Full wwPDB X-ray Structure Validation Report (i)

Feb 25, 2024 – 05:16 AM EST

PDB ID	:	4YZ0
Title	:	C. bescii Family 3 pectate lyase double mutant K108A/E39Q in complex with trigalacturonic acid
Authors	:	Alahuhta, P.M.; Lunin, V.V.
Deposited on	:	2015-03-24
Resolution	:	1.15 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 (i) 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 (i)) were used in the production of this report:

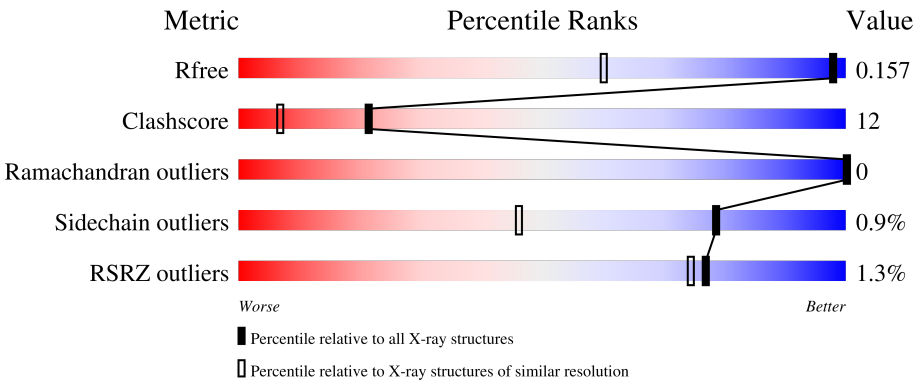
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

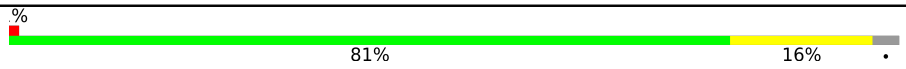
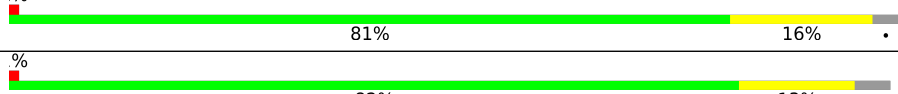
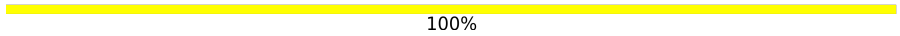
The reported resolution of this entry is 1.15 Å.

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	1492 (1.18-1.10)
Clashscore	141614	1537 (1.18-1.10)
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)
RSRZ outliers	127900	1464 (1.18-1.10)

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 <=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	204	
1	B	204	
2	C	3	
3	D	3	

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
7	MRD	A	208[B]	-	-	X	-
7	MRD	A	209	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 4283 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 Pectate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	198	1735	1083	302	343	7	0	28	0
1	B	195	1702	1066	294	336	6	0	27	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP B9MKT4
A	-9	ALA	-	expression tag	UNP B9MKT4
A	-8	HIS	-	expression tag	UNP B9MKT4
A	-7	HIS	-	expression tag	UNP B9MKT4
A	-6	HIS	-	expression tag	UNP B9MKT4
A	-5	HIS	-	expression tag	UNP B9MKT4
A	-4	HIS	-	expression tag	UNP B9MKT4
A	-3	HIS	-	expression tag	UNP B9MKT4
A	-2	VAL	-	expression tag	UNP B9MKT4
A	-1	GLY	-	expression tag	UNP B9MKT4
A	0	THR	-	expression tag	UNP B9MKT4
A	39	GLN	GLU	engineered mutation	UNP B9MKT4
A	108	ALA	LYS	engineered mutation	UNP B9MKT4
B	-10	MET	-	expression tag	UNP B9MKT4
B	-9	ALA	-	expression tag	UNP B9MKT4
B	-8	HIS	-	expression tag	UNP B9MKT4
B	-7	HIS	-	expression tag	UNP B9MKT4
B	-6	HIS	-	expression tag	UNP B9MKT4
B	-5	HIS	-	expression tag	UNP B9MKT4
B	-4	HIS	-	expression tag	UNP B9MKT4
B	-3	HIS	-	expression tag	UNP B9MKT4
B	-2	VAL	-	expression tag	UNP B9MKT4
B	-1	GLY	-	expression tag	UNP B9MKT4
B	0	THR	-	expression tag	UNP B9MKT4
B	39	GLN	GLU	engineered mutation	UNP B9MKT4

Continued on next page...

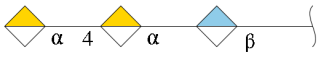
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	108	ALA	LYS	engineered mutation	UNP B9MKT4

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranuronic acid-(1-4)-alpha-D-galactopyranuronic acid-(1-4)-alpha-D-talopyranuronic acid.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	3	37	18	19	0	3	0

- Molecule 3 is an oligosaccharide called alpha-D-galactopyranuronic acid-(1-4)-alpha-D-galactopyranuronic acid-(1-4)-beta-D-talopyranuronic acid.

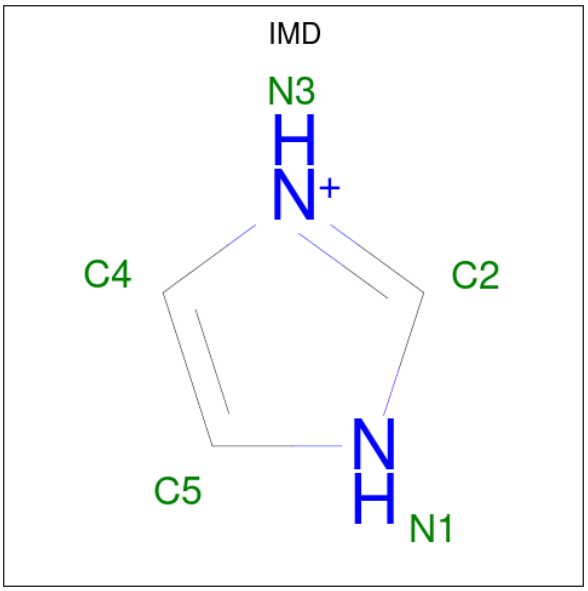


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	D	3	37	18	19	0	3	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

