



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2022 – 06:42 PM JST

PDB ID : 7EXJ
Title : Crystal structure of alkaline alpha-galctosidase D383A mutant from *Arabidopsis thaliana* complexed with Raffinose
Authors : Chuankhayan, P.; Guan, H.H.; Lin, C.C.; Chen, N.C.; Huang, Y.C.; Yoshimura, M.; Nakagawa, A.; Lee, R.H.; Chen, C.J.
Deposited on : 2021-05-27
Resolution : 2.47 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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	:	2.31.3
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)	:	2.31.3

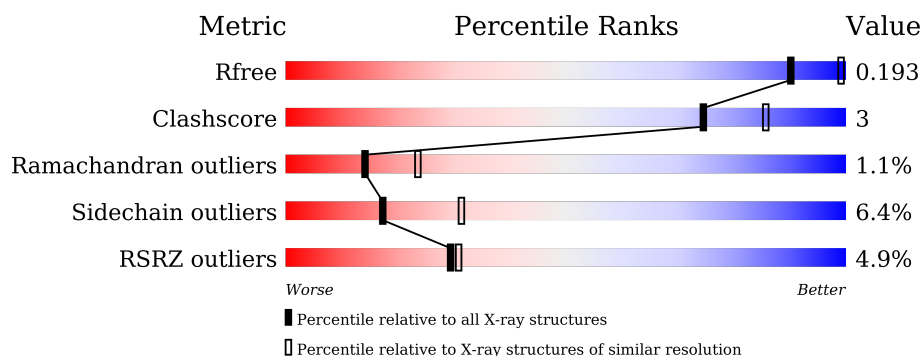
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 $\leq 5\%$. 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	749	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	749	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>
2	C	3	<div> <div>67%</div> <div>33%</div> </div>
2	D	3	<div> <div>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
2	FRU	C	1	X	-	-	-
2	GLC	C	2	X	-	-	-
2	GLA	C	3	X	-	-	-
2	FRU	D	1	X	-	-	-
2	GLC	D	2	X	-	-	-
2	GLA	D	3	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11324 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 Probable galactinol–sucrose galactosyltransferase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	718	Total	C	N	O	S	0	0	0
			5620	3573	969	1049	29			
1	A	718	Total	C	N	O	S	0	0	0
			5620	3573	969	1049	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	302	ARG	LYS	conflict	UNP Q8RX87
B	383	ALA	ASP	engineered mutation	UNP Q8RX87
A	302	ARG	LYS	conflict	UNP Q8RX87
A	383	ALA	ASP	engineered mutation	UNP Q8RX87

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranoside-(1-2)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			34	18	16			
2	D	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	9	Total	O	0	0
			9	9		

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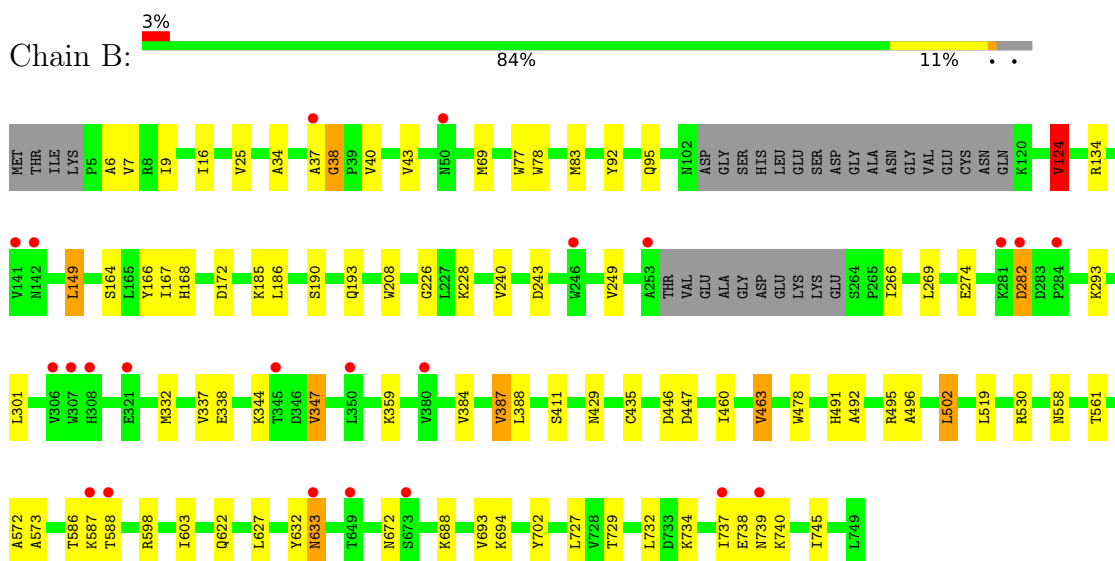
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		

