



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:56 AM GMT

PDB ID : 3GXN
Title : Crystal structure of apo alpha-galactosidase A at pH 4.5
Authors : Lieberman, R.L.
Deposited on : 2009-04-02
Resolution : 3.01 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>

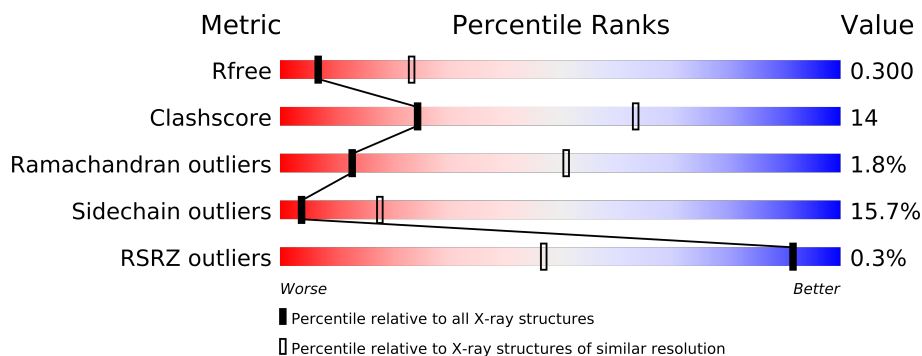
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.01 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	1332 (3.04-3.00)
Clashscore	79885	1732 (3.04-3.00)
Ramachandran outliers	78287	1669 (3.04-3.00)
Sidechain outliers	78261	1672 (3.04-3.00)
RSRZ outliers	66119	1333 (3.04-3.00)

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 ≥ 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	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6305 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	390	Total	C	N	O	S	0	0	0
			3122	1988	534	574	26			

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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



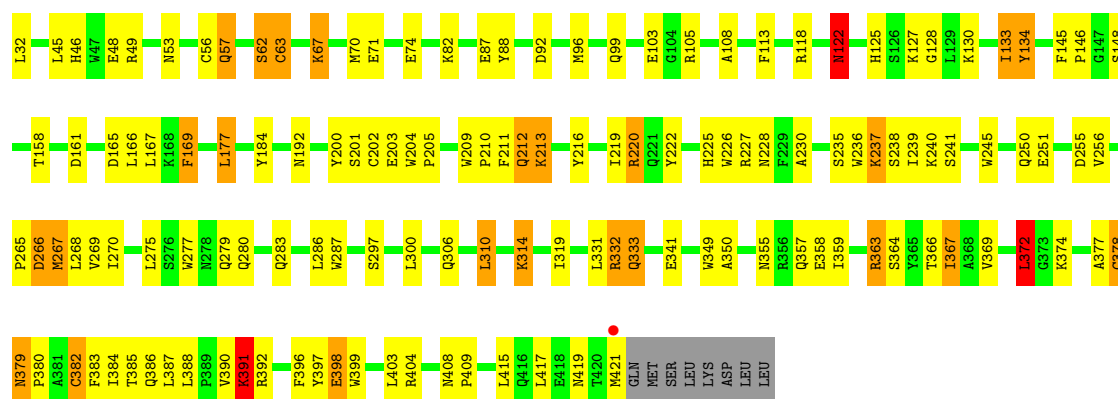
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

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.