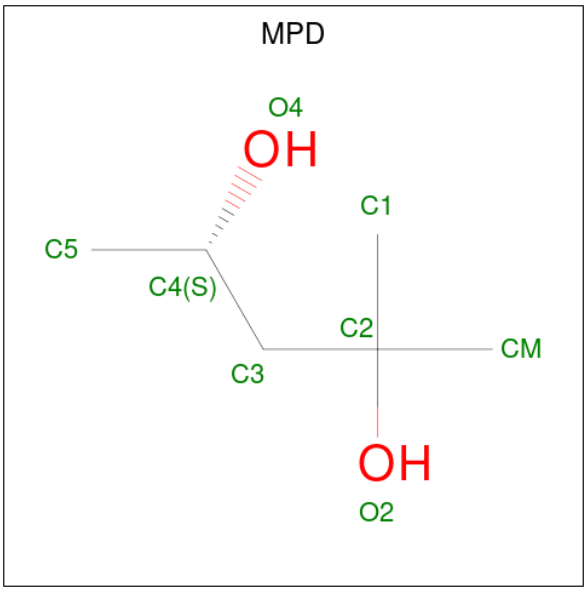
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	4	4	4	0	0
			Total	Ca		
4	B	4	4	4	0	0

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 5 3 2	0	1

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



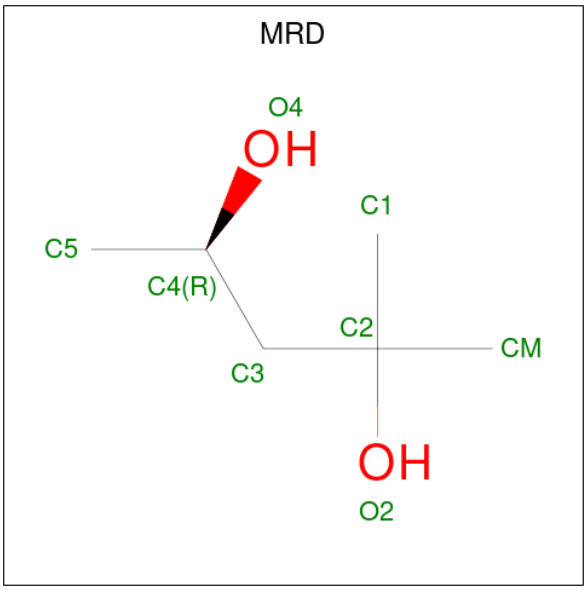
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	1

Continued on next page...

Continued from previous page...

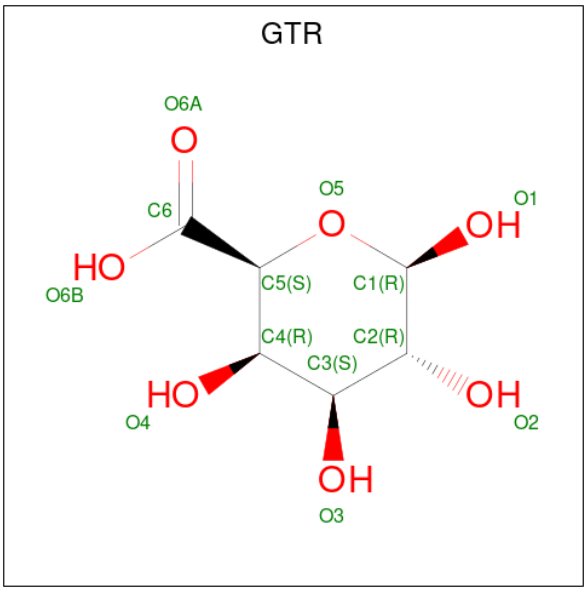
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	8	6	2	0	0

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



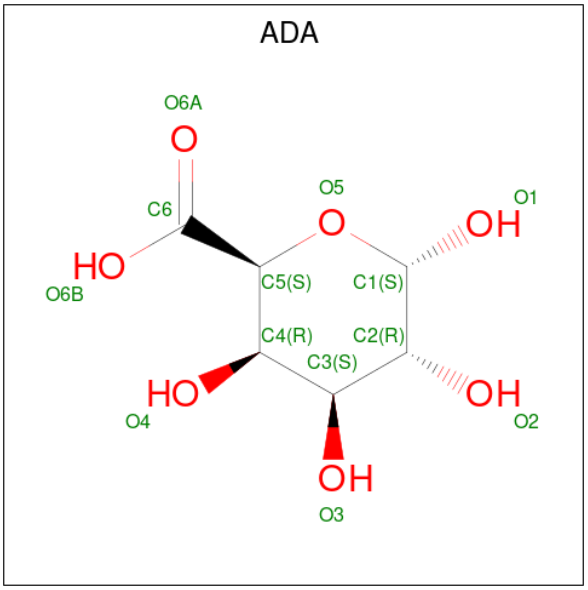
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	8	6	2	0	1
			Total	C	O		
7	A	1	8	6	2	0	0
			Total	C	O		
7	A	1	8	6	2	0	0
			Total	C	O		
7	A	1	8	6	2	0	0
			Total	C	O		
7	B	1	8	6	2	0	0

- Molecule 8 is beta-D-galactopyranuronic acid (three-letter code: GTR) (formula: $C_6H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	13	6	7	0	1
			Total	C	O		
8	B	1	13	6	7	0	1

- Molecule 9 is alpha-D-galactopyranuronic acid (three-letter code: ADA) (formula: $C_6H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	12	6	6	0	1
			Total	C	O		
9	A	1	12	6	6	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	B	1	13	6	7	0	1
			Total	C	O		
9	B	1	12	6	6	0	1
			Total	C	O		
9	B	1	12	6	6	0	1
			Total	C	O		
9	B	1	12	6	6	0	1
			Total	C	O		
9	B	1	12	6	6	0	1

- Molecule 10 is water.

