Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID	:	3OGR
Title	:	Complex structure of beta-galactosidase from Trichoderma reesei with galactose
Authors	:	Maksimainen, M.; Rouvinen, J.
Deposited on	:	2010-08-17
Resolution	:	1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ①) were used in the production of this report:

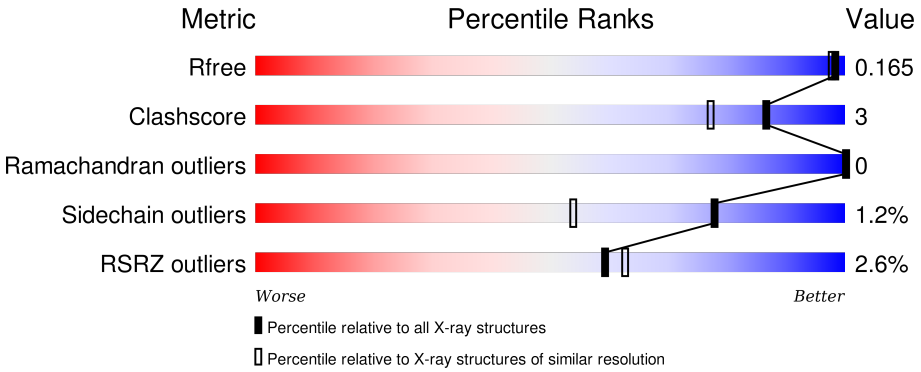
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	1003	3% 90% 8%

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
3	MAN	A	1031	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	1042	-	-	-	X
5	NAG	A	1043	-	-	-	X
6	NAG	A	1044	-	-	-	X
6	NAG	A	1045	-	-	-	X

2 Entry composition

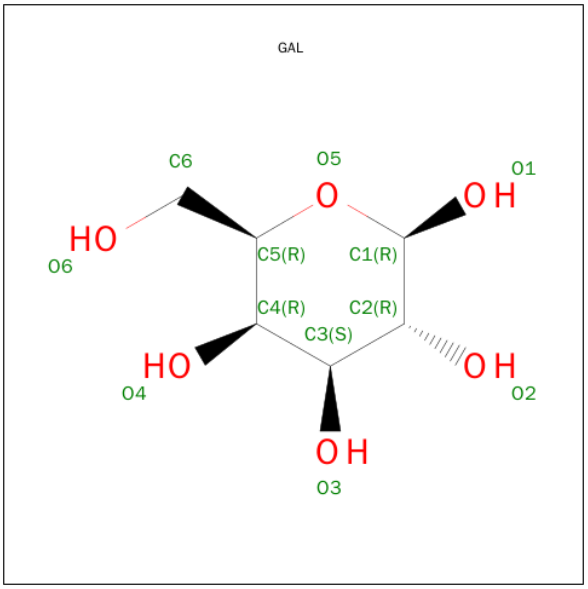
There are 7 unique types of molecules in this entry. The entry contains 8986 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	986	Total	C	N	O	S	0	9	0
			7688	4939	1298	1443	8			

- Molecule 2 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



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

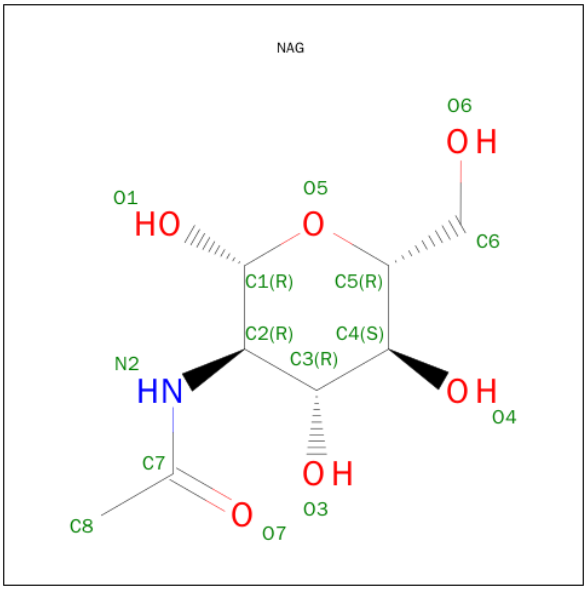
- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is water.

