



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:17 PM UTC

PDB ID : 3NSN / pdb_00003nsn
Title : Crystal Structure of insect beta-N-acetyl-D-hexosaminidase OfHex1 complexed with TMG-chitotriomycin
Authors : Zhang, H.; Liu, T.; Liu, F.; Yang, Q.; Shen, X.
Deposited on : 2010-07-02
Resolution : 2.10 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

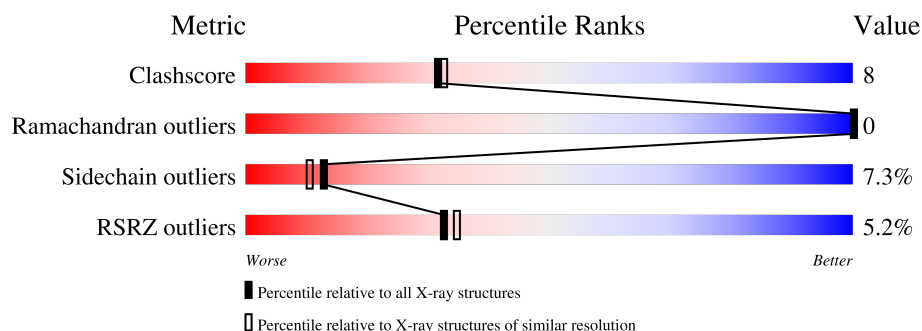
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	572	5% 58% 36% 6%
2	B	4	50% 25% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5097 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 N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4615	2944	776	870	25			

- Molecule 2 is an oligosaccharide called 2-deoxy-2-(trimethylammonio)-beta-D-glucopyranoside-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	0	0	0
			57	33	4	20			

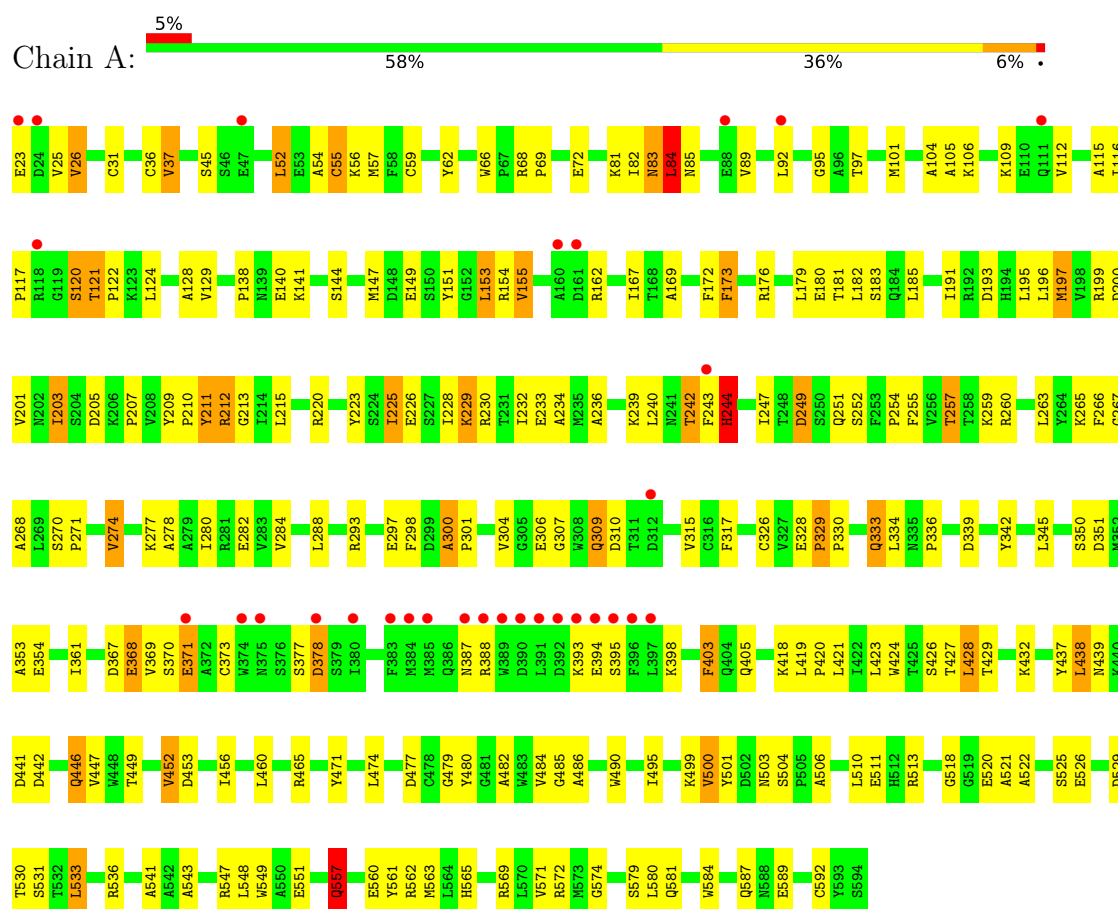
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	425	Total	O	0	0
			425	425		

