



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:40 PM UTC

PDB ID : 3CZN / pdb_00003czn
Title : Golgi alpha-mannosidase II (D204A nucleophile mutant) in complex with Gn-Man5Gn
Authors : Shah, N.; Rose, D.R.
Deposited on : 2008-04-29
Resolution : 1.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

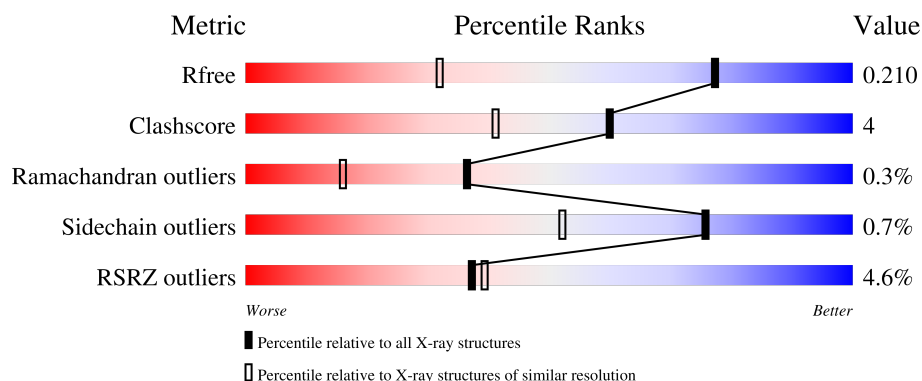
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

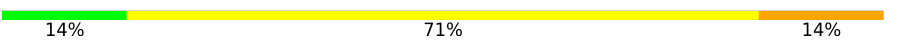
The reported resolution of this entry is 1.40 Å.

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}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	1045	
2	B	7	

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.

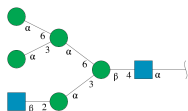
- Molecule 1 is a protein called Alpha-mannosidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1014	Total	C	N	O	S	0	35	0
			8434	5363	1484	1547	40			

There are 14 discrepancies between the modelled and reference sequences:

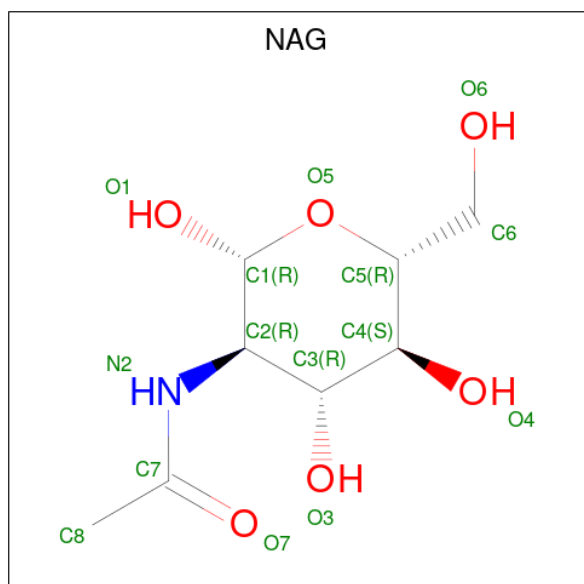
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	expression tag	UNP Q24451
A	2	SER	-	expression tag	UNP Q24451
A	3	SER	-	expression tag	UNP Q24451
A	4	HIS	-	expression tag	UNP Q24451
A	5	HIS	-	expression tag	UNP Q24451
A	6	HIS	-	expression tag	UNP Q24451
A	7	HIS	-	expression tag	UNP Q24451
A	8	HIS	-	expression tag	UNP Q24451
A	9	HIS	-	expression tag	UNP Q24451
A	10	GLY	-	expression tag	UNP Q24451
A	11	GLU	-	expression tag	UNP Q24451
A	12	PHE	-	expression tag	UNP Q24451
A	204	ALA	ASP	engineered mutation	UNP Q24451
A	907	LYS	GLU	SEE REMARK 999	UNP Q24451