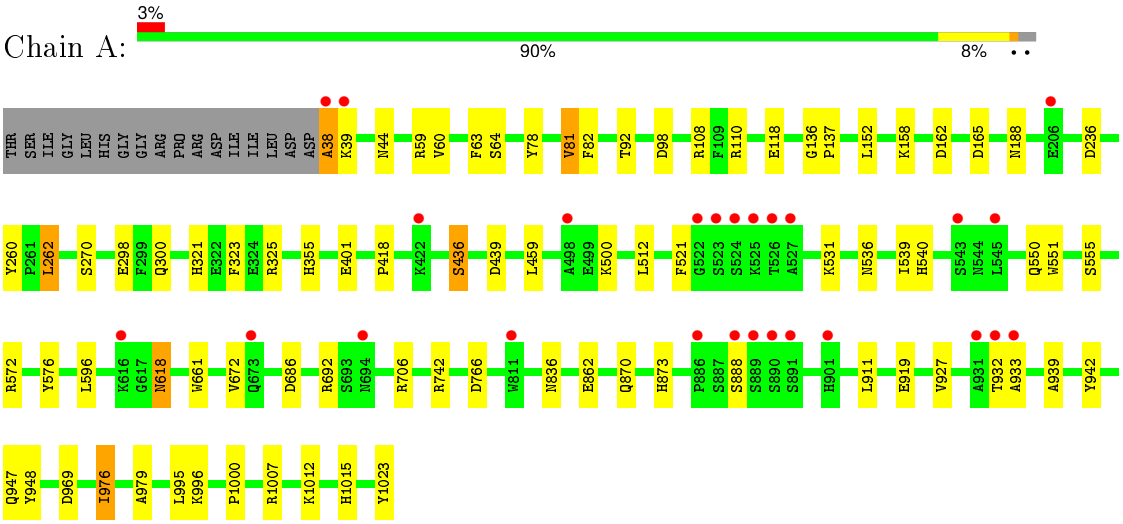
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1031	Total	O	0	0
			1031	1031		

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: Beta-galactosidase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.43Å 69.28Å 81.50Å 109.03° 97.34° 114.38°	Depositor
Resolution (Å)	19.78 – 1.50 19.78 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.78-1.50) 79.8 (19.78-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.128 , 0.168 0.145 , 0.165	Depositor DCC
R_{free} test set	8981 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	9.6	Xtriage
Anisotropy	0.758	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 55.2	EDS
Estimated twinning fraction	0.014 for k,h,-h-k-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 179614 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8986	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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

