



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2024 – 08:54 PM EST

PDB ID : 4G68  
Title : Biochemical and structural insights into xylan utilization by the thermophilic bacterium *Caldanaerobius polysaccharolyticus*  
Authors : Agarwal, V.; Nair, S.K.  
Deposited on : 2012-07-18  
Resolution : 1.80 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.

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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

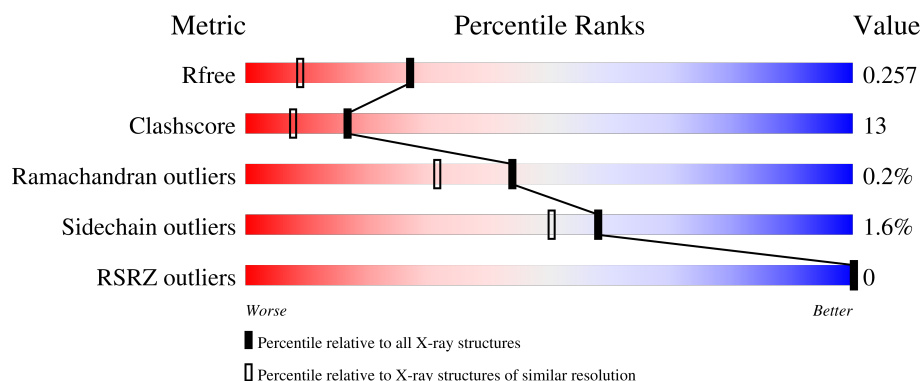
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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 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	456	
2	B	432	
3	C	432	
4	D	3	
4	E	3	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10210 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 ABC transporter.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	Se	0	2	0
			3058	1957	494	597	4	6			

- Molecule 2 is a protein called ABC transporter.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	392	Total	C	N	O	S	Se	0	0	0
			3050	1951	494	596	4	5			

- Molecule 3 is a protein called ABC transporter.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	392	Total	C	N	O	S	Se	0	0	0
			3050	1951	494	596	8	1			

- Molecule 4 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	D	3	Total	C	O	0	0	0
			28	15	13			
4	E	3	Total	C	O	0	0	0
			28	15	13			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	364	Total 364	O 364	0	0
5	B	363	Total 363	O 363	0	0
5	C	269	Total 269	O 269	0	0





- Molecule 4: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose



- Molecule 4: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.33Å 150.86Å 150.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.80 25.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-1.80) 99.7 (25.00-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.42 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0056	Depositor
R, $R_{free}$	0.230 , 0.261 0.215 , 0.257	Depositor DCC
$R_{free}$ test set	6314 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 20.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.478 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.11	4/3125 (0.1%)	0.99	6/4224 (0.1%)
2	B	1.08	5/3112 (0.2%)	0.97	9/4209 (0.2%)
3	C	0.91	5/3116 (0.2%)	0.87	3/4221 (0.1%)
All	All	1.04	14/9353 (0.1%)	0.94	18/12654 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	GLU	CD-OE1	6.94	1.33	1.25
2	B	406	GLU	CD-OE2	-6.76	1.18	1.25
2	B	346	TRP	CD2-CE2	6.33	1.49	1.41
2	B	320	GLU	CD-OE1	6.33	1.32	1.25
2	B	64	GLU	CD-OE1	6.33	1.32	1.25
3	C	30	TRP	CD2-CE2	6.29	1.48	1.41
1	A	300	GLU	CD-OE1	-6.13	1.19	1.25
3	C	346	TRP	CD2-CE2	5.81	1.48	1.41
3	C	49	TRP	CD2-CE2	5.48	1.48	1.41
1	A	346	TRP	CD2-CE2	5.36	1.47	1.41
3	C	378	TRP	CD2-CE2	5.33	1.47	1.41
3	C	191	TRP	CD2-CE2	5.31	1.47	1.41
2	B	300	GLU	CD-OE1	-5.16	1.20	1.25
1	A	252	GLU	CD-OE2	-5.12	1.20	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	195	MET	CG-SD-CE	-11.49	81.82	100.20
1	A	323	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	323	ARG	NE-CZ-NH2	-7.25	116.67	120.30
3	C	207	ARG	NE-CZ-NH2	-6.72	116.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	MSE	CG-SE-CE	-6.64	84.30	98.90
2	B	316	LYS	CD-CE-NZ	-6.33	97.14	111.70
2	B	323	ARG	NE-CZ-NH2	-6.29	117.16	120.30
2	B	319	ASP	CB-CG-OD2	-5.86	113.03	118.30
2	B	336	ASP	CB-CG-OD1	5.65	123.38	118.30
3	C	207	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	392	ASP	CB-CG-OD1	5.36	123.12	118.30
2	B	300	GLU	OE1-CD-OE2	-5.34	116.89	123.30
2	B	323	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	B	319	ASP	CB-CG-OD1	5.22	123.00	118.30
2	B	364	MET	CG-SD-CE	-5.17	91.94	100.20
1	A	336	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	320	GLU	CG-CD-OE1	5.11	128.53	118.30
3	C	352	ASP	CB-CG-OD1	5.04	122.83	118.30

