Full wwPDB X-ray Structure Validation Report ⓘ

Jun 29, 2025 – 08:33 am BST

PDB ID	:	9FHZ / pdb_00009fhz
Title	:	Bacteroides ovatus polysaccharide lyase family 38 (BoPL38) wild type in complex unsaturated guluronic acid tetramer at pH 3.5
Authors	:	Tandrup, T.; Wilkens, C.
Deposited on	:	2024-05-28
Resolution	:	1.88 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:

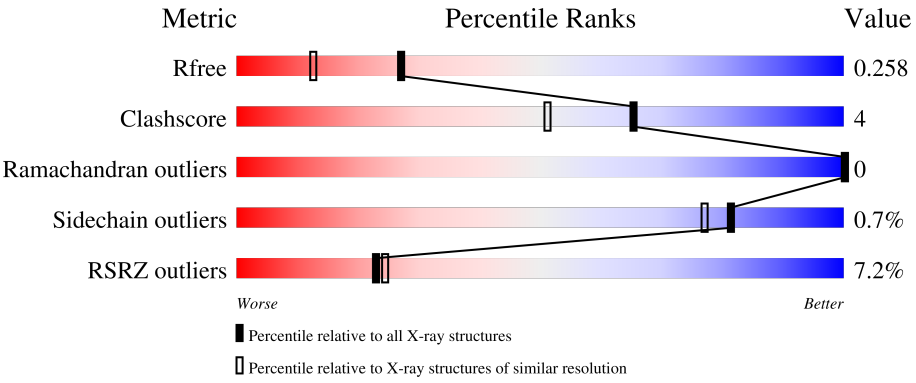
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 1.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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	404	4% 85% 9% 6%
1	B	404	7% 86% 8% 6%
1	C	404	7% 87% 6% 6%
1	D	404	10% 83% 11% 6%
2	E	3	67% 33%

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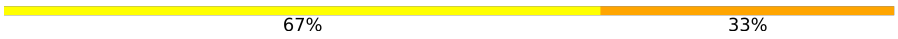
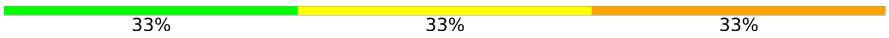
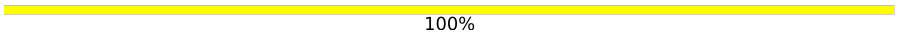
Mol	Chain	Length	Quality of chain
3	F	3	
3	G	3	
4	H	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12802 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 Alginate lyase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	1	0
			3054	1954	518	569	13			
1	B	380	Total	C	N	O	S	0	1	0
			3057	1955	517	572	13			
1	C	380	Total	C	N	O	S	0	0	0
			3052	1952	516	571	13			
1	D	380	Total	C	N	O	S	0	0	0
			3052	1952	516	571	13			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5M5BWR5
A	2	GLY	-	expression tag	UNP A0A5M5BWR5
A	3	SER	-	expression tag	UNP A0A5M5BWR5
A	4	SER	-	expression tag	UNP A0A5M5BWR5
A	5	HIS	-	expression tag	UNP A0A5M5BWR5
A	6	HIS	-	expression tag	UNP A0A5M5BWR5
A	7	HIS	-	expression tag	UNP A0A5M5BWR5
A	8	HIS	-	expression tag	UNP A0A5M5BWR5
A	9	HIS	-	expression tag	UNP A0A5M5BWR5
A	10	HIS	-	expression tag	UNP A0A5M5BWR5
A	11	SER	-	expression tag	UNP A0A5M5BWR5
A	12	SER	-	expression tag	UNP A0A5M5BWR5
A	13	GLY	-	expression tag	UNP A0A5M5BWR5
A	14	LEU	-	expression tag	UNP A0A5M5BWR5
A	15	VAL	-	expression tag	UNP A0A5M5BWR5
A	16	PRO	-	expression tag	UNP A0A5M5BWR5
A	17	ARG	-	expression tag	UNP A0A5M5BWR5
A	18	GLY	-	expression tag	UNP A0A5M5BWR5
A	19	SER	-	expression tag	UNP A0A5M5BWR5
A	20	HIS	-	expression tag	UNP A0A5M5BWR5
A	21	MET	-	expression tag	UNP A0A5M5BWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP A0A5M5BWR5
A	23	SER	-	expression tag	UNP A0A5M5BWR5
B	1	MET	-	initiating methionine	UNP A0A5M5BWR5
B	2	GLY	-	expression tag	UNP A0A5M5BWR5
B	3	SER	-	expression tag	UNP A0A5M5BWR5
B	4	SER	-	expression tag	UNP A0A5M5BWR5
B	5	HIS	-	expression tag	UNP A0A5M5BWR5
B	6	HIS	-	expression tag	UNP A0A5M5BWR5
B	7	HIS	-	expression tag	UNP A0A5M5BWR5
B	8	HIS	-	expression tag	UNP A0A5M5BWR5
B	9	HIS	-	expression tag	UNP A0A5M5BWR5
B	10	HIS	-	expression tag	UNP A0A5M5BWR5
B	11	SER	-	expression tag	UNP A0A5M5BWR5
B	12	SER	-	expression tag	UNP A0A5M5BWR5
B	13	GLY	-	expression tag	UNP A0A5M5BWR5
B	14	LEU	-	expression tag	UNP A0A5M5BWR5
B	15	VAL	-	expression tag	UNP A0A5M5BWR5
B	16	PRO	-	expression tag	UNP A0A5M5BWR5
B	17	ARG	-	expression tag	UNP A0A5M5BWR5
B	18	GLY	-	expression tag	UNP A0A5M5BWR5
B	19	SER	-	expression tag	UNP A0A5M5BWR5
B	20	HIS	-	expression tag	UNP A0A5M5BWR5
B	21	MET	-	expression tag	UNP A0A5M5BWR5
B	22	ALA	-	expression tag	UNP A0A5M5BWR5
B	23	SER	-	expression tag	UNP A0A5M5BWR5
C	1	MET	-	initiating methionine	UNP A0A5M5BWR5
C	2	GLY	-	expression tag	UNP A0A5M5BWR5
C	3	SER	-	expression tag	UNP A0A5M5BWR5
C	4	SER	-	expression tag	UNP A0A5M5BWR5
C	5	HIS	-	expression tag	UNP A0A5M5BWR5
C	6	HIS	-	expression tag	UNP A0A5M5BWR5
C	7	HIS	-	expression tag	UNP A0A5M5BWR5
C	8	HIS	-	expression tag	UNP A0A5M5BWR5
C	9	HIS	-	expression tag	UNP A0A5M5BWR5
C	10	HIS	-	expression tag	UNP A0A5M5BWR5
C	11	SER	-	expression tag	UNP A0A5M5BWR5
C	12	SER	-	expression tag	UNP A0A5M5BWR5
C	13	GLY	-	expression tag	UNP A0A5M5BWR5
C	14	LEU	-	expression tag	UNP A0A5M5BWR5
C	15	VAL	-	expression tag	UNP A0A5M5BWR5
C	16	PRO	-	expression tag	UNP A0A5M5BWR5
C	17	ARG	-	expression tag	UNP A0A5M5BWR5

