



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:25 AM BST

PDB ID : 4YZA
Title : C. bescii Family 3 pectate lyase double mutant K108A/Q111A in complex with trigalacturonic acid
Authors : Alahuhta, P.M.; Lunin, V.V.
Deposited on : 2015-03-24
Resolution : 1.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

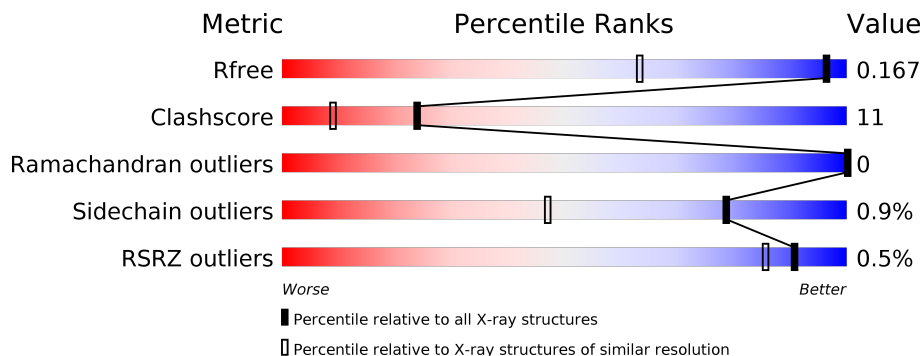
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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 ≥ 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	204	
1	B	204	
2	C	3	
3	D	3	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 4280 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	1678	1049	289	333	7	0	23	0
1	B	196	1691	1057	290	338	6	0	25	0

There are 26 discrepancies between the modelled and reference sequences:

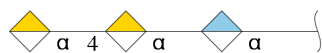
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP B9MKT4
A	-9	ALA	-	expression tag	UNP B9MKT4
A	-8	HIS	-	expression tag	UNP B9MKT4
A	-7	HIS	-	expression tag	UNP B9MKT4
A	-6	HIS	-	expression tag	UNP B9MKT4
A	-5	HIS	-	expression tag	UNP B9MKT4
A	-4	HIS	-	expression tag	UNP 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	108	ALA	LYS	engineered mutation	UNP B9MKT4
A	111	ALA	GLN	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	108	ALA	LYS	engineered mutation	UNP B9MKT4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	111	ALA	GLN	engineered mutation	UNP B9MKT4

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

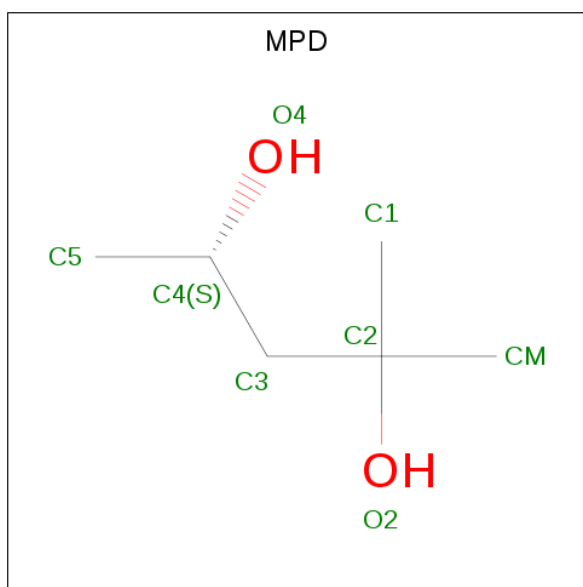


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	D	3	37	18	19	0	3	0

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

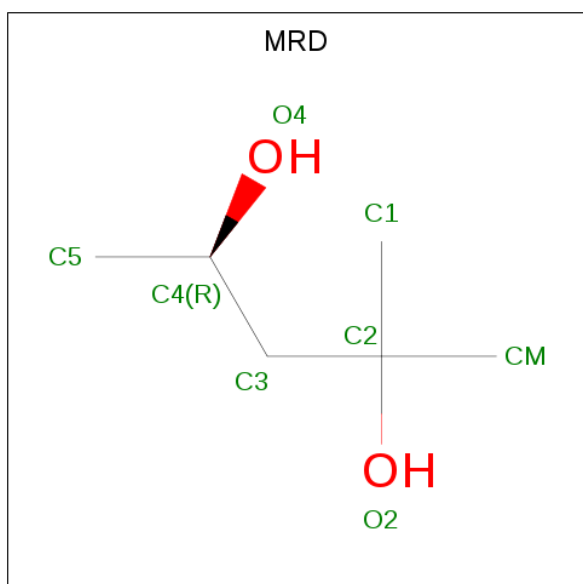
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Ca	0	0
			4	4		
4	A	5	Total	Ca	0	0
			5	5		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