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	3058	0	2995	32	1
2	B	3050	0	2981	34	1
3	C	3050	0	2981	165	2
4	D	28	0	9	0	0
4	E	28	0	9	0	0
5	A	364	0	0	14	0
5	B	363	0	0	14	0
5	C	269	0	0	126	0
All	All	10210	0	8975	229	2

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 13.

All (229) 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)
2:B:218:ASN:HB3	5:B:1245:HOH:O	1.21	1.29
3:C:69:LYS:HD2	5:C:701:HOH:O	1.25	1.27
3:C:363:ILE:HG22	5:C:764:HOH:O	1.13	1.27
3:C:198:LEU:HG	5:C:765:HOH:O	1.28	1.27
3:C:279:VAL:HG21	5:C:584:HOH:O	1.26	1.26
3:C:45:ILE:HG22	5:C:596:HOH:O	1.36	1.20
3:C:222:THR:HA	5:C:577:HOH:O	1.43	1.16
1:A:364:MET:SD	5:A:1255:HOH:O	2.07	1.12
3:C:382:LEU:HD22	5:C:727:HOH:O	1.49	1.10
3:C:396:GLN:HB3	5:C:757:HOH:O	1.53	1.09
3:C:348:TYR:HA	5:C:518:HOH:O	1.52	1.09
3:C:395:ALA:HB1	5:C:746:HOH:O	1.52	1.08
3:C:191:TRP:HA	5:C:633:HOH:O	1.53	1.08
3:C:387:ALA:HA	5:C:590:HOH:O	1.56	1.05
1:A:25:ILE:N	5:A:1249:HOH:O	1.88	1.04
3:C:169:LYS:HB3	5:C:600:HOH:O	1.54	1.03
3:C:253:PHE:HB2	5:C:677:HOH:O	1.59	1.02
3:C:114:LYS:HG3	5:C:607:HOH:O	1.61	1.00
3:C:178:PRO:HG2	5:C:604:HOH:O	1.61	0.98
3:C:155:VAL:HG12	5:C:535:HOH:O	1.60	0.98
3:C:386:ALA:HB1	5:C:711:HOH:O	1.62	0.98
3:C:172:LYS:HB2	5:C:604:HOH:O	1.64	0.96
1:A:413:GLN:HG3	5:A:1163:HOH:O	1.65	0.96
3:C:45:ILE:HG21	5:C:674:HOH:O	1.65	0.94
3:C:244:LEU:HD22	5:C:673:HOH:O	1.68	0.94
3:C:381:TYR:CB	5:C:742:HOH:O	2.14	0.94
3:C:395:ALA:CB	5:C:746:HOH:O	2.12	0.92
3:C:294:GLY:HA3	5:C:605:HOH:O	1.68	0.91
3:C:330:LYS:HD2	5:C:767:HOH:O	1.71	0.90
3:C:90:GLY:HA3	5:C:748:HOH:O	1.72	0.89
2:B:79:ASN:HD21	2:B:101:LYS:HE3	1.38	0.88
3:C:139:GLN:HB2	5:C:648:HOH:O	1.72	0.88
3:C:400:LYS:NZ	5:C:766:HOH:O	2.04	0.88
3:C:48:GLN:NE2	5:C:693:HOH:O	2.05	0.87
3:C:161:PHE:CE2	5:C:526:HOH:O	2.28	0.86
3:C:166:ASP:HB2	5:C:672:HOH:O	1.75	0.85
1:A:218:ASN:HB3	5:A:1256:HOH:O	1.78	0.84
3:C:143:LEU:HD21	3:C:260:MET:CE	2.09	0.82
3:C:356:VAL:HB	5:C:654:HOH:O	1.80	0.80
1:A:147:LYS:HE3	1:A:284:GLU:HB2	1.64	0.80
3:C:161:PHE:HE2	5:C:526:HOH:O	1.63	0.80
3:C:32:LEU:HG	5:C:516:HOH:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:ILE:HB	5:C:564:HOH:O	1.82	0.79
3:C:355:LYS:HB2	5:C:627:HOH:O	1.83	0.78
2:B:25:ILE:N	5:B:1258:HOH:O	2.17	0.77
3:C:199:ARG:CB	3:C:291:ILE:HD12	2.15	0.76
3:C:365:ASN:HB3	5:C:565:HOH:O	1.86	0.76
3:C:199:ARG:HB2	3:C:291:ILE:HD12	1.69	0.75
3:C:388:GLN:HA	5:C:687:HOH:O	1.85	0.75
3:C:346:TRP:HB2	5:C:767:HOH:O	1.86	0.74
3:C:370:ASN:ND2	5:C:659:HOH:O	2.19	0.74
3:C:190:MET:HE2	5:C:580:HOH:O	1.86	0.74
