



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 12:46 PM BST

PDB ID : 4YZX
Title : C. bescii Family 3 pectate lyase double mutant K108A/D107N in complex with trigalacturonic acid
Authors : Alahuhta, P.M.; Lunin, V.V.
Deposited on : 2015-03-25
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

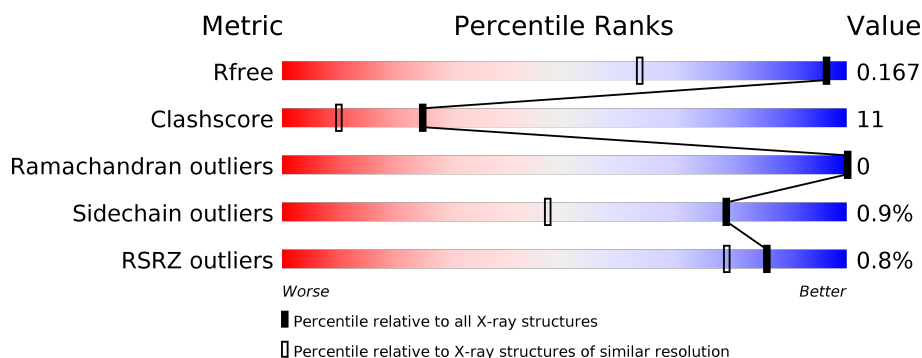
1 Overall quality at a glance

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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 82%, green 14%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 14% . </div> </div>
1	B	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 84%, green 12%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 84% 12% . </div> </div>
2	C	3	<div> <div style="width: 100%; height: 10px; background: yellow;"></div> <div style="text-align: center;">100%</div> </div>
2	D	3	<div> <div style="width: 100%; height: 10px; background: yellow;"></div> <div style="text-align: center;">100%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IMD	B	206	-	-	X	-
6	MRD	A	209	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4150 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
1	A	198	Total	C	N	O	S	0	23	0
			1680	1050	290	333	7			
1	B	195	Total	C	N	O	S	0	22	0
			1656	1039	282	329	6			

There are 26 discrepancies between the modelled and reference sequences:

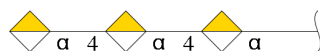
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP B9MKT4
A	-9	ALA	-	expression tag	UNP B9MKT4
A	-8	HIS	-	expression tag	UNP B9MKT4
A	-7	HIS	-	expression tag	UNP B9MKT4
A	-6	HIS	-	expression tag	UNP B9MKT4
A	-5	HIS	-	expression tag	UNP B9MKT4
A	-4	HIS	-	expression tag	UNP 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	107	ASN	ASP	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	107	ASN	ASP	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-galactopyranuronic acid.

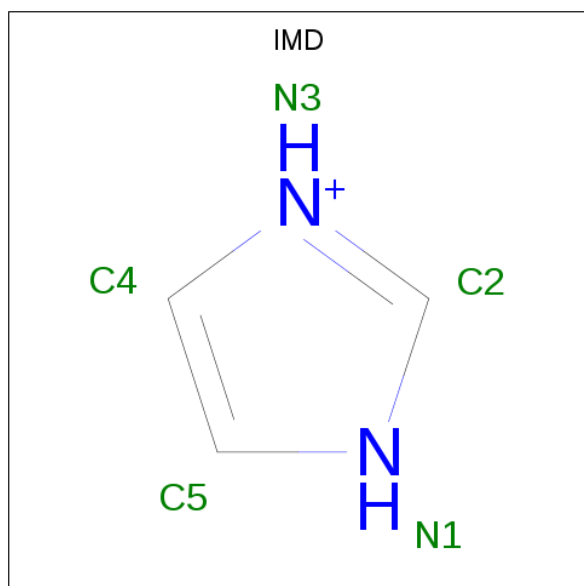


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			37	18	19			
2	D	3	Total	C	O	0	3	0
			37	18	19			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

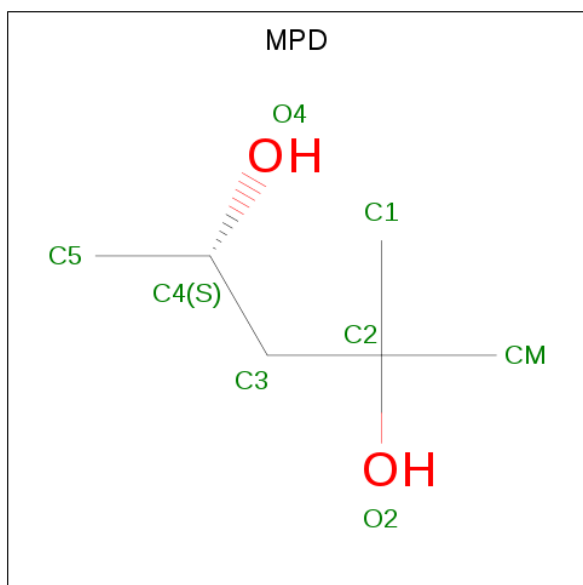
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Ca	0	0
			4	4		
3	A	4	Total	Ca	0	0
			4	4		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



