



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:20 PM UTC

PDB ID : 3BVX / pdb_00003bvx
Title : GOLGI MANNOSIDASE II D204A catalytic nucleophile mutant complex with Methyl (2-deoxy-2-acetamido-beta-D-glucopyranosyl)-(1->2)-(alpha-D-mannopyranosyl)- (1->3)-[(alpha-D-mannopyranosyl)-(1->6)-(alpha-D-mannopyranosyl)-(1->6)]-beta-D-mannopyranoside
Authors : Kuntz, D.A.; Rose, D.R.
Deposited on : 2008-01-07
Resolution : 1.10 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

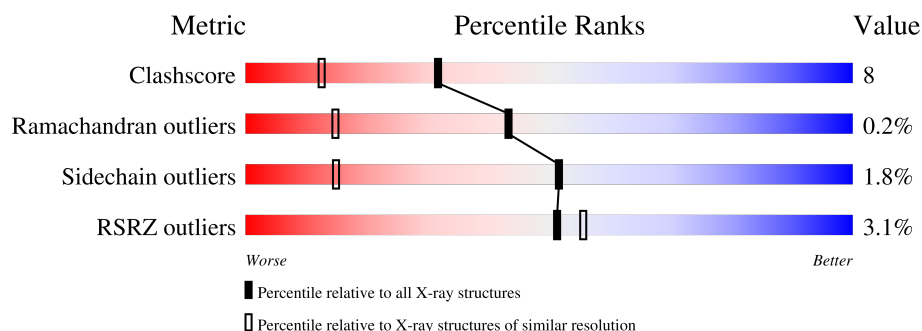
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 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	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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% 84% 12% ..
2	B	5	80% 20%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10180 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.

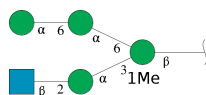
- Molecule 1 is a protein called Alpha-mannosidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1016	8585	5446	1518	1577	44	0	45	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 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]methyl beta-D-mannopyranoside.

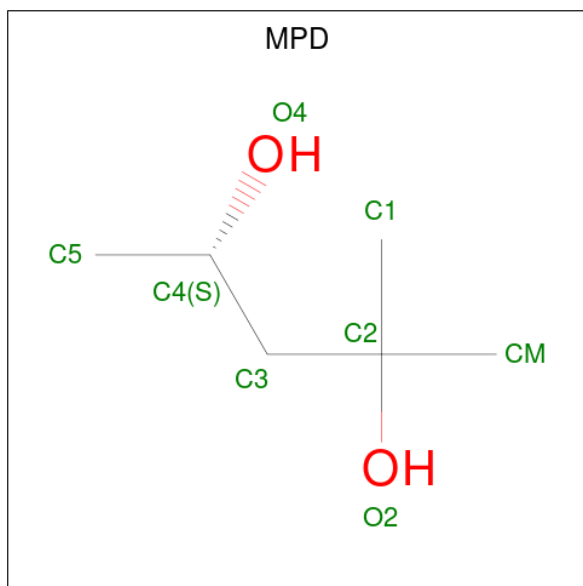


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	60	33	1	26	0	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