3:C:198:LEU:HD21	3:C:300:GLU:HB2	1.69	0.73
3:C:167:ALA:HB2	5:C:535:HOH:O	1.88	0.73
2:B:147:LYS:HE2	2:B:284:GLU:HB2	1.71	0.73
3:C:350:ASN:HD22	3:C:350:ASN:H	1.37	0.73
3:C:172:LYS:HD3	5:C:560:HOH:O	1.87	0.73
3:C:144:TYR:CD1	5:C:730:HOH:O	2.42	0.73
3:C:227:LYS:HD3	5:C:526:HOH:O	1.88	0.72
3:C:103:LEU:HA	5:C:660:HOH:O	1.89	0.72
3:C:115:ASP:HB3	5:C:700:HOH:O	1.90	0.72
3:C:284:GLU:HB3	5:C:564:HOH:O	1.88	0.72
3:C:181:LEU:HA	5:C:682:HOH:O	1.89	0.72
3:C:382:LEU:HD13	5:C:711:HOH:O	1.88	0.72
2:B:287:ARG:HD2	5:B:1242:HOH:O	1.89	0.72
3:C:381:TYR:HB2	5:C:742:HOH:O	1.85	0.71
2:B:413:GLN:HG2	5:B:1160:HOH:O	1.90	0.71
3:C:143:LEU:HD21	3:C:260:MET:HE1	1.73	0.70
3:C:162:SER:HB2	5:C:563:HOH:O	1.89	0.70
1:A:350:ASN:H	1:A:350:ASN:HD22	1.40	0.70
3:C:385:ASP:HB2	5:C:569:HOH:O	1.92	0.70
2:B:41:LYS:HD3	5:B:1235:HOH:O	1.92	0.70
3:C:156:LYS:HE3	5:C:716:HOH:O	1.92	0.70
3:C:178:PRO:CG	5:C:604:HOH:O	2.27	0.70
3:C:285:ALA:H	3:C:362:GLN:NE2	1.90	0.69
3:C:378:TRP:HH2	5:C:758:HOH:O	1.76	0.69
3:C:143:LEU:HD11	3:C:260:MET:CE	2.23	0.69
3:C:244:LEU:HB3	5:C:661:HOH:O	1.94	0.68
3:C:198:LEU:HD21	3:C:300:GLU:CB	2.24	0.67
3:C:147:LYS:HB2	5:C:710:HOH:O	1.94	0.67
1:A:218:ASN:CB	5:A:1256:HOH:O	2.35	0.67
1:A:218:ASN:OD1	5:A:1256:HOH:O	2.13	0.67
3:C:381:TYR:HB3	5:C:742:HOH:O	1.81	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:285:ALA:HB2	5:C:730:HOH:O	1.96	0.66
3:C:331:GLN:HA	5:C:506:HOH:O	1.94	0.66
3:C:167:ALA:CB	5:C:535:HOH:O	2.43	0.65
3:C:291:ILE:HB	5:C:605:HOH:O	1.97	0.65
3:C:376:PRO:CG	5:C:656:HOH:O	2.45	0.64
1:A:413:GLN:CG	5:A:1163:HOH:O	2.32	0.64
3:C:155:VAL:CG1	5:C:535:HOH:O	2.29	0.64
3:C:180:ALA:N	5:C:678:HOH:O	2.29	0.64
2:B:218:ASN:CB	5:B:1245:HOH:O	2.03	0.64
3:C:194:ASP:HA	5:C:763:HOH:O	1.97	0.63
3:C:207:ARG:NH2	5:C:576:HOH:O	2.17	0.63
3:C:391:LYS:HD3	5:C:687:HOH:O	1.98	0.63
2:B:285:ALA:H	2:B:362:GLN:NE2	1.98	0.62
1:A:416:ASN:C	5:A:1261:HOH:O	2.39	0.61
3:C:198:LEU:CD2	3:C:300:GLU:OE1	2.49	0.61
3:C:143:LEU:HD11	3:C:260:MET:HE2	1.82	0.61
1:A:218:ASN:CG	5:A:1256:HOH:O	2.39	0.61
2:B:287:ARG:CD	5:B:1242:HOH:O	2.47	0.61
3:C:187:TRP:HB2	5:C:580:HOH:O	2.01	0.61
3:C:359:LEU:HD11	5:C:730:HOH:O	2.01	0.61
1:A:337:TYR:HE1	5:A:1233:HOH:O	1.84	0.61
3:C:350:ASN:ND2	5:C:518:HOH:O	2.30	0.60
3:C:378:TRP:CH2	5:C:758:HOH:O	2.52	0.60
3:C:376:PRO:HG2	5:C:656:HOH:O	2.02	0.60
3:C:90:GLY:CA	5:C:748:HOH:O	2.39	0.59
3:C:240:GLY:HA3	5:C:722:HOH:O	2.01	0.59
3:C:66:ASP:HA	5:C:701:HOH:O	2.03	0.58
3:C:194:ASP:HB2	5:C:633:HOH:O	2.03	0.58
3:C:183:GLU:HG3	5:C:629:HOH:O	2.04	0.58
1:A:372:LYS:HD3	5:A:1137:HOH:O	2.04	0.58