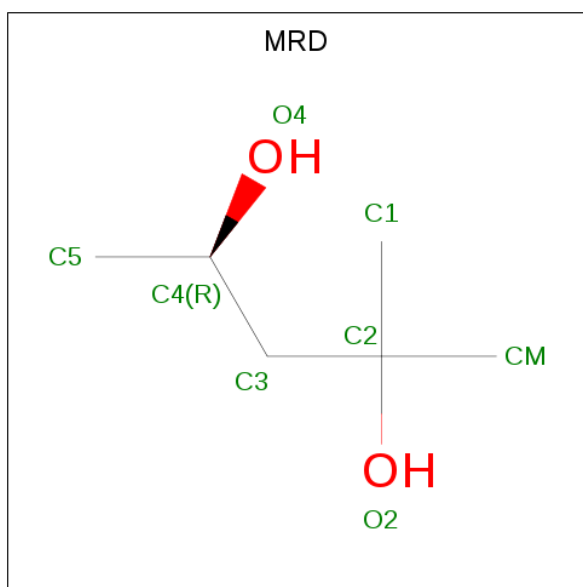
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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: $C_6H_{14}O_2$).

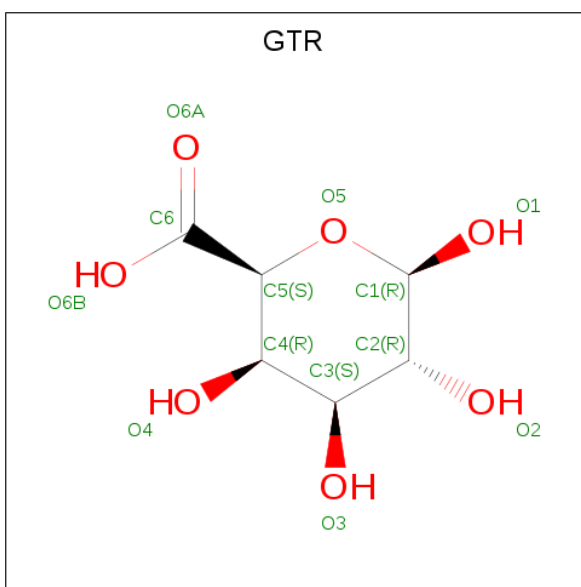


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

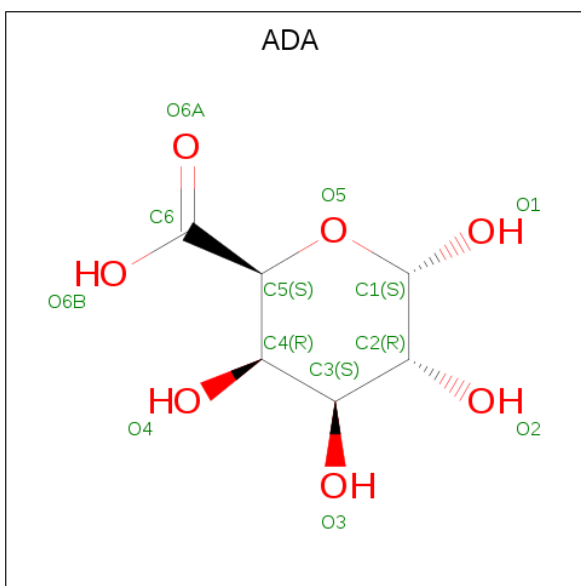
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is beta-D-galactopyranuronic acid (three-letter code: GTR) (formula: C₆H₁₀O₇).



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

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



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

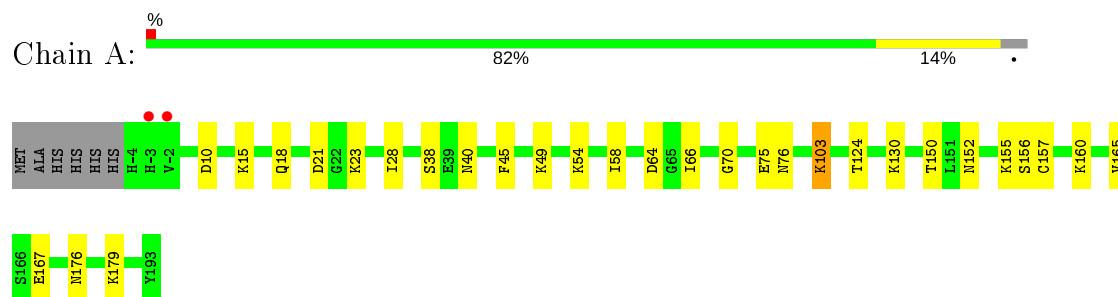
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	292	Total 324	O 324	0	32
10	B	286	Total 311	O 311	0	25

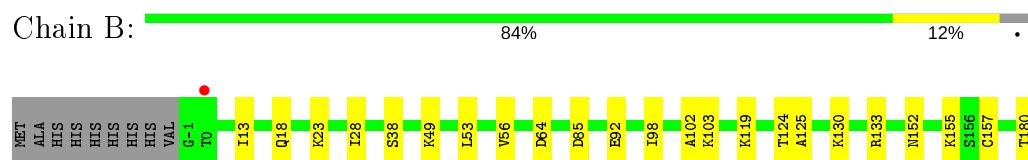
3 Residue-property plots [i](#)

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.