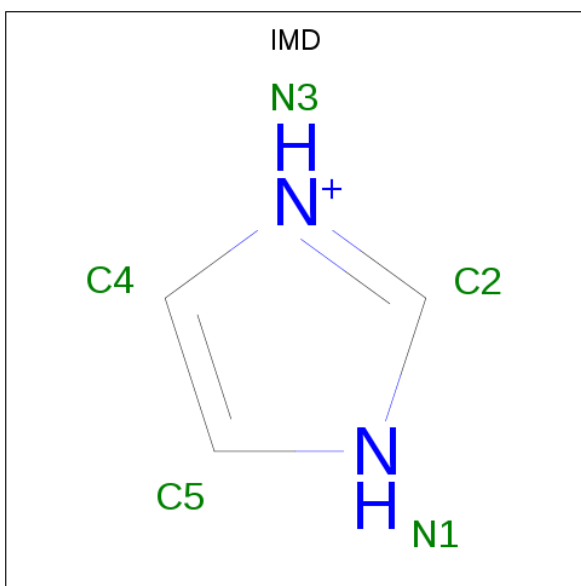
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



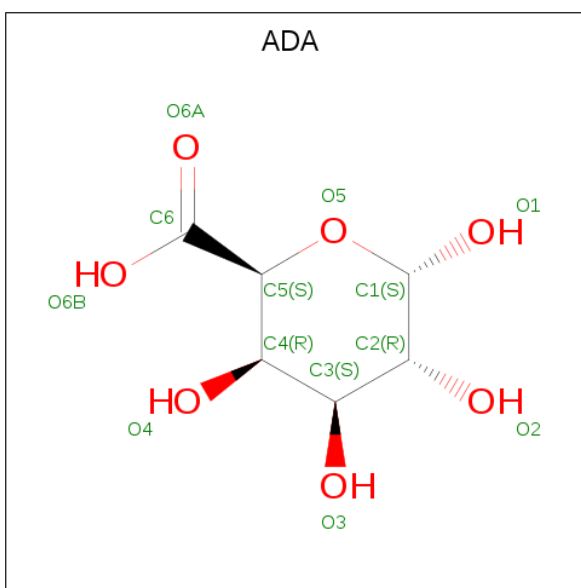
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



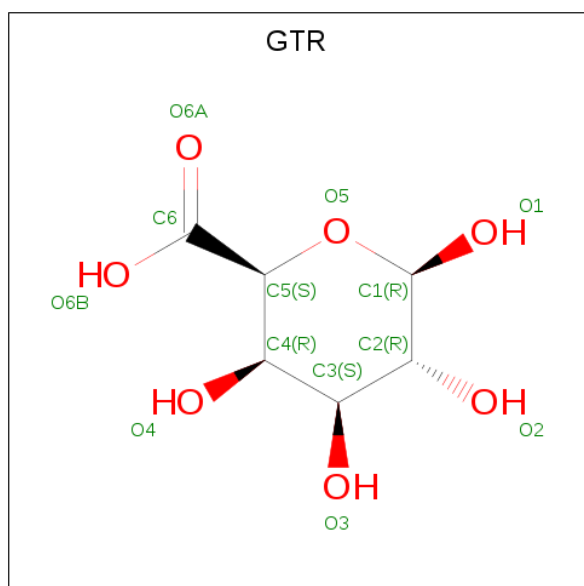
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			5	3	2		

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



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

- Molecule 9 is beta-D-galactopyranuronic acid (three-letter code: GTR) (formula: C₆H₁₀O₇).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	305	Total O 333 333	0	28

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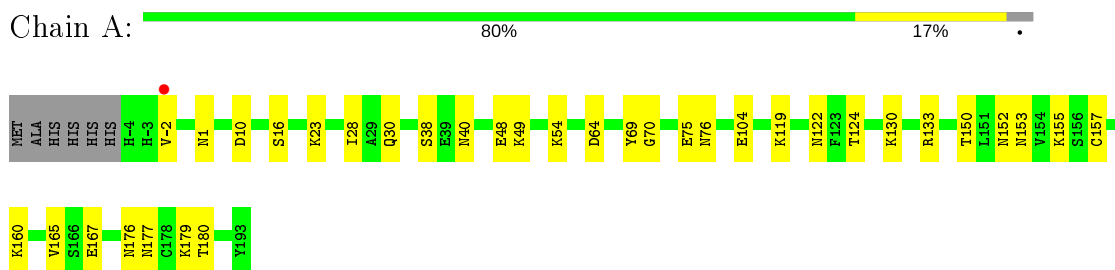
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	306	Total 339	O 339	0	33