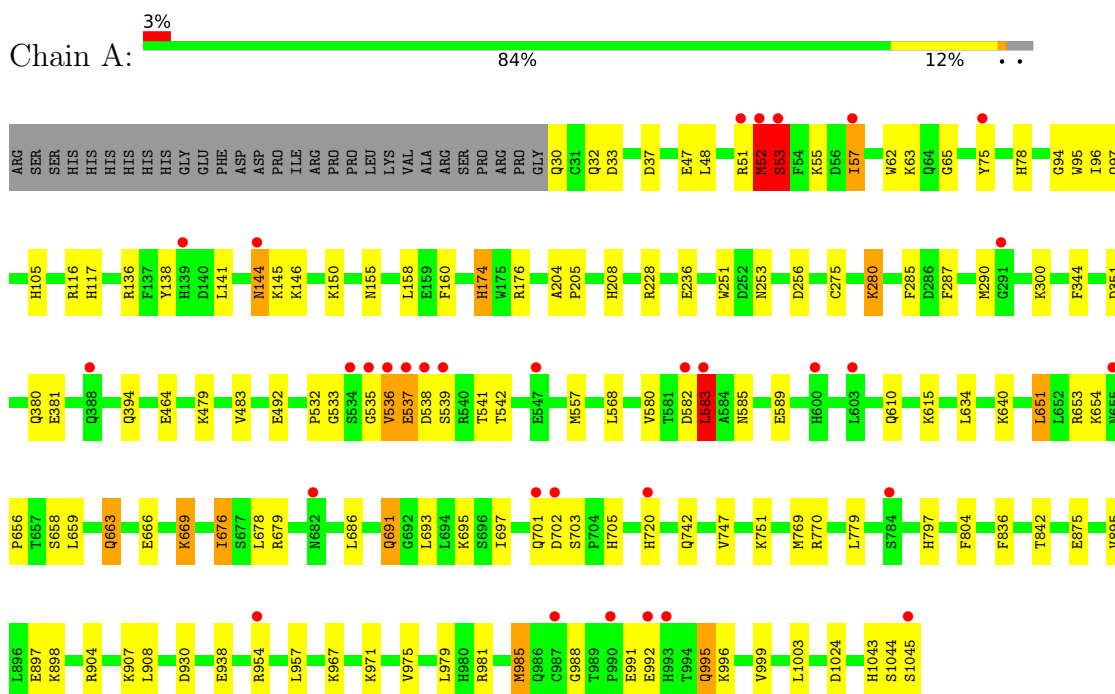
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1500	Total	O	0	26
			1526	1526		

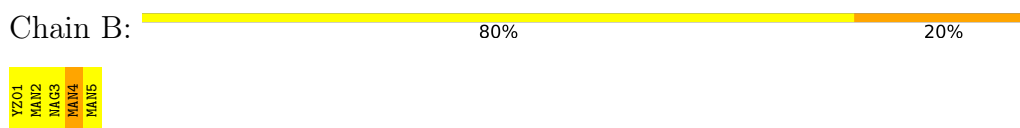
3 Residue-property plots

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-(1-6)-alpha-D-mannopyranose-(1-6)]methyl beta-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	68.81Å 109.55Å 138.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.10 20.00 – 1.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-1.10) 73.8 (20.00-1.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.10Å)	Xtriage
Refinement program	SHELX, SHELXL-97	Depositor
R, R_{free}	0.153 , 0.190 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	10.2	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10180	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: YZ0, MPD, ZN, NAG, MAN

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	0.88	0/8824	1.25	31/11971 (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 (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52[A]	MET	N-CA-C	8.40	122.92	110.48
1	A	52[B]	MET	N-CA-C	8.40	122.92	110.48
1	A	836	PHE	CA-CB-CG	7.60	121.40	113.80
1	A	676	ILE	CA-CB-CG2	6.98	122.36	110.50
1	A	1024	ASP	CA-CB-CG	6.97	119.57	112.60
1	A	995	GLN	OE1-CD-NE2	6.65	129.25	122.60
1	A	875	GLU	CB-CG-CD	6.54	123.71	112.60
1	A	285	PHE	CA-CB-CG	-6.37	107.43	113.80
1	A	78	HIS	CA-CB-CG	-6.34	107.46	113.80
1	A	705	HIS	CA-CB-CG	-6.16	107.64	113.80
1	A	174	HIS	CA-CB-CG	-6.14	107.66	113.80
1	A	381	GLU	CB-CG-CD	-6.03	102.34	112.60
1	A	985[A]	MET	O-C-N	5.89	129.81	122.86
1	A	985[B]	MET	O-C-N	5.89	129.81	122.86
1	A	804	PHE	CA-CB-CG	5.89	119.69	113.80
1	A	394	GLN	N-CA-C	5.85	120.26	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	GLN	CB-CG-CD	-5.76	102.81	112.60
1	A	208	HIS	ND1-CE1-NE2	5.65	114.05	108.40
1	A	53	SER	N-CA-C	5.39	119.96	112.90
1	A	160	PHE	CA-CB-CG	-5.39	108.41	113.80
1	A	988	GLY	CA-C-N	-5.35	114.17	121.61
1	A	988	GLY	C-N-CA	-5.35	114.17	121.61
1	A	464	GLU	CB-CG-CD	5.32	121.64	112.60
1	A	287	PHE	CA-CB-CG	-5.26	108.54	113.80
1	A	797	HIS	CA-CB-CG	-5.21	108.59	113.80
1	A	539	SER	N-CA-C	-5.19	106.10	112.90
1	A	144	ASN	CA-CB-CG	5.18	117.78	112.60
1	A	658	SER	O-C-N	5.10	128.60	122.79
1	A	1043	HIS	CA-C-N	-5.08	114.24	121.50
1	A	1043	HIS	C-N-CA	-5.08	114.24	121.50
1	A	344	PHE	CA-CB-CG	-5.01	108.78	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	583	LEU	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	8585	0	8334	132	0
2	B	60	0	39	5	0
3	A	1	0	0	0	0
4	A	8	0	14	1	0
5	A	1526	0	0	62	0
All	All	10180	0	8387	138	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 8.