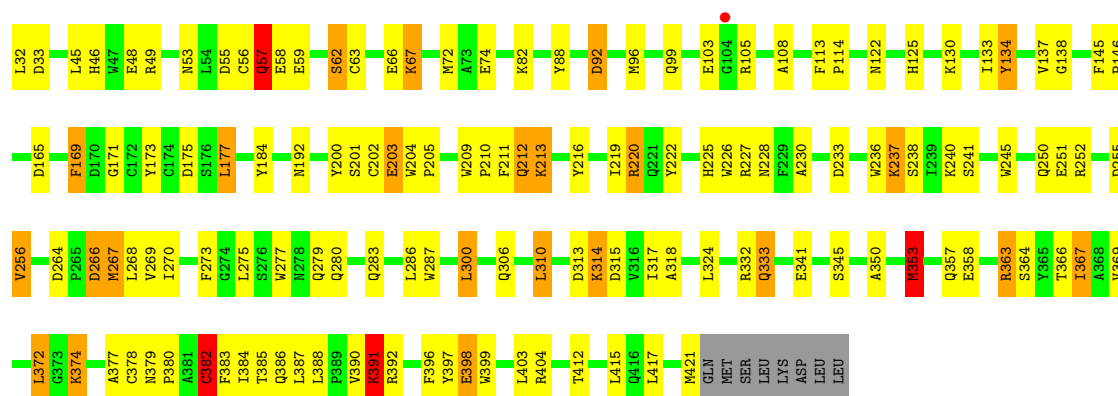
- Molecule 1: Alpha-galactosidase A

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	90.38Å 90.38Å 217.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.66 – 3.01 44.66 – 3.01	Depositor EDS
% Data completeness (in resolution range)	88.1 (44.66-3.01) 88.1 (44.66-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.236 , 0.301 0.236 , 0.300	Depositor DCC
R_{free} test set	971 reflections (5.48%)	DCC
Wilson B-factor (Å ²)	103.2	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 104.8	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 18676 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6305	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: NAG, 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	0.86	1/3209 (0.0%)	0.92	4/4358 (0.1%)
1	B	0.82	1/3209 (0.0%)	0.88	3/4358 (0.1%)
All	All	0.84	2/6418 (0.0%)	0.90	7/8716 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	CYS	CB-SG	-7.64	1.69	1.82
1	A	382	CYS	CB-SG	-7.38	1.69	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	286	LEU	CA-CB-CG	-6.59	100.14	115.30
1	B	286	LEU	CA-CB-CG	-6.50	100.36	115.30
1	A	332	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	266	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	353	MET	CG-SD-CE	5.12	108.38	100.20
1	A	388	LEU	CB-CG-CD2	-5.06	102.40	111.00

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	2984	91	0
1	B	3122	0	2984	87	1
2	A	28	0	25	3	1
2	B	28	0	25	4	0
3	A	5	0	0	0	0
All	All	6305	0	6018	172	1

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 14.

