



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:22 PM UTC

PDB ID : 3BVU / pdb_00003bvu
Title : GOLGI MANNOSIDASE II D204A catalytic nucleophile mutant complex with Methyl(alpha-D-mannopyranosyl)-(1->3)-S-[(alpha-D-mannopyranosyl)-(1->6)]-alpha-D-mannopyranoside
Authors : Kuntz, D.A.; Rose, D.R.
Deposited on : 2008-01-07
Resolution : 1.12 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

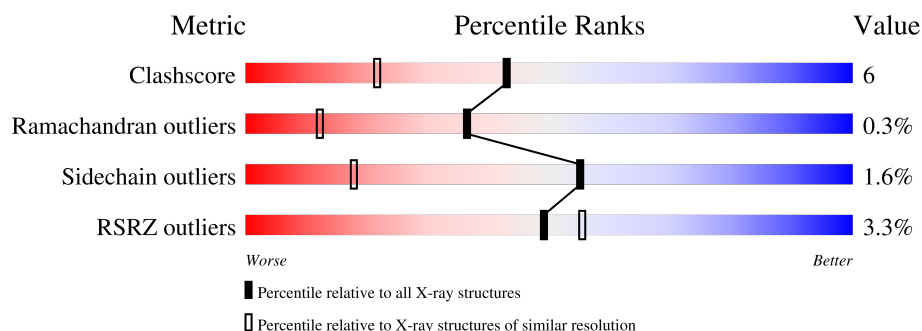
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.12 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))
Clashscore	190562	2021 (1.14-1.10)
Ramachandran outliers	187476	1978 (1.14-1.10)
Sidechain outliers	187428	1974 (1.14-1.10)
RSRZ outliers	180081	1984 (1.14-1.10)

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	3% 85% 11% ..
2	B	3	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10001 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-mannosidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1015	Total	C	N	O	S	3	42	0
			8422	5373	1466	1539	44			

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 alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl 3-thio-alpha-D-mannopyranoside.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	O	S	0	1	0
			36	19	16	1			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