5.1 Standard geometry

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

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	1.29	31/7908 (0.4%)	1.05	30/10777 (0.3%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	555[A]	SER	CB-OG	-13.59	1.24	1.42
1	A	555[B]	SER	CB-OG	-13.59	1.24	1.42
1	A	270[A]	SER	CA-CB	-9.74	1.38	1.52
1	A	270[B]	SER	CA-CB	-9.74	1.38	1.52
1	A	942	TYR	CD2-CE2	7.96	1.51	1.39
1	A	919	GLU	CD-OE1	7.79	1.34	1.25
1	A	551	TRP	CE3-CZ3	-7.58	1.25	1.38
1	A	862	GLU	CB-CG	-7.05	1.38	1.52
1	A	82[A]	PHE	CG-CD2	6.96	1.49	1.38
1	A	82[B]	PHE	CG-CD2	6.96	1.49	1.38
1	A	555[A]	SER	C-N	6.72	1.49	1.34
1	A	555[B]	SER	C-N	6.72	1.49	1.34
1	A	118	GLU	CD-OE1	6.69	1.33	1.25
1	A	500	LYS	CD-CE	6.40	1.67	1.51
1	A	500	LYS	CE-NZ	6.40	1.65	1.49
1	A	118	GLU	CD-OE2	6.29	1.32	1.25
1	A	862	GLU	CD-OE2	-6.14	1.18	1.25
1	A	108	ARG	CZ-NH1	5.84	1.40	1.33
1	A	661	TRP	CE3-CZ3	5.75	1.48	1.38
1	A	81	VAL	CB-CG2	-5.62	1.41	1.52
1	A	38	ALA	CA-CB	5.60	1.64	1.52
1	A	536	ASN	CB-CG	-5.40	1.38	1.51
1	A	44	ASN	CB-CG	-5.33	1.38	1.51
1	A	158	LYS	CD-CE	5.30	1.64	1.51
1	A	551	TRP	CB-CG	5.28	1.59	1.50
1	A	521	PHE	CE1-CZ	5.20	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	ARG	CB-CG	-5.18	1.38	1.52
1	A	551	TRP	CG-CD1	5.06	1.43	1.36
1	A	976[A]	ILE	C-O	5.03	1.32	1.23
1	A	976[B]	ILE	C-O	5.03	1.32	1.23
1	A	436	SER	CB-OG	5.01	1.48	1.42

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	572	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	A	323	PHE	CB-CG-CD1	-7.22	115.75	120.80
1	A	706	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	942	TYR	CG-CD2-CE2	-6.97	115.73	121.30
1	A	969	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	108	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	262	LEU	CB-CG-CD1	6.47	122.00	111.00
1	A	325	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	152	LEU	CB-CG-CD2	6.18	121.51	111.00
1	A	82[A]	PHE	CB-CG-CD2	-6.18	116.48	120.80
1	A	82[B]	PHE	CB-CG-CD2	-6.18	116.48	120.80
1	A	766	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	576	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	A	572	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	82[A]	PHE	CB-CG-CD1	5.97	124.98	120.80
1	A	82[B]	PHE	CB-CG-CD1	5.97	124.98	120.80
1	A	236	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	165	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	766	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	976[A]	ILE	CB-CG1-CD1	-5.75	97.79	113.90
1	A	976[B]	ILE	CB-CG1-CD1	-5.75	97.79	113.90
1	A	439	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	1007	ARG	NE-CZ-NH1	-5.65	117.48	120.30
1	A	995	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	933	ALA	N-CA-C	-5.55	96.02	111.00
1	A	98	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	162	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	572	ARG	CD-NE-CZ	5.31	131.04	123.60
1	A	59	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	162	ASP	CB-CG-OD2	-5.15	113.67	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	7688	0	7472	41	0
2	A	12	0	12	1	0
3	A	83	0	70	1	0
4	A	116	0	95	1	0
5	A	28	0	26	0	0
6	A	28	0	25	2	0
7	A	1031	0	0	12	0
All	All	8986	0	7700	42	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 3.

