wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:17 PM GMT

PDB ID	:	1T0O
Title	:	The structure of alpha-galactosidase from Trichoderma reesei complexed with beta-D-galactose
Authors	:	Golubev, A.M.; Nagem, R.A.P.; Brandao Neto, J.R.; Neustroev, K.N.; Eneyskaya, E.V.; Kulminskaya, A.A.; Shabalin, K.A.; Savel'ev, A.N.; Polikarpov, I.
Deposited on	:	2004-04-12
Resolution	:	1.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

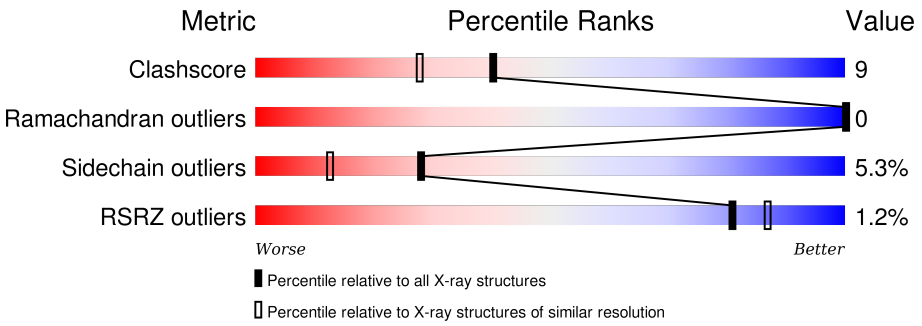
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

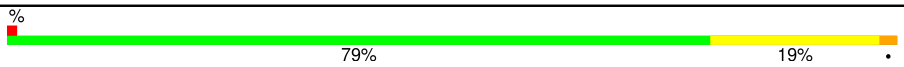
The reported resolution of this entry is 1.96 Å.

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	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	417	

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
5	GAL	A	901	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3798 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 alpha-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	3213	2039	539	618	17	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	LEU	VAL	SEE REMARK 999	GB 1580816
A	70	PRO	VAL	SEE REMARK 999	GB 1580816
A	72	ALA	THR	SEE REMARK 999	GB 1580816
A	88	ALA	ASP	SEE REMARK 999	GB 1580816
A	148	ASN	ALA	SEE REMARK 999	GB 1580816
A	151	PHE	ALA	SEE REMARK 999	GB 1580816
A	153	LYS	GLN	SEE REMARK 999	GB 1580816
A	161	THR	SER	SEE REMARK 999	GB 1580816
A	165	ASP	GLU	SEE REMARK 999	GB 1580816
A	167	THR	ASN	SEE REMARK 999	GB 1580816
A	185	GLY	ASN	SEE REMARK 999	GB 1580816
A	196	HIS	ARG	SEE REMARK 999	GB 1580816
A	202	MET	LEU	SEE REMARK 999	GB 1580816
A	207	GLN	VAL	SEE REMARK 999	GB 1580816
A	216	SER	GLU	SEE REMARK 999	GB 1580816
A	225	ASP	GLY	SEE REMARK 999	GB 1580816
A	230	ASN	GLU	SEE REMARK 999	GB 1580816
A	236	ARG	HIS	SEE REMARK 999	GB 1580816
A	238	LEU	ILE	SEE REMARK 999	GB 1580816
A	240	LEU	MET	SEE REMARK 999	GB 1580816
A	245	LEU	MET	SEE REMARK 999	GB 1580816
A	249	ASP	GLY	SEE REMARK 999	GB 1580816
A	258	MET	ILE	SEE REMARK 999	GB 1580816
A	297	ASN	GLU	SEE REMARK 999	GB 1580816
A	300	ASN	GLU	SEE REMARK 999	GB 1580816
A	327	ILE	VAL	SEE REMARK 999	GB 1580816
A	335	VAL	TYR	SEE REMARK 999	GB 1580816

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	TYR	ASN	SEE REMARK 999	GB 1580816
A	341	PHE	TYR	SEE REMARK 999	GB 1580816
A	355	VAL	MET	SEE REMARK 999	GB 1580816
A	360	ILE	HIS	SEE REMARK 999	GB 1580816
A	362	ALA	VAL	SEE REMARK 999	GB 1580816
A	363	THR	ARG	SEE REMARK 999	GB 1580816
A	369	ASN	SER	SEE REMARK 999	GB 1580816
A	378	HIS	ARG	SEE REMARK 999	GB 1580816
A	386	SER	THR	SEE REMARK 999	GB 1580816
A	389	ASP	SER	SEE REMARK 999	GB 1580816
A	398	ALA	THR	SEE REMARK 999	GB 1580816
A	415	GLN	ARG	SEE REMARK 999	GB 1580816
A	416	ARG	ASN	SEE REMARK 999	GB 1580816