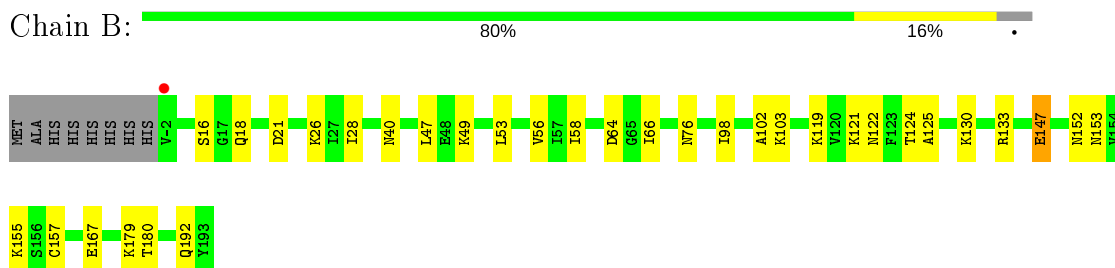
3 Residue-property plots [i](#)

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



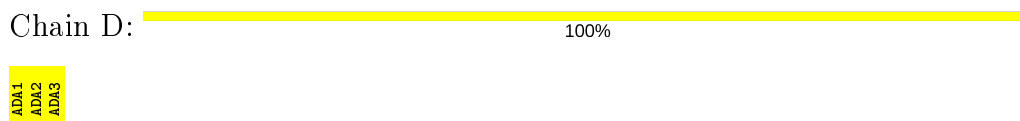
- Molecule 1: Pectate lyase



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.82Å 36.43Å 100.52Å 90.00° 132.85° 90.00°	Depositor
Resolution (Å)	50.89 – 1.25 50.89 – 1.25	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.89-1.25) 98.3 (50.89-1.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.25Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.108 , 0.151 0.126 , 0.167	Depositor DCC
R_{free} test set	4803 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	9.6	Xtrriage
Anisotropy	0.236	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4280	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: MPD, IMD, CA, X1X, GTR, ADA, 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	1.02	3/1703 (0.2%)	1.04	2/2303 (0.1%)
1	B	0.95	0/1714	1.04	7/2317 (0.3%)
All	All	0.98	3/3417 (0.1%)	1.04	9/4620 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	GLU	CD-OE2	-6.38	1.18	1.25
1	A	167[A]	GLU	CD-OE2	-5.22	1.20	1.25
1	A	167[B]	GLU	CD-OE2	-5.22	1.20	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	B	133	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	21	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	21	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	10	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	103	LYS	CA-CB-CG	5.26	124.98	113.40
1	B	147	GLU	OE1-CD-OE2	-5.13	117.15	123.30
1	B	133	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	47	LEU	CB-CG-CD2	5.05	119.58	111.00

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	1678	0	1658	37	0
1	B	1691	0	1675	38	0
2	C	37	0	10	1	0
3	D	37	0	12	0	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
5	A	16	0	28	6	0
5	B	16	0	28	5	0
6	A	8	0	14	0	0
7	A	5	0	4	1	0
8	A	61	0	19	0	0
8	B	24	0	8	0	0
9	A	13	0	4	0	0
9	B	13	0	3	0	0
10	A	333	0	0	18	0
10	B	339	0	0	34	0
All	All	4280	0	3463	79	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 11.

