



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 04:33 PM GMT

PDB ID : 4IUG  
Title : Crystal structure of beta-galactosidase from *Aspergillus oryzae* in complex with galactose  
Authors : Maksimainen, M.; Rouvinen, J.  
Deposited on : 2013-01-21  
Resolution : 2.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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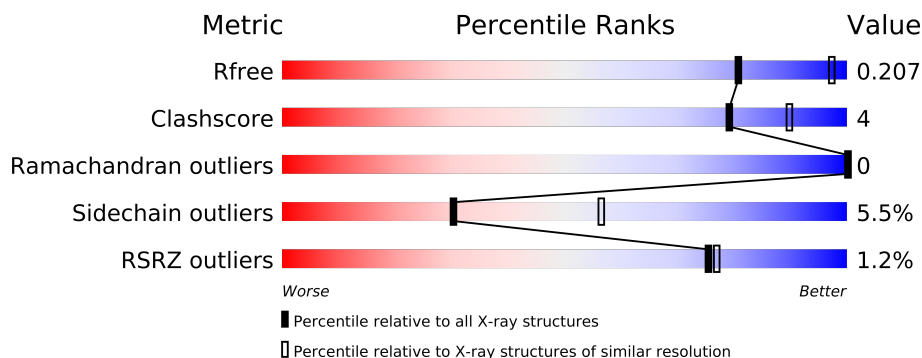
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1005	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	M6D	A	1163	-	X
2	CD	A	1101	-	X
3	GAL	A	1130	-	X
5	NAG	A	1136	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8208 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

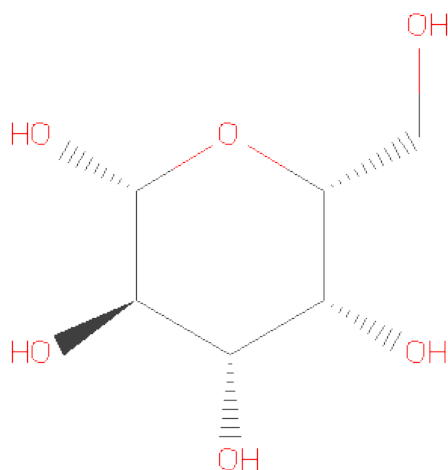
- Molecule 1 is a protein called Beta-galactosidase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	957	Total	C	N	O	P	S	0	0	0
			7441	4752	1227	1452	1	9			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	Cd	0	0
			29	29		

- Molecule 3 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

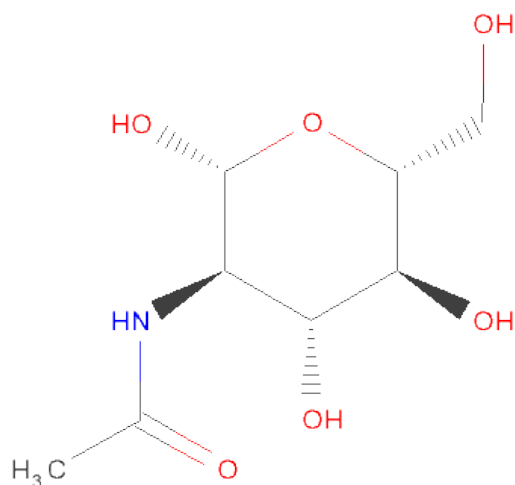


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		

- 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		

- Molecule 6 is a polymer of unknown type called SUGAR (7-MER).

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

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

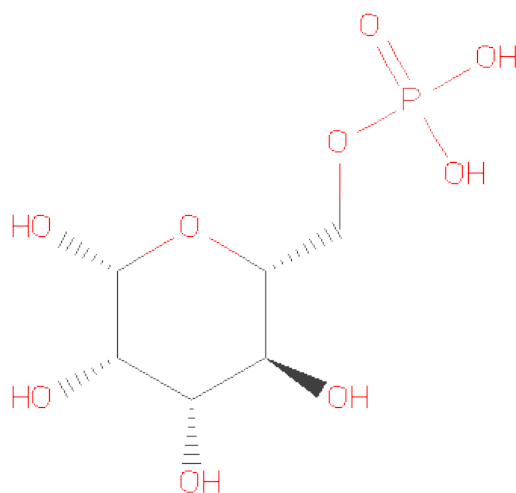
- Molecule 8 is a polymer of unknown type called SUGAR (10-MER).