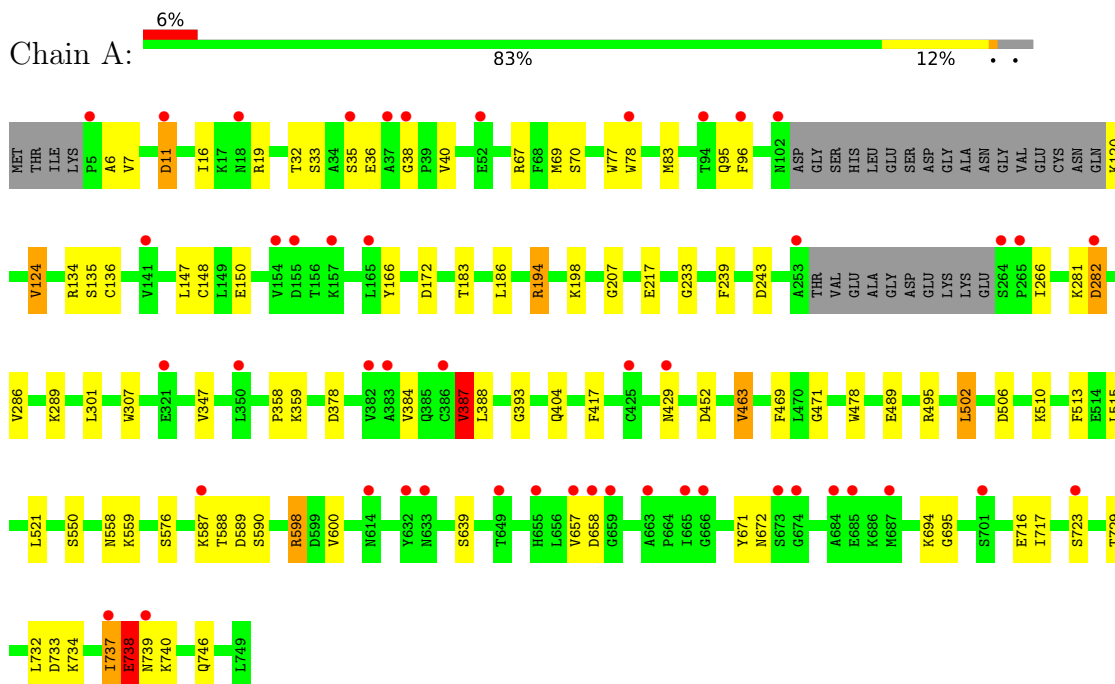
3 Residue-property plots

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: Probable galactinol–sucrose galactosyltransferase 6



- Molecule 1: Probable galactinol–sucrose galactosyltransferase 6



- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain C:  67% 33%

FRU1
GLC2
GLA3

- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain D:  100%

FRU1
GLC2
GLA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.60Å 103.30Å 181.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.47 29.95 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.47) 99.3 (29.95-2.47)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.191 , 0.249 0.199 , 0.193	Depositor DCC
R_{free} test set	3138 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11324	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: GLC, GLA, FRU

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	0.61	0/5754	0.81	6/7793 (0.1%)
1	B	0.71	0/5754	0.87	4/7793 (0.1%)
All	All	0.66	0/11508	0.84	10/15586 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	B	447	ASP	CB-CG-OD1	7.04	124.64	118.30
1	B	149	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	124	VAL	CB-CA-C	-5.73	100.52	111.40
1	A	194	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	172	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	598	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	124	VAL	CB-CA-C	-5.16	101.59	111.40
1	A	387	VAL	CB-CA-C	-5.09	101.73	111.40
1	A	506	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ASP	Peptide
1	B	34	ALA	Peptide
1	B	740	LYS	Peptide

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	5620	0	5539	33	0
1	B	5620	0	5539	38	0
2	C	34	0	28	1	0
2	D	34	0	29	1	0
3	A	7	0	0	0	0
3	B	9	0	0	0	0
All	All	11324	0	11135	72	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 3.