All (138) 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:532:PRO:HB2	1:A:536:VAL:CG1	1.69	1.22
1:A:532:PRO:C	1:A:536:VAL:HG11	1.65	1.20
5:A:2544:HOH:O	2:B:4:MAN:H3	1.50	1.08
1:A:136[B]:ARG:O	1:A:136[B]:ARG:HD2	1.55	1.07
1:A:532:PRO:HB2	1:A:536:VAL:HG13	1.40	1.01
1:A:96:ILE:HG22	5:A:2330:HOH:O	1.59	0.99
1:A:380:GLN:HG2	5:A:2186:HOH:O	1.63	0.96
1:A:532:PRO:CB	1:A:536:VAL:CG1	2.45	0.94
1:A:532:PRO:CB	1:A:536:VAL:HG11	1.98	0.93
1:A:532:PRO:O	1:A:536:VAL:HG11	1.71	0.91
1:A:532:PRO:C	1:A:536:VAL:CG1	2.45	0.89
1:A:57:ILE:HG12	5:A:2158:HOH:O	1.73	0.86
1:A:136[B]:ARG:HD2	1:A:136[B]:ARG:C	2.01	0.85
1:A:136[B]:ARG:HG2	1:A:136[B]:ARG:HH21	1.40	0.84
5:A:2142[B]:HOH:O	2:B:4:MAN:H62	1.79	0.81
1:A:654:LYS:HD2	1:A:742[A]:GLN:HE22	1.44	0.81
1:A:954:ARG:NH2	1:A:981[B]:ARG:HH21	1.79	0.81
1:A:954:ARG:NH2	1:A:981[B]:ARG:NH2	2.31	0.78
1:A:971[B]:LYS:HZ2	1:A:1045:SER:H	1.30	0.77
1:A:532:PRO:CA	1:A:536:VAL:HG11	2.15	0.77
1:A:96:ILE:CG2	5:A:2330:HOH:O	2.24	0.76
1:A:742[A]:GLN:HG3	5:A:1786:HOH:O	1.85	0.76
1:A:659:LEU:HB3	5:A:2047:HOH:O	1.85	0.76
1:A:136[A]:ARG:HD3	5:A:1065[A]:HOH:O	1.88	0.74
1:A:116:ARG:HD2	5:A:2420:HOH:O	1.87	0.73
1:A:693:LEU:HD13	5:A:1949:HOH:O	1.88	0.73
1:A:679:ARG:HH12	1:A:701:GLN:HG2	1.53	0.73
1:A:666:GLU:HB2	5:A:1837:HOH:O	1.88	0.71
1:A:47[B]:GLU:HG3	5:A:1169:HOH:O	1.91	0.70
1:A:770[B]:ARG:NE	5:A:1465:HOH:O	2.24	0.70
1:A:971[B]:LYS:HZ2	1:A:1045:SER:N	1.89	0.70
1:A:533:GLY:O	1:A:536:VAL:HG12	1.90	0.69
1:A:651:LEU:HD13	1:A:653:ARG:HG2	1.74	0.69
1:A:653:ARG:HD2	1:A:656:PRO:HA	1.76	0.68
1:A:53:SER:OG	1:A:55:LYS:HG2	1.96	0.66
1:A:610:GLN:HB3	5:A:2241:HOH:O	1.94	0.66
1:A:136[B]:ARG:HH21	1:A:136[B]:ARG:CG	2.09	0.66
1:A:742[B]:GLN:HG3	5:A:2442:HOH:O	1.95	0.65
1:A:904:ARG:HG2	1:A:985[A]:MET:SD	2.38	0.64
4:A:1048:MPD:HM2	5:A:1365:HOH:O	1.96	0.64
1:A:583:LEU:HA	5:A:2059:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105[B]:HIS:ND1	5:A:1955:HOH:O	2.31	0.62
1:A:256:ASP:HB2	5:A:1961:HOH:O	1.99	0.61
1:A:720:HIS:CE1	5:A:2526:HOH:O	2.52	0.61
1:A:1044:SER:HB3	5:A:2490:HOH:O	2.01	0.61