3:C:284:GLU:CB	5:C:564:HOH:O	2.48	0.57
3:C:376:PRO:HG3	5:C:656:HOH:O	2.04	0.57
3:C:333:SER:HB3	5:C:767:HOH:O	2.03	0.57
3:C:157:VAL:HG21	5:C:579:HOH:O	2.05	0.56
3:C:398:PHE:CE1	5:C:520:HOH:O	2.58	0.56
2:B:320:GLU:HG3	5:B:1015:HOH:O	2.05	0.56
2:B:287:ARG:NH2	5:B:1234:HOH:O	2.39	0.56
2:B:79:ASN:ND2	2:B:101:LYS:HE3	2.17	0.55
2:B:198:LEU:HD21	2:B:300:GLU:CB	2.36	0.55
3:C:179:PHE:HB3	5:C:678:HOH:O	2.07	0.55
3:C:216:PHE:HD2	5:C:735:HOH:O	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:334:ASP:HB2	5:C:506:HOH:O	2.06	0.55
3:C:412:GLN:HA	5:C:735:HOH:O	2.06	0.55
3:C:199:ARG:HB3	3:C:291:ILE:HD12	1.88	0.55
3:C:355:LYS:HD2	5:C:627:HOH:O	2.07	0.54
3:C:198:LEU:HD23	3:C:300:GLU:OE1	2.07	0.54
3:C:156:LYS:HB2	5:C:618:HOH:O	2.06	0.54
2:B:126:THR:OG1	2:B:131:ILE:HD13	2.08	0.54
1:A:297:ASP:HB3	1:A:300:GLU:HG3	1.89	0.54
3:C:110:ASN:ND2	5:C:670:HOH:O	2.40	0.54
3:C:383:SER:HA	5:C:740:HOH:O	2.08	0.54
3:C:45:ILE:HD13	5:C:674:HOH:O	2.08	0.53
3:C:356:VAL:CG2	5:C:654:HOH:O	2.56	0.53
3:C:253:PHE:CB	5:C:677:HOH:O	2.36	0.53
2:B:298:PRO:HG3	5:B:1207:HOH:O	2.09	0.53
3:C:388:GLN:CA	5:C:687:HOH:O	2.50	0.53
1:A:285:ALA:H	1:A:362:GLN:NE2	2.06	0.53
3:C:198:LEU:CD2	3:C:300:GLU:HB2	2.39	0.52
1:A:29:PHE:O	1:A:60:GLU:HA	2.09	0.52
2:B:330:LYS:NZ	2:B:350:ASN:HD21	2.07	0.52
3:C:353:GLN:O	3:C:356:VAL:HG22	2.10	0.52
2:B:41:LYS:HE3	5:B:949:HOH:O	2.10	0.52
2:B:198:LEU:HD21	2:B:300:GLU:HB2	1.91	0.52
2:B:337:TYR:HE1	2:B:364:MET:CE	2.23	0.52
1:A:360:GLU:HG3	5:A:1233:HOH:O	2.10	0.51
3:C:25:ILE:HG12	5:C:550:HOH:O	2.10	0.51
3:C:25:ILE:CG1	5:C:550:HOH:O	2.58	0.51
2:B:25:ILE:HD12	2:B:317:TYR:CE1	2.46	0.51
3:C:92:PHE:CA	5:C:769:HOH:O	2.60	0.50
3:C:161:PHE:CE2	3:C:227:LYS:HD3	2.46	0.50
3:C:198:LEU:HD21	3:C:300:GLU:OE1	2.10	0.50
3:C:254:ASN:HA	5:C:584:HOH:O	2.12	0.50
2:B:350:ASN:HD22	2:B:350:ASN:H	1.60	0.49
3:C:143:LEU:HD11	3:C:260:MET:HE1	1.95	0.49
3:C:32:LEU:CG	5:C:516:HOH:O	2.51	0.49
2:B:337:TYR:HE1	2:B:364:MET:HE2	1.78	0.48
3:C:386:ALA:N	5:C:569:HOH:O	2.46	0.48
1:A:353:GLN:O	1:A:356:VAL:HG22	2.14	0.47
2:B:218:ASN:OD1	5:B:1002:HOH:O	2.20	0.47
3:C:81:ALA:HB1	3:C:82:PRO:HD2	1.97	0.47
3:C:217:ASP:HA	3:C:408:SER:HB3	1.97	0.47
3:C:290:THR:HG22	3:C:298:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:380:ILE:O	3:C:380:ILE:HG22	2.14	0.47
3:C:143:LEU:HB2	5:C:509:HOH:O	2.14	0.46
3:C:225:ALA:HB3	5:C:577:HOH:O	2.14	0.46
3:C:40:THR:O	3:C:44:GLU:HG3	2.15	0.46
2:B:62:VAL:HG12	5:B:948:HOH:O	2.15	0.46
3:C:79:ASN:HD21	3:C:101:LYS:NZ	2.14	0.46
1:A:195:MSE:HB2	1:A:195:MSE:HE2	1.66	0.45
