Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 03:11 AM EDT

PDB ID	:	3BVU
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 (i) 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 (i)) were used in the production of this report:

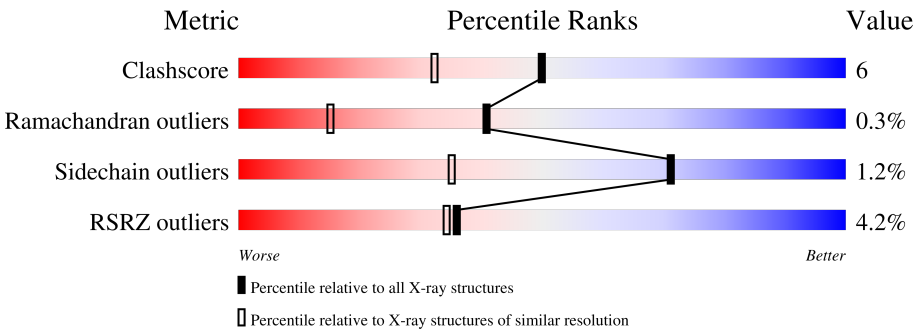
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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	141614	1205 (1.14-1.10)
Ramachandran outliers	138981	1168 (1.14-1.10)
Sidechain outliers	138945	1165 (1.14-1.10)
RSRZ outliers	127900	1146 (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 <=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	4% 85% 11% • •
2	B	3	100%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	1015	8422	5373	1466	1539	44	3	42	0

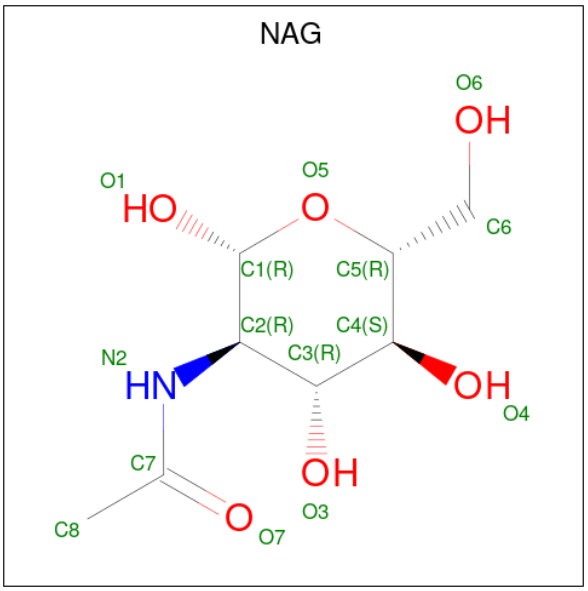
There are 14 discrepancies between the modelled and reference sequences:

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.

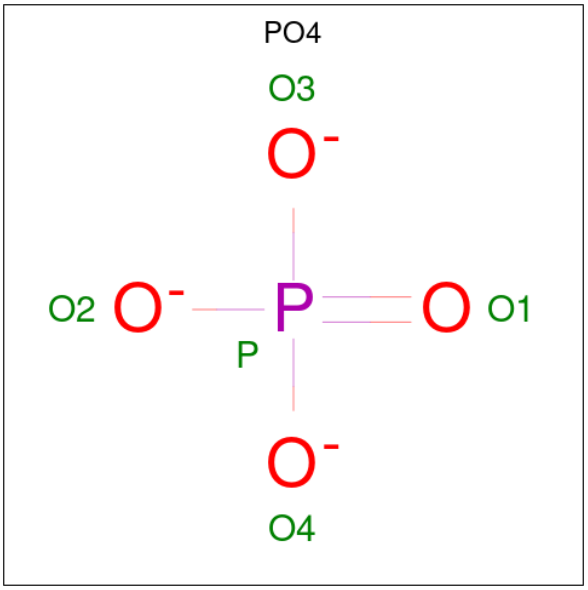
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
2	B	3	36	19	16	1	0	1	0