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: N-acetylglucosaminidase



• Molecule 2: 2-deoxy-2-(trimethylammonio)-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.50Å 108.50Å 175.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.13 – 2.10 28.13 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.13-2.10) 79.2 (28.13-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.10Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0072	Depositor
R, R_{free}	0.202 , (Not available) 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5097	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: TMX, NAG

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	2.12	147/4737 (3.1%)	1.22	29/6432 (0.5%)

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	551	GLU	C-O	-10.71	1.18	1.23
1	A	361	ILE	C-O	-8.59	1.15	1.24
1	A	530	THR	C-O	-7.65	1.15	1.24
1	A	180	GLU	C-O	-7.19	1.15	1.24
1	A	304	VAL	C-O	-7.18	1.16	1.24
1	A	486	ALA	CA-CB	-7.00	1.43	1.53
1	A	328	GLU	C-O	-6.99	1.16	1.24
1	A	561	TYR	C-O	-6.98	1.16	1.24
1	A	268	ALA	CA-CB	-6.92	1.41	1.53
1	A	265	LYS	C-O	-6.74	1.16	1.24
1	A	249	ASP	C-O	-6.64	1.17	1.24
1	A	236	ALA	CA-CB	-6.62	1.43	1.53
1	A	31	CYS	C-O	-6.58	1.16	1.23
1	A	419	LEU	C-O	-6.57	1.17	1.24
1	A	112	VAL	C-O	-6.50	1.16	1.24
1	A	531	SER	C-O	-6.48	1.16	1.24
1	A	257	THR	C-O	-6.46	1.16	1.24
1	A	220	ARG	C-O	-6.45	1.16	1.24
1	A	212	ARG	CD-NE	-6.45	1.37	1.46
1	A	484	VAL	C-O	-6.44	1.17	1.24
1	A	306	GLU	C-O	-6.41	1.16	1.23
1	A	232	ILE	C-O	-6.35	1.16	1.24
1	A	247	ILE	C-O	-6.34	1.15	1.24
1	A	418	LYS	C-O	-6.33	1.16	1.24
1	A	282	GLU	C-O	-6.33	1.16	1.24
1	A	263	LEU	C-O	-6.31	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	PRO	C-O	-6.29	1.16	1.24
1	A	569	ARG	C-O	-6.27	1.16	1.24
1	A	191	ILE	C-O	-6.27	1.17	1.24
1	A	252	SER	C-O	-6.26	1.16	1.23
1	A	274	VAL	C-O	-6.26	1.17	1.23
1	A	89	VAL	C-O	-6.25	1.17	1.24
1	A	350	SER	C-O	-6.22	1.16	1.24
1	A	571	VAL	C-O	-6.17	1.17	1.24
1	A	526	GLU	C-O	-6.15	1.16	1.24
1	A	426	SER	C-O	-6.14	1.18	1.24
1	A	427	THR	C-O	-6.13	1.17	1.24
1	A	300	ALA	C-O	-6.04	1.18	1.24
1	A	106	LYS	C-O	-6.01	1.17	1.24
1	A	233	GLU	C-O	-6.00	1.17	1.24
1	A	105	ALA	CA-CB	-5.99	1.44	1.53
1	A	432	LYS	C-O	-5.96	1.17	1.24
1	A	104	ALA	CA-CB	-5.94	1.44	1.53
1	A	55	CYS	C-O	-5.94	1.17	1.24
1	A	504	SER	C-O	-5.93	1.18	1.24
