



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:48 PM GMT

PDB ID : 3S5Z  
Title : Pharmacological Chaperoning in Human alpha-Galactosidase  
Authors : Guce, A.I.; Clark, N.E.; Garman, S.C.  
Deposited on : 2011-05-23  
Resolution : 2.00 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](mailto: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.

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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 : 1.7 (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

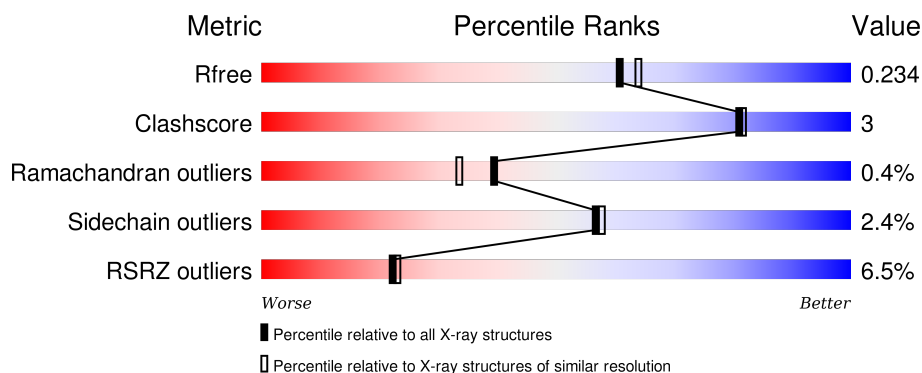
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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  $\geq 3$ , 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	398	<div> <div>7%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	B	398	<div> <div>6%</div> <div>86%</div> <div>11%</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	XYP	A	698	X	-	-	-
5	GAL	A	804	-	-	-	X
7	XYP	B	698	X	-	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6930 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 A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	5	0
			3143	2000	536	578	29			
1	B	390	Total	C	N	O	S	0	6	0
			3157	2008	540	579	30			

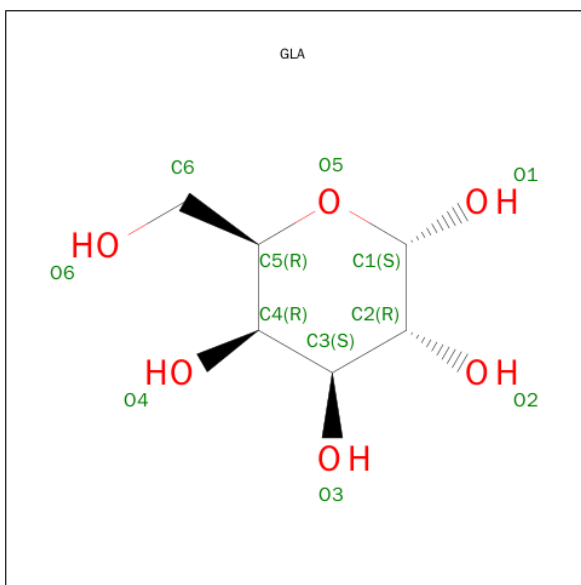
- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	7	Total	C	N	O	0	0
			80	45	2	33		

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

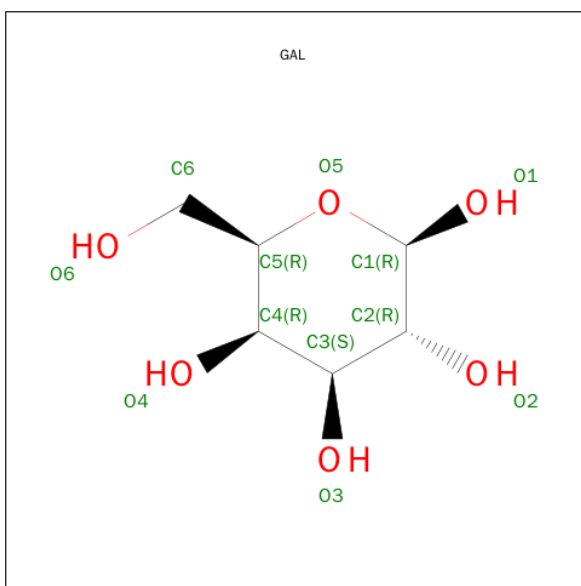
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is SUGAR (ALPHA D-GALACTOSE) (three-letter code: GLA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



