



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID : 3LRM
Title : Structure of alfa-galactosidase from Saccharomyces cerevisiae with raffinose
Authors : Fernandez-Leiro, R.; Pereira-Rodriguez, A.; Cerdan, M.E.; Becerra, M.; Sanz-Aparicio, J.
Deposited on : 2010-02-11
Resolution : 2.70 Å(reported)

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

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

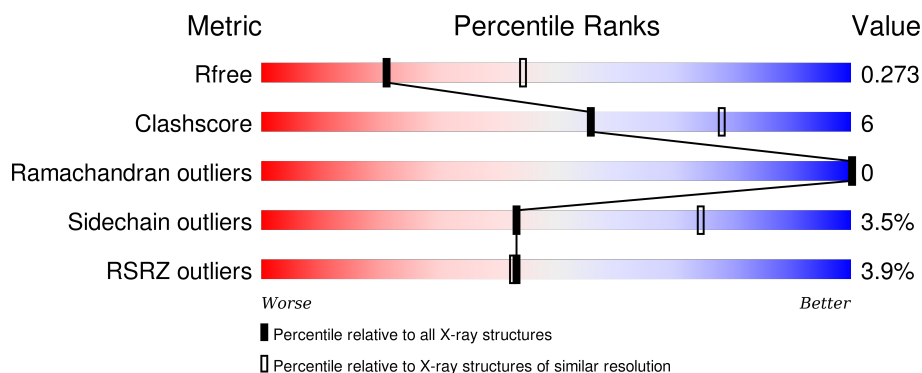
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 $\leq 5\%$. 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	479	<div> <div>82%12%6%</div> <div> <div>0%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>
1	B	479	<div> <div>8%81%13%6%</div> <div> <div>8%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
1	C	479	<div> <div>3%81%13%6%</div> <div> <div>3%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
1	D	479	<div> <div>2%82%11%6%</div> <div> <div>2%</div> <div>82%</div> <div>11%</div> <div>6%</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
3	NAG	A	3001	X	-	-	X
3	NAG	B	3001	X	-	-	-
3	NAG	C	3001	X	-	-	-
4	GLA	A	9002	-	-	-	X
4	SUC	D	9001	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15512 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3515	2203	596	695	21			
1	B	452	Total	C	N	O	S	0	0	0
			3515	2203	596	695	21			
1	C	452	Total	C	N	O	S	0	0	0
			3515	2203	596	695	21			
1	D	452	Total	C	N	O	S	0	0	0
			3515	2203	596	695	21			

There are 40 discrepancies between the modelled and reference sequences:

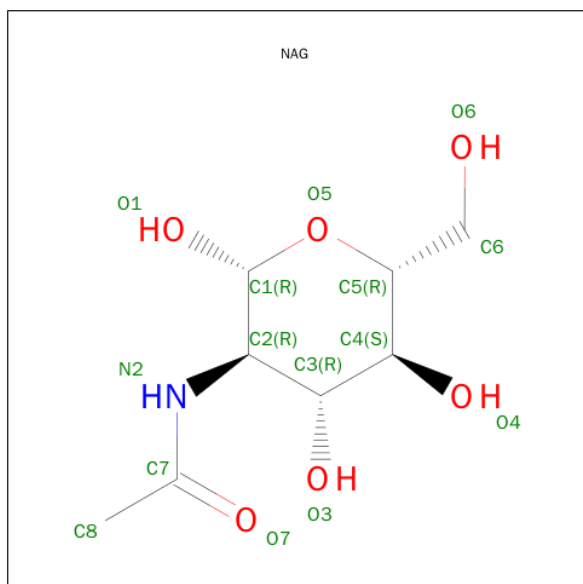
Chain	Residue	Modelled	Actual	Comment	Reference
A	149	ALA	ASP	ENGINEERED	UNP P04824
A	181	VAL	ILE	ENGINEERED	UNP P04824
A	472	ASP	-	EXPRESSION TAG	UNP P04824
A	473	TYR	-	EXPRESSION TAG	UNP P04824
A	474	LYS	-	EXPRESSION TAG	UNP P04824
A	475	ASP	-	EXPRESSION TAG	UNP P04824
A	476	ASP	-	EXPRESSION TAG	UNP P04824
A	477	ASP	-	EXPRESSION TAG	UNP P04824
A	478	ASP	-	EXPRESSION TAG	UNP P04824
A	479	LYS	-	EXPRESSION TAG	UNP P04824
B	149	ALA	ASP	ENGINEERED	UNP P04824
B	181	VAL	ILE	ENGINEERED	UNP P04824
B	472	ASP	-	EXPRESSION TAG	UNP P04824
B	473	TYR	-	EXPRESSION TAG	UNP P04824
B	474	LYS	-	EXPRESSION TAG	UNP P04824
B	475	ASP	-	EXPRESSION TAG	UNP P04824
B	476	ASP	-	EXPRESSION TAG	UNP P04824
B	477	ASP	-	EXPRESSION TAG	UNP P04824
B	478	ASP	-	EXPRESSION TAG	UNP P04824
B	479	LYS	-	EXPRESSION TAG	UNP P04824
C	149	ALA	ASP	ENGINEERED	UNP P04824

