



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:44 PM UTC

PDB ID : 3OGS / pdb\_00003ogs  
Title : Complex structure of beta-galactosidase from *Trichoderma reesei* with IPTG  
Authors : Maksimainen, M.; Rouvinen, J.  
Deposited on : 2010-08-17  
Resolution : 1.75 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](mailto: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>.

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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

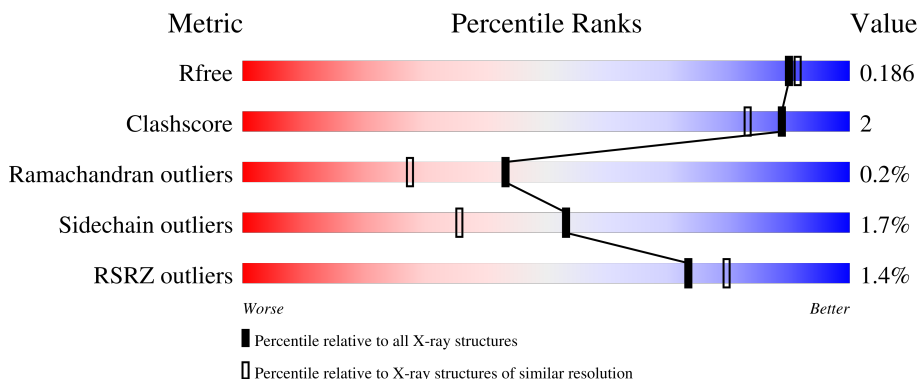
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



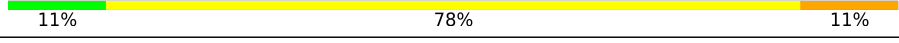
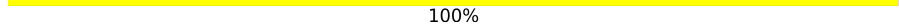
The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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  $\geq 3$ , 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	1003	 78% 20% ..
2	B	7	 14% 86%
3	C	9	 11% 78% 11%
4	D	2	 100%

## 2 Entry composition i

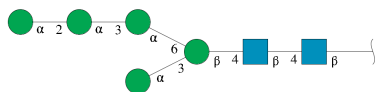
There are 7 unique types of molecules in this entry. The entry contains 8819 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-galactosidase.

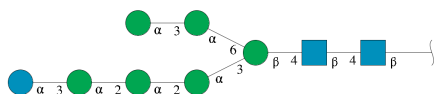
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	986	7634	4906	1289	1431	8	0	3	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(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
			Total	C	N	O			
2	B	7	83	46	2	35	0	0	0

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



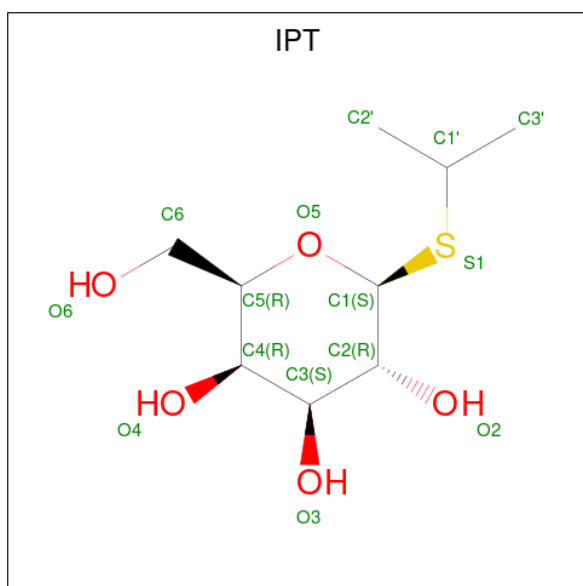
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	105	58	2	45	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	28	16	2	10	0	0	0

- Molecule 5 is 1-methylethyl 1-thio-beta-D-galactopyranoside (CCD ID: IPT) (formula:  $C_9H_{18}O_5S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	A	1	15	9	5	1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

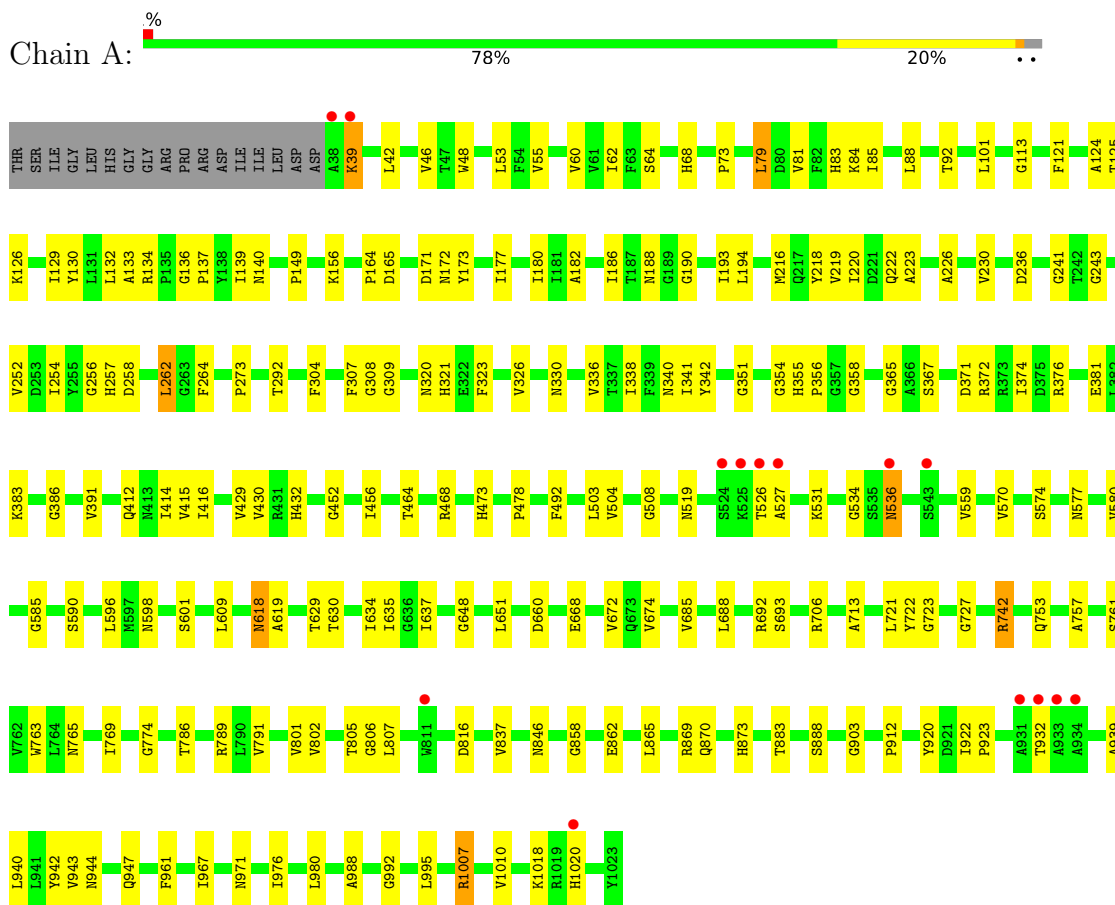
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	926	Total	O	0	0
			926	926		