5:A:2544:HOH:O	2:B:4:MAN:H5	2.01	0.60
1:A:532:PRO:CB	1:A:536:VAL:HG13	2.22	0.59
1:A:663:GLN:HG3	5:A:2043:HOH:O	2.02	0.58
1:A:48:LEU:HG	1:A:52[A]:MET:HE2	1.86	0.58
1:A:380:GLN:CG	5:A:2186:HOH:O	2.36	0.58
1:A:654:LYS:HD2	1:A:742[A]:GLN:NE2	2.17	0.57
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.40	0.57
1:A:96:ILE:HG23	1:A:479:LYS:HE2	1.85	0.57
1:A:678:LEU:HD12	1:A:769[A]:MET:HE1	1.87	0.57
1:A:538:ASP:HA	5:A:2475:HOH:O	2.03	0.57
1:A:300:LYS:NZ	5:A:2487:HOH:O	2.27	0.57
1:A:535:GLY:HA3	1:A:779:LEU:HD21	1.87	0.57
1:A:691:GLN:NE2	5:A:1117:HOH:O	2.29	0.57
1:A:75[A]:TYR:HD1	5:A:1266:HOH:O	1.87	0.56
1:A:770[B]:ARG:NH2	5:A:1465:HOH:O	2.38	0.56
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.34	0.56
1:A:30:GLN:N	5:A:2450:HOH:O	2.38	0.56
1:A:117[B]:HIS:HE1	1:A:351:ASP:OD1	1.88	0.56
1:A:720:HIS:HB3	5:A:2319:HOH:O	2.04	0.55
1:A:967:LYS:HE2	5:A:2507:HOH:O	2.04	0.55
1:A:116:ARG:CD	5:A:2420:HOH:O	2.48	0.55
1:A:536:VAL:CG1	1:A:537:GLU:N	2.69	0.55
1:A:938:GLU:HG3	5:A:2402:HOH:O	2.06	0.55
1:A:532:PRO:O	1:A:536:VAL:CG1	2.50	0.55
1:A:537:GLU:CD	5:A:2359:HOH:O	2.50	0.55
1:A:954:ARG:HH22	1:A:981[B]:ARG:NH2	2.02	0.55
1:A:280:LYS:NZ	1:A:280:LYS:HB2	2.22	0.55
1:A:589:GLU:OE2	1:A:751:LYS:HE3	2.07	0.55
1:A:483:VAL:HG11	5:A:2136:HOH:O	2.07	0.54
1:A:653:ARG:HD3	1:A:654:LYS:O	2.06	0.54
1:A:51[B]:ARG:NH2	5:A:1162:HOH:O	2.42	0.52
1:A:583:LEU:HG	5:A:1918:HOH:O	2.09	0.52
1:A:770[B]:ARG:CZ	5:A:1465:HOH:O	2.58	0.52
1:A:492:GLU:HG3	5:A:2263:HOH:O	2.08	0.51
1:A:37:ASP:HB2	5:A:2444:HOH:O	2.11	0.51
1:A:96:ILE:HG23	1:A:479:LYS:CE	2.40	0.50
1:A:535:GLY:N	5:A:2408:HOH:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:GLN:HG3	5:A:1502:HOH:O	2.10	0.50
1:A:96:ILE:HG22	1:A:96:ILE:O	2.11	0.50
1:A:538:ASP:OD1	1:A:538:ASP:O	2.30	0.49
1:A:136[B]:ARG:CG	1:A:136[B]:ARG:NH2	2.69	0.49
1:A:907:LYS:HD3	5:A:2454:HOH:O	2.12	0.49
1:A:954:ARG:CZ	1:A:981[B]:ARG:NH2	2.75	0.49
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.47	0.49
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.93	0.49
1:A:51[A]:ARG:NH2	5:A:1162:HOH:O	2.46	0.49