1	A	172	PHE	C-O	-5.92	1.17	1.24
1	A	278	ALA	C-O	-5.90	1.17	1.24
1	A	503	ASN	C-O	-5.90	1.16	1.24
1	A	562	ARG	C-O	-5.88	1.17	1.24
1	A	173	PHE	C-O	-5.85	1.17	1.24
1	A	212	ARG	CZ-NH2	-5.85	1.25	1.33
1	A	128	ALA	CA-CB	-5.84	1.44	1.53
1	A	579	SER	C-O	-5.84	1.16	1.24
1	A	557	GLN	C-O	-5.81	1.16	1.24
1	A	490	TRP	C-O	-5.80	1.17	1.24
1	A	288	LEU	C-O	-5.77	1.17	1.24
1	A	298	PHE	C-O	-5.76	1.17	1.23
1	A	565	HIS	C-O	-5.75	1.17	1.24
1	A	240	LEU	C-O	-5.74	1.16	1.23
1	A	482	ALA	C-O	-5.73	1.16	1.23
1	A	242	THR	C-O	-5.71	1.17	1.24
1	A	254	PRO	C-O	-5.70	1.16	1.24
1	A	284	VAL	C-O	-5.65	1.17	1.24
1	A	536	ARG	C-O	-5.64	1.17	1.24
1	A	54	ALA	CA-CB	-5.63	1.44	1.53
1	A	522	ALA	C-O	-5.63	1.17	1.24
1	A	115	ALA	CA-CB	-5.62	1.43	1.53
1	A	354	GLU	C-O	-5.62	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	LYS	C-O	-5.61	1.17	1.24
1	A	167	ILE	C-O	-5.61	1.18	1.24
1	A	572	ARG	C-O	-5.61	1.17	1.24
1	A	563	MET	C-O	-5.60	1.17	1.24
1	A	446	GLN	C-O	-5.59	1.17	1.24
1	A	228	ILE	C-O	-5.59	1.17	1.24
1	A	447	VAL	C-O	-5.58	1.18	1.24
1	A	506	ALA	C-O	-5.58	1.17	1.24
1	A	518	GLY	C-O	-5.58	1.16	1.23
1	A	140	GLU	C-O	-5.58	1.17	1.24
1	A	329	PRO	C-O	-5.57	1.18	1.24
1	A	373	CYS	C-O	-5.56	1.17	1.24
1	A	203	ILE	C-O	-5.54	1.18	1.24
1	A	584	TRP	C-O	-5.54	1.17	1.24
1	A	333	GLN	C-O	-5.54	1.17	1.23
1	A	251	GLN	C-O	-5.52	1.17	1.24
1	A	244	HIS	C-O	-5.51	1.17	1.24
1	A	351	ASP	C-O	-5.51	1.17	1.24
1	A	317	PHE	C-O	-5.50	1.17	1.23
1	A	182	LEU	C-O	-5.49	1.17	1.24
1	A	181	THR	C-O	-5.48	1.17	1.24
1	A	59	CYS	C-O	-5.46	1.17	1.24
1	A	548	LEU	C-O	-5.45	1.17	1.24
1	A	420	PRO	C-O	-5.44	1.17	1.23
1	A	66	TRP	C-O	-5.44	1.17	1.24
1	A	153	LEU	C-O	-5.44	1.17	1.24
1	A	211	TYR	C-O	-5.44	1.17	1.24
1	A	260	ARG	C-O	-5.44	1.17	1.24
1	A	226	GLU	C-O	-5.42	1.17	1.24
1	A	403	PHE	C-O	-5.42	1.17	1.24
1	A	429	THR	C-O	-5.40	1.16	1.24
1	A	195	LEU	C-O	-5.39	1.17	1.24
1	A	521	ALA	C-O	-5.38	1.17	1.24
1	A	243	PHE	C-O	-5.37	1.17	1.24
1	A	547	ARG	C-O	-5.37	1.17	1.24
1	A	183	SER	C-O	-5.37	1.17	1.24
1	A	229	LYS	C-O	-5.37	1.17	1.24
1	A	101	MET	C-O	-5.37	1.17	1.24
1	A	529	ASP	C-O	-5.35	1.19	1.24
1	A	587	GLN	C-O	-5.35	1.17	1.24
1	A	369	VAL	C-O	-5.33	1.18	1.24
1	A	234	ALA	C-O	-5.32	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	592	CYS	C-O	-5.31	1.17	1.24
1	A	277	LYS	C-O	-5.30	1.18	1.24
1	A	499	LYS	C-O	-5.30	1.17	1.24