All (72) 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:95:GLN:HE22	1:B:429:ASN:HA	1.49	0.76
1:A:558:ASN:HD21	1:A:672:ASN:HD21	1.33	0.75
1:B:558:ASN:HD21	1:B:672:ASN:HD21	1.37	0.72
1:B:627:LEU:HD21	1:B:702:TYR:HB2	1.76	0.67
1:B:95:GLN:HE21	1:B:134:ARG:HH21	1.47	0.62
1:B:492:ALA:HB1	1:B:519:LEU:HD11	1.84	0.60
1:B:738:GLU:HB3	1:B:739:ASN:C	2.23	0.59
1:A:737:ILE:O	1:A:738:GLU:HB2	2.02	0.58
1:A:7:VAL:HG13	1:A:16:ILE:CD1	2.33	0.58
1:A:95:GLN:HE21	1:A:134:ARG:HH21	1.50	0.58
1:B:463:VAL:HG13	1:B:478:TRP:CE2	2.40	0.56
1:A:307:TRP:HE1	2:C:3:GLA:H4	1.71	0.55
1:B:693:VAL:HG21	1:B:745:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:TYR:O	1:B:633:ASN:HB2	2.08	0.54
1:B:495:ARG:HB3	1:B:502:LEU:HD22	1.90	0.54
1:A:738:GLU:HB3	1:A:740:LYS:N	2.24	0.53
1:A:95:GLN:HE22	1:A:429:ASN:HA	1.74	0.53
1:A:495:ARG:HB3	1:A:502:LEU:HD22	1.89	0.52
1:A:384:VAL:O	1:A:387:VAL:HG22	2.10	0.51
2:D:1:FRU:H61	2:D:2:GLC:H62	1.92	0.51
1:A:233:GLY:HA3	1:A:513:PHE:CE1	2.45	0.51
1:B:496:ALA:HB2	1:B:519:LEU:CD2	2.41	0.50
1:A:266:ILE:HD12	1:A:347:VAL:HG12	1.92	0.50
1:B:502:LEU:HD21	1:B:519:LEU:HD22	1.94	0.50
1:A:95:GLN:HE21	1:A:134:ARG:NH2	2.11	0.49
1:B:95:GLN:HE21	1:B:134:ARG:NH2	2.10	0.49
1:B:7:VAL:HG22	1:B:16:ILE:HD12	1.94	0.49
1:B:693:VAL:CG2	1:B:745:ILE:HD12	2.43	0.49
1:A:77:TRP:HB2	1:A:78:TRP:CD1	2.49	0.48
1:A:358:PRO:HB3	1:A:404:GLN:OE1	2.14	0.48
1:B:384:VAL:HG12	1:B:387:VAL:HG22	1.96	0.47
1:A:96:PHE:HB3	1:A:469:PHE:CE2	2.50	0.47
1:A:558:ASN:ND2	1:A:672:ASN:HD21	2.08	0.47
1:A:40:VAL:HG21	1:A:183:THR:CG2	2.46	0.46
1:B:737:ILE:O	1:B:738:GLU:HB2	2.17	0.45
1:B:124:VAL:O	1:B:167:ILE:HA	2.17	0.45
1:B:266:ILE:HD12	1:B:347:VAL:HG12	1.98	0.45
1:B:572:ALA:O	1:B:573:ALA:HB2	2.17	0.45
1:A:489:GLU:OE1	1:A:671:TYR:OH	2.36	0.44
1:B:7:VAL:HG13	1:B:16:ILE:CD1	2.47	0.44
1:A:96:PHE:HB3	1:A:469:PHE:CD2	2.52	0.44
1:A:194:ARG:HD3	1:A:471:GLY:O	2.19	0.43
1:B:77:TRP:HB2	1:B:78:TRP:CD1	2.54	0.43
1:A:134:ARG:NH1	1:A:136:CYS:SG	2.92	0.43
1:B:332:MET:HB3	1:B:337:VAL:HG21	2.01	0.43
1:A:286:VAL:HG13	1:A:289:LYS:HE2	2.01	0.43
1:A:521:LEU:HD13	1:A:695:GLY:HA2	2.01	0.43
1:B:37:ALA:N	1:B:38:GLY:HA2	2.34	0.43
1:B:190:SER:O	1:B:435:CYS:HA	2.18	0.43
1:A:378:ASP:O	1:A:417:PHE:HB3	2.19	0.42
1:B:738:GLU:HG3	1:B:739:ASN:HB2	2.02	0.42
1:B:491:HIS:O	1:B:495:ARG:HG2	2.20	0.42
1:B:491:HIS:HD1	1:B:495:ARG:HH12	1.67	0.42
1:A:40:VAL:HG21	1:A:183:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ILE:HD13	1:B:25:VAL:HG11	2.02	0.42
1:A:135:SER:HB3	1:A:147:LEU:HD11	2.00	0.42
1:A:510:LYS:HA	1:A:510:LYS:HE2	2.02	0.42
1:B:627:LEU:HD22	1:B:727:LEU:HD13	2.00	0.42
1:A:463:VAL:HG22	1:A:478:TRP:CD1	2.55	0.41
1:B:208:TRP:O	1:B:240:VAL:HA	2.21	0.41
1:A:166:TYR:CZ	1:A:183:THR:HG21	2.56	0.41
1:A:281:LYS:O	1:A:282:ASP:CB	2.68	0.41
1:B:172:ASP:OD1	1:B:172:ASP:C	2.59	0.41
1:B:185:LYS:NZ	1:B:193:GLN:HE21	2.19	0.41
1:B:92:TYR:CE1	1:B:338:GLU:HG2	2.56	0.41
1:B:92:TYR:CD1	1:B:338:GLU:HG2	2.56	0.40
1:B:208:TRP:CH2	1:B:226:GLY:HA3	2.56	0.40
1:B:249:VAL:HG12	1:B:269:LEU:HA	2.02	0.40
1:A:207:GLY:HA3	1:A:239:PHE:CE2	2.56	0.40
1:A:281:LYS:O	1:A:282:ASP:HB2	2.22	0.40
1:B:166:TYR:CE1	1:B:168:HIS:HB2	2.57	0.40
1:A:717:ILE:O	1:A:717:ILE:HD12	2.22	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	712/749 (95%)	660 (93%)	43 (6%)	9 (1%)	12	19
1	B	712/749 (95%)	669 (94%)	37 (5%)	6 (1%)	19	33
All	All	1424/1498 (95%)	1329 (93%)	80 (6%)	15 (1%)	14	23