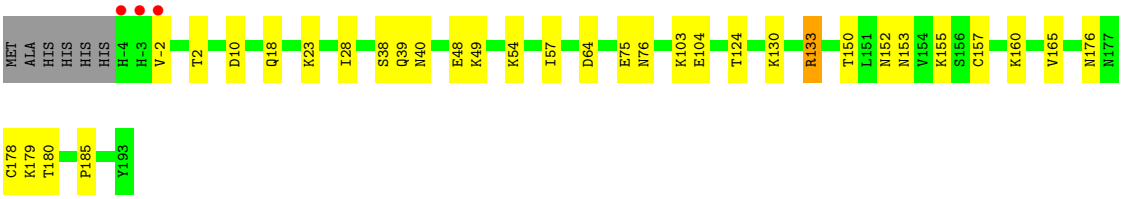
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	278	298	298	0	29
			Total	O		
10	B	265	286	286	0	28

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.

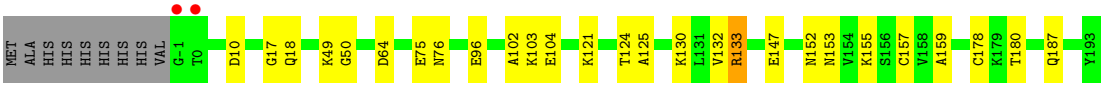
• Molecule 1: Pectate lyase

Chain A:



• Molecule 1: Pectate lyase

Chain B:

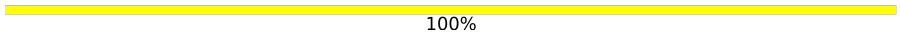


• Molecule 2: alpha-D-galactopyranuronic acid-(1-4)-alpha-D-galactopyranuronic acid-(1-4)-alpha-D-talopyranuronic acid

Chain C:

• Molecule 3: alpha-D-galactopyranuronic acid-(1-4)-alpha-D-galactopyranuronic acid-(1-4)-beta-D-talopyranuronic acid

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.29Å 36.47Å 100.07Å 90.00° 132.63° 90.00°	Depositor
Resolution (Å)	50.00 – 1.15 50.87 – 1.15	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-1.15) 95.2 (50.87-1.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 1.15Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.116 , 0.148 0.133 , 0.157	Depositor DCC
R_{free} test set	6269 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	8.9	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	4283	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MPD, GTR, CA, ADA, X0X, IMD, X1X, MRD

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	1.05	5/1760 (0.3%)	1.21	7/2381 (0.3%)
1	B	1.01	0/1726	1.05	3/2332 (0.1%)
All	All	1.03	5/3486 (0.1%)	1.13	10/4713 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	GLU	CD-OE2	-7.48	1.17	1.25
1	A	39	GLN	CD-NE2	6.01	1.47	1.32
1	A	39	GLN	CG-CD	5.37	1.63	1.51
1	A	18	GLN	CD-OE1	5.17	1.35	1.24
1	A	104	GLU	CD-OE1	5.06	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133[A]	ARG	NE-CZ-NH1	15.70	128.15	120.30
1	A	133[B]	ARG	NE-CZ-NH1	15.70	128.15	120.30
1	A	133[A]	ARG	NE-CZ-NH2	-13.17	113.72	120.30
1	A	133[B]	ARG	NE-CZ-NH2	-13.17	113.72	120.30
1	B	133[A]	ARG	NE-CZ-NH1	10.47	125.53	120.30
1	B	133[B]	ARG	NE-CZ-NH1	10.47	125.53	120.30
1	A	23	LYS	CD-CE-NZ	9.50	133.54	111.70
1	A	10	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	10	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	10	ASP	CB-CG-OD2	-6.31	112.62	118.30

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	1735	0	1715	41	0
1	B	1702	0	1690	29	0
2	C	37	0	11	2	0
3	D	37	0	11	1	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	5	0	5	2	0
6	A	16	0	28	5	0
6	B	8	0	14	1	0
7	A	32	0	56	17	0
7	B	8	0	14	0	0
8	A	13	0	3	0	0
8	B	13	0	4	0	0
9	A	24	0	8	0	0
9	B	61	0	18	3	0
10	A	298	0	0	31	0
10	B	286	0	0	24	0
All	All	4283	0	3577	88	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 12.

