



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:48 AM UTC

PDB ID : 4EB2 / pdb_00004eb2
Title : Crystal structure Mistletoe Lectin I from *Viscum album* in complex with n-acetyl-d-glucosamine at 1.94 Å resolution.
Authors : Laskov, A.A.; Prokofev, I.I.; Gabdoulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.
Deposited on : 2012-03-23
Resolution : 1.94 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

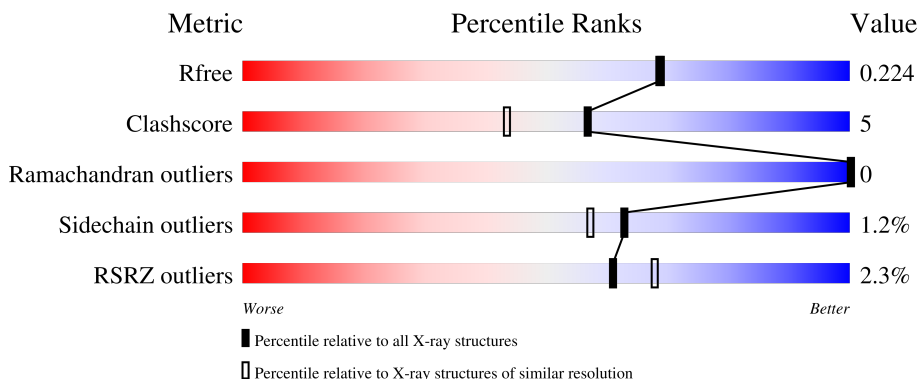
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

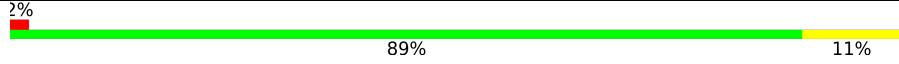
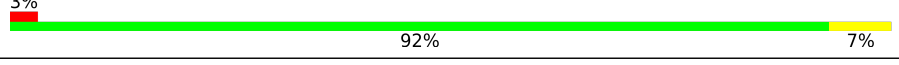
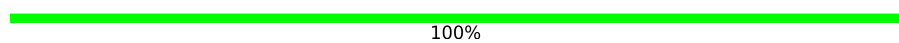
The reported resolution of this entry is 1.94 Å.

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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	249	 2% 89% 11%
2	B	263	 3% 92% 7%
3	C	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	AZI	B	301	-	X	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4392 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-galactoside-specific lectin 1 chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	249	1964	1245	342	373	4	0	4	0

- Molecule 2 is a protein called Beta-galactoside-specific lectin 1 chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	263	2020	1250	359	399	12	0	4	0

- Molecule 3 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			
3	C	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

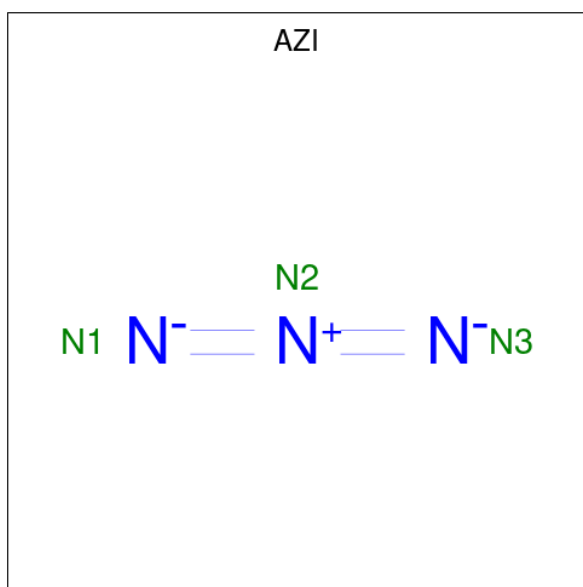
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 7 4 3	0	0

- Molecule 10 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total N 3 3	0	0