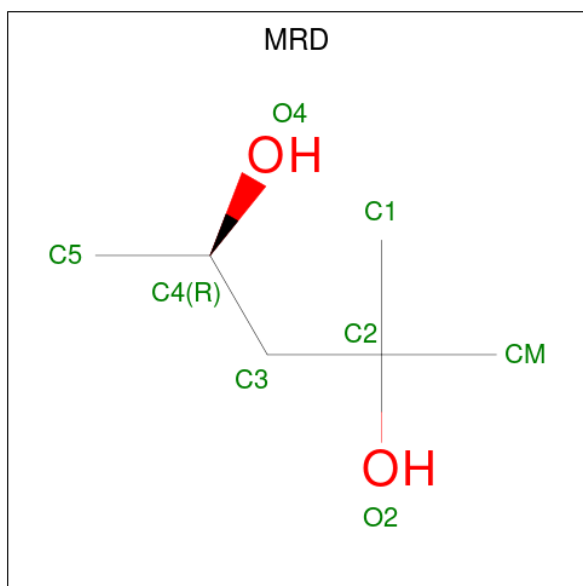


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

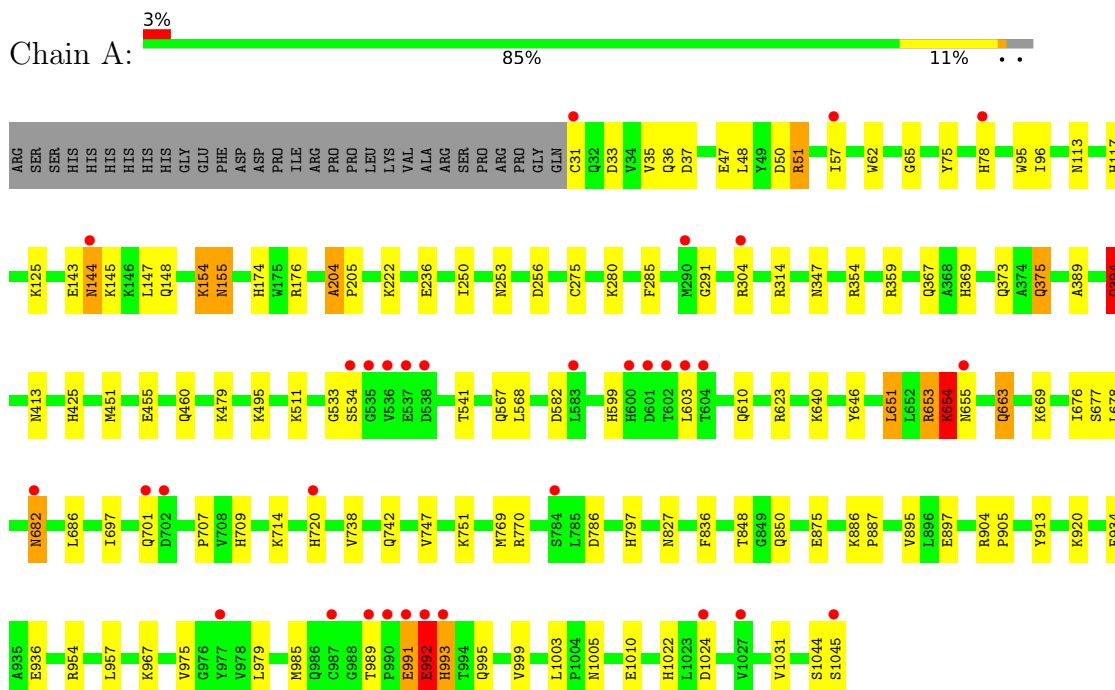
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1499	Total	O	0	16
			1515	1515		

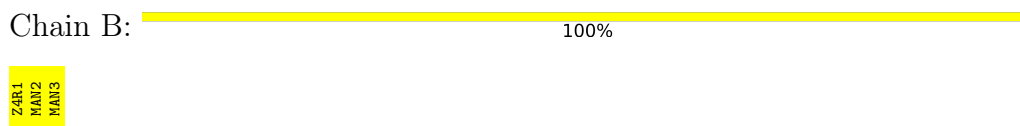
3 Residue-property plots [i](#)

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: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl 3-thio-alpha-D-mannopyranoside



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.99Å 109.79Å 139.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.12 20.00 – 1.12	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-1.12) 93.4 (20.00-1.12)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.12Å)	Xtriage
Refinement program	SHELX, SHELXL-97	Depositor
R, R_{free}	0.114 , 0.155 0.122 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10001	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Z4R, MRD, NAG, MAN, PO4, 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	0.86	0/8772	1.20	37/11903 (0.3%)