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



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

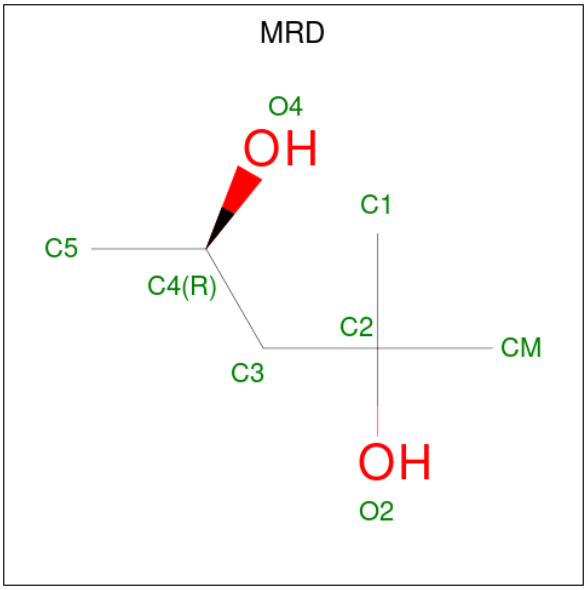


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
4	A	1	5	4	1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



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

- Molecule 7 is water.

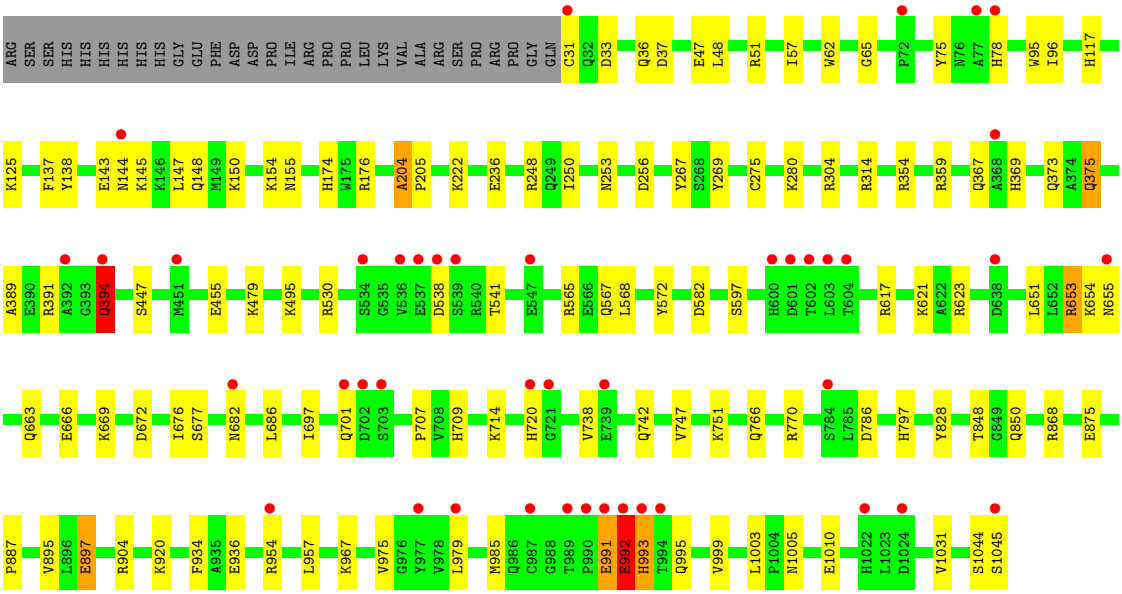
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1499	Total O 1515 1515	0	16

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.

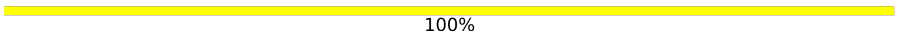
• Molecule 1: Alpha-mannosidase 2

Chain A:



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl 3-thio-alpha-D-mannopyranoside

Chain B:



4 Data and refinement statistics (i)

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 19.84 – 1.12	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-1.12) 93.4 (19.84-1.12)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.37 , 68.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, ZN, PO4, MRD, MAN, Z4R

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	0.70	1/8772 (0.0%)	1.08	30/11903 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	597	SER	CB-OG	-5.40	1.35	1.42