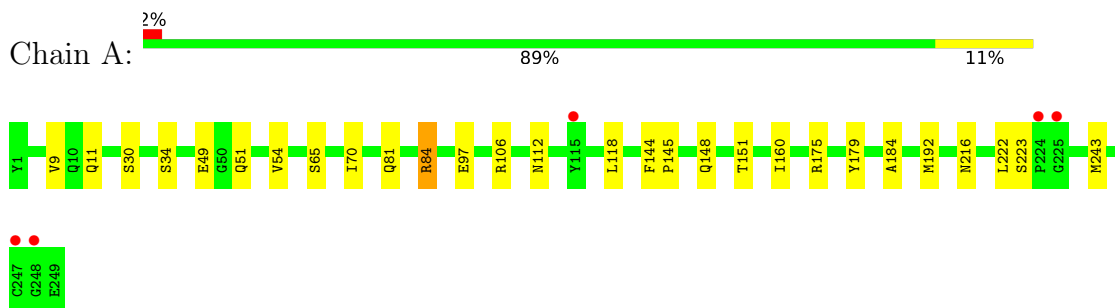
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	72	Total O 72 72	0	0
11	B	159	Total O 159 159	0	0

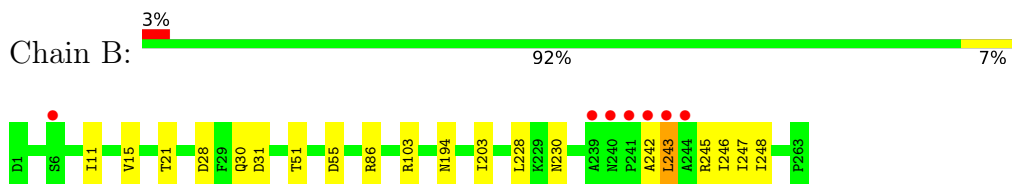
3 Residue-property plots [i](#)

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.

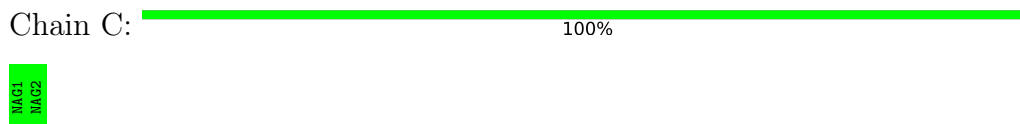
- Molecule 1: Beta-galactoside-specific lectin 1 chain A



- Molecule 2: Beta-galactoside-specific lectin 1 chain B



- Molecule 3: 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 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	107.06Å 107.06Å 311.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 1.94 8.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.2 (8.00-1.94) 96.6 (8.00-1.94)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.93Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.180 , 0.226 0.181 , 0.224	Depositor DCC
R_{free} test set	3873 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtrriage
Anisotropy	0.235	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 74.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4392	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GOL, SO4, CL, AZI, PEG, EDO

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	0.42	0/2009	0.73	0/2734
2	B	0.43	0/2063	0.74	1/2813 (0.0%)
All	All	0.43	0/4072	0.73	1/5547 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	242	ALA	N-CA-C	-5.11	105.13	112.13

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	1964	0	1954	19	0
2	B	2020	0	1962	15	0
3	C	28	0	25	0	0
4	A	14	0	13	2	0
4	B	28	0	26	2	0
5	A	10	0	0	1	0
6	A	24	0	32	1	0
6	B	18	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	4	0	6	0	0
7	B	16	0	24	2	0
8	A	1	0	0	0	0
9	A	16	0	20	1	0
9	B	15	0	20	1	0
10	B	3	0	0	0	0
11	A	72	0	0	1	0
11	B	159	0	0	3	0
All	All	4392	0	4106	37	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 5.

