



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:25 PM BST

PDB ID : 3AHT  
Title : Crystal structure of rice BGlu1 E176Q mutant in complex with laminaribiose  
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Deposited on : 2010-04-29  
Resolution : 2.80 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

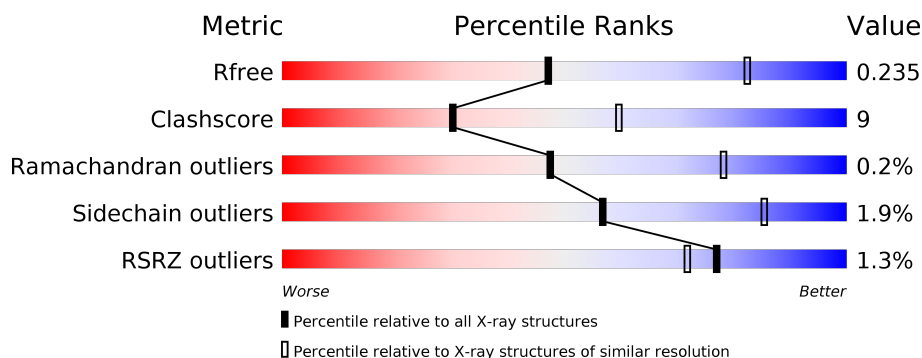
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	481	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	481	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7754 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-glucosidase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3801	2446	654	688	13			
1	B	471	Total	C	N	O	S	0	0	0
			3801	2446	654	688	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ALA	-	expression tag	UNP Q75I93
A	-3	MET	-	expression tag	UNP Q75I93
A	-2	ALA	-	expression tag	UNP Q75I93
A	-1	ASP	-	expression tag	UNP Q75I93
A	0	VAL	-	expression tag	UNP Q75I93
A	24	VAL	ALA	SEE REMARK 999	UNP Q75I93
A	176	GLN	GLU	engineered mutation	UNP Q75I93
B	-4	ALA	-	expression tag	UNP Q75I93
B	-3	MET	-	expression tag	UNP Q75I93
B	-2	ALA	-	expression tag	UNP Q75I93
B	-1	ASP	-	expression tag	UNP Q75I93
B	0	VAL	-	expression tag	UNP Q75I93
B	24	VAL	ALA	SEE REMARK 999	UNP Q75I93
B	176	GLN	GLU	engineered mutation	UNP Q75I93

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			

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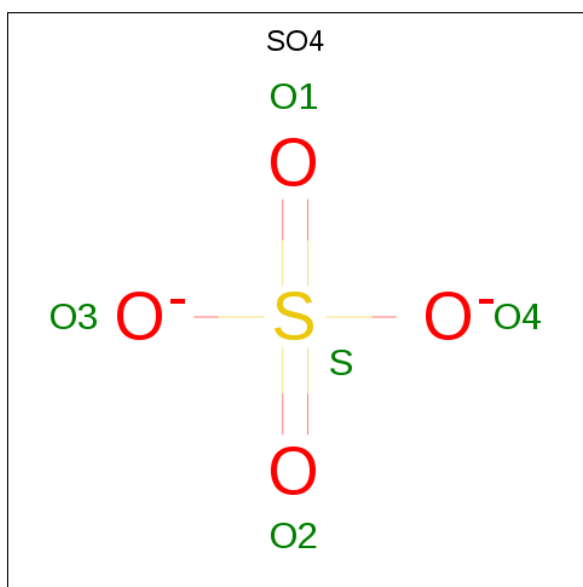
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

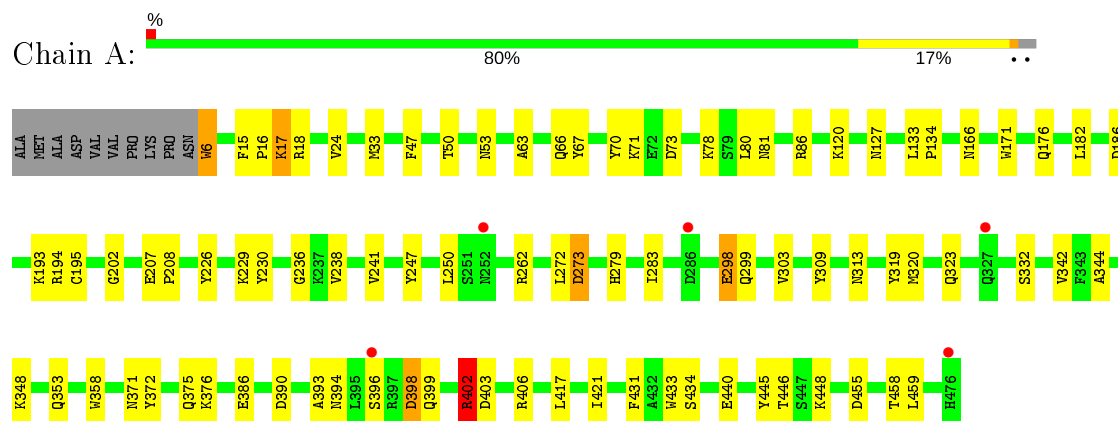
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total	O	0	0
			39	39		
6	B	32	Total	O	0	0
			32	32		