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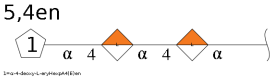
Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLY	-	expression tag	UNP A0A5M5BWR5
C	19	SER	-	expression tag	UNP A0A5M5BWR5
C	20	HIS	-	expression tag	UNP A0A5M5BWR5
C	21	MET	-	expression tag	UNP A0A5M5BWR5
C	22	ALA	-	expression tag	UNP A0A5M5BWR5
C	23	SER	-	expression tag	UNP A0A5M5BWR5
D	1	MET	-	initiating methionine	UNP A0A5M5BWR5
D	2	GLY	-	expression tag	UNP A0A5M5BWR5
D	3	SER	-	expression tag	UNP A0A5M5BWR5
D	4	SER	-	expression tag	UNP A0A5M5BWR5
D	5	HIS	-	expression tag	UNP A0A5M5BWR5
D	6	HIS	-	expression tag	UNP A0A5M5BWR5
D	7	HIS	-	expression tag	UNP A0A5M5BWR5
D	8	HIS	-	expression tag	UNP A0A5M5BWR5
D	9	HIS	-	expression tag	UNP A0A5M5BWR5
D	10	HIS	-	expression tag	UNP A0A5M5BWR5
D	11	SER	-	expression tag	UNP A0A5M5BWR5
D	12	SER	-	expression tag	UNP A0A5M5BWR5
D	13	GLY	-	expression tag	UNP A0A5M5BWR5
D	14	LEU	-	expression tag	UNP A0A5M5BWR5
D	15	VAL	-	expression tag	UNP A0A5M5BWR5
D	16	PRO	-	expression tag	UNP A0A5M5BWR5
D	17	ARG	-	expression tag	UNP A0A5M5BWR5
D	18	GLY	-	expression tag	UNP A0A5M5BWR5
D	19	SER	-	expression tag	UNP A0A5M5BWR5
D	20	HIS	-	expression tag	UNP A0A5M5BWR5
D	21	MET	-	expression tag	UNP A0A5M5BWR5
D	22	ALA	-	expression tag	UNP A0A5M5BWR5
D	23	SER	-	expression tag	UNP A0A5M5BWR5

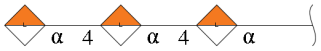
- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			36	18	18			

- Molecule 3 is an oligosaccharide called alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyr

anuronic acid-(1-4)-alpha-L-gulopyranuronic acid.

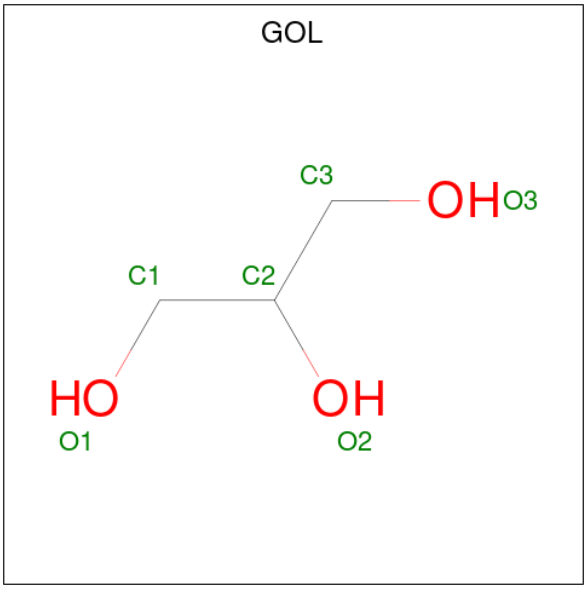


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	3	Total C O 37 18 19	0	0	0
3	G	3	Total C O 37 18 19	0	0	0

- Molecule 4 is an oligosaccharide called 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	H	2	Total C O 23 12 11	0	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 12 6 6	0	1

- Molecule 6 is water.

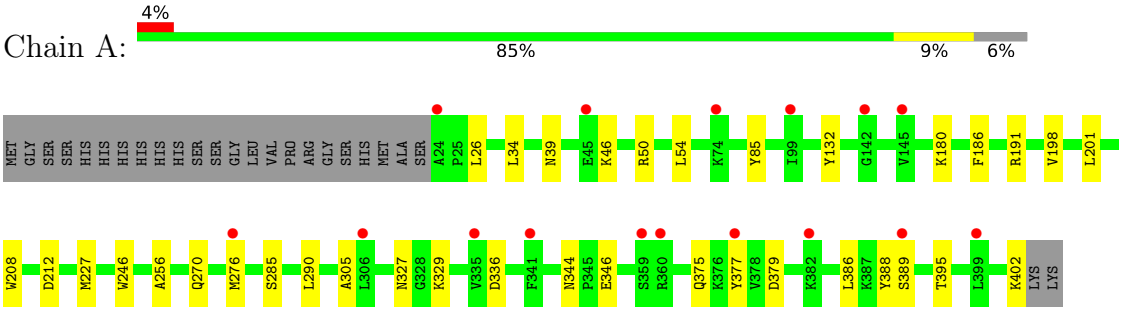
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	154	Total O 154 154	0	0
6	B	124	Total O 124 124	0	0
6	C	85	Total O 85 85	0	0
6	D	73	Total O 73 73	0	0

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.

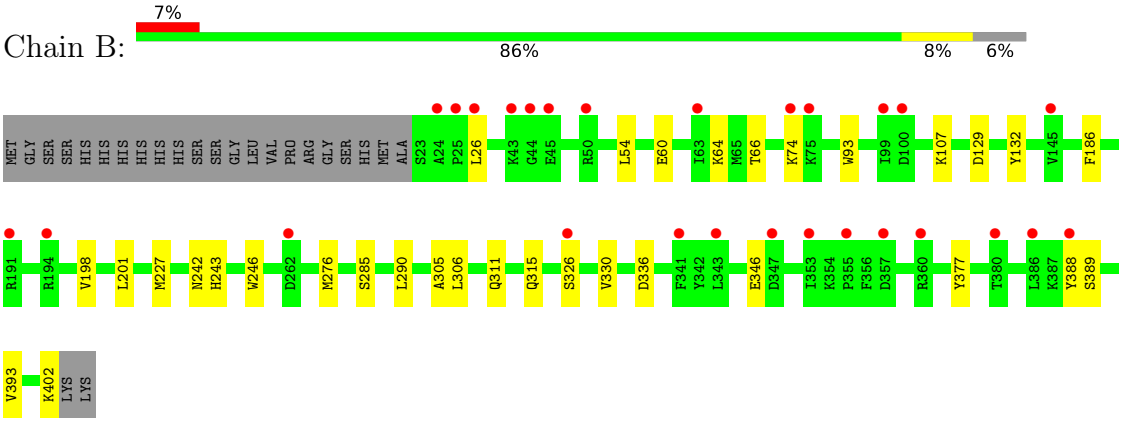
• Molecule 1: Alginate lyase family protein

Chain A:



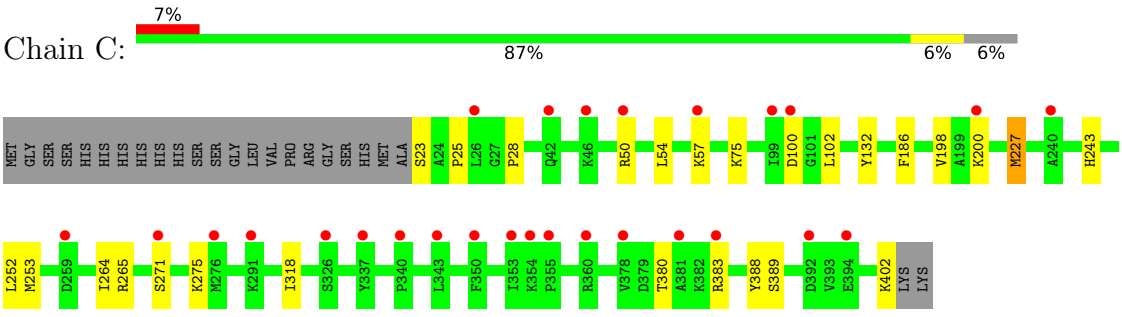
• Molecule 1: Alginate lyase family protein

Chain B:



