



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:25 PM UTC

PDB ID : 1JS4 / pdb_00001js4
Title : ENDO/EXOCELLULASE:CELLOBIOSE FROM THERMOMONOSPORA
Authors : Sakon, J.; Wilson, D.B.; Karplus, P.A.
Deposited on : 1997-05-30
Resolution : 2.00 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

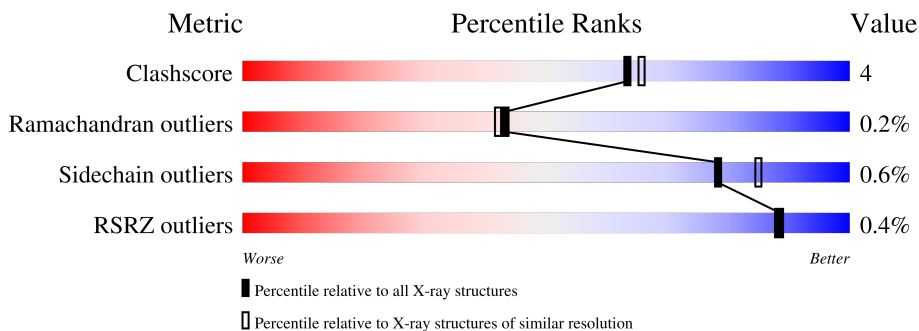
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	145.68Å 145.68Å 157.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	80.0 (8.00-2.00) 79.2 (8.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.99Å)	Xtrriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.199 , (Not available) 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 102.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11127	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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.

3 Model quality i

3.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BGC

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	0/4912	0.87	8/6716 (0.1%)
1	B	0.41	0/4912	0.86	7/6716 (0.1%)
All	All	0.42	0/9824	0.87	15/13432 (0.1%)

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	B	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	55	ASP	N-CA-C	7.60	119.25	110.97
1	A	55	ASP	N-CA-C	7.58	119.23	110.97
1	B	54	TYR	N-CA-C	-5.94	100.81	110.20
1	A	423	ASN	N-CA-C	5.67	119.89	112.92
1	A	228	GLY	N-CA-C	-5.62	107.50	115.43
1	B	63	GLY	N-CA-C	5.55	119.39	112.73
1	B	400	GLY	N-CA-C	5.44	122.58	115.40
1	B	228	GLY	N-CA-C	-5.42	107.79	115.43
1	A	335	ASP	CA-C-N	5.37	125.01	119.05
1	A	335	ASP	C-N-CA	5.37	125.01	119.05
1	A	54	TYR	N-CA-C	-5.35	101.74	110.20
1	A	591	ILE	N-CA-C	-5.31	100.10	107.80
1	A	378	ARG	N-CA-C	5.24	116.68	110.97
1	B	555	GLU	N-CA-C	5.20	116.95	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	ARG	N-CA-C	5.04	117.16	111.02

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	86	ARG	Sidechain

3.2 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	4757	0	4384	37	0
1	B	4757	0	4384	34	0
2	C	34	0	30	3	0
3	D	23	0	21	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	B	12	0	12	0	0
6	A	785	0	0	12	0
6	B	755	0	0	4	0
All	All	11127	0	8831	74	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 4.

