W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Mar 1, 2014 – 04:25 AM GMT

PDB ID : 3HG3
Title : Human alpha-galactosidase catalytic mechanism 2. Substrate bound
Authors : Guce, A.I.; Clark, N.E.; Garman, S.C.
Deposited on : 2009-05-13
Resolution : 1.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html

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 (i)

The reported resolution of this entry is 1.90 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.
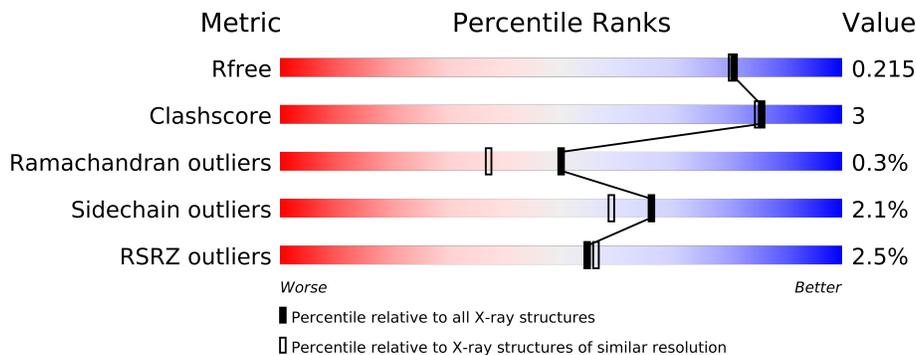
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. 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	404	
1	B	404	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	B	639	-	X
2	NAG	B	715	-	X
6	2PE	A	822	-	X
6	2PE	A	823	-	X
6	2PE	A	824	-	X
6	2PE	A	825	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 7537 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 Alpha-galactosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total 3204	C 2035	N 548	O 592	S 29	0	11	0
1	B	394	Total 3171	C 2020	N 542	O 582	S 27	0	6	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ALA	ASP	ENGINEERED	UNP P06280
A	430	HIS	-	EXPRESSION TAG	UNP P06280
A	431	HIS	-	EXPRESSION TAG	UNP P06280
A	432	HIS	-	EXPRESSION TAG	UNP P06280
A	433	HIS	-	EXPRESSION TAG	UNP P06280
A	434	HIS	-	EXPRESSION TAG	UNP P06280
A	435	HIS	-	EXPRESSION TAG	UNP P06280
B	170	ALA	ASP	ENGINEERED	UNP P06280
B	430	HIS	-	EXPRESSION TAG	UNP P06280
B	431	HIS	-	EXPRESSION TAG	UNP P06280
B	432	HIS	-	EXPRESSION TAG	UNP P06280
B	433	HIS	-	EXPRESSION TAG	UNP P06280
B	434	HIS	-	EXPRESSION TAG	UNP P06280
B	435	HIS	-	EXPRESSION TAG	UNP P06280

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
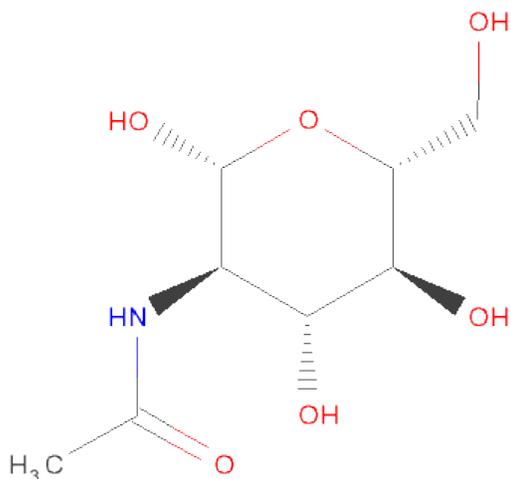
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

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

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ALA	ASP	ENGINEERED	UNP P06280
A	430	HIS	-	EXPRESSION TAG	UNP P06280
A	431	HIS	-	EXPRESSION TAG	UNP P06280
A	432	HIS	-	EXPRESSION TAG	UNP P06280
A	433	HIS	-	EXPRESSION TAG	UNP P06280
A	434	HIS	-	EXPRESSION TAG	UNP P06280
A	435	HIS	-	EXPRESSION TAG	UNP P06280
B	170	ALA	ASP	ENGINEERED	UNP P06280
B	430	HIS	-	EXPRESSION TAG	UNP P06280