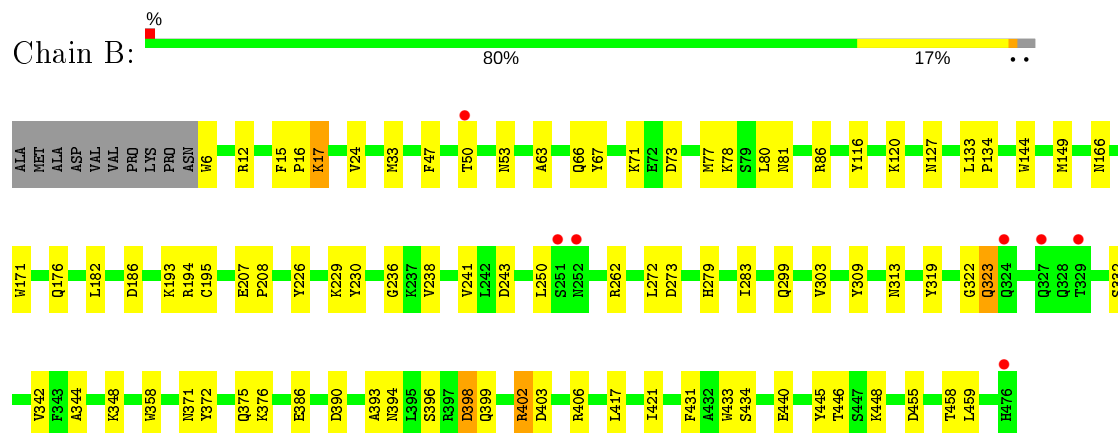
### 3 Residue-property plots [i](#)

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-glucosidase 7



- Molecule 1: Beta-glucosidase 7



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.70Å 101.48Å 128.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.70 – 2.80 25.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (25.70-2.80) 99.0 (25.70-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.44 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.0 (rigid body refinement for isomorphous crystal)	Depositor
R, $R_{free}$	0.205 , 0.248 0.200 , 0.235	Depositor DC
$R_{free}$ test set	1273 reflections (4.90%)	wwPDB
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 31.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7754	wwPDB
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5794e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ZN, BGC, SO4, MES

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	0.36	1/3917 (0.0%)	0.48	0/5324
1	B	0.34	0/3917	0.48	2/5324 (0.0%)
All	All	0.35	1/7834 (0.0%)	0.48	2/10648 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	ARG	CZ-NH1	7.58	1.43	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	ARG	CG-CD-NE	7.08	126.66	111.80
1	B	402	ARG	NE-CZ-NH1	5.07	122.83	120.30

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	3801	0	3640	70	0
1	B	3801	0	3640	68	0
2	C	23	0	21	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	23	0	21	5	0
3	A	1	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
5	A	12	0	12	1	0
5	B	12	0	12	1	0
6	A	39	0	0	3	0
6	B	32	0	0	3	0
All	All	7754	0	7346	140	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 9.