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	ALA
1	A	393	GLY
1	A	6	ALA
1	A	282	ASP
1	B	282	ASP
1	A	738	GLU
1	B	446	ASP
1	A	11	ASP
1	A	36	GLU
1	A	38	GLY
1	B	347	VAL
1	B	603	ILE
1	B	38	GLY
1	A	657	VAL
1	A	600	VAL

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	614/640 (96%)	569 (93%)	45 (7%)	14	25
1	B	614/640 (96%)	580 (94%)	34 (6%)	21	39
All	All	1228/1280 (96%)	1149 (94%)	79 (6%)	17	31

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	40	VAL
1	B	43	VAL
1	B	69	MET
1	B	83	MET
1	B	124	VAL
1	B	149	LEU
1	B	164	SER
1	B	186	LEU
1	B	228	LYS

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Mol	Chain	Res	Type
1	B	243	ASP
1	B	274	GLU
1	B	282	ASP
1	B	293	LYS
1	B	301	LEU
1	B	344	LYS
1	B	359	LYS
1	B	387	VAL
1	B	388	LEU
1	B	411	SER
1	B	460	ILE
1	B	463	VAL
1	B	502	LEU
1	B	561	THR
1	B	586	THR
1	B	587	LYS
1	B	588	THR
1	B	598	ARG
1	B	622	GLN
1	B	633	ASN
1	B	688	LYS
1	B	694	LYS
1	B	729	THR
1	B	732	LEU
1	B	734	LYS
1	A	19	ARG
1	A	32	THR
1	A	33	SER
1	A	35	SER
1	A	67	ARG
1	A	69	MET
1	A	70	SER
1	A	83	MET
1	A	120	LYS
1	A	124	VAL
1	A	148	CYS
1	A	150	GLU
1	A	186	LEU
1	A	198	LYS
1	A	217	GLU
1	A	243	ASP
1	A	301	LEU

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Mol	Chain	Res	Type
1	A	359	LYS
1	A	387	VAL
1	A	388	LEU
1	A	452	ASP
1	A	463	VAL
1	A	502	LEU
1	A	515	LEU
1	A	550	SER
1	A	559	LYS
1	A	576	SER
1	A	587	LYS
1	A	588	THR
1	A	589	ASP
1	A	590	SER
1	A	598	ARG
1	A	639	SER
1	A	658	ASP
1	A	694	LYS
1	A	716	GLU
1	A	723	SER
1	A	729	THR
1	A	732	LEU
1	A	733	ASP
1	A	734	LYS
1	A	737	ILE
1	A	738	GLU
1	A	739	ASN
1	A	746	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	65	ASN
1	B	95	GLN
1	B	138	GLN
1	B	175	GLN
1	B	193	GLN
1	B	385	GLN
1	B	406	HIS
1	B	456	HIS
1	B	475	GLN
1	B	558	ASN

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Mol	Chain	Res	Type
1	A	95	GLN
1	A	193	GLN
1	A	385	GLN
1	A	406	HIS
1	A	456	HIS
1	A	475	GLN
1	A	558	ASN
1	A	743	HIS