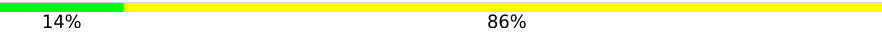
### 3 Residue-property plots

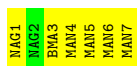
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-galactosidase



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

Chain B: 



- Molecule 3: alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-

6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  11% 78% 11%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
GLC7  
MAN8  
MAN9

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

Chain D:  100%

MAG1  
MAG2

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.50Å 70.30Å 82.40Å 108.50° 97.80° 114.40°	Depositor
Resolution (Å)	43.54 – 1.75 43.54 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.0 (43.54-1.75) 91.2 (43.54-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.145 , 0.200 0.157 , 0.186	Depositor DCC
$R_{free}$ test set	5893 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtrriage
Anisotropy	0.590	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for k,h,-h-k-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GLC, BMA, MAN, IPT

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	2.10	176/7862 (2.2%)	1.18	16/10715 (0.1%)

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	GLY	N-CA	8.62	1.54	1.45
1	A	922	ILE	CA-CB	8.27	1.61	1.54
1	A	48	TRP	N-CA	7.89	1.55	1.46
1	A	920	TYR	N-CA	7.79	1.55	1.46
1	A	132	LEU	C-O	7.62	1.33	1.24
1	A	252	VAL	N-CA	7.57	1.55	1.46
1	A	336	VAL	N-CA	7.48	1.55	1.46
1	A	590	SER	N-CA	7.38	1.55	1.46
1	A	139	ILE	N-CA	7.31	1.53	1.46
1	A	713	ALA	CA-CB	7.29	1.63	1.53
1	A	376	ARG	N-CA	7.16	1.55	1.45
1	A	354	GLY	N-CA	7.13	1.54	1.45
1	A	942	TYR	CA-C	7.13	1.61	1.52
1	A	219	VAL	CA-CB	7.12	1.62	1.54
1	A	939	ALA	N-CA	7.10	1.54	1.45
1	A	508	GLY	N-CA	7.08	1.53	1.45
1	A	816	ASP	CA-C	7.06	1.61	1.53
1	A	134	ARG	N-CA	7.04	1.54	1.46
1	A	84	LYS	C-O	6.91	1.32	1.24
1	A	846	ASN	N-CA	6.80	1.54	1.46
1	A	503	LEU	CA-C	6.78	1.60	1.52
1	A	791	VAL	C-O	6.77	1.31	1.24
1	A	391	VAL	CA-CB	6.75	1.62	1.54
1	A	292	THR	CA-CB	6.67	1.62	1.54
1	A	862	GLU	CA-CB	6.67	1.62	1.53
1	A	79	LEU	C-O	6.66	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	ASN	N-CA	6.64	1.54	1.45
1	A	230	VAL	CA-CB	6.62	1.62	1.54
1	A	674	VAL	CA-CB	6.62	1.60	1.55
1	A	769	ILE	CA-CB	6.58	1.61	1.55
1	A	180	ILE	CA-CB	6.54	1.62	1.54
1	A	355	HIS	CA-C	6.50	1.60	1.52
1	A	807	LEU	N-CA	6.49	1.54	1.46
1	A	177	ILE	CA-CB	6.48	1.62	1.54
1	A	88	LEU	N-CA	6.46	1.54	1.46
1	A	416	ILE	CA-CB	6.44	1.62	1.54
1	A	193	ILE	CA-CB	6.43	1.62	1.54
1	A	81	VAL	CA-CB	6.43	1.62	1.54
1	A	858	GLY	N-CA	6.43	1.53	1.44
1	A	429	VAL	CA-CB	6.40	1.61	1.54
1	A	193	ILE	CA-C	6.36	1.61	1.52
1	A	574	SER	C-O	6.35	1.31	1.24
1	A	46	VAL	C-O	6.34	1.31	1.24
1	A	326	VAL	CA-CB	6.34	1.61	1.54
1	A	508	GLY	CA-C	6.33	1.57	1.52
1	A	101	LEU	N-CA	6.31	1.54	1.46
1	A	125	THR	CA-CB	6.29	1.63	1.53
1	A	577	ASN	N-CA	6.26	1.53	1.46
1	A	220	ILE	N-CA	6.26	1.53	1.46
1	A	83	HIS	N-CA	6.24	1.53	1.46
1	A	356	PRO	N-CA	6.20	1.55	1.47
1	A	765	ASN	N-CA	6.20	1.54	1.46
1	A	223	ALA	CA-CB	6.20	1.63	1.53
1	A	415	VAL	CA-CB	6.11	1.62	1.54
1	A	358	GLY	N-CA	6.10	1.50	1.45
1	A	182	ALA	N-CA	6.07	1.53	1.46
1	A	865	LEU	N-CA	6.05	1.53	1.45
1	A	802	VAL	C-O	6.03	1.30	1.24
1	A	304	PHE	C-O	5.99	1.31	1.23
1	A	257	HIS	CA-CB	5.95	1.63	1.53
1	A	473	HIS	CA-CB	5.94	1.62	1.53
1	A	630	THR	CA-CB	5.94	1.62	1.53
1	A	580	VAL	CA-C	5.92	1.59	1.52
1	A	182	ALA	CA-CB	5.92	1.62	1.53
1	A	256	GLY	C-O	5.89	1.30	1.23
1	A	940	LEU	CA-C	5.89	1.59	1.52
1	A	478	PRO	CA-C	5.87	1.59	1.52
1	A	341	ILE	CA-CB	5.87	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	LEU	CA-C	5.86	1.60	1.52
1	A	769	ILE	C-O	5.83	1.29	1.23
1	A	226	ALA	N-CA	5.82	1.53	1.46
1	A	504	VAL	C-O	5.82	1.30	1.24
1	A	171	ASP	C-O	5.82	1.30	1.24
1	A	801	VAL	CA-CB	5.82	1.61	1.54
1	A	254	ILE	CA-CB	5.81	1.62	1.54
1	A	598	ASN	N-CA	5.80	1.54	1.46
1	A	786	THR	C-O	5.79	1.30	1.23
1	A	660	ASP	N-CA	5.78	1.53	1.45
1	A	256	GLY	CA-C	5.76	1.56	1.51
1	A	414	ILE	N-CA	5.75	1.52	1.46
1	A	723	GLY	N-CA	5.74	1.53	1.45
1	A	805	THR	CA-CB	5.73	1.61	1.53
1	A	46	VAL	CA-CB	5.71	1.61	1.54
1	A	570	VAL	C-O	5.70	1.30	1.23