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

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	5	Total	C	N	O	0	0
			62	34	2	26		

- Molecule 10 is 6-O-PHOSPHONO-BETA-D-MANNOPYRANOSE (three-letter code: M6D) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	P	0	0
			15	6	8	1		

- Molecule 11 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is water.

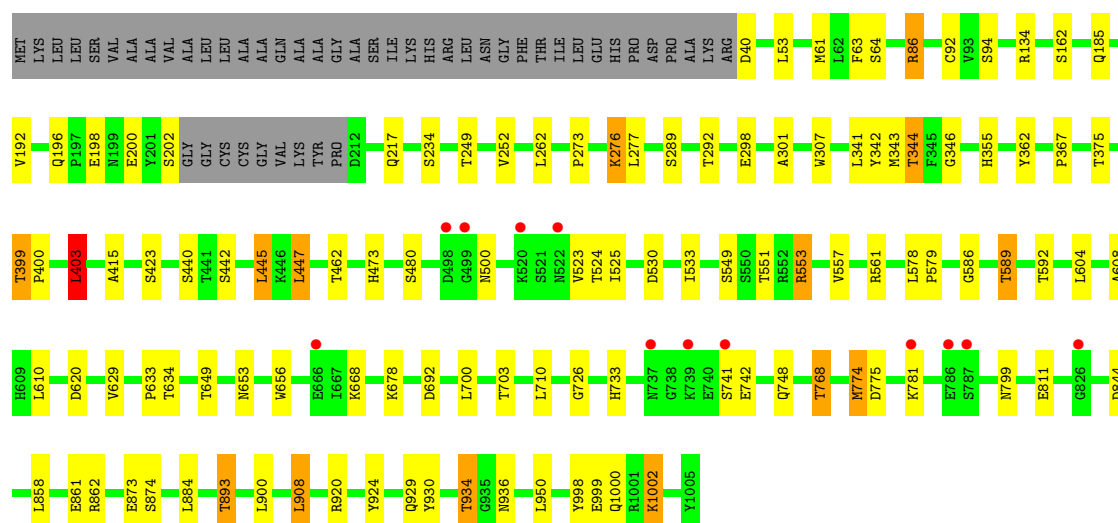
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	280	Total	O	0	0
			280	280		

### 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: Beta-galactosidase A

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.38Å 146.38Å 136.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.91 – 2.60 47.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.91-2.60) 99.9 (47.91-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.180 , 0.214 0.174 , 0.207	Depositor DCC
$R_{free}$ test set	2607 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 26.5	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 52147 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8208	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, SEP, CD, GAL, M6D, 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	0.44	0/7640	0.59	1/10408 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	LEU	CA-CB-CG	6.28	129.75	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7441	0	7109	52	0
2	A	29	0	0	0	0
3	A	12	0	12	2	0
4	A	61	0	52	1	0
5	A	14	0	13	0	0
6	A	83	0	70	1	0
7	A	56	0	50	0	0
8	A	116	0	97	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	62	0	52	0	0
10	A	15	0	8	1	0
11	A	39	0	33	1	0
12	A	280	0	0	1	0
All	All	8208	0	7496	54	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 54 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:134:ARG:NH2	1:A:298:GLU:OE2	2.20	0.70
1:A:589:THR:HG22	1:A:592:THR:H	1.61	0.67
1:A:861:GLU:OE2	1:A:924:TYR:OH	2.14	0.65
1:A:298:GLU:OE1	3:A:1130:GAL:H1	1.95	0.65
1:A:134:ARG:HG2	1:A:196:GLN:HB3	1.85	0.58

There are no symmetry-related clashes.

## 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	952/1005 (95%)	907 (95%)	45 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	794/828 (96%)	750 (94%)	44 (6%)	30 56

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	THR
1	A	634	THR
1	A	930	TYR
1	A	551	THR
1	A	578	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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	$\# Z  > 2$
1	SEP	A	569	1	9,9,10	6.05	5 (55%)	10,12,14	1.92	3 (30%)

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
1	SEP	A	569	1	-	0/6/8/10	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	SEP	O-C	17.05	1.23	1.11
1	A	569	SEP	CA-C	3.77	1.55	1.48
1	A	569	SEP	P-O1P	3.10	1.61	1.51
1	A	569	SEP	P-O3P	2.25	1.62	1.54
1	A	569	SEP	P-OG	2.22	1.67	1.60