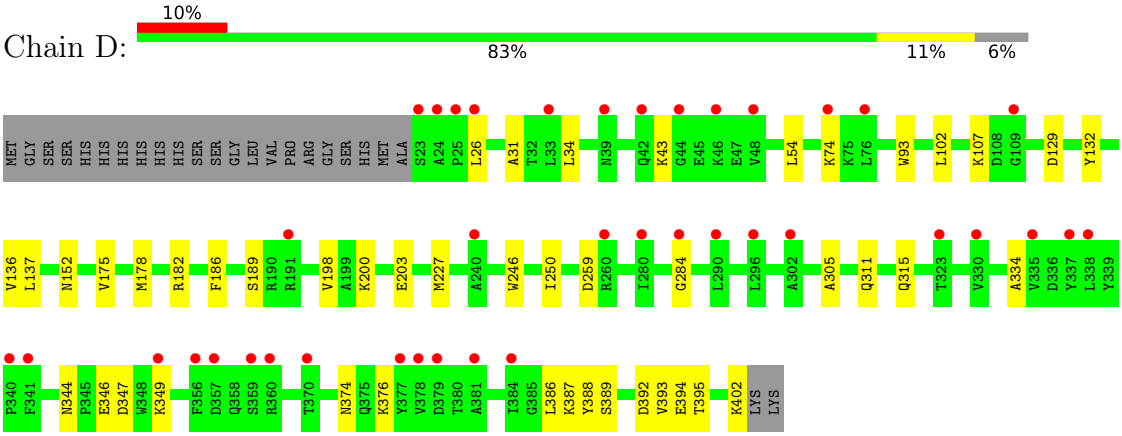
• Molecule 1: Alginate lyase family protein

Chain C:



• Molecule 1: Alginate lyase family protein

Chain D:



• Molecule 2: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid

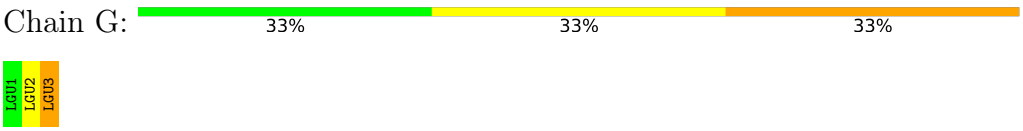
Chain E:

• Molecule 3: alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid

Chain F:

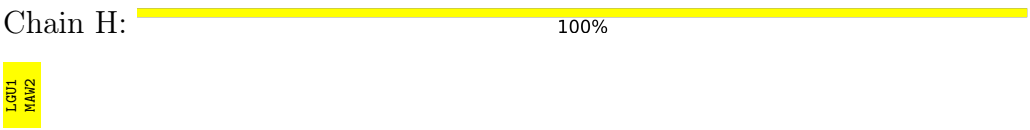
• Molecule 3: alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid

Chain G:



• Molecule 4: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	198.42Å 88.65Å 147.31Å 90.00° 120.42° 90.00°	Depositor
Resolution (Å)	52.94 – 1.88 52.94 – 1.88	Depositor EDS
% Data completeness (in resolution range)	92.5 (52.94-1.88) 92.6 (52.94-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.227 , 0.258 0.227 , 0.258	Depositor DCC
R_{free} test set	8926 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 27.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12802	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.36% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAW, GOL, LGU

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	0.38	0/3135	0.55	0/4248
1	B	0.36	0/3138	0.54	0/4253
1	C	0.36	0/3130	0.53	1/4242 (0.0%)
1	D	0.33	0/3130	0.53	0/4242
All	All	0.36	0/12533	0.54	1/16985 (0.0%)

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	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	227	MET	CB-CG-SD	-5.16	97.21	112.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	50	ARG	Sidechain

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	3054	0	3030	24	0
1	B	3057	0	3028	22	0
1	C	3052	0	3022	13	0
1	D	3052	0	3022	29	0
2	E	36	0	19	1	0
3	F	37	0	21	2	0
3	G	37	0	21	1	0
4	H	23	0	11	0	0
5	B	6	0	8	0	0
5	D	12	0	16	2	0
6	A	154	0	0	7	0
6	B	124	0	0	1	0
6	C	85	0	0	0	0
6	D	73	0	0	1	0
All	All	12802	0	12198	90	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 4.