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Chain	Residue	Modelled	Actual	Comment	Reference
B	431	HIS	-	EXPRESSION TAG	UNP P06280
B	432	HIS	-	EXPRESSION TAG	UNP P06280
B	433	HIS	-	EXPRESSION TAG	UNP P06280
B	434	HIS	-	EXPRESSION TAG	UNP P06280
B	435	HIS	-	EXPRESSION TAG	UNP P06280

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ALA	ASP	ENGINEERED	UNP P06280
A	430	HIS	-	EXPRESSION TAG	UNP P06280
A	431	HIS	-	EXPRESSION TAG	UNP P06280
A	432	HIS	-	EXPRESSION TAG	UNP P06280
A	433	HIS	-	EXPRESSION TAG	UNP P06280
A	434	HIS	-	EXPRESSION TAG	UNP P06280
A	435	HIS	-	EXPRESSION TAG	UNP P06280

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	2	23	12	11	0	0
5	B	2	23	12	11	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ALA	ASP	ENGINEERED	UNP P06280
A	430	HIS	-	EXPRESSION TAG	UNP P06280
A	431	HIS	-	EXPRESSION TAG	UNP P06280
A	432	HIS	-	EXPRESSION TAG	UNP P06280
A	433	HIS	-	EXPRESSION TAG	UNP P06280
A	434	HIS	-	EXPRESSION TAG	UNP P06280
A	435	HIS	-	EXPRESSION TAG	UNP P06280
B	170	ALA	ASP	ENGINEERED	UNP P06280

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Chain	Residue	Modelled	Actual	Comment	Reference
B	430	HIS	-	EXPRESSION TAG	UNP P06280
B	431	HIS	-	EXPRESSION TAG	UNP P06280
B	432	HIS	-	EXPRESSION TAG	UNP P06280
B	433	HIS	-	EXPRESSION TAG	UNP P06280
B	434	HIS	-	EXPRESSION TAG	UNP P06280
B	435	HIS	-	EXPRESSION TAG	UNP P06280

- Molecule 6 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).
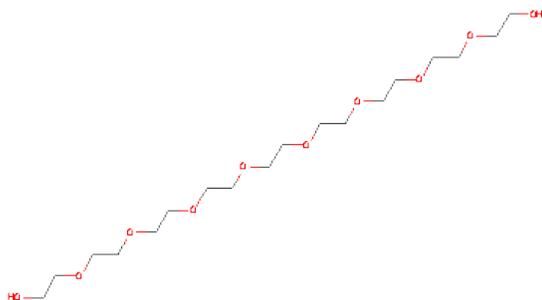
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 19	C 12	O 7	0	0
6	A	1	Total 7	C 4	O 3	0	0
6	A	1	Total 7	C 4	O 3	0	0
6	A	1	Total 7	C 4	O 3	0	0
6	A	1	Total 13	C 8	O 5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	421	Total 421	O 421	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	472	Total 472	O 472	0	0

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: Alpha-galactosidase A

Chain A:
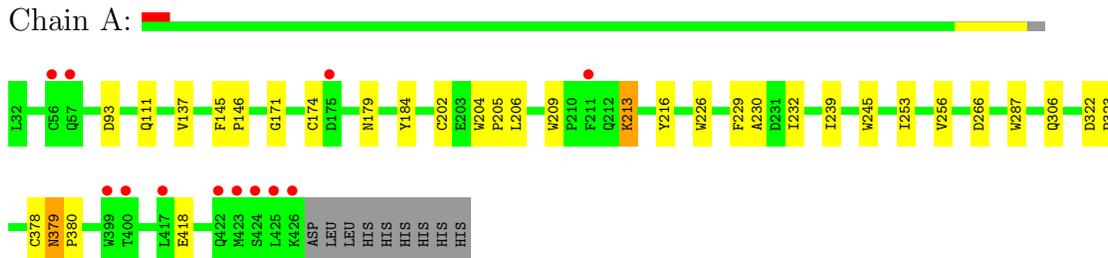
• Molecule 1: Alpha-galactosidase A