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	SEP	C-CA-N	-3.96	109.87	113.83
1	A	569	SEP	OG-CB-CA	3.30	113.36	108.69
1	A	569	SEP	O3P-P-OG	2.04	112.27	106.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

34 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$
4	NAG	A	1131	1,4	12,14,15	0.88	1 (8%)	15,19,21	0.81	0
4	NAG	A	1132	4	12,14,15	0.88	1 (8%)	15,19,21	1.92	3 (20%)
4	BMA	A	1133	4	10,11,12	1.74	3 (30%)	11,15,17	1.74	3 (27%)
4	MAN	A	1134	4	10,11,12	0.97	1 (10%)	11,15,17	1.00	0
4	MAN	A	1135	4	10,11,12	0.72	0	11,15,17	0.96	1 (9%)
6	NAG	A	1137	1,6	12,14,15	0.74	1 (8%)	15,19,21	1.50	2 (13%)
6	NAG	A	1138	6	12,14,15	0.73	0	15,19,21	0.81	1 (6%)
6	BMA	A	1139	6	10,11,12	1.92	2 (20%)	11,15,17	3.09	7 (63%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	A	1140	6	10,11,12	0.83	1 (10%)	11,15,17	1.18	1 (9%)
6	MAN	A	1141	6	10,11,12	0.81	1 (10%)	11,15,17	1.10	1 (9%)
6	MAN	A	1142	6	10,11,12	0.86	0	11,15,17	1.15	0
6	MAN	A	1143	6	10,11,12	0.75	0	11,15,17	1.57	1 (9%)
7	NAG	A	1144	1,7	12,14,15	0.64	0	15,19,21	1.33	2 (13%)
7	NAG	A	1145	7	12,14,15	0.59	0	15,19,21	1.09	1 (6%)
7	NAG	A	1146	1,7	12,14,15	0.62	0	15,19,21	0.90	0
7	NAG	A	1147	7	12,14,15	0.61	0	15,19,21	1.00	0
8	NAG	A	1148	1,8	12,14,15	0.92	1 (8%)	15,19,21	0.89	0
8	NAG	A	1149	8	12,14,15	0.85	1 (8%)	15,19,21	0.92	1 (6%)
8	BMA	A	1150	8	10,11,12	1.89	3 (30%)	11,15,17	1.23	1 (9%)
8	MAN	A	1151	8	10,11,12	0.78	0	11,15,17	2.47	5 (45%)
8	MAN	A	1152	8	10,11,12	0.66	0	11,15,17	1.65	1 (9%)
8	MAN	A	1153	8	10,11,12	0.80	1 (10%)	11,15,17	1.09	0
8	MAN	A	1154	8	10,11,12	0.65	0	11,15,17	0.79	0
8	MAN	A	1155	8	10,11,12	0.69	0	11,15,17	1.54	2 (18%)
8	MAN	A	1156	8	10,11,12	0.54	0	11,15,17	1.48	1 (9%)
8	MAN	A	1157	8	10,11,12	0.72	0	11,15,17	1.93	3 (27%)
9	NAG	A	1158	9	12,14,15	0.72	0	15,19,21	1.40	3 (20%)
9	BMA	A	1159	9	10,11,12	0.96	1 (10%)	11,15,17	2.17	3 (27%)
9	BMA	A	1160	9,2	10,11,12	1.09	1 (10%)	11,15,17	2.00	3 (27%)
9	NAG	A	1161	9,10	12,14,15	0.77	1 (8%)	15,19,21	0.99	1 (6%)
9	BMA	A	1162	9	12,12,12	1.49	2 (16%)	17,17,17	1.74	5 (29%)
11	NAG	A	1164	11,10	12,14,15	0.69	1 (8%)	15,19,21	1.30	1 (6%)
11	BMA	A	1165	11,2	10,11,12	1.24	1 (10%)	11,15,17	1.85	3 (27%)
11	NAG	A	1166	11	12,14,15	0.84	1 (8%)	15,19,21	1.75	5 (33%)