All (37) 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:112:ASN:ND2	4:A:301:NAG:O5	1.96	0.95
1:A:9:VAL:HG23	1:A:11:GLN:H	1.31	0.95
1:A:112:ASN:CG	4:A:301:NAG:C1	2.51	0.84
1:A:30:SER:HB2	9:A:310:PEG:H12	1.71	0.72
2:B:31:ASP:H	7:B:312:EDO:H21	1.51	0.72
1:A:97:GLU:HG2	1:A:106:ARG:HD2	1.73	0.70
1:A:148:GLN:HG3	1:A:151:THR:H	1.56	0.70
1:A:175:ARG:HH12	1:A:192:MET:HB2	1.59	0.68
1:A:216:ASN:ND2	5:A:303:SO4:O2	2.28	0.61
2:B:194:ASN:HD22	2:B:248:ILE:HD13	1.66	0.60
1:A:65:SER:HB2	6:A:306:GOL:H12	1.85	0.59
1:A:9:VAL:HG23	1:A:11:GLN:N	2.09	0.58
1:A:34:SER:HB3	1:A:243:MET:HE1	1.86	0.58
1:A:175:ARG:NH1	1:A:192:MET:HB2	2.19	0.56
4:B:302:NAG:H81	11:B:527:HOH:O	2.06	0.55
2:B:11:ILE:HG12	2:B:51:THR:OG1	2.06	0.55
2:B:55:ASP:HB2	2:B:86:ARG:HH22	1.71	0.55
2:B:194:ASN:ND2	2:B:230:ASN:HD21	2.10	0.50
2:B:103:ARG:HB2	6:B:308:GOL:H11	1.92	0.49
1:A:49:GLU:HG2	1:A:51:GLN:H	1.77	0.48
2:B:28:ASP:OD1	2:B:30:GLN:HG2	2.14	0.47
2:B:243:LEU:HB3	2:B:245:ARG:HG3	1.96	0.47
2:B:203:ILE:HD12	2:B:246:ILE:HG22	1.95	0.47
2:B:247:ILE:HD13	7:B:311:EDO:H22	1.97	0.46
2:B:103:ARG:HD3	6:B:308:GOL:H32	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:HG13	1:A:70:ILE:HB	1.98	0.44
1:A:144:PHE:HA	1:A:145:PRO:HD3	1.86	0.44
2:B:15[A]:VAL:HG22	2:B:21:THR:HG22	2.00	0.43
2:B:228:LEU:HD12	9:B:314:PEG:H41	2.02	0.42
1:A:179:TYR:HD1	1:A:184:ALA:HB3	1.85	0.42
4:B:302:NAG:O4	11:B:528:HOH:O	2.21	0.42
1:A:118:LEU:HD11	1:A:160:ILE:HD12	2.01	0.41
6:B:307:GOL:H11	11:B:432:HOH:O	2.19	0.41
1:A:84:ARG:H	1:A:84:ARG:CD	2.34	0.40
2:B:194:ASN:HD21	2:B:230:ASN:HD21	1.68	0.40
2:B:243:LEU:HD23	2:B:245:ARG:HD3	2.03	0.40
1:A:84:ARG:NH2	11:A:441:HOH:O	2.47	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	251/249 (101%)	245 (98%)	6 (2%)	0	100	100
2	B	265/263 (101%)	257 (97%)	8 (3%)	0	100	100
All	All	516/512 (101%)	502 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	213/209 (102%)	209 (98%)	4 (2%)	50	40
2	B	221/217 (102%)	220 (100%)	1 (0%)	81	82
All	All	434/426 (102%)	429 (99%)	5 (1%)	63	57

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	84	ARG
1	A	222	LEU
1	A	223	SER
2	B	243	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	81	GLN
2	B	169	GLN
2	B	188	GLN

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](#)

2 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$
3	NAG	C	1	2,3	14,14,15	0.58	0	17,19,21	0.71	0
3	NAG	C	2	3	14,14,15	0.60	0	17,19,21	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