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	FRU	C	1	2	11,12,12	4.04	8 (72%)	10,18,18	0.98	0
2	GLC	C	2	2	11,11,12	3.04	6 (54%)	15,15,17	1.93	3 (20%)
2	GLA	C	3	2	11,11,12	2.37	2 (18%)	15,15,17	3.39	7 (46%)
2	FRU	D	1	2	11,12,12	4.22	8 (72%)	10,18,18	1.23	2 (20%)
2	GLC	D	2	2	11,11,12	3.24	6 (54%)	15,15,17	2.49	5 (33%)
2	GLA	D	3	2	11,11,12	2.14	2 (18%)	15,15,17	2.21	7 (46%)

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	FRU	C	1	2	1/1/4/4	3/5/24/24	0/1/1/1
2	GLC	C	2	2	1/1/4/5	1/2/19/22	0/1/1/1
2	GLA	C	3	2	3/3/4/5	0/2/19/22	0/1/1/1
2	FRU	D	1	2	1/1/4/4	1/5/24/24	0/1/1/1
2	GLC	D	2	2	1/1/4/5	2/2/19/22	0/1/1/1
2	GLA	D	3	2	3/3/4/5	0/2/19/22	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	C2-C3	-6.90	1.42	1.52
2	D	1	FRU	C4-C5	6.29	1.69	1.53
2	C	1	FRU	C4-C3	-5.93	1.27	1.52
2	D	1	FRU	C4-C3	-5.84	1.28	1.52
2	D	1	FRU	O5-C2	5.83	1.52	1.43
2	C	2	GLC	C2-C3	-5.71	1.44	1.52
2	C	1	FRU	C4-C5	5.70	1.67	1.53
2	D	1	FRU	C1-C2	-5.68	1.43	1.52
2	C	2	GLC	O5-C5	5.45	1.54	1.43
2	C	1	FRU	O5-C2	5.43	1.51	1.43
2	C	3	GLA	O5-C1	5.13	1.51	1.43
2	D	3	GLA	C2-C3	-5.11	1.45	1.52
2	C	1	FRU	C1-C2	-5.11	1.44	1.52
2	D	2	GLC	O5-C5	4.99	1.53	1.43
2	C	3	GLA	C2-C3	-4.92	1.45	1.52
2	D	1	FRU	O5-C5	-4.65	1.33	1.43
2	C	1	FRU	O2-C2	4.17	1.47	1.40
2	C	1	FRU	O5-C5	-4.15	1.34	1.43
2	C	2	GLC	O3-C3	3.89	1.52	1.43
2	D	3	GLA	O5-C1	3.87	1.49	1.43
2	D	2	GLC	O5-C1	3.71	1.49	1.43
2	C	1	FRU	O3-C3	3.45	1.49	1.42
2	D	1	FRU	O4-C4	3.43	1.51	1.43
2	D	2	GLC	O3-C3	3.32	1.50	1.43
2	D	1	FRU	O3-C3	3.27	1.49	1.42
2	D	1	FRU	O2-C2	3.17	1.46	1.40
2	D	2	GLC	O2-C2	3.04	1.49	1.43
2	C	2	GLC	C4-C5	3.03	1.59	1.53
2	C	1	FRU	O4-C4	2.88	1.49	1.43
2	C	2	GLC	O2-C2	2.87	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	C4-C5	2.58	1.58	1.53
2	C	2	GLC	O5-C1	2.46	1.47	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	GLA	C1-C2-C3	9.45	121.29	109.67
2	D	2	GLC	C1-O5-C5	5.46	119.59	112.19
2	D	2	GLC	O5-C1-C2	4.63	117.92	110.77
2	C	3	GLA	O2-C2-C1	4.44	118.23	109.15
2	D	3	GLA	O3-C3-C2	-4.35	101.67	109.99
2	C	3	GLA	O3-C3-C2	-4.15	102.06	109.99
2	C	2	GLC	C1-O5-C5	4.07	117.71	112.19
2	C	2	GLC	C3-C4-C5	4.02	117.40	110.24
2	D	3	GLA	C1-C2-C3	3.86	114.42	109.67
2	D	2	GLC	C3-C4-C5	3.86	117.13	110.24
2	C	3	GLA	O2-C2-C3	-3.65	102.82	110.14
2	D	2	GLC	O5-C5-C6	3.58	112.81	107.20
2	D	3	GLA	O5-C1-C2	2.91	115.27	110.77
2	C	3	GLA	C2-C3-C4	2.85	115.82	110.89
2	D	3	GLA	C1-O5-C5	2.82	116.01	112.19
2	C	3	GLA	O4-C4-C3	-2.52	104.53	110.35
2	D	3	GLA	O5-C5-C4	-2.50	104.74	110.83
2	C	2	GLC	C6-C5-C4	2.42	118.67	113.00
2	D	3	GLA	C2-C3-C4	2.39	115.03	110.89
2	D	1	FRU	O4-C4-C5	2.19	117.38	111.05
2	D	2	GLC	O6-C6-C5	-2.11	104.07	111.29
2	D	1	FRU	C5-C4-C3	2.06	108.51	101.91
2	C	3	GLA	O4-C4-C5	2.05	114.38	109.30
2	D	3	GLA	O2-C2-C3	-2.02	106.10	110.14