All (74) 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:255:ARG:HH21	1:A:298:GLN:HE22	1.41	0.68
1:A:298:GLN:HG2	6:A:2001:HOH:O	1.94	0.68
1:B:255:ARG:NH1	1:B:298:GLN:HE22	1.93	0.66
1:B:247:GLN:NE2	1:B:255:ARG:HH22	1.95	0.63
1:B:420:TYR:O	1:B:424:GLU:HB2	1.98	0.63
1:A:259:ALA:HB3	6:A:2034:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:NH2	1:A:298:GLN:HE22	1.98	0.60
1:A:388:ILE:HG22	6:A:4855:HOH:O	2.01	0.59
1:B:195:VAL:HG13	1:B:208:SER:HB3	1.85	0.58
1:B:1:GLU:HB3	1:B:2:PRO:HD2	1.88	0.55
1:A:273:LYS:HG3	1:A:332:VAL:HG11	1.89	0.55
1:A:195:VAL:HG13	1:A:208:SER:HB3	1.89	0.54
1:A:506:ASP:HB3	6:A:4972:HOH:O	2.08	0.54
1:B:273:LYS:HG3	1:B:332:VAL:HG11	1.92	0.51
1:B:597:GLY:HA2	6:B:4509:HOH:O	2.09	0.51
1:B:255:ARG:HH11	1:B:298:GLN:HE22	1.59	0.50
1:A:414:THR:HB	6:A:4259:HOH:O	2.12	0.50
1:A:144:ASP:HB2	1:A:145:PRO:CD	2.42	0.49
1:A:327:LEU:HB3	1:A:439:MET:HE2	1.93	0.49
1:B:203:GLY:O	1:B:207:ASN:HB2	2.11	0.49
1:B:144:ASP:HB2	1:B:145:PRO:CD	2.42	0.49
1:A:263:LYS:N	1:A:263:LYS:HD2	2.26	0.49
1:A:530:HIS:HB3	6:A:4312:HOH:O	2.13	0.48
1:A:127:TRP:CD1	6:A:5384:HOH:O	2.67	0.48
1:B:505:LEU:HD21	1:B:511:PRO:HD3	1.96	0.48
1:A:247:GLN:HG3	1:A:248:GLN:H	1.79	0.47
1:B:497:GLY:HA2	1:B:594:TYR:O	2.15	0.47
1:A:330:ALA:O	1:A:339:LYS:HE2	2.14	0.47
1:B:263:LYS:N	1:B:263:LYS:HD2	2.29	0.47
1:B:552:GLY:HA3	1:B:555:GLU:OE1	2.14	0.47
1:A:203:GLY:O	1:A:207:ASN:HB2	2.16	0.46
1:A:56:ALA:HB1	1:A:425:VAL:O	2.16	0.46
1:B:180:GLN:HG3	6:B:5036:HOH:O	2.15	0.46
1:B:195:VAL:CG1	1:B:208:SER:HB3	2.45	0.46
1:A:90:MET:N	1:A:91:PRO:HD2	2.31	0.45
1:B:247:GLN:HG3	1:B:248:GLN:H	1.80	0.45
1:B:396:HIS:CE1	1:B:488:GLY:O	2.68	0.45
1:A:110:SER:HB2	1:A:111:PRO:HD2	1.98	0.45
1:B:64:PHE:HB3	1:B:65:PRO:CD	2.46	0.45
6:A:4185:HOH:O	2:C:1:BGC:H1	2.16	0.45
1:B:462:GLU:HB3	1:B:487:SER:HA	1.99	0.44
1:B:90:MET:N	1:B:91:PRO:HD2	2.33	0.44
6:A:4185:HOH:O	2:C:1:BGC:C1	2.65	0.44
1:B:576:TRP:CG	1:B:605:PRO:HG3	2.52	0.44
1:A:587:PRO:O	1:A:589:PRO:HD3	2.17	0.44
1:B:16:PHE:CD1	1:B:401:ALA:HB2	2.53	0.44
1:A:307:MET:HE2	1:A:309:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASP:HB2	1:A:145:PRO:HD2	2.00	0.43
1:B:116:VAL:HG11	1:B:152:VAL:HG11	2.00	0.43
1:B:144:ASP:HB2	1:B:145:PRO:HD2	2.01	0.43
1:A:255:ARG:HH21	1:A:298:GLN:NE2	2.14	0.43
1:A:64:PHE:HB3	1:A:65:PRO:CD	2.49	0.43
1:B:245:THR:HA	1:B:252:ARG:HA	2.01	0.43
1:A:25:LEU:HA	1:A:26:PRO:HD3	1.88	0.43
1:A:101:ASN:O	1:A:105:ILE:HG13	2.19	0.43
1:A:116:VAL:HG11	1:A:152:VAL:HG11	2.01	0.42
1:A:497:GLY:HA2	1:A:594:TYR:O	2.19	0.42
1:B:72:MET:HE3	1:B:432:GLY:HA2	1.99	0.42
1:A:245:THR:HA	1:A:252:ARG:HA	2.02	0.42
1:B:195:VAL:HG13	1:B:208:SER:CB	2.48	0.42
1:A:324:PHE:CE1	1:A:435:SER:HB3	2.54	0.42
1:B:414:THR:HA	6:B:3018:HOH:O	2.18	0.42
1:A:420:TYR:O	1:A:424:GLU:HB2	2.20	0.42
1:A:195:VAL:CG1	1:A:208:SER:HB3	2.49	0.42
1:A:502:TRP:CD1	1:A:538:TYR:HB3	2.55	0.42
1:A:307:MET:HB2	1:A:352:TYR:CE2	2.56	0.41
1:B:110:SER:HB2	1:B:111:PRO:HD2	2.03	0.41
1:B:8:GLU:HG3	1:B:449:LEU:HG	2.02	0.41
1:B:1:GLU:N	6:B:5083:HOH:O	2.54	0.41
1:B:576:TRP:CD1	1:B:605:PRO:HG3	2.56	0.41
1:A:251:LEU:HD12	6:A:4194:HOH:O	2.20	0.41
1:B:271:LEU:HD23	1:B:271:LEU:HA	1.87	0.41
1:A:127:TRP:HD1	6:A:5384:HOH:O	2.02	0.40
6:A:4893:HOH:O	2:C:1:BGC:H4	2.21	0.40