All (90) 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:85:TYR:OH	1:A:191[B]:ARG:NH2	2.12	0.82
1:A:344:ASN:ND2	1:A:346:GLU:OE2	2.17	0.78
1:A:39:ASN:OD1	6:A:501:HOH:O	2.10	0.70
1:C:388:TYR:HA	1:C:402:LYS:HB3	1.75	0.68
1:D:31:ALA:H	5:D:501[B]:GOL:H12	1.58	0.67
1:B:336:ASP:OD1	1:B:377:TYR:OH	2.13	0.66
1:D:394:GLU:CD	1:D:394:GLU:H	2.05	0.64
1:A:336:ASP:OD1	1:A:377:TYR:OH	2.14	0.64
1:B:60:GLU:HG3	1:B:64:LYS:HE3	1.79	0.63
1:B:388:TYR:HA	1:B:402:LYS:HB3	1.83	0.61
1:A:388:TYR:HA	1:A:402:LYS:HB3	1.84	0.59
1:A:386:LEU:HD13	1:A:395:THR:HB	1.85	0.58
1:A:54:LEU:HD21	1:A:389:SER:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:PHE:CZ	1:C:227:MET:HG2	2.39	0.57
1:B:243:HIS:NE2	3:F:3:LGU:H5	2.20	0.56
1:D:189:SER:HB2	1:D:250:ILE:HD13	1.87	0.56
1:D:74:LYS:H	1:D:74:LYS:CD	2.19	0.55
1:D:93:TRP:CD1	1:D:107:LYS:HE3	2.42	0.55
1:A:186:PHE:CZ	1:A:227:MET:HG2	2.41	0.55
1:D:392:ASP:HB3	1:D:394:GLU:OE2	2.06	0.55
1:A:270:GLN:OE1	6:A:503:HOH:O	2.18	0.55
1:B:186:PHE:CZ	1:B:227:MET:HG2	2.42	0.55
1:D:388:TYR:HA	1:D:402:LYS:HB3	1.90	0.54
1:A:375:GLN:O	1:A:375:GLN:NE2	2.40	0.54
1:B:74:LYS:H	1:B:74:LYS:CD	2.21	0.54
1:B:93:TRP:CD1	1:B:107:LYS:HE3	2.43	0.53
1:D:347:ASP:O	1:D:349:LYS:HE3	2.07	0.53
1:D:178:MET:SD	1:D:182:ARG:HD3	2.49	0.53
1:C:57:LYS:HD2	1:C:57:LYS:N	2.23	0.52
1:D:344:ASN:ND2	1:D:346:GLU:OE2	2.24	0.52
1:D:394:GLU:OE1	1:D:394:GLU:N	2.32	0.52
1:A:191[A]:ARG:NH2	6:A:510:HOH:O	2.43	0.52
1:B:276:MET:SD	1:B:306:LEU:HD13	2.50	0.51
1:D:374:ASN:OD1	1:D:376:LYS:HG2	2.10	0.51
1:A:276:MET:HE1	6:A:535:HOH:O	2.09	0.51
1:B:54:LEU:HD21	1:B:389:SER:HA	1.92	0.51
1:D:311:GLN:O	5:D:501[B]:GOL:O1	2.27	0.50
1:C:132:TYR:CD1	1:C:198:VAL:HG21	2.47	0.50
1:A:46:LYS:O	1:A:50:ARG:HG3	2.12	0.50
1:B:66:THR:O	6:B:601:HOH:O	2.19	0.49
1:A:26:LEU:HG	1:A:256:ALA:HB1	1.94	0.49
1:D:186:PHE:CZ	1:D:227:MET:HG2	2.49	0.48
1:B:276:MET:HA	1:B:276:MET:HE3	1.95	0.47
1:A:39:ASN:HB3	6:A:634:HOH:O	2.14	0.47
1:B:74:LYS:H	1:B:74:LYS:HD3	1.79	0.47
1:D:34:LEU:HD11	1:D:136:VAL:HG13	1.97	0.47
1:A:327:ASN:HD21	1:A:329:LYS:HD2	1.80	0.47
1:C:54:LEU:HD21	1:C:389:SER:HA	1.96	0.46
1:C:265:ARG:HG2	1:C:318:ILE:HD11	1.96	0.46
1:D:386:LEU:HD13	1:D:395:THR:HB	1.97	0.46
1:A:285:SER:HB2	1:A:290:LEU:HD11	1.98	0.46
1:C:271:SER:HG	1:C:275:LYS:HZ1	1.55	0.45
1:B:198:VAL:HG13	1:B:201:LEU:HD12	1.98	0.45
1:C:243:HIS:NE2	3:G:3:LGU:H5	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:TRP:CE2	1:D:305:ALA:HB2	2.51	0.44
1:A:375:GLN:NE2	1:A:379:ASP:OD1	2.50	0.44
1:B:285:SER:HB2	1:B:290:LEU:HD11	1.99	0.44
1:B:346:GLU:H	1:B:346:GLU:CD	2.26	0.44
1:B:26:LEU:CD2	1:B:315:GLN:HB3	2.48	0.44
1:B:60:GLU:HG3	1:B:64:LYS:CE	2.47	0.43
1:A:132:TYR:CD1	1:A:198:VAL:HG21	2.53	0.43
1:D:284:GLY:O	1:D:334:ALA:HA	2.18	0.43
1:D:346:GLU:H	1:D:346:GLU:CD	2.26	0.43
1:A:198:VAL:HG13	1:A:201:LEU:HD12	1.99	0.43
6:A:654:HOH:O	2:E:1:LGU:O1	2.21	0.43
1:C:28:PRO:HB3	1:C:253:MET:HG2	2.00	0.43
1:A:375:GLN:HE21	1:A:379:ASP:CG	2.26	0.43
1:B:129:ASP:HA	1:B:393:VAL:HG21	2.00	0.42
1:C:380:THR:HG23	1:C:383:ARG:NH2	2.33	0.42
1:D:43:LYS:HE3	1:D:43:LYS:HB3	1.83	0.42
1:D:137:LEU:HD23	1:D:137:LEU:HA	1.75	0.42
1:C:25:PRO:HB3	1:C:200:LYS:HE3	2.02	0.42
1:D:26:LEU:HA	1:D:315:GLN:OE1	2.20	0.42
1:D:186:PHE:CZ	1:D:227:MET:HE3	2.54	0.42
1:B:242:ASN:ND2	3:F:3:LGU:O6A	2.34	0.42
1:D:132:TYR:CD1	1:D:198:VAL:HG21	2.54	0.42
1:D:129:ASP:HA	1:D:393:VAL:HG21	2.02	0.41
1:D:200:LYS:HD3	1:D:203:GLU:CD	2.45	0.41
1:A:208:TRP:CZ3	1:A:212:ASP:HB3	2.55	0.41
1:B:132:TYR:CD1	1:B:198:VAL:HG21	2.55	0.41
1:B:246:TRP:CD1	1:B:305:ALA:HB2	2.54	0.41
1:D:54:LEU:HD21	1:D:389:SER:HA	2.02	0.41
1:A:186:PHE:CZ	1:A:227:MET:HE3	2.55	0.41
1:C:100:ASP:O	1:C:102:LEU:HD22	2.21	0.41
1:D:387:LYS:HA	1:D:387:LYS:HD3	1.80	0.41
1:C:252:LEU:HD22	1:C:264:ILE:HG23	2.02	0.40
1:A:246:TRP:CE2	1:A:305:ALA:HB2	2.56	0.40
1:B:311:GLN:O	1:B:315:GLN:NE2	2.55	0.40
1:D:152:ASN:ND2	6:D:611:HOH:O	2.54	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	378/404 (94%)	372 (98%)	6 (2%)	0	100	100
1	B	379/404 (94%)	373 (98%)	6 (2%)	0	100	100
1	C	378/404 (94%)	372 (98%)	6 (2%)	0	100	100
1	D	378/404 (94%)	373 (99%)	5 (1%)	0	100	100
All	All	1513/1616 (94%)	1490 (98%)	23 (2%)	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	324/344 (94%)	322 (99%)	2 (1%)	84	80
1	B	325/344 (94%)	323 (99%)	2 (1%)	84	80
1	C	324/344 (94%)	322 (99%)	2 (1%)	84	80
1	D	324/344 (94%)	321 (99%)	3 (1%)	75	69
All	All	1297/1376 (94%)	1288 (99%)	9 (1%)	81	77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	180	LYS

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Mol	Chain	Res	Type
1	B	326	SER
1	B	330	VAL
1	C	23	SER
1	C	75	LYS
1	D	102	LEU
1	D	175	VAL
1	D	259	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	173	GLN
1	A	279	GLN
1	A	358	GLN
1	A	375	GLN
1	B	173	GLN
1	B	279	GLN
1	C	39	ASN
1	C	358	GLN
1	D	36	GLN
1	D	173	GLN

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)

11 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	LGU	E	1	2	13,13,13	0.94	0	18,19,19	1.26	1 (5%)
2	LGU	E	2	2	12,12,13	1.06	1 (8%)	14,17,19	1.34	3 (21%)
2	MAW	E	3	2	10,11,12	1.32	1 (10%)	13,15,17	2.32	4 (30%)
3	LGU	F	1	3	13,13,13	0.88	1 (7%)	18,19,19	1.45	4 (22%)
3	LGU	F	2	3	12,12,13	1.09	1 (8%)	14,17,19	1.20	2 (14%)
3	LGU	F	3	3	12,12,13	1.18	1 (8%)	14,17,19	1.52	4 (28%)
3	LGU	G	1	3	13,13,13	0.92	0	18,19,19	1.08	0
3	LGU	G	2	3	12,12,13	1.10	1 (8%)	14,17,19	1.29	1 (7%)
3	LGU	G	3	3	12,12,13	1.05	0	14,17,19	1.25	1 (7%)
4	LGU	H	1	4	12,12,13	1.00	1 (8%)	14,17,19	1.39	2 (14%)
4	MAW	H	2	4	10,11,12	1.38	2 (20%)	13,15,17	2.16	3 (23%)

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	LGU	E	1	2	-	0/4/24/24	0/1/1/1
2	LGU	E	2	2	-	0/4/21/24	0/1/1/1
2	MAW	E	3	2	-	0/4/17/20	0/1/1/1
3	LGU	F	1	3	-	0/4/24/24	0/1/1/1
3	LGU	F	2	3	-	0/4/21/24	0/1/1/1
3	LGU	F	3	3	-	1/4/21/24	0/1/1/1
3	LGU	G	1	3	-	0/4/24/24	0/1/1/1
3	LGU	G	2	3	-	1/4/21/24	0/1/1/1
3	LGU	G	3	3	-	1/4/21/24	0/1/1/1
4	LGU	H	1	4	-	0/4/21/24	0/1/1/1
4	MAW	H	2	4	-	0/4/17/20	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	LGU	O6B-C6	-2.50	1.22	1.30
3	G	2	LGU	O6B-C6	-2.44	1.22	1.30
4	H	1	LGU	O6B-C6	-2.33	1.22	1.30
2	E	3	MAW	C5-C6	2.33	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	LGU	O6B-C6	-2.32	1.23	1.30
4	H	2	MAW	O6B-C6	-2.28	1.23	1.30
2	E	2	LGU	O6B-C6	-2.25	1.23	1.30
3	F	1	LGU	O6B-C6	-2.09	1.23	1.30
4	H	2	MAW	C5-C6	2.00	1.53	1.48