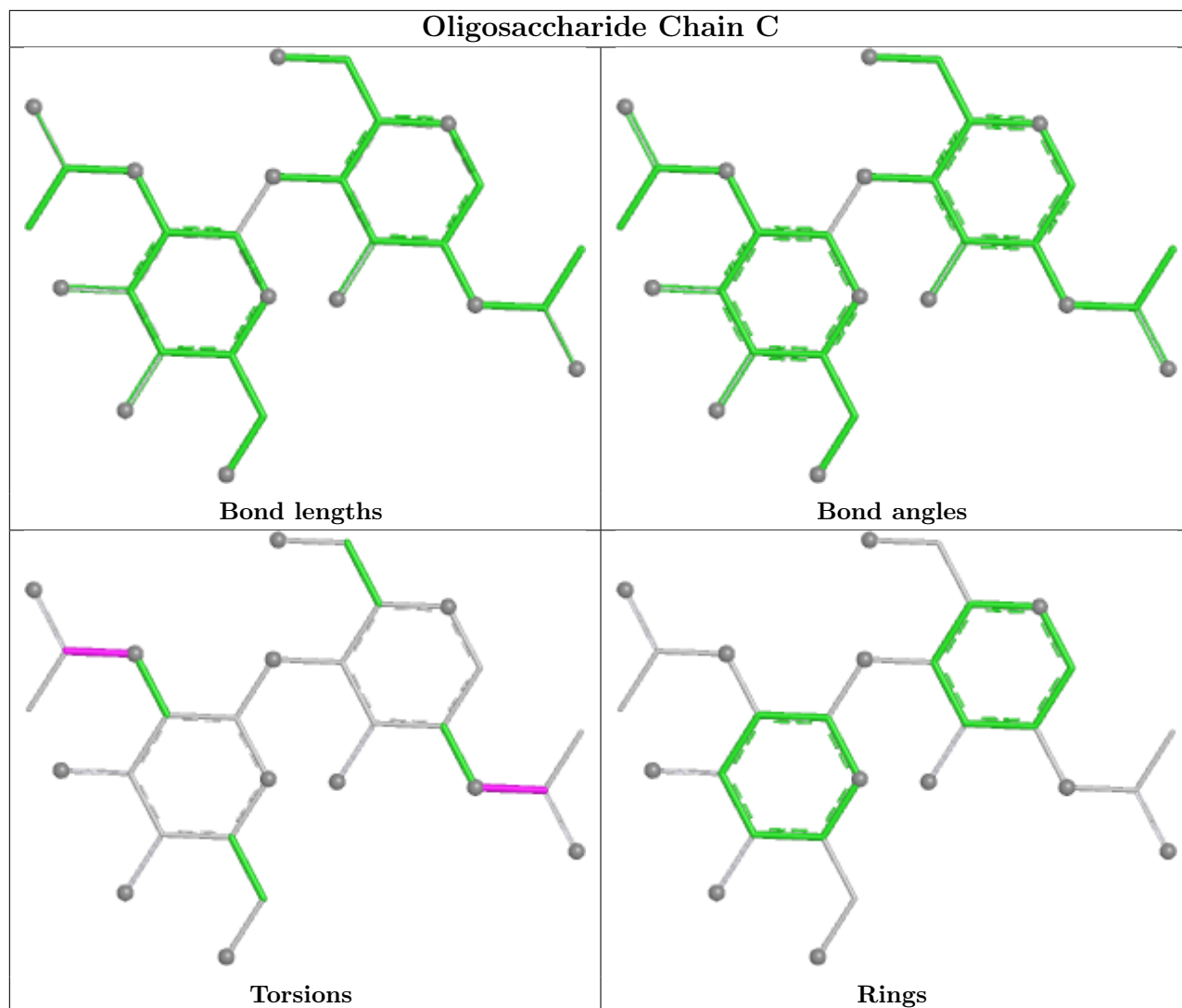
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	$\# Z > 2$
7	EDO	B	310	-	3,3,3	0.47	0	2,2,2	0.39	0
9	PEG	B	313	-	3,3,6	0.58	0	2,2,5	0.32	0
4	NAG	B	305	2	14,14,15	0.49	0	17,19,21	1.31	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	B	311	-	3,3,3	0.44	0	2,2,2	0.35	0
7	EDO	A	308	-	3,3,3	0.45	0	2,2,2	0.34	0
9	PEG	A	310	-	3,3,6	0.62	0	2,2,5	0.68	0
9	PEG	A	312	-	3,3,6	0.57	0	2,2,5	0.35	0
6	GOL	B	306	-	5,5,5	0.49	0	5,5,5	0.24	0
6	GOL	B	307	-	5,5,5	0.48	0	5,5,5	0.25	0
9	PEG	B	315	-	6,6,6	0.62	0	5,5,5	0.60	0
6	GOL	B	308	-	5,5,5	0.37	0	5,5,5	0.28	0
4	NAG	A	301	1	14,14,15	0.47	0	17,19,21	0.80	1 (5%)
6	GOL	A	305	-	5,5,5	0.33	0	5,5,5	0.38	0
7	EDO	B	309	-	3,3,3	0.44	0	2,2,2	0.38	0
5	SO4	A	303	-	4,4,4	0.23	0	6,6,6	0.10	0
9	PEG	A	313	-	3,3,6	0.58	0	2,2,5	0.36	0
9	PEG	B	314	-	3,3,6	0.59	0	2,2,5	0.34	0
10	AZI	B	301	-	2,2,2	3.15	2 (100%)	0,1,1	-	-
6	GOL	A	304	-	5,5,5	0.39	0	5,5,5	0.27	0
6	GOL	A	306	-	5,5,5	0.35	0	5,5,5	0.36	0
7	EDO	B	312	-	3,3,3	0.37	0	2,2,2	0.55	0
5	SO4	A	302	-	4,4,4	0.22	0	6,6,6	0.15	0
9	PEG	A	311	-	3,3,6	0.61	0	2,2,5	0.39	0
