



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:30 AM GMT

PDB ID : 3HG4
Title : Human alpha-galactosidase catalytic mechanism 3. Covalent intermediate
Authors : Guce, A.I.; Clark, N.E.; Garman, S.C.
Deposited on : 2009-05-13
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

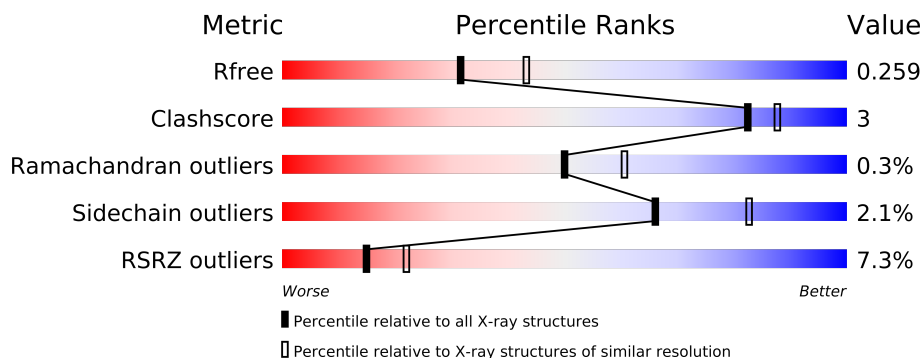
The following versions of software and data (see [references](#)) were used in the production of this report:

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



The reported resolution of this entry is 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	398	
1	B	398	

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

Mol	Type	Chain	Res	Geometry	Electron density
6	SO4	B	822	-	X
7	ACY	A	843	-	X
7	ACY	B	841	-	X
8	NAG	B	715	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7250 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	390	Total	C	N	O	S	0	0	0
			3122	1988	534	574	26			
1	B	392	Total	C	N	O	S	0	0	0
			3139	1998	537	577	27			

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

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

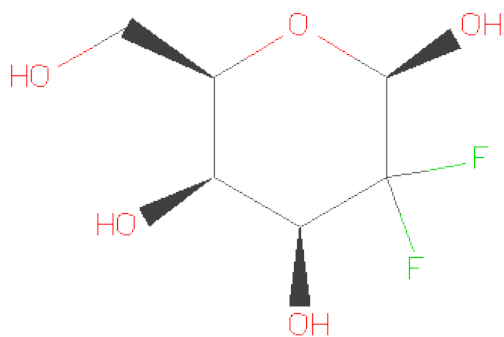
- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

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

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

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

- Molecule 5 is 2,6-ANHYDRO-5-DEOXY-5,5-DIFLUORO-D-ARABINO-HEXITOL (three-letter code: 7JZ) (formula: C₆H₁₀F₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	F	O	0	0
			12	6	2	4		
5	B	1	Total	C	F	O	0	0
			12	6	2	4		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



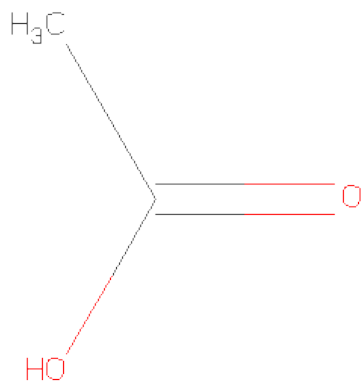
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

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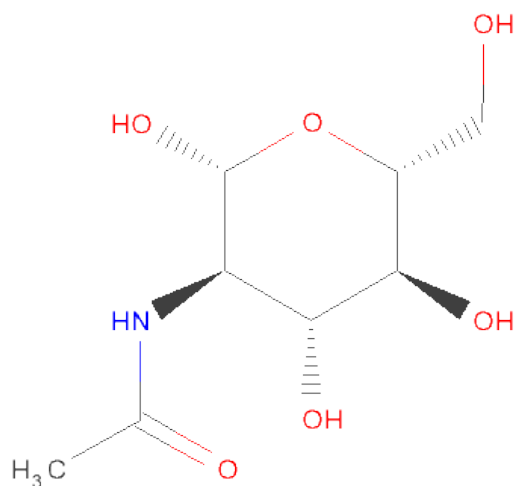
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