All (172) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:ASN:HD21	2:A:692:NAG:C1	1.60	1.15
1:B:192:ASN:HD21	2:B:692:NAG:C1	1.68	1.04
1:B:57:GLN:NE2	1:B:57:GLN:HA	1.88	0.89
1:A:386:GLN:NE2	1:A:390:VAL:HG22	1.90	0.87
1:B:53:ASN:HD22	1:B:62:SER:HB2	1.39	0.87
1:A:386:GLN:O	1:A:391:LYS:HA	1.74	0.86
1:B:53:ASN:ND2	1:B:62:SER:HB2	1.91	0.84
1:B:210:PRO:HD2	1:B:211:PHE:CE2	2.14	0.83
1:B:386:GLN:NE2	1:B:390:VAL:HG22	1.95	0.82
1:A:57:GLN:NE2	1:A:57:GLN:HA	1.96	0.79
1:B:386:GLN:O	1:B:391:LYS:HA	1.81	0.79
1:A:192:ASN:ND2	2:A:692:NAG:C1	2.43	0.79
1:A:386:GLN:HE22	1:A:390:VAL:HG22	1.48	0.78
1:A:366:THR:HG22	1:A:404:ARG:HA	1.63	0.78
1:A:46:HIS:CD2	1:A:92:ASP:H	2.03	0.77
1:A:53:ASN:HD22	1:A:62:SER:HB2	1.53	0.74
1:A:251:GLU:OE1	1:A:251:GLU:N	2.15	0.74
1:A:363:ARG:HG2	1:A:363:ARG:HH11	1.51	0.74
1:B:192:ASN:ND2	2:B:692:NAG:C1	2.48	0.73
1:A:314:LYS:N	1:A:314:LYS:HD3	2.04	0.73
1:A:145:PHE:HB3	1:A:146:PRO:HD2	1.71	0.73
1:A:384:ILE:HG12	1:A:417:LEU:HG	1.70	0.71
1:A:125:HIS:HE1	1:A:165:ASP:OD2	1.71	0.71
1:A:237:LYS:HE3	1:B:237:LYS:HE3	1.71	0.71
1:B:314:LYS:HD3	1:B:314:LYS:N	2.06	0.71
1:B:251:GLU:N	1:B:251:GLU:OE1	2.18	0.70
1:B:384:ILE:HG12	1:B:417:LEU:HG	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:LEU:N	1:A:220:ARG:O	2.25	0.70
1:B:46:HIS:CD2	1:B:92:ASP:H	2.09	0.70
1:B:386:GLN:HE22	1:B:390:VAL:HG22	1.58	0.69
1:A:367:ILE:HD12	1:A:403:LEU:HB3	1.74	0.69
1:B:210:PRO:HD2	1:B:211:PHE:CZ	2.28	0.68
1:B:145:PHE:HB3	1:B:146:PRO:HD2	1.74	0.68
1:B:57:GLN:HE21	1:B:57:GLN:HA	1.59	0.67
1:B:366:THR:HG22	1:B:404:ARG:HA	1.77	0.66
1:A:216:TYR:HA	1:A:219:ILE:HD12	1.77	0.64
1:A:239:ILE:HD12	1:A:275:LEU:HD21	1.80	0.63
1:A:213:LYS:HD2	1:A:213:LYS:H	1.63	0.63
1:B:192:ASN:HD21	2:B:692:NAG:C2	2.10	0.63
1:A:367:ILE:CD1	1:A:403:LEU:HB3	2.28	0.62
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.33	0.62
1:A:409:PRO:HD2	1:B:273:PHE:CD2	2.34	0.62
1:B:367:ILE:HD12	1:B:403:LEU:HB3	1.80	0.62
1:A:32:LEU:HD22	1:A:222:TYR:O	1.98	0.62
1:B:383:PHE:HD1	1:B:396:PHE:CE1	2.18	0.62
1:B:390:VAL:O	1:B:391:LYS:CB	2.47	0.61
1:B:367:ILE:CD1	1:B:403:LEU:HB3	2.30	0.61
1:A:225:HIS:HA	1:A:226:TRP:CE3	2.35	0.61
1:B:177:LEU:H	1:B:177:LEU:HD12	1.64	0.61
1:B:57:GLN:CA	1:B:57:GLN:NE2	2.63	0.61
1:B:213:LYS:H	1:B:213:LYS:HD2	1.66	0.60
1:A:210:PRO:HD2	1:A:211:PHE:CE2	2.36	0.60
1:A:269:VAL:HG23	1:A:275:LEU:HD11	1.84	0.60
1:A:177:LEU:H	1:A:177:LEU:HD12	1.67	0.59
1:A:277:TRP:HA	1:A:280:GLN:HE21	1.67	0.59
1:B:227:ARG:HH11	1:B:227:ARG:HG3	1.67	0.59
1:A:270:ILE:HD13	1:A:310:LEU:HD13	1.86	0.58