All (79) 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:179[B]:LYS:HB2	10:A:306:HOH:O	1.29	1.30
1:A:76[B]:ASN:ND2	10:A:303:HOH:O	1.65	1.25
1:B:119[A]:LYS:HE2	10:B:302:HOH:O	1.15	1.24
1:B:153[B]:ASN:ND2	10:B:306:HOH:O	1.71	1.22
1:B:167[B]:GLU:OE2	10:B:305:HOH:O	1.53	1.21
1:B:122[B]:ASN:ND2	10:B:466[B]:HOH:O	1.77	1.15
1:A:179[B]:LYS:N	10:A:306:HOH:O	1.80	1.15
1:A:152[B]:ASN:ND2	10:A:305:HOH:O	1.78	1.13
1:A:179[B]:LYS:CB	10:A:306:HOH:O	1.82	1.12
1:B:152[B]:ASN:ND2	10:B:307:HOH:O	1.85	1.09
1:B:119[A]:LYS:CE	10:B:302:HOH:O	1.76	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176[A]:ASN:OD1	10:A:304:HOH:O	1.76	1.03
1:B:76[B]:ASN:ND2	10:B:308:HOH:O	1.88	1.03
1:B:76[B]:ASN:ND2	10:B:533[B]:HOH:O	1.63	1.03
1:B:155[B]:LYS:HD3	10:B:536:HOH:O	1.61	1.00
1:A:155[A]:LYS:NZ	10:A:308:HOH:O	1.94	0.99
1:B:119[A]:LYS:NZ	10:B:309:HOH:O	1.94	0.98
1:A:179[B]:LYS:CA	10:A:306:HOH:O	2.01	0.92
1:A:48:GLU:OE1	10:A:307:HOH:O	1.86	0.92
1:A:28[B]:ILE:CD1	10:B:328:HOH:O	2.17	0.90
1:B:122[B]:ASN:OD1	5:B:206:MPD:H52	1.71	0.90
1:B:179[A]:LYS:NZ	10:B:310:HOH:O	2.06	0.88
1:A:119[B]:LYS:CE	5:A:206:MPD:HM1	2.05	0.86
1:A:38[A]:SER:OG	1:A:40:ASN:OD1	1.95	0.82
1:A:119[B]:LYS:HE2	5:A:206:MPD:CM	2.10	0.82
1:A:124[B]:THR:HG21	10:A:487:HOH:O	1.80	0.81
1:A:119[B]:LYS:HE2	5:A:206:MPD:HM1	1.61	0.80
1:A:119[B]:LYS:CD	5:A:206:MPD:HM1	2.15	0.77
1:A:119[B]:LYS:HD3	5:A:206:MPD:HM1	1.67	0.77
1:B:119[A]:LYS:NZ	10:B:302:HOH:O	2.05	0.75
5:B:201:MPD:H51	10:B:483:HOH:O	1.85	0.75
1:B:40[B]:ASN:HB2	10:B:304:HOH:O	1.88	0.73
1:B:180[B]:THR:OG1	10:B:311:HOH:O	2.07	0.73
1:A:180[B]:THR:N	10:A:310:HOH:O	2.21	0.72
1:A:23:LYS:HE3	10:A:354:HOH:O	1.91	0.71
1:A:16[A]:SER:OG	10:A:307:HOH:O	2.09	0.69
1:A:28[B]:ILE:HD11	10:B:328:HOH:O	1.88	0.67
1:B:124[B]:THR:HG21	10:B:493:HOH:O	1.94	0.66
1:B:49[A]:LYS:HD3	10:B:384:HOH:O	1.96	0.66
1:B:18[A]:GLN:OE1	10:B:312:HOH:O	2.14	0.66
1:B:76[B]:ASN:CG	10:B:533[B]:HOH:O	2.17	0.66
1:A:122[A]:ASN:OD1	10:A:309:HOH:O	2.13	0.65
1:A:30[B]:GLN:HG2	10:A:388[B]:HOH:O	1.95	0.65
1:B:124[A]:THR:CG2	10:B:307:HOH:O	2.44	0.64
1:A:-2:VAL:HG11	10:B:591:HOH:O	2.00	0.62
1:A:165:VAL:HG22	10:A:455:HOH:O	2.01	0.60
1:A:124[B]:THR:HG23	10:A:322:HOH:O	2.02	0.59
1:A:49[A]:LYS:HG2	1:A:69:TYR:O	2.03	0.59
1:B:122[B]:ASN:OD1	5:B:206:MPD:C5	2.49	0.58
1:A:124[B]:THR:HG22	1:A:150:THR:HB	1.84	0.57
1:A:54:LYS:HA	1:A:75[B]:GLU:O	2.07	0.54
5:B:201:MPD:O2	5:B:201:MPD:H52	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40[B]:ASN:HB2	10:B:542[B]:HOH:O	2.08	0.54
2:C:1[C]:X1X:O2	2:C:2[C]:ADA:H5	2.07	0.54
1:A:28[B]:ILE:HD12	10:B:328:HOH:O	2.00	0.52
1:B:124[A]:THR:HG23	10:B:307:HOH:O	2.08	0.50
1:B:18[A]:GLN:HB3	10:B:312:HOH:O	2.11	0.49
1:B:58:ILE:HD11	1:B:66[B]:ILE:HD11	1.95	0.49
1:B:155[A]:LYS:NZ	10:B:319[A]:HOH:O	2.46	0.47
5:B:206:MPD:C1	10:B:322:HOH:O	2.63	0.47
1:B:192:GLN:HG2	10:B:447[A]:HOH:O	2.14	0.47
1:B:130:LYS:HA	1:B:157:CYS:O	2.15	0.46
1:B:18[A]:GLN:CG	10:B:312:HOH:O	2.65	0.45
1:A:130:LYS:HE2	1:A:160[A]:LYS:HD3	1.98	0.45
1:B:49[A]:LYS:HB2	1:B:49[A]:LYS:HE2	1.78	0.45
1:B:53:LEU:HD11	1:B:56[B]:VAL:HG21	1.99	0.44
1:A:130:LYS:HA	1:A:157:CYS:O	2.17	0.44
1:B:26:LYS:HE2	1:B:28[B]:ILE:HD11	1.99	0.43
1:B:102:ALA:O	1:B:125:ALA:HA	2.18	0.43
1:A:155[A]:LYS:HD2	7:A:209:IMD:C4	2.48	0.43
1:B:121[B]:LYS:HA	1:B:147:GLU:O	2.19	0.42
1:B:98[B]:ILE:CD1	10:B:584:HOH:O	2.67	0.42
1:B:53:LEU:HD23	1:B:66[A]:ILE:HD13	2.02	0.41
1:A:124[A]:THR:CG2	10:A:305:HOH:O	2.68	0.41
1:B:76[B]:ASN:OD1	10:B:533[B]:HOH:O	2.22	0.41
1:B:49[B]:LYS:NZ	10:B:315:HOH:O	2.34	0.41
1:A:49[A]:LYS:HA	1:A:70:GLY:O	2.20	0.40
1:A:153:ASN:HA	1:A:177[B]:ASN:O	2.21	0.40
1:A:1:ASN:OD1	5:A:207:MPD:H31	2.21	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	219/204 (107%)	205 (94%)	14 (6%)	0	100	100
1	B	221/204 (108%)	205 (93%)	16 (7%)	0	100	100
All	All	440/408 (108%)	410 (93%)	30 (7%)	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	189/171 (110%)	188 (100%)	1 (0%)	88	66
1	B	190/171 (111%)	187 (98%)	3 (2%)	62	25
All	All	379/342 (111%)	375 (99%)	4 (1%)	78	39