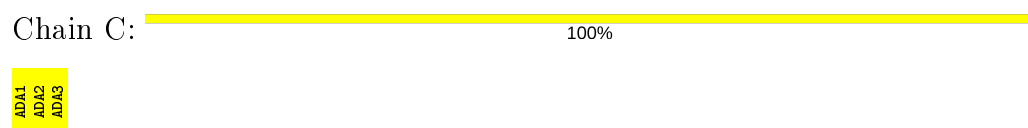
- Molecule 1: Pectate lyase



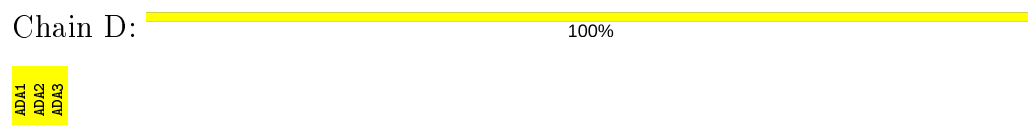
- Molecule 1: Pectate lyase



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



- Molecule 2: 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	138.33 Å 36.35 Å 100.11 Å 90.00° 132.67° 90.00°	Depositor
Resolution (Å)	34.58 – 1.25 34.58 – 1.25	Depositor EDS
% Data completeness (in resolution range)	94.7 (34.58-1.25) 94.7 (34.58-1.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.25 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.110 , 0.156 0.127 , 0.167	Depositor DCC
R_{free} test set	4592 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	10.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4150	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, IMD, CL, CA, 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	0.99	0/1705	0.98	3/2305 (0.1%)
1	B	0.95	0/1679	0.99	2/2269 (0.1%)
All	All	0.97	0/3384	0.98	5/4574 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	133	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	10	ASP	CB-CG-OD1	6.88	124.50	118.30
1	A	21	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	103	LYS	CD-CE-NZ	-5.44	99.18	111.70