All (42) 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:976[A]:ILE:CG1	1:A:976[A]:ILE:CD1	1.76	1.62
1:A:976[B]:ILE:CB	1:A:976[B]:ILE:CG2	1.79	1.59
1:A:38:ALA:HB3	7:A:1704:HOH:O	1.73	0.89
1:A:976[A]:ILE:CB	1:A:976[A]:ILE:CD1	2.53	0.85
1:A:110:ARG:NE	7:A:2064:HOH:O	2.16	0.77
1:A:976[A]:ILE:HG21	1:A:976[A]:ILE:HD13	1.69	0.74
1:A:976[B]:ILE:CA	1:A:976[B]:ILE:CG2	2.71	0.66
1:A:78:TYR:O	1:A:81:VAL:HG22	1.96	0.65
4:A:1041:GLC:H61	7:A:1968:HOH:O	1.97	0.64
1:A:911:LEU:HD22	1:A:976[A]:ILE:HD11	1.81	0.63
1:A:512:LEU:HD11	1:A:550:GLN:HG2	1.83	0.59
1:A:188:ASN:HB3	7:A:1560:HOH:O	2.05	0.57
1:A:976[A]:ILE:CG2	1:A:976[A]:ILE:CD1	2.83	0.56
1:A:976[A]:ILE:HG21	1:A:976[A]:ILE:CD1	2.35	0.56
1:A:873:HIS:CD2	1:A:873:HIS:H	2.26	0.54
1:A:436:SER:OG	6:A:1044:NAG:H5	2.07	0.53
1:A:976[B]:ILE:CG1	1:A:976[B]:ILE:CG2	2.78	0.51
1:A:976[A]:ILE:CG2	1:A:976[A]:ILE:HD13	2.40	0.50
1:A:870:GLN:NE2	7:A:1757:HOH:O	2.45	0.49
1:A:459:LEU:HD13	1:A:540:HIS:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60[B]:VAL:HG21	1:A:596:LEU:HD12	1.95	0.48
1:A:321:HIS:HD2	7:A:1182:HOH:O	1.96	0.48
1:A:298:GLU:OE1	2:A:1024:GAL:H1	2.15	0.47
1:A:531:LYS:HE3	1:A:539:ILE:HD12	1.98	0.46
1:A:742:ARG:HG2	7:A:1772:HOH:O	2.14	0.46
1:A:401:GLU:HB2	1:A:418:PRO:HG2	1.98	0.46
1:A:1023:TYR:HB2	7:A:1711:HOH:O	2.14	0.46
1:A:136:GLY:HA3	1:A:137:PRO:C	2.36	0.46
1:A:692:ARG:NH1	7:A:1635:HOH:O	2.39	0.46
1:A:1012:LYS:HE3	7:A:1586:HOH:O	2.16	0.46
1:A:618:ASN:C	1:A:618:ASN:HD22	2.19	0.45
1:A:836:ASN:ND2	7:A:1913:HOH:O	2.48	0.45
1:A:64:SER:HA	1:A:92:THR:O	2.18	0.44
1:A:321:HIS:HE1	3:A:1029:MAN:O4	2.02	0.42
1:A:873:HIS:HE1	7:A:1135:HOH:O	2.00	0.42
1:A:686:ASP:OD2	1:A:692:ARG:CZ	2.68	0.42
1:A:436:SER:O	6:A:1044:NAG:H62	2.20	0.41
1:A:672:VAL:HG23	1:A:1000:PRO:HG3	2.00	0.41
1:A:459:LEU:HD13	1:A:540:HIS:CD2	2.55	0.41
1:A:927:VAL:HG21	1:A:996:LYS:HG3	2.02	0.41
1:A:260:TYR:HA	1:A:300:GLN:HB2	2.01	0.41
1:A:939:ALA:HA	1:A:979:ALA:O	2.21	0.41

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	993/1003 (99%)	964 (97%)	29 (3%)	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	814/819 (99%)	804 (99%)	10 (1%)	78 54

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	63	PHE
1	A	262	LEU
1	A	355	HIS
1	A	618	ASN
1	A	888	SER
1	A	932	THR
1	A	947	GLN
1	A	948	TYR
1	A	1015	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	321	HIS
1	A	540	HIS
1	A	618	ASN
1	A	664	HIS
1	A	836	ASN
1	A	873	HIS
1	A	884	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)

