4-C4	2.49	1.48	1.43
2	A	1232	BGC	O5-C1	2.56	1.47	1.43

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1233	GAL	C1-C2-C3	-6.85	101.43	109.54
2	C	1232	BGC	C1-C2-C3	-6.68	100.49	110.43
2	B	1233	GAL	C1-C2-C3	-4.85	103.80	109.54
2	A	1232	BGC	C1-C2-C3	-4.69	103.46	110.43
2	A	1233	GAL	C1-C2-C3	-4.12	104.67	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1232	BGC	5	0
2	A	1233	GAL	4	0
2	B	1233	GAL	2	0
2	C	1232	BGC	6	0
2	C	1233	GAL	4	0
2	D	1232	BGC	1	0
2	D	1233	GAL	2	0
2	D	1234	FUC	1	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	231/246 (93%)	2.94	151 (65%) 0 0	16, 28, 50, 67	1 (0%)
1	B	235/246 (95%)	2.80	146 (62%) 0 0	17, 34, 60, 74	0
1	C	233/246 (94%)	2.82	151 (64%) 0 0	18, 41, 63, 96	1 (0%)
1	D	236/246 (95%)	2.91	148 (62%) 0 0	20, 37, 60, 83	0
All	All	935/984 (95%)	2.87	596 (63%) 0 0	16, 34, 60, 96	2 (0%)

The worst 5 of 596 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	174	CYS	11.2
1	B	166	TYR	10.3
1	C	116	GLY	10.0
1	B	108	ILE	9.7
1	A	85	GLU	9.6

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
2	BGC	D	1232	12/12	0.30	0.84	2.46	42,53,59,60	0
2	GAL	D	1233	11/12	0.28	0.66	1.72	44,47,58,62	0
2	GAL	B	1233	11/12	0.31	0.69	1.49	27,29,30,32	0
2	BGC	B	1232	12/12	0.34	0.59	0.82	26,29,33,33	0
2	BGC	A	1232	12/12	0.44	0.57	0.27	25,28,32,36	0
2	FUC	B	1234	10/11	0.51	0.52	0.16	26,35,41,41	0
2	FUC	D	1234	10/11	0.54	0.57	0.08	48,54,62,64	0
2	GAL	A	1233	11/12	0.44	0.44	-0.82	21,23,26,27	0
2	FUC	C	1234	10/11	0.55	0.41	-0.95	23,31,36,41	0
2	BGC	C	1232	12/12	0.45	0.38	-1.14	28,33,39,46	0
2	FUC	A	1234	10/11	0.51	0.37	-1.57	13,19,30,33	0
2	GAL	C	1233	11/12	0.55	0.33	-2.55	31,33,39,43	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.