1:A:356:VAL:CG2	1:A:361:ILE:HD11	2.47	0.45
1:A:137:ASP:OD1	1:A:307:GLY:HA3	2.17	0.45
2:B:25:ILE:HD12	2:B:317:TYR:CZ	2.52	0.45
3:C:328:LEU:CD2	5:C:596:HOH:O	2.64	0.45
2:B:193:TYR:CD2	2:B:193:TYR:C	2.90	0.45
3:C:244:LEU:HD13	5:C:673:HOH:O	2.17	0.45
2:B:284:GLU:HA	2:B:362:GLN:HE22	1.81	0.45
3:C:92:PHE:HB2	5:C:769:HOH:O	2.16	0.45
3:C:124:ASN:ND2	5:C:656:HOH:O	2.49	0.44
3:C:380:ILE:O	3:C:380:ILE:CG2	2.65	0.44
3:C:284:GLU:HA	3:C:362:GLN:HE22	1.81	0.44
2:B:138:GLN:HG3	2:B:343:LEU:HB2	1.99	0.44
3:C:193:TYR:CD2	3:C:193:TYR:C	2.90	0.44
3:C:261:TYR:HD1	5:C:677:HOH:O	2.00	0.44
3:C:402:ILE:HB	5:C:757:HOH:O	2.18	0.44
3:C:295:LYS:HD3	3:C:295:LYS:HA	1.81	0.44
3:C:161:PHE:HB2	3:C:291:ILE:HG12	1.99	0.43
1:A:350:ASN:H	1:A:350:ASN:ND2	2.11	0.43
3:C:109:LEU:HB3	5:C:607:HOH:O	2.19	0.43
3:C:115:ASP:CG	5:C:522:HOH:O	2.57	0.43
2:B:251:ALA:O	2:B:255:GLN:HG2	2.19	0.43
2:B:364:MET:HG2	5:B:1125:HOH:O	2.19	0.43
3:C:138:GLN:O	3:C:343:LEU:HB2	2.19	0.43
3:C:78:ALA:O	3:C:80:GLU:HG3	2.19	0.42
3:C:156:LYS:HE2	5:C:618:HOH:O	2.19	0.42
1:A:90:GLY:HA3	5:A:1186:HOH:O	2.18	0.42
5:A:1036:HOH:O	3:C:213:LYS:CE	2.68	0.42
2:B:29:PHE:O	2:B:60:GLU:HA	2.18	0.42
3:C:131:ILE:HD11	5:C:675:HOH:O	2.19	0.42
3:C:226:GLN:HB2	5:C:752:HOH:O	2.18	0.42
3:C:316:LYS:N	5:C:613:HOH:O	2.50	0.42
3:C:322:VAL:HG12	3:C:326:LYS:HE3	2.01	0.42
1:A:49:TRP:CD1	1:A:58:ILE:HD12	2.54	0.42
1:A:292:GLU:OE2	3:C:207:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:228:LEU:HD11	3:C:398:PHE:CE1	2.55	0.42
2:B:330:LYS:HZ3	2:B:350:ASN:HD21	1.67	0.42
3:C:156:LYS:CE	5:C:716:HOH:O	2.59	0.42
3:C:398:PHE:CD1	5:C:520:HOH:O	2.57	0.42
3:C:398:PHE:CG	5:C:520:HOH:O	2.73	0.42
3:C:303:GLY:HA2	5:C:537:HOH:O	2.19	0.42
3:C:328:LEU:HD23	5:C:596:HOH:O	2.20	0.42
3:C:195:MET:HG2	3:C:288:PHE:CG	2.55	0.41
3:C:382:LEU:CD2	5:C:727:HOH:O	2.32	0.41
3:C:388:GLN:N	5:C:687:HOH:O	2.52	0.41
1:A:190:MSE:HE2	1:A:190:MSE:HB3	1.92	0.41
1:A:187:TRP:CG	1:A:188:PRO:HD3	2.56	0.41
3:C:350:ASN:HD22	3:C:350:ASN:N	2.10	0.41
3:C:287:ARG:NH2	5:C:706:HOH:O	2.52	0.41
1:A:147:LYS:CE	1:A:284:GLU:HB2	2.42	0.41
1:A:159:THR:HG21	3:C:128:ASN:C	2.42	0.41
1:A:199:ARG:HB2	1:A:291:ILE:HD12	2.03	0.41
1:A:284:GLU:HA	1:A:362:GLN:HE22	1.86	0.41
2:B:297:ASP:HB3	2:B:300:GLU:HG3	2.02	0.41
3:C:92:PHE:N	5:C:769:HOH:O	2.54	0.41
1:A:94:GLN:N	1:A:95:PRO:CD	2.84	0.40
3:C:356:VAL:CB	5:C:654:HOH:O	2.53	0.40
3:C:198:LEU:HD23	3:C:198:LEU:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:SER:O	3:C:154:ASN:ND2[1_455]	2.02	0.18
1:A:347:LYS:NZ	3:C:295:LYS:NZ[1_455]	2.13	0.07