4	NAG	B	302	2	14,14,15	0.44	0	17,19,21	0.92	1 (5%)
6	GOL	A	307	-	5,5,5	0.38	0	5,5,5	0.35	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
7	EDO	B	310	-	-	1/1/1/1	-
9	PEG	B	313	-	-	1/1/1/4	-
4	NAG	B	305	2	-	4/6/23/26	0/1/1/1
7	EDO	B	311	-	-	0/1/1/1	-
7	EDO	A	308	-	-	0/1/1/1	-
9	PEG	A	310	-	-	1/1/1/4	-
9	PEG	A	312	-	-	0/1/1/4	-
6	GOL	B	306	-	-	1/4/4/4	-
6	GOL	B	307	-	-	3/4/4/4	-
9	PEG	B	315	-	-	1/4/4/4	-
6	GOL	B	308	-	-	2/4/4/4	-
6	GOL	A	305	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	301	1	-	2/6/23/26	0/1/1/1
7	EDO	B	309	-	-	0/1/1/1	-
9	PEG	A	313	-	-	1/1/1/4	-
9	PEG	B	314	-	-	1/1/1/4	-
6	GOL	A	304	-	-	2/4/4/4	-
6	GOL	A	306	-	-	2/4/4/4	-
7	EDO	B	312	-	-	0/1/1/1	-
9	PEG	A	311	-	-	0/1/1/4	-
4	NAG	B	302	2	-	2/6/23/26	0/1/1/1
6	GOL	A	307	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	301	AZI	N3-N2	-3.16	1.16	1.23
10	B	301	AZI	N1-N2	-3.14	1.16	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	305	NAG	C1-O5-C5	3.21	116.49	112.19
4	A	301	NAG	C1-O5-C5	2.40	115.40	112.19
4	B	305	NAG	C2-N2-C7	2.33	126.02	122.90
4	B	302	NAG	C2-N2-C7	-2.12	120.06	122.90