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Chain	Residue	Modelled	Actual	Comment	Reference
C	181	VAL	ILE	ENGINEERED	UNP P04824
C	472	ASP	-	EXPRESSION TAG	UNP P04824
C	473	TYR	-	EXPRESSION TAG	UNP P04824
C	474	LYS	-	EXPRESSION TAG	UNP P04824
C	475	ASP	-	EXPRESSION TAG	UNP P04824
C	476	ASP	-	EXPRESSION TAG	UNP P04824
C	477	ASP	-	EXPRESSION TAG	UNP P04824
C	478	ASP	-	EXPRESSION TAG	UNP P04824
C	479	LYS	-	EXPRESSION TAG	UNP P04824
D	149	ALA	ASP	ENGINEERED	UNP P04824
D	181	VAL	ILE	ENGINEERED	UNP P04824
D	472	ASP	-	EXPRESSION TAG	UNP P04824
D	473	TYR	-	EXPRESSION TAG	UNP P04824
D	474	LYS	-	EXPRESSION TAG	UNP P04824
D	475	ASP	-	EXPRESSION TAG	UNP P04824
D	476	ASP	-	EXPRESSION TAG	UNP P04824
D	477	ASP	-	EXPRESSION TAG	UNP P04824
D	478	ASP	-	EXPRESSION TAG	UNP P04824
D	479	LYS	-	EXPRESSION TAG	UNP P04824

- 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	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	2	Total	C	O	0	0
			34	18	16		
4	B	2	Total	C	O	0	0
			34	18	16		
4	C	2	Total	C	O	0	0
			34	18	16		

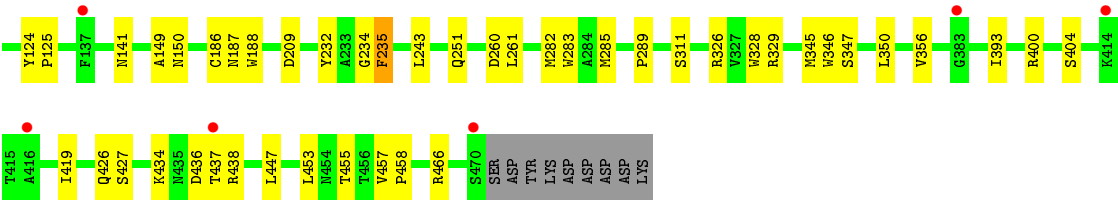
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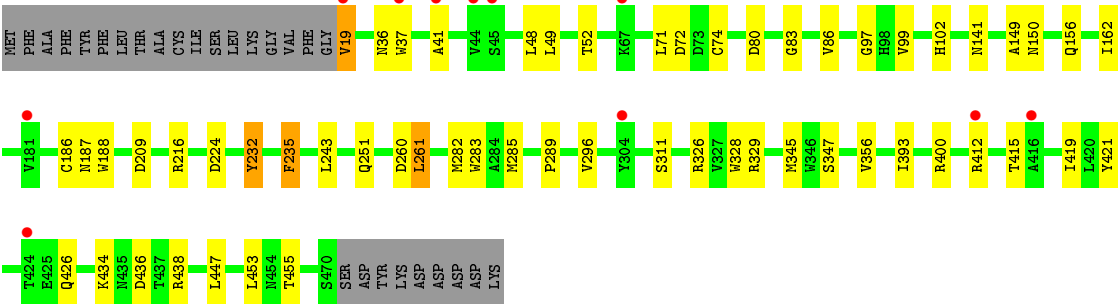
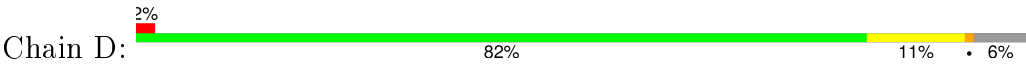
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	2	Total	C	O	0	0
			34	18	16		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	286	Total	O	0	0
			286	286		
5	B	235	Total	O	0	0
			235	235		
5	C	264	Total	O	0	0
			264	264		
5	D	237	Total	O	0	0
			237	237		