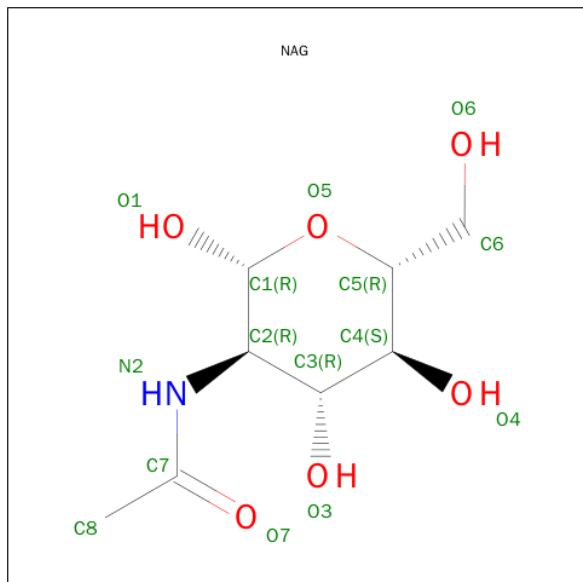
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		

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



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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	5	Total	C	N	O	0	0
			59	33	2	24		

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		

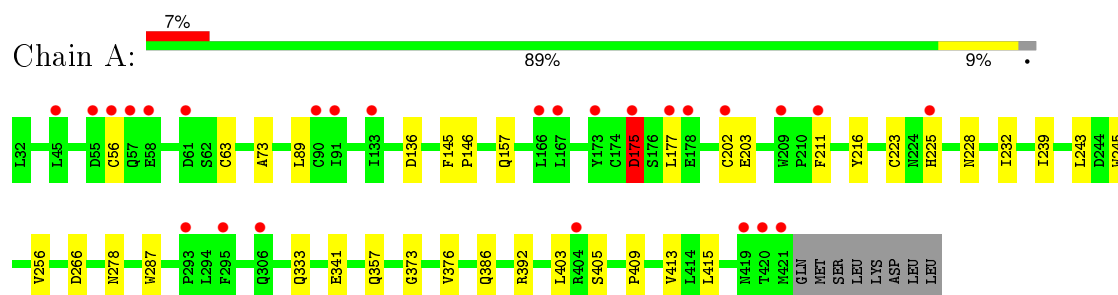
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	175	Total	O	0	0
			175	175		
10	B	161	Total	O	0	0
			161	161		

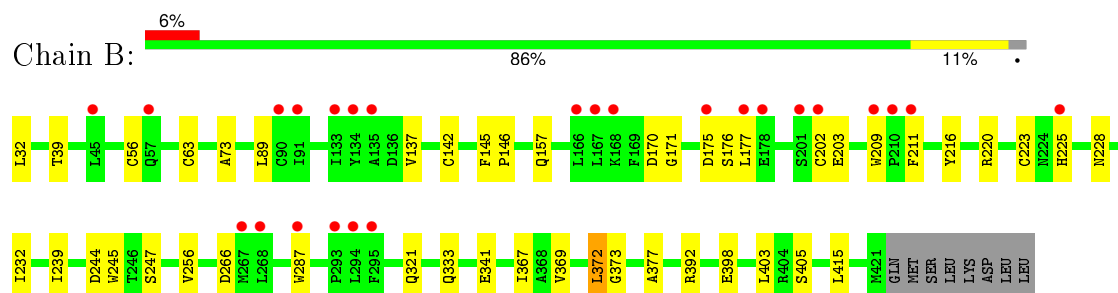
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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 A



#### • Molecule 1: Alpha-galactosidase A





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.31Å 140.61Å 182.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.44 – 2.00 30.44 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.44-2.00) 99.3 (30.44-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.210 , 0.234 0.213 , 0.234	Depositor DCC
$R_{free}$ test set	3867 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 77025 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, GOL, BMA, NAG, GLA, GAL, FUC, 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	0.49	3/3243 (0.1%)	0.62	3/4403 (0.1%)
1	B	0.46	3/3255 (0.1%)	0.60	2/4418 (0.0%)
All	All	0.47	6/6498 (0.1%)	0.61	5/8821 (0.1%)