There are no symmetry-related clashes.

3.3 Torsion angles [i](#)

3.3.1 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	603/605 (100%)	579 (96%)	23 (4%)	1 (0%)	43	42
1	B	603/605 (100%)	581 (96%)	21 (4%)	1 (0%)	43	42
All	All	1206/1210 (100%)	1160 (96%)	44 (4%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	GLN
1	B	247	GLN

3.3.2 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	485/485 (100%)	482 (99%)	3 (1%)	78	85
1	B	485/485 (100%)	482 (99%)	3 (1%)	78	85
All	All	970/970 (100%)	964 (99%)	6 (1%)	78	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	312	THR
1	A	360	ASN
1	B	86	ARG
1	B	312	THR
1	B	360	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	247	GLN
1	A	248	GLN

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Mol	Chain	Res	Type
1	A	278	GLN
1	A	285	ASN
1	A	296	ASN
1	A	298	GLN
1	A	468	GLN
1	A	486	GLN
1	A	553	GLN
1	A	561	GLN
1	B	101	ASN
1	B	180	GLN
1	B	247	GLN
1	B	248	GLN
1	B	278	GLN
1	B	285	ASN
1	B	298	GLN
1	B	468	GLN
1	B	486	GLN
1	B	561	GLN

3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

3.5 Carbohydrates [i](#)

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	BGC	C	1	2	12,12,12	1.14	1 (8%)	17,17,17	1.25	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	C	2	2	11,11,12	0.70	0	15,15,17	0.71	0
2	BGC	C	3	2	11,11,12	0.35	0	15,15,17	0.50	0
3	BGC	D	1	3	12,12,12	0.74	0	17,17,17	0.82	0
3	BGC	D	2	3	11,11,12	0.28	0	15,15,17	0.72	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
2	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1
3	BGC	D	1	3	-	0/2/22/22	0/1/1/1
3	BGC	D	2	3	-	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	C	1	BGC	O4-C4	2.28	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	BGC	O5-C5-C4	4.32	117.48	109.70

There are no chirality outliers.