1:A:138[A]:TYR:OH	1:A:150:LYS:HE2	2.13	0.49
1:A:908:LEU:HG	5:A:2485:HOH:O	2.13	0.49
1:A:32:GLN:HG3	5:A:2203:HOH:O	2.13	0.49
1:A:679:ARG:NH1	1:A:701:GLN:HG2	2.24	0.49
1:A:536:VAL:HG12	1:A:537:GLU:N	2.28	0.48
1:A:37:ASP:HB2	1:A:253[B]:ASN:ND2	2.29	0.48
1:A:290:MET:HE1	5:A:1951[B]:HOH:O	2.13	0.48
1:A:47[A]:GLU:HG2	5:A:1067:HOH:O	2.14	0.48
1:A:533:GLY:O	1:A:536:VAL:CG1	2.61	0.47
1:A:954:ARG:HD2	1:A:991:GLU:OE2	2.15	0.47
1:A:640:LYS:HE3	5:A:2497:HOH:O	2.14	0.47
1:A:48:LEU:HD11	1:A:236:GLU:HG2	1.96	0.47
1:A:582:ASP:C	1:A:582:ASP:OD2	2.58	0.46
1:A:33:ASP:O	5:A:2444:HOH:O	2.21	0.46
1:A:542:THR:OG1	1:A:615:LYS:HE3	2.16	0.45
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.98	0.45
1:A:676:ILE:HD13	1:A:747:VAL:HG21	1.99	0.45
1:A:141:LEU:O	1:A:146:LYS:NZ	2.49	0.45
1:A:979[B]:LEU:HD21	1:A:999:VAL:HG11	1.98	0.45
1:A:615:LYS:HD2	5:A:1847:HOH:O	2.17	0.45
1:A:582:ASP:O	1:A:585:ASN:N	2.36	0.45
5:A:2544:HOH:O	2:B:4:MAN:C3	2.29	0.44
1:A:63:LYS:HE2	5:A:1947:HOH:O	2.17	0.44
1:A:702:ASP:OD2	1:A:703:SER:N	2.50	0.44
1:A:996[B]:LYS:HE3	1:A:996[B]:LYS:HA	1.98	0.44
1:A:568:LEU:HD12	1:A:770[A]:ARG:HD3	2.00	0.44
1:A:907:LYS:NZ	5:A:2459:HOH:O	2.50	0.44
1:A:536:VAL:HG12	1:A:537:GLU:H	1.82	0.44
1:A:663:GLN:HG2	5:A:2422:HOH:O	2.17	0.44
1:A:678:LEU:CD1	1:A:769[A]:MET:HE1	2.47	0.43
1:A:57:ILE:HG12	1:A:57:ILE:H	1.69	0.43
1:A:656:PRO:HB3	5:A:1074:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:GLY:HA3	1:A:779:LEU:CD2	2.49	0.43
1:A:720:HIS:HB3	5:A:2271:HOH:O	2.18	0.43
1:A:280:LYS:NZ	5:A:1681:HOH:O	2.50	0.42
1:A:48:LEU:O	1:A:52[A]:MET:HB2	2.19	0.42
1:A:251:TRP:CD1	1:A:251:TRP:C	2.97	0.42
1:A:957:LEU:HD11	1:A:979[A]:LEU:HG	2.02	0.42
1:A:94:GLY:HA2	1:A:97[B]:GLN:O	2.21	0.41
5:A:2544:HOH:O	2:B:4:MAN:C4	2.64	0.41
1:A:669:LYS:HZ3	1:A:669:LYS:HG3	1.53	0.41
1:A:155[A]:ASN:OD1	1:A:155[A]:ASN:C	2.64	0.41
1:A:205:PRO:O	1:A:228:ARG:HB2	2.21	0.40
1:A:615:LYS:HD2	5:A:1848:HOH:O	2.20	0.40
1:A:842:THR:OG1	1:A:898:LYS:NZ	2.54	0.40
1:A:557:MET:HA	1:A:930:ASP:O	2.21	0.40
1:A:580:VAL:HG22	1:A:634:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