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
1	A	0	2

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASN	OD1-CG-ND2	11.69	134.29	122.60
1	A	78	HIS	CA-CB-CG	-9.54	104.25	113.80
1	A	144	ASN	CA-CB-CG	9.24	121.84	112.60
1	A	155	ASN	OD1-CG-ND2	-9.04	113.56	122.60
1	A	155	ASN	CB-CG-ND2	7.68	127.92	116.40
1	A	347	ASN	CA-CB-CG	-7.53	105.08	112.60
1	A	1024	ASP	CA-CB-CG	-7.41	105.19	112.60
1	A	836	PHE	CA-CB-CG	6.92	120.72	113.80
1	A	413	ASN	CA-CB-CG	6.81	119.41	112.60
1	A	663	GLN	OE1-CD-NE2	6.59	129.19	122.60
1	A	113	ASN	CA-CB-CG	-6.53	106.07	112.60
1	A	533	GLY	O-C-N	6.45	128.06	122.64
1	A	875	GLU	CB-CG-CD	6.30	123.32	112.60
1	A	50	ASP	CA-CB-CG	6.24	118.83	112.60
1	A	989	THR	CB-CA-C	-5.93	101.50	110.87
1	A	534	SER	CB-CA-C	5.92	119.14	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	1022	HIS	CA-C-N	-5.81	114.71	122.72
1	A	1022	HIS	C-N-CA	-5.81	114.71	122.72
1	A	603	LEU	CA-C-O	5.78	126.66	120.24
1	A	654	LYS	O-C-N	-5.68	116.32	122.79
1	A	1024	ASP	CA-C-O	5.62	127.38	121.19
1	A	285	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	599	HIS	CA-CB-CG	-5.54	108.26	113.80
1	A	610	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	682	ASN	N-CA-C	-5.34	106.08	112.59
1	A	663	GLN	CB-CG-CD	-5.33	103.53	112.60
1	A	827	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	35	VAL	N-CA-C	5.29	116.11	111.56
1	A	291	GLY	O-C-N	-5.27	115.85	122.70
1	A	394	GLN	OE1-CD-NE2	5.26	127.86	122.60
1	A	460	GLN	OE1-CD-NE2	5.22	127.82	122.60
1	A	582	ASP	CA-C-N	-5.12	114.16	122.65
1	A	582	ASP	C-N-CA	-5.12	114.16	122.65
1	A	646	TYR	CA-CB-CG	-5.05	104.81	113.90
1	A	425	HIS	CA-CB-CG	-5.03	108.77	113.80
1	A	394	GLN	CG-CD-OE1	-5.00	110.80	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1044	SER	Peptide
1	A	992	GLU	Peptide

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	8422	0	8296	99	1
2	B	36	0	12	0	0
3	A	14	0	13	5	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
6	A	8	0	14	0	0
7	A	1515	0	0	46	0
All	All	10001	0	8335	104	1

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.

