



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 11:08 AM BST

PDB ID : 6JR8
Title : Flavobacterium johnsoniae GH31 dextranase, FjDex31A, mutant D412A complexed with isomaltotriose
Authors : Tonozuka, T.
Deposited on : 2019-04-02
Resolution : 1.80 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

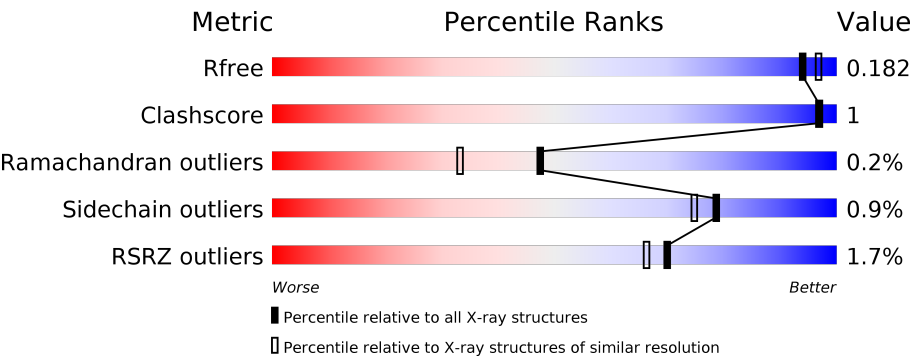
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	838	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>94%</div><div>. .</div></div>
1	B	838	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>94%</div><div>. .</div></div>
1	C	838	<div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>93%</div><div>. .</div></div>
1	D	838	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>93%</div><div>. .</div></div>
2	E	3	<div><div></div><div><div></div></div><div>100%</div><div></div></div>
2	F	3	<div><div></div><div><div></div></div><div>100%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	3	<div><div></div><div>33%</div><div>67%</div></div>
2	H	3	<div><div></div><div>33%</div><div>33%</div><div>33%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30205 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 Candidate alpha-glycosidase Glycoside hydrolase family 31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	812	Total	C	N	O	S	0	0	0
			6582	4220	1103	1228	31			
1	B	812	Total	C	N	O	S	0	0	0
			6582	4220	1103	1228	31			
1	C	812	Total	C	N	O	S	0	0	0
			6582	4220	1103	1228	31			
1	D	812	Total	C	N	O	S	0	0	0
			6582	4220	1103	1228	31			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP A5FBI1
A	0	GLY	-	expression tag	UNP A5FBI1
A	1	SER	-	expression tag	UNP A5FBI1
A	2	SER	-	expression tag	UNP A5FBI1
A	3	HIS	-	expression tag	UNP A5FBI1
A	4	HIS	-	expression tag	UNP A5FBI1
A	5	HIS	-	expression tag	UNP A5FBI1
A	6	