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	MAW	O5-C5-C4	-5.55	120.12	124.81
4	H	2	MAW	O5-C5-C4	-4.99	120.59	124.81
4	H	2	MAW	C2-C3-C4	-4.14	106.66	112.32
3	F	1	LGU	O2-C2-C3	-3.37	102.56	110.35
2	E	3	MAW	C2-C3-C4	-3.23	107.90	112.32
3	F	3	LGU	O4-C4-C5	3.03	116.53	109.74
2	E	3	MAW	C3-C4-C5	-2.69	117.05	121.60
2	E	2	LGU	O2-C2-C1	2.69	114.65	109.15
2	E	3	MAW	O6A-C6-C5	-2.58	113.63	120.48
3	F	3	LGU	O4-C4-C3	-2.52	104.53	110.35
4	H	1	LGU	O2-C2-C3	-2.46	105.22	110.14
2	E	1	LGU	O2-C2-C1	2.43	114.78	109.16
3	F	3	LGU	O2-C2-C1	2.41	114.09	109.15
3	G	2	LGU	C1-C2-C3	2.35	112.56	109.67
3	F	3	LGU	O3-C3-C4	-2.34	104.95	110.35
4	H	2	MAW	C3-C4-C5	-2.33	117.67	121.60
4	H	1	LGU	O2-C2-C1	2.32	113.89	109.15
3	F	1	LGU	C3-C4-C5	-2.24	105.42	109.25
2	E	2	LGU	O3-C3-C4	-2.24	105.17	110.35
2	E	2	LGU	O2-C2-C3	-2.21	105.70	110.14
3	F	2	LGU	O2-C2-C1	2.20	113.64	109.15
3	F	1	LGU	O4-C4-C5	2.17	114.61	109.74
3	F	2	LGU	O3-C3-C4	-2.12	105.44	110.35
3	G	3	LGU	O2-C2-C1	2.12	113.50	109.15
3	F	1	LGU	C1-O5-C5	2.06	115.25	112.22

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	LGU	O5-C5-C6-O6B
3	F	3	LGU	C4-C5-C6-O6B
3	G	3	LGU	C4-C5-C6-O6B

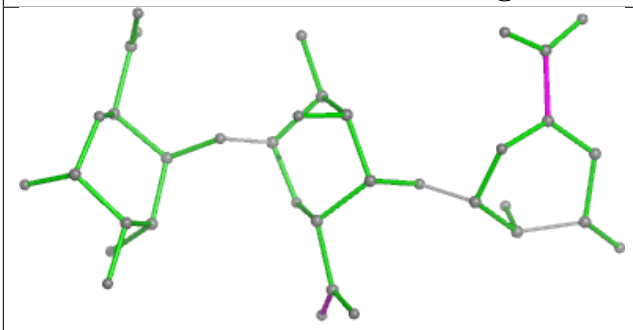
There are no ring outliers.

3 monomers are involved in 4 short contacts:

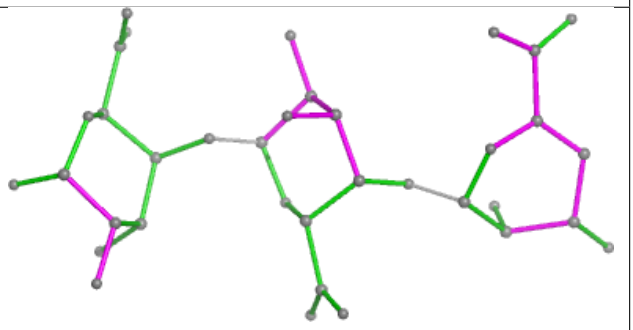
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	LGU	2	0
2	E	1	LGU	1	0
3	G	3	LGU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