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			84	46	2	36			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

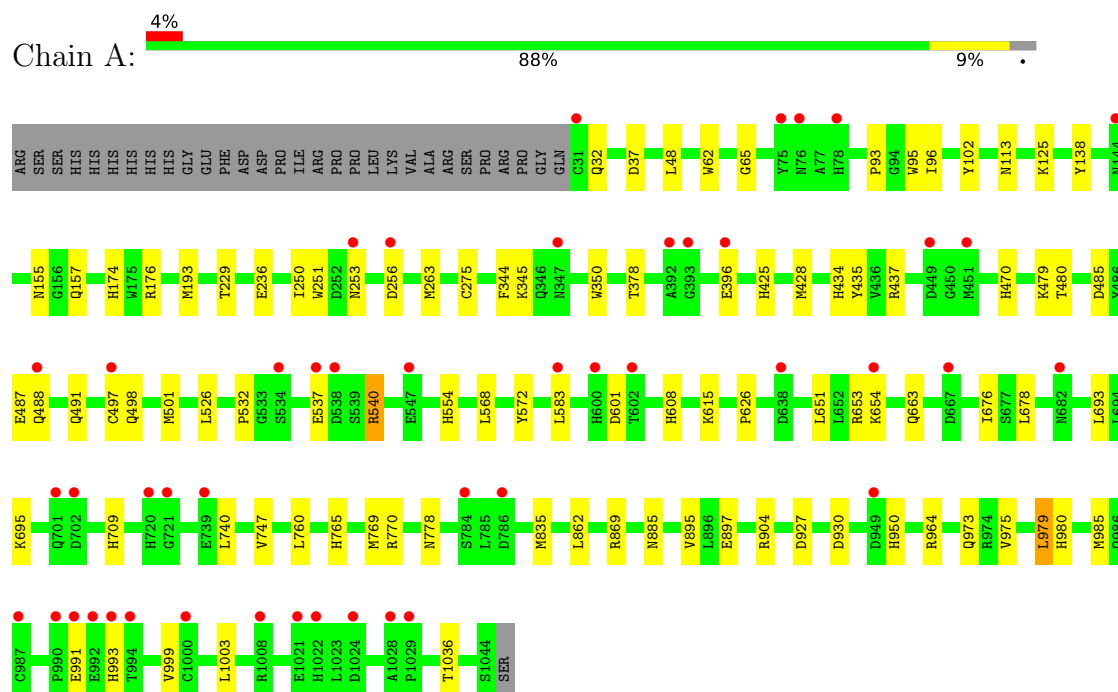
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1158	Total	O	0	0
			1158	1158		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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-mannosidase 2



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.93Å 109.58Å 138.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.54 – 1.40 10.54 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.54-1.40) 99.7 (10.54-1.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.24 (at 1.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.197 (Not available) , 0.210	Depositor DCC
R_{free} test set	10286 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9691	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: BMA, NDG, NAG, MAN, ZN

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	0.47	0/8696	0.68	1/11803 (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	654	LYS	N-CA-C	-5.42	102.46	110.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	8434	0	8249	71	0
2	B	84	0	68	1	0
3	A	14	0	13	0	0
4	A	1	0	0	0	0
5	A	1158	0	0	19	0
All	All	9691	0	8330	72	0

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 4.