1:A:220:ARG:NH1	1:A:256:VAL:O	2.35	0.58
1:A:386:GLN:NE2	1:A:390:VAL:CG2	2.66	0.57
1:A:53:ASN:ND2	1:A:62:SER:HB2	2.19	0.57
1:B:250:GLN:O	1:B:251:GLU:C	2.42	0.57
1:A:363:ARG:HG2	1:A:363:ARG:NH1	2.20	0.56
1:B:277:TRP:HA	1:B:280:GLN:HE21	1.71	0.56
1:A:366:THR:HG22	1:A:404:ARG:CA	2.35	0.56
1:A:57:GLN:CA	1:A:57:GLN:NE2	2.69	0.55
1:B:137:VAL:HG12	1:B:171:GLY:HA2	1.89	0.55
1:A:384:ILE:HD12	1:A:397:TYR:CD1	2.41	0.55
1:B:138:GLY:HA3	1:B:173:TYR:O	2.07	0.55
1:B:225:HIS:HA	1:B:226:TRP:CE3	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:237:LYS:CE	1:B:237:LYS:HE3	2.37	0.54
1:B:57:GLN:CA	1:B:57:GLN:HE21	2.21	0.53
1:A:158:THR:O	1:A:161:ASP:HB2	2.08	0.53
1:A:125:HIS:O	1:A:128:GLY:N	2.33	0.53
1:B:108:ALA:HB1	1:B:113:PHE:HB2	1.91	0.53
1:A:103:GLU:CD	1:A:105:ARG:HH12	2.12	0.53
1:B:32:LEU:N	1:B:220:ARG:O	2.41	0.53
1:B:363:ARG:HG2	1:B:363:ARG:HH11	1.74	0.52
1:B:66:GLU:OE1	1:B:114:PRO:HG2	2.09	0.52
1:A:398:GLU:HA	1:A:398:GLU:OE2	2.08	0.52
1:A:355:ASN:HB3	1:A:408:ASN:O	2.10	0.52
1:B:403:LEU:HD21	1:B:415:LEU:HD13	1.92	0.52
1:B:216:TYR:HA	1:B:219:ILE:HD12	1.90	0.51
1:A:366:THR:HA	1:A:403:LEU:O	2.10	0.51
1:B:201:SER:HB2	1:B:225:HIS:CE1	2.46	0.51
1:B:386:GLN:HA	1:B:415:LEU:HD23	1.92	0.51
1:B:269:VAL:HG23	1:B:275:LEU:HD11	1.93	0.50
1:B:270:ILE:HD13	1:B:310:LEU:HD13	1.94	0.50
1:A:211:PHE:O	1:A:212:GLN:HB3	2.11	0.50
1:B:203:GLU:HG3	1:B:227:ARG:HB2	1.93	0.50
1:A:235:SER:OG	1:A:238:SER:HB2	2.12	0.50
1:B:32:LEU:HD22	1:B:222:TYR:O	2.12	0.50
1:A:319:ILE:HD11	1:A:387:LEU:CD2	2.42	0.49
1:B:72:MET:SD	1:B:300:LEU:HB2	2.52	0.49
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.93	0.49
1:A:386:GLN:HA	1:A:415:LEU:HD23	1.95	0.49
1:A:268:LEU:HA	1:A:283:GLN:HE22	1.78	0.49
1:A:390:VAL:O	1:A:391:LYS:CB	2.61	0.48
1:A:108:ALA:HB1	1:A:113:PHE:HB2	1.95	0.48
1:B:125:HIS:HE1	1:B:165:ASP:OD2	1.96	0.48
1:B:382:CYS:HB3	1:B:397:TYR:HB2	1.96	0.48
1:A:236:TRP:NE1	1:A:240:LYS:HD2	2.28	0.48
1:A:359:ILE:HD12	1:B:233:ASP:HB3	1.95	0.48
1:B:236:TRP:CE3	1:B:279:GLN:HG2	2.48	0.48
1:A:203:GLU:HG3	1:A:227:ARG:HB2	1.96	0.48
1:A:134:TYR:CD2	1:A:134:TYR:C	2.87	0.47
1:B:353:MET:O	1:B:412:THR:HA	2.14	0.47
1:B:67:LYS:HD3	1:B:67:LYS:H	1.79	0.47
1:A:88:TYR:CZ	1:A:130:LYS:HD2	2.49	0.47
1:A:331:LEU:HD22	1:A:341:GLU:OE2	2.15	0.47
1:B:55:ASP:OD2	1:B:57:GLN:HB2	2.14	0.47
1:B:386:GLN:NE2	1:B:390:VAL:CG2	2.73	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:166:LEU:HD23	1:A:167:LEU:N	2.29	0.47
1:B:372:LEU:HA	1:B:372:LEU:HD12	1.70	0.47
1:A:403:LEU:HD21	1:A:415:LEU:HD13	1.97	0.47