Chain B:
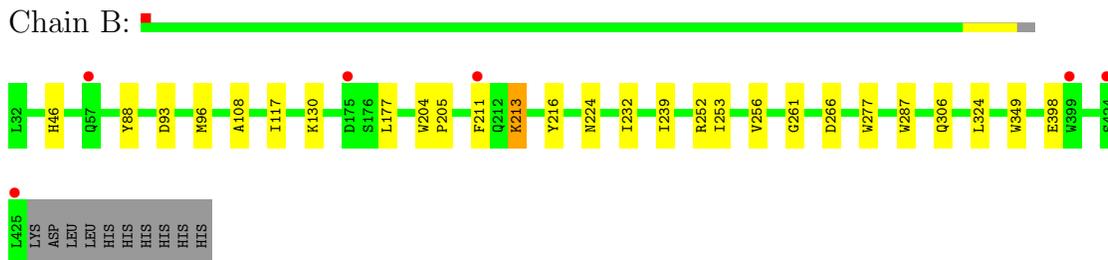
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.55Å 106.11Å 181.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.71 – 1.90 21.71 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (21.71-1.90) 98.6 (21.71-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$<I/\sigma(I)>$ [1]	2.80 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.165 , 0.197 0.182 , 0.215	Depositor DCC
R_{free} test set	4521 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 32.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	0 of 90229 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7537	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]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, GLA, GLC, 2PE, 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	0.35	0/3330	0.51	0/4518
1	B	0.35	0/3285	0.51	0/4459
All	All	0.35	0/6615	0.51	0/8977

There are no bond length outliers.

There are no bond angle outliers.

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	3204	0	3052	21	0
1	B	3171	0	3025	13	0
2	A	14	0	13	0	0
2	B	28	0	26	0	0
3	A	50	0	43	0	0
3	B	50	0	43	0	0
4	A	28	0	25	0	0
5	A	23	0	21	1	0
5	B	23	0	21	1	0
6	A	53	0	69	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	421	0	0	2	0
7	B	472	0	0	1	0
All	All	7537	0	6338	35	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 3.

The worst 5 of 35 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:379:ASN:HD22	1:A:380:PRO:HA	1.47	0.79
1:A:230:ALA:H	6:A:821:2PE:H111	1.50	0.77
6:A:824:2PE:H52	1:B:277:TRP:H	1.48	0.77
1:A:230:ALA:HB3	6:A:821:2PE:H81	1.68	0.75
1:B:232:ILE:HD11	1:B:239[A]:ILE:HD13	1.80	0.64

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	404/404 (100%)	393 (97%)	10 (2%)	1 (0%)	56	44
1	B	398/404 (98%)	388 (98%)	9 (2%)	1 (0%)	50	37
All	All	802/808 (99%)	781 (97%)	19 (2%)	2 (0%)	50	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	266	ASP
1	A	266	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	346/344 (101%)	339 (98%)	7 (2%)	68	61
1	B	340/344 (99%)	332 (98%)	8 (2%)	61	53
All	All	686/688 (100%)	671 (98%)	15 (2%)	66	57

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	GLU
1	B	46	HIS
1	B	324	LEU
1	A	379	ASN
1	B	287	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	B	228	ASN
1	A	379	ASN
1	A	119	GLN
1	B	179	ASN

5.3.3 RNA (i)

There are no RNA chains 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)

14 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	692	1,3	12,14,15	0.60	0	15,19,21	0.89	1 (6%)
3	NAG	A	693	3	12,14,15	0.63	0	15,19,21	1.05	1 (6%)
3	BMA	A	694	3	10,11,12	0.46	0	11,15,17	0.74	0
3	MAN	A	695	3	10,11,12	0.74	0	11,15,17	1.01	2 (18%)
4	NAG	A	715	1,4	12,14,15	0.62	0	15,19,21	0.92	1 (6%)
4	NAG	A	716	4	12,14,15	0.64	0	15,19,21	0.81	0
5	GLA	A	801	5	10,11,12	0.38	0	11,15,17	0.84	1 (9%)
5	GLC	A	811	5	12,12,12	0.51	0	17,17,17	0.84	0
3	NAG	B	692	1,3	12,14,15	0.60	0	15,19,21	0.97	1 (6%)
3	NAG	B	693	3	12,14,15	0.65	0	15,19,21	0.94	1 (6%)
3	BMA	B	694	3	10,11,12	0.56	0	11,15,17	1.19	2 (18%)
3	MAN	B	695	3	10,11,12	0.71	0	11,15,17	0.81	1 (9%)
5	GLA	B	802	5	10,11,12	0.44	0	11,15,17	0.46	0
5	GLC	B	812	5	12,12,12	0.52	0	17,17,17	0.72	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
3	NAG	A	692	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	693	3	-	0/6/23/26	0/1/1/1
3	BMA	A	694	3	-	0/2/19/22	0/1/1/1
3	MAN	A	695	3	-	0/2/19/22	0/1/1/1
4	NAG	A	715	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	716	4	-	0/6/23/26	0/1/1/1
5	GLA	A	801	5	-	0/2/19/22	0/1/1/1
5	GLC	A	811	5	-	0/2/22/22	0/1/1/1
3	NAG	B	692	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	693	3	-	0/6/23/26	0/1/1/1
3	BMA	B	694	3	-	0/2/19/22	0/1/1/1
3	MAN	B	695	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLA	B	802	5	-	0/2/19/22	0/1/1/1
5	GLC	B	812	5	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	692	NAG	O5-C5-C6	2.89	110.02	106.98
3	A	693	NAG	O5-C5-C6	2.84	109.96	106.98
5	A	801	GLA	O5-C5-C6	2.51	109.61	106.98
3	A	692	NAG	O5-C5-C6	2.41	109.51	106.98
3	B	695	MAN	O5-C5-C4	2.26	113.52	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