All (140) 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:398:ASP:HB3	1:A:402:ARG:HH12	1.39	0.87
1:B:17:LYS:H	1:B:17:LYS:HD3	1.45	0.80
1:A:17:LYS:HD3	1:A:17:LYS:H	1.46	0.80
1:A:17:LYS:HD3	1:A:17:LYS:N	1.98	0.79
1:B:17:LYS:N	1:B:17:LYS:HD3	1.97	0.79
1:B:17:LYS:H	1:B:17:LYS:CD	1.99	0.74
1:A:398:ASP:CB	1:A:402:ARG:HH12	1.99	0.74
1:A:17:LYS:CD	1:A:17:LYS:H	2.01	0.74
1:B:47:PHE:HE1	1:B:193:LYS:HD2	1.54	0.71
1:A:398:ASP:OD1	1:A:402:ARG:NH1	2.24	0.70
1:B:398:ASP:HB3	1:B:402:ARG:HH12	1.56	0.70
1:A:47:PHE:HE1	1:A:193:LYS:HD2	1.56	0.69
1:A:78:LYS:CD	1:A:120:LYS:HE3	2.24	0.67
1:A:78:LYS:HD2	1:A:120:LYS:HE3	1.76	0.67
1:B:398:ASP:CB	1:B:402:ARG:HH12	2.09	0.66
1:A:229:LYS:HD3	1:A:230:TYR:CE2	2.32	0.65
1:A:358:TRP:CZ2	2:C:1:BGC:H5	2.32	0.64
1:B:78:LYS:CD	1:B:120:LYS:HE3	2.27	0.64
1:B:78:LYS:HD2	1:B:120:LYS:HE3	1.81	0.63
1:A:6:TRP:N	6:A:514:HOH:O	2.33	0.62
1:A:344:ALA:HB1	1:A:348:LYS:O	2.00	0.61
1:B:229:LYS:HD3	1:B:230:TYR:CE2	2.37	0.60
1:B:166:ASN:HB2	4:B:1002:SO4:O4	2.02	0.60
1:A:319:TYR:HB2	1:A:342:VAL:HG23	1.84	0.59
1:B:319:TYR:HB2	1:B:342:VAL:HG23	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:TYR:OH	1:B:236:GLY:HA3	2.03	0.59
1:A:166:ASN:HB2	4:A:1002:SO4:O4	2.03	0.59
1:A:358:TRP:CE2	2:C:1:BGC:H6C2	2.38	0.59
1:B:273:ASP:HB3	1:B:279:HIS:O	2.05	0.57
1:B:386:GLU:OE2	2:D:2:BGC:O2	2.21	0.57
1:A:386:GLU:OE2	2:C:2:BGC:O2	2.23	0.57
1:A:50:THR:HB	1:A:53:ASN:ND2	2.20	0.57
1:A:372:TYR:CZ	1:A:376:LYS:HD2	2.40	0.57
1:B:50:THR:HB	1:B:53:ASN:ND2	2.20	0.57
1:A:273:ASP:HB3	1:A:279:HIS:O	2.05	0.56
1:A:47:PHE:CE1	1:A:193:LYS:HD2	2.40	0.56
1:B:77:MET:SD	6:B:494:HOH:O	2.58	0.56
1:A:226:TYR:OH	1:A:236:GLY:HA3	2.06	0.56
1:B:47:PHE:CE1	1:B:193:LYS:HD2	2.39	0.55
1:B:398:ASP:OD1	1:B:402:ARG:NH1	2.39	0.55
1:A:66:GLN:NE2	1:A:73:ASP:OD2	2.40	0.55
1:B:372:TYR:CZ	1:B:376:LYS:HD2	2.42	0.55
1:B:344:ALA:HB1	1:B:348:LYS:O	2.07	0.54
1:B:66:GLN:NE2	1:B:73:ASP:OD2	2.38	0.54
1:A:133:LEU:HD12	1:A:134:PRO:HD2	1.89	0.54
1:A:313:ASN:OD1	1:A:386:GLU:HB2	2.08	0.54
1:B:417:LEU:O	1:B:421:ILE:HG13	2.08	0.53
1:B:358:TRP:CZ2	2:D:1:BGC:H5	2.44	0.53
1:B:319:TYR:CB	1:B:342:VAL:HG23	2.39	0.52
1:A:393:ALA:O	1:A:394:ASN:HB2	2.09	0.52
1:B:396:SER:OG	1:B:399:GLN:HG3	2.09	0.52
1:A:417:LEU:O	1:A:421:ILE:HG13	2.10	0.52
1:A:319:TYR:CB	1:A:342:VAL:HG23	2.40	0.52
1:B:17:LYS:H	1:B:17:LYS:CE	2.22	0.52
1:B:24:VAL:CG2	1:B:431:PHE:HB3	2.40	0.51
1:B:207:GLU:N	1:B:208:PRO:CD	2.74	0.51
1:B:133:LEU:HD12	1:B:134:PRO:HD2	1.91	0.51
1:A:182:LEU:O	1:A:186:ASP:HB3	2.11	0.51
1:A:372:TYR:OH	1:A:376:LYS:HD2	2.11	0.51
1:A:24:VAL:CG2	1:A:431:PHE:HB3	2.41	0.50
1:A:15:PHE:HB3	1:A:16:PRO:CD	2.41	0.50
1:B:313:ASN:OD1	1:B:386:GLU:HB2	2.11	0.50
1:A:17:LYS:CE	1:A:17:LYS:H	2.25	0.49
1:B:15:PHE:HB3	1:B:16:PRO:CD	2.42	0.49
1:A:207:GLU:N	1:A:208:PRO:CD	2.74	0.49
1:A:455:ASP:O	1:A:459:LEU:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:MET:HG3	1:B:67:TYR:CD2	2.47	0.49
1:A:262:ARG:HG2	1:A:283:ILE:HG12	1.95	0.49
1:A:33:MET:HG3	1:A:67:TYR:CD2	2.47	0.49
1:A:396:SER:OG	1:A:399:GLN:HG3	2.13	0.49
1:B:455:ASP:O	1:B:459:LEU:N	2.41	0.49
1:A:358:TRP:CH2	2:C:1:BGC:H5	2.48	0.48