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	NAG	A	1131	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1132	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1133	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1134	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	1135	4	-	0/2/19/22	0/1/1/1
6	NAG	A	1137	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1138	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1139	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1140	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1141	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1142	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1143	6	-	0/2/19/22	0/1/1/1
7	NAG	A	1144	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1145	7	-	0/6/23/26	0/1/1/1
7	NAG	A	1146	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1147	7	-	0/6/23/26	0/1/1/1
8	NAG	A	1148	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	1149	8	-	0/6/23/26	0/1/1/1
8	BMA	A	1150	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1151	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1152	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1153	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1154	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1155	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1156	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1157	8	-	0/2/19/22	0/1/1/1
9	NAG	A	1158	9	-	0/6/23/26	0/1/1/1
9	BMA	A	1159	9	-	0/2/19/22	0/1/1/1
9	BMA	A	1160	9,2	-	0/2/19/22	0/1/1/1
9	NAG	A	1161	9,10	-	0/6/23/26	0/1/1/1
9	BMA	A	1162	9	-	0/2/22/22	0/1/1/1
11	NAG	A	1164	11,10	-	0/6/23/26	0/1/1/1
11	BMA	A	1165	11,2	-	0/2/19/22	0/1/1/1
11	NAG	A	1166	11	-	0/6/23/26	0/1/1/1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1139	BMA	C4-C3	-4.35	1.40	1.52
8	A	1150	BMA	C4-C3	-4.09	1.41	1.52
4	A	1133	BMA	C4-C3	-3.73	1.42	1.52
9	A	1162	BMA	C4-C3	-3.67	1.42	1.52
11	A	1165	BMA	O5-C5	-3.13	1.39	1.45

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1139	BMA	C6-C5-C4	-5.73	99.16	113.00
9	A	1160	BMA	C4-C3-C2	5.18	117.45	110.50
8	A	1151	MAN	O5-C5-C4	5.16	117.20	110.65
9	A	1159	BMA	C4-C3-C2	5.09	117.34	110.50
4	A	1132	NAG	C2-N2-C7	-4.91	114.85	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

Of 32 ligands modelled in this entry, 29 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GAL	A	1130	-	12,12,12	0.87	1 (8%)	17,17,17	1.15	1 (5%)
5	NAG	A	1136	1	12,14,15	0.69	0	15,19,21	1.24	3 (20%)
10	M6D	A	1163	9,11	14,15,16	1.16	2 (14%)	18,22,24	0.87	1 (5%)

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	GAL	A	1130	-	-	0/2/22/22	0/1/1/1
5	NAG	A	1136	1	-	0/6/23/26	0/1/1/1
10	M6D	A	1163	9,11	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1163	M6D	O4-C4	-2.52	1.36	1.43
10	A	1163	M6D	C4-C5	-2.13	1.48	1.53
3	A	1130	GAL	O2-C2	-2.10	1.37	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1136	NAG	C2-N2-C7	-2.73	118.50	123.09
5	A	1136	NAG	O5-C5-C6	2.31	109.40	106.98
10	A	1163	M6D	O5-C5-C6	2.21	109.39	107.07
3	A	1130	GAL	O5-C5-C4	-2.18	105.72	109.76
5	A	1136	NAG	C3-C4-C5	-2.01	106.61	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	957/1005 (95%)	-0.38	12 (1%) 74 75	24, 32, 47, 64	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	ASP	4.5
1	A	739	LYS	3.4
1	A	499	GLY	3.2
1	A	781	LYS	2.8
1	A	737	ASN	2.7

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

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	569	10/11	0.13	-0.60	32,34,39,41	0