All (72) 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:498[B]:GLN:HG2	1:A:526:LEU:HD12	1.26	1.17
1:A:434:HIS:HE1	1:A:930:ASP:OD1	1.61	0.82
1:A:651:LEU:HD11	1:A:653[B]:ARG:HE	1.46	0.81
1:A:435:TYR:HB3	1:A:497[A]:CYS:SG	2.22	0.79
1:A:497[A]:CYS:SG	1:A:501:MET:SD	2.81	0.78
1:A:964:ARG:HH11	1:A:973:GLN:HE21	1.34	0.76
1:A:709[A]:HIS:CD2	5:A:2137:HOH:O	2.44	0.70
1:A:155:ASN:HD21	1:A:157:GLN:HE21	1.42	0.67
1:A:498[A]:GLN:HE21	1:A:526:LEU:H	1.41	0.67
1:A:678:LEU:HD12	1:A:769:MET:HE1	1.78	0.65
1:A:532[B]:PRO:CG	1:A:537:GLU:HB3	2.27	0.65
1:A:979:LEU:HD21	1:A:999:VAL:HG11	1.79	0.64
1:A:434:HIS:HD2	1:A:927:ASP:OD1	1.81	0.64
1:A:678:LEU:CD1	1:A:769:MET:HE1	2.29	0.63
1:A:980:HIS:HE1	5:A:1217:HOH:O	1.81	0.62
1:A:765:HIS:HE1	5:A:1245:HOH:O	1.85	0.59
1:A:950:HIS:HE1	5:A:1495:HOH:O	1.87	0.58
1:A:980:HIS:HD2	1:A:1036:THR:OG1	1.88	0.57
1:A:434:HIS:CE1	1:A:930:ASP:OD1	2.51	0.57
1:A:174:HIS:CE1	1:A:176[A]:ARG:HD3	2.39	0.57
1:A:498[B]:GLN:HG2	1:A:526:LEU:CD1	2.18	0.56
1:A:626:PRO:O	1:A:950:HIS:HD2	1.89	0.56
1:A:532[B]:PRO:HG3	1:A:537:GLU:HB3	1.86	0.55
1:A:693:LEU:HD13	5:A:1586:HOH:O	2.07	0.55
1:A:572:TYR:CD2	1:A:615:LYS:HD3	2.42	0.55
1:A:532[B]:PRO:HG2	1:A:537:GLU:HB3	1.87	0.54
1:A:765:HIS:HD2	1:A:778:ASN:OD1	1.90	0.54
1:A:869:ARG:HH11	1:A:885:ASN:HD22	1.56	0.54
1:A:904:ARG:HG2	1:A:985:MET:SD	2.48	0.53
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.90	0.53
1:A:125[A]:LYS:HD3	1:A:157:GLN:HA	1.91	0.53
1:A:32:GLN:NE2	5:A:1903:HOH:O	2.41	0.52
1:A:256:ASP:HB2	5:A:1903:HOH:O	2.09	0.51
1:A:540:ARG:HG2	5:A:1841:HOH:O	2.10	0.51
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.46	0.51
1:A:491[B]:GLN:NE2	5:A:1562:HOH:O	2.44	0.49
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.42	0.49
1:A:125[A]:LYS:HD2	1:A:378:THR:HG23	1.95	0.49
1:A:113:ASN:HB2	5:A:2229:HOH:O	2.13	0.49
1:A:176[B]:ARG:HH22	1:A:437:ARG:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:HIS:HD2	5:A:1499:HOH:O	1.95	0.49
1:A:663:GLN:HG3	5:A:1881:HOH:O	2.13	0.48
1:A:96:ILE:HG13	1:A:102:TYR:OH	2.12	0.48
1:A:96:ILE:HA	1:A:479:LYS:HG3	1.95	0.48
1:A:37:ASP:HB3	1:A:253:ASN:ND2	2.29	0.47
1:A:540:ARG:HG3	1:A:572:TYR:CE2	2.48	0.47
1:A:428:MET:HE1	1:A:491[B]:GLN:HG2	1.96	0.47
1:A:498[A]:GLN:NE2	1:A:526:LEU:H	2.10	0.47
1:A:174:HIS:CE1	1:A:176[B]:ARG:HG3	2.49	0.46
1:A:709[A]:HIS:HD2	5:A:2137:HOH:O	1.86	0.46
1:A:425:HIS:HE1	1:A:487:GLU:OE1	1.99	0.45
1:A:601:ASP:HB2	1:A:608:HIS:CE1	2.52	0.45
1:A:653[B]:ARG:NH2	5:A:1734:HOH:O	2.44	0.45
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.52	0.45
1:A:229:THR:HG21	1:A:263:MET:HE2	1.99	0.45
5:A:1875:HOH:O	2:B:1:NDG:H6C2	2.17	0.44
1:A:488:GLN:NE2	5:A:2130:HOH:O	2.42	0.44
1:A:48:LEU:HD11	1:A:236:GLU:HG2	2.00	0.43
1:A:344:PHE:HB3	1:A:350:TRP:CE2	2.54	0.43
1:A:568:LEU:HD12	1:A:770:ARG:HD3	2.01	0.43
1:A:480:THR:HG23	5:A:1717:HOH:O	2.19	0.42
1:A:485:ASP:HA	1:A:488:GLN:HE21	1.84	0.42
1:A:250:ILE:HD11	5:A:1796:HOH:O	2.19	0.42
1:A:676:ILE:HD13	1:A:747:VAL:HG21	2.03	0.41
1:A:251:TRP:CD1	1:A:251:TRP:C	2.97	0.41
1:A:975:VAL:HG21	1:A:1003:LEU:HD12	2.02	0.41
1:A:651:LEU:CD1	1:A:653[A]:ARG:HG2	2.50	0.41
1:A:345:LYS:C	5:A:2229:HOH:O	2.64	0.41
1:A:835:MET:HE2	1:A:862:LEU:HD22	2.01	0.41
1:A:885:ASN:H	1:A:885:ASN:ND2	2.19	0.40
1:A:138:TYR:CE1	1:A:193:MET:HE1	2.56	0.40
1:A:740:LEU:HD22	1:A:760:LEU:HD22	2.03	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	1047/1045 (100%)	1020 (97%)	24 (2%)	3 (0%)	36	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	991	GLU
1	A	993	HIS