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	304	GOL	O1-C1-C2-C3
6	A	306	GOL	O1-C1-C2-C3
6	A	307	GOL	O1-C1-C2-C3
6	B	308	GOL	O1-C1-C2-C3
4	B	302	NAG	C8-C7-N2-C2
4	B	302	NAG	O7-C7-N2-C2
4	B	305	NAG	O7-C7-N2-C2
4	B	305	NAG	C8-C7-N2-C2
6	B	307	GOL	C1-C2-C3-O3
6	A	307	GOL	O1-C1-C2-O2
6	B	307	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	308	GOL	O1-C1-C2-O2
4	A	301	NAG	O5-C5-C6-O6
6	A	304	GOL	O1-C1-C2-O2
9	A	313	PEG	O1-C1-C2-O2
4	B	305	NAG	O5-C5-C6-O6
9	B	315	PEG	O1-C1-C2-O2
6	A	306	GOL	O1-C1-C2-O2
6	B	307	GOL	O1-C1-C2-O2
6	A	305	GOL	O2-C2-C3-O3
4	B	305	NAG	C3-C2-N2-C7
9	B	313	PEG	O1-C1-C2-O2
4	A	301	NAG	C1-C2-N2-C7
6	B	306	GOL	O1-C1-C2-O2
7	B	310	EDO	O1-C1-C2-O2
9	A	310	PEG	O1-C1-C2-O2
9	B	314	PEG	O2-C3-C4-O4