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	FRU	C4
2	C	2	GLC	C5
2	C	3	GLA	C2
2	C	3	GLA	C3
2	C	3	GLA	C4
2	D	1	FRU	C4
2	D	2	GLC	C5
2	D	3	GLA	C2

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Mol	Chain	Res	Type	Atom
2	D	3	GLA	C3
2	D	3	GLA	C4

All (7) torsion outliers are listed below:

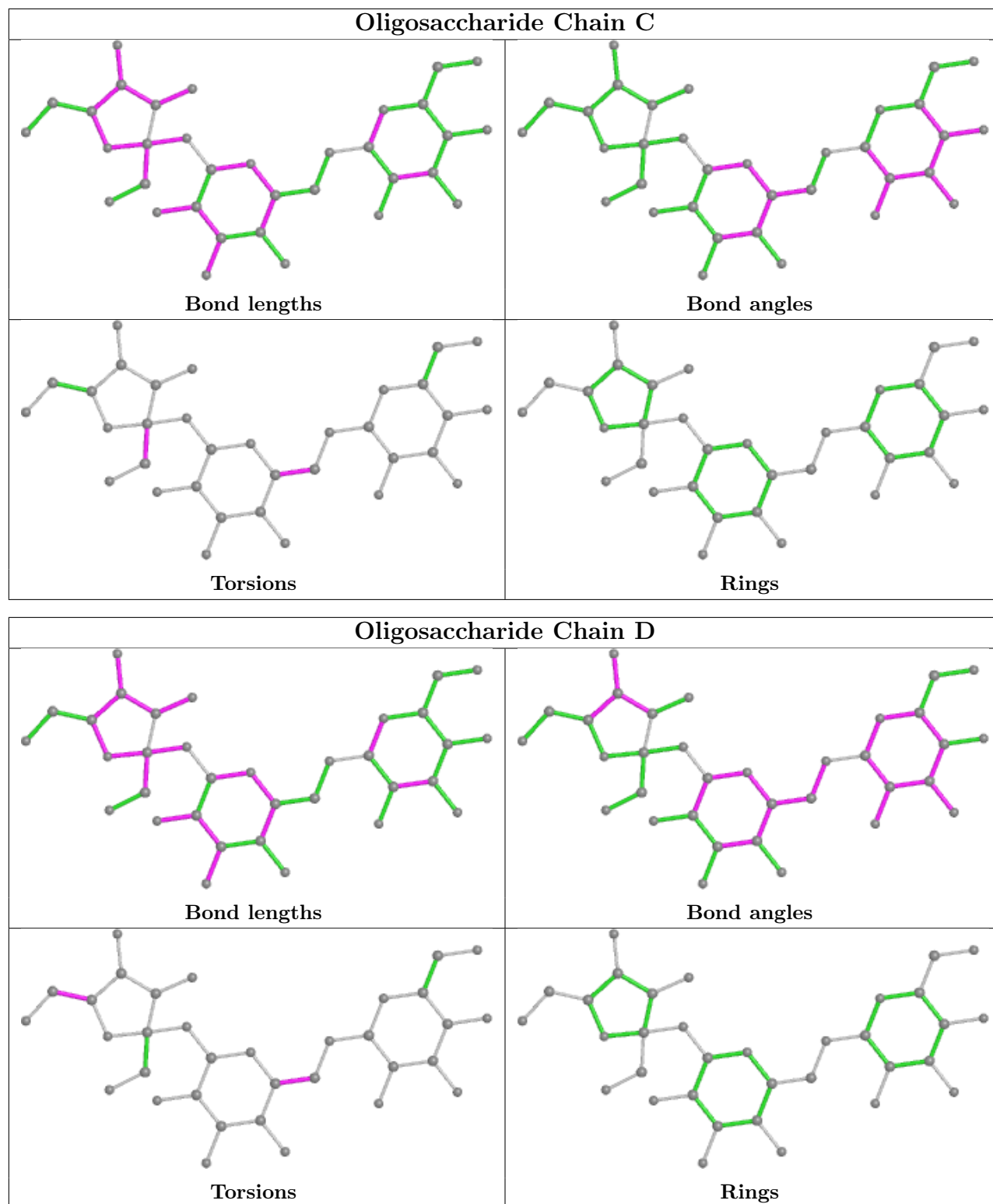
Mol	Chain	Res	Type	Atoms
2	C	1	FRU	O1-C1-C2-C3
2	C	1	FRU	O1-C1-C2-O2
2	C	1	FRU	O1-C1-C2-O5
2	D	2	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	D	1	FRU	C4-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	FRU	1	0
2	C	3	GLA	1	0
2	D	2	GLC	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	718/749 (95%)	0.16	48 (6%)	17 17	48, 73, 111, 143	0
1	B	718/749 (95%)	-0.03	23 (3%)	47 50	40, 62, 94, 132	0
All	All	1436/1498 (95%)	0.07	71 (4%)	29 31	40, 68, 106, 143	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	739	ASN	6.2
1	B	253	ALA	4.9
1	A	37	ALA	4.9
1	A	141	VAL	4.6
1	A	658	ASP	4.5
1	B	281	LYS	4.4
1	B	282	ASP	4.2
1	A	18	ASN	4.2
1	A	154	VAL	3.9
1	A	587	LYS	3.9
1	A	632	TYR	3.7
1	A	665	ILE	3.6
1	A	102	ASN	3.6
1	B	142	ASN	3.5
1	B	588	THR	3.5
1	A	321	GLU	3.5
1	A	425	CYS	3.4
1	A	350	LEU	3.3
1	B	284	PRO	3.3
1	B	380	VAL	3.2
1	A	685	GLU	3.2
1	B	141	VAL	3.2
1	A	674	GLY	3.2
1	B	739	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	666	GLY	3.1
1	A	52	GLU	3.1
1	A	684	ALA	3.0
1	A	659	GLY	3.0
1	A	265	PRO	2.9
1	A	383	ALA	2.9
1	B	737	ILE	2.9
1	A	657	VAL	2.9
1	A	5	PRO	2.9
1	B	321	GLU	2.8
1	B	306	VAL	2.8
1	A	157	LYS	2.8
1	B	587	LYS	2.8
1	B	633	ASN	2.8
1	A	649	THR	2.7
1	A	687	MET	2.7
1	A	35	SER	2.7
1	A	155	ASP	2.6
1	A	673	SER	2.6
1	A	253	ALA	2.5
1	A	165	LEU	2.5
1	A	382	VAL	2.5
1	A	655	HIS	2.5
1	A	701	SER	2.4
1	A	78	TRP	2.4
1	B	307	TRP	2.4
1	A	282	ASP	2.4
1	A	264	SER	2.3
1	B	308	HIS	2.3
1	A	38	GLY	2.3
1	B	345	THR	2.3
1	A	723	SER	2.3
1	A	633	ASN	2.2
1	A	614	ASN	2.2
1	B	246	TRP	2.2
1	A	11	ASP	2.1
1	B	50	ASN	2.1
1	B	350	LEU	2.1
1	A	663	ALA	2.1
1	B	649	THR	2.1
1	A	94	THR	2.1
1	B	673	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	429	ASN	2.1
1	B	37	ALA	2.0
1	A	737	ILE	2.0
1	A	386	CYS	2.0
1	A	96	PHE	2.0