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	935/928 (101%)	929 (99%)	6 (1%)	78	56

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	CYS
1	A	396	GLU
1	A	540	ARG
1	A	583	LEU
1	A	695	LYS
1	A	979	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	79	HIS
1	A	91	ASN

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Mol	Chain	Res	Type
1	A	119	HIS
1	A	148	GLN
1	A	157	GLN
1	A	191	GLN
1	A	347	ASN
1	A	371	ASN
1	A	394	GLN
1	A	434	HIS
1	A	460	GLN
1	A	470	HIS
1	A	488	GLN
1	A	554	HIS
1	A	585	ASN
1	A	586	ASN
1	A	608	HIS
1	A	765	HIS
1	A	778	ASN
1	A	812	GLN
1	A	866	GLN
1	A	880	GLN
1	A	885	ASN
1	A	919	HIS
1	A	950	HIS
1	A	973	GLN
1	A	980	HIS
1	A	995	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 ⓘ

7 monosaccharides 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	NDG	B	1	2	15,15,15	2.32	1 (6%)	21,21,21	1.57	5 (23%)
2	BMA	B	2	2	11,11,12	0.26	0	15,15,17	0.83	0
2	MAN	B	3	2	11,11,12	0.30	0	15,15,17	0.83	1 (6%)
2	NAG	B	4	2	14,14,15	0.31	0	17,19,21	1.23	2 (11%)
2	MAN	B	5	2	11,11,12	0.40	0	15,15,17	0.96	1 (6%)
2	MAN	B	6	2	11,11,12	0.20	0	15,15,17	0.90	1 (6%)
2	MAN	B	7	2,4	11,11,12	0.53	0	15,15,17	1.14	2 (13%)