1	A	85	ILE	N-CA	5.68	1.53	1.46
1	A	121	PHE	N-CA	5.68	1.53	1.46
1	A	464	THR	C-O	5.67	1.30	1.24
1	A	688	LEU	N-CA	5.66	1.52	1.46
1	A	216	MET	C-O	5.65	1.30	1.24
1	A	338	ILE	C-O	5.65	1.30	1.24
1	A	763	TRP	CA-C	5.63	1.59	1.52
1	A	372	ARG	CA-CB	5.62	1.61	1.53
1	A	173	TYR	CA-CB	5.61	1.62	1.53
1	A	601	SER	CA-C	5.61	1.59	1.52
1	A	62	ILE	CA-CB	5.60	1.60	1.54
1	A	492	PHE	N-CA	5.60	1.53	1.46
1	A	218	TYR	N-CA	5.57	1.53	1.46
1	A	42	LEU	C-O	5.55	1.31	1.23
1	A	171	ASP	CA-C	5.55	1.59	1.52
1	A	789	ARG	CA-CB	5.54	1.61	1.53
1	A	967	ILE	C-O	5.54	1.30	1.24
1	A	134	ARG	C-N	5.54	1.38	1.33
1	A	121	PHE	CA-C	5.54	1.59	1.52
1	A	816	ASP	N-CA	5.49	1.53	1.46
1	A	68	HIS	CA-CB	5.48	1.60	1.53
1	A	371	ASP	N-CA	5.48	1.53	1.46
1	A	172	ASN	CA-C	5.47	1.59	1.52
1	A	757	ALA	CA-CB	5.43	1.61	1.53
1	A	236	ASP	N-CA	5.42	1.52	1.46
1	A	124	ALA	N-CA	5.42	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	LYS	C-O	5.40	1.30	1.23
1	A	598	ASN	CA-C	5.40	1.59	1.52
1	A	129	ILE	N-CA	5.40	1.52	1.46
1	A	336	VAL	CA-C	5.40	1.59	1.52
1	A	338	ILE	CA-CB	5.39	1.61	1.54
1	A	381	GLU	N-CA	5.38	1.52	1.46
1	A	870	GLN	N-CA	5.38	1.53	1.46
1	A	73	PRO	N-CA	5.36	1.51	1.47
1	A	961	PHE	CA-CB	5.36	1.60	1.53
1	A	944	ASN	CA-C	5.35	1.59	1.53
1	A	55	VAL	C-O	5.34	1.29	1.24
1	A	113	GLY	N-CA	5.33	1.53	1.45
1	A	806	GLY	N-CA	5.33	1.51	1.45
1	A	130	TYR	N-CA	5.32	1.52	1.45
1	A	761	SER	N-CA	5.32	1.52	1.45
1	A	456	ILE	CA-CB	5.32	1.61	1.54
1	A	988	ALA	N-CA	5.31	1.52	1.46
1	A	774	GLY	N-CA	5.30	1.50	1.45
1	A	140	ASN	N-CA	5.30	1.53	1.46
1	A	468	ARG	N-CA	5.28	1.54	1.46
1	A	165	ASP	CA-C	5.28	1.59	1.52
1	A	149	PRO	C-O	5.26	1.30	1.23
1	A	180	ILE	N-CA	5.25	1.52	1.46
1	A	219	VAL	N-CA	5.24	1.52	1.46
1	A	53	LEU	C-O	5.24	1.31	1.23
1	A	340	ASN	C-O	5.22	1.30	1.24
1	A	992	GLY	N-CA	5.22	1.50	1.45
1	A	761	SER	CA-C	5.21	1.58	1.52
1	A	943	VAL	N-CA	5.20	1.53	1.46
1	A	721	LEU	N-CA	5.20	1.52	1.46
1	A	132	LEU	CA-CB	5.19	1.59	1.53
1	A	351	GLY	N-CA	5.18	1.53	1.45
1	A	559	VAL	C-O	5.18	1.29	1.24
1	A	869	ARG	CZ-NH1	5.17	1.40	1.32
1	A	635	ILE	CA-CB	5.17	1.60	1.54
1	A	648	GLY	N-CA	5.17	1.52	1.45
1	A	365	GLY	N-CA	5.16	1.52	1.45
1	A	629	THR	N-CA	5.16	1.52	1.46
1	A	1018	LYS	CA-C	5.16	1.59	1.52
1	A	258	ASP	C-O	5.15	1.30	1.23
1	A	330	ASN	CA-CB	5.15	1.61	1.53
1	A	243	GLY	N-CA	5.14	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	672	VAL	CA-CB	5.14	1.60	1.54
1	A	452	GLY	N-CA	5.14	1.51	1.45
1	A	133	ALA	CA-CB	5.12	1.60	1.53
1	A	164	PRO	C-O	5.12	1.30	1.24
1	A	903	GLY	N-CA	5.12	1.50	1.45
1	A	980	LEU	CA-C	5.11	1.58	1.52
1	A	139	ILE	CA-CB	5.11	1.61	1.54
1	A	292	THR	CA-C	5.11	1.57	1.52
1	A	241	GLY	CA-C	5.10	1.58	1.51
1	A	722	TYR	C-O	5.10	1.30	1.24
1	A	432	HIS	N-CA	5.08	1.52	1.45
1	A	685	VAL	N-CA	5.05	1.52	1.46
1	A	386	GLY	C-O	5.05	1.29	1.23
1	A	753	GLN	C-O	5.05	1.29	1.23
1	A	308	GLY	N-CA	5.04	1.53	1.45
1	A	383	LYS	N-CA	5.04	1.52	1.46
1	A	922	ILE	CA-C	5.04	1.58	1.52
1	A	619	ALA	N-CA	5.03	1.52	1.46
1	A	194	LEU	N-CA	5.03	1.52	1.45
1	A	430	VAL	CA-CB	5.03	1.60	1.54
1	A	1010	VAL	CA-CB	5.03	1.59	1.54
1	A	967	ILE	CA-C	5.02	1.59	1.52
1	A	307	PHE	N-CA	5.02	1.52	1.46
1	A	222	GLN	C-O	5.00	1.29	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	637	ILE	CB-CA-C	-7.16	103.16	110.89
1	A	976	ILE	CA-C-N	6.99	126.40	121.65
1	A	976	ILE	C-N-CA	6.99	126.40	121.65
1	A	156	LYS	N-CA-C	6.94	118.84	111.28
1	A	534	GLY	N-CA-C	6.31	119.35	112.29
1	A	367	SER	N-CA-C	6.29	118.13	111.28
1	A	769	ILE	N-CA-C	5.69	117.08	111.67
1	A	273	PRO	N-CA-C	5.64	119.94	111.14
1	A	912	PRO	CB-CA-C	-5.38	104.95	111.46
1	A	923	PRO	CB-CA-C	-5.38	104.95	111.46
1	A	88	LEU	N-CA-C	-5.21	106.76	113.01
1	A	727	GLY	N-CA-C	5.17	122.72	115.43
1	A	264	PHE	N-CA-C	5.11	121.27	113.61
1	A	342	TYR	CA-C-N	5.06	130.81	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	TYR	C-N-CA	5.06	130.81	121.70
1	A	585	GLY	N-CA-C	-5.02	105.33	112.55

There are no chirality outliers.

There are no planarity outliers.

## 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	7634	0	7435	27	0
2	B	83	0	70	0	0
3	C	105	0	88	2	0
4	D	28	0	25	0	0
5	A	15	0	18	0	0
6	A	28	0	26	0	0
7	A	926	0	0	15	0
All	All	8819	0	7662	29	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 2.