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	1059/1045 (101%)	1030 (97%)	27 (2%)	2 (0%)	43 15

All (2) Ramachandran outliers are listed below:

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

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	946/928 (102%)	928 (98%)	18 (2%)	50 13

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52[A]	MET
1	A	52[B]	MET
1	A	53	SER
1	A	57	ILE
1	A	144	ASN
1	A	145	LYS
1	A	158[A]	LEU
1	A	158[B]	LEU
1	A	275	CYS
1	A	280	LYS
1	A	536	VAL
1	A	537	GLU
1	A	541	THR
1	A	583	LEU
1	A	651	LEU
1	A	669	LYS
1	A	691	GLN
1	A	695	LYS

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	371	ASN
1	A	610	GLN
1	A	643	HIS
1	A	901	ASN
1	A	923	GLN
1	A	943	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 ⓘ

5 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	YZ0	B	1	2	13,13,13	0.94	1 (7%)	18,18,18	1.50	4 (22%)
2	MAN	B	2	2	11,11,12	0.23	0	15,15,17	1.14	1 (6%)
2	NAG	B	3	2	14,14,15	0.51	0	17,19,21	1.24	3 (17%)
2	MAN	B	4	2	11,11,12	0.40	0	15,15,17	1.73	2 (13%)
2	MAN	B	5	3,2	11,11,12	0.81	0	15,15,17	1.11	1 (6%)

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	YZ0	B	1	2	-	0/4/24/24	0/1/1/1
2	MAN	B	2	2	-	0/2/19/22	0/1/1/1
2	NAG	B	3	2	-	0/6/23/26	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	0/1/1/1
2	MAN	B	5	3,2	-	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	YZ0	O1-C1	2.94	1.45	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	MAN	O5-C5-C6	-4.54	98.82	107.66
2	B	2	MAN	C6-C5-C4	-3.02	105.61	113.02
2	B	1	YZ0	O5-C1-O1	-2.89	104.22	110.94
2	B	5	MAN	C1-C2-C3	2.79	113.71	109.64
2	B	4	MAN	C1-C2-C3	2.64	113.48	109.64
2	B	3	NAG	O3-C3-C2	2.51	114.61	109.40
2	B	1	YZ0	O1-C1-C2	2.44	110.96	108.14
2	B	1	YZ0	O5-C1-C2	-2.34	105.55	110.37
2	B	3	NAG	C4-C3-C2	-2.15	107.87	111.02
2	B	3	NAG	C6-C5-C4	-2.08	107.92	113.02
2	B	1	YZ0	C4-C3-C2	-2.00	107.32	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