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	1680	0	1663	29	0
1	B	1656	0	1651	33	0
2	C	37	0	21	0	0
2	D	37	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	5	0	5	2	0
4	B	5	0	5	4	0
5	A	16	0	28	0	0
5	B	16	0	28	3	0
6	A	16	0	28	8	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	13	0	3	1	0
9	B	24	0	8	0	0
10	A	324	0	0	24	0
10	B	311	0	0	29	0
All	All	4150	0	3450	76	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 (76) 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[A]:LYS:N	10:A:303:HOH:O	1.64	1.27
1:B:38[A]:SER:OG	10:B:302:HOH:O	1.52	1.23
1:A:179[A]:LYS:CB	10:A:303:HOH:O	1.78	1.23
1:B:103[B]:LYS:HE2	10:B:512[B]:HOH:O	1.31	1.23
1:A:152[B]:ASN:ND2	10:A:305:HOH:O	1.72	1.21
1:A:179[A]:LYS:HB2	10:A:303:HOH:O	1.36	1.16
6:A:209:MRD:H1C3	10:A:534:HOH:O	1.42	1.15
1:A:176[B]:ASN:ND2	10:A:306:HOH:O	1.84	1.09
1:A:167[A]:GLU:OE1	10:A:304:HOH:O	1.68	1.08
6:A:209:MRD:HMC3	10:A:527[A]:HOH:O	1.55	1.06
6:A:209:MRD:C1	10:A:534:HOH:O	2.00	1.05
1:B:155[B]:LYS:NZ	10:B:303:HOH:O	1.66	1.01
1:B:152[A]:ASN:ND2	10:B:307:HOH:O	1.94	1.00
1:B:155[B]:LYS:CE	10:B:303:HOH:O	2.02	0.99
1:A:28[A]:ILE:CD1	10:A:414:HOH:O	2.10	0.97
4:B:206:IMD:N1	10:B:308:HOH:O	1.99	0.95
1:A:179[A]:LYS:CA	10:A:303:HOH:O	1.89	0.92
1:A:76[A]:ASN:ND2	10:A:307:HOH:O	2.02	0.91
8:B:212[B]:GTR:O2	10:B:306:HOH:O	1.89	0.91
1:B:180[A]:THR:OG1	10:B:305[A]:HOH:O	1.88	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:206:IMD:C5	10:B:308:HOH:O	2.21	0.89
1:A:155[A]:LYS:NZ	10:A:308:HOH:O	2.08	0.87
1:A:124[B]:THR:HG21	10:A:463:HOH:O	1.76	0.84
1:B:155[A]:LYS:HD2	10:B:425:HOH:O	1.78	0.83
1:A:38[A]:SER:OG	1:A:40:ASN:OD1	1.96	0.82
5:B:201:MPD:H51	10:B:478:HOH:O	1.81	0.79
1:A:28[A]:ILE:HD11	10:A:414:HOH:O	1.75	0.79
1:B:103[B]:LYS:NZ	10:B:309:HOH:O	2.10	0.73
6:A:209:MRD:H5C3	10:A:498:HOH:O	1.89	0.72
1:B:155[B]:LYS:HD3	1:B:155[B]:LYS:N	2.05	0.71
1:B:124[A]:THR:CG2	10:B:307:HOH:O	2.39	0.69
1:B:155[A]:LYS:HD2	10:B:344:HOH:O	1.93	0.68
1:B:183:GLU:OE2	10:B:310:HOH:O	2.14	0.65
1:B:119[C]:LYS:NZ	4:B:206:IMD:HN1	1.95	0.64
6:A:209:MRD:CM	10:A:527[A]:HOH:O	2.30	0.64
6:A:209:MRD:CM	10:A:571:HOH:O	2.45	0.63
1:B:103[B]:LYS:CE	10:B:512[B]:HOH:O	2.09	0.62
1:B:103[A]:LYS:HD2	10:B:384:HOH:O	2.00	0.62
1:B:124[A]:THR:HG23	10:B:307:HOH:O	1.97	0.61
1:B:124[B]:THR:HG21	10:B:463:HOH:O	2.00	0.60
1:A:155[A]:LYS:HD3	4:A:205:IMD:N3	2.17	0.59
1:B:155[B]:LYS:HE3	10:B:303:HOH:O	1.87	0.59
6:A:209:MRD:HMC1	10:A:571:HOH:O	2.04	0.58
1:B:103[B]:LYS:CG	10:B:512[B]:HOH:O	2.50	0.56
1:A:23:LYS:NZ	10:A:312:HOH:O	2.37	0.56
1:B:119[C]:LYS:HZ3	4:B:206:IMD:HN1	1.54	0.54
1:A:165:VAL:HG22	10:A:469:HOH:O	2.07	0.54
1:B:155[A]:LYS:CD	10:B:344:HOH:O	2.53	0.53
1:A:103:LYS:CE	10:A:325[B]:HOH:O	2.56	0.52
1:A:124[B]:THR:HG22	1:A:150:THR:HB	1.91	0.51
1:A:58:ILE:HD11	1:A:66[B]:ILE:HD11	1.93	0.50
1:A:15[B]:LYS:HB2	1:A:18:GLN:HG3	1.94	0.49
5:B:207:MPD:C1	10:B:315:HOH:O	2.61	0.49
1:B:28[B]:ILE:HG22	1:B:28[B]:ILE:O	2.12	0.49
1:B:23:LYS:HE2	10:B:381:HOH:O	2.14	0.48
6:A:209:MRD:H1C2	10:A:375:HOH:O	2.14	0.48
1:A:45:PHE:HB2	1:A:66[B]:ILE:HD12	1.94	0.47
1:A:155[A]:LYS:CD	4:A:205:IMD:N3	2.78	0.46
1:A:130:LYS:HE2	1:A:160[A]:LYS:HD3	1.98	0.46
1:A:49[A]:LYS:HA	1:A:70:GLY:O	2.15	0.45
1:A:54:LYS:HA	1:A:75[B]:GLU:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:201:MPD:H52	5:B:201:MPD:O2	2.17	0.45
1:B:53:LEU:HD11	1:B:56[B]:VAL:HG21	1.98	0.45
1:B:49[B]:LYS:HE2	10:B:554:HOH:O	2.17	0.44
1:A:179[B]:LYS:HE3	1:A:179[B]:LYS:HB2	1.37	0.44
1:B:98[B]:ILE:HG23	1:B:98[B]:ILE:O	2.17	0.44
1:B:13:ILE:CD1	10:B:564:HOH:O	2.65	0.43
1:B:130:LYS:HA	1:B:157:CYS:O	2.19	0.43
1:B:103[B]:LYS:HG3	10:B:512[B]:HOH:O	2.16	0.43
1:A:156[A]:SER:O	1:A:179[A]:LYS:HB3	2.19	0.42
1:A:124[B]:THR:CG2	10:A:463:HOH:O	2.51	0.42
1:B:49[B]:LYS:NZ	10:B:324:HOH:O	2.53	0.42
1:B:102:ALA:O	1:B:125:ALA:HA	2.20	0.42
1:B:49[A]:LYS:NZ	1:B:92:GLU:O	2.54	0.41
1:B:18[A]:GLN:NE2	10:B:318:HOH:O	2.47	0.41
1:A:130:LYS:HA	1:A:157:CYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/204 (107%)	207 (94%)	12 (6%)	0	100	100
1	B	216/204 (106%)	202 (94%)	14 (6%)	0	100	100
All	All	435/408 (107%)	409 (94%)	26 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	190/172 (110%)	189 (100%)	1 (0%)	88	66
1	B	187/172 (109%)	185 (99%)	2 (1%)	73	39
All	All	377/344 (110%)	374 (99%)	3 (1%)	78	53