All (104) 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:669:LYS:HE2	7:A:1461:HOH:O	1.45	1.13
3:A:1046:NAG:H83	3:A:1046:NAG:H3	1.31	1.07
3:A:1046:NAG:H3	3:A:1046:NAG:C8	2.03	0.88
1:A:655:ASN:HB2	7:A:2201:HOH:O	1.76	0.85
1:A:954[B]:ARG:HG2	7:A:1092:HOH:O	1.76	0.85
1:A:117[B]:HIS:HE1	1:A:354:ARG:HE	1.26	0.82
1:A:567:GLN:HB2	7:A:2528:HOH:O	1.82	0.78
1:A:455:GLU:HG2	1:A:967:LYS:HZ2	1.48	0.78
1:A:47:GLU:OE2	1:A:51:ARG:CD	2.33	0.76
1:A:663:GLN:HG3	7:A:2524:HOH:O	1.85	0.76
1:A:47:GLU:OE2	1:A:51:ARG:HD3	1.85	0.76
1:A:117[B]:HIS:CE1	1:A:354:ARG:HE	2.04	0.76
1:A:256:ASP:HB2	7:A:1113:HOH:O	1.86	0.74
1:A:995:GLN:HG3	7:A:1207:HOH:O	1.87	0.73
1:A:47:GLU:CD	1:A:51:ARG:HD3	2.13	0.72
1:A:913:TYR:HB2	1:A:985[B]:MET:HE3	1.71	0.71
1:A:957:LEU:HD11	1:A:979[A]:LEU:HG	1.73	0.70
1:A:144:ASN:HB3	7:A:1593:HOH:O	1.92	0.69
1:A:1010:GLU:HG2	7:A:1190:HOH:O	1.93	0.69
1:A:991:GLU:HA	1:A:991:GLU:OE1	1.94	0.67
1:A:954[B]:ARG:HD2	7:A:1091:HOH:O	1.94	0.67
1:A:250:ILE:HD11	7:A:1935:HOH:O	1.94	0.67
1:A:954[B]:ARG:CD	7:A:1091:HOH:O	2.41	0.67
1:A:848[B]:THR:CG2	1:A:850:GLN:NE2	2.59	0.66
3:A:1046:NAG:H83	3:A:1046:NAG:C3	2.18	0.65
1:A:154:LYS:HE3	7:A:1584:HOH:O	1.96	0.65
1:A:954[B]:ARG:CG	7:A:1091:HOH:O	2.44	0.65
1:A:993:HIS:O	1:A:993:HIS:ND1	2.30	0.64
1:A:905:PRO:HD3	1:A:985[B]:MET:HE1	1.80	0.64
1:A:455:GLU:HG2	1:A:967:LYS:NZ	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ASN:CB	7:A:2201:HOH:O	2.41	0.61
1:A:75:TYR:HD1	7:A:1982:HOH:O	1.84	0.60
1:A:96:ILE:HG23	1:A:479:LYS:HE2	1.84	0.60
1:A:678:LEU:HD12	1:A:769[A]:MET:HE1	1.84	0.60
1:A:96:ILE:HG22	7:A:2349:HOH:O	2.00	0.59
1:A:314:ARG:NH2	7:A:2024:HOH:O	2.34	0.59
1:A:125:LYS:HE2	7:A:2295:HOH:O	2.03	0.59
3:A:1046:NAG:C1	3:A:1046:NAG:H82	2.32	0.59
1:A:904:ARG:HG2	1:A:985[A]:MET:SD	2.43	0.58
1:A:920:LYS:HG3	7:A:1506:HOH:O	2.03	0.58
1:A:541:THR:HG21	7:A:1389:HOH:O	2.04	0.57
1:A:797[B]:HIS:HA	7:A:2119:HOH:O	2.03	0.57
1:A:848[B]:THR:HG23	1:A:850:GLN:NE2	2.19	0.57
1:A:47:GLU:OE2	1:A:51:ARG:HD2	2.04	0.57
1:A:676[A]:ILE:HD13	1:A:747:VAL:HG21	1.87	0.56
1:A:848[B]:THR:HG22	1:A:850:GLN:H	1.70	0.56
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.36	0.55
1:A:709[A]:HIS:ND1	7:A:2232:HOH:O	2.33	0.55
1:A:222:LYS:HD2	7:A:2281:HOH:O	2.06	0.54
1:A:37:ASP:HB2	7:A:1109:HOH:O	2.07	0.54
1:A:57:ILE:HG12	7:A:1804:HOH:O	2.07	0.54
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.89	0.54
1:A:751:LYS:HE3	7:A:1447:HOH:O	2.07	0.54
1:A:145:LYS:HE2	7:A:2525:HOH:O	2.08	0.53
1:A:707:PRO:HG2	1:A:797[A]:HIS:CE1	2.43	0.53