1:A:250:LEU:HD22	1:A:342:VAL:HG21	1.95	0.48
1:A:440:GLU:HG3	1:A:440:GLU:O	2.14	0.48
1:B:371:ASN:O	1:B:375:GLN:HG2	2.14	0.48
1:B:182:LEU:O	1:B:186:ASP:HB3	2.13	0.48
1:B:262:ARG:HG2	1:B:283:ILE:HG12	1.96	0.47
1:A:194:ARG:O	1:A:195:CYS:HB3	2.15	0.47
1:A:403:ASP:OD2	1:A:406:ARG:HD2	2.15	0.47
1:A:433:TRP:HA	1:A:434:SER:HA	1.63	0.47
1:A:393:ALA:HB2	1:A:446:THR:HA	1.97	0.47
1:A:78:LYS:HD3	1:A:120:LYS:HE3	1.95	0.47
1:B:393:ALA:O	1:B:394:ASN:HB2	2.16	0.47
1:A:86:ARG:NH2	1:A:241:VAL:HG21	2.30	0.46
1:B:390:ASP:HA	1:B:448:LYS:O	2.16	0.46
1:B:403:ASP:OD2	1:B:406:ARG:HD2	2.16	0.46
1:B:440:GLU:HG3	1:B:440:GLU:O	2.15	0.46
1:A:398:ASP:CB	1:A:402:ARG:NH1	2.73	0.46
1:B:372:TYR:OH	1:B:376:LYS:HD2	2.16	0.46
1:B:458:THR:O	1:B:459:LEU:HB2	2.15	0.46
1:B:393:ALA:HB2	1:B:446:THR:HA	1.97	0.45
1:A:299:GLN:O	1:A:303:VAL:HG23	2.16	0.45
1:A:390:ASP:HA	1:A:448:LYS:O	2.15	0.45
5:B:1003:MES:H72	6:B:508:HOH:O	2.16	0.45
1:A:402:ARG:HH11	1:A:402:ARG:HD3	1.72	0.45
1:B:15:PHE:HB3	1:B:16:PRO:HD2	1.98	0.45
1:B:63:ALA:HA	1:B:445:TYR:OH	2.16	0.45
1:A:15:PHE:HB3	1:A:16:PRO:HD2	1.98	0.45
1:A:398:ASP:CG	1:A:402:ARG:NH1	2.70	0.45
1:B:86:ARG:NH2	1:B:241:VAL:HG21	2.32	0.45
1:B:78:LYS:HD3	1:B:120:LYS:HE3	1.96	0.45
5:A:1003:MES:H52	5:A:1003:MES:H82	1.34	0.44
1:A:298:GLU:HG2	1:A:298:GLU:H	1.22	0.44
1:A:63:ALA:HA	1:A:445:TYR:OH	2.16	0.44
1:B:194:ARG:O	1:B:195:CYS:HB3	2.18	0.44
1:B:433:TRP:HA	1:B:434:SER:HA	1.62	0.44
1:A:458:THR:O	1:A:459:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:GLU:OE1	2:D:2:BGC:C1	2.66	0.43
1:B:176:GLN:HA	6:B:479:HOH:O	2.19	0.43
1:A:371:ASN:O	1:A:375:GLN:HG2	2.18	0.43
1:A:398:ASP:CG	1:A:402:ARG:HH12	2.22	0.43
1:B:250:LEU:HD22	1:B:342:VAL:HG21	1.99	0.43
1:A:70:TYR:CE2	1:A:71:LYS:HG3	2.54	0.42
1:B:272:LEU:HA	1:B:272:LEU:HD23	1.75	0.42
1:B:299:GLN:O	1:B:303:VAL:HG23	2.18	0.42
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.76	0.42
1:A:247:TYR:CE2	1:A:320:MET:HE3	2.54	0.42
1:B:71:LYS:HG2	1:B:116:TYR:CD2	2.54	0.42
1:B:171:TRP:HB2	1:B:238:VAL:HG22	2.01	0.42
1:B:80:LEU:O	1:B:81:ASN:HB2	2.18	0.42
1:B:226:TYR:OH	1:B:236:GLY:CA	2.67	0.42
1:B:358:TRP:CH2	2:D:1:BGC:H5	2.55	0.42
1:A:353:GLN:HG3	6:A:508:HOH:O	2.20	0.41
1:A:176:GLN:HA	6:A:481:HOH:O	2.19	0.41
1:A:229:LYS:HD3	1:A:230:TYR:CZ	2.54	0.41
1:A:80:LEU:O	1:A:81:ASN:HB2	2.20	0.41
1:A:194:ARG:NH2	1:A:202:GLY:HA2	2.35	0.41
1:B:348:LYS:HD3	1:B:348:LYS:HA	1.94	0.41
1:B:398:ASP:CG	1:B:402:ARG:HH12	2.24	0.41
1:B:358:TRP:CE2	2:D:1:BGC:H6C2	2.56	0.41
1:B:207:GLU:N	1:B:208:PRO:HD2	2.36	0.41
1:B:176:GLN:HG2	1:B:243:ASP:HB3	2.03	0.41
1:B:398:ASP:O	1:B:402:ARG:NH1	2.54	0.41
1:A:193:LYS:HB3	1:A:193:LYS:HE2	1.92	0.40
1:A:171:TRP:HB2	1:A:238:VAL:HG22	2.03	0.40
1:A:17:LYS:O	1:A:18:ARG:HB2	2.21	0.40
1:B:144:TRP:HA	1:B:149:MET:HG3	2.03	0.40
1:B:322:GLY:O	1:B:323:GLN:HB3	2.21	0.40
1:A:226:TYR:OH	1:A:236:GLY:CA	2.69	0.40
1:B:12:ARG:NH2	1:B:81:ASN:O	2.54	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	469/481 (98%)	451 (96%)	17 (4%)	1 (0%)	47	78
1	B	469/481 (98%)	448 (96%)	20 (4%)	1 (0%)	47	78
All	All	938/962 (98%)	899 (96%)	37 (4%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
1	B	323	GLN