All (29) 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:1020:HIS:HB2	7:A:1807:HOH:O	1.20	1.34
1:A:188:ASN:HB3	7:A:1881:HOH:O	1.48	1.14
1:A:531:LYS:HB3	7:A:1575:HOH:O	1.62	0.97
1:A:971:ASN:HB3	7:A:1816:HOH:O	1.67	0.95
7:A:1952:HOH:O	3:C:7:GLC:H61	1.79	0.82
1:A:536:ASN:OD1	1:A:536:ASN:C	2.33	0.71
1:A:971:ASN:ND2	7:A:1816:HOH:O	2.21	0.67
1:A:971:ASN:CB	7:A:1816:HOH:O	2.36	0.64
1:A:692:ARG:NH1	7:A:1666:HOH:O	2.30	0.64
1:A:706:ARG:NH1	7:A:1805:HOH:O	2.34	0.60
1:A:262:LEU:HD22	1:A:323:PHE:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD22	1:A:323:PHE:CD1	2.42	0.54
1:A:321:HIS:HD2	7:A:1189:HOH:O	1.91	0.53
1:A:668:GLU:HB3	7:A:1882:HOH:O	2.12	0.49
1:A:60[B]:VAL:HG11	1:A:596:LEU:CD1	2.43	0.48
1:A:1007:ARG:HD2	7:A:1607:HOH:O	2.12	0.48
1:A:651:LEU:HD23	1:A:651:LEU:N	2.28	0.48
1:A:883:THR:HG21	7:A:1721:HOH:O	2.14	0.48
1:A:651:LEU:HD23	1:A:651:LEU:H	1.80	0.47
1:A:618:ASN:HD22	1:A:618:ASN:C	2.23	0.46
1:A:79:LEU:HD22	1:A:126:LYS:HD3	2.00	0.44
1:A:64:SER:HA	1:A:92:THR:O	2.18	0.43
7:A:1952:HOH:O	3:C:7:GLC:C6	2.53	0.43
1:A:742:ARG:HG3	1:A:837:VAL:HG22	2.01	0.42
1:A:873:HIS:H	1:A:873:HIS:CD2	2.38	0.42
1:A:136:GLY:HA3	1:A:137:PRO:C	2.45	0.41
1:A:883:THR:CG2	7:A:1721:HOH:O	2.67	0.41
1:A:374:ILE:HD11	1:A:609:LEU:HB2	2.03	0.41
1:A:186:ILE:HA	1:A:190:GLY:O	2.21	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	987/1003 (98%)	957 (97%)	28 (3%)	2 (0%)	43 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	ALA
1	A	519	ASN

### 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	808/819 (99%)	794 (98%)	14 (2%)	53 36

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

Mol	Chain	Res	Type
1	A	39	LYS
1	A	262	LEU
1	A	412	GLN
1	A	526	THR
1	A	536	ASN
1	A	618	ASN
1	A	634	ILE
1	A	693	SER
1	A	742	ARG
1	A	888	SER
1	A	932	THR
1	A	947	GLN
1	A	995	LEU
1	A	1007	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	225	ASN
1	A	321	HIS
1	A	340	ASN
1	A	412	GLN
1	A	573	ASN
1	A	577	ASN
1	A	618	ASN
1	A	664	HIS
1	A	846	ASN
1	A	873	HIS

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Mol	Chain	Res	Type
1	A	884	HIS
1	A	918	GLN
1	A	1015	HIS

### 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](#)

18 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	1,2	14,14,15	1.28	1 (7%)	17,19,21	1.77	4 (23%)
2	NAG	B	2	2	14,14,15	1.04	0	17,19,21	0.93	0
2	BMA	B	3	2	11,11,12	1.53	2 (18%)	15,15,17	1.13	2 (13%)
2	MAN	B	4	2	11,11,12	1.62	3 (27%)	15,15,17	1.46	2 (13%)
2	MAN	B	5	2	11,11,12	1.26	2 (18%)	15,15,17	1.51	4 (26%)
2	MAN	B	6	2	11,11,12	0.68	0	15,15,17	1.35	3 (20%)
2	MAN	B	7	2	11,11,12	1.22	2 (18%)	15,15,17	1.94	4 (26%)
3	NAG	C	1	1,3	14,14,15	1.88	2 (14%)	17,19,21	1.61	4 (23%)
3	NAG	C	2	3	14,14,15	0.79	0	17,19,21	1.41	2 (11%)
3	BMA	C	3	3	11,11,12	1.08	1 (9%)	15,15,17	1.29	2 (13%)
3	MAN	C	4	3	11,11,12	1.21	1 (9%)	15,15,17	2.24	4 (26%)
3	MAN	C	5	3	11,11,12	0.96	0	15,15,17	1.71	4 (26%)
3	MAN	C	6	3	11,11,12	0.90	1 (9%)	15,15,17	2.10	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLC	C	7	3	11,11,12	0.67	0	15,15,17	2.54	4 (26%)
3	MAN	C	8	3	11,11,12	0.85	0	15,15,17	1.84	2 (13%)
3	MAN	C	9	3	11,11,12	0.62	0	15,15,17	0.94	0
4	NAG	D	1	1,4	14,14,15	0.57	0	17,19,21	1.59	5 (29%)
4	NAG	D	2	4	14,14,15	0.65	0	17,19,21	1.22	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	1/2/19/22	0/1/1/1
2	MAN	B	6	2	-	2/2/19/22	0/1/1/1
2	MAN	B	7	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	GLC	C	7	3	-	0/2/19/22	0/1/1/1
3	MAN	C	8	3	-	0/2/19/22	0/1/1/1
3	MAN	C	9	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C1-C2	5.50	1.59	1.52
3	C	1	NAG	C3-C2	2.86	1.58	1.52
2	B	4	MAN	C2-C3	2.76	1.56	1.52
2	B	7	MAN	C2-C3	2.62	1.56	1.52
2	B	5	MAN	O2-C2	2.61	1.48	1.43
2	B	3	BMA	O4-C4	2.61	1.49	1.43
2	B	4	MAN	C6-C5	2.44	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	MAN	C2-C3	2.42	1.56	1.52
2	B	7	MAN	O5-C1	-2.37	1.39	1.43
2	B	3	BMA	C2-C3	2.35	1.56	1.52
3	C	6	MAN	C2-C3	2.22	1.55	1.52
2	B	1	NAG	C2-N2	2.19	1.49	1.46
3	C	3	BMA	O2-C2	2.10	1.47	1.43
2	B	4	MAN	O5-C5	2.08	1.47	1.43
2	B	5	MAN	C2-C3	2.07	1.55	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	7	GLC	C1-O5-C5	7.18	121.81	112.19
3	C	4	MAN	C6-C5-C4	-6.60	96.82	113.02
2	B	7	MAN	C1-O5-C5	5.68	119.80	112.19
3	C	8	MAN	O5-C5-C6	5.06	117.51	107.66
3	C	7	GLC	C1-C2-C3	4.83	116.68	109.64
3	C	6	MAN	O3-C3-C2	4.30	118.83	110.05
3	C	6	MAN	O3-C3-C4	-4.17	100.55	110.38
3	C	5	MAN	C1-O5-C5	4.02	117.57	112.19
2	B	1	NAG	C4-C3-C2	3.79	116.58	111.02
4	D	1	NAG	O5-C5-C6	3.78	115.01	107.66
3	C	4	MAN	C3-C4-C5	3.55	116.66	110.23
3	C	6	MAN	O2-C2-C1	-3.44	101.34	109.22
2	B	1	NAG	O5-C1-C2	-3.43	105.99	111.29
2	B	5	MAN	C1-O5-C5	3.40	116.75	112.19
2	B	4	MAN	C1-O5-C5	3.33	116.66	112.19
3	C	8	MAN	O3-C3-C2	3.18	116.55	110.05
2	B	4	MAN	O2-C2-C3	-3.15	103.63	110.15
3	C	1	NAG	C2-N2-C7	3.14	127.11	122.90
3	C	3	BMA	O3-C3-C2	3.06	116.31	110.05
3	C	2	NAG	C1-O5-C5	3.04	116.27	112.19
3	C	7	GLC	O3-C3-C2	-3.04	103.85	110.05
3	C	1	NAG	O5-C1-C2	-3.00	106.65	111.29
2	B	7	MAN	C6-C5-C4	-2.83	106.06	113.02
2	B	3	BMA	O4-C4-C3	-2.81	103.76	110.38
3	C	3	BMA	O3-C3-C4	-2.80	103.77	110.38
3	C	2	NAG	O7-C7-C8	-2.75	117.16	122.05
3	C	5	MAN	O2-C2-C1	2.67	115.33	109.22
2	B	6	MAN	O2-C2-C3	-2.66	104.64	110.15
4	D	1	NAG	O3-C3-C2	-2.62	103.96	109.40
2	B	5	MAN	O6-C6-C5	-2.56	102.61	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C8-C7-N2	2.56	120.36	116.12
4	D	1	NAG	C3-C4-C5	-2.54	105.63	110.23
3	C	1	NAG	C6-C5-C4	-2.48	106.92	113.02
3	C	5	MAN	O2-C2-C3	-2.43	105.13	110.15
3	C	7	GLC	O5-C5-C6	2.38	112.29	107.66
2	B	6	MAN	O6-C6-C5	-2.37	103.25	111.33
3	C	6	MAN	O2-C2-C3	2.30	114.91	110.15
4	D	1	NAG	C4-C3-C2	2.27	114.35	111.02
3	C	5	MAN	O5-C5-C6	2.27	112.09	107.66
2	B	3	BMA	O3-C3-C2	-2.25	105.47	110.05
3	C	4	MAN	C2-C3-C4	-2.23	106.94	110.86
2	B	1	NAG	O5-C5-C6	2.23	111.99	107.66
2	B	5	MAN	O3-C3-C2	2.20	114.54	110.05
4	D	2	NAG	C1-O5-C5	2.20	115.13	112.19
2	B	1	NAG	C1-O5-C5	2.16	115.08	112.19
3	C	4	MAN	O4-C4-C3	2.16	115.46	110.38
2	B	5	MAN	O2-C2-C1	2.14	114.13	109.22
2	B	6	MAN	C2-C3-C4	-2.13	107.11	110.86
2	B	7	MAN	O3-C3-C2	2.02	114.18	110.05
2	B	7	MAN	O5-C5-C6	-2.01	103.75	107.66
4	D	1	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