1	A	495	ILE	C-O	-5.30	1.17	1.23
1	A	521	ALA	CA-CB	-5.29	1.45	1.53
1	A	45	SER	C-O	-5.28	1.17	1.23
1	A	501	TYR	C-O	-5.26	1.18	1.24
1	A	449	THR	C-O	-5.26	1.17	1.23
1	A	541	ALA	C-O	-5.26	1.17	1.24
1	A	210	PRO	C-O	-5.24	1.18	1.24
1	A	270	SER	C-O	-5.24	1.17	1.24
1	A	421	LEU	C-O	-5.22	1.17	1.23
1	A	574	GLY	C-O	-5.21	1.17	1.24
1	A	460	LEU	C-O	-5.21	1.18	1.24
1	A	471	TYR	C-O	-5.20	1.17	1.24
1	A	480	TYR	C-O	-5.19	1.18	1.23
1	A	315	VAL	C-O	-5.18	1.18	1.24
1	A	155	VAL	C-O	-5.18	1.18	1.24
1	A	193	ASP	C-O	-5.18	1.17	1.23
1	A	353	ALA	C-O	-5.18	1.18	1.24
1	A	342	TYR	C-O	-5.17	1.17	1.24
1	A	196	LEU	C-O	-5.16	1.17	1.23
1	A	230	ARG	C-O	-5.16	1.18	1.24
1	A	293	ARG	C-O	-5.15	1.17	1.23
1	A	37	VAL	C-O	-5.14	1.18	1.24
1	A	280	ILE	C-O	-5.13	1.18	1.24
1	A	255	PHE	C-O	-5.11	1.17	1.23
1	A	57	MET	C-O	-5.09	1.18	1.24
1	A	485	GLY	C-O	-5.08	1.16	1.23
1	A	179	LEU	N-CA	-5.07	1.40	1.46
1	A	236	ALA	C-O	-5.07	1.18	1.24
1	A	326	CYS	C-O	-5.06	1.18	1.23
1	A	26	VAL	C-O	-5.05	1.19	1.24
1	A	405	GLN	C-O	-5.04	1.18	1.24
1	A	581	GLN	C-O	-5.03	1.19	1.24
1	A	84	LEU	C-O	-5.01	1.18	1.24
1	A	197	MET	C-O	-5.00	1.18	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	N-CA-C	7.83	119.60	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	GLY	N-CA-C	7.52	122.11	111.14
1	A	479	GLY	N-CA-C	7.47	124.63	114.92
1	A	267	GLY	N-CA-C	7.37	122.20	112.77
1	A	92	LEU	N-CA-C	7.28	119.29	111.36
1	A	456	ILE	N-CA-C	6.94	117.08	110.42
1	A	525	SER	N-CA-C	6.75	120.82	112.59
1	A	548	LEU	N-CA-C	6.21	118.13	111.36
1	A	209	TYR	CA-C-N	6.02	125.57	119.19
1	A	209	TYR	C-N-CA	6.02	125.57	119.19
1	A	251	GLN	N-CA-C	6.00	117.90	111.36
1	A	452	VAL	N-CA-CB	-5.90	104.69	112.36
1	A	266	PHE	CA-C-N	5.88	126.46	120.00
1	A	266	PHE	C-N-CA	5.88	126.46	120.00
1	A	378	ASP	N-CA-CB	-5.76	101.66	110.01
1	A	368	GLU	N-CA-C	5.64	119.17	111.39
1	A	477	ASP	N-CA-C	5.57	118.29	111.82
1	A	560	GLU	N-CA-C	5.46	116.91	111.07
1	A	377	SER	CA-C-N	5.43	127.49	120.44
1	A	377	SER	C-N-CA	5.43	127.49	120.44
1	A	26	VAL	N-CA-CB	-5.28	104.05	112.07
1	A	239	LYS	N-CA-C	5.22	119.60	113.23
1	A	116	ILE	CB-CA-C	-5.19	104.81	110.78
1	A	169	ALA	N-CA-C	5.09	117.12	109.23
1	A	259	LYS	N-CA-C	5.06	116.87	111.36
1	A	162	ARG	N-CA-C	5.02	116.44	108.96
1	A	339	ASP	N-CA-C	5.02	116.75	111.28
1	A	453	ASP	CA-C-N	5.00	124.78	119.28
1	A	453	ASP	C-N-CA	5.00	124.78	119.28