1:B:372:LEU:O	1:B:374:LYS:N	2.42	0.47
1:A:67:LYS:H	1:A:67:LYS:HD3	1.80	0.47
1:A:202:CYS:O	1:A:226:TRP:HA	2.15	0.46
1:A:372:LEU:HA	1:A:372:LEU:HD12	1.75	0.46
1:B:398:GLU:OE2	1:B:398:GLU:HA	2.15	0.46
1:B:378:CYS:O	1:B:399:TRP:HD1	1.99	0.46
1:B:341:GLU:HA	1:B:350:ALA:O	2.15	0.46
1:B:211:PHE:O	1:B:212:GLN:HB3	2.16	0.46
1:A:210:PRO:HD2	1:A:211:PHE:CZ	2.51	0.45
1:B:88:TYR:CZ	1:B:130:LYS:HD2	2.52	0.45
1:B:228:ASN:HB3	1:B:245:TRP:CH2	2.51	0.45
1:B:33:ASP:O	2:B:692:NAG:H4	2.16	0.45
1:A:250:GLN:O	1:A:251:GLU:C	2.55	0.45
1:B:377:ALA:O	1:B:378:CYS:SG	2.75	0.45
1:A:404:ARG:HH12	1:B:58:GLU:HB3	1.82	0.44
1:A:237:LYS:NZ	1:B:237:LYS:HE3	2.33	0.44
1:A:236:TRP:CE3	1:A:279:GLN:HG2	2.53	0.44
1:B:315:ASP:O	1:B:318:ALA:HB3	2.18	0.44
1:A:267:MET:SD	1:A:297:SER:HB2	2.57	0.44
1:A:118:ARG:O	1:A:122:ASN:HB2	2.16	0.44
1:B:313:ASP:O	1:B:317:ILE:HG13	2.18	0.44
1:B:268:LEU:HA	1:B:283:GLN:HE22	1.82	0.44
1:B:366:THR:HG22	1:B:404:ARG:CA	2.46	0.44
1:B:384:ILE:HD12	1:B:397:TYR:CD1	2.52	0.44
1:B:236:TRP:CD1	1:B:240:LYS:HD2	2.53	0.44
1:A:201:SER:HB2	1:A:225:HIS:CE1	2.53	0.44
1:A:378:CYS:O	1:A:399:TRP:HD1	2.01	0.43
1:B:390:VAL:O	1:B:391:LYS:HB2	2.17	0.43
1:B:333:GLN:HB2	1:B:333:GLN:HE21	1.55	0.43
1:A:265:PRO:O	1:A:266:ASP:CB	2.67	0.43
1:A:57:GLN:HE21	1:A:57:GLN:HA	1.81	0.43
1:A:228:ASN:HB3	1:A:245:TRP:CZ3	2.54	0.43
1:A:277:TRP:HA	1:A:280:GLN:NE2	2.32	0.43
1:A:67:LYS:O	1:A:71:GLU:HB2	2.19	0.43
1:B:48:GLU:N	1:B:267:MET:HE1	2.33	0.43
1:A:383:PHE:HD1	1:A:396:PHE:CE1	2.37	0.42
1:B:379:ASN:HA	1:B:380:PRO:HA	1.87	0.42
1:A:200:TYR:CE2	1:A:202:CYS:SG	3.12	0.42
1:A:341:GLU:HA	1:A:350:ALA:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:200:TYR:CE2	1:B:202:CYS:SG	3.12	0.42
1:B:134:TYR:CD2	1:B:134:TYR:C	2.93	0.42
1:B:220:ARG:NH1	1:B:256:VAL:O	2.53	0.42
1:A:417:LEU:HD12	1:A:417:LEU:N	2.34	0.42
1:A:169:PHE:HB3	1:A:184:TYR:HE1	1.85	0.42
1:A:192:ASN:ND2	2:A:692:NAG:O7	2.53	0.42
1:A:379:ASN:HA	1:A:380:PRO:HA	1.81	0.41
1:A:48:GLU:N	1:A:267:MET:HE1	2.36	0.41
1:B:366:THR:HA	1:B:403:LEU:O	2.20	0.41
1:B:237:LYS:HB2	1:B:237:LYS:HE2	1.69	0.41
1:A:333:GLN:HE21	1:A:333:GLN:HB2	1.60	0.41
1:B:226:TRP:O	1:B:264:ASP:HB3	2.21	0.41
1:B:169:PHE:HB3	1:B:184:TYR:HE1	1.86	0.41
1:A:349:TRP:CD1	1:A:377:ALA:HB2	2.56	0.41
1:A:378:CYS:O	1:A:399:TRP:CD1	2.74	0.40
1:B:204:TRP:HB3	1:B:205:PRO:HD3	2.02	0.40
1:B:103:GLU:CD	1:B:105:ARG:HH12	2.25	0.40
1:A:62:SER:O	1:A:63:CYS:C	2.60	0.40
1:A:133:ILE:HG13	1:A:134:TYR:H	1.86	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:B:210:PRO:CB	2:A:692:NAG:O5[4_545]	2.05	0.15