19 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	$\#\|Z\| > 2$
3	NAG	A	1025	1,3	14,14,15	1.53	2 (14%)	15,19,21	0.85	0
3	NAG	A	1026	3	14,14,15	0.57	0	15,19,21	0.99	1 (6%)
3	BMA	A	1027	3	11,11,12	1.03	1 (9%)	14,15,17	1.59	3 (21%)
3	MAN	A	1028	3	11,11,12	0.94	0	14,15,17	0.87	0
3	MAN	A	1029	3	11,11,12	1.09	1 (9%)	14,15,17	1.08	1 (7%)
3	MAN	A	1030	3	11,11,12	0.78	0	14,15,17	1.33	2 (14%)
3	MAN	A	1031	3	11,11,12	1.48	1 (9%)	14,15,17	2.14	3 (21%)
4	NAG	A	1032	1,4	14,14,15	1.05	1 (7%)	15,19,21	1.12	1 (6%)
4	NAG	A	1033	4	14,14,15	0.91	0	15,19,21	1.13	1 (6%)
4	BMA	A	1034	4	11,11,12	1.00	0	14,15,17	1.22	2 (14%)
4	MAN	A	1035	4	11,11,12	0.69	0	14,15,17	2.20	4 (28%)
4	MAN	A	1036	4	11,11,12	1.02	0	14,15,17	1.97	7 (50%)
4	MAN	A	1037	4	11,11,12	0.81	0	14,15,17	1.58	4 (28%)
4	MAN	A	1038	4	11,11,12	0.94	0	14,15,17	2.96	8 (57%)
4	MAN	A	1039	4	11,11,12	0.39	0	14,15,17	1.70	3 (21%)
4	MAN	A	1040	4	11,11,12	0.99	1 (9%)	14,15,17	1.78	5 (35%)
4	GLC	A	1041	4	11,11,12	1.61	3 (27%)	14,15,17	4.27	5 (35%)
6	NAG	A	1044	1,6	14,14,15	1.38	1 (7%)	15,19,21	3.07	9 (60%)
6	NAG	A	1045	6	14,14,15	0.85	1 (7%)	15,19,21	1.37	3 (20%)