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	B	16[A]	SER
1	B	16[B]	SER
1	B	64	ASP

Some 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[C]	2,4	10,13,13	1.17	0	15,19,19	1.80	6 (40%)
2	ADA	C	2[C]	2,4	9,12,13	0.80	0	12,17,19	1.56	3 (25%)
2	ADA	C	3[C]	2,4	9,12,13	0.76	0	12,17,19	0.93	0
3	ADA	D	1[A]	3	10,13,13	1.05	1 (10%)	15,19,19	1.73	2 (13%)
3	ADA	D	2[A]	3,4	9,12,13	1.32	1 (11%)	12,17,19	1.86	3 (25%)
3	ADA	D	3[A]	3,4	9,12,13	1.49	1 (11%)	12,17,19	0.98	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[C]	2,4	-	0/0/24/24	0/1/1/1
2	ADA	C	2[C]	2,4	-	0/0/21/24	0/1/1/1
2	ADA	C	3[C]	2,4	-	0/0/21/24	0/1/1/1
3	ADA	D	1[A]	3	-	0/0/24/24	0/1/1/1
3	ADA	D	2[A]	3,4	-	0/0/21/24	0/1/1/1
3	ADA	D	3[A]	3,4	-	0/0/21/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3[A]	ADA	O5-C5	3.89	1.47	1.43
3	D	2[A]	ADA	O5-C5	3.32	1.47	1.43
3	D	1[A]	ADA	O1-C1	2.00	1.46	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1[A]	ADA	C1-O5-C5	4.39	118.86	112.31
3	D	2[A]	ADA	O4-C4-C5	4.08	117.86	110.05
2	C	1[C]	X1X	C1-O5-C5	3.83	118.04	112.31
2	C	1[C]	X1X	O5-C1-C2	-3.12	104.72	110.28
2	C	2[C]	ADA	O4-C4-C5	2.59	115.01	110.05
3	D	2[A]	ADA	C6-C5-C4	2.54	119.40	113.04
3	D	1[A]	ADA	O4-C4-C5	-2.49	105.29	110.05
2	C	1[C]	X1X	O2-C2-C1	-2.38	103.63	109.16
2	C	2[C]	ADA	O4-C4-C3	-2.28	105.08	110.35
2	C	1[C]	X1X	C6-C5-C4	-2.21	107.50	113.04
2	C	2[C]	ADA	C1-O5-C5	-2.11	108.45	112.17
2	C	1[C]	X1X	O5-C5-C4	2.05	112.29	108.91
2	C	1[C]	X1X	O2-C2-C3	2.03	115.03	110.35
3	D	2[A]	ADA	O4-C4-C3	-2.01	105.70	110.35

There are no chirality outliers.