## 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	392/456 (86%)	386 (98%)	5 (1%)	1 (0%)	37	25
2	B	390/432 (90%)	382 (98%)	8 (2%)	0	100	100
3	C	390/432 (90%)	379 (97%)	10 (3%)	1 (0%)	37	25
All	All	1172/1320 (89%)	1147 (98%)	23 (2%)	2 (0%)	44	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	154	ASN
1	A	65	ASN

### 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	321/375 (86%)	317 (99%)	4 (1%)	67	62
2	B	319/352 (91%)	315 (99%)	4 (1%)	65	59
3	C	319/356 (90%)	312 (98%)	7 (2%)	47	36
All	All	959/1083 (89%)	944 (98%)	15 (2%)	58	50

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

Mol	Chain	Res	Type
1	A	25	ILE
1	A	32	LEU
1	A	228	LEU
1	A	350	ASN
2	B	32	LEU
2	B	244	LEU
2	B	356	VAL
2	B	372	LYS
3	C	25	ILE

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Mol	Chain	Res	Type
3	C	32	LEU
3	C	138	GLN
3	C	198	LEU
3	C	228	LEU
3	C	350	ASN
3	C	372	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	65	ASN
1	A	79	ASN
1	A	110	ASN
1	A	219	GLN
1	A	229	GLN
1	A	350	ASN
1	A	353	GLN
1	A	362	GLN
2	B	57	GLN
2	B	65	ASN
2	B	79	ASN
2	B	110	ASN
2	B	219	GLN
2	B	229	GLN
2	B	350	ASN
2	B	353	GLN
2	B	362	GLN
3	C	57	GLN
3	C	79	ASN
3	C	229	GLN
3	C	350	ASN
3	C	362	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

6 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$
4	XYS	D	1	4	10,10,10	2.01	3 (30%)	14,14,14	2.63	8 (57%)
4	XYP	D	2	4	9,9,10	0.97	0	10,12,14	2.09	4 (40%)
4	XYP	D	3	4	9,9,10	1.00	0	10,12,14	1.31	1 (10%)
4	XYS	E	1	4	10,10,10	1.93	3 (30%)	14,14,14	2.45	7 (50%)
4	XYP	E	2	4	9,9,10	1.19	1 (11%)	10,12,14	2.06	2 (20%)
4	XYP	E	3	4	9,9,10	0.92	0	10,12,14	1.03	1 (10%)