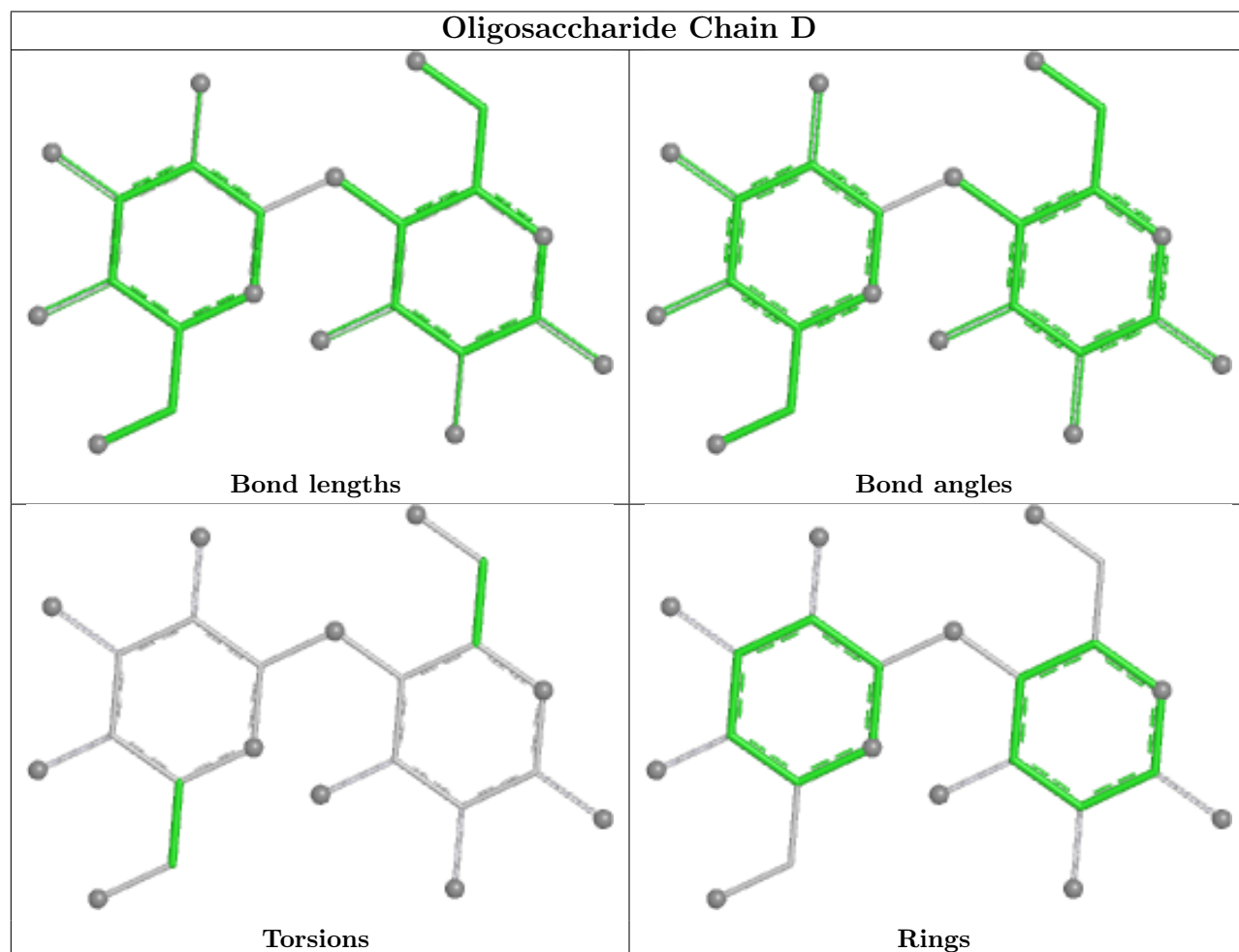
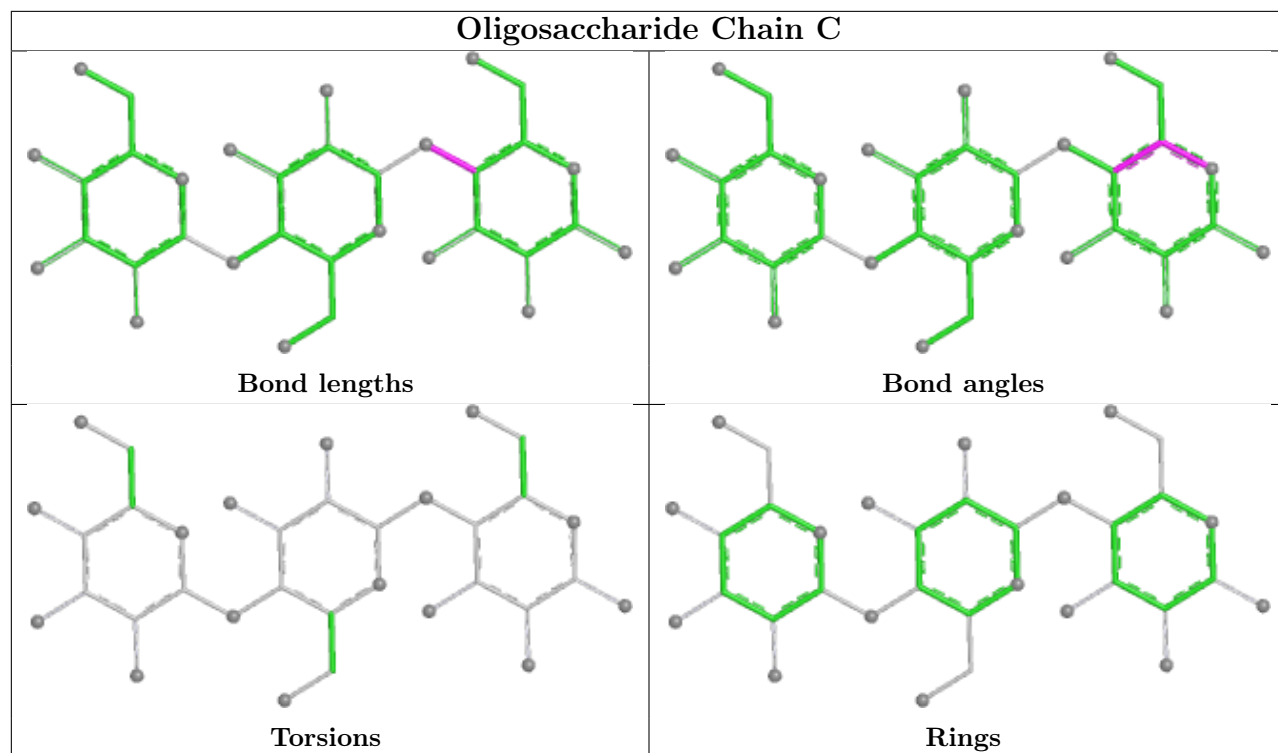
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	BGC	3	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.