All (88) 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:B:153[B]:ASN:ND2	10:B:303:HOH:O	1.63	1.32
1:B:187:GLN:OE1	10:B:302:HOH:O	1.55	1.25
1:A:76[A]:ASN:ND2	10:A:304:HOH:O	1.72	1.23
7:A:208[B]:MRD:H1C1	10:A:322[B]:HOH:O	1.39	1.23
1:A:179[A]:LYS:CB	10:A:305:HOH:O	1.87	1.22
6:A:207[A]:MPD:O4	10:A:301:HOH:O	1.56	1.21
1:A:179[A]:LYS:HB2	10:A:305:HOH:O	1.37	1.18
7:A:208[B]:MRD:H4	10:A:301:HOH:O	1.47	1.14
1:A:179[A]:LYS:N	10:A:305:HOH:O	1.76	1.14
1:A:48[B]:GLU:OE1	10:A:302:HOH:O	1.66	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180[A]:THR:OG1	10:B:304:HOH:O	1.68	1.11
1:A:176[B]:ASN:OD1	10:A:303[B]:HOH:O	1.71	1.07
1:B:152[A]:ASN:ND2	10:B:305:HOH:O	1.90	1.04
1:A:152[B]:ASN:OD1	10:A:306:HOH:O	1.77	1.02
1:B:76[A]:ASN:ND2	10:B:307:HOH:O	1.97	0.97
1:A:57[A]:ILE:HD13	7:A:209:MRD:C1	1.96	0.95
1:A:152[A]:ASN:OD1	10:A:307[A]:HOH:O	1.84	0.94
1:A:179[A]:LYS:CA	10:A:305:HOH:O	2.01	0.93
1:A:124[B]:THR:HG23	10:A:319:HOH:O	1.69	0.92
1:A:155[A]:LYS:NZ	10:A:308:HOH:O	2.04	0.89
1:B:155[A]:LYS:HG2	10:B:308[A]:HOH:O	1.73	0.88
1:A:133[A]:ARG:NH2	10:A:310:HOH:O	2.06	0.87
1:A:57[A]:ILE:HD13	7:A:209:MRD:H1C1	1.55	0.86
1:A:28[B]:ILE:CD1	10:A:416:HOH:O	2.23	0.85
1:A:57[A]:ILE:CD1	7:A:209:MRD:H1C1	2.08	0.84
7:A:209:MRD:HMC2	10:A:440[B]:HOH:O	1.79	0.81
1:A:28[B]:ILE:HD11	10:A:416:HOH:O	1.84	0.78
1:B:76[A]:ASN:ND2	10:B:306:HOH:O	1.96	0.78
6:A:207[A]:MPD:HM3	10:A:363:HOH:O	1.83	0.77
7:A:208[B]:MRD:HMC2	7:A:208[B]:MRD:O4	1.85	0.77
1:A:38[A]:SER:OG	1:A:40[A]:ASN:OD1	2.02	0.75
1:A:103:LYS:NZ	9:B:214[B]:ADA:O6A	2.20	0.74
1:A:103:LYS:NZ	9:B:211[A]:ADA:O6A	2.20	0.73
1:B:103[C]:LYS:HD3	10:B:382:HOH:O	1.87	0.73
1:A:153[B]:ASN:OD1	5:A:205[B]:IMD:N3	2.23	0.72
1:A:178[B]:CYS:O	10:A:311:HOH:O	2.06	0.72
1:A:57[A]:ILE:HD13	7:A:209:MRD:H1C3	1.71	0.71
1:A:180[A]:THR:N	10:A:313:HOH:O	2.22	0.71
7:A:209:MRD:HMC3	10:B:535:HOH:O	1.88	0.71
1:B:155[A]:LYS:CE	10:B:308[A]:HOH:O	2.38	0.71
1:B:155[A]:LYS:NZ	10:B:308[A]:HOH:O	2.13	0.71
1:B:155[A]:LYS:CG	10:B:308[A]:HOH:O	2.36	0.69
1:A:75[B]:GLU:OE1	10:A:312:HOH:O	2.10	0.69
6:B:205:MPD:H51	10:B:486:HOH:O	1.92	0.69
1:B:103[A]:LYS:HD3	10:B:382:HOH:O	1.91	0.69
7:A:209:MRD:H5C2	10:A:498:HOH:O	1.93	0.68
1:A:103:LYS:NZ	3:D:2[C]:ADA:O6A	2.27	0.67
1:A:124[B]:THR:HG21	10:A:465:HOH:O	1.94	0.66
1:B:124[B]:THR:HG23	10:B:311:HOH:O	1.96	0.66
1:B:18[B]:GLN:OE1	10:B:309:HOH:O	2.13	0.65
1:B:124[A]:THR:CG2	10:B:305:HOH:O	2.46	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1[A]:X1X:O2	2:C:2[A]:ADA:H5	1.98	0.62
1:B:96[B]:GLU:OE2	1:B:121[B]:LYS:HD2	2.00	0.60
1:B:103[A]:LYS:HG2	1:B:104:GLU:HG2	1.82	0.60
1:A:153[B]:ASN:OD1	5:A:205[B]:IMD:C2	2.50	0.59
1:B:103[A]:LYS:CD	10:B:382:HOH:O	2.52	0.57
1:A:124[B]:THR:HG22	1:A:150:THR:HB	1.86	0.57
1:B:17[B]:GLY:HA2	1:B:50:GLY:O	2.05	0.56
1:A:57[A]:ILE:HD12	7:A:209:MRD:H1C1	1.88	0.55
1:A:185:PRO:HA	7:A:208[B]:MRD:HMC2	1.89	0.54
7:A:209:MRD:H1C3	10:B:360[B]:HOH:O	2.08	0.53
1:B:124[B]:THR:HG21	10:B:497:HOH:O	2.10	0.52
1:B:178:CYS:SG	1:B:180[B]:THR:O	2.69	0.51
7:A:208[B]:MRD:O4	7:A:208[B]:MRD:CM	2.58	0.50
1:B:133[A]:ARG:NH2	10:B:315:HOH:O	2.43	0.49
1:A:130:LYS:HE2	1:A:160[A]:LYS:HD3	1.95	0.49
1:B:124[A]:THR:HG23	10:B:305:HOH:O	2.12	0.48
1:A:185:PRO:HA	7:A:208[B]:MRD:CM	2.44	0.48
1:A:54:LYS:HA	1:A:75[A]:GLU:O	2.14	0.47
1:B:130:LYS:HA	1:B:157:CYS:O	2.15	0.47
1:B:155[B]:LYS:HD3	10:B:373:HOH:O	2.15	0.47
1:B:102:ALA:O	1:B:125:ALA:HA	2.15	0.46
9:B:210[A]:ADA:O6B	10:B:310[A]:HOH:O	2.21	0.45
1:A:130:LYS:HA	1:A:157:CYS:O	2.16	0.45
1:A:185:PRO:HA	6:A:207[A]:MPD:H12	1.99	0.44
2:C:1[A]:X1X:O2	2:C:2[A]:ADA:C5	2.67	0.42
1:A:49[A]:LYS:HB2	1:A:49[A]:LYS:HE2	1.90	0.42
1:A:155[A]:LYS:CE	10:A:308:HOH:O	2.56	0.42
1:A:165:VAL:HG22	10:A:449:HOH:O	2.19	0.42
1:B:132[B]:VAL:O	1:B:159:ALA:HA	2.19	0.42
7:A:208[B]:MRD:C1	10:A:322[B]:HOH:O	2.22	0.41
7:A:209:MRD:H5C1	10:A:543:HOH:O	2.19	0.41
1:B:121[A]:LYS:HA	1:B:147:GLU:O	2.20	0.41
1:A:155[A]:LYS:HE2	10:A:308:HOH:O	2.22	0.40
6:A:207[A]:MPD:H51	10:A:516:HOH:O	2.21	0.40
1:A:-2:VAL:HG22	1:A:2:THR:OG1	2.21	0.40
6:A:207[A]:MPD:C3	10:A:301:HOH:O	2.69	0.40
1:B:75[A]:GLU:O	1:B:76[A]:ASN:C	2.60	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	225/204 (110%)	208 (92%)	17 (8%)	0	100	100
1	B	221/204 (108%)	209 (95%)	12 (5%)	0	100	100
All	All	446/408 (109%)	417 (94%)	29 (6%)	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	196/172 (114%)	195 (100%)	1 (0%)	88	64
1	B	191/172 (111%)	189 (99%)	2 (1%)	76	42
All	All	387/344 (112%)	384 (99%)	3 (1%)	78	50

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	B	49	LYS
1	B	64	ASP

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

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)