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](#)

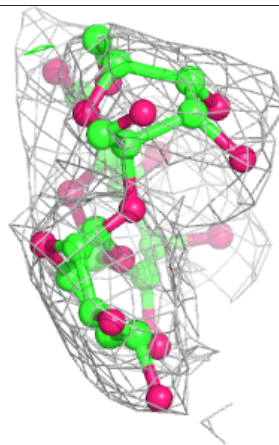
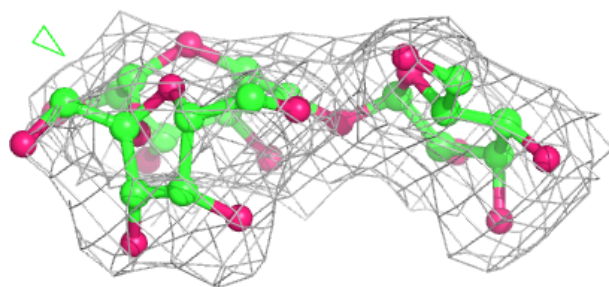
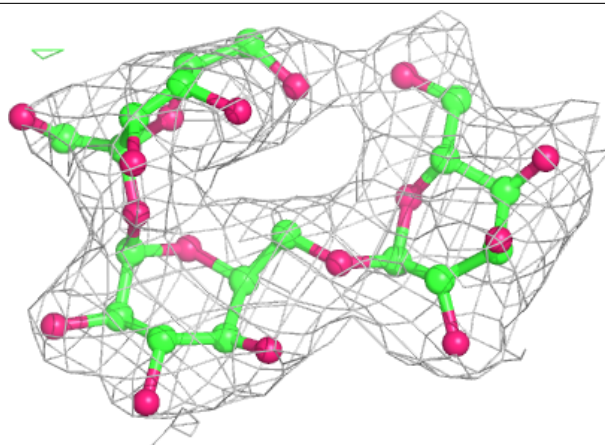
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