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	766[A]	GLN	CG-CD-OE1	-5.90	109.80	121.60
1	A	766[B]	GLN	CG-CD-OE1	-5.90	109.80	121.60
1	A	868	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	138[A]	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	A	138[B]	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	A	269	TYR	CB-CG-CD1	5.82	124.49	121.00
1	A	267	TYR	CB-CG-CD2	-5.81	117.52	121.00
1	A	248	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	572	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	A	565	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	617	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	78	HIS	CA-CB-CG	-5.50	104.25	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	672	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	137	PHE	CB-CG-CD1	-5.42	117.01	120.80
1	A	394	GLN	CG-CD-OE1	-5.40	110.80	121.60
1	A	253	ASN	OD1-CG-ND2	5.39	134.29	121.90
1	A	138[A]	TYR	CG-CD1-CE1	-5.31	117.05	121.30
1	A	138[B]	TYR	CG-CD1-CE1	-5.31	117.05	121.30
1	A	391	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	617	ARG	CD-NE-CZ	5.29	131.00	123.60
1	A	766[A]	GLN	CG-CD-NE2	5.21	129.21	116.70
1	A	766[B]	GLN	CG-CD-NE2	5.21	129.21	116.70
1	A	447[A]	SER	N-CA-CB	-5.19	102.71	110.50
1	A	447[B]	SER	N-CA-CB	-5.19	102.71	110.50
1	A	875	GLU	OE1-CD-OE2	-5.11	117.16	123.30
1	A	572	TYR	CB-CG-CD1	5.05	124.03	121.00
1	A	582	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	897	GLU	OE1-CD-OE2	5.04	129.35	123.30
1	A	538	ASP	CB-CG-OD2	5.02	122.81	118.30

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 (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	8422	0	8296	93	1
2	B	36	0	12	0	0
3	A	14	0	13	5	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
6	A	8	0	14	0	0
7	A	1515	0	0	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10001	0	8335	98	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 (98) 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: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:455:GLU:HG2	1:A:967:LYS:HZ2	1.51	0.75
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: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:47:GLU:CD	1:A:51:ARG:HD3	2.13	0.68
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:455:GLU:HG2	1:A:967:LYS:NZ	2.15	0.62
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:621:LYS:NZ	7:A:1231:HOH:O	2.49	0.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:389:ALA:HB1	1:A:394:GLN:CD	2.39	0.42
1:A:31:CYS:N	7:A:1202:HOH:O	2.52	0.42
1:A:150:LYS:NZ	7:A:1590:HOH:O	2.51	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%)	41 15

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%)	929 (98%)	14 (2%)	65 26

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

Mol	Chain	Res	Type
1	A	275	CYS
1	A	375	GLN
1	A	394	GLN
1	A	653	ARG
1	A	666[A]	GLU
1	A	666[B]	GLU
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	828	TYR
1	A	991	GLU
1	A	992	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

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	1.04	1 (8%)	13,18,18	1.79	2 (15%)
2	MAN	B	2[A]	-	11,11,12	0.93	1 (9%)	15,15,17	1.28	2 (13%)
2	MAN	B	2[B]	-	11,11,12	0.77	0	15,15,17	1.22	2 (13%)
2	MAN	B	3	5,2	11,11,12	1.44	1 (9%)	15,15,17	1.57	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	3.49	1.50	1.43
2	B	2[A]	MAN	O6-C6	-2.47	1.32	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	Z4R	O1-C1	2.30	1.44	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	Z4R	C1M-O1-C1	-5.16	105.31	113.27
2	B	3	MAN	C1-C2-C3	3.99	114.56	109.67
2	B	1	Z4R	O1-C1-C2	2.29	110.83	108.15
2	B	2[A]	MAN	C2-C3-C4	-2.20	107.09	110.89
2	B	2[B]	MAN	C2-C3-C4	-2.20	107.09	110.89
2	B	3	MAN	O5-C5-C4	-2.11	105.70	110.83
2	B	2[A]	MAN	O5-C5-C6	2.09	110.47	107.20
2	B	2[B]	MAN	O5-C5-C6	2.09	110.47	107.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