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	NAG	A	1025	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1026	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1027	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1028	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1029	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1030	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1031	3	-	0/2/19/22	0/1/1/1
4	NAG	A	1032	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1033	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1034	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1035	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1036	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1037	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1038	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1039	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1040	4	-	0/2/19/22	0/1/1/1
4	GLC	A	1041	4	-	0/2/19/22	0/1/1/1
6	NAG	A	1044	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1045	6	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1025	NAG	O5-C1	-4.75	1.35	1.43
6	A	1044	NAG	C1-C2	-4.08	1.46	1.52
4	A	1041	GLC	O5-C1	-3.66	1.37	1.43
3	A	1029	MAN	O5-C1	-2.68	1.39	1.43
4	A	1041	GLC	O4-C4	-2.62	1.36	1.43
4	A	1041	GLC	C2-C3	-2.60	1.49	1.52
4	A	1040	MAN	C2-C3	2.10	1.55	1.52
3	A	1027	BMA	C2-C3	2.14	1.55	1.52
6	A	1045	NAG	C1-C2	2.25	1.55	1.52
4	A	1032	NAG	C1-C2	2.50	1.55	1.52
3	A	1025	NAG	C1-C2	2.54	1.56	1.52
3	A	1031	MAN	C2-C3	3.66	1.57	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1041	GLC	O3-C3-C2	-6.67	97.96	110.00
4	A	1041	GLC	C2-C3-C4	-5.68	101.39	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1035	MAN	O3-C3-C4	-4.45	100.32	110.34
4	A	1038	MAN	C6-C5-C4	-4.00	103.15	113.02
6	A	1044	NAG	O3-C3-C2	-3.74	101.71	109.11
4	A	1036	MAN	O2-C2-C1	-3.44	102.31	109.21
3	A	1027	BMA	C1-O5-C5	-3.43	107.89	112.25
4	A	1038	MAN	C1-C2-C3	-3.21	105.74	109.54
3	A	1031	MAN	O5-C1-C2	-3.19	105.68	110.86
4	A	1038	MAN	O2-C2-C3	-3.18	103.72	110.12
3	A	1027	BMA	O3-C3-C2	-3.02	104.54	110.00
3	A	1030	MAN	O6-C6-C5	-2.71	102.37	111.33
3	A	1030	MAN	O3-C3-C2	-2.70	105.11	110.00
4	A	1039	MAN	C1-C2-C3	-2.67	106.38	109.54
4	A	1040	MAN	O5-C1-C2	-2.60	106.64	110.86
6	A	1044	NAG	O4-C4-C5	-2.59	102.37	109.24
6	A	1045	NAG	O7-C7-C8	-2.57	117.35	122.06
6	A	1044	NAG	O7-C7-C8	-2.56	117.37	122.06
4	A	1038	MAN	O4-C4-C5	-2.55	102.49	109.24
4	A	1039	MAN	O3-C3-C2	-2.47	105.54	110.00
4	A	1037	MAN	O6-C6-C5	-2.46	103.19	111.33
3	A	1031	MAN	C6-C5-C4	-2.46	106.95	113.02
4	A	1037	MAN	C1-C2-C3	-2.44	106.66	109.54
3	A	1027	BMA	O4-C4-C3	-2.32	105.11	110.34
4	A	1035	MAN	C6-C5-C4	-2.31	107.31	113.02
4	A	1038	MAN	O5-C5-C6	-2.30	102.38	107.35
4	A	1040	MAN	O3-C3-C4	-2.23	105.31	110.34
4	A	1033	NAG	O4-C4-C3	-2.22	105.33	110.34
3	A	1026	NAG	C4-C3-C2	-2.22	107.78	111.23
4	A	1034	BMA	C1-C2-C3	-2.12	107.03	109.54
4	A	1040	MAN	C6-C5-C4	-2.10	107.83	113.02
4	A	1036	MAN	O3-C3-C2	-2.09	106.22	110.00
4	A	1041	GLC	O4-C4-C5	-2.06	103.79	109.24
4	A	1036	MAN	O2-C2-C3	-2.04	106.02	110.12
4	A	1040	MAN	O3-C3-C2	2.06	113.71	110.00
4	A	1037	MAN	C3-C4-C5	2.07	113.81	110.20
4	A	1036	MAN	C2-C3-C4	2.07	114.56	111.04
6	A	1044	NAG	O3-C3-C4	2.08	115.02	110.34
4	A	1034	BMA	O3-C3-C2	2.09	113.77	110.00
4	A	1036	MAN	C1-C2-C3	2.41	112.39	109.54
6	A	1045	NAG	C8-C7-N2	2.42	120.75	116.11
4	A	1032	NAG	C1-O5-C5	2.45	115.35	112.25
4	A	1036	MAN	O5-C5-C6	2.56	112.89	107.35
6	A	1044	NAG	O7-C7-N2	2.67	127.31	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1029	MAN	C1-O5-C5	2.74	115.72	112.25
4	A	1035	MAN	O3-C3-C2	2.75	114.97	110.00
4	A	1037	MAN	C1-O5-C5	3.07	116.15	112.25
6	A	1045	NAG	C2-N2-C7	3.16	127.11	123.04
6	A	1044	NAG	C4-C3-C2	3.26	116.30	111.23
4	A	1036	MAN	C1-O5-C5	3.27	116.40	112.25
6	A	1044	NAG	C1-O5-C5	3.42	116.58	112.25
4	A	1038	MAN	O5-C1-C2	4.10	117.51	110.86
4	A	1040	MAN	C1-C2-C3	4.12	114.42	109.54
4	A	1038	MAN	C3-C4-C5	4.18	117.49	110.20
4	A	1039	MAN	C1-O5-C5	4.60	118.08	112.25
4	A	1035	MAN	O5-C5-C6	5.26	118.73	107.35
6	A	1044	NAG	O5-C5-C6	5.40	119.03	107.35
4	A	1038	MAN	C1-O5-C5	5.97	119.83	112.25
3	A	1031	MAN	C1-O5-C5	6.10	119.99	112.25
6	A	1044	NAG	C2-N2-C7	6.31	131.15	123.04
4	A	1041	GLC	C1-O5-C5	8.53	123.08	112.25
4	A	1041	GLC	C1-C2-C3	9.59	120.89	109.54

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	1029	MAN	1	0
4	A	1041	GLC	1	0
6	A	1044	NAG	2	0