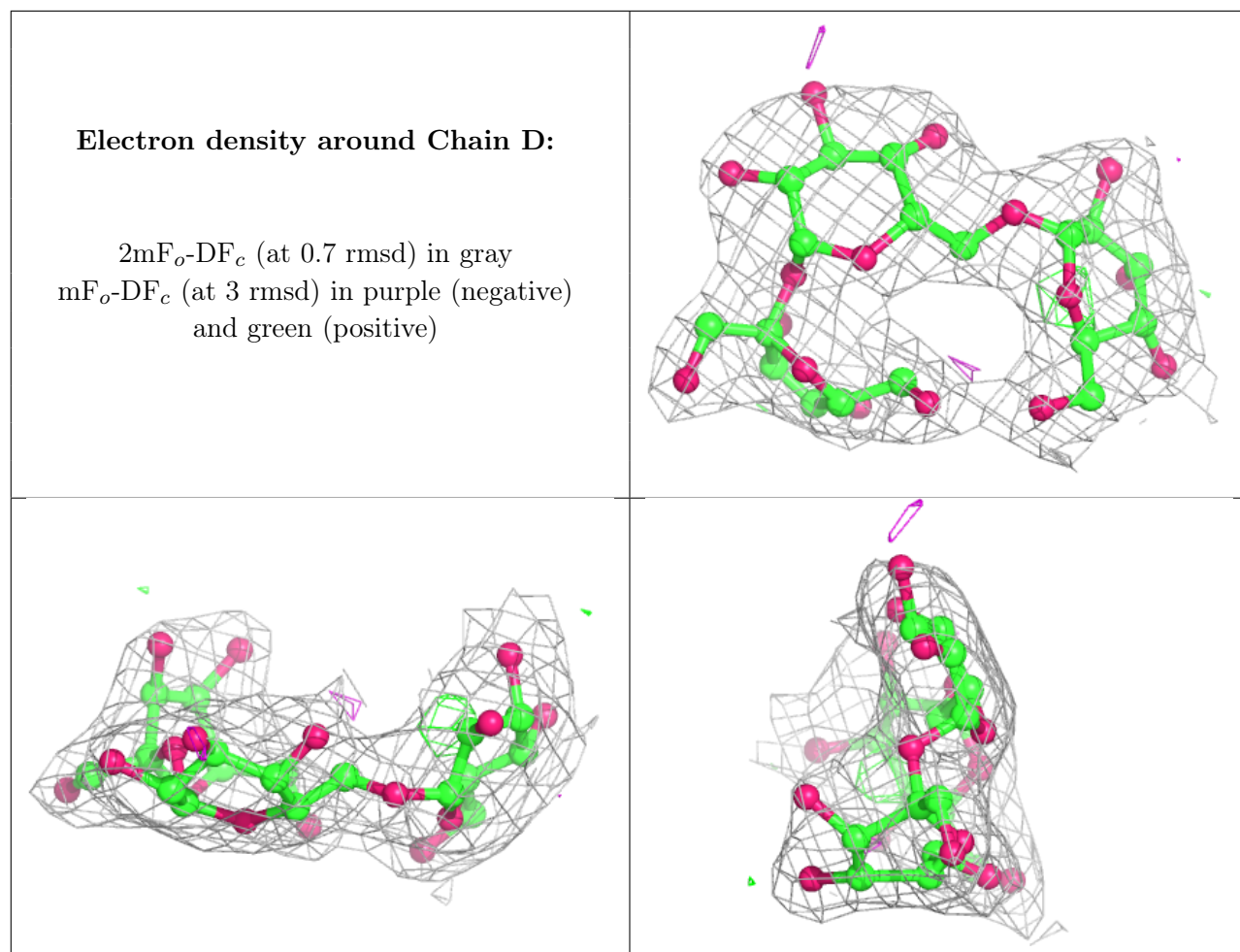
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FRU	C	1	12/12	0.87	0.17	79,99,111,114	0
2	GLC	C	2	11/12	0.88	0.16	76,86,104,110	0
2	FRU	D	1	12/12	0.93	0.15	53,69,73,75	0
2	GLA	D	3	11/12	0.96	0.21	51,56,63,85	0
2	GLC	D	2	11/12	0.97	0.10	51,61,65,67	0
2	GLA	C	3	11/12	0.97	0.23	52,59,63,66	0

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

Electron density around Chain C:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.