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	4615	0	4448	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	57	0	56	1	0
3	A	425	0	0	0	0
All	All	5097	0	4504	71	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 (71) 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:510:LEU:O	1:A:513:ARG:HG3	1.54	1.08
1:A:333:GLN:NE2	1:A:370:SER:H	1.59	1.00
1:A:333:GLN:HE22	1:A:370:SER:N	1.70	0.88
1:A:36:CYS:HG	1:A:55:CYS:HG	1.02	0.87
1:A:333:GLN:HE22	1:A:370:SER:H	0.90	0.87
1:A:371:GLU:H	1:A:371:GLU:CD	1.82	0.86
1:A:52:LEU:HD21	1:A:56:LYS:HE2	1.64	0.79
1:A:371:GLU:HG3	1:A:393:LYS:HE2	1.65	0.78
1:A:307:GLY:H	1:A:309:GLN:HE22	1.32	0.74
1:A:424:TRP:CZ3	1:A:446:GLN:HG2	2.23	0.73
1:A:82:ILE:HG13	1:A:197:MET:HE3	1.68	0.73
1:A:52:LEU:CD2	1:A:56:LYS:HE2	2.19	0.73
1:A:309:GLN:HE21	1:A:309:GLN:H	1.35	0.73
1:A:387:ASN:O	1:A:388:ARG:HG2	1.92	0.70
1:A:149:GLU:OE1	1:A:212:ARG:NH2	2.27	0.68
1:A:129:VAL:CG2	1:A:197:MET:HE1	2.27	0.64
1:A:367:ASP:OD1	1:A:367:ASP:N	2.29	0.64
1:A:215:LEU:C	1:A:215:LEU:HD23	2.23	0.63
1:A:83:ASN:C	1:A:83:ASN:HD22	2.05	0.63
1:A:511:GLU:H	1:A:511:GLU:CD	2.09	0.60
1:A:83:ASN:HD22	1:A:84:LEU:N	2.00	0.60
1:A:371:GLU:CD	1:A:371:GLU:N	2.56	0.60
1:A:82:ILE:HG13	1:A:197:MET:CE	2.33	0.59
1:A:225:ILE:CD1	1:A:229:LYS:HE3	2.36	0.56
1:A:129:VAL:HG22	1:A:197:MET:HE1	1.88	0.56
1:A:155:VAL:HB	1:A:201:VAL:HB	1.89	0.54
1:A:439:ASN:HD22	1:A:441:ASP:H	1.54	0.54
1:A:244:HIS:HD2	1:A:520:GLU:OE1	1.91	0.53
1:A:307:GLY:H	1:A:309:GLN:NE2	2.02	0.52
1:A:52:LEU:HD22	1:A:56:LYS:HD2	1.90	0.52
1:A:95:GLY:HA3	1:A:138:PRO:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ASN:O	1:A:388:ARG:CG	2.57	0.51
1:A:439:ASN:ND2	1:A:442:ASP:H	2.09	0.51
1:A:211:TYR:CZ	1:A:242:THR:HG21	2.47	0.50
1:A:121:THR:HG22	1:A:122:PRO:HD2	1.93	0.50
1:A:83:ASN:ND2	1:A:85:ASN:H	2.11	0.49
1:A:81:LYS:O	1:A:82:ILE:HD13	2.12	0.49
1:A:129:VAL:HG21	1:A:197:MET:HE1	1.93	0.49
1:A:154:ARG:HH21	1:A:154:ARG:HB3	1.79	0.48
1:A:368:GLU:CD	2:B:4:TMX:H27	2.39	0.47
1:A:129:VAL:HG21	1:A:197:MET:CE	2.45	0.46
1:A:334:LEU:O	1:A:336:PRO:HD3	2.16	0.46
1:A:437:TYR:C	1:A:438:LEU:HD13	2.40	0.46
1:A:223:TYR:HE1	1:A:533:LEU:HB2	1.80	0.46
1:A:151:TYR:CE2	1:A:205:ASP:HB3	2.51	0.45
1:A:72:GLU:O	1:A:203:ILE:HA	2.16	0.45
1:A:117:PRO:O	1:A:120:SER:HB2	2.16	0.45
1:A:185:LEU:HD13	1:A:201:VAL:HG21	1.97	0.45
1:A:336:PRO:HB3	1:A:403:PHE:HB2	1.99	0.45
1:A:500:VAL:HG22	1:A:543:ALA:HB3	1.98	0.45
1:A:309:GLN:O	1:A:310:ASP:HB2	2.17	0.44
1:A:36:CYS:HG	1:A:55:CYS:CB	2.30	0.44
1:A:52:LEU:HD22	1:A:56:LYS:HE2	2.00	0.43
1:A:207:PRO:HB3	1:A:549:TRP:CE3	2.53	0.43
1:A:244:HIS:HE1	1:A:297:GLU:OE1	2.02	0.43
1:A:62:TYR:CE2	1:A:68:ARG:HD2	2.53	0.43
1:A:56:LYS:NZ	1:A:589:GLU:OE1	2.47	0.43
1:A:97:THR:HG22	1:A:141:LYS:HB3	2.01	0.43
1:A:300:ALA:HB1	1:A:301:PRO:HA	2.01	0.43
1:A:244:HIS:CE1	1:A:297:GLU:OE1	2.73	0.42
1:A:83:ASN:HD22	1:A:85:ASN:H	1.68	0.42
1:A:329:PRO:HA	1:A:330:PRO:HA	1.77	0.42
1:A:309:GLN:H	1:A:309:GLN:NE2	2.11	0.42
1:A:428:LEU:HD22	1:A:437:TYR:CD2	2.55	0.42
1:A:557:GLN:NE2	1:A:557:GLN:H	2.18	0.41
1:A:225:ILE:HD11	1:A:229:LYS:HE3	2.00	0.41
1:A:82:ILE:HD13	1:A:82:ILE:HA	1.76	0.41
1:A:68:ARG:HA	1:A:69:PRO:HD3	1.87	0.41
1:A:147:MET:HE3	1:A:173:PHE:CD2	2.55	0.41
1:A:144:SER:O	1:A:147:MET:HG2	2.21	0.40
1:A:215:LEU:HD12	1:A:244:HIS:CD2	2.56	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	570/572 (100%)	560 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	495/495 (100%)	459 (93%)	36 (7%)	13	10