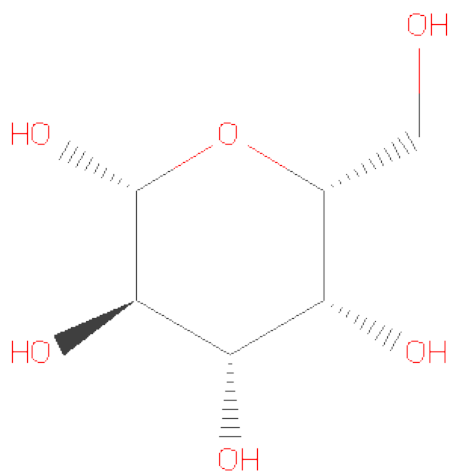
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 9 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: C₆H₁₂O₆).



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

- Molecule 10 is water.

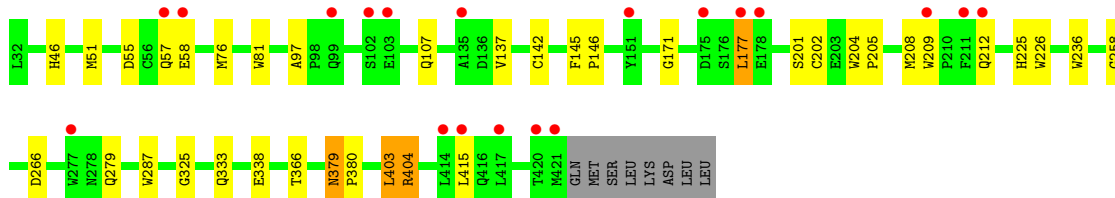
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	370	Total 370	O 370	0	0
10	B	312	Total 312	O 312	0	0

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.

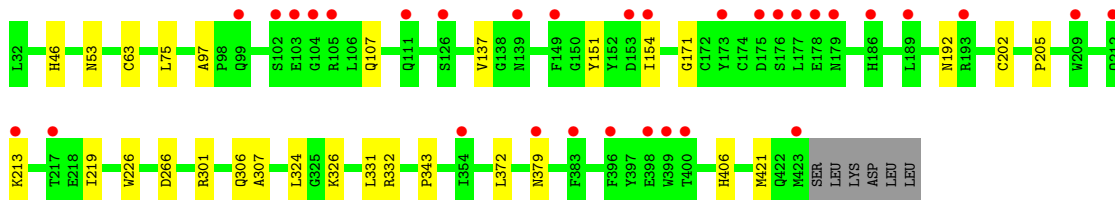
- Molecule 1: Alpha-galactosidase A

Chain A: 



- Molecule 1: Alpha-galactosidase A

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.22Å 90.22Å 216.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.05 – 2.30 18.05 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (18.05-2.30) 99.8 (18.05-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.221 0.212 , 0.259	Depositor DCC
R_{free} test set	949 reflections (2.09%)	DCC
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.7	EDS
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 46268 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7250	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, GAL, 7JZ, FUC, ACY, MAN, SO4

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	0.41	0/3209	0.56	1/4358 (0.0%)
1	B	0.40	0/3226	0.53	0/4380
All	All	0.41	0/6435	0.54	1/8738 (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	177	LEU	CA-CB-CG	5.72	128.46	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	3122	0	2981	20	0
1	B	3139	0	2998	15	0
2	A	38	0	34	1	0
2	B	38	0	34	0	0
3	A	61	0	52	0	0
3	B	61	0	52	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	28	0	25	0	0
5	A	12	0	8	1	0
5	B	12	0	8	0	0
6	A	5	0	0	0	0
6	B	10	0	0	1	0
7	A	8	0	6	0	0
7	B	8	0	6	0	0
8	B	14	0	13	0	0
9	B	12	0	12	0	0
10	A	370	0	0	2	0
10	B	312	0	0	3	0
All	All	7250	0	6229	40	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.