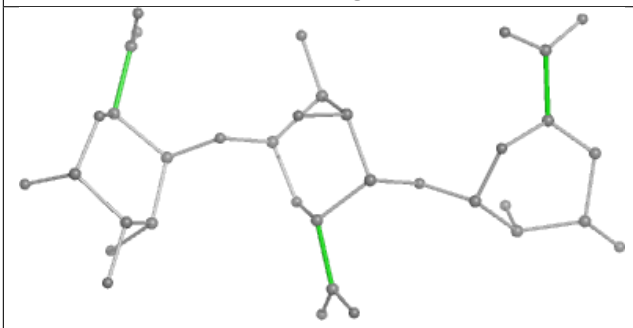
Oligosaccharide Chain E



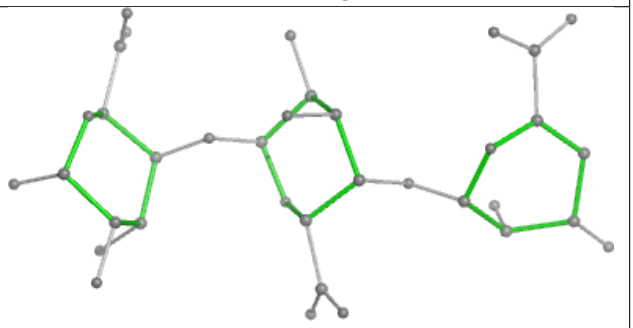
Bond lengths



Bond angles

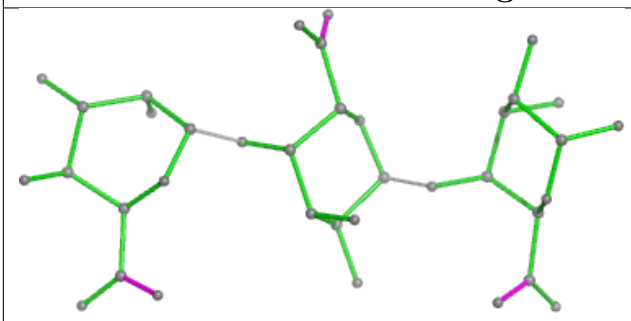


Torsions

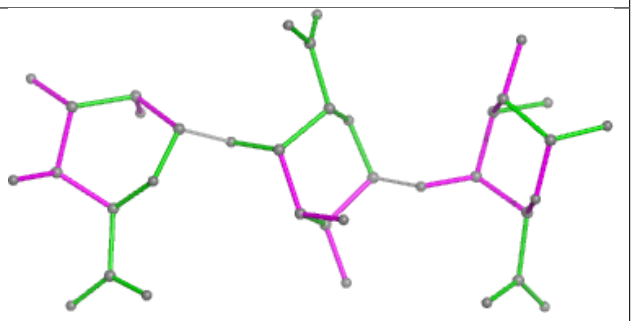


Rings

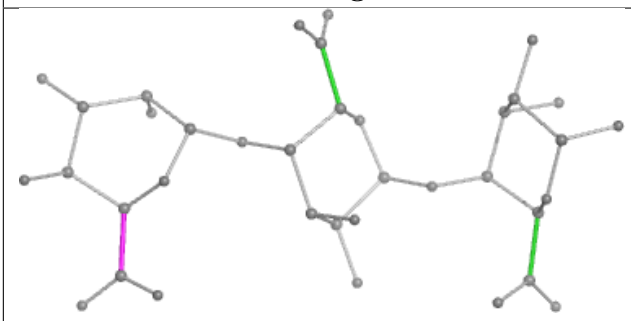
Oligosaccharide Chain F



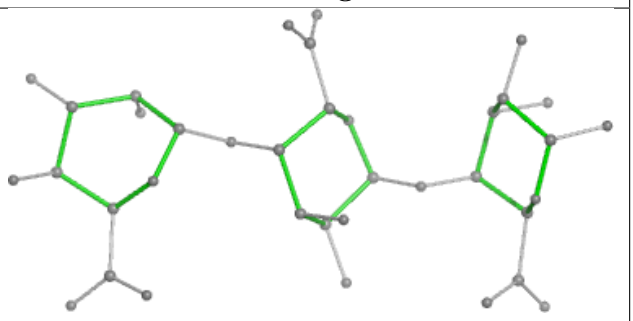
Bond lengths



Bond angles

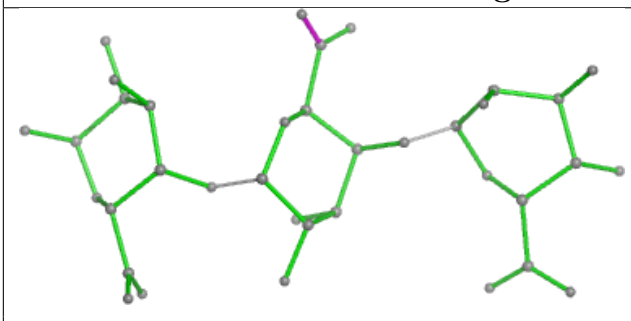


Torsions

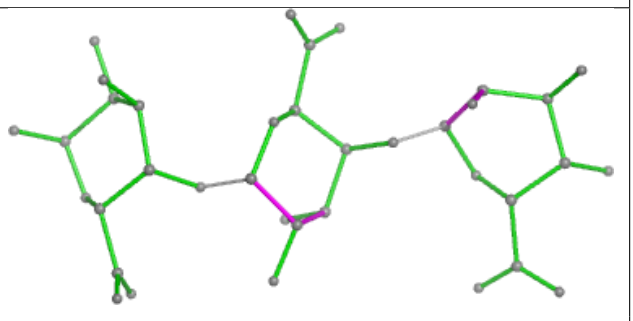


Rings

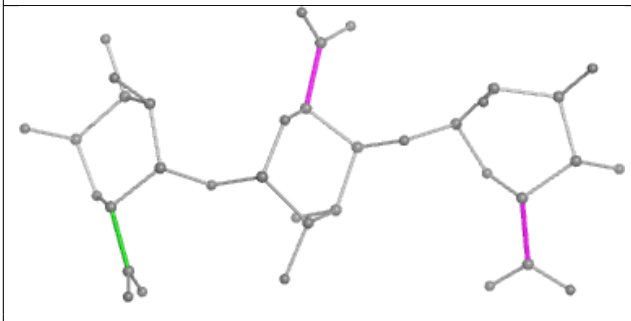
Oligosaccharide Chain G



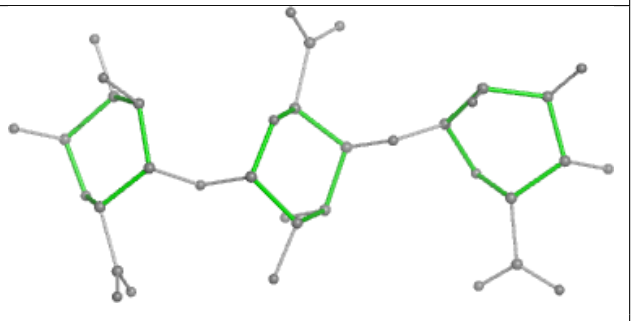
Bond lengths



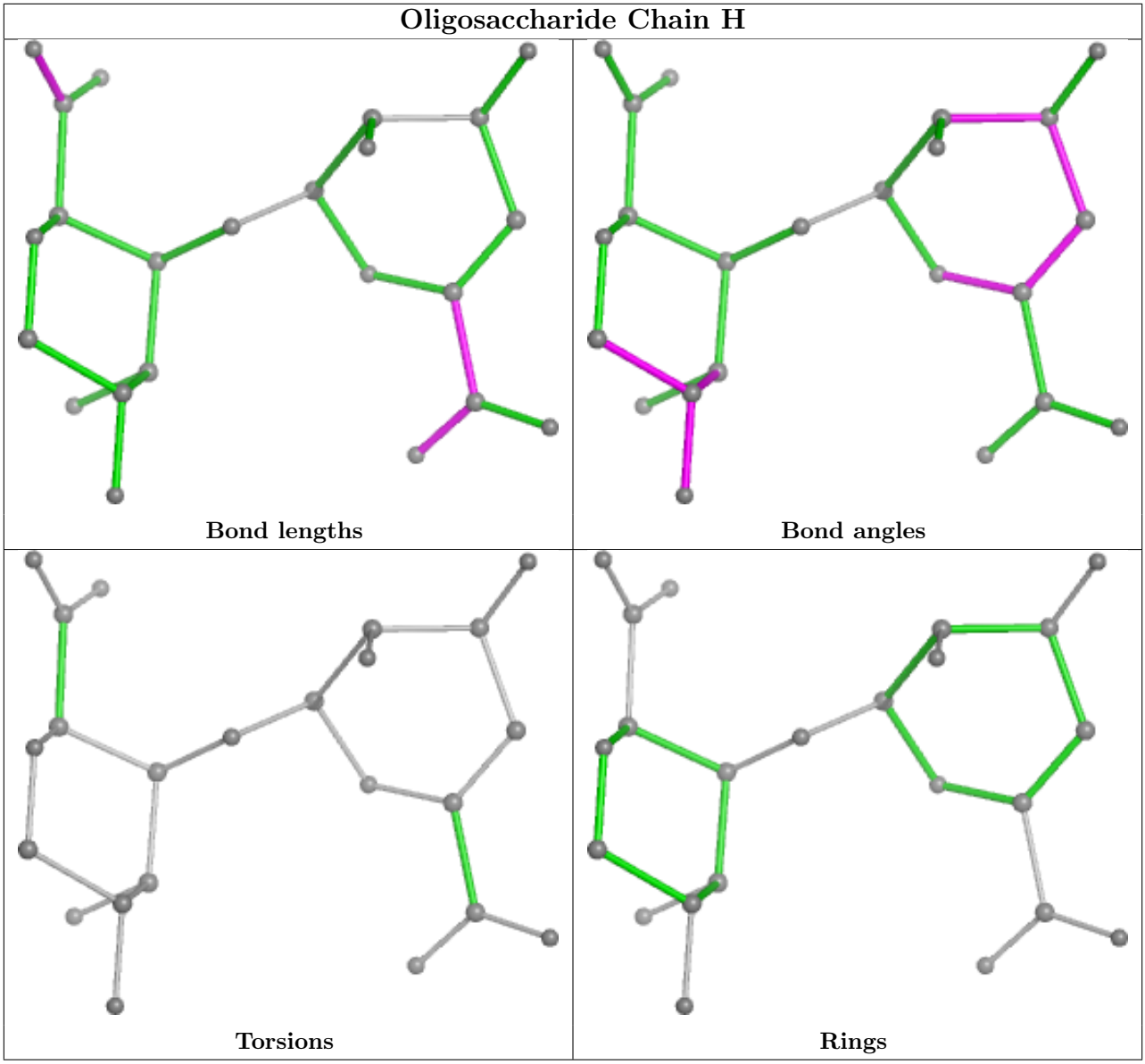
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

3 ligands 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	$\#\|Z\| > 2$
5	GOL	D	501[A]	-	5,5,5	0.30	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	B	501	-	5,5,5	0.46	0	5,5,5	0.76	0
5	GOL	D	501[B]	-	5,5,5	0.36	0	5,5,5	0.31	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	GOL	D	501[A]	-	-	2/4/4/4	-
5	GOL	B	501	-	-	0/4/4/4	-
5	GOL	D	501[B]	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	501[A]	GOL	O1-C1-C2-C3
5	D	501[A]	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501[B]	GOL	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