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	25	VAL
1	A	26	VAL
1	A	37	VAL
1	A	52	LEU
1	A	83	ASN
1	A	84	LEU
1	A	109	LYS
1	A	120	SER
1	A	121	THR
1	A	124	LEU
1	A	153	LEU
1	A	176	ARG

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Mol	Chain	Res	Type
1	A	200	ASP
1	A	225	ILE
1	A	244	HIS
1	A	249	ASP
1	A	257	THR
1	A	274	VAL
1	A	309	GLN
1	A	345	LEU
1	A	371	GLU
1	A	378	ASP
1	A	394	GLU
1	A	395	SER
1	A	398	LYS
1	A	423	LEU
1	A	428	LEU
1	A	438	LEU
1	A	452	VAL
1	A	465	ARG
1	A	474	LEU
1	A	500	VAL
1	A	533	LEU
1	A	557	GLN
1	A	580	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	41	ASN
1	A	83	ASN
1	A	170	ASN
1	A	244	HIS
1	A	309	GLN
1	A	333	GLN
1	A	381	GLN
1	A	439	ASN
1	A	512	HIS
1	A	515	GLN
1	A	557	GLN
1	A	581	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	NAG	B	1	2	15,15,15	1.65	3 (20%)	21,21,21	2.11	5 (23%)
2	NAG	B	2	2	14,14,15	0.73	0	17,19,21	1.04	0
2	NAG	B	3	2	14,14,15	0.70	0	17,19,21	0.89	0
2	TMX	B	4	2	12,14,15	1.01	1 (8%)	18,21,23	1.25	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2	-	4/6/26/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	B	3	2	-	2/6/23/26	0/1/1/1
2	TMX	B	4	2	-	0/8/25/28	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	3.99	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C3-C2	3.02	1.58	1.53
2	B	1	NAG	O4-C4	2.16	1.48	1.43
2	B	4	TMX	O5-C1	2.15	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O5-C1-C2	5.60	115.14	109.52
2	B	1	NAG	C1-C2-C3	4.80	117.09	110.54
2	B	4	TMX	C1-O5-C5	4.24	117.86	112.19
2	B	1	NAG	C4-C3-C2	3.11	114.93	110.40
2	B	1	NAG	C1-C2-N2	-2.74	107.55	110.73
2	B	1	NAG	C1-O5-C5	-2.07	109.64	113.65

There are no chirality outliers.