• Molecule 1: Alpha-galactosidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.17Å 129.53Å 136.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.05 – 2.70 71.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (94.05-2.70) 100.0 (71.80-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.241 , 0.284 0.237 , 0.273	Depositor DCC
R_{free} test set	2781 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 54890 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15512	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, SUC, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/3602	0.52	1/4891 (0.0%)
1	B	0.37	0/3602	0.52	1/4891 (0.0%)
1	C	0.37	0/3602	0.51	0/4891
1	D	0.37	0/3602	0.51	1/4891 (0.0%)
All	All	0.37	0/14408	0.51	3/19564 (0.0%)

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
3	A	1	0
3	B	1	0
3	C	1	0
All	All	3	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	436	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	261	LEU	CA-CB-CG	5.15	127.15	115.30
1	D	261	LEU	CA-CB-CG	5.05	126.91	115.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	3001	NAG	C1
3	B	3001	NAG	C1

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Mol	Chain	Res	Type	Atom
3	C	3001	NAG	C1

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	3515	0	3283	44	2
1	B	3515	0	3283	46	2
1	C	3515	0	3283	42	0
1	D	3515	0	3284	42	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
2	C	42	0	39	1	0
2	D	28	0	26	0	0
3	A	56	0	50	0	0
3	B	56	0	50	0	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	34	0	31	1	0
4	B	34	0	31	1	0
4	C	34	0	31	2	0
4	D	34	0	31	1	0
5	A	286	0	0	13	0
5	B	235	0	0	21	0
5	C	264	0	0	10	0
5	D	237	0	0	8	0
All	All	15512	0	13524	173	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 6.

The worst 5 of 173 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:79:ARG:HA	5:A:1534:HOH:O	1.31	1.26
1:B:435:ASN:HB2	5:B:537:HOH:O	1.47	1.12
1:C:42:CYS:HB3	5:C:1121:HOH:O	1.58	1.01
1:A:438:ARG:CZ	5:A:1610:HOH:O	2.20	0.88
1:A:85:LEU:HA	5:A:1534:HOH:O	1.72	0.87

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:A:434:LYS:CG	1:B:438:ARG:NH1[2_454]	1.84	0.36
1:A:433:SER:CB	1:B:436:ASP:OD1[2_454]	2.11	0.09

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	450/479 (94%)	430 (96%)	20 (4%)	0	100	100
1	B	450/479 (94%)	430 (96%)	20 (4%)	0	100	100
1	C	450/479 (94%)	429 (95%)	21 (5%)	0	100	100
1	D	450/479 (94%)	429 (95%)	21 (5%)	0	100	100
All	All	1800/1916 (94%)	1718 (95%)	82 (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	375/398 (94%)	362 (96%)	13 (4%)	43	74
1	B	375/398 (94%)	361 (96%)	14 (4%)	41	72
1	C	375/398 (94%)	362 (96%)	13 (4%)	43	74
1	D	375/398 (94%)	362 (96%)	13 (4%)	43	74
All	All	1500/1592 (94%)	1447 (96%)	53 (4%)	43	74

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	400	ARG
1	C	102	HIS
1	D	311	SER
1	B	438	ARG
1	B	455	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	413	ASN
1	C	36	ASN
1	D	355	GLN
1	B	426	GLN
1	A	355	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 ⓘ