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	2	28	16	2	10	0	0
			Total	C	N	O		
2	A	2	28	16	2	10	0	0

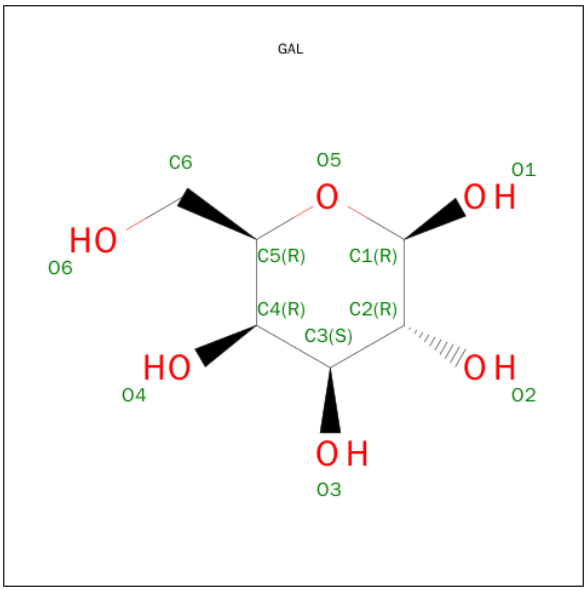
- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	7	83	46	2	35	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	4	50	28	2	20	0	0

- Molecule 5 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	12	6	6	0	0

- Molecule 6 is water.

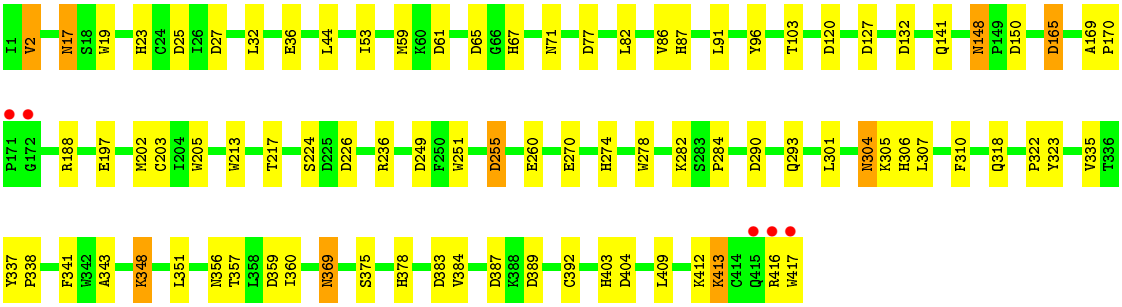
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	384	384	384	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: alpha-galactosidase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.83Å 58.31Å 153.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 1.96 9.86 – 1.96	Depositor EDS
% Data completeness (in resolution range)	72.3 (9.00-1.96) 70.4 (9.86-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.151 , 0.205 0.158 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 54.9	EDS
Estimated twinning fraction	0.078 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 26738 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3798	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, GAL, BMA, NAG

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	0.52	0/3304	0.85	10/4512 (0.2%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	61	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	77	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	255	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	404	ASP	CB-CG-OD2	5.50	123.25	118.30

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	3213	0	3045	56	0
2	A	56	0	50	1	0
3	A	83	0	70	2	0
4	A	50	0	43	1	0
5	A	12	0	12	1	0
6	A	384	0	0	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3798	0	3220	58	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 9.

The worst 5 of 58 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:A:306:HIS:HD2	6:A:1060:HOH:O	1.56	0.87
1:A:260:GLU:H	1:A:274:HIS:HE1	1.24	0.85
1:A:270:GLU:OE2	1:A:403:HIS:HD2	1.62	0.81
1:A:87:HIS:HE1	1:A:127:ASP:OD2	1.65	0.79
1:A:165:ASP:HB2	6:A:945:HOH:O	1.84	0.77

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	415/417 (100%)	407 (98%)	8 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	340/340 (100%)	322 (95%)	18 (5%)	28 13

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	305	LYS
1	A	412	LYS
1	A	278	TRP
1	A	301	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	246	ASN
1	A	369	ASN
1	A	141	GLN
1	A	306	HIS

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)