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
2	A	3	0
7	B	3	0
All	All	6	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	341	GLU	CD-OE2	-5.71	1.19	1.25
1	B	341	GLU	CD-OE1	-5.65	1.19	1.25
1	A	341	GLU	CD-OE1	-5.25	1.19	1.25
1	A	203	GLU	CD-OE2	-5.23	1.19	1.25
1	B	203	GLU	CD-OE2	-5.12	1.20	1.25
1	A	341	GLU	CD-OE2	-5.08	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	GLU	OE1-CD-OE2	-7.69	114.07	123.30
1	A	203	GLU	OE1-CD-OE2	-6.76	115.19	123.30
1	A	341	GLU	OE1-CD-OE2	-6.64	115.33	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	GLU	OE1-CD-OE2	-6.08	116.00	123.30
1	A	136	ASP	CB-CG-OD2	5.22	123.00	118.30

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	698	XYP	C4B,C2B,C3B
7	B	698	XYP	C4B,C2B,C3B

There are no planarity outliers.

## 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	3143	0	2996	21	0
1	B	3157	0	3013	21	2
2	A	80	0	67	0	0
3	A	38	0	34	0	0
4	A	12	0	12	0	0
4	B	12	0	12	0	0
5	A	12	0	12	0	0
5	B	12	0	12	0	0
6	B	14	0	13	0	0
7	B	59	0	49	0	0
8	B	49	0	43	0	0
9	B	6	0	8	0	0
10	A	175	0	0	6	0
10	B	161	0	0	1	2
All	All	6930	0	6271	42	2

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:413:VAL:CG1	10:A:454:HOH:O	2.25	0.84
1:B:216:TYR:HB3	1:B:256:VAL:HG11	1.60	0.84
1:A:413:VAL:HG13	10:A:454:HOH:O	1.81	0.80
1:A:216:TYR:HB3	1:A:256:VAL:HG11	1.76	0.67
1:A:413:VAL:HG12	10:A:454:HOH:O	1.93	0.64
1:A:403:LEU:HD21	1:A:415:LEU:CD1	2.28	0.62
1:B:177:LEU:HD11	1:B:211:PHE:HB2	1.81	0.61
1:B:403:LEU:HD21	1:B:415:LEU:CD1	2.31	0.61
1:A:177:LEU:HD11	1:A:211:PHE:HB2	1.86	0.57
1:B:177:LEU:HD11	1:B:211:PHE:CB	2.36	0.55
1:B:403:LEU:HD21	1:B:415:LEU:HD13	1.88	0.55
1:B:39:THR:OG1	1:B:321:GLN:NE2	2.40	0.54
1:A:403:LEU:HD21	1:A:415:LEU:HD13	1.90	0.52
1:A:386:GLN:HG3	10:A:454:HOH:O	2.12	0.48
1:B:373:GLY:HA3	1:B:377:ALA:HB2	1.96	0.48
1:B:369:VAL:HA	1:B:372:LEU:HD22	1.96	0.47
1:B:232:ILE:HD11	1:B:239:ILE:CD1	2.45	0.47
1:A:278:ASN:ND2	10:A:561:HOH:O	2.30	0.47
1:A:202[B]:CYS:SG	1:A:223:CYS:SG	3.12	0.46
1:A:373:GLY:O	1:A:376:VAL:HG22	2.16	0.46
1:B:56[B]:CYS:HB3	1:B:63:CYS:SG	2.55	0.46
1:A:175:ASP:N	1:A:175:ASP:OD1	2.48	0.46
1:A:232:ILE:HD11	1:A:239:ILE:CD1	2.46	0.46
1:A:403:LEU:HD21	1:A:415:LEU:HD11	1.98	0.46
1:B:367:ILE:HD13	1:B:372:LEU:HD11	2.00	0.44
1:A:56[B]:CYS:HB3	1:A:63:CYS:SG	2.57	0.44
1:B:228:ASN:HB3	1:B:245:TRP:CH2	2.54	0.43
1:A:357:GLN:O	1:A:409:PRO:HB3	2.19	0.43
1:A:415:LEU:HD23	10:A:454:HOH:O	2.19	0.42
1:A:145:PHE:HB3	1:A:146:PRO:CD	2.49	0.42
1:B:209:TRP:HA	10:B:523:HOH:O	2.19	0.42
1:B:73:ALA:HB2	1:B:89:LEU:HD22	2.02	0.41
1:B:145:PHE:HB3	1:B:146:PRO:CD	2.48	0.41
1:A:243:LEU:HA	1:A:243:LEU:HD23	1.86	0.41
1:B:73:ALA:HB2	1:B:89:LEU:CD2	2.50	0.41
1:B:175:ASP:N	1:B:175:ASP:OD2	2.54	0.41
1:B:202[B]:CYS:SG	1:B:223:CYS:SG	3.15	0.41
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.56	0.41
1:A:73:ALA:HB2	1:A:89:LEU:HD22	2.02	0.41
1:B:137:VAL:HG12	1:B:171:GLY:HA2	2.03	0.40
1:B:32:LEU:N	1:B:220:ARG:O	2.53	0.40
1:B:142[A]:CYS:SG	1:B:170:ASP:OD2	2.80	0.40