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.39	0.53
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.44	0.52
1:A:623:ARG:NH1	7:A:1212:HOH:O	2.42	0.52
1:A:389:ALA:HB1	1:A:394:GLN:HG2	1.91	0.52
1:A:359:ARG:HD3	7:A:2527:HOH:O	2.10	0.52
1:A:373:GLN:HG3	1:A:375:GLN:HE22	1.75	0.51
1:A:678:LEU:CD1	1:A:769[A]:MET:HE1	2.40	0.51
1:A:934:PHE:CE2	1:A:936[A]:GLU:HB2	2.45	0.50
1:A:96:ILE:HG23	1:A:479:LYS:CE	2.41	0.50
1:A:155:ASN:ND2	7:A:2313:HOH:O	2.43	0.48
1:A:568:LEU:HD12	1:A:770[A]:ARG:HD3	1.96	0.48
1:A:848[B]:THR:CG2	1:A:850:GLN:HE21	2.25	0.48
1:A:848[B]:THR:HG22	1:A:850:GLN:NE2	2.28	0.47
1:A:280:LYS:HE3	7:A:2506:HOH:O	2.14	0.47
1:A:389:ALA:HB1	1:A:394:GLN:CD	2.39	0.47
1:A:886:LYS:NZ	7:A:1478:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979[B]:LEU:HD21	1:A:999:VAL:HG11	1.97	0.46
3:A:1046:NAG:C8	3:A:1046:NAG:C1	2.93	0.46
1:A:511:LYS:NZ	7:A:1328:HOH:O	2.49	0.45
1:A:47:GLU:OE1	1:A:51:ARG:HD3	2.16	0.45
1:A:48:LEU:HD11	1:A:236:GLU:HG2	1.97	0.45
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.51	0.45
1:A:742:GLN:HG3	7:A:2135:HOH:O	2.16	0.45
1:A:954[B]:ARG:HG3	7:A:1091:HOH:O	2.13	0.45
1:A:143:GLU:OE2	1:A:147:LEU:HG	2.17	0.45
1:A:682:ASN:ND2	7:A:2480:HOH:O	2.50	0.45
1:A:848[B]:THR:CG2	1:A:850:GLN:O	2.64	0.45
1:A:653:ARG:HD3	1:A:654:LYS:O	2.18	0.44
1:A:848[B]:THR:HG21	1:A:850:GLN:O	2.18	0.44
1:A:786:ASP:HA	7:A:2355:HOH:O	2.17	0.44
1:A:992:GLU:HB3	1:A:993:HIS:H	1.68	0.43
1:A:451[A]:MET:HA	1:A:451[A]:MET:HE2	2.01	0.43
1:A:714:LYS:HG3	1:A:738:VAL:HG22	2.00	0.43
1:A:33:ASP:O	7:A:1109:HOH:O	2.21	0.42
1:A:75:TYR:HE1	7:A:1981:HOH:O	2.02	0.42
1:A:367:GLN:HB3	1:A:369:HIS:CD2	2.55	0.42
1:A:992:GLU:O	1:A:993:HIS:C	2.62	0.42
1:A:686:LEU:HD22	1:A:697:ILE:HG12	2.00	0.42
1:A:654:LYS:HE3	1:A:654:LYS:HB3	1.63	0.42
1:A:887:PRO:HG2	7:A:2188:HOH:O	2.18	0.42
1:A:1005:ASN:CB	1:A:1045:SER:HA	2.50	0.42
1:A:31:CYS:N	7:A:1202:HOH:O	2.52	0.42
1:A:204:ALA:H	1:A:205:PRO:HD3	1.86	0.41
1:A:96:ILE:HG21	7:A:2543:HOH:O	2.21	0.41
1:A:145:LYS:HD3	1:A:148:GLN:OE1	2.20	0.41
1:A:51:ARG:HG3	7:A:1879:HOH:O	2.21	0.40
1:A:979[A]:LEU:HD23	1:A:1031:VAL:HG13	2.03	0.40
1:A:495:LYS:NZ	7:A:1525:HOH:O	2.50	0.40
1:A:304:ARG:NH2	7:A:1750:HOH:O	2.55	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLN:O	1:A:669:LYS:NZ[3_644]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1055/1045 (101%)	1023 (97%)	29 (3%)	3 (0%)	36	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	993	HIS
1	A	204	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	943/928 (102%)	927 (98%)	16 (2%)	53	16