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
4	XYS	D	1	4	-	-	0/1/1/1
4	XYP	D	2	4	-	-	0/1/1/1
4	XYP	D	3	4	-	-	0/1/1/1
4	XYS	E	1	4	-	-	0/1/1/1
4	XYP	E	2	4	-	-	0/1/1/1
4	XYP	E	3	4	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	XYS	O5-C5	-4.87	1.35	1.43
4	E	1	XYS	O5-C5	-4.30	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	XYS	O5-C1	-2.69	1.38	1.43
4	E	2	XYP	C2-C3	2.46	1.56	1.52
4	E	1	XYS	O2-C2	-2.32	1.37	1.43
4	D	1	XYS	O5-C1	-2.21	1.39	1.43
4	D	1	XYS	O2-C2	-2.02	1.38	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	XYS	C5-O5-C1	6.29	125.54	112.46
4	E	1	XYS	C5-O5-C1	5.63	124.17	112.46
4	E	2	XYP	C4-C3-C2	-4.77	105.26	110.92
4	D	2	XYP	C4-C3-C2	-4.40	105.70	110.92
4	D	1	XYS	O5-C5-C4	3.44	118.99	110.79
4	E	1	XYS	O5-C1-C2	3.27	119.49	109.94
4	D	1	XYS	O2-C2-C1	3.14	116.49	109.25
4	D	2	XYP	O3-C3-C2	-3.02	103.89	110.05
4	E	1	XYS	O2-C2-C1	2.88	115.90	109.25
4	D	1	XYS	O4-C4-C5	2.75	115.53	109.22
4	E	2	XYP	O2-C2-C3	-2.74	104.47	110.15
4	E	3	XYP	O3-C3-C2	-2.73	104.49	110.05
4	E	1	XYS	O4-C4-C5	2.69	115.38	109.22
4	D	2	XYP	C1-C2-C3	-2.55	105.93	109.64
4	E	1	XYS	O1-C1-C2	2.46	116.11	108.98
4	D	1	XYS	O1-C1-C2	2.33	115.74	108.98
4	D	1	XYS	O4-C4-C3	2.30	114.91	110.15
4	D	1	XYS	O5-C1-C2	2.24	116.48	109.94
4	E	1	XYS	O5-C5-C4	2.23	116.11	110.79
4	E	1	XYS	O3-C3-C4	2.18	114.50	110.05
4	D	2	XYP	O4-C4-C3	-2.12	105.75	110.15
4	D	1	XYS	C1-C2-C3	2.11	114.65	110.36
4	D	3	XYP	C5-C4-C3	2.07	112.66	109.64

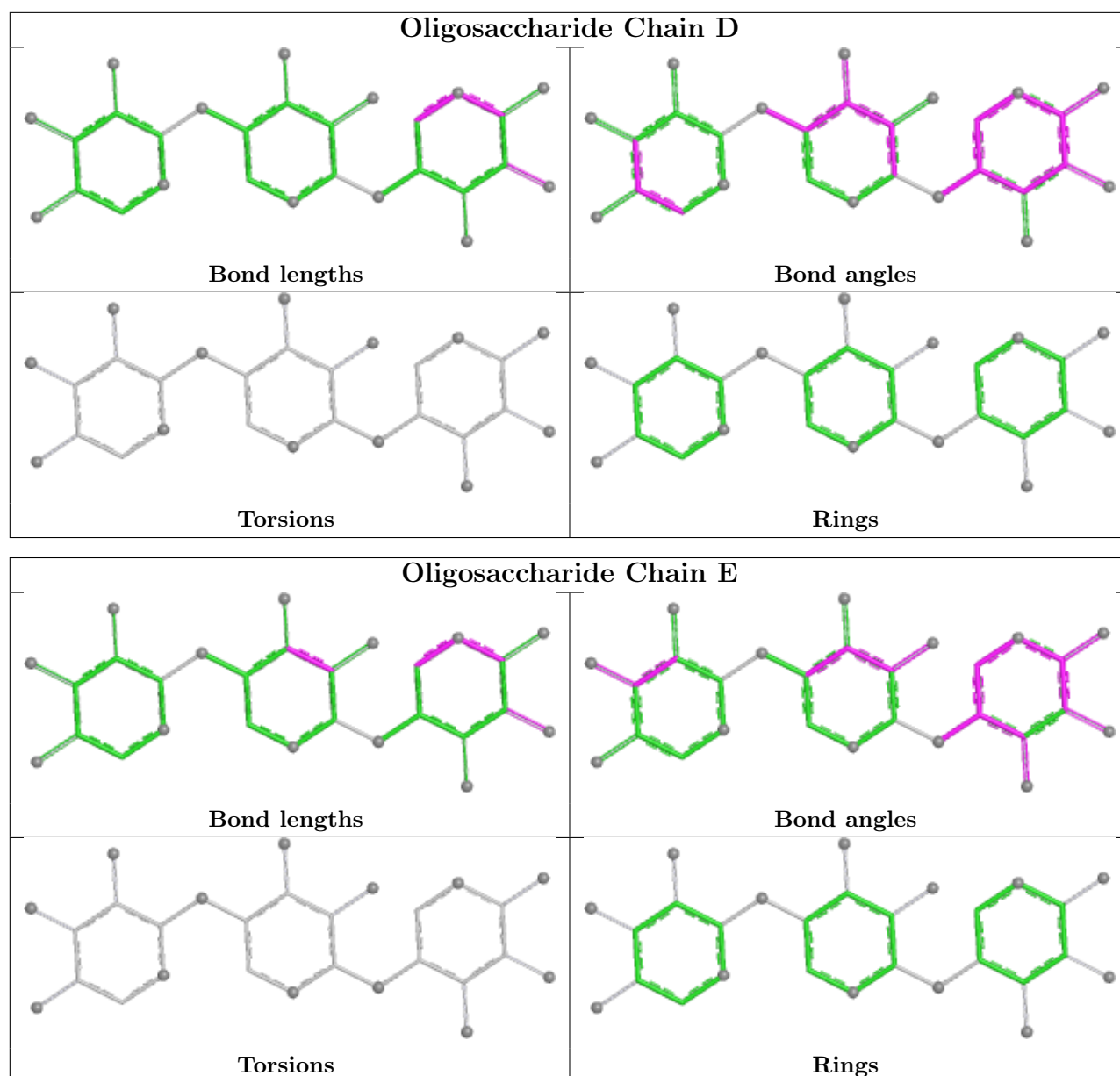
There are no chirality outliers.