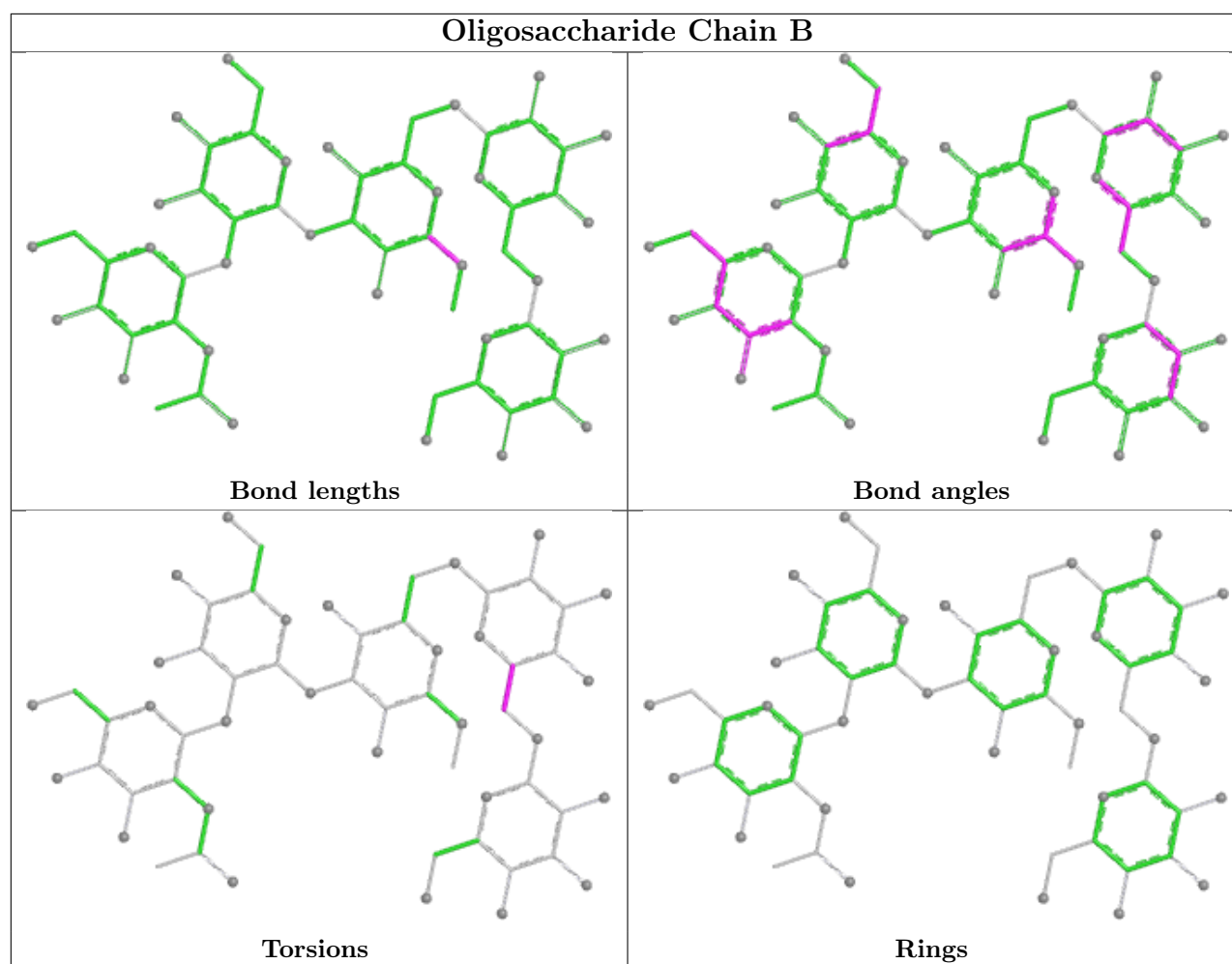
Mol	Chain	Res	Type	Atoms
2	B	4	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	MAN	5	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	$\# Z > 2$
4	MPD	A	1048	-	7,7,7	0.72	0	9,10,10	0.59	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
4	MPD	A	1048	-	-	0/5/5/5	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1048	MPD	1	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	1016/1045 (97%)	-0.01	32 (3%) 51 55	5, 14, 33, 97	45 (4%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	VAL	14.3
1	A	537	GLU	9.2
1	A	538	ASP	8.5
1	A	535	GLY	8.3
1	A	534	SER	5.8
1	A	539	SER	5.0
1	A	583	LEU	4.9
1	A	53	SER	3.9
1	A	954	ARG	3.5
1	A	603	LEU	3.3
1	A	144	ASN	3.2
1	A	57	ILE	3.2
1	A	993	HIS	3.0
1	A	784	SER	3.0
1	A	51[A]	ARG	2.8
1	A	582	ASP	2.8
1	A	990	PRO	2.6
1	A	139[A]	HIS	2.6
1	A	720	HIS	2.6
1	A	1045	SER	2.5
1	A	992	GLU	2.5
1	A	702	ASP	2.5
1	A	682	ASN	2.4
1	A	291	GLY	2.3
1	A	987	CYS	2.3
1	A	388	GLN	2.3
1	A	547	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	600	HIS	2.3
1	A	701	GLN	2.2
1	A	52[A]	MET	2.1
1	A	75[A]	TYR	2.1
1	A	655[A]	ASN	2.1