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%)	347 (89%)	33 (8%)	8 (2%)	11	45
1	B	388/398 (98%)	342 (88%)	40 (10%)	6 (2%)	15	56
All	All	776/796 (98%)	689 (89%)	73 (9%)	14 (2%)	13	51

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	230	ALA
1	B	266	ASP
1	A	266	ASP
1	A	391	LYS
1	B	212	GLN
1	B	230	ALA
1	B	391	LYS
1	A	122	ASN
1	B	57	GLN
1	B	175	ASP
1	A	57	GLN
1	A	372	LEU
1	A	378	CYS

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%)	282 (85%)	49 (15%)	4	20
1	B	331/339 (98%)	276 (83%)	55 (17%)	3	15
All	All	662/678 (98%)	558 (84%)	104 (16%)	4	18

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	49	ARG
1	A	56	CYS
1	A	62	SER
1	A	63	CYS
1	A	67	LYS
1	A	70	MET
1	A	74	GLU
1	A	82	LYS
1	A	87	GLU
1	A	96	MET
1	A	99	GLN

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Mol	Chain	Res	Type
1	A	122	ASN
1	A	127	LYS
1	A	133	ILE
1	A	134	TYR
1	A	148	SER
1	A	169	PHE
1	A	177	LEU
1	A	209	TRP
1	A	213	LYS
1	A	220	ARG
1	A	237	LYS
1	A	241	SER
1	A	255	ASP
1	A	267	MET
1	A	287	TRP
1	A	300	LEU
1	A	306	GLN
1	A	310	LEU
1	A	314	LYS
1	A	332	ARG
1	A	333	GLN
1	A	357	GLN
1	A	358	GLU
1	A	363	ARG
1	A	364	SER
1	A	367	ILE
1	A	369	VAL
1	A	372	LEU
1	A	374	LYS
1	A	379	ASN
1	A	382	CYS
1	A	385	THR
1	A	391	LYS
1	A	392	ARG
1	A	398	GLU
1	A	419	ASN
1	A	421	MET
1	B	45	LEU
1	B	49	ARG
1	B	56	CYS
1	B	57	GLN
1	B	59	GLU