All (2) 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:247:SER:N	10:B:507:HOH:O[3_655]	1.93	0.27
1:B:244:ASP:O	10:B:507:HOH:O[3_655]	1.96	0.24

## 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	393/398 (99%)	380 (97%)	11 (3%)	2 (0%)	34	26
1	B	394/398 (99%)	381 (97%)	12 (3%)	1 (0%)	46	41
All	All	787/796 (99%)	761 (97%)	23 (3%)	3 (0%)	39	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ASP
1	B	266	ASP
1	A	175	ASP

### 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	336/339 (99%)	329 (98%)	7 (2%)	61	63
1	B	337/339 (99%)	328 (97%)	9 (3%)	52	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	673/678 (99%)	657 (98%)	16 (2%)	57 58

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	175	ASP
1	A	225	HIS
1	A	287	TRP
1	A	333	GLN
1	A	392	ARG
1	A	405	SER
1	B	157	GLN
1	B	176	SER
1	B	225	HIS
1	B	287	TRP
1	B	333	GLN
1	B	372	LEU
1	B	392	ARG
1	B	398	GLU
1	B	405	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	ASN
1	A	416	GLN
1	B	228	ASN
1	B	321	GLN
1	B	416	GLN

### 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 ⓘ

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
2	NAG	A	692	1,2	14,14,15	0.48	0	15,19,21	1.49	1 (6%)
2	NAG	A	693	2	14,14,15	0.60	0	15,19,21	0.80	0
2	BMA	A	694	2	11,11,12	0.40	0	14,15,17	1.36	2 (14%)
2	MAN	A	695	2	11,11,12	0.56	0	14,15,17	0.66	0
2	MAN	A	696	2	11,11,12	0.56	0	14,15,17	0.92	1 (7%)
2	FUC	A	697	2	10,10,11	0.55	0	14,14,16	1.10	2 (14%)
2	XYP	A	698	2	9,9,10	1.29	1 (11%)	12,12,14	0.62	0
3	NAG	A	715	1,3	14,14,15	0.52	0	15,19,21	0.70	0
3	NAG	A	716	3	14,14,15	0.49	0	15,19,21	0.84	0
3	FUC	A	720	3	10,10,11	0.53	0	14,14,16	0.89	2 (14%)
7	NAG	B	692	1,7	14,14,15	0.38	0	15,19,21	1.48	2 (13%)
7	NAG	B	693	7	14,14,15	0.54	0	15,19,21	1.05	1 (6%)
7	BMA	B	694	7	11,11,12	0.54	0	14,15,17	1.55	2 (14%)
7	MAN	B	695	7	11,11,12	0.54	0	14,15,17	1.06	1 (7%)
7	XYP	B	698	7	9,9,10	1.27	1 (11%)	12,12,14	0.82	0
8	NAG	B	715	1,8	14,14,15	0.55	0	15,19,21	1.18	2 (13%)
8	NAG	B	716	8	14,14,15	0.62	0	15,19,21	0.98	1 (6%)
8	BMA	B	717	8	11,11,12	0.38	0	14,15,17	0.69	0
8	FUC	B	720	8	10,10,11	0.63	0	14,14,16	1.08	1 (7%)