8 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	NAG	A	639	1	12,14,15	0.56	0	15,19,21	0.88	1 (6%)
6	2PE	A	821	-	18,18,27	0.55	0	17,17,26	0.44	0
6	2PE	A	822	-	6,6,27	0.68	0	5,5,26	0.70	0
6	2PE	A	823	-	6,6,27	0.67	0	5,5,26	0.70	0
6	2PE	A	824	-	6,6,27	0.66	0	5,5,26	0.67	0
6	2PE	A	825	-	12,12,27	0.58	0	11,11,26	0.57	0
2	NAG	B	639	1	12,14,15	0.59	0	15,19,21	0.78	1 (6%)
2	NAG	B	715	1	12,14,15	0.61	0	15,19,21	0.82	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	639	1	-	0/6/23/26	0/1/1/1
6	2PE	A	821	-	-	0/16/16/25	0/0/0/0
6	2PE	A	822	-	-	0/4/4/25	0/0/0/0
6	2PE	A	823	-	-	0/4/4/25	0/0/0/0
6	2PE	A	824	-	-	0/4/4/25	0/0/0/0
6	2PE	A	825	-	-	0/10/10/25	0/0/0/0
2	NAG	B	639	1	-	0/6/23/26	0/1/1/1
2	NAG	B	715	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	639	NAG	O5-C5-C6	2.66	109.77	106.98
2	B	639	NAG	O5-C5-C6	2.02	109.10	106.98
2	B	715	NAG	O5-C5-C6	2.02	109.10	106.98

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, 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	395/404 (97%)	0.03	12 (3%)	48	49	12, 18, 33, 84	0
1	B	394/404 (97%)	-0.01	6 (1%)	70	72	10, 17, 31, 66	0
All	All	789/808 (97%)	0.01	18 (2%)	54	59	10, 18, 32, 84	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	PHE	6.2
1	B	424	SER	5.9
1	A	426	LYS	5.4
1	B	425	LEU	4.0
1	A	424	SER	3.8

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, 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MAN	B	695	11/12	0.36	83.86	74,77,78,80	0
5	GLC	A	811	12/12	0.36	11.85	37,66,70,71	0
4	NAG	A	715	14/15	0.35	10.67	50,59,63,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
4	NAG	A	716	14/15	0.38	9.36	71,74,76,76	0
3	NAG	A	693	14/15	0.15	6.83	46,54,58,62	0
3	NAG	B	693	14/15	0.16	2.25	46,51,55,55	0
3	MAN	A	695	11/12	0.24	2.06	78,80,81,81	0
3	NAG	B	692	14/15	0.12	1.84	32,40,45,46	0
3	NAG	A	692	14/15	0.09	1.64	33,36,43,44	0
5	GLC	B	812	12/12	0.35	1.34	42,59,62,65	0
5	GLA	A	801	11/12	0.09	-0.20	24,29,33,34	0
5	GLA	B	802	11/12	0.06	-0.82	32,35,39,41	0
3	BMA	A	694	11/12	0.23	-	69,74,75,76	0
3	BMA	B	694	11/12	0.28	-	58,64,66,69	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, 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	RSR	LLDF	B-factors(Å²)	Q<0.9
6	2PE	A	825	13/28	0.38	24.97	68,72,74,74	0
6	2PE	A	824	7/28	0.27	10.91	45,53,60,62	0
6	2PE	A	822	7/28	0.38	10.32	40,52,64,64	0
2	NAG	B	715	14/15	0.39	7.29	58,68,72,73	0
6	2PE	A	823	7/28	0.25	2.74	69,71,72,73	0
2	NAG	B	639	14/15	0.25	2.01	44,50,56,57	0
2	NAG	A	639	14/15	0.23	1.91	49,53,61,63	0
6	2PE	A	821	19/28	0.17	1.44	26,41,57,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.