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, 95^{th} 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	379/404 (93%)	0.49	16 (4%)	41	42	22, 36, 48, 58	1 (0%)
1	B	380/404 (94%)	0.63	27 (7%)	23	25	21, 37, 51, 59	1 (0%)
1	C	380/404 (94%)	0.72	27 (7%)	23	25	29, 40, 55, 62	0
1	D	380/404 (94%)	0.87	39 (10%)	13	15	28, 42, 58, 65	0
All	All	1519/1616 (93%)	0.68	109 (7%)	23	24	21, 38, 53, 65	2 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	360	ARG	4.8
1	D	74	LYS	4.8
1	D	24	ALA	4.3
1	D	337	TYR	3.7
1	B	24	ALA	3.6
1	C	57	LYS	3.5
1	C	343	LEU	3.5
1	C	26	LEU	3.4
1	A	74	LYS	3.3
1	A	360	ARG	3.3
1	B	26	LEU	3.2
1	B	74	LYS	3.2
1	C	350	PHE	3.0
1	B	191	ARG	2.9
1	C	392	ASP	2.9
1	D	370	THR	2.9
1	B	326	SER	2.9
1	D	335	VAL	2.9
1	D	341	PHE	2.8
1	D	240	ALA	2.8
1	D	26	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	25	PRO	2.8
1	C	383	ARG	2.8
1	B	63	ILE	2.8
1	D	378	VAL	2.8
1	B	99	ILE	2.8
1	D	290	LEU	2.7
1	A	306	LEU	2.7
1	D	359	SER	2.7
1	C	360	ARG	2.7
1	B	43	LYS	2.7
1	D	39	ASN	2.6
1	C	381	ALA	2.6
1	D	23	SER	2.6
1	B	25	PRO	2.6
1	D	296	LEU	2.6
1	C	326	SER	2.6
1	A	24	ALA	2.6
1	C	46	LYS	2.6
1	A	99	ILE	2.6
1	B	353	ILE	2.6
1	B	355	PRO	2.5
1	C	340	PRO	2.5
1	D	284	GLY	2.5
1	C	259	ASP	2.5
1	D	340	PRO	2.5
1	D	76	LEU	2.5
1	B	194	ARG	2.5
1	A	45	GLU	2.5
1	D	48	VAL	2.5
1	D	330	VAL	2.5
1	B	341	PHE	2.4
1	D	356	PHE	2.4
1	D	280	ILE	2.4
1	D	46	LYS	2.4
1	D	109	GLY	2.4
1	B	262	ASP	2.4
1	C	42	GLN	2.4
1	A	377	TYR	2.4
1	D	377	TYR	2.4
1	D	191	ARG	2.3
1	A	359	SER	2.3
1	B	50	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	240	ALA	2.3
1	C	291	LYS	2.3
1	A	335	VAL	2.3
1	C	99	ILE	2.2
1	D	381	ALA	2.2
1	A	276	MET	2.2
1	B	388	TYR	2.2
1	C	353	ILE	2.2
1	C	394	GLU	2.2
1	B	100	ASP	2.2
1	C	378	VAL	2.2
1	B	343	LEU	2.2
1	D	349	LYS	2.2
1	C	100	ASP	2.2
1	D	260	ARG	2.2
1	A	389	SER	2.2
1	A	145	VAL	2.2
1	C	200	LYS	2.2
1	B	386	LEU	2.2
1	B	45	GLU	2.2
1	B	75	LYS	2.1
1	C	354	LYS	2.1
1	D	42	GLN	2.1
1	D	338	LEU	2.1
1	C	355	PRO	2.1
1	B	357	ASP	2.1
1	D	384	ILE	2.1
1	B	380	THR	2.1
1	B	145	VAL	2.1
1	A	341	PHE	2.1
1	D	379	ASP	2.1
1	C	337	TYR	2.1
1	A	382	LYS	2.1
1	B	44	GLY	2.1
1	C	50	ARG	2.1
1	D	357	ASP	2.1
1	D	33	LEU	2.1
1	C	276	MET	2.1
1	D	44	GLY	2.1
1	A	399	LEU	2.0
1	D	323	THR	2.0
1	A	142	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	347	ASP	2.0
1	D	302	ALA	2.0
1	C	271	SER	2.0
1	B	360	ARG	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)

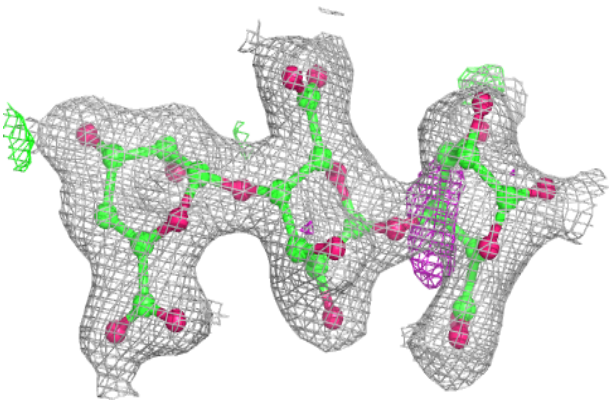
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

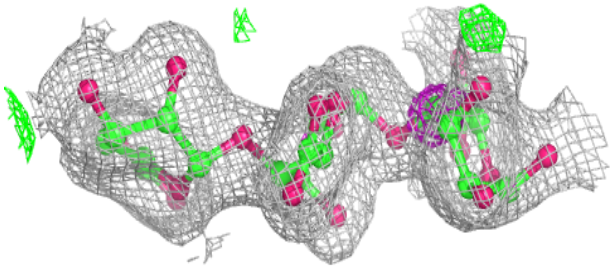
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LGU	F	1	13/13	0.71	0.17	47,60,70,72	0
3	LGU	G	1	13/13	0.74	0.15	52,58,65,67	0
2	LGU	E	1	13/13	0.77	0.14	47,52,60,63	0
4	LGU	H	1	12/13	0.85	0.12	40,43,48,49	0
4	MAW	H	2	11/12	0.92	0.10	34,40,43,43	0
3	LGU	G	3	12/13	0.93	0.09	33,38,41,48	0
3	LGU	F	2	12/13	0.93	0.09	34,39,45,47	0
2	MAW	E	3	11/12	0.93	0.09	28,31,33,34	0
3	LGU	F	3	12/13	0.94	0.08	31,34,36,42	0
3	LGU	G	2	12/13	0.95	0.08	37,42,48,48	0
2	LGU	E	2	12/13	0.96	0.06	32,35,41,46	0

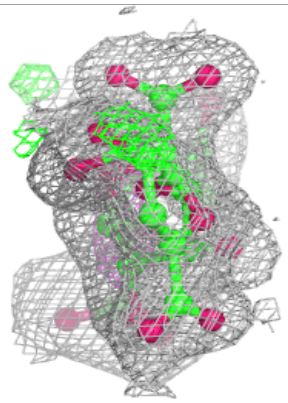
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