### 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	389/397 (98%)	380 (98%)	9 (2%)	50	82
1	B	389/397 (98%)	383 (98%)	6 (2%)	65	89
All	All	778/794 (98%)	763 (98%)	15 (2%)	57	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TRP
1	A	17	LYS
1	A	127	ASN
1	A	273	ASP

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Mol	Chain	Res	Type
1	A	298	GLU
1	A	309	TYR
1	A	332	SER
1	A	398	ASP
1	A	402	ARG
1	B	6	TRP
1	B	17	LYS
1	B	127	ASN
1	B	309	TYR
1	B	332	SER
1	B	398	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	BGC	C	1	2	12,12,12	0.49	0	17,17,17	0.69	0
2	BGC	C	2	2	11,11,12	0.51	0	15,15,17	2.48	4 (26%)
2	BGC	D	1	2	12,12,12	0.51	0	17,17,17	0.64	0
2	BGC	D	2	2	11,11,12	0.50	0	15,15,17	2.44	4 (26%)

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	-	2/2/22/22	0/1/1/1
2	BGC	C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	D	1	2	-	2/2/22/22	0/1/1/1
2	BGC	D	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	BGC	C1-C2-C3	5.54	116.47	109.67
2	C	2	BGC	C1-O5-C5	5.35	119.45	112.19
2	C	2	BGC	C1-C2-C3	5.06	115.89	109.67
2	C	2	BGC	O5-C1-C2	5.02	118.52	110.77
2	D	2	BGC	O5-C1-C2	4.89	118.32	110.77
2	D	2	BGC	C1-O5-C5	4.59	118.41	112.19
2	D	2	BGC	C3-C4-C5	-2.74	105.35	110.24
2	C	2	BGC	C3-C4-C5	-2.26	106.20	110.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	BGC	O5-C5-C6-O6
2	D	1	BGC	O5-C5-C6-O6
2	C	1	BGC	O5-C5-C6-O6
2	C	2	BGC	C4-C5-C6-O6
2	D	1	BGC	C4-C5-C6-O6
2	C	1	BGC	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	BGC	1	0
2	D	2	BGC	2	0
2	D	1	BGC	3	0