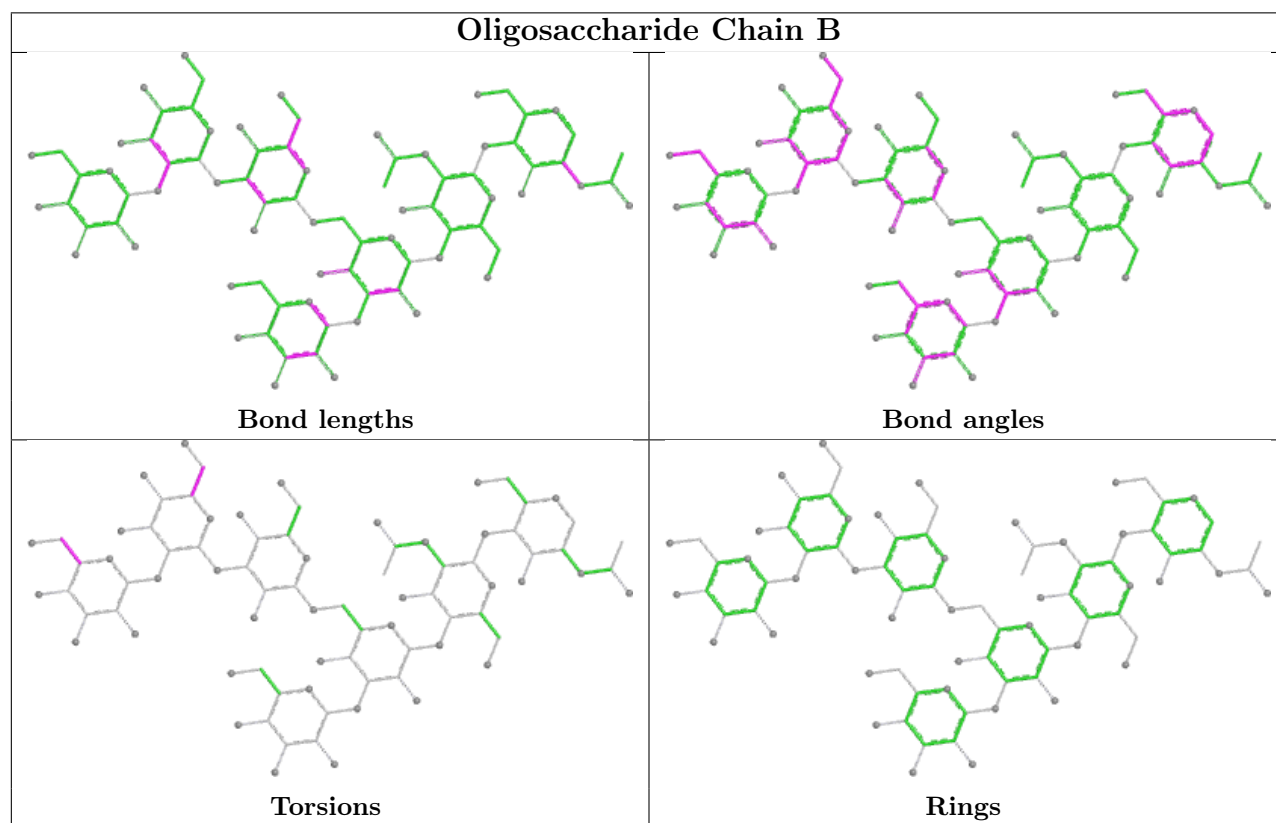
Mol	Chain	Res	Type	Atoms
3	C	9	MAN	C4-C5-C6-O6
3	C	9	MAN	O5-C5-C6-O6
2	B	6	MAN	O5-C5-C6-O6
2	B	6	MAN	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6
4	D	1	NAG	C1-C2-N2-C7
3	C	1	NAG	C4-C5-C6-O6