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

Mol	Chain	Res	Type
1	A	64	ASP
1	B	64	ASP
1	B	85	ASP

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	ADA	C	1	2	10,13,13	1.59	2 (20%)	15,19,19	1.55	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADA	C	2	3,2	9,12,13	1.74	2 (22%)	12,17,19	1.73	4 (33%)
2	ADA	C	3	3,2	9,12,13	2.18	2 (22%)	12,17,19	1.30	1 (8%)
2	ADA	D	1[A]	2	10,13,13	0.87	0	15,19,19	1.41	2 (13%)
2	ADA	D	2[A]	3,2	9,12,13	2.25	2 (22%)	12,17,19	1.65	3 (25%)
2	ADA	D	3[A]	3,2	9,12,13	1.44	1 (11%)	12,17,19	0.91	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
2	ADA	C	1	2	-	0/0/24/24	0/1/1/1
2	ADA	C	2	3,2	-	0/0/21/24	0/1/1/1
2	ADA	C	3	3,2	-	0/0/21/24	0/1/1/1
2	ADA	D	1[A]	2	-	0/0/24/24	0/1/1/1
2	ADA	D	2[A]	3,2	-	0/0/21/24	0/1/1/1
2	ADA	D	3[A]	3,2	-	0/0/21/24	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	ADA	O5-C5	-5.36	1.37	1.43
2	D	2[A]	ADA	C2-C3	4.40	1.59	1.52
2	D	2[A]	ADA	O5-C5	4.05	1.47	1.43
2	C	2	ADA	O5-C5	3.69	1.47	1.43
2	D	3[A]	ADA	O5-C5	3.65	1.47	1.43
2	C	1	ADA	C3-C2	2.73	1.59	1.52
2	C	3	ADA	C2-C3	-2.55	1.48	1.52
2	C	1	ADA	O2-C2	2.53	1.48	1.43
2	C	2	ADA	O4-C4	2.02	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	ADA	C1-O5-C5	4.58	119.15	112.31
2	C	2	ADA	O4-C4-C5	3.87	117.46	110.05
2	D	2[A]	ADA	O4-C4-C5	3.40	116.55	110.05
2	C	3	ADA	C1-O5-C5	2.90	117.29	112.17
2	D	2[A]	ADA	O4-C4-C3	-2.69	104.13	110.35
2	C	1	ADA	C6-C5-C4	-2.45	106.91	113.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3[A]	ADA	C1-O5-C5	2.43	116.45	112.17
2	C	2	ADA	O4-C4-C3	-2.34	104.93	110.35
2	C	2	ADA	C1-C2-C3	2.30	112.50	109.67
2	D	1[A]	ADA	O3-C3-C4	2.30	115.66	110.35
2	D	2[A]	ADA	C6-C5-C4	2.27	118.72	113.04
2	D	1[A]	ADA	C1-C2-C3	-2.25	105.65	110.31
2	C	1	ADA	O3-C3-C4	2.06	115.12	110.35
2	C	2	ADA	C1-O5-C5	-2.01	108.62	112.17

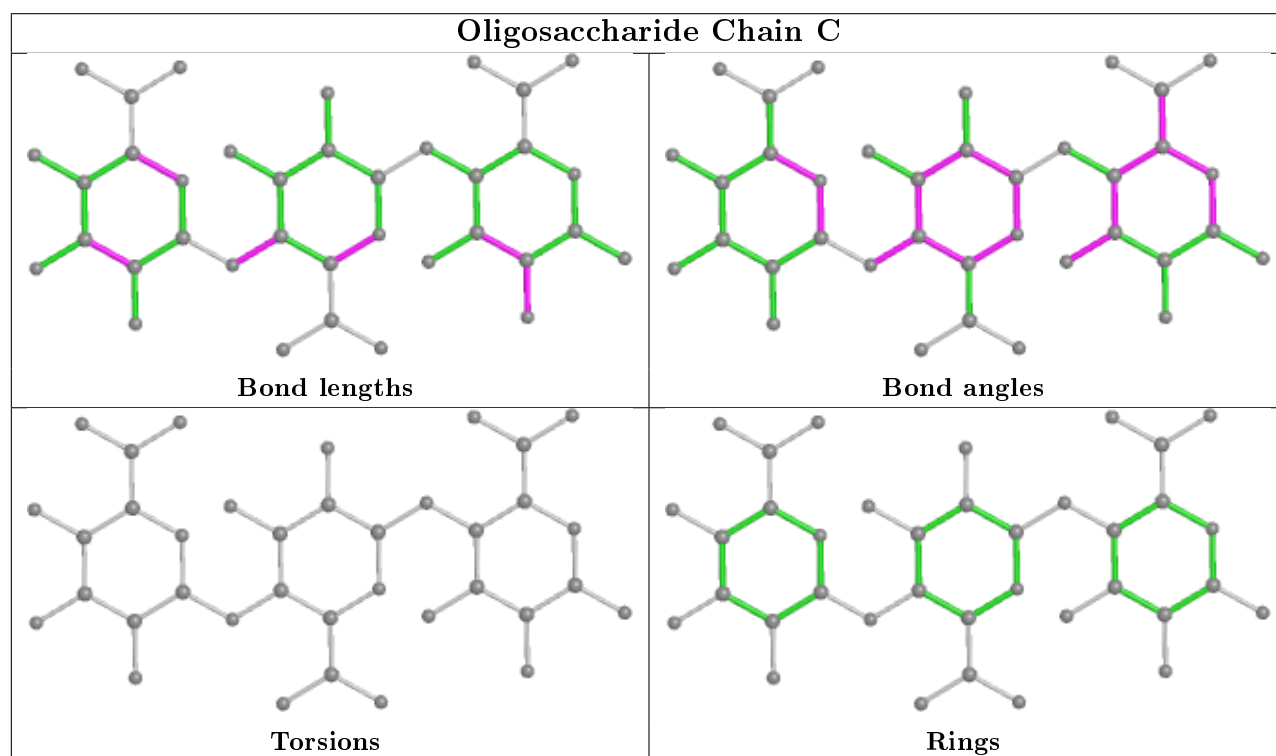
There are no chirality outliers.