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	154	LYS
1	A	275	CYS
1	A	375	GLN
1	A	394	GLN
1	A	640	LYS
1	A	651	LEU
1	A	653	ARG

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Mol	Chain	Res	Type
1	A	654	LYS
1	A	677[A]	SER
1	A	677[B]	SER
1	A	701	GLN
1	A	720[A]	HIS
1	A	720[B]	HIS
1	A	991	GLU
1	A	992	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	A	347	ASN
1	A	375	GLN
1	A	610	GLN
1	A	812	GLN
1	A	923	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 ⓘ

4 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	Z4R	B	1	2	12,13,13	1.05	1 (8%)	13,18,18	1.81	2 (15%)
2	MAN	B	2[A]	-	11,11,12	0.93	1 (9%)	15,15,17	1.17	1 (6%)
2	MAN	B	2[B]	-	11,11,12	0.76	0	15,15,17	1.10	1 (6%)
2	MAN	B	3	5,2	11,11,12	1.44	1 (9%)	15,15,17	1.46	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	Z4R	B	1	2	-	1/4/24/24	0/1/1/1
2	MAN	B	2[A]	-	-	0/2/19/22	0/1/1/1
2	MAN	B	2[B]	-	-	0/2/19/22	0/1/1/1
2	MAN	B	3	5,2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	MAN	O2-C2	3.53	1.50	1.43
2	B	2[A]	MAN	O6-C6	-2.49	1.32	1.42
2	B	1	Z4R	O1-C1	2.33	1.44	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	Z4R	C1M-O1-C1	-5.23	105.31	113.26
2	B	3	MAN	C1-C2-C3	3.38	114.56	109.64
2	B	1	Z4R	O1-C1-C2	2.34	110.83	108.14
2	B	2[A]	MAN	C2-C3-C4	-2.14	107.09	110.86
2	B	2[B]	MAN	C2-C3-C4	-2.14	107.09	110.86
2	B	3	MAN	O5-C5-C4	-2.11	105.70	110.83

There are no chirality outliers.

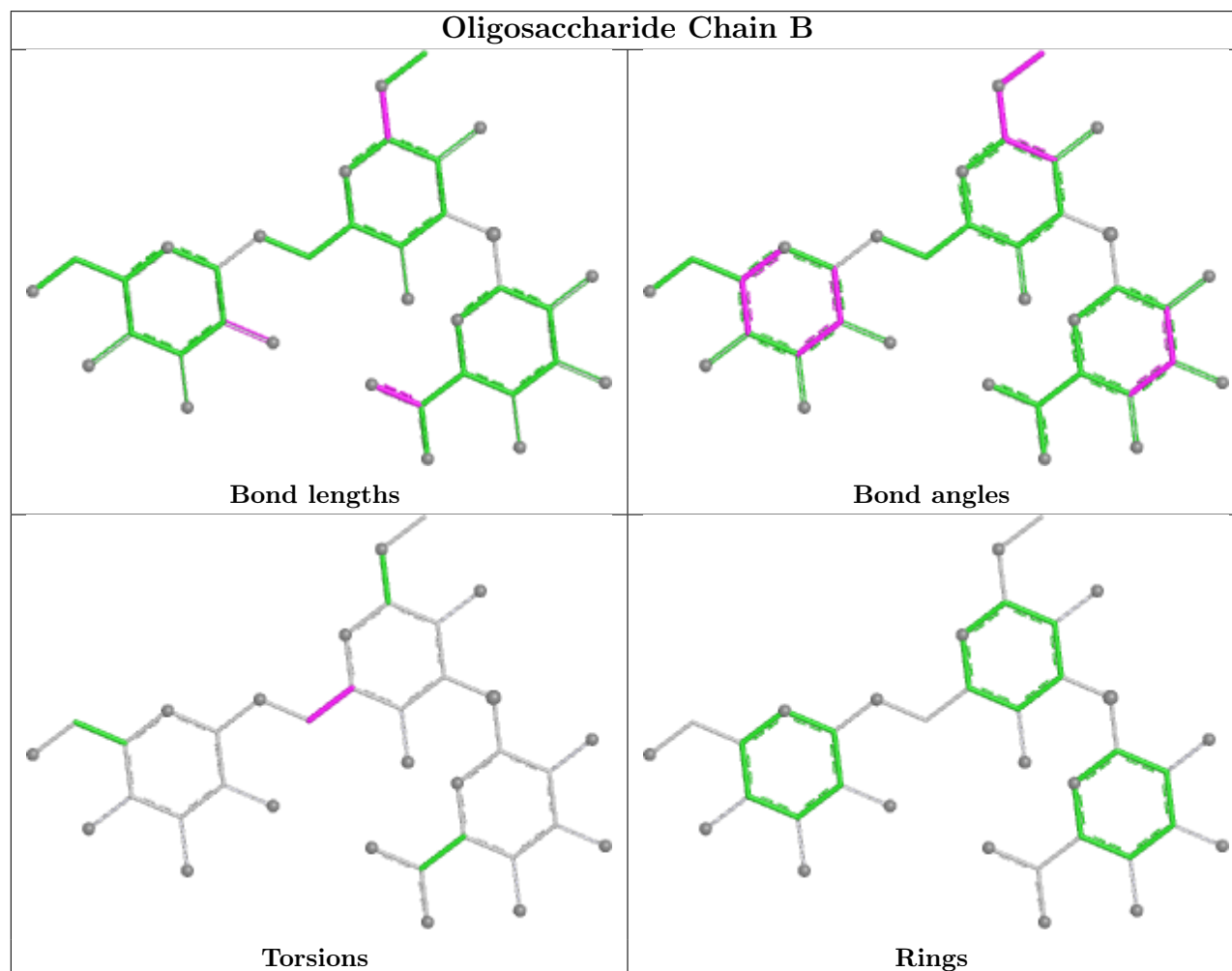
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	Z4R	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	1046	1	14,14,15	0.73	0	17,19,21	1.39	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	A	1047	-	4,4,4	1.86	2 (50%)	6,6,6	0.74	0
6	MRD	A	1049	-	7,7,7	0.76	0	9,10,10	0.88	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	1046	1	-	4/6/23/26	0/1/1/1
6	MRD	A	1049	-	-	3/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1047	PO4	P-O4	-2.44	1.47	1.54
4	A	1047	PO4	P-O3	2.33	1.61	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1046	NAG	C6-C5-C4	-2.35	107.25	113.02
3	A	1046	NAG	O5-C1-C2	-2.29	107.75	111.29
3	A	1046	NAG	C4-C3-C2	-2.03	108.05	111.02