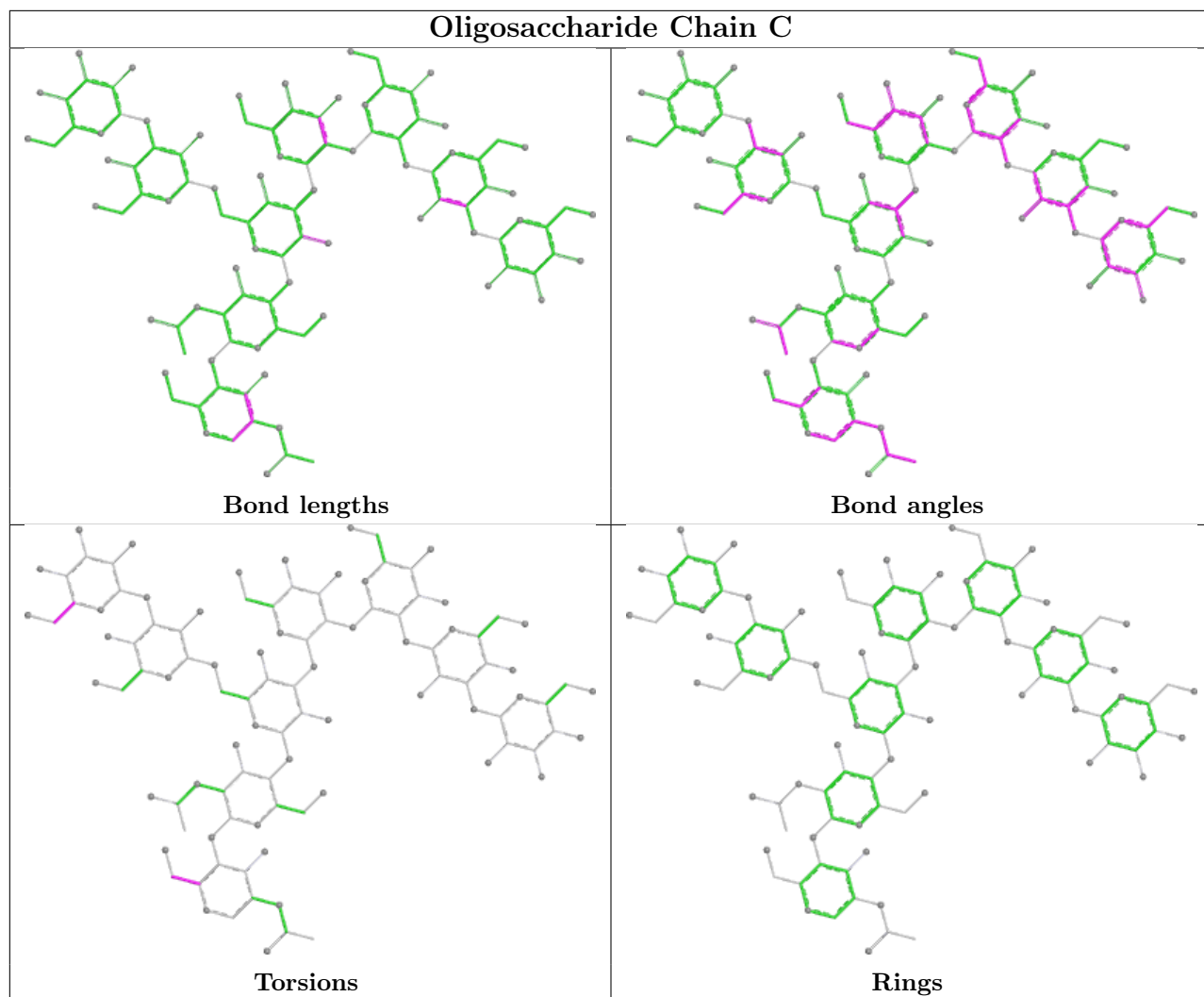
There are no ring outliers.

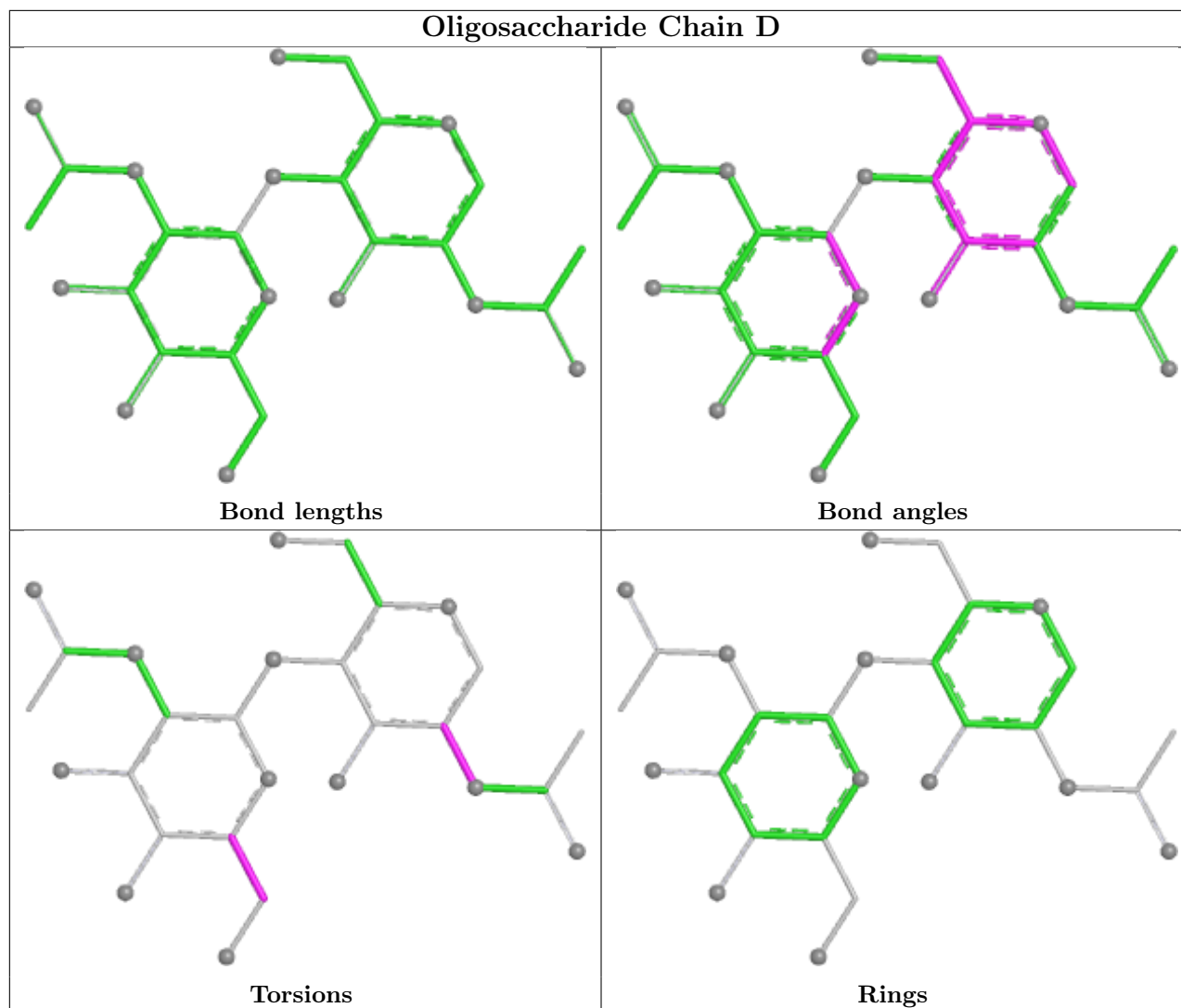
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	7	GLC	2	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](#)