15 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	NAG	A	500	1,2	14,14,15	0.59	0	15,19,21	0.87	0
2	NAG	A	501	2	14,14,15	0.57	0	15,19,21	0.73	0
3	NAG	A	600	1,3	14,14,15	0.72	0	15,19,21	0.85	0
3	NAG	A	601	3	14,14,15	0.75	0	15,19,21	1.26	1 (6%)
3	BMA	A	602	3	11,11,12	0.74	0	14,15,17	1.61	4 (28%)
3	MAN	A	603	3	11,11,12	0.64	0	14,15,17	1.46	2 (14%)
3	MAN	A	604	3	11,11,12	0.92	1 (9%)	14,15,17	1.35	3 (21%)
3	MAN	A	605	3	11,11,12	0.52	0	14,15,17	0.91	1 (7%)
3	MAN	A	606	3	11,11,12	0.68	0	14,15,17	1.53	2 (14%)
4	NAG	A	700	1,4	14,14,15	0.73	0	15,19,21	0.99	1 (6%)
4	NAG	A	701	4	14,14,15	0.81	1 (7%)	15,19,21	0.64	0
4	BMA	A	702	4	11,11,12	0.51	0	14,15,17	1.13	1 (7%)
4	MAN	A	703	4	11,11,12	0.60	0	14,15,17	1.36	2 (14%)
2	NAG	A	800	1,2	14,14,15	0.79	0	15,19,21	1.15	1 (6%)
2	NAG	A	801	2	14,14,15	0.65	0	15,19,21	1.17	1 (6%)

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	NAG	A	500	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	501	2	-	0/6/23/26	0/1/1/1
3	NAG	A	600	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	601	3	-	0/6/23/26	0/1/1/1
3	BMA	A	602	3	-	0/2/19/22	0/1/1/1
3	MAN	A	603	3	-	0/2/19/22	0/1/1/1
3	MAN	A	604	3	-	0/2/19/22	0/1/1/1
3	MAN	A	605	3	-	0/2/19/22	0/1/1/1
3	MAN	A	606	3	-	0/2/19/22	0/1/1/1
4	NAG	A	700	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	701	4	-	0/6/23/26	0/1/1/1
4	BMA	A	702	4	-	0/2/19/22	0/1/1/1
4	MAN	A	703	4	-	0/2/19/22	0/1/1/1
2	NAG	A	800	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	801	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	NAG	O5-C1	-2.20	1.40	1.43
3	A	604	MAN	O5-C1	-2.07	1.40	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	MAN	C1-O5-C5	-4.02	107.15	112.25
3	A	602	BMA	C3-C4-C5	-3.17	104.68	110.20
3	A	606	MAN	O2-C2-C1	-2.72	103.74	109.21
3	A	602	BMA	C1-O5-C5	-2.59	108.97	112.25
3	A	604	MAN	O2-C2-C1	-2.58	104.04	109.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	MAN	2	0
4	A	700	NAG	1	0
2	A	800	NAG	1	0

5.6 Ligand geometry (i)

1 ligand is 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	GAL	A	901	-	12,12,12	2.41	3 (25%)	17,17,17	2.01	4 (23%)

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	GAL	A	901	-	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	GAL	C3-C2	-4.42	1.40	1.52
5	A	901	GAL	O3-C3	3.74	1.51	1.43
5	A	901	GAL	C1-C2	5.19	1.62	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	901	GAL	O4-C4-C5	-4.18	98.17	109.24
5	A	901	GAL	O4-C4-C3	-3.00	103.57	110.34
5	A	901	GAL	O3-C3-C4	-2.12	105.56	110.34
5	A	901	GAL	O5-C5-C4	4.09	117.36	109.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	GAL	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	417/417 (100%)	-0.46	5 (1%) 81 87	12, 21, 35, 71	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	417	TRP	11.6
1	A	416	ARG	4.1
1	A	415	GLN	2.8
1	A	172	GLY	2.4
1	A	171	PRO	2.0

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(Å^2)	Q<0.9
3	MAN	A	606	11/12	0.97	0.08	0.90	13,16,19,24	0
4	NAG	A	700	14/15	0.96	0.08	-0.21	22,23,26,26	0
4	NAG	A	701	14/15	0.96	0.08	-0.52	23,26,31,35	0
2	NAG	A	500	14/15	0.94	0.09	-0.70	37,39,41,45	0
3	BMA	A	602	11/12	0.95	0.10	-	27,31,37,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MAN	A	604	11/12	0.96	0.08	-	20,25,34,40	0
3	NAG	A	600	14/15	0.95	0.09	-	24,27,34,37	0
3	MAN	A	605	11/12	0.89	0.24	-	47,50,52,53	0
2	NAG	A	800	14/15	0.96	0.08	-	21,27,32,33	0
2	NAG	A	501	14/15	0.86	0.28	-	48,51,53,54	0
4	BMA	A	702	11/12	0.91	0.14	-	42,48,50,55	0
2	NAG	A	801	14/15	0.91	0.16	-	36,37,43,44	0
3	NAG	A	601	14/15	0.97	0.08	-	21,24,27,28	0
3	MAN	A	603	11/12	0.76	0.27	-	49,53,55,57	0
4	MAN	A	703	11/12	0.80	0.36	-	60,64,65,66	0

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(Å^2)	Q<0.9
5	GAL	A	901	12/12	0.90	0.14	6.64	20,22,24,25	0

6.5 Other polymers (i)

There are no such residues in this entry.