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1049	MRD	C2-C3-C4-O4
6	A	1049	MRD	C2-C3-C4-C5
3	A	1046	NAG	C8-C7-N2-C2
3	A	1046	NAG	O7-C7-N2-C2
3	A	1046	NAG	C3-C2-N2-C7
3	A	1046	NAG	C1-C2-N2-C7
6	A	1049	MRD	O2-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1046	NAG	5	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 ⓘ

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	1015/1045 (97%)	-0.06	33 (3%) 49 55	5, 13, 34, 85	42 (4%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1045	SER	5.4
1	A	990	PRO	4.9
1	A	977	TYR	4.5
1	A	993	HIS	4.4
1	A	992	GLU	3.9
1	A	144	ASN	3.5
1	A	991	GLU	3.3
1	A	602	THR	3.3
1	A	538	ASP	3.2
1	A	655	ASN	3.2
1	A	987	CYS	3.2
1	A	534	SER	3.1
1	A	989	THR	3.0
1	A	702	ASP	3.0
1	A	600	HIS	2.9
1	A	720[A]	HIS	2.8
1	A	57	ILE	2.8
1	A	1024	ASP	2.7
1	A	583	LEU	2.6
1	A	784	SER	2.6
1	A	536	VAL	2.6
1	A	603	LEU	2.5
1	A	1027	VAL	2.4
1	A	78	HIS	2.3
1	A	304	ARG	2.2
1	A	31	CYS	2.2
1	A	701	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	682	ASN	2.1
1	A	601	ASP	2.1
1	A	290	MET	2.1
1	A	604	THR	2.1
1	A	537	GLU	2.0
1	A	535	GLY	2.0