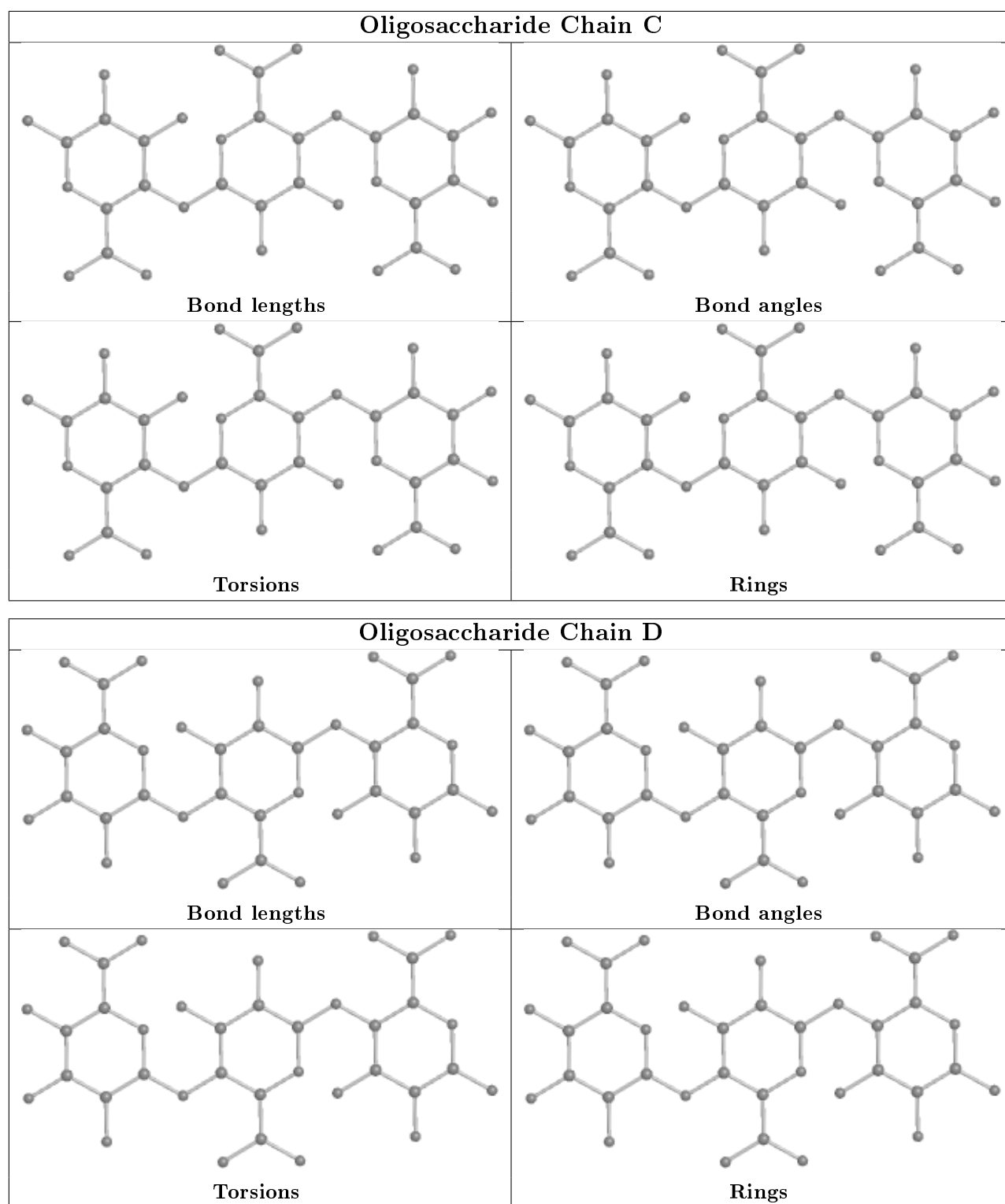
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1[C]	X1X	1	0
2	C	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.



5.6 Ligand geometry [\(i\)](#)

Of 24 ligands modelled in this entry, 9 are monoatomic - leaving 15 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
9	GTR	A	216[B]	8,4	10,13,13	1.06	0	15,19,19	1.21	2 (13%)
6	MRD	A	208	-	7,7,7	0.37	0	9,10,10	1.15	1 (11%)
8	ADA	A	213[A]	8,4	10,13,13	1.37	1 (10%)	15,19,19	1.98	2 (13%)
8	ADA	A	214[A]	8,4	9,12,13	1.94	2 (22%)	12,17,19	1.55	2 (16%)
7	IMD	A	209	1	3,5,5	0.32	0	4,5,5	0.69	0
5	MPD	B	201	-	7,7,7	0.38	0	9,10,10	0.85	0
5	MPD	A	207	-	7,7,7	0.78	0	9,10,10	2.12	2 (22%)
9	GTR	B	210[B]	8	10,13,13	1.06	1 (10%)	15,19,19	1.39	2 (13%)
8	ADA	A	215[A]	8,4	9,12,13	1.29	1 (11%)	12,17,19	1.21	1 (8%)
8	ADA	B	211[B]	9,8,4	9,12,13	1.13	0	12,17,19	1.73	2 (16%)
5	MPD	A	206	-	7,7,7	1.09	1 (14%)	9,10,10	1.75	2 (22%)
8	ADA	A	217[B]	9,8,4	9,12,13	1.01	0	12,17,19	1.63	3 (25%)
5	MPD	B	206	-	7,7,7	1.01	1 (14%)	9,10,10	2.18	2 (22%)
8	ADA	A	218[B]	8,4	9,12,13	0.50	0	12,17,19	0.99	0
8	ADA	B	212[B]	8,4	9,12,13	1.44	1 (11%)	12,17,19	0.94	1 (8%)