3.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are 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
5	BGC	B	6015	-	12,12,12	0.45	0	17,17,17	0.49	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
5	BGC	B	6015	-	-	0/2/22/22	0/1/1/1

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.

No monomer is involved in short contacts.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data [i](#)

4.1 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	604/605 (99%)	-0.83	3 (0%) 87 87	5, 18, 40, 105	0
1	B	605/605 (100%)	-0.75	2 (0%) 90 89	6, 20, 42, 106	0
All	All	1209/1210 (99%)	-0.79	5 (0%) 88 88	5, 19, 41, 106	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	GLU	4.2
1	A	246	GLU	2.5
1	A	249	THR	2.4
1	B	248	GLN	2.1
1	A	248	GLN	2.1

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

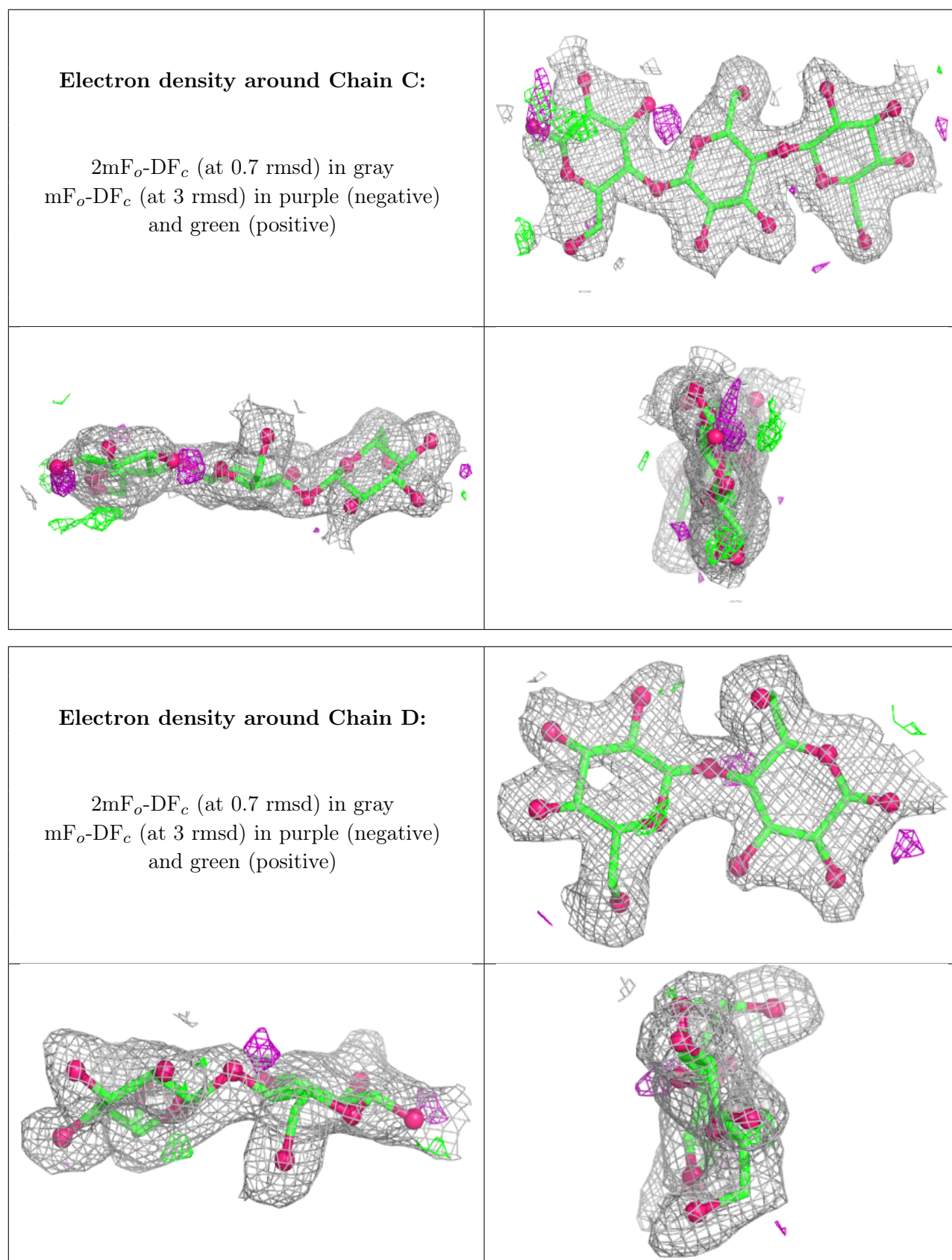
There are no non-standard protein/DNA/RNA residues in this entry.

4.3 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	BGC	C	1	12/12	0.84	0.11	34,49,63,64	0
3	BGC	D	2	11/12	0.88	0.09	8,16,20,23	11
3	BGC	D	1	12/12	0.91	0.07	19,38,43,47	0
2	BGC	C	3	11/12	0.93	0.06	23,30,39,45	0
2	BGC	C	2	11/12	0.95	0.05	16,26,30,34	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.



4.4 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
5	BGC	B	6015	12/12	0.80	0.10	31,40,48,49	1
4	CA	A	6168	1/1	0.97	0.05	26,26,26,26	0
4	CA	B	7166	1/1	0.99	0.03	12,12,12,12	0
4	CA	B	7168	1/1	1.00	0.02	13,13,13,13	0
4	CA	A	6166	1/1	1.00	0.04	9,9,9,9	0

4.5 Other polymers [i](#)

There are no such residues in this entry.