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	692	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	693	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	A	694	2	-	0/2/19/22	0/1/1/1
2	MAN	A	695	2	-	0/2/19/22	0/1/1/1
2	MAN	A	696	2	-	0/2/19/22	0/1/1/1
2	FUC	A	697	2	-	0/0/17/20	0/1/1/1
2	XYP	A	698	2	3/3/3/4	0/0/14/17	0/1/1/1
3	NAG	A	715	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	716	3	-	0/6/23/26	0/1/1/1
3	FUC	A	720	3	-	0/0/17/20	0/1/1/1
7	NAG	B	692	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	693	7	-	0/6/23/26	0/1/1/1
7	BMA	B	694	7	-	0/2/19/22	0/1/1/1
7	MAN	B	695	7	-	0/2/19/22	0/1/1/1
7	XYP	B	698	7	3/3/3/4	0/0/14/17	0/1/1/1
8	NAG	B	715	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	716	8	-	0/6/23/26	0/1/1/1
8	BMA	B	717	8	-	0/2/19/22	0/1/1/1
8	FUC	B	720	8	-	0/0/17/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	698	XYP	O5B-C5B	-3.48	1.36	1.42
7	B	698	XYP	O5B-C5B	-3.40	1.36	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	694	BMA	O5-C1-C2	-2.71	106.47	110.86
2	A	694	BMA	C1-C2-C3	-2.46	106.63	109.54
7	B	692	NAG	C6-C5-C4	-2.32	107.30	113.02
3	A	720	FUC	C1-O5-C5	2.01	115.48	112.38
2	A	697	FUC	C1-C2-C3	2.09	112.01	109.54
8	B	715	NAG	O3-C3-C2	2.12	113.32	109.11
3	A	720	FUC	O5-C5-C6	2.12	109.64	106.13
8	B	720	FUC	C1-O5-C5	2.14	115.68	112.38
2	A	694	BMA	C3-C4-C5	2.17	113.98	110.20
8	B	716	NAG	C4-C3-C2	2.27	114.75	111.23
8	B	715	NAG	C2-N2-C7	2.52	126.28	123.04
2	A	696	MAN	C1-C2-C3	2.53	112.54	109.54
2	A	697	FUC	C1-O5-C5	2.60	116.40	112.38
7	B	695	MAN	C1-O5-C5	2.76	115.75	112.25
7	B	693	NAG	C1-O5-C5	3.12	116.20	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	694	BMA	C3-C4-C5	3.32	115.99	110.20
2	A	692	NAG	C1-O5-C5	4.43	117.87	112.25
7	B	692	NAG	C1-O5-C5	4.77	118.30	112.25

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	698	XYP	C4B
2	A	698	XYP	C2B
2	A	698	XYP	C3B
7	B	698	XYP	C4B
7	B	698	XYP	C2B
7	B	698	XYP	C3B

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
4	GLA	A	801	-	12,12,12	0.47	0	17,17,17	0.94	1 (5%)
5	GAL	A	804	-	12,12,12	0.48	0	17,17,17	0.54	0
9	GOL	B	1001	-	5,5,5	0.33	0	5,5,5	0.30	0
6	NAG	B	639	1	14,14,15	0.53	0	15,19,21	0.79	0
4	GLA	B	802	-	12,12,12	0.51	0	17,17,17	0.93	0
5	GAL	B	803	-	12,12,12	0.43	0	17,17,17	0.61	0