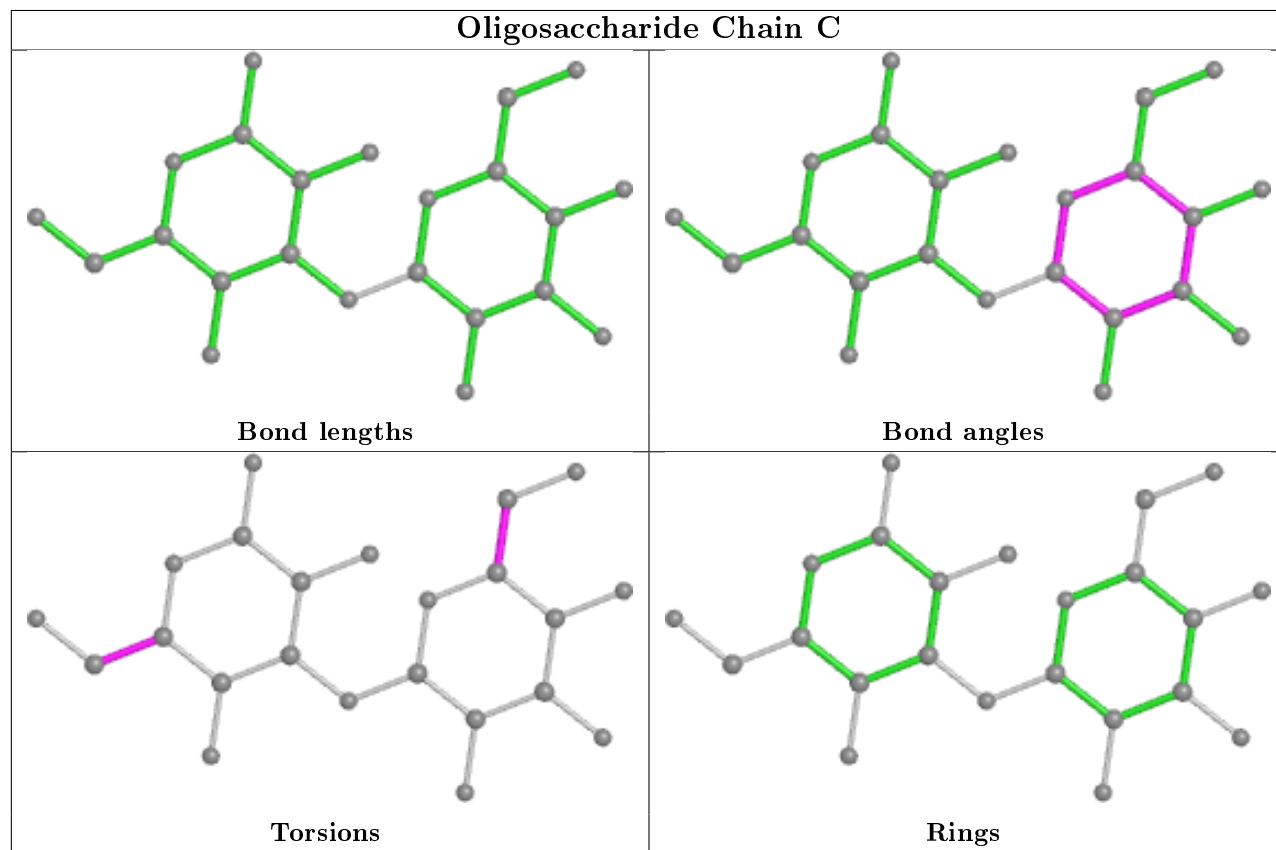
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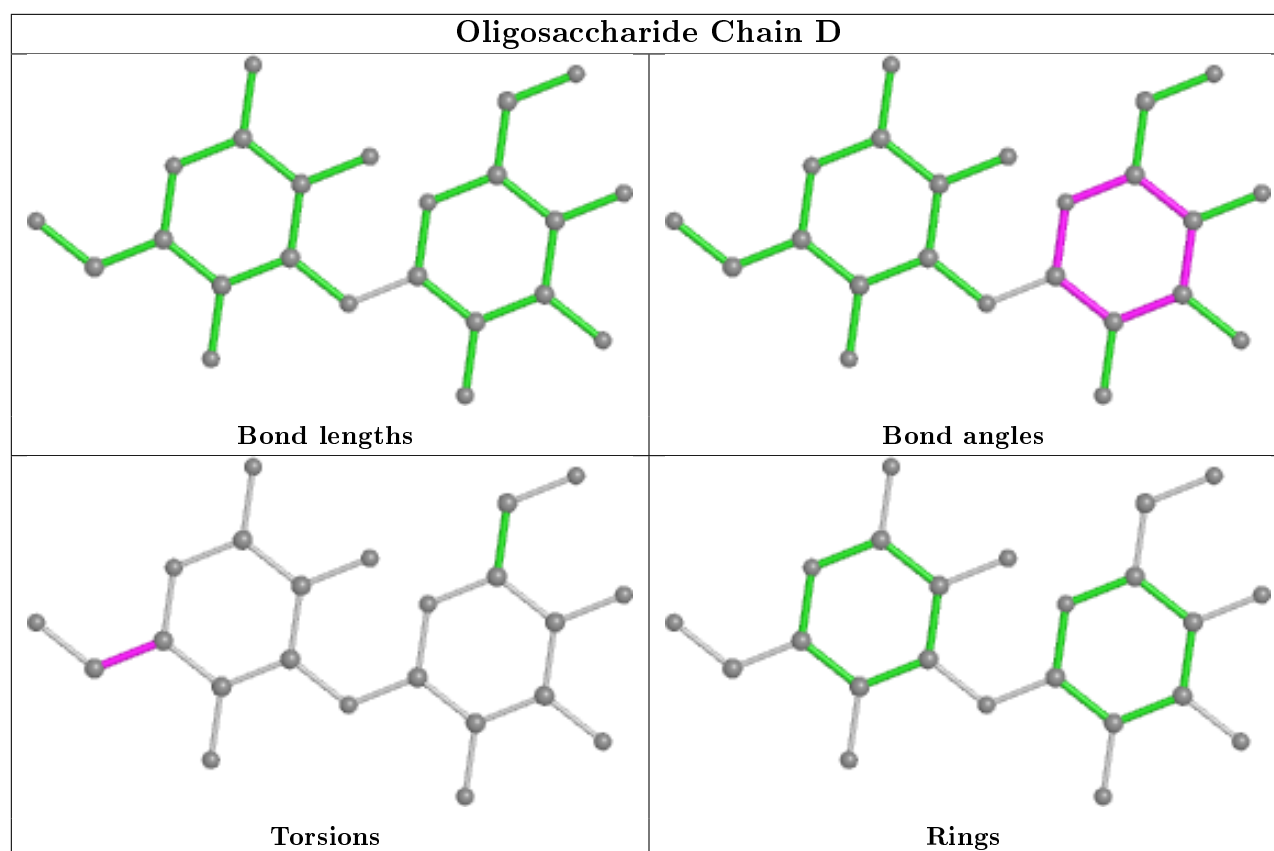


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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	BGC	3	0

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





## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	B	1002	-	4,4,4	0.14	0	6,6,6	0.14	0
5	MES	A	1003	-	12,12,12	2.19	1 (8%)	14,16,16	7.67	10 (71%)
4	SO4	A	1002	-	4,4,4	0.13	0	6,6,6	0.17	0
5	MES	B	1003	-	12,12,12	2.17	1 (8%)	14,16,16	7.54	10 (71%)

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	MES	A	1003	-	-	5/6/14/14	0/1/1/1
5	MES	B	1003	-	-	5/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1003	MES	C8-S	-7.17	1.67	1.77
5	A	1003	MES	C8-S	-7.13	1.67	1.77

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	MES	O2S-S-C8	-18.43	84.72	106.92
5	B	1003	MES	O1S-S-C8	-17.96	85.29	106.92
5	A	1003	MES	O1S-S-C8	-15.25	88.55	106.92
5	B	1003	MES	O2S-S-C8	-15.18	88.64	106.92
5	A	1003	MES	O3S-S-C8	-12.84	85.00	105.77
5	B	1003	MES	O3S-S-C8	-12.16	86.10	105.77
5	A	1003	MES	C5-N4-C3	5.18	120.48	108.83
5	B	1003	MES	C5-N4-C3	5.15	120.42	108.83
5	B	1003	MES	O3S-S-O1S	4.49	122.24	111.27
5	A	1003	MES	O3S-S-O2S	3.84	120.67	111.27
5	A	1003	MES	C7-N4-C5	3.47	120.10	111.23
5	B	1003	MES	C7-N4-C3	3.36	119.84	111.23
5	B	1003	MES	C7-N4-C5	3.33	119.75	111.23
5	A	1003	MES	C7-N4-C3	3.20	119.42	111.23
5	A	1003	MES	O3S-S-O1S	3.13	118.93	111.27
5	B	1003	MES	C2-C3-N4	-2.99	105.58	110.10
5	B	1003	MES	O3S-S-O2S	2.47	117.31	111.27
5	B	1003	MES	C6-C5-N4	-2.35	106.53	110.10
5	A	1003	MES	C6-C5-N4	-2.25	106.69	110.10
5	A	1003	MES	C2-C3-N4	-2.22	106.73	110.10