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	$\#\|Z\| > 2$
2	X1X	C	1[A]	2	13,13,13	1.49	3 (23%)	18,19,19	1.30	3 (16%)
2	ADA	C	2[A]	2,4	12,12,13	1.29	2 (16%)	14,17,19	1.55	2 (14%)
2	ADA	C	3[A]	2,4	12,12,13	1.93	4 (33%)	14,17,19	1.20	1 (7%)
3	X0X	D	1[C]	3	13,13,13	1.69	4 (30%)	18,19,19	1.93	6 (33%)
3	ADA	D	2[C]	3,4	12,12,13	0.84	0	14,17,19	1.18	0
3	ADA	D	3[C]	3,4	12,12,13	0.84	1 (8%)	14,17,19	0.76	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	X1X	C	1[A]	2	-	0/4/24/24	0/1/1/1
2	ADA	C	2[A]	2,4	-	0/4/21/24	0/1/1/1
2	ADA	C	3[A]	2,4	-	0/4/21/24	0/1/1/1
3	X0X	D	1[C]	3	-	0/4/24/24	0/1/1/1
3	ADA	D	2[C]	3,4	-	0/4/21/24	0/1/1/1
3	ADA	D	3[C]	3,4	-	0/4/21/24	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3[A]	ADA	C2-C3	-4.33	1.46	1.52
3	D	1[C]	X0X	O5-C5	-3.23	1.38	1.43
3	D	1[C]	X0X	O5-C1	-3.13	1.35	1.42
2	C	1[A]	X1X	O1-C1	2.95	1.49	1.39
2	C	3[A]	ADA	C1-C2	-2.61	1.46	1.52
3	D	1[C]	X0X	C5-C6	-2.58	1.47	1.53
2	C	2[A]	ADA	C1-C2	2.57	1.58	1.52
2	C	1[A]	X1X	O4-C4	2.51	1.48	1.43
2	C	1[A]	X1X	O5-C5	2.36	1.47	1.43
2	C	3[A]	ADA	O3-C3	2.21	1.48	1.43
3	D	3[C]	ADA	O6B-C6	-2.07	1.23	1.30
2	C	3[A]	ADA	C4-C5	-2.03	1.49	1.53
3	D	1[C]	X0X	O3-C3	2.01	1.47	1.43
2	C	2[A]	ADA	O4-C4	2.00	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1[C]	X0X	C1-O5-C5	-5.18	104.60	112.22
2	C	2[A]	ADA	O4-C4-C5	3.25	117.03	109.74
2	C	3[A]	ADA	C1-C2-C3	2.62	112.89	109.67
3	D	1[C]	X0X	O6A-C6-C5	-2.53	111.53	120.81
3	D	1[C]	X0X	O1-C1-O5	-2.46	102.99	110.38
2	C	2[A]	ADA	O2-C2-C3	2.25	114.64	110.14
2	C	1[A]	X1X	C1-O5-C5	2.23	115.51	112.22
3	D	1[C]	X0X	O3-C3-C4	2.20	115.44	110.35
2	C	1[A]	X1X	O5-C5-C4	2.14	113.39	109.57
2	C	1[A]	X1X	O1-C1-O5	2.08	116.62	110.38
3	D	1[C]	X0X	O6B-C6-O6A	2.04	128.72	124.09
3	D	1[C]	X0X	O5-C5-C4	2.04	113.21	109.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

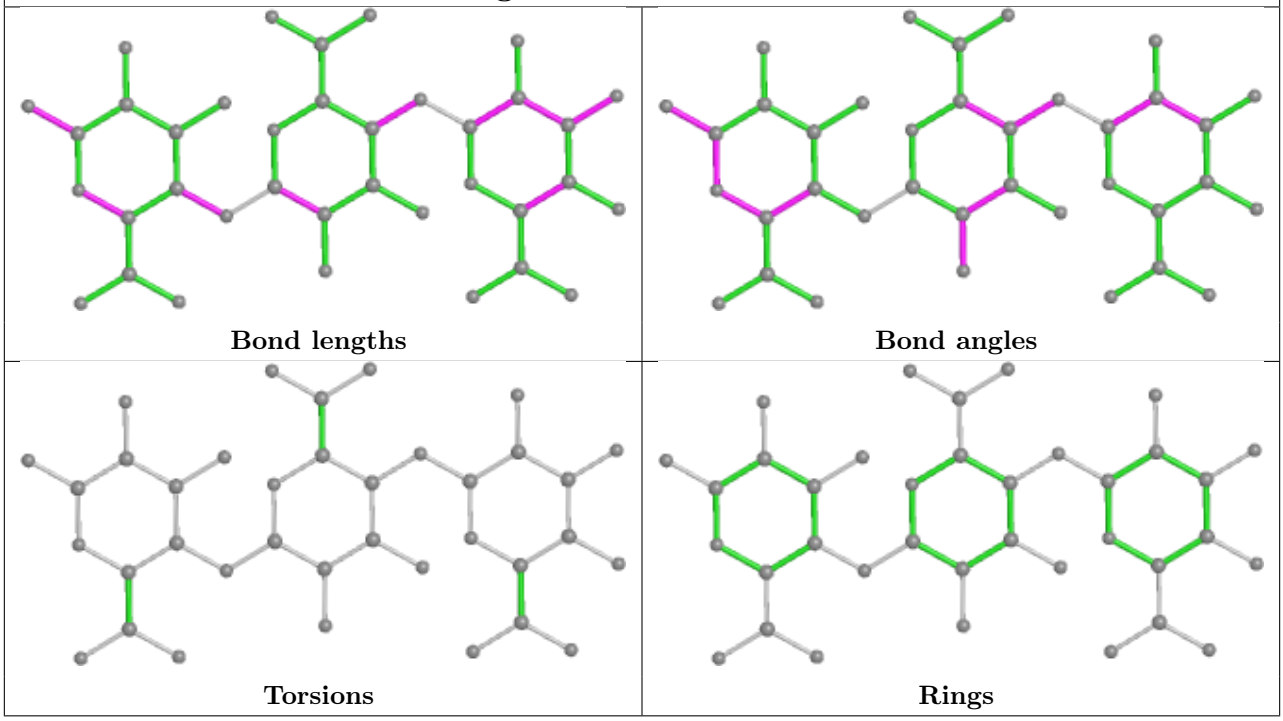
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1[A]	X1X	2	0
2	C	2[A]	ADA	2	0
3	D	2[C]	ADA	1	0