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
9	GTR	A	216[B]	8,4	-	0/0/24/24	0/1/1/1
6	MRD	A	208	-	-	0/5/5/5	-
8	ADA	A	213[A]	8,4	-	0/0/24/24	0/1/1/1
8	ADA	A	214[A]	8,4	-	0/0/21/24	0/1/1/1
9	GTR	B	210[B]	8	-	0/0/24/24	0/1/1/1
5	MPD	B	201	-	-	1/5/5/5	-
5	MPD	A	207	-	-	0/5/5/5	-
7	IMD	A	209	1	-	-	0/1/1/1
8	ADA	A	215[A]	8,4	-	0/0/21/24	0/1/1/1
8	ADA	B	211[B]	9,8,4	-	0/0/21/24	0/1/1/1
5	MPD	A	206	-	-	1/5/5/5	-
8	ADA	A	217[B]	9,8,4	-	0/0/21/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	B	206	-	-	0/5/5/5	-
8	ADA	A	218[B]	8,4	-	0/0/21/24	0/1/1/1
8	ADA	B	212[B]	8,4	-	0/0/21/24	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	214[A]	ADA	O5-C5	4.27	1.48	1.43
8	B	212[B]	ADA	O5-C5	3.94	1.47	1.43
8	A	215[A]	ADA	O5-C5	-3.23	1.40	1.43
8	A	213[A]	ADA	O2-C2	2.66	1.49	1.43
8	A	214[A]	ADA	C2-C3	2.57	1.56	1.52
5	B	206	MPD	C3-C2	-2.20	1.47	1.53
9	B	210[B]	GTR	O1-C1	2.20	1.46	1.39
5	A	206	MPD	O2-C2	-2.10	1.39	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	213[A]	ADA	C1-O5-C5	6.25	121.64	112.31
5	A	207	MPD	CM-C2-C1	-5.54	99.04	110.57
5	B	206	MPD	O2-C2-C1	4.72	123.22	108.08
8	B	211[B]	ADA	O4-C4-C5	3.93	117.56	110.05
8	A	214[A]	ADA	O4-C4-C5	3.52	116.77	110.05
5	B	206	MPD	C5-C4-C3	-3.50	95.19	111.69
5	A	206	MPD	O2-C2-C1	3.25	118.50	108.08
9	B	210[B]	GTR	C1-C2-C3	-3.11	103.86	110.31
8	A	217[B]	ADA	O4-C4-C5	3.01	115.80	110.05
9	A	216[B]	GTR	O5-C1-C2	-2.67	105.52	110.28
5	A	206	MPD	C5-C4-C3	-2.60	99.42	111.69
5	A	207	MPD	O2-C2-C1	2.58	116.37	108.08
8	A	214[A]	ADA	C3-C4-C5	-2.40	104.09	109.02
8	B	212[B]	ADA	C1-O5-C5	2.39	116.39	112.17
8	B	211[B]	ADA	C3-C4-C5	-2.34	104.21	109.02
9	B	210[B]	GTR	O4-C4-C5	-2.32	105.62	110.05
8	A	217[B]	ADA	C1-O5-C5	-2.29	108.14	112.17
6	A	208	MRD	O2-C2-C1	2.25	115.28	108.08
8	A	213[A]	ADA	O4-C4-C5	-2.21	105.83	110.05
8	A	217[B]	ADA	O4-C4-C3	-2.19	105.28	110.35
8	A	215[A]	ADA	O2-C2-C3	2.10	114.34	110.14
9	A	216[B]	GTR	C6-C5-C4	-2.02	108.00	113.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	201	MPD	C2-C3-C4-C5
5	A	206	MPD	C1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	209	IMD	1	0
5	B	201	MPD	2	0
5	A	207	MPD	1	0
5	A	206	MPD	5	0
5	B	206	MPD	3	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%)	-0.75	1 (0%) 91 85	7, 11, 23, 57	4 (2%)
1	B	196/204 (96%)	-0.70	1 (0%) 91 85	6, 12, 25, 87	0
All	All	394/408 (96%)	-0.73	2 (0%) 91 85	6, 11, 25, 87	4 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-2	VAL	5.6
1	A	-2	VAL	4.0