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	NDG	B	1	2	-	2/6/26/26	0/1/1/1
2	BMA	B	2	2	-	0/2/19/22	0/1/1/1
2	MAN	B	3	2	-	0/2/19/22	0/1/1/1
2	NAG	B	4	2	-	0/6/23/26	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
2	MAN	B	7	2,4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NDG	C8-C7	-8.76	1.32	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NDG	O5-C5-C4	3.36	115.75	109.70
2	B	1	NDG	C1-C2-N2	-3.29	106.91	110.73
2	B	5	MAN	C1-O5-C5	2.95	116.13	112.19
2	B	7	MAN	C1-C2-C3	2.83	113.76	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NDG	C3-C4-C5	2.81	115.33	110.23
2	B	4	NAG	C4-C3-C2	-2.80	106.92	111.02
2	B	6	MAN	C1-O5-C5	2.76	115.89	112.19
2	B	4	NAG	C2-N2-C7	-2.61	119.41	122.90
2	B	1	NDG	C1-O5-C5	2.51	118.52	113.65
2	B	7	MAN	C1-O5-C5	2.26	115.21	112.19
2	B	3	MAN	C1-O5-C5	2.06	114.94	112.19
2	B	1	NDG	C3-C2-N2	-2.05	106.84	110.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

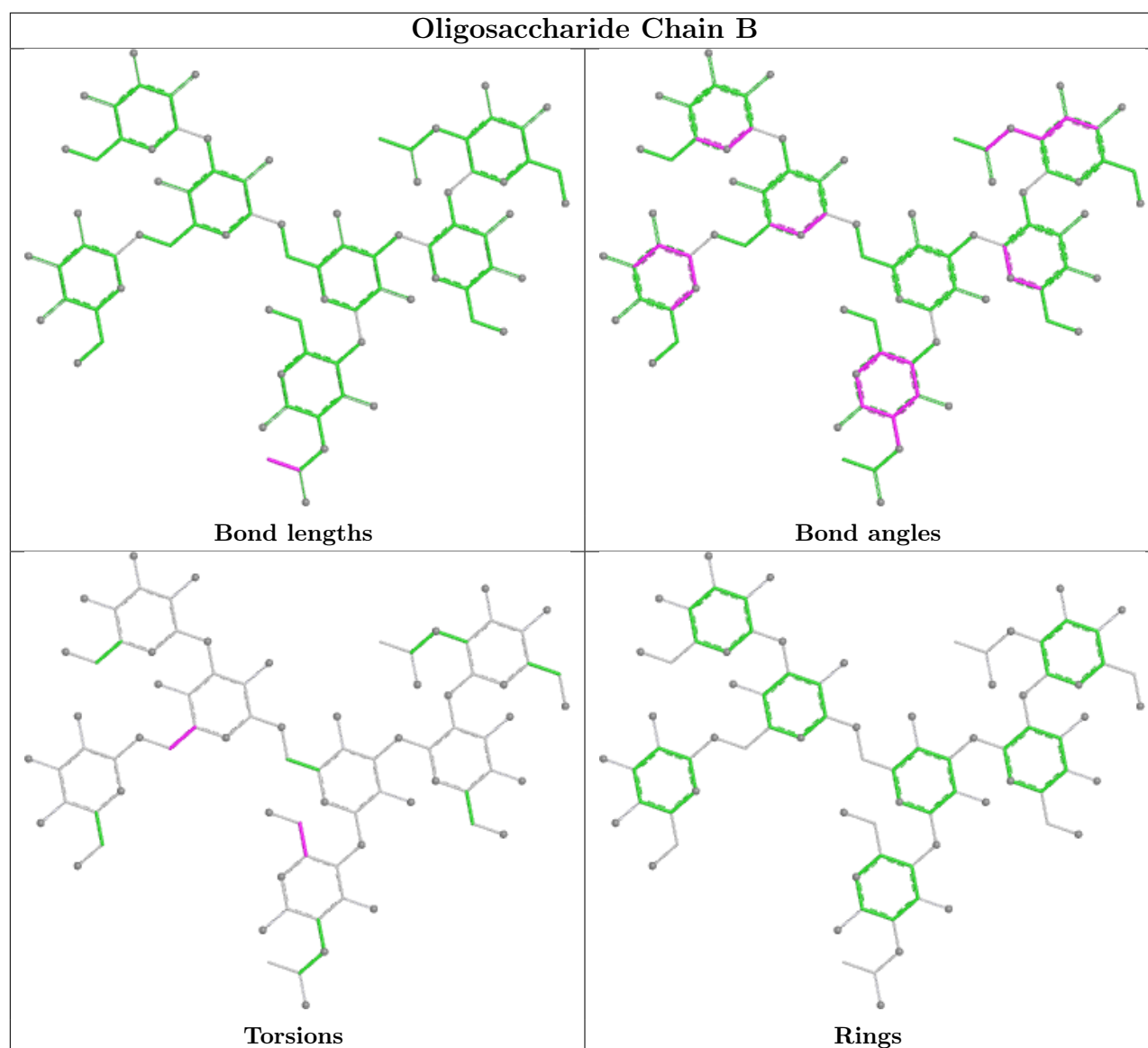
Mol	Chain	Res	Type	Atoms
2	B	1	NDG	C4-C5-C6-O6
2	B	1	NDG	O5-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NDG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	1101	1	14,14,15	0.51	0	17,19,21	0.80	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	1101	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	NAG	C8-C7-N2-C2