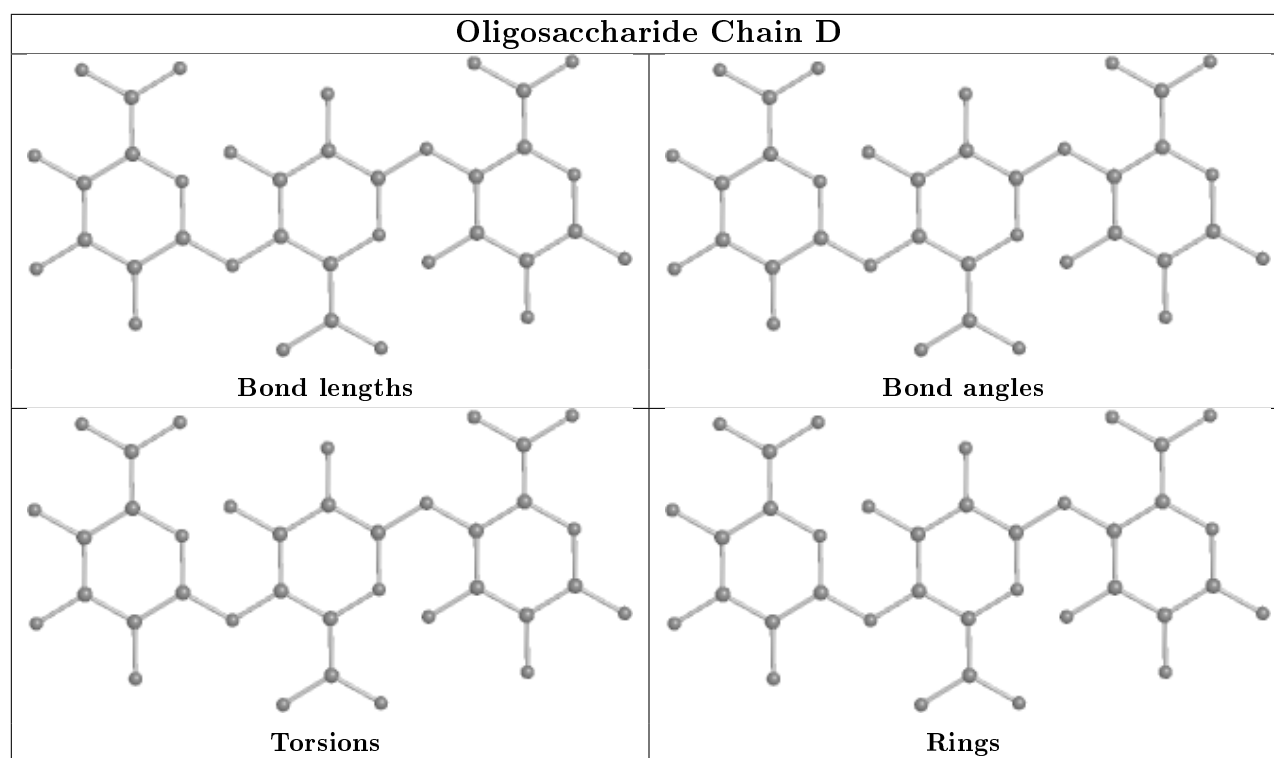
There are no torsion outliers.

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](#)

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	A	207	-	7,7,7	0.53	0	9,10,10	1.08	1 (11%)
5	MPD	B	201	-	7,7,7	0.55	0	9,10,10	0.84	0
4	IMD	B	206	-	3,5,5	0.44	0	4,5,5	0.94	0
9	ADA	B	214[B]	9,3	9,12,13	1.29	1 (11%)	12,17,19	0.88	1 (8%)
8	GTR	B	212[B]	9	10,13,13	0.84	0	15,19,19	1.55	1 (6%)
5	MPD	B	207	-	7,7,7	0.91	1 (14%)	9,10,10	1.69	2 (22%)
6	MRD	A	209	-	7,7,7	0.56	0	9,10,10	1.11	0
5	MPD	A	206	-	7,7,7	0.88	0	9,10,10	2.15	1 (11%)
9	ADA	B	213[B]	9,8,3	9,12,13	1.01	0	12,17,19	1.74	4 (33%)
4	IMD	A	205	-	3,5,5	0.24	0	4,5,5	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MRD	A	208	-	7,7,7	0.39	0	9,10,10	0.87	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	A	207	-	-	0/5/5/5	-
5	MPD	B	201	-	-	1/5/5/5	-
4	IMD	B	206	-	-	-	0/1/1/1
9	ADA	B	214[B]	9,3	-	0/0/21/24	0/1/1/1
8	GTR	B	212[B]	9	-	0/0/24/24	0/1/1/1
5	MPD	B	207	-	-	0/5/5/5	-
6	MRD	A	209	-	-	0/5/5/5	-
5	MPD	A	206	-	-	0/5/5/5	-
9	ADA	B	213[B]	9,8,3	-	0/0/21/24	0/1/1/1
4	IMD	A	205	-	-	-	0/1/1/1
6	MRD	A	208	-	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	214[B]	ADA	O5-C5	3.19	1.47	1.43
5	B	207	MPD	C3-C2	-2.09	1.48	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	206	MPD	CM-C2-C1	-5.82	98.44	110.57
8	B	212[B]	GTR	C1-O5-C5	-4.76	105.21	112.31
9	B	213[B]	ADA	C1-O5-C5	-3.50	106.00	112.17
5	B	207	MPD	O2-C2-C1	3.32	118.73	108.08
5	B	207	MPD	C5-C4-C3	-3.31	96.10	111.69
9	B	213[B]	ADA	O4-C4-C5	3.13	116.03	110.05
9	B	213[B]	ADA	C1-C2-C3	2.35	112.55	109.67
5	A	207	MPD	CM-C2-C1	-2.24	105.90	110.57
9	B	214[B]	ADA	C6-C5-C4	-2.02	107.99	113.04
9	B	213[B]	ADA	O4-C4-C3	-2.00	105.72	110.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	201	MPD	2	0
4	B	206	IMD	4	0
8	B	212[B]	GTR	1	0
5	B	207	MPD	1	0
6	A	209	MRD	8	0
4	A	205	IMD	2	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%)	-0.60	2 (1%) 82 73	9, 12, 27, 57	3 (1%)
1	B	195/204 (95%)	-0.63	1 (0%) 91 85	8, 14, 27, 48	0
All	All	393/408 (96%)	-0.62	3 (0%) 86 79	8, 13, 27, 57	3 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	HIS	5.0
1	A	-2	VAL	4.6
1	B	0	THR	2.4