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1003	MES	C8-C7-N4-C5
5	A	1003	MES	C7-C8-S-O1S
5	A	1003	MES	C7-C8-S-O2S
5	A	1003	MES	C7-C8-S-O3S
5	B	1003	MES	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
5	B	1003	MES	C7-C8-S-O3S
5	A	1003	MES	N4-C7-C8-S
5	B	1003	MES	N4-C7-C8-S
5	B	1003	MES	C7-C8-S-O1S
5	B	1003	MES	C7-C8-S-O2S

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1002	SO4	1	0
5	A	1003	MES	1	0
4	A	1002	SO4	1	0
5	B	1003	MES	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	471/481 (97%)	-0.31	5 (1%) 80 75	16, 21, 30, 41	0
1	B	471/481 (97%)	-0.29	7 (1%) 73 68	16, 21, 30, 41	0
All	All	942/962 (97%)	-0.30	12 (1%) 77 72	16, 21, 30, 41	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	ASN	4.0
1	B	476	HIS	4.0
1	A	476	HIS	3.6
1	B	324	GLN	3.1
1	B	251	SER	2.7
1	B	329	THR	2.6
1	A	396	SER	2.4
1	A	327	GLN	2.3
1	A	286	ASP	2.2
1	B	327	GLN	2.2
1	B	252	ASN	2.1
1	B	50	THR	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains

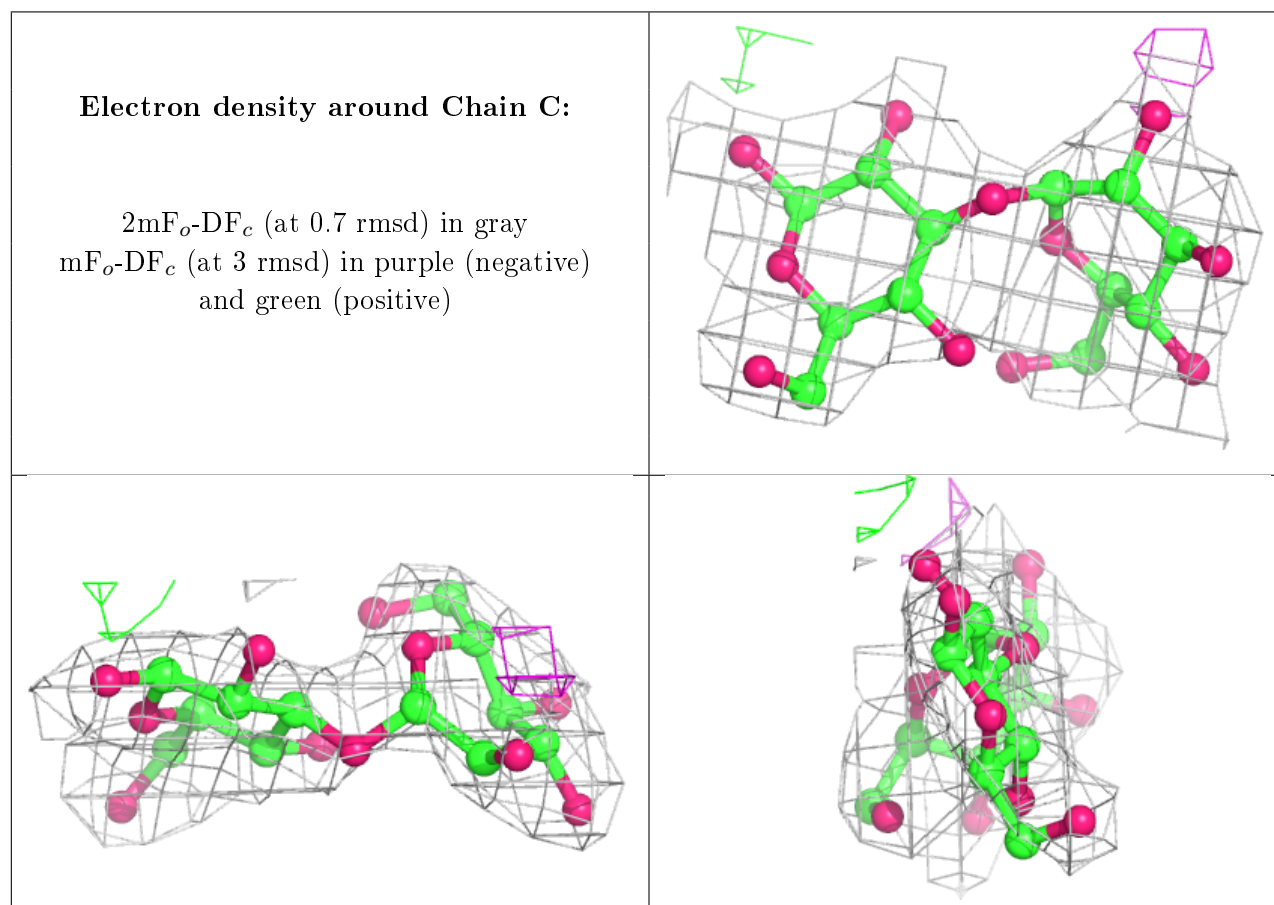
There are no non-standard protein/DNA/RNA residues in this entry.