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

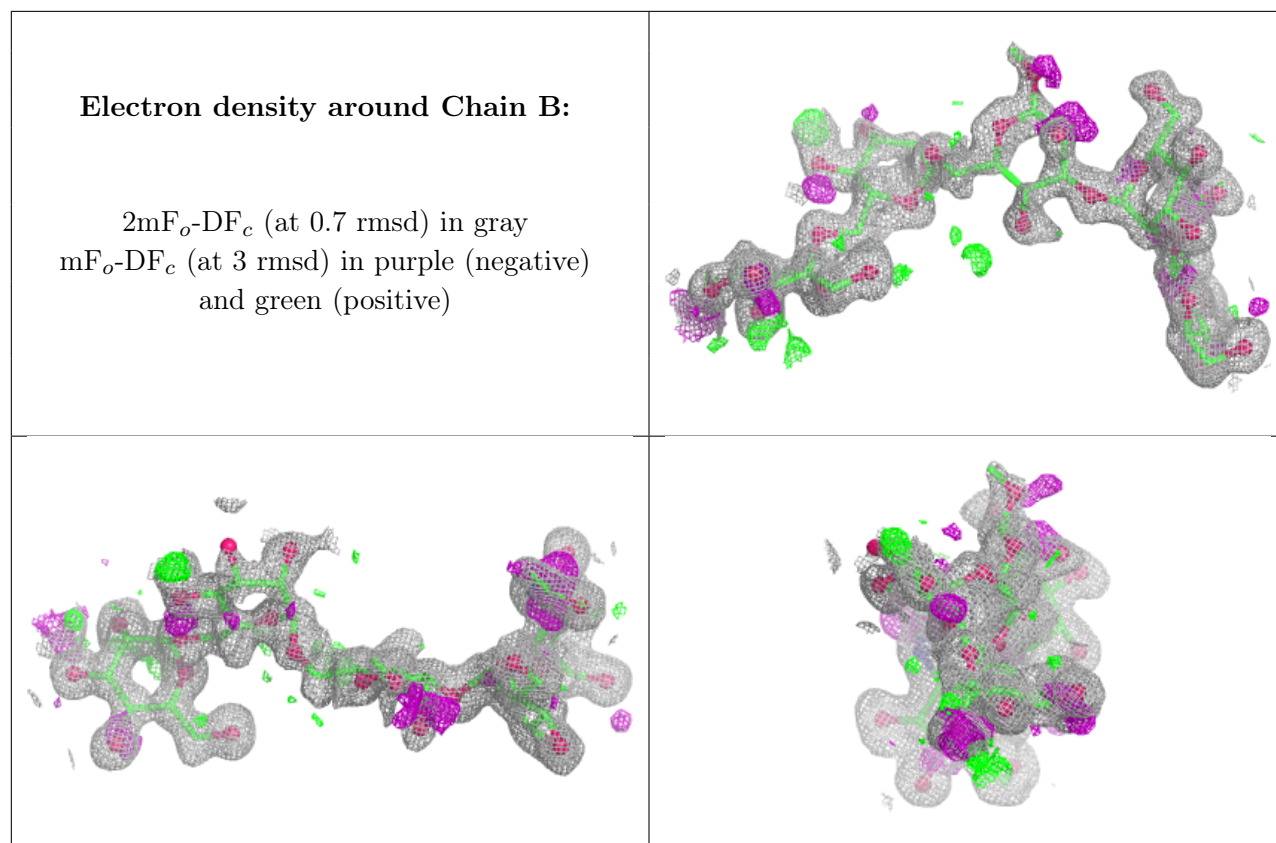
There are no non-standard protein/DNA/RNA residues in this entry.

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	YZ0	B	1	13/13	0.81	0.14	24,45,62,66	0
2	MAN	B	4	11/12	0.88	0.12	19,51,58,81	0
2	NAG	B	3	14/15	0.94	0.09	16,20,31,42	0
2	MAN	B	2	11/12	0.94	0.08	19,27,33,41	0
2	MAN	B	5	11/12	0.98	0.05	10,12,14,15	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
4	MPD	A	1048	8/8	0.83	0.13	23,33,40,40	0
3	ZN	A	1046	1/1	1.00	0.02	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.