All (40) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:692:NAG:H81	10:B:1431:HOH:O	1.95	0.66
1:A:403:LEU:HD11	1:A:415:LEU:HD13	1.83	0.60
1:A:379:ASN:HD22	1:A:380:PRO:HA	1.67	0.59
1:B:151:TYR:HD1	1:B:154:ILE:HD11	1.68	0.59
1:B:75:LEU:HD11	1:B:301:ARG:HG2	1.85	0.59
1:B:137:VAL:HG12	1:B:171:GLY:HA2	1.86	0.57
1:B:192:ASN:HA	3:B:692:NAG:H83	1.86	0.56
1:B:205:PRO:HG3	1:B:219:ILE:HD13	1.86	0.56
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.88	0.56
1:A:201:SER:HB2	1:A:225:HIS:CE1	2.41	0.56
3:B:694:BMA:H62	3:B:696:MAN:H5	1.89	0.54
1:B:75:LEU:CD1	1:B:301:ARG:HG2	2.38	0.53
3:B:694:BMA:C6	3:B:696:MAN:H5	2.39	0.53
1:A:366:THR:HG22	1:A:404:ARG:HB3	1.91	0.53
2:A:639:NAG:H61	2:A:640:NAG:H82	1.92	0.51
1:B:202:CYS:O	1:B:226:TRP:HA	2.11	0.50
1:A:177:LEU:HD22	10:A:1374:HOH:O	2.10	0.50
1:A:236:TRP:CE3	1:A:279:GLN:HG2	2.48	0.49
1:A:137:VAL:HG12	1:A:171:GLY:HA2	1.96	0.47
1:B:97:ALA:HB3	1:B:107:GLN:HG3	1.97	0.47
1:B:406:HIS:ND1	6:B:822:SO4:O4	2.33	0.47
1:A:333:GLN:HG3	1:A:338:GLU:HG2	1.97	0.46
1:B:306:GLN:HG2	10:B:1468:HOH:O	2.14	0.46
1:A:97:ALA:HB3	1:A:107:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:TRP:HE1	1:A:208:MET:CE	2.29	0.45
1:B:151:TYR:CD1	1:B:154:ILE:HD11	2.49	0.45
1:B:331:LEU:HG	1:B:332:ARG:HG3	1.99	0.45
1:A:142:CYS:HB2	5:A:801:7JZ:O6	2.18	0.44
1:A:202:CYS:O	1:A:226:TRP:HA	2.18	0.44
1:B:307:ALA:HA	10:B:1670:HOH:O	2.18	0.42
1:A:55:ASP:OD2	1:A:58:GLU:HB2	2.18	0.42
1:A:57:GLN:HG2	10:A:1511:HOH:O	2.21	0.41
1:A:145:PHE:HB3	1:A:146:PRO:CD	2.50	0.41
1:B:326:LYS:HG2	1:B:343:PRO:HG2	2.01	0.41
1:A:379:ASN:HD22	1:A:380:PRO:CA	2.31	0.41
1:A:258:GLY:HA2	1:A:325:GLY:O	2.20	0.41
1:A:76:MET:HA	1:A:81:TRP:HB2	2.03	0.40
1:A:403:LEU:HD11	1:A:415:LEU:CD1	2.49	0.40
3:B:694:BMA:H62	3:B:696:MAN:C5	2.51	0.40
1:B:53:ASN:HB3	1:B:63:CYS:HA	2.04	0.40

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	388/398 (98%)	377 (97%)	10 (3%)	1 (0%)	50	60
1	B	390/398 (98%)	378 (97%)	11 (3%)	1 (0%)	50	60
All	All	778/796 (98%)	755 (97%)	21 (3%)	2 (0%)	50	60