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Mol	Chain	Res	Type
1	B	62	SER
1	B	63	CYS
1	B	67	LYS
1	B	74	GLU
1	B	82	LYS
1	B	92	ASP
1	B	96	MET
1	B	99	GLN
1	B	122	ASN
1	B	133	ILE
1	B	134	TYR
1	B	169	PHE
1	B	177	LEU
1	B	203	GLU
1	B	209	TRP
1	B	213	LYS
1	B	220	ARG
1	B	237	LYS
1	B	238	SER
1	B	241	SER
1	B	252	ARG
1	B	255	ASP
1	B	256	VAL
1	B	267	MET
1	B	287	TRP
1	B	300	LEU
1	B	306	GLN
1	B	310	LEU
1	B	314	LYS
1	B	324	LEU
1	B	332	ARG
1	B	333	GLN
1	B	345	SER
1	B	353	MET
1	B	357	GLN
1	B	358	GLU
1	B	363	ARG
1	B	364	SER
1	B	367	ILE
1	B	369	VAL
1	B	372	LEU
1	B	374	LYS

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Mol	Chain	Res	Type
1	B	382	CYS
1	B	385	THR
1	B	387	LEU
1	B	388	LEU
1	B	391	LYS
1	B	392	ARG
1	B	398	GLU
1	B	421	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	57	GLN
1	A	125	HIS
1	A	192	ASN
1	A	212	GLN
1	A	280	GLN
1	A	333	GLN
1	A	379	ASN
1	A	386	GLN
1	B	46	HIS
1	B	57	GLN
1	B	125	HIS
1	B	179	ASN
1	B	186	HIS
1	B	192	ASN
1	B	212	GLN
1	B	280	GLN
1	B	333	GLN
1	B	379	ASN
1	B	386	GLN

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 ⓘ

4 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	2	12,14,15	0.49	0	15,19,21	2.41	4 (26%)
2	NAG	A	693	2	12,14,15	0.56	0	15,19,21	1.88	4 (26%)
2	NAG	B	692	2	12,14,15	0.63	0	15,19,21	1.10	2 (13%)
2	NAG	B	693	2	12,14,15	0.94	1 (8%)	15,19,21	2.47	6 (40%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	693	NAG	O5-C5	-2.17	1.41	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	693	NAG	O5-C5-C6	-7.01	99.62	106.98
2	A	692	NAG	O5-C5-C6	6.49	113.79	106.98
2	A	693	NAG	O5-C5-C4	4.36	116.18	110.65
2	A	692	NAG	C2-N2-C7	-4.02	116.34	123.09
2	A	692	NAG	C3-C2-N2	3.82	117.58	111.76
2	A	693	NAG	O7-C7-N2	3.29	128.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	693	NAG	C3-C4-C5	3.25	116.01	110.20
2	B	693	NAG	C2-N2-C7	-3.08	117.92	123.09
2	B	693	NAG	O5-C5-C4	2.82	114.24	110.65
2	A	693	NAG	C2-N2-C7	2.76	127.73	123.09
2	B	692	NAG	C2-N2-C7	2.55	127.38	123.09
2	A	693	NAG	C8-C7-N2	-2.23	111.75	116.11
2	A	692	NAG	O5-C5-C4	2.22	113.47	110.65
2	B	693	NAG	O3-C3-C2	2.07	113.44	109.09
2	B	693	NAG	O4-C4-C3	-2.03	105.80	110.35
2	B	692	NAG	O5-C5-C4	2.00	113.19	110.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	692	NAG	O7-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	1	-	4,4,4	0.17	0	6,6,6	0.63	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	SO4	A	1	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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	390/398 (97%)	-0.21	1 (0%)	91 47	117, 121, 123, 128	0
1	B	390/398 (97%)	-0.13	1 (0%)	91 47	117, 121, 123, 128	0
All	All	780/796 (97%)	-0.17	2 (0%)	91 47	117, 121, 123, 128	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	GLY	3.4
1	A	421	MET	2.1

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
2	NAG	B	692	14/15	0.27	-0.28	142,144,147,150	0
2	NAG	A	692	14/15	0.13	-1.06	126,130,134,136	0
2	NAG	B	693	14/15	0.24	-1.12	141,143,144,144	0
2	NAG	A	693	14/15	0.13	-1.26	136,138,140,141	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(Å ²)	Q<0.9
3	SO4	A	1	5/5	0.08	-1.82	125,126,127,127	0

6.5 Other polymers

There are no such residues in this entry.