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GAL	A	1024	-	12,12,12	0.87	1 (8%)	17,17,17	1.32	1 (5%)
5	NAG	A	1042	1	14,14,15	0.96	0	15,19,21	1.70	3 (20%)
5	NAG	A	1043	1	14,14,15	0.62	0	15,19,21	1.39	2 (13%)

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	GAL	A	1024	-	-	0/2/22/22	0/1/1/1
5	NAG	A	1042	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1043	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1024	GAL	C1-C2	2.08	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1024	GAL	O1-C1-O5	-4.38	98.28	110.25
5	A	1042	NAG	O6-C6-C5	-4.28	97.20	111.33
5	A	1043	NAG	O7-C7-C8	-3.17	116.25	122.06
5	A	1043	NAG	O6-C6-C5	-2.88	101.82	111.33
5	A	1042	NAG	O3-C3-C2	-2.06	105.03	109.11
5	A	1042	NAG	C1-O5-C5	3.34	116.49	112.25

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
2	A	1024	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

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	986/1003 (98%)	-0.31	26 (2%) 59 63	6, 11, 24, 45	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	933	ALA	11.7
1	A	523	SER	7.1
1	A	811	TRP	7.0
1	A	932	THR	6.5
1	A	498	ALA	6.0
1	A	38	ALA	5.6
1	A	543	SER	5.6
1	A	526	THR	5.5
1	A	525	LYS	5.5
1	A	890	SER	5.1
1	A	931	ALA	4.4
1	A	888	SER	4.4
1	A	889	SER	4.3
1	A	522	GLY	4.0
1	A	524	SER	3.6
1	A	886	PRO	3.4
1	A	39	LYS	3.1
1	A	545	LEU	3.0
1	A	527	ALA	2.9
1	A	673	GLN	2.6
1	A	422	LYS	2.6
1	A	891	SER	2.5
1	A	901	HIS	2.5
1	A	206	GLU	2.2
1	A	694	ASN	2.2
1	A	616	LYS	2.1

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, 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	LLDF	B-factors(Å^2)	Q<0.9
6	NAG	A	1045	14/15	0.62	0.34	19.51	40,48,53,54	0
6	NAG	A	1044	14/15	0.82	0.17	3.79	25,35,42,43	0
3	MAN	A	1031	11/12	0.97	0.11	3.10	15,17,20,21	0
3	NAG	A	1026	14/15	0.98	0.06	0.06	7,9,14,15	0
4	MAN	A	1039	11/12	0.97	0.07	-0.08	13,15,19,22	0
3	MAN	A	1029	11/12	0.98	0.06	-0.17	9,10,17,27	0
4	NAG	A	1032	14/15	0.96	0.07	-0.22	11,14,20,29	0
3	NAG	A	1025	14/15	0.99	0.05	-1.07	8,10,19,20	0
4	MAN	A	1040	11/12	0.94	0.09	-	13,16,25,25	0
4	MAN	A	1037	11/12	0.72	0.34	-	46,48,52,55	0
4	BMA	A	1034	11/12	0.97	0.06	-	12,15,17,18	0
3	MAN	A	1028	11/12	0.99	0.05	-	7,9,12,18	0
3	MAN	A	1030	11/12	0.92	0.23	-	22,27,35,41	0
3	BMA	A	1027	11/12	0.98	0.06	-	8,9,14,14	0
4	NAG	A	1033	14/15	0.94	0.10	-	10,16,26,26	0
4	MAN	A	1036	11/12	0.68	0.32	-	38,46,49,50	0
4	GLC	A	1041	11/12	0.81	0.16	-	27,30,32,35	0
4	MAN	A	1038	11/12	0.94	0.09	-	15,18,23,28	0
4	MAN	A	1035	11/12	0.87	0.15	-	24,30,37,41	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, 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	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	1043	14/15	0.92	0.20	6.70	22,27,34,41	0
5	NAG	A	1042	14/15	0.76	0.26	6.04	32,39,45,49	0
2	GAL	A	1024	12/12	0.99	0.05	-0.33	5,7,10,14	0

6.5 Other polymers (i)

There are no such residues in this entry.