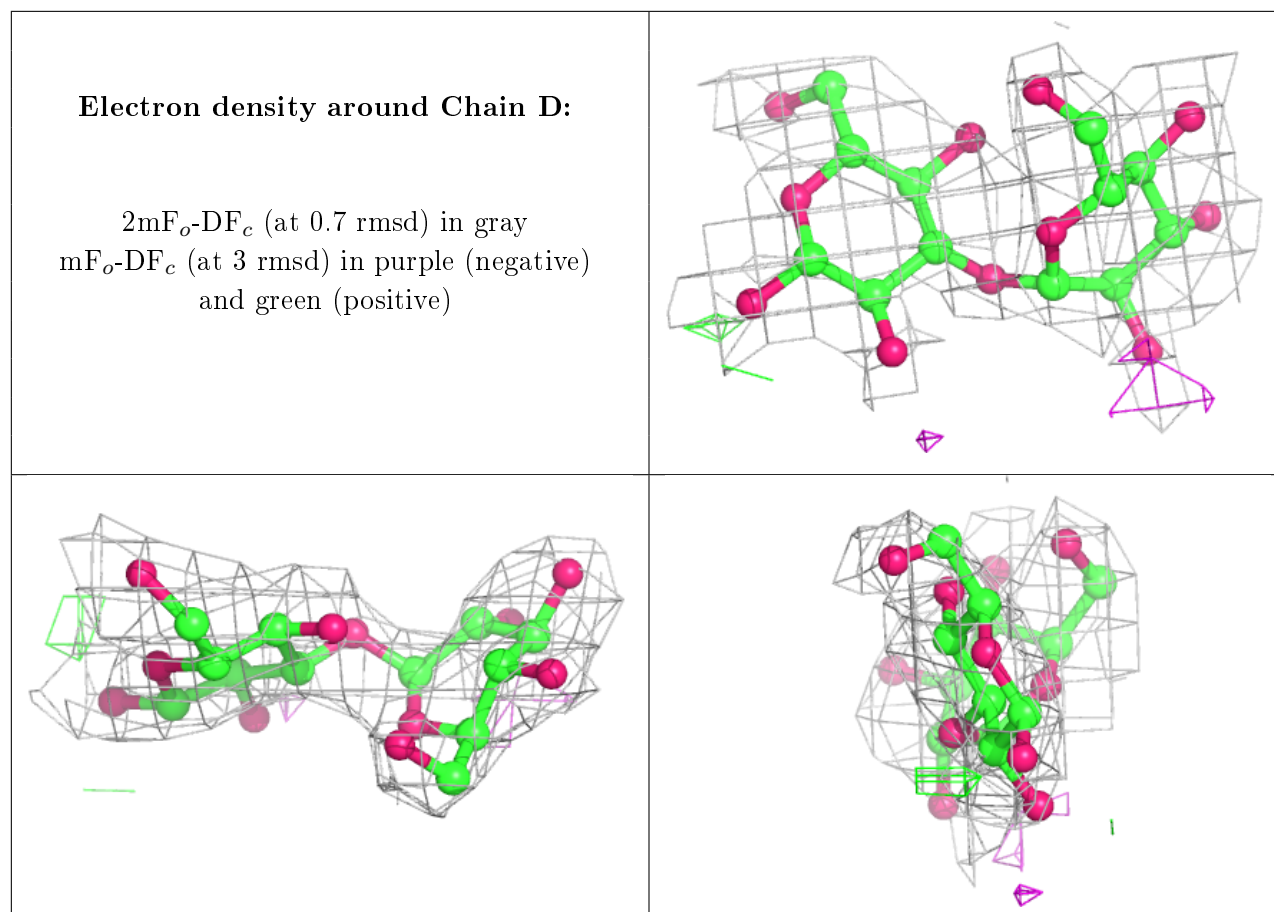
### 6.3 Carbohydrates

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
2	BGC	C	1	12/12	0.84	0.24	43,44,45,45	0
2	BGC	D	1	12/12	0.87	0.24	43,44,44,44	0
2	BGC	C	2	11/12	0.91	0.17	39,40,42,42	0
2	BGC	D	2	11/12	0.91	0.21	40,41,43,43	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 ⓘ

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
5	MES	A	1003	12/12	0.91	0.28	52,53,54,54	0
5	MES	B	1003	12/12	0.94	0.24	43,44,45,45	0
4	SO4	A	1002	5/5	0.97	0.17	61,62,62,62	0
4	SO4	B	1002	5/5	0.97	0.15	61,62,62,62	0
3	ZN	A	1001	1/1	0.99	0.05	15,15,15,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.