All (2) Ramachandran outliers are listed below:

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

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	331/339 (98%)	323 (98%)	8 (2%)	61	79
1	B	333/339 (98%)	327 (98%)	6 (2%)	71	86
All	All	664/678 (98%)	650 (98%)	14 (2%)	66	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	51	MET
1	A	209	TRP
1	A	212	GLN
1	A	287	TRP
1	A	379	ASN
1	A	403	LEU
1	A	404	ARG
1	B	46	HIS
1	B	213	LYS
1	B	324	LEU
1	B	372	LEU
1	B	379	ASN
1	B	421	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	225	HIS
1	A	379	ASN
1	B	179	ASN
1	B	212	GLN
1	B	228	ASN
1	B	379	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

18 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	639	1,2	12,14,15	0.59	0	15,19,21	0.82	0
2	NAG	A	640	2	12,14,15	0.64	0	15,19,21	1.03	1 (6%)
2	FUC	A	644	2	9,10,11	0.76	0	10,14,16	0.99	0
3	NAG	A	692	1,3	12,14,15	0.62	0	15,19,21	0.94	1 (6%)
3	NAG	A	693	3	12,14,15	0.59	0	15,19,21	0.88	1 (6%)
3	BMA	A	694	3	10,11,12	0.44	0	11,15,17	0.82	0
3	MAN	A	695	3	10,11,12	0.82	0	11,15,17	2.02	3 (27%)
3	MAN	A	696	3	10,11,12	0.71	0	11,15,17	0.82	0
4	NAG	A	715	1,4	12,14,15	0.58	0	15,19,21	0.93	0
4	NAG	A	716	4	12,14,15	0.56	0	15,19,21	1.04	1 (6%)
2	NAG	B	639	1,2	12,14,15	0.69	0	15,19,21	0.98	1 (6%)
2	NAG	B	640	2	12,14,15	0.63	0	15,19,21	0.89	1 (6%)
2	FUC	B	644	2	9,10,11	0.79	0	10,14,16	0.84	0
3	NAG	B	692	1,3	12,14,15	0.60	0	15,19,21	0.61	0
3	NAG	B	693	3	12,14,15	0.62	0	15,19,21	1.05	1 (6%)
3	BMA	B	694	3	10,11,12	0.54	0	11,15,17	2.13	4 (36%)
3	MAN	B	695	3	10,11,12	0.71	0	11,15,17	0.90	1 (9%)
3	MAN	B	696	3	10,11,12	0.65	0	11,15,17	1.01	1 (9%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	640	2	-	0/6/23/26	0/1/1/1
2	FUC	A	644	2	-	0/0/17/20	0/1/1/1
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
3	MAN	A	696	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
2	NAG	B	639	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	640	2	-	0/6/23/26	0/1/1/1
2	FUC	B	644	2	-	0/0/17/20	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
3	MAN	B	696	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	695	MAN	C4-C3-C2	4.89	117.07	110.50
3	B	694	BMA	C3-C4-C5	4.29	117.86	110.20
3	B	694	BMA	O5-C5-C4	4.04	115.78	110.65
3	A	695	MAN	O5-C5-C6	3.61	110.77	106.98
3	B	693	NAG	O5-C5-C6	2.78	109.90	106.98
3	A	692	NAG	O5-C5-C6	2.75	109.87	106.98
3	B	694	BMA	C4-C3-C2	2.64	114.04	110.50
2	B	640	NAG	O5-C5-C6	2.47	109.57	106.98
3	B	696	MAN	O5-C5-C6	2.39	109.49	106.98
3	B	695	MAN	O5-C5-C6	2.33	109.43	106.98
3	A	695	MAN	C3-C4-C5	2.33	114.36	110.20
2	A	640	NAG	O5-C5-C6	2.31	109.41	106.98
4	A	716	NAG	O5-C5-C6	2.25	109.34	106.98
3	B	694	BMA	C6-C5-C4	-2.15	107.81	113.00
3	A	693	NAG	O5-C5-C6	2.06	109.14	106.98
2	B	639	NAG	C3-C4-C5	2.03	113.83	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