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

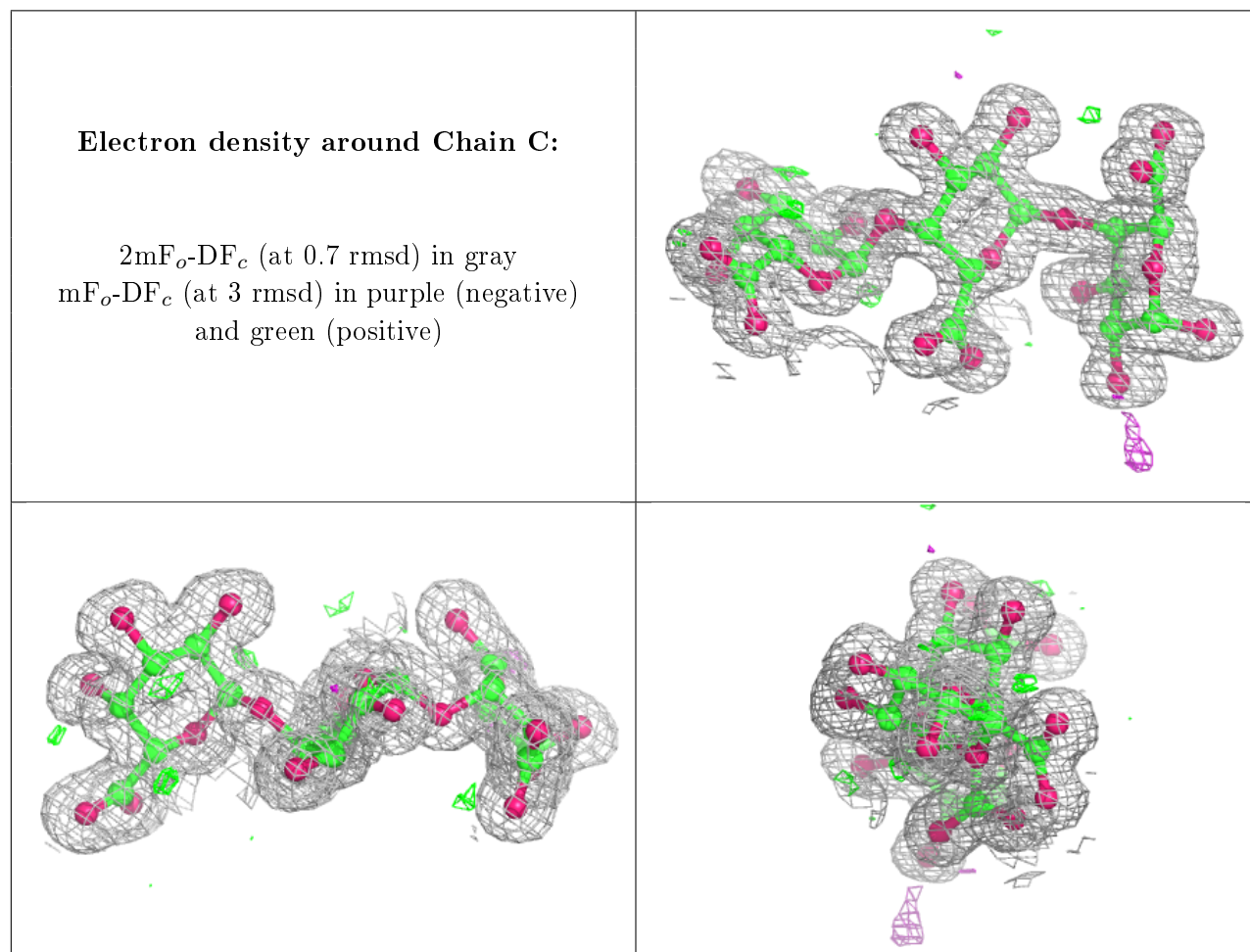
There are no non-standard protein/DNA/RNA residues in this entry.