### 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. 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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	MAN	A	1157	11/12	0.22	29.86	48,50,51,52	0
9	BMA	A	1162	12/12	0.24	5.82	50,55,60,65	0
8	MAN	A	1156	11/12	0.24	3.19	38,41,46,49	0
7	NAG	A	1145	14/15	0.29	2.95	50,58,62,62	0
8	MAN	A	1151	11/12	0.13	2.87	37,41,43,44	0
11	NAG	A	1164	14/15	0.15	2.00	51,52,54,55	0
11	NAG	A	1166	14/15	0.16	1.28	45,50,51,52	0
9	BMA	A	1160	11/12	0.14	0.95	42,44,47,48	0
7	NAG	A	1146	14/15	0.13	0.88	36,43,50,52	0
4	MAN	A	1134	11/12	0.12	0.39	38,41,44,47	0
6	MAN	A	1143	11/12	0.20	0.34	49,54,57,57	0
9	BMA	A	1159	11/12	0.10	-0.25	35,37,39,42	0
7	NAG	A	1144	14/15	0.15	-0.30	42,46,51,52	0
8	NAG	A	1149	14/15	0.13	-0.42	28,31,35,35	0
6	MAN	A	1140	11/12	0.12	-0.49	30,32,34,34	0
8	MAN	A	1153	11/12	0.10	-0.59	32,33,34,38	0
9	NAG	A	1158	14/15	0.10	-0.62	36,39,41,42	0
8	MAN	A	1155	11/12	0.11	-0.68	31,32,34,35	0
8	MAN	A	1154	11/12	0.11	-0.70	31,33,34,35	0
8	BMA	A	1150	11/12	0.10	-0.94	30,31,33,37	0
4	NAG	A	1131	14/15	0.11	-0.96	25,28,31,33	0
4	NAG	A	1132	14/15	0.10	-0.96	30,32,34,37	0
6	NAG	A	1137	14/15	0.09	-0.99	26,29,30,30	0
9	NAG	A	1161	14/15	0.09	-1.25	36,40,42,43	0
8	NAG	A	1148	14/15	0.10	-1.26	27,30,35,37	0
6	MAN	A	1141	11/12	0.09	-1.36	31,32,35,38	0
4	BMA	A	1133	11/12	0.09	-1.56	35,38,39,39	0
11	BMA	A	1165	11/12	0.11	-1.77	51,53,53,54	0
8	MAN	A	1152	11/12	0.07	-2.02	31,32,33,34	0
6	NAG	A	1138	14/15	0.09	-2.36	27,29,30,30	0
6	BMA	A	1139	11/12	0.11	-2.83	29,32,35,35	0
6	MAN	A	1142	11/12	0.09	-3.44	35,36,41,45	0
4	MAN	A	1135	11/12	0.30	-	50,53,56,56	0
7	NAG	A	1147	14/15	0.28	-	55,58,61,63	0

## 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. 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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	1136	14/15	0.36	10.02	42,47,50,50	0
10	M6D	A	1163	15/16	0.20	5.27	47,52,59,60	0
2	CD	A	1101	1/1	0.17	3.67	104,104,104,104	0
3	GAL	A	1130	12/12	0.19	2.89	27,30,34,35	0
2	CD	A	1117	1/1	0.18	1.06	119,119,119,119	0
2	CD	A	1127	1/1	0.18	0.84	113,113,113,113	0
2	CD	A	1105	1/1	0.11	-0.07	42,42,42,42	0
2	CD	A	1123	1/1	0.15	-0.27	105,105,105,105	0
2	CD	A	1121	1/1	0.13	-0.33	104,104,104,104	0
2	CD	A	1104	1/1	0.10	-0.53	42,42,42,42	0
2	CD	A	1116	1/1	0.20	-0.81	113,113,113,113	0
2	CD	A	1124	1/1	0.11	-0.86	91,91,91,91	0
2	CD	A	1126	1/1	0.16	-1.09	110,110,110,110	0
2	CD	A	1129	1/1	0.06	-1.60	108,108,108,108	0
2	CD	A	1106	1/1	0.02	-1.82	85,85,85,85	0
2	CD	A	1115	1/1	0.04	-2.17	78,78,78,78	0
2	CD	A	1109	1/1	0.14	-2.52	95,95,95,95	0
2	CD	A	1120	1/1	0.07	-2.62	98,98,98,98	0
2	CD	A	1119	1/1	0.06	-2.67	88,88,88,88	0
2	CD	A	1118	1/1	0.10	-3.15	110,110,110,110	0
2	CD	A	1103	1/1	0.05	-3.38	47,47,47,47	0
2	CD	A	1110	1/1	0.05	-3.82	91,91,91,91	0
2	CD	A	1108	1/1	0.06	-4.03	70,70,70,70	0
2	CD	A	1122	1/1	0.07	-4.14	95,95,95,95	0
2	CD	A	1102	1/1	0.09	-4.26	49,49,49,49	0
2	CD	A	1112	1/1	0.08	-4.30	96,96,96,96	0
2	CD	A	1114	1/1	0.08	-4.42	84,84,84,84	0
2	CD	A	1128	1/1	0.06	-7.64	73,73,73,73	0
2	CD	A	1125	1/1	0.04	-8.41	89,89,89,89	0
2	CD	A	1113	1/1	0.08	-12.43	94,94,94,94	0
2	CD	A	1111	1/1	0.30	-	108,108,108,108	0
2	CD	A	1107	1/1	0.06	-	97,97,97,97	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.