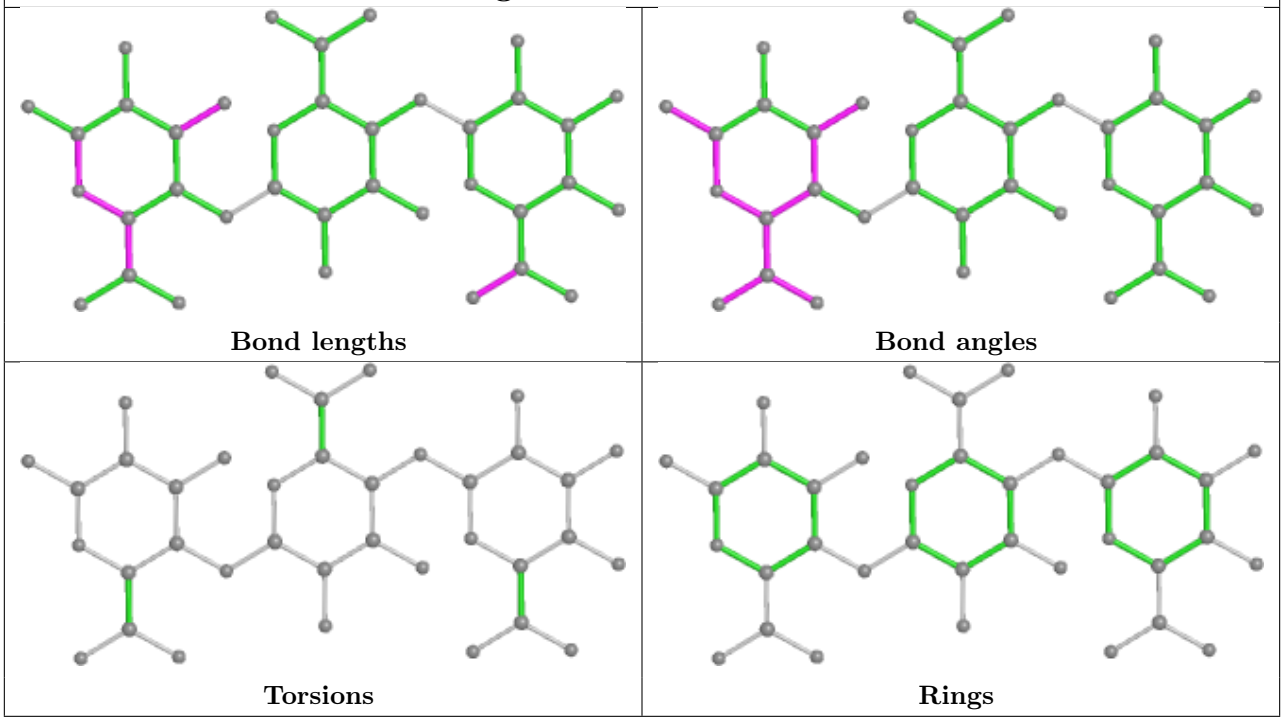
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
6	MPD	A	207[A]	-	7,7,7	0.60	0	9,10,10	0.97	0
7	MRD	B	206	-	7,7,7	0.76	0	9,10,10	1.31	1 (11%)
9	ADA	B	214[B]	8,4,9	12,12,13	1.09	0	14,17,19	1.55	5 (35%)
8	GTR	A	215[B]	9	13,13,13	2.27	5 (38%)	18,19,19	2.15	7 (38%)
9	ADA	B	212[A]	4,9	12,12,13	1.06	1 (8%)	14,17,19	0.80	0
5	IMD	A	205[B]	-	3,5,5	0.31	0	4,5,5	1.02	0
7	MRD	A	209	-	7,7,7	1.00	1 (14%)	9,10,10	2.17	2 (22%)
9	ADA	A	216[B]	8,4,9	12,12,13	1.18	1 (8%)	14,17,19	1.52	2 (14%)
9	ADA	A	217[B]	4,9	12,12,13	1.89	4 (33%)	14,17,19	1.27	1 (7%)
9	ADA	B	215[B]	4,9	12,12,13	1.14	1 (8%)	14,17,19	0.88	0
6	MPD	A	206	-	7,7,7	1.34	1 (14%)	9,10,10	2.40	3 (33%)
8	GTR	B	213[B]	9	13,13,13	0.88	1 (7%)	18,19,19	1.29	2 (11%)
9	ADA	B	211[A]	4,9	12,12,13	0.85	0	14,17,19	1.44	4 (28%)
7	MRD	A	210	-	7,7,7	1.04	1 (14%)	9,10,10	1.39	1 (11%)
6	MPD	B	205	-	7,7,7	0.58	0	9,10,10	0.96	0
7	MRD	A	208[B]	-	7,7,7	1.26	1 (14%)	9,10,10	0.77	0
7	MRD	A	211	-	7,7,7	0.64	0	9,10,10	1.05	1 (11%)
9	ADA	B	210[A]	9	13,13,13	1.48	3 (23%)	18,19,19	1.63	5 (27%)