There are no torsion outliers.

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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	386/456 (84%)	-1.76	0 100 100	4, 9, 19, 36	2 (0%)
2	B	387/432 (89%)	-1.77	0 100 100	4, 9, 18, 35	0
3	C	391/432 (90%)	-1.45	0 100 100	15, 28, 41, 54	0
All	All	1164/1320 (88%)	-1.66	0 100 100	4, 13, 36, 54	2 (0%)

There are no RSRZ outliers to report.

### 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](#)

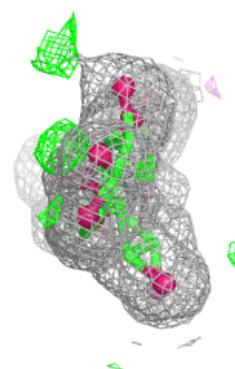
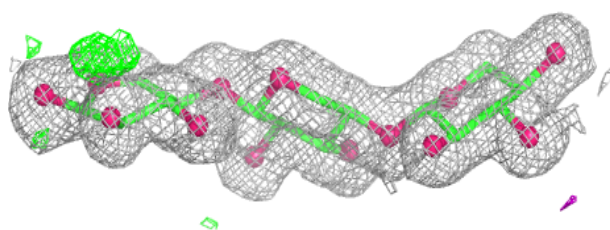
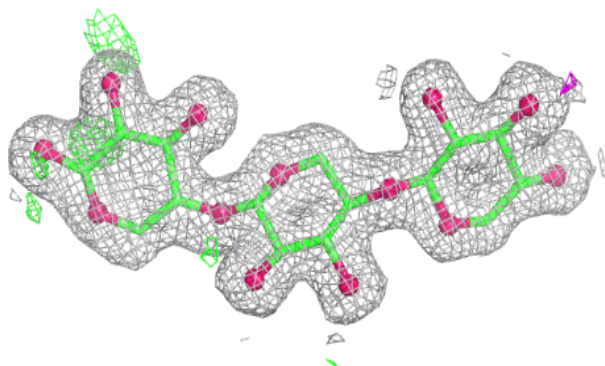
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	XYS	D	1	10/10	0.99	0.02	8,10,15,17	0
4	XYP	D	2	9/10	1.00	0.01	5,5,6,6	0
4	XYP	D	3	9/10	1.00	0.01	4,4,4,4	0
4	XYS	E	1	10/10	1.00	0.02	9,11,14,19	0
4	XYP	E	2	9/10	1.00	0.01	4,5,5,5	0
4	XYP	E	3	9/10	1.00	0.01	3,3,4,4	0

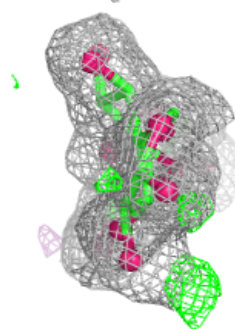
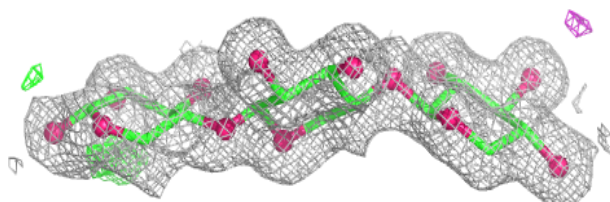
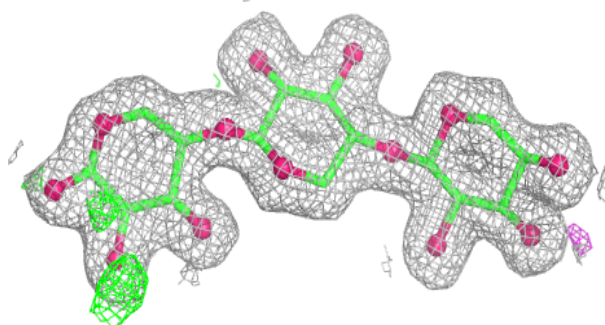
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain D:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain E:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.