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	GLA	A	801	-	-	0/2/22/22	0/1/1/1
5	GAL	A	804	-	-	0/2/22/22	0/1/1/1
9	GOL	B	1001	-	-	0/4/4/4	0/0/0/0
6	NAG	B	639	1	-	0/6/23/26	0/1/1/1
4	GLA	B	802	-	-	0/2/22/22	0/1/1/1
5	GAL	B	803	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	GLA	C1-O5-C5	2.09	117.34	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<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	390/398 (97%)	0.16	26 (6%) 21 22	17, 36, 63, 105	0
1	B	390/398 (97%)	0.19	25 (6%) 23 24	23, 36, 60, 88	0
All	All	780/796 (97%)	0.18	51 (6%) 22 23	17, 36, 62, 105	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	TRP	6.7
1	B	211	PHE	6.0
1	B	210	PRO	6.0
1	A	211	PHE	5.2
1	B	295	PHE	5.0
1	B	167	LEU	4.2
1	A	56[A]	CYS	3.7
1	A	419	ASN	3.6
1	B	133	ILE	3.5
1	A	421	MET	3.4
1	B	45	LEU	3.4
1	A	175	ASP	3.3
1	A	91	ILE	3.3
1	B	175	ASP	3.3
1	B	201	SER	3.2
1	A	295	PHE	3.2
1	B	91	ILE	3.2
1	A	57	GLN	3.1
1	B	166	LEU	3.0
1	B	178	GLU	2.9
1	A	133	ILE	2.9
1	A	45	LEU	2.9
1	A	177	LEU	2.9
1	A	58	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	178	GLU	2.8
1	B	267	MET	2.7
1	B	57	GLN	2.6
1	A	420	THR	2.5
1	A	202[A]	CYS	2.5
1	B	293	PRO	2.5
1	B	168	LYS	2.4
1	B	294	LEU	2.4
1	A	225	HIS	2.3
1	A	293	PRO	2.3
1	A	166	LEU	2.3
1	B	268	LEU	2.3
1	A	167	LEU	2.3
1	B	135	ALA	2.2
1	B	134	TYR	2.2
1	A	90	CYS	2.2
1	A	55	ASP	2.2
1	B	202[A]	CYS	2.2
1	B	287	TRP	2.2
1	A	404	ARG	2.2
1	B	177	LEU	2.1
1	A	173	TYR	2.1
1	A	306	GLN	2.1
1	A	209	TRP	2.1
1	B	225	HIS	2.0
1	A	61	ASP	2.0
1	B	90	CYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	692	14/15	0.93	0.14	1.67	36,44,56,60	0
7	NAG	B	692	14/15	0.92	0.16	0.55	39,47,54,64	0
8	NAG	B	715	14/15	0.95	0.13	0.50	28,39,50,51	0
3	FUC	A	720	10/11	0.87	0.39	-	90,94,96,97	0
2	XYP	A	698	9/10	0.74	0.28	-	64,81,86,87	0
7	BMA	B	694	11/12	0.80	0.31	-	90,97,101,107	0
7	XYP	B	698	9/10	0.77	0.37	-	95,98,101,104	0
2	MAN	A	695	11/12	0.78	0.33	-	81,89,92,95	0
2	MAN	A	696	11/12	0.78	0.39	-	96,101,107,107	0
3	NAG	A	715	14/15	0.86	0.28	-	68,78,93,95	0
7	NAG	B	693	14/15	0.84	0.26	-	55,69,78,85	0
8	FUC	B	720	10/11	0.95	0.19	-	37,40,47,47	0
8	BMA	B	717	11/12	0.70	0.27	-	82,87,91,92	0
3	NAG	A	716	14/15	0.88	0.34	-	81,93,96,99	0
8	NAG	B	716	14/15	0.92	0.20	-	40,49,67,75	0
2	FUC	A	697	10/11	0.79	0.60	-	82,90,93,94	0
2	BMA	A	694	11/12	0.86	0.27	-	78,88,99,103	0
7	MAN	B	695	11/12	0.77	0.32	-	80,91,94,95	0
2	NAG	A	693	14/15	0.93	0.17	-	47,60,71,73	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<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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GAL	A	804	12/12	0.89	0.23	3.12	56,60,65,69	0
9	GOL	B	1001	6/6	0.90	0.17	1.31	69,78,78,82	0
5	GAL	B	803	12/12	0.89	0.16	1.05	59,66,73,76	0
4	GLA	A	801	12/12	0.95	0.13	-0.35	29,34,39,46	0
4	GLA	B	802	12/12	0.95	0.11	-0.76	18,26,31,37	0
6	NAG	B	639	14/15	0.63	0.40	-	76,83,92,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.