3 ligands 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$
5	IPT	A	1024	-	15,15,15	1.27	1 (6%)	18,21,21	1.78	5 (27%)
6	NAG	A	1042	1	14,14,15	0.54	0	17,19,21	1.77	5 (29%)
6	NAG	A	1041	1	14,14,15	0.58	0	17,19,21	2.38	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
5	IPT	A	1024	-	-	3/6/26/26	0/1/1/1
6	NAG	A	1042	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1041	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1024	IPT	C4-C5	3.09	1.59	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1041	NAG	C1-O5-C5	7.40	122.11	112.19
5	A	1024	IPT	C1-O5-C5	4.37	120.39	112.56
6	A	1041	NAG	O5-C1-C2	3.81	117.19	111.29
6	A	1042	NAG	C1-O5-C5	3.73	117.19	112.19
6	A	1041	NAG	C1-C2-N2	-3.39	105.09	110.43
5	A	1024	IPT	C2'-C1'-S1	3.20	119.34	110.12
6	A	1042	NAG	O3-C3-C2	-3.20	102.75	109.40
6	A	1042	NAG	O7-C7-C8	-3.09	116.55	122.05
5	A	1024	IPT	O2-C2-C3	-2.48	104.54	110.38
6	A	1042	NAG	C8-C7-N2	2.41	120.11	116.12
6	A	1041	NAG	O5-C5-C4	2.17	116.10	110.83
5	A	1024	IPT	O4-C4-C3	-2.12	105.37	110.38
6	A	1042	NAG	O6-C6-C5	-2.12	104.10	111.33
5	A	1024	IPT	O5-C5-C4	-2.09	105.93	109.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1024	IPT	C2'-C1'-S1-C1
5	A	1024	IPT	C3'-C1'-S1-C1
6	A	1041	NAG	O5-C5-C6-O6
5	A	1024	IPT	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	986/1003 (98%)	-0.31	14 (1%) 73 80	9, 17, 33, 64	3 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	933	ALA	5.4
1	A	932	THR	3.9
1	A	526	THR	3.8
1	A	811	TRP	3.5
1	A	931	ALA	3.3
1	A	38	ALA	3.2
1	A	527	ALA	2.6
1	A	39	LYS	2.6
1	A	1020	HIS	2.6
1	A	543	SER	2.5
1	A	934	ALA	2.5
1	A	524	SER	2.4
1	A	536	ASN	2.3
1	A	525	LYS	2.3

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

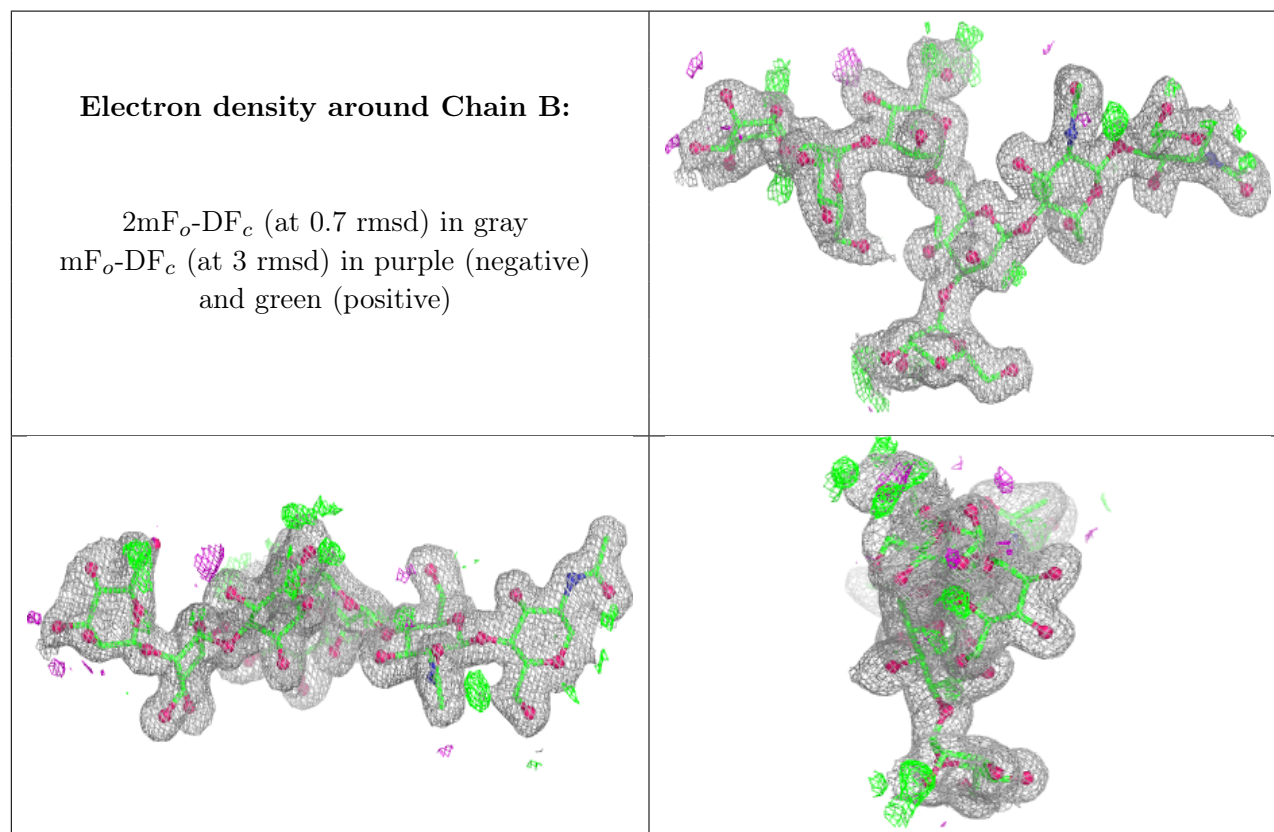
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 95<sup>th</sup> 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.