All (8) torsion outliers are listed below:

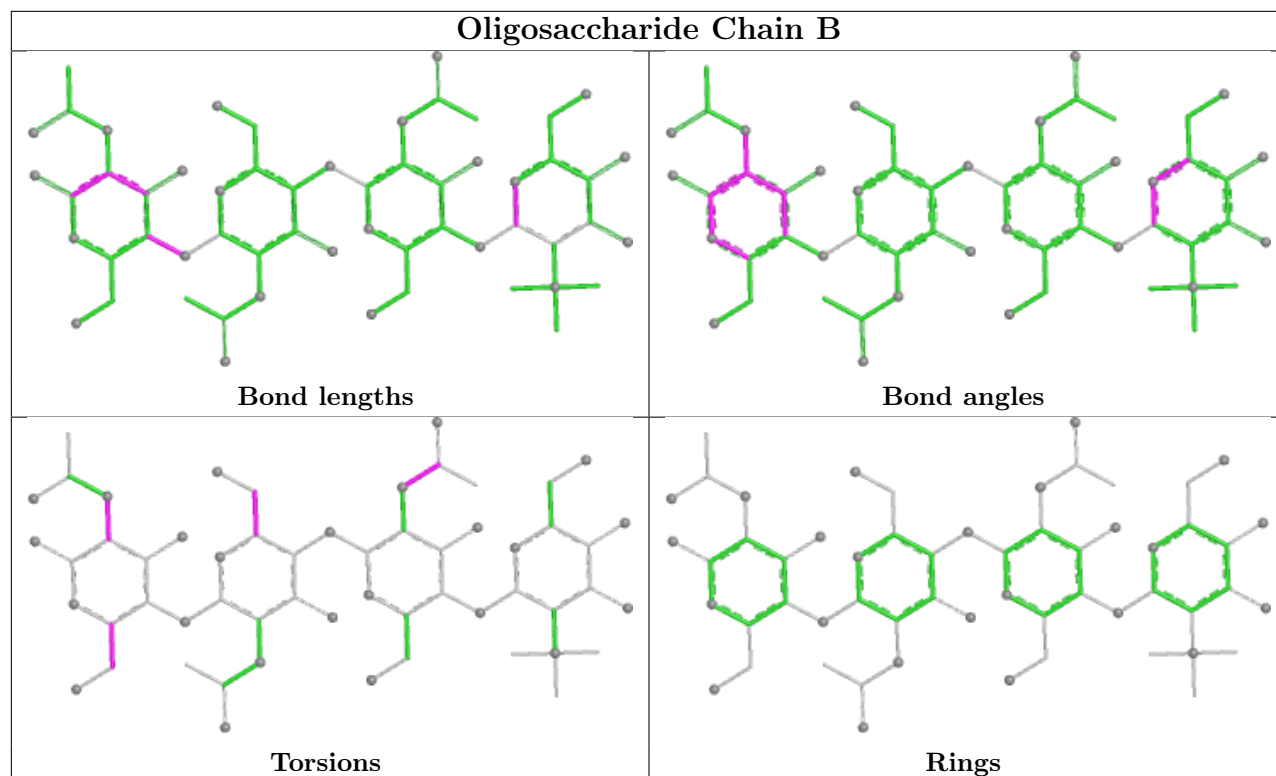
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	3	NAG	C8-C7-N2-C2
2	B	3	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C1-C2-N2-C7
2	B	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	TMX	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](#)

There are no ligands in this entry.