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

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

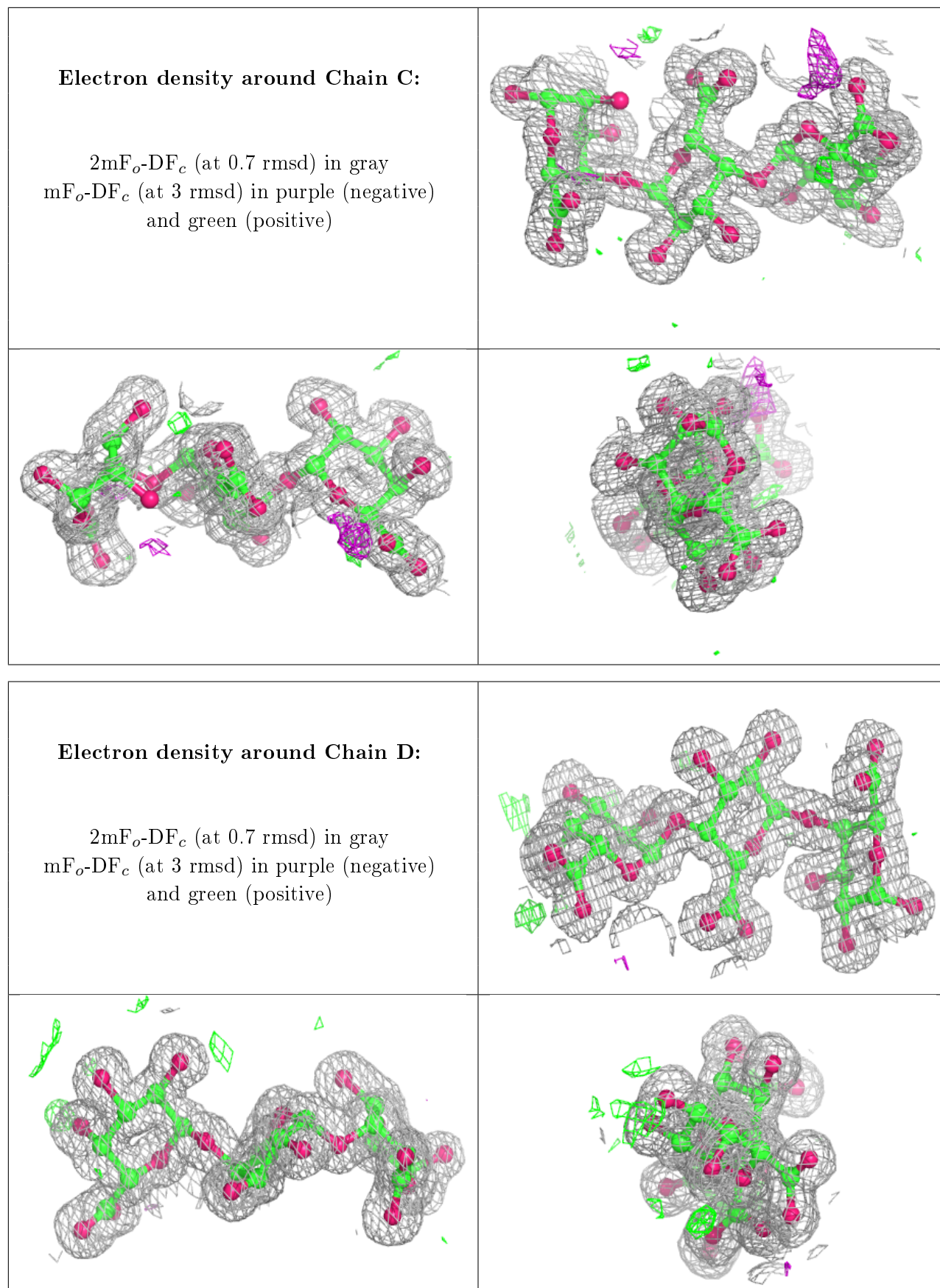
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	X1X	C	1[C]	13/13	0.98	0.08	14,16,21,21	13
2	ADA	C	3[C]	12/13	0.98	0.06	10,12,16,20	12
3	ADA	D	2[A]	12/13	0.99	0.03	9,10,11,12	12
3	ADA	D	1[A]	13/13	0.99	0.04	11,12,16,21	13
2	ADA	C	2[C]	12/13	0.99	0.06	12,14,15,16	12
3	ADA	D	3[A]	12/13	0.99	0.04	9,11,15,16	12

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MPD	B	206	8/8	0.81	0.14	21,35,40,49	8
7	IMD	A	209	5/5	0.83	0.16	26,29,34,42	5
5	MPD	B	201	8/8	0.86	0.14	28,35,53,61	0
5	MPD	A	206	8/8	0.91	0.09	22,25,31,36	0
5	MPD	A	207	8/8	0.92	0.08	22,31,37,39	0
9	GTR	A	216[B]	13/13	0.97	0.08	12,15,17,21	13
8	ADA	A	213[A]	13/13	0.97	0.07	12,16,23,24	13
6	MRD	A	208	8/8	0.97	0.06	19,20,28,30	0
8	ADA	A	218[B]	12/13	0.98	0.06	11,13,17,19	12
8	ADA	A	215[A]	12/13	0.98	0.06	9,13,19,21	12
8	ADA	B	212[B]	12/13	0.99	0.04	10,11,14,18	12
8	ADA	B	211[B]	12/13	0.99	0.03	10,11,14,15	12
8	ADA	A	214[A]	12/13	0.99	0.06	9,11,13,15	12
8	ADA	A	217[B]	12/13	0.99	0.06	13,14,16,20	12
9	GTR	B	210[B]	13/13	0.99	0.04	13,14,20,21	13
4	CA	A	202	1/1	1.00	0.02	9,9,9,9	0
4	CA	A	204	1/1	1.00	0.03	13,13,13,13	1
4	CA	B	203	1/1	1.00	0.04	10,10,10,10	0
4	CA	A	205	1/1	1.00	0.07	16,16,16,16	1
4	CA	A	201	1/1	1.00	0.02	9,9,9,9	0
4	CA	B	204	1/1	1.00	0.04	10,10,10,10	0
4	CA	B	205	1/1	1.00	0.02	11,11,11,11	1
4	CA	B	202	1/1	1.00	0.02	9,9,9,9	0
4	CA	A	203	1/1	1.00	0.03	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.