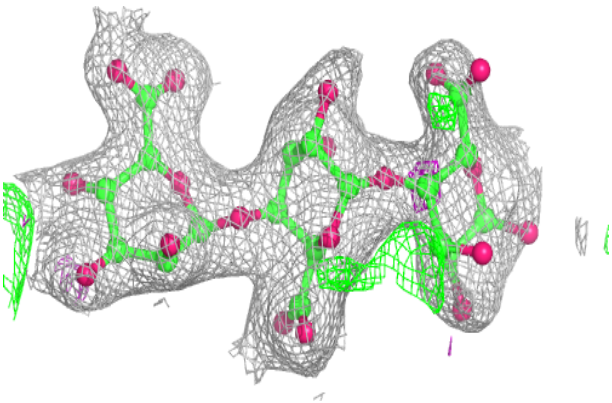


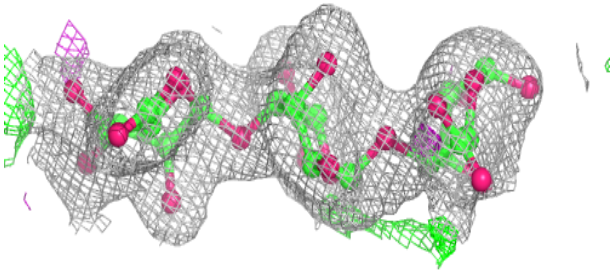


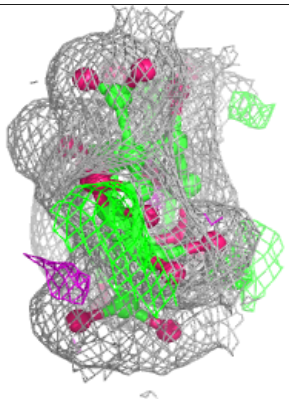


Electron density around Chain F:

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

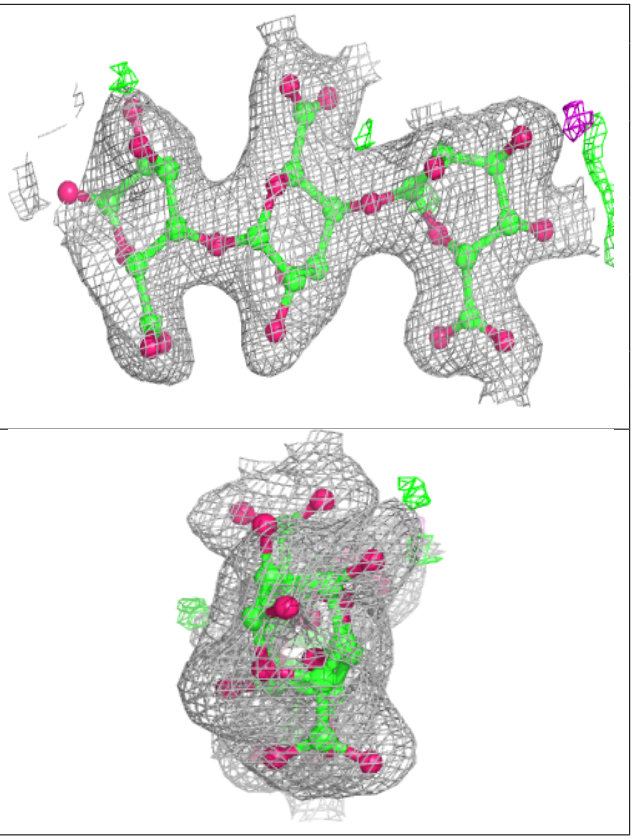


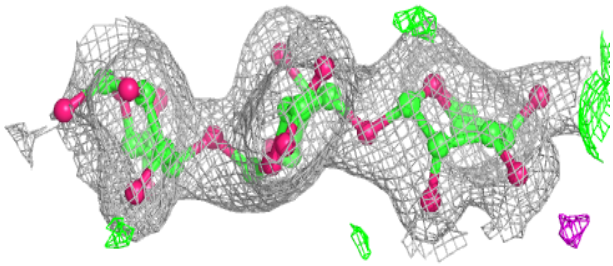




Electron density around Chain G:

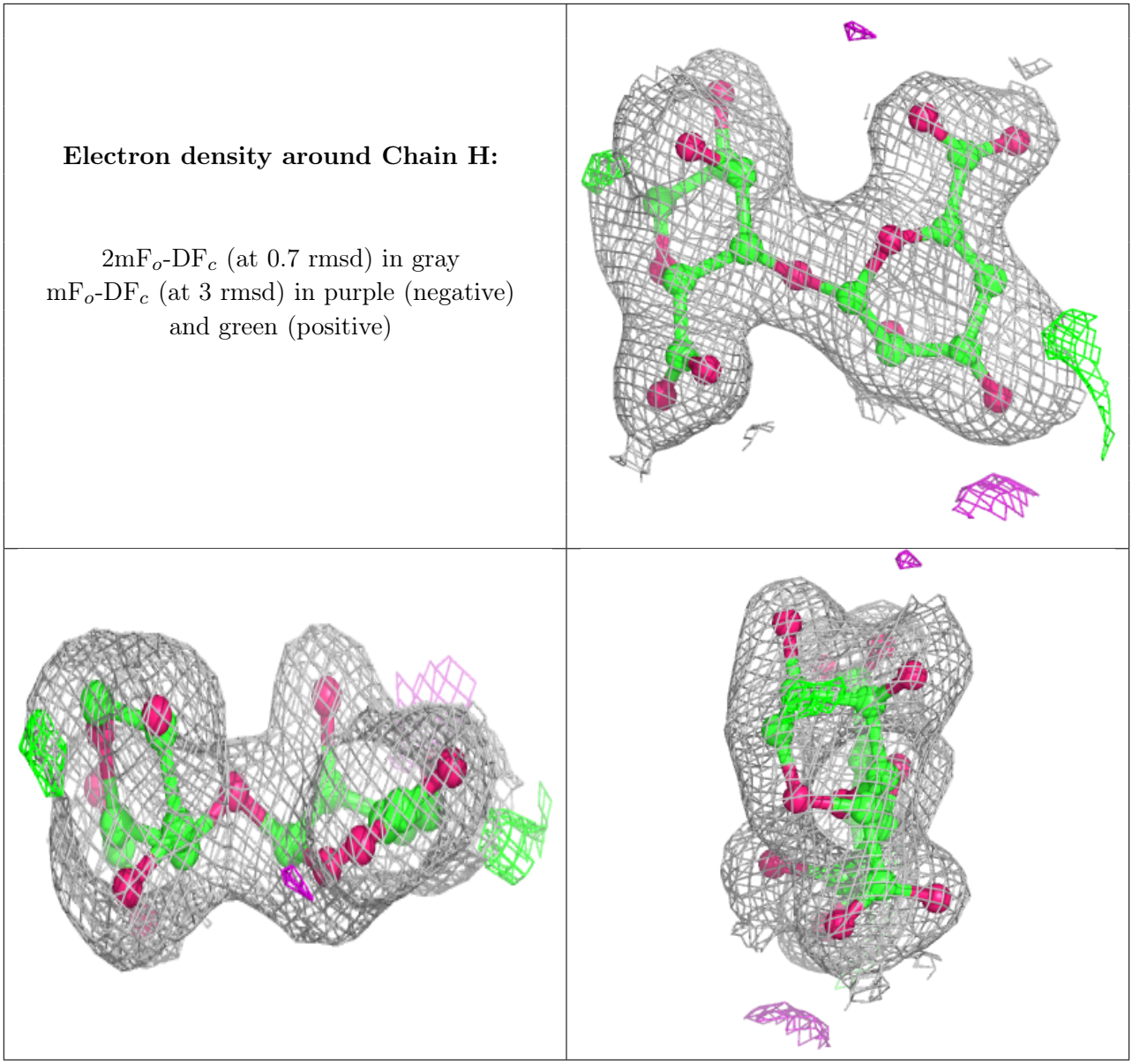
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around Chain H:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	GOL	D	501[A]	6/6	0.60	0.29	39,42,43,44	6
5	GOL	D	501[B]	6/6	0.60	0.29	37,41,43,44	6
5	GOL	B	501	6/6	0.79	0.20	42,46,46,47	0

6.5 Other polymers (i)

There are no such residues in this entry.