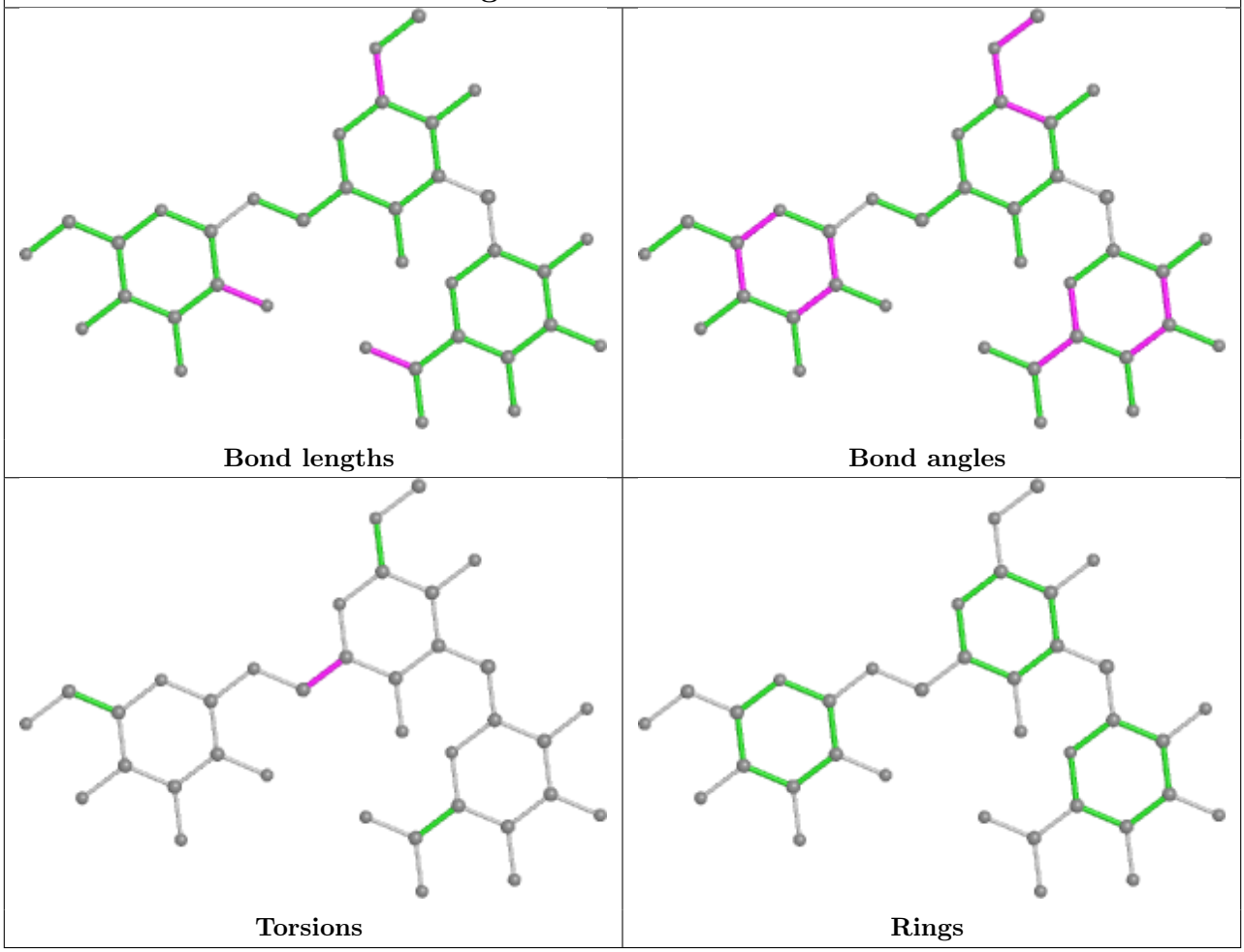
Mol	Chain	Res	Type	Atoms
2	B	1	Z4R	O5-C5-C6-O6

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.

Oligosaccharide Chain B



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	$\#\|Z\| > 2$
6	MRD	A	1049	-	7,7,7	0.72	0	9,10,10	0.89	0
4	PO4	A	1047	-	4,4,4	1.80	2 (50%)	6,6,6	0.72	0
3	NAG	A	1046	1	14,14,15	0.72	0	17,19,21	1.45	4 (23%)