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
6	MPD	A	207[A]	-	-	0/5/5/5	-
7	MRD	B	206	-	-	0/5/5/5	-
9	ADA	B	214[B]	8,4,9	-	0/4/21/24	0/1/1/1
8	GTR	A	215[B]	9	-	1/4/24/24	0/1/1/1
9	ADA	B	212[A]	4,9	-	0/4/21/24	0/1/1/1
7	MRD	A	209	-	-	0/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADA	A	216[B]	8,4,9	-	1/4/21/24	0/1/1/1
9	ADA	A	217[B]	4,9	-	0/4/21/24	0/1/1/1
9	ADA	B	215[B]	4,9	-	0/4/21/24	0/1/1/1
5	IMD	A	205[B]	-	-	-	0/1/1/1
6	MPD	A	206	-	-	2/5/5/5	-
8	GTR	B	213[B]	9	-	0/4/24/24	0/1/1/1
9	ADA	B	211[A]	4,9	-	0/4/21/24	0/1/1/1
7	MRD	A	210	-	-	2/5/5/5	-
6	MPD	B	205	-	-	1/5/5/5	-
7	MRD	A	208[B]	-	-	0/5/5/5	-
7	MRD	A	211	-	-	0/5/5/5	-
9	ADA	B	210[A]	9	-	0/4/24/24	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	215[B]	GTR	O2-C2	4.71	1.54	1.43
8	A	215[B]	GTR	O4-C4	4.11	1.52	1.43
9	A	217[B]	ADA	C2-C3	-3.68	1.47	1.52
8	A	215[B]	GTR	O5-C1	-3.56	1.34	1.42
9	A	217[B]	ADA	C1-C2	-3.07	1.45	1.52
9	A	217[B]	ADA	C4-C5	-2.98	1.48	1.53
9	B	210[A]	ADA	O1-C1	2.71	1.48	1.39
9	A	216[B]	ADA	C1-C2	2.53	1.58	1.52
9	B	212[A]	ADA	O6B-C6	-2.52	1.22	1.30
9	B	215[B]	ADA	O6B-C6	-2.49	1.22	1.30
7	A	208[B]	MRD	O2-C2	-2.46	1.38	1.44
6	A	206	MPD	C1-C2	-2.44	1.44	1.52
8	B	213[B]	GTR	O5-C1	-2.41	1.36	1.42
9	B	210[A]	ADA	O2-C2	2.38	1.48	1.43
8	A	215[B]	GTR	O6B-C6	-2.29	1.23	1.30
7	A	210	MRD	O2-C2	-2.28	1.38	1.44
9	A	217[B]	ADA	O3-C3	2.24	1.48	1.43
9	B	210[A]	ADA	O5-C5	-2.22	1.39	1.43
8	A	215[B]	GTR	C1-C2	-2.12	1.47	1.52
7	A	209	MRD	O2-C2	2.02	1.49	1.44

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	209	MRD	O2-C2-CM	5.64	126.17	108.08
6	A	206	MPD	O2-C2-CM	-5.33	90.98	108.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	215[B]	GTR	O1-C1-O5	-4.68	96.33	110.38
8	A	215[B]	GTR	O5-C1-C2	-3.81	103.49	110.28
9	B	210[A]	ADA	C1-O5-C5	3.61	117.53	112.22
8	A	215[B]	GTR	C1-C2-C3	-3.24	103.58	110.31
7	A	210	MRD	CM-C2-C1	-3.19	103.93	110.57
9	A	217[B]	ADA	C1-C2-C3	3.16	113.55	109.67
9	B	214[B]	ADA	O6B-C6-O6A	2.99	130.87	124.09
9	A	216[B]	ADA	O4-C4-C5	2.98	116.43	109.74
6	A	206	MPD	CM-C2-C3	2.96	123.74	109.96
7	B	206	MRD	O2-C2-C1	2.86	117.27	108.08
9	B	211[A]	ADA	C3-C4-C5	-2.71	104.61	109.25
8	A	215[B]	GTR	C3-C4-C5	-2.62	104.76	109.25
8	A	215[B]	GTR	O4-C4-C3	2.44	115.99	110.35
8	B	213[B]	GTR	C1-O5-C5	-2.40	108.70	112.22
7	A	209	MRD	O2-C2-C1	-2.39	100.42	108.08
9	B	214[B]	ADA	C3-C4-C5	-2.35	105.23	109.25
6	A	206	MPD	O2-C2-C1	2.34	115.60	108.08
8	B	213[B]	GTR	O1-C1-O5	-2.32	103.42	110.38
8	A	215[B]	GTR	O3-C3-C4	2.25	115.54	110.35
9	B	210[A]	ADA	O5-C5-C4	2.21	113.53	109.57
9	B	210[A]	ADA	O6A-C6-C5	-2.21	112.69	120.81
7	A	211	MRD	CM-C2-C1	-2.20	105.99	110.57
9	B	211[A]	ADA	C1-C2-C3	2.19	112.36	109.67
8	A	215[B]	GTR	O3-C3-C2	-2.16	105.36	110.35
9	B	211[A]	ADA	O5-C1-C2	-2.15	107.44	110.77
9	B	214[B]	ADA	O4-C4-C5	2.15	114.57	109.74
9	A	216[B]	ADA	O2-C2-C1	-2.14	104.77	109.15
9	B	210[A]	ADA	O6B-C6-C5	2.10	121.36	113.65
9	B	214[B]	ADA	O5-C1-C2	-2.10	107.53	110.77
9	B	214[B]	ADA	C1-C2-C3	2.07	112.21	109.67
9	B	210[A]	ADA	O1-C1-O5	2.01	116.42	110.38
9	B	211[A]	ADA	O4-C4-C5	2.01	114.25	109.74

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	206	MPD	C2-C3-C4-C5
6	B	205	MPD	C2-C3-C4-C5
6	A	206	MPD	C2-C3-C4-O4
7	A	210	MRD	C1-C2-C3-C4
7	A	210	MRD	O2-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	215[B]	GTR	O5-C5-C6-O6B
9	A	216[B]	ADA	C4-C5-C6-O6B

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	207[A]	MPD	5	0
9	B	214[B]	ADA	1	0
5	A	205[B]	IMD	2	0
7	A	209	MRD	10	0
9	B	211[A]	ADA	1	0
6	B	205	MPD	1	0
7	A	208[B]	MRD	7	0
9	B	210[A]	ADA	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 (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	198/204 (97%)	-0.43	3 (1%)	73	71	5, 8, 22, 98	3 (1%)
1	B	195/204 (95%)	-0.44	2 (1%)	82	80	5, 10, 23, 58	1 (0%)
All	All	393/408 (96%)	-0.43	5 (1%)	77	74	5, 9, 23, 98	4 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-4	HIS	3.5
1	A	-3	HIS	3.0
1	B	-1	GLY	2.9
1	B	0	THR	2.7
1	A	-2	VAL	2.4

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(Å^2)	Q<0.9
2	X1X	C	1[A]	13/13	0.96	0.12	28,49,121,138	13
2	ADA	C	2[A]	12/13	0.98	0.06	7,10,18,19	12
3	X0X	D	1[C]	13/13	0.98	0.05	9,11,13,14	13
2	ADA	C	3[A]	12/13	0.99	0.05	8,10,12,12	12

Continued on next page...