3	A	1101	NAG	O7-C7-N2-C2
3	A	1101	NAG	O5-C5-C6-O6
3	A	1101	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1014/1045 (97%)	0.07	47 (4%) 37 39	5, 14, 26, 41	35 (3%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	7.0
1	A	702	ASP	5.4
1	A	583	LEU	4.9
1	A	1024	ASP	4.6
1	A	497[A]	CYS	4.4
1	A	987	CYS	4.1
1	A	992	GLU	4.1
1	A	990	PRO	4.1
1	A	78	HIS	3.7
1	A	537	GLU	3.7
1	A	396	GLU	3.7
1	A	701	GLN	3.6
1	A	600	HIS	3.6
1	A	638	ASP	3.5
1	A	538	ASP	3.4
1	A	451	MET	3.4
1	A	784[A]	SER	3.1
1	A	256	ASP	3.1
1	A	547	GLU	3.1
1	A	602	THR	3.0
1	A	682	ASN	3.0
1	A	991	GLU	2.9
1	A	721	GLY	2.8
1	A	786[A]	ASP	2.8
1	A	31	CYS	2.7
1	A	1028	ALA	2.6
1	A	534	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	144	ASN	2.5
1	A	720[A]	HIS	2.5
1	A	76	ASN	2.5
1	A	253	ASN	2.4
1	A	347	ASN	2.4
1	A	654	LYS	2.3
1	A	1021	GLU	2.3
1	A	1008	ARG	2.2
1	A	393	GLY	2.2
1	A	75	TYR	2.2
1	A	949	ASP	2.2
1	A	392	ALA	2.2
1	A	1022	HIS	2.2
1	A	994	THR	2.2
1	A	488	GLN	2.1
1	A	1029	PRO	2.1
1	A	739	GLU	2.1
1	A	1000	CYS	2.1
1	A	667	ASP	2.1
1	A	449	ASP	2.0