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	572/572 (100%)	0.41	30 (5%) 33 35	15, 27, 44, 72	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	PHE	4.8
1	A	385	MET	4.8
1	A	389	TRP	4.7
1	A	391	LEU	4.7
1	A	394	GLU	4.3
1	A	388	ARG	4.1
1	A	378	ASP	3.9
1	A	396	PHE	3.9
1	A	392	ASP	3.6
1	A	393	LYS	3.4
1	A	395	SER	3.3
1	A	161	ASP	2.9
1	A	118	ARG	2.9
1	A	243	PHE	2.8
1	A	23	GLU	2.7
1	A	371	GLU	2.7
1	A	24	ASP	2.6
1	A	312	ASP	2.5
1	A	384	MET	2.5
1	A	160	ALA	2.4
1	A	390	ASP	2.4
1	A	111	GLN	2.4
1	A	88	GLU	2.3
1	A	387	ASN	2.3
1	A	397	LEU	2.3
1	A	380	ILE	2.2
1	A	92	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	47	GLU	2.2
1	A	374	TRP	2.1
1	A	375	ASN	2.0

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

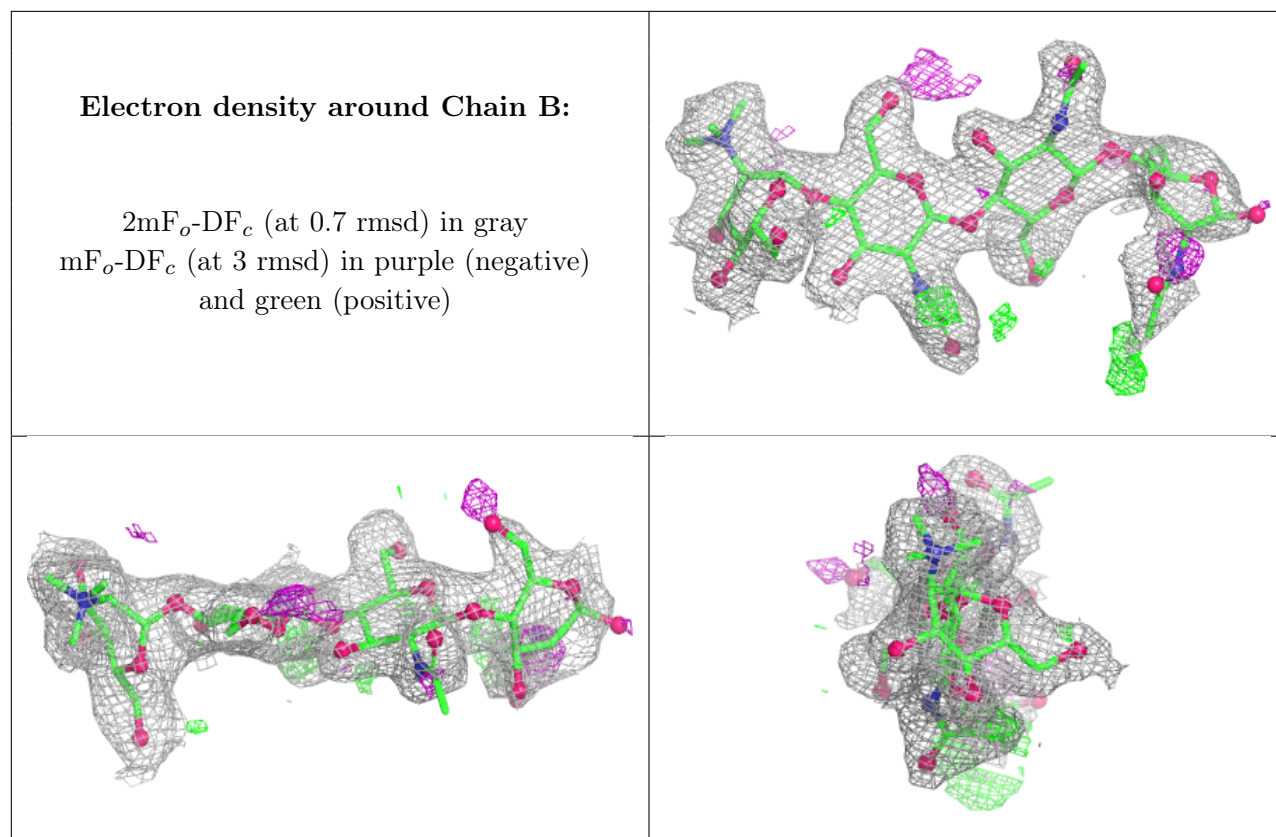
There are no non-standard protein/DNA/RNA residues in this entry.

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	NAG	B	1	15/15	0.58	0.21	49,56,58,58	0
2	NAG	B	2	14/15	0.88	0.13	32,41,44,44	0
2	NAG	B	3	14/15	0.91	0.10	23,26,28,29	0
2	TMX	B	4	14/15	0.95	0.07	21,22,23,23	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.