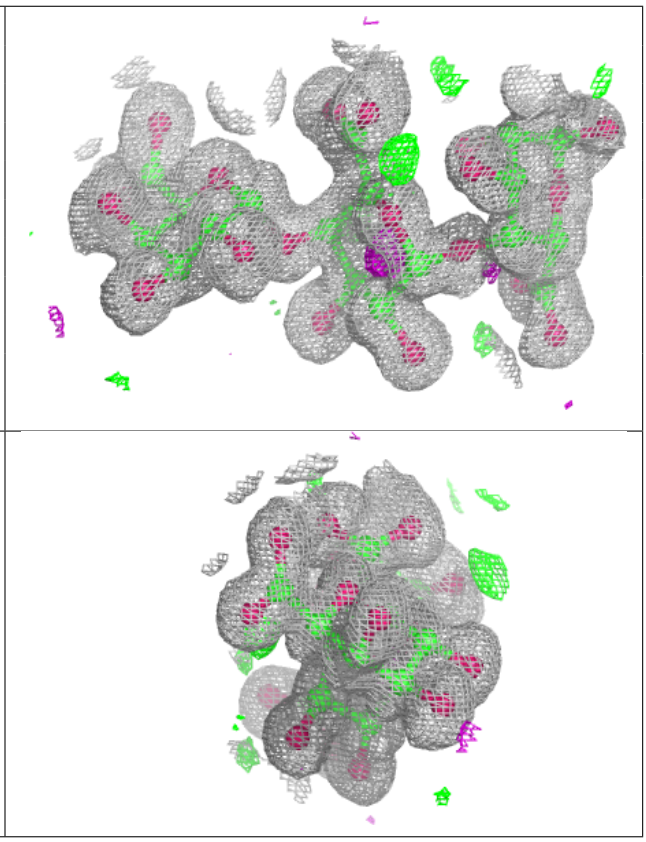
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADA	D	2[C]	12/13	0.99	0.04	9,12,14,20	12
3	ADA	D	3[C]	12/13	0.99	0.05	7,8,13,14	12

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

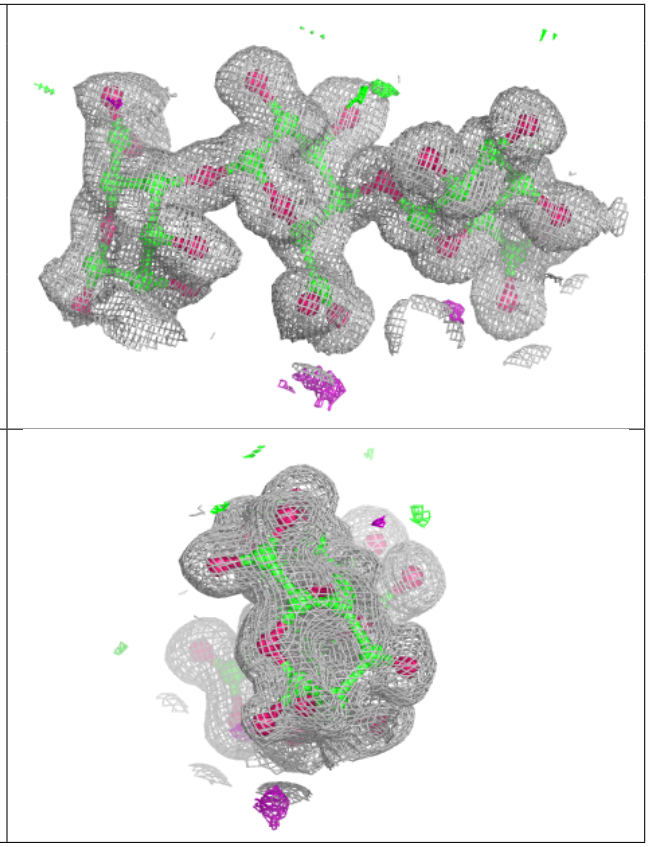
Electron density around Chain C:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)



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(Å^2)	Q<0.9
7	MRD	B	206	8/8	0.81	0.17	16,26,34,37	0
6	MPD	B	205	8/8	0.88	0.11	27,43,51,58	0
6	MPD	A	207[A]	8/8	0.88	0.18	20,31,36,68	8
7	MRD	A	208[B]	8/8	0.90	0.19	7,9,15,21	8
7	MRD	A	209	8/8	0.91	0.15	16,22,25,26	8
7	MRD	A	210	8/8	0.93	0.10	22,33,37,46	0
5	IMD	A	205[B]	5/5	0.94	0.12	19,29,37,38	5
6	MPD	A	206	8/8	0.94	0.09	19,25,32,39	0
8	GTR	A	215[B]	13/13	0.96	0.12	9,14,21,23	13
7	MRD	A	211	8/8	0.97	0.08	17,20,23,25	8
8	GTR	B	213[B]	13/13	0.98	0.05	11,26,39,41	13
9	ADA	A	216[B]	12/13	0.98	0.06	9,12,21,25	12
9	ADA	B	210[A]	13/13	0.98	0.05	12,20,27,28	13
9	ADA	A	217[B]	12/13	0.99	0.05	8,11,22,27	12

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	201	1/1	0.99	0.04	16,16,16,16	1
9	ADA	B	211[A]	12/13	0.99	0.04	10,12,15,18	12
9	ADA	B	212[A]	12/13	0.99	0.05	8,9,13,14	12
9	ADA	B	214[B]	12/13	0.99	0.04	6,8,11,15	12
9	ADA	B	215[B]	12/13	0.99	0.05	6,8,11,14	12
4	CA	B	202	1/1	1.00	0.05	10,10,10,10	1
4	CA	B	203	1/1	1.00	0.03	7,7,7,7	0
4	CA	B	204	1/1	1.00	0.02	7,7,7,7	0
4	CA	A	202	1/1	1.00	0.04	11,11,11,11	1
4	CA	A	203	1/1	1.00	0.02	8,8,8,8	0
4	CA	A	204	1/1	1.00	0.03	8,8,8,8	0
4	CA	B	201	1/1	1.00	0.05	13,13,13,13	1

6.5 Other polymers (i)

There are no such residues in this entry.