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

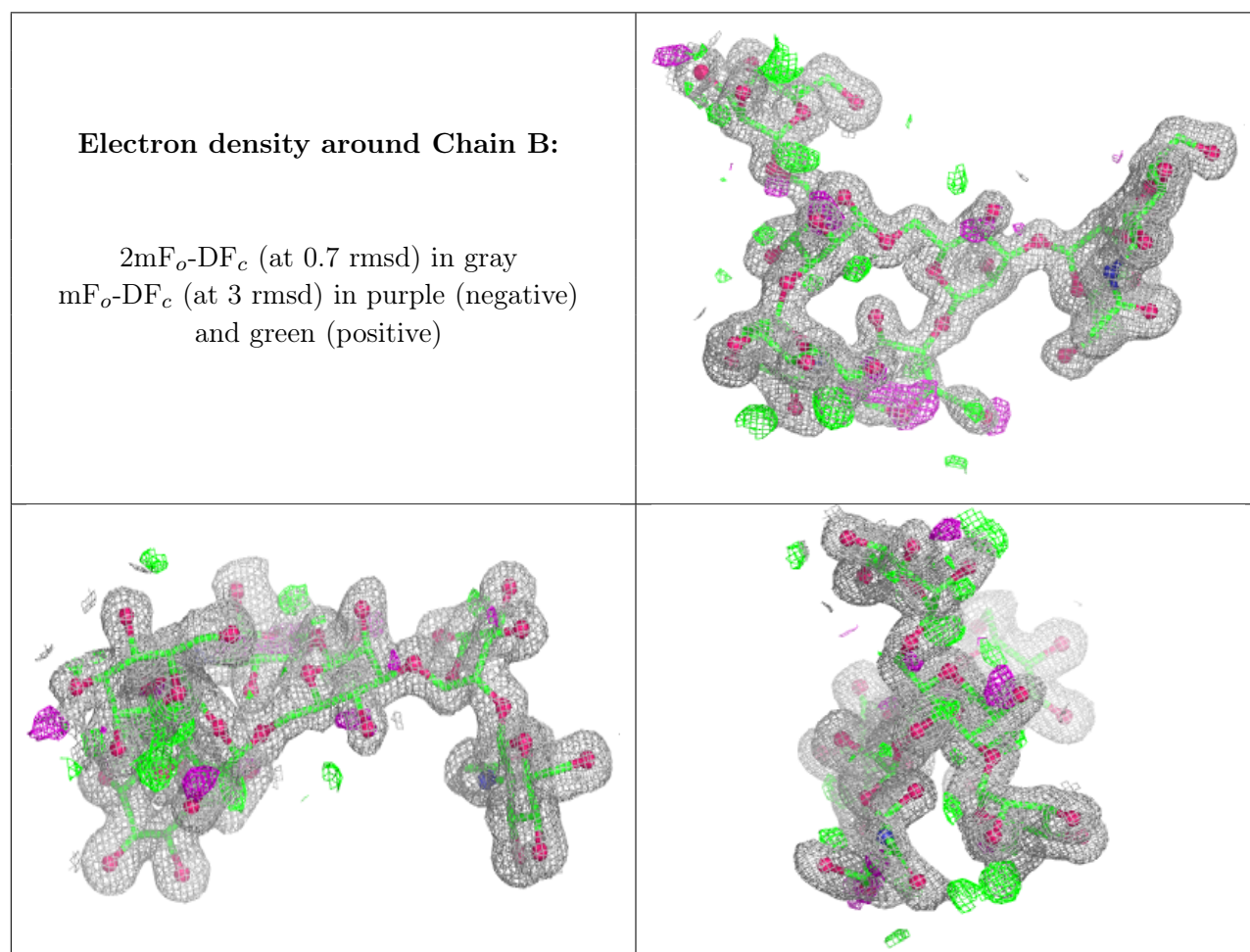
There are no non-standard protein/DNA/RNA residues in this entry.

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. 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	B-factors(Å ²)	Q<0.9
2	NDG	B	1	15/15	0.73	0.14	27,31,34,35	0
2	BMA	B	2	11/12	0.90	0.08	17,20,24,24	0
2	MAN	B	5	11/12	0.90	0.08	15,16,18,18	0
2	MAN	B	3	11/12	0.94	0.06	13,17,21,24	0
2	MAN	B	6	11/12	0.94	0.06	13,14,16,22	0
2	NAG	B	4	14/15	0.95	0.07	12,13,19,19	0
2	MAN	B	7	11/12	0.95	0.06	11,13,16,18	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	1101	14/15	0.54	0.14	31,37,38,39	0
4	ZN	A	1102	1/1	0.99	0.02	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.