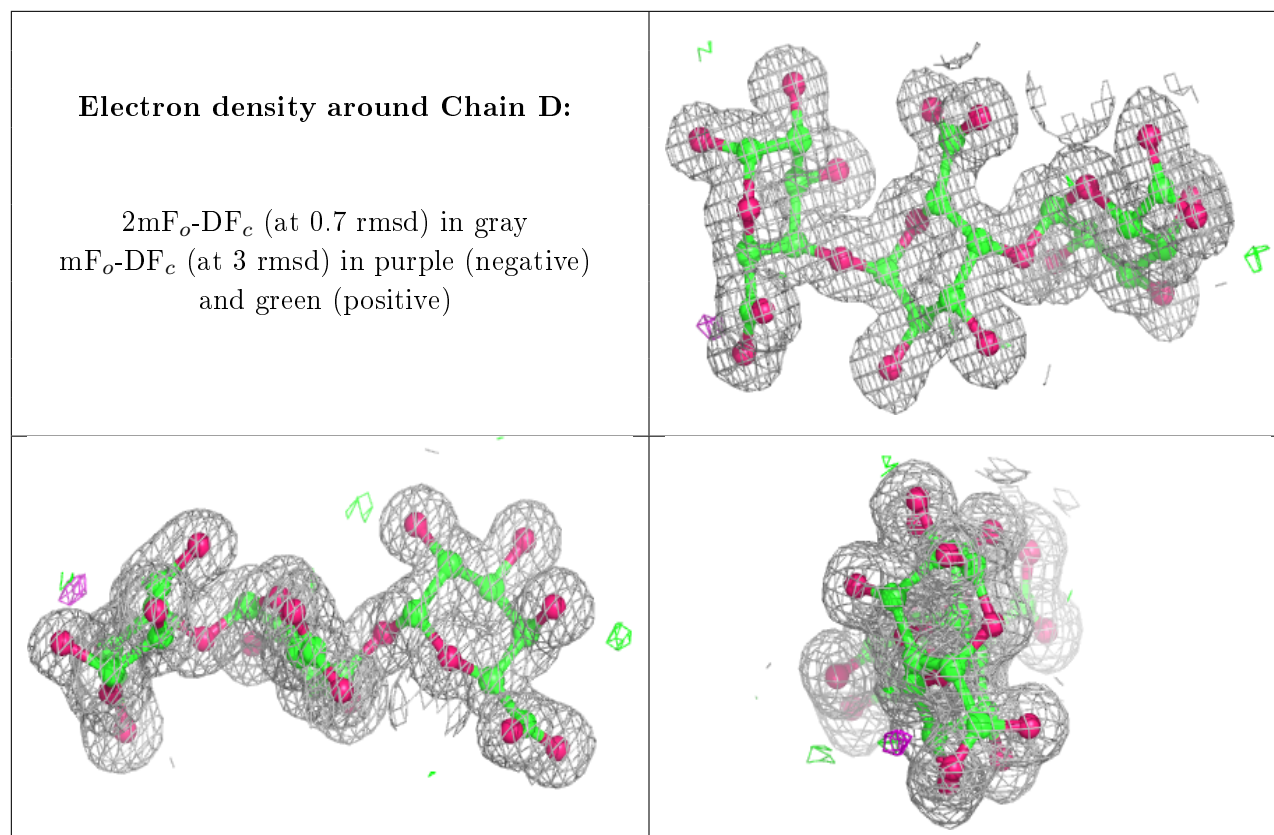
6.3 Carbohydrates [i](#)

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	ADA	C	1	13/13	0.98	0.06	15,18,24,27	0
2	ADA	C	2	12/13	0.98	0.04	11,13,16,16	0
2	ADA	C	3	12/13	0.98	0.05	11,12,18,18	0
2	ADA	D	3[A]	12/13	0.99	0.04	9,10,13,15	12
2	ADA	D	2[A]	12/13	0.99	0.04	9,10,11,11	12
2	ADA	D	1[A]	13/13	0.99	0.04	11,13,15,16	13

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





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	IMD	A	205	5/5	0.80	0.22	25,29,43,51	5
6	MRD	A	209	8/8	0.87	0.16	16,23,25,27	8
5	MPD	B	207	8/8	0.87	0.17	16,27,32,41	8
4	IMD	B	206	5/5	0.89	0.10	43,50,59,65	5
5	MPD	B	201	8/8	0.89	0.16	30,40,63,70	0
5	MPD	A	207	8/8	0.93	0.09	26,37,46,49	0
5	MPD	A	206	8/8	0.93	0.11	28,36,54,95	0
6	MRD	A	208	8/8	0.95	0.09	22,24,34,37	0
8	GTR	B	212[B]	13/13	0.99	0.04	23,27,32,32	13
9	ADA	B	214[B]	12/13	0.99	0.04	16,18,21,21	12
9	ADA	B	213[B]	12/13	0.99	0.04	17,19,25,29	12
3	CA	B	204	1/1	1.00	0.06	11,11,11,11	0
3	CA	A	202	1/1	1.00	0.04	12,12,12,12	0
3	CA	B	205	1/1	1.00	0.03	11,11,11,11	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	B	202	1/1	1.00	0.03	13,13,13,13	1
7	CL	B	208	1/1	1.00	0.03	14,14,14,14	0
7	CL	A	210	1/1	1.00	0.03	16,16,16,16	1
3	CA	A	201	1/1	1.00	0.06	16,16,16,16	1
3	CA	A	204	1/1	1.00	0.03	11,11,11,11	0
3	CA	A	203	1/1	1.00	0.04	11,11,11,11	0
3	CA	B	203	1/1	1.00	0.04	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.