11 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$
5	7JZ	A	801	1	10,12,13	1.84	2 (20%)	13,18,20	1.48	2 (15%)
6	SO4	A	823	-	4,4,4	0.37	0	6,6,6	0.21	0
7	ACY	A	842	-	3,3,3	0.64	0	3,3,3	0.65	0
7	ACY	A	843	-	3,3,3	0.63	0	3,3,3	0.71	0
8	NAG	B	715	1	12,14,15	0.56	0	15,19,21	1.04	2 (13%)
5	7JZ	B	802	1	10,12,13	1.88	2 (20%)	13,18,20	1.80	2 (15%)
9	GAL	B	803	-	12,12,12	0.55	0	17,17,17	0.96	1 (5%)
6	SO4	B	821	-	4,4,4	0.24	0	6,6,6	0.12	0
6	SO4	B	822	-	4,4,4	2.89	3 (75%)	6,6,6	0.38	0
7	ACY	B	841	-	3,3,3	0.64	0	3,3,3	0.67	0
7	ACY	B	844	-	3,3,3	0.65	0	3,3,3	0.73	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
5	7JZ	A	801	1	-	0/2/22/26	1/1/1/1
6	SO4	A	823	-	-	0/0/0/0	0/0/0/0
7	ACY	A	842	-	-	0/0/0/0	0/0/0/0
7	ACY	A	843	-	-	0/0/0/0	0/0/0/0
8	NAG	B	715	1	-	0/6/23/26	0/1/1/1
5	7JZ	B	802	1	1/1/4/5	0/2/22/26	1/1/1/1
9	GAL	B	803	-	1/1/5/5	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	B	821	-	-	0/0/0/0	0/0/0/0
6	SO4	B	822	-	-	0/0/0/0	0/0/0/0
7	ACY	B	841	-	-	0/0/0/0	0/0/0/0
7	ACY	B	844	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	801	7JZ	F2A-C2	-4.45	1.32	1.37
5	B	802	7JZ	F2A-C2	-4.10	1.33	1.37
6	B	822	SO4	O3-S	3.76	1.60	1.47
5	B	802	7JZ	F2B-C2	-3.74	1.33	1.37
5	A	801	7JZ	F2B-C2	-3.29	1.34	1.37
6	B	822	SO4	O4-S	3.25	1.58	1.47
6	B	822	SO4	O1-S	2.92	1.56	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	802	7JZ	F2B-C2-F2A	4.31	110.26	104.89
5	B	802	7JZ	O5-C5-C6	4.20	111.39	106.98
5	A	801	7JZ	F2B-C2-F2A	3.79	109.63	104.89
5	A	801	7JZ	O5-C5-C6	3.08	110.22	106.98
8	B	715	NAG	C3-C4-C5	2.45	114.58	110.20
8	B	715	NAG	O5-C5-C4	2.15	113.38	110.65
9	B	803	GAL	C3-C4-C5	2.06	113.89	110.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	802	7JZ	C1
9	B	803	GAL	C4

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	802	7JZ	C1-C2-C3-C4-C5-O5
5	A	801	7JZ	C1-C2-C3-C4-C5-O5