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

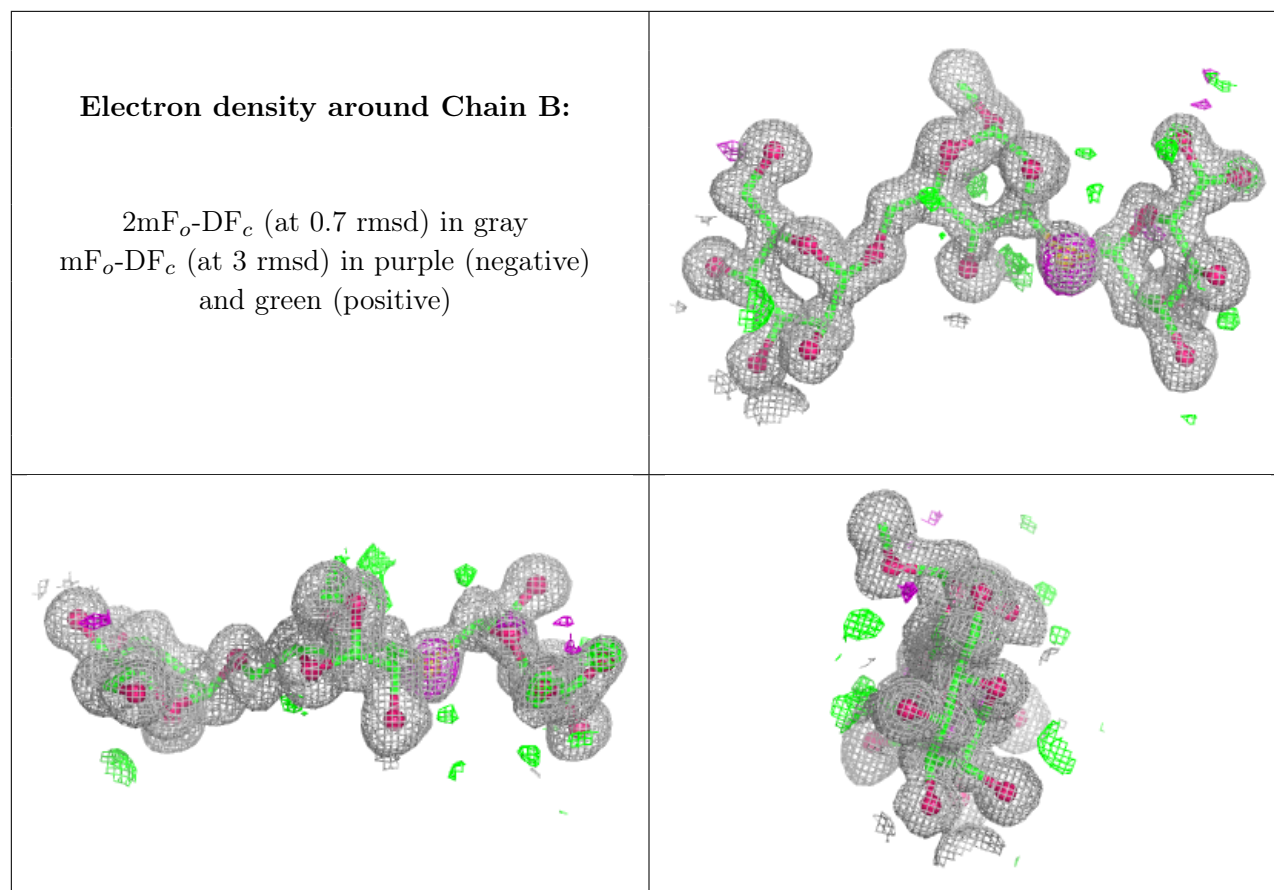
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	Z4R	B	1	13/13	0.98	0.06	13,15,20,25	0
2	MAN	B	2[A]	11/12	0.98	0.06	14,15,17,18	1
2	MAN	B	2[B]	11/12	0.98	0.06	14,15,17,18	1
2	MAN	B	3	11/12	0.99	0.03	9,10,11,12	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	1046	14/15	0.71	0.15	39,61,77,89	0
4	PO4	A	1047	5/5	0.92	0.14	22,34,47,48	0
6	MRD	A	1049	8/8	0.98	0.06	13,16,19,22	0
5	ZN	A	1048	1/1	1.00	0.00	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.