20 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	3001	1,3	14,14,15	0.82	0	15,19,21	1.13	2 (13%)
3	NAG	A	3002	3	14,14,15	0.47	0	15,19,21	1.01	1 (6%)
3	NAG	A	5001	1,3	14,14,15	0.42	0	15,19,21	1.27	2 (13%)
3	NAG	A	5002	3	14,14,15	0.55	0	15,19,21	0.88	0
4	SUC	A	9001	4	24,24,24	0.45	0	36,36,36	0.94	1 (2%)
4	GLA	A	9002	4	11,11,12	0.45	0	14,15,17	0.60	0
3	NAG	B	3001	1,3	14,14,15	0.80	0	15,19,21	1.25	2 (13%)
3	NAG	B	3002	3	14,14,15	0.52	0	15,19,21	1.14	1 (6%)
3	NAG	B	5001	1,3	14,14,15	0.45	0	15,19,21	1.38	2 (13%)
3	NAG	B	5002	3	14,14,15	0.52	0	15,19,21	1.05	1 (6%)
4	SUC	B	9001	4	24,24,24	0.43	0	36,36,36	1.01	2 (5%)
4	GLA	B	9002	4	11,11,12	0.55	0	14,15,17	0.99	1 (7%)
3	NAG	C	3001	1,3	14,14,15	0.64	0	15,19,21	0.91	0
3	NAG	C	3002	3	14,14,15	0.44	0	15,19,21	1.07	1 (6%)
4	SUC	C	9001	4	24,24,24	0.45	0	36,36,36	0.94	1 (2%)
4	GLA	C	9002	4	11,11,12	0.40	0	14,15,17	0.74	0
3	NAG	D	5001	1,3	14,14,15	0.44	0	15,19,21	1.17	3 (20%)
3	NAG	D	5002	3	14,14,15	0.51	0	15,19,21	1.43	1 (6%)
4	SUC	D	9001	4	24,24,24	0.41	0	36,36,36	0.95	0
4	GLA	D	9002	4	11,11,12	0.42	0	14,15,17	0.64	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	3001	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	3002	3	-	0/6/23/26	0/1/1/1
3	NAG	A	5001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	5002	3	-	0/6/23/26	0/1/1/1
4	SUC	A	9001	4	-	0/12/51/51	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLA	A	9002	4	-	0/2/19/22	0/1/1/1
3	NAG	B	3001	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	3002	3	-	0/6/23/26	0/1/1/1
3	NAG	B	5001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	5002	3	-	0/6/23/26	0/1/1/1
4	SUC	B	9001	4	-	0/12/51/51	0/2/2/2
4	GLA	B	9002	4	-	0/2/19/22	0/1/1/1
3	NAG	C	3001	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	3002	3	-	0/6/23/26	0/1/1/1
4	SUC	C	9001	4	-	0/12/51/51	0/2/2/2
4	GLA	C	9002	4	-	0/2/19/22	0/1/1/1
3	NAG	D	5001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	5002	3	-	0/6/23/26	0/1/1/1
4	SUC	D	9001	4	-	0/12/51/51	0/2/2/2
4	GLA	D	9002	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3001	NAG	C1-O5-C5	-3.23	108.14	112.25
3	A	3001	NAG	C3-C2-N2	-3.22	102.84	110.56
3	D	5001	NAG	C3-C4-C5	2.02	113.72	110.20
4	C	9001	SUC	O1-C2'-C3'	2.05	115.19	108.04
3	A	5001	NAG	C4-C3-C2	2.18	114.61	111.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	3001	NAG	C1
3	C	3001	NAG	C1
3	A	3001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	9001	SUC	1	0
4	B	9001	SUC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	9001	SUC	2	0
4	D	9001	SUC	1	0