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
6	MRD	A	1049	-	-	2/5/5/5	-
3	NAG	A	1046	1	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1047	PO4	P-O4	-2.35	1.47	1.54
4	A	1047	PO4	P-O3	2.27	1.61	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1046	NAG	O5-C5-C6	2.55	111.20	107.20
3	A	1046	NAG	C6-C5-C4	-2.46	107.25	113.00
3	A	1046	NAG	O5-C1-C2	-2.24	107.75	111.29
3	A	1046	NAG	C4-C3-C2	-2.03	108.05	111.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1015/1045 (97%)	0.26	43 (4%) 36 34	7, 14, 34, 85	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	702	ASP	8.1
1	A	602	THR	7.9
1	A	991	GLU	7.7
1	A	992	GLU	7.5
1	A	993	HIS	7.3
1	A	701	GLN	7.2
1	A	990	PRO	7.1
1	A	603	LEU	5.7
1	A	78	HIS	5.7
1	A	1045	SER	5.6
1	A	538	ASP	5.3
1	A	1024	ASP	5.2
1	A	720[A]	HIS	5.0
1	A	977	TYR	4.7
1	A	144	ASN	4.5
1	A	989	THR	4.1
1	A	600	HIS	4.1
1	A	638	ASP	4.1
1	A	682	ASN	4.0
1	A	534	SER	3.6
1	A	536	VAL	3.5
1	A	721	GLY	3.4
1	A	601	ASP	3.2
1	A	539	SER	3.1
1	A	784	SER	3.0
1	A	994	THR	2.9
1	A	77	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	451[A]	MET	2.7
1	A	987	CYS	2.6
1	A	655	ASN	2.6
1	A	31	CYS	2.6
1	A	537	GLU	2.6
1	A	703	SER	2.5
1	A	394	GLN	2.3
1	A	1022	HIS	2.3
1	A	604	THR	2.3
1	A	979[A]	LEU	2.3
1	A	547	GLU	2.2
1	A	368	ALA	2.2
1	A	392	ALA	2.2
1	A	739	GLU	2.1
1	A	954[A]	ARG	2.1
1	A	72	PRO	2.1

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)

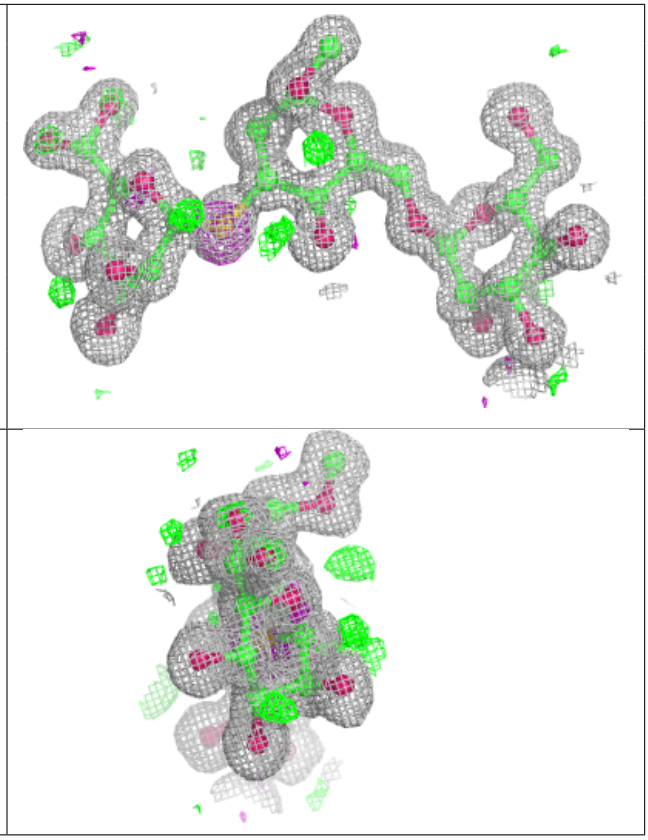
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MAN	B	2[A]	11/12	0.94	0.11	14,15,17,18	1
2	MAN	B	2[B]	11/12	0.94	0.11	14,15,17,18	1
2	Z4R	B	1	13/13	0.98	0.09	13,15,20,25	0
2	MAN	B	3	11/12	0.98	0.07	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.

Electron density around Chain B:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(Å^2)	Q<0.9
3	NAG	A	1046	14/15	0.76	0.36	39,61,77,89	0
4	PO4	A	1047	5/5	0.95	0.21	22,34,47,48	0
6	MRD	A	1049	8/8	0.96	0.07	13,16,19,22	0
5	ZN	A	1048	1/1	1.00	0.05	8,8,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.