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	311	EDO	1	0
9	A	310	PEG	1	0
6	B	307	GOL	1	0
6	B	308	GOL	2	0
4	A	301	NAG	2	0
5	A	303	SO4	1	0
9	B	314	PEG	1	0
6	A	306	GOL	1	0
7	B	312	EDO	1	0
4	B	302	NAG	2	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	249/249 (100%)	-0.68	5 (2%) 65 72	25, 51, 86, 113	4 (1%)
2	B	263/263 (100%)	-0.91	7 (2%) 56 63	21, 42, 72, 122	6 (2%)
All	All	512/512 (100%)	-0.80	12 (2%) 61 68	21, 46, 83, 122	10 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	243	LEU	4.8
2	B	244	ALA	3.8
2	B	241	PRO	3.5
2	B	240	ASN	3.4
1	A	225	GLY	2.8
2	B	242	ALA	2.7
1	A	247	CYS	2.2
1	A	224	PRO	2.2
1	A	248	GLY	2.1
2	B	239	ALA	2.1
2	B	6	SER	2.0
1	A	115[A]	TYR	2.0

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

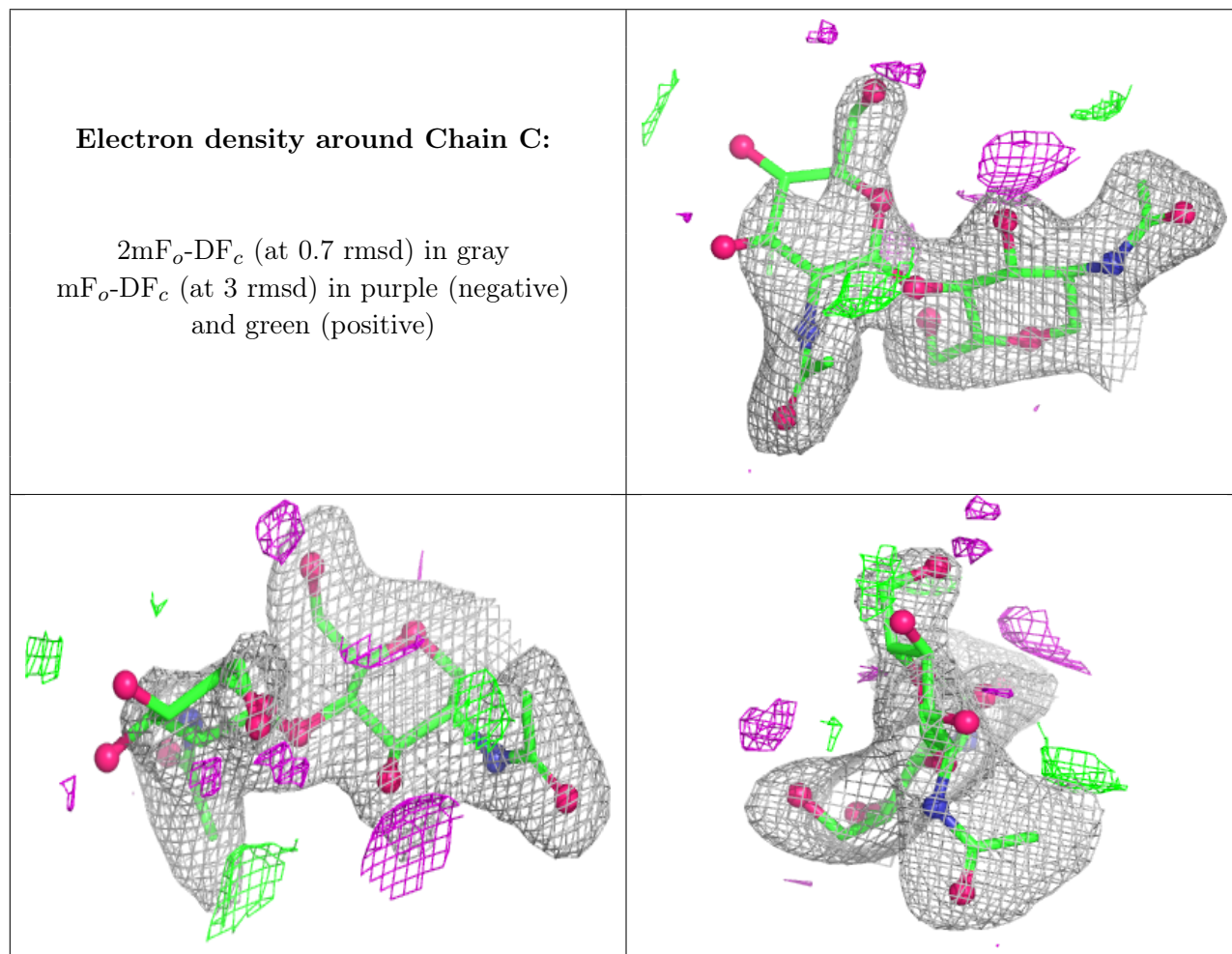
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
3	NAG	C	2	14/15	0.87	0.10	63,74,84,85	0
3	NAG	C	1	14/15	0.98	0.04	39,48,55,60	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(\AA^2)	Q<0.9
7	EDO	B	312	4/4	0.72	0.16	57,63,73,77	0
9	PEG	B	315	7/7	0.77	0.10	87,88,97,97	0
4	NAG	B	305	14/15	0.78	0.10	58,69,75,78	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PEG	A	312	4/7	0.81	0.13	87,88,88,89	0
6	GOL	A	306	6/6	0.84	0.11	68,75,82,91	0
4	NAG	A	301	14/15	0.85	0.10	83,89,99,102	14
6	GOL	A	307	6/6	0.86	0.08	80,87,90,92	0
9	PEG	B	313	4/7	0.87	0.09	70,73,75,75	0
9	PEG	A	313	4/7	0.87	0.08	78,79,83,86	0
4	NAG	B	302	14/15	0.88	0.09	54,66,73,74	14
7	EDO	B	310	4/4	0.89	0.09	55,61,71,74	0
6	GOL	B	308	6/6	0.90	0.11	81,85,87,88	0
7	EDO	B	309	4/4	0.90	0.07	76,77,80,84	0
9	PEG	B	314	4/7	0.91	0.06	74,77,78,78	0
9	PEG	A	311	4/7	0.91	0.08	79,84,84,84	0
7	EDO	B	311	4/4	0.92	0.04	77,81,84,86	0
7	EDO	A	308	4/4	0.93	0.05	82,83,85,85	0
6	GOL	A	304	6/6	0.95	0.07	53,70,85,90	0
6	GOL	A	305	6/6	0.96	0.05	59,65,70,74	0
5	SO4	A	303	5/5	0.97	0.04	58,64,65,69	5
6	GOL	B	306	6/6	0.97	0.05	35,39,50,55	0
10	AZI	B	301	3/3	0.97	0.06	63,63,72,74	0
6	GOL	B	307	6/6	0.98	0.04	38,52,58,62	0
9	PEG	A	310	4/7	0.98	0.06	71,71,73,79	0
5	SO4	A	302	5/5	0.98	0.06	70,70,73,78	0
8	CL	A	309	1/1	0.99	0.03	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.