5.6 Ligand geometry

9 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	2001	1	14,14,15	0.44	0	15,19,21	0.71	0
2	NAG	A	4001	1	14,14,15	0.54	0	15,19,21	1.23	1 (6%)
2	NAG	B	2001	1	14,14,15	0.42	0	15,19,21	2.35	2 (13%)
2	NAG	B	4001	1	14,14,15	0.52	0	15,19,21	1.10	1 (6%)
2	NAG	C	2001	1	14,14,15	0.43	0	15,19,21	1.32	1 (6%)
2	NAG	C	4001	1	14,14,15	0.46	0	15,19,21	0.64	0
2	NAG	C	5001	1	14,14,15	0.43	0	15,19,21	0.94	1 (6%)
2	NAG	D	2001	1	14,14,15	0.58	0	15,19,21	1.08	1 (6%)
2	NAG	D	4001	1	14,14,15	0.46	0	15,19,21	0.80	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	2001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	4001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	2001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	4001	1	-	0/6/23/26	0/1/1/1
2	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
2	NAG	C	4001	1	-	0/6/23/26	0/1/1/1
2	NAG	C	5001	1	-	0/6/23/26	0/1/1/1
2	NAG	D	2001	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	4001	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4001	NAG	C1-O5-C5	2.18	115.01	112.25
2	C	5001	NAG	C1-O5-C5	2.28	115.14	112.25
2	D	2001	NAG	C2-N2-C7	2.43	126.16	123.04
2	A	4001	NAG	C1-O5-C5	2.89	115.92	112.25
2	B	4001	NAG	C1-O5-C5	3.01	116.07	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	C	4001	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	452/479 (94%)	0.22	6 (1%) 79 79	33, 40, 45, 48	0
1	B	452/479 (94%)	0.55	38 (8%) 14 11	32, 40, 45, 48	0
1	C	452/479 (94%)	0.28	15 (3%) 50 50	33, 40, 45, 48	0
1	D	452/479 (94%)	0.30	11 (2%) 62 62	33, 40, 45, 48	0
All	All	1808/1916 (94%)	0.34	70 (3%) 43 43	32, 40, 45, 48	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	VAL	4.8
1	D	41	ALA	4.1
1	B	39	THR	4.0
1	B	412	ARG	4.0
1	B	37	TRP	3.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	3001	14/15	0.91	0.23	2.88	48,51,53,53	0
4	SUC	D	9001	23/23	0.76	0.35	2.29	97,99,101,102	0
4	GLA	A	9002	11/12	0.82	0.32	2.04	74,75,75,75	0
3	NAG	C	3001	14/15	0.90	0.20	1.50	50,53,57,58	0
4	GLA	B	9002	11/12	0.73	0.32	1.42	81,82,82,83	0
4	SUC	A	9001	23/23	0.82	0.30	1.42	75,76,78,78	0
4	SUC	C	9001	23/23	0.72	0.34	1.29	83,86,89,89	0
4	SUC	B	9001	23/23	0.85	0.35	1.23	82,82,83,83	0
4	GLA	C	9002	11/12	0.90	0.20	0.66	79,80,80,81	0
4	GLA	D	9002	11/12	0.79	0.21	0.52	96,97,97,97	0
3	NAG	B	3001	14/15	0.88	0.21	0.21	50,53,57,57	0
3	NAG	A	5001	14/15	0.92	0.17	0.08	55,57,61,64	0
3	NAG	D	5001	14/15	0.89	0.17	-0.71	55,58,60,61	0
3	NAG	B	5001	14/15	0.90	0.17	-1.11	54,57,61,66	0
3	NAG	D	5002	14/15	0.87	0.20	-	63,64,67,67	0
3	NAG	C	3002	14/15	0.91	0.15	-	57,57,58,58	0
3	NAG	B	3002	14/15	0.81	0.24	-	60,61,64,64	0
3	NAG	B	5002	14/15	0.68	0.40	-	70,73,74,74	0
3	NAG	A	5002	14/15	0.86	0.22	-	68,70,71,71	0
3	NAG	A	3002	14/15	0.88	0.19	-	56,57,59,61	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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	D	4001	14/15	0.89	0.22	1.32	53,56,57,57	0
2	NAG	B	2001	14/15	0.92	0.22	0.71	49,51,52,53	0
2	NAG	C	5001	14/15	0.90	0.19	0.18	51,53,54,55	0
2	NAG	A	2001	14/15	0.93	0.15	-0.04	46,48,49,49	0
2	NAG	C	2001	14/15	0.92	0.19	-0.25	45,47,48,48	0
2	NAG	B	4001	14/15	0.88	0.26	-	52,55,57,57	0
2	NAG	D	2001	14/15	0.91	0.19	-	47,49,51,51	0
2	NAG	C	4001	14/15	0.86	0.27	-	53,55,56,57	0
2	NAG	A	4001	14/15	0.88	0.20	-	50,52,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.