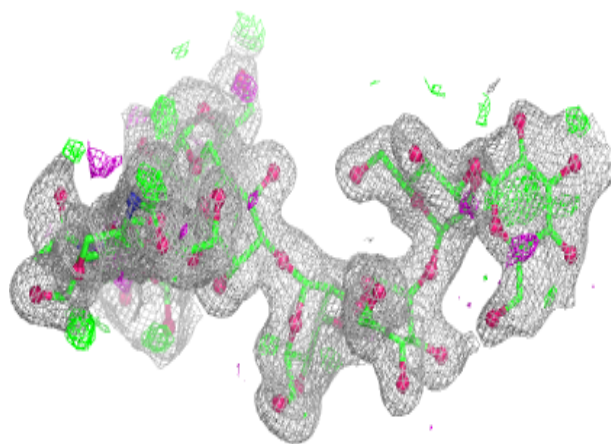
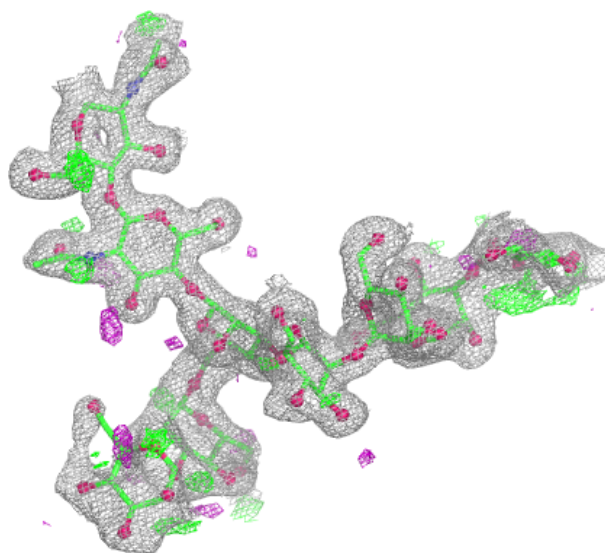
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MAN	C	9	11/12	0.73	0.14	55,62,64,65	0
4	NAG	D	2	14/15	0.77	0.14	46,56,63,63	0
3	GLC	C	7	11/12	0.80	0.15	41,47,48,49	0
3	MAN	C	8	11/12	0.85	0.13	34,40,45,48	0
2	MAN	B	6	11/12	0.87	0.15	30,35,41,47	0
3	MAN	C	4	11/12	0.91	0.09	22,25,31,34	0
4	NAG	D	1	14/15	0.92	0.10	32,37,44,46	0
3	MAN	C	6	11/12	0.92	0.09	24,30,35,38	0
3	NAG	C	1	14/15	0.94	0.07	13,18,24,30	0
2	MAN	B	7	11/12	0.94	0.07	24,26,28,30	0
3	NAG	C	2	14/15	0.95	0.07	16,23,37,39	0
2	BMA	B	3	11/12	0.96	0.06	13,16,19,19	0
3	MAN	C	5	11/12	0.96	0.06	17,22,26,27	0
2	MAN	B	4	11/12	0.96	0.05	13,15,18,25	0
3	BMA	C	3	11/12	0.96	0.07	19,21,25,29	0
2	NAG	B	2	14/15	0.97	0.05	13,15,21,22	0
2	MAN	B	5	11/12	0.97	0.06	15,16,28,35	0
2	NAG	B	1	14/15	0.97	0.05	13,15,25,27	0

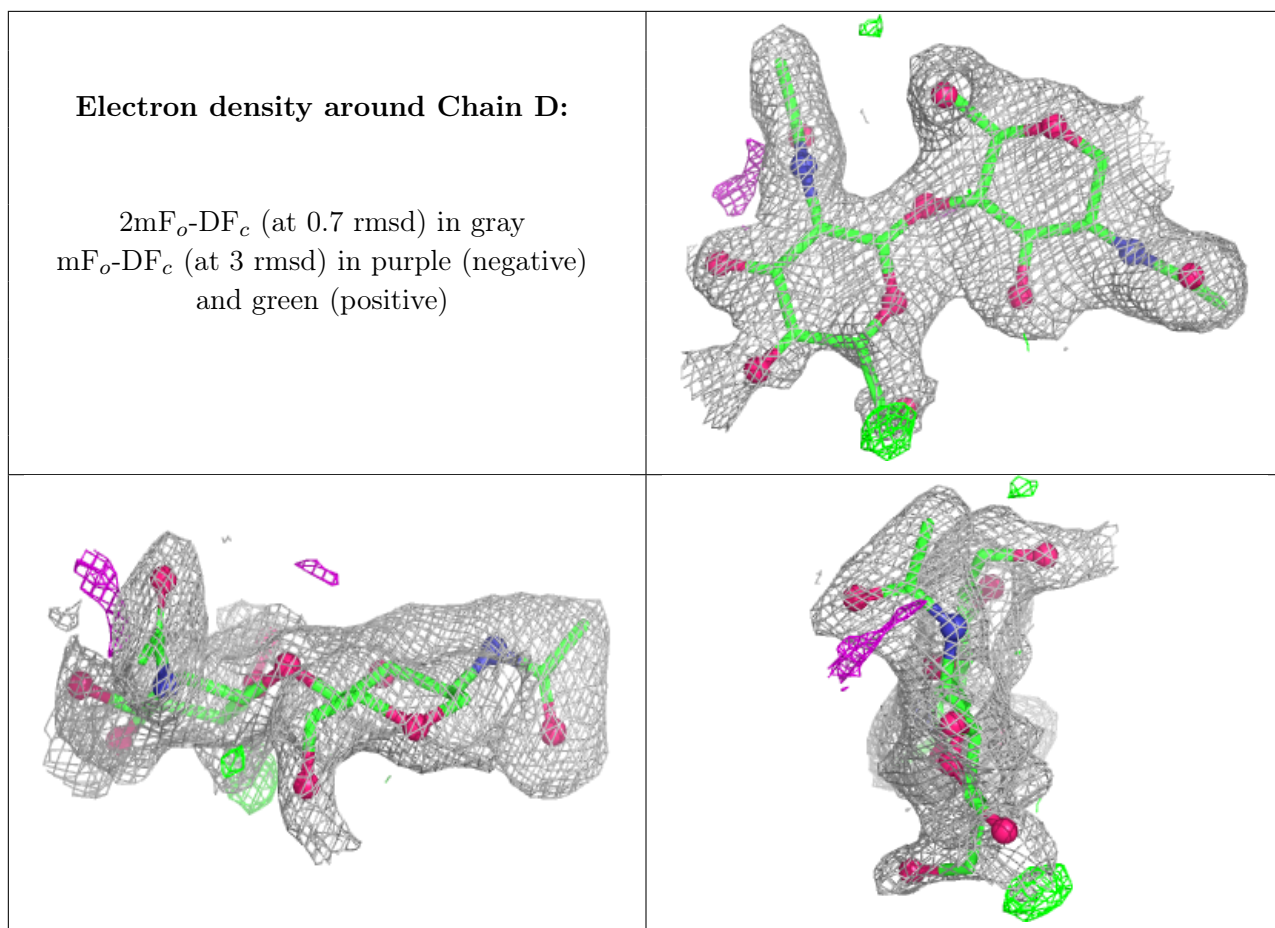
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain C:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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
6	NAG	A	1041	14/15	0.78	0.15	39,48,56,59	0
6	NAG	A	1042	14/15	0.85	0.11	33,39,48,52	0
5	IPT	A	1024	15/15	0.97	0.06	9,12,26,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.