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	390/398 (97%)	0.34	19 (4%) 28 39	41, 47, 53, 63	0
1	B	392/398 (98%)	0.43	32 (8%) 12 18	41, 47, 54, 68	0
All	All	782/796 (98%)	0.39	51 (6%) 15 26	41, 47, 53, 68	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	MET	7.2
1	B	102	SER	6.0
1	A	211	PHE	4.9
1	B	423	MET	4.5
1	A	57	GLN	4.4
1	B	173	TYR	4.1
1	B	103	GLU	3.9
1	A	102	SER	3.8
1	B	209	TRP	3.6
1	B	149	PHE	3.5
1	B	193	ARG	3.4
1	A	177	LEU	3.4
1	B	177	LEU	3.4
1	B	399	TRP	3.3
1	B	175	ASP	3.3
1	B	178	GLU	3.1
1	A	415	LEU	3.0
1	B	99	GLN	3.0
1	B	213	LYS	2.9
1	A	178	GLU	2.9
1	A	175	ASP	2.8
1	A	212	GLN	2.8
1	B	154	ILE	2.6
1	A	58	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	383	PHE	2.5
1	A	151	TYR	2.4
1	B	126	SER	2.4
1	B	139	ASN	2.3
1	A	99	GLN	2.3
1	B	400	THR	2.3
1	B	153	ASP	2.3
1	B	111	GLN	2.3
1	B	179	ASN	2.3
1	A	417	LEU	2.2
1	B	105	ARG	2.2
1	B	212	GLN	2.2
1	B	189	LEU	2.2
1	B	104	GLY	2.2
1	A	277	TRP	2.1
1	B	354	ILE	2.1
1	A	414	LEU	2.1
1	A	135	ALA	2.1
1	A	209	TRP	2.1
1	B	379	ASN	2.1
1	B	398	GLU	2.1
1	B	217	THR	2.0
1	A	103	GLU	2.0
1	B	186	HIS	2.0
1	B	176	SER	2.0
1	B	396	PHE	2.0
1	A	420	THR	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, 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(\AA^2)	Q<0.9
3	MAN	B	695	11/12	0.28	15.00	87,88,88,89	0
4	NAG	A	716	14/15	0.45	4.54	84,86,87,87	0
4	NAG	A	715	14/15	0.29	3.04	72,77,78,81	0
2	FUC	B	644	10/11	0.53	2.56	88,90,90,90	0
3	MAN	A	696	11/12	0.49	2.38	93,94,94,94	0
3	NAG	B	693	14/15	0.26	1.77	74,77,79,82	0
2	NAG	A	639	14/15	0.26	0.93	70,74,80,81	0
2	NAG	B	639	14/15	0.31	0.78	73,77,85,86	0
3	NAG	A	693	14/15	0.22	0.01	66,70,73,78	0
3	NAG	B	692	14/15	0.16	-0.27	61,65,66,70	0
3	NAG	A	692	14/15	0.12	-0.55	52,54,57,62	0
2	NAG	B	640	14/15	0.58	-	87,90,90,91	0
3	BMA	A	694	11/12	0.40	-	83,87,89,91	0
3	MAN	A	695	11/12	0.44	-	91,91,92,92	0
2	NAG	A	640	14/15	0.44	-	82,84,84,84	0
2	FUC	A	644	10/11	0.38	-	83,85,85,85	0
3	BMA	B	694	11/12	0.40	-	86,88,91,94	0
3	MAN	B	696	11/12	0.56	-	96,97,97,97	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(\AA^2)	Q<0.9
7	ACY	B	841	4/4	0.46	7.45	109,109,109,109	0
8	NAG	B	715	14/15	0.41	7.15	73,77,78,78	0
7	ACY	A	843	4/4	0.43	4.55	100,100,100,100	0
6	SO4	B	822	5/5	0.47	4.04	158,158,158,158	0
5	7JZ	B	802	12/13	0.17	1.14	45,49,50,50	0
7	ACY	A	842	4/4	0.25	0.87	100,100,100,100	0
9	GAL	B	803	12/12	0.22	0.82	74,76,76,77	0
5	7JZ	A	801	12/13	0.14	0.08	42,44,45,45	0
7	ACY	B	844	4/4	0.16	-0.17	83,83,83,83	0
6	SO4	B	821	5/5	0.14	-0.19	70,70,70,71	0
6	SO4	A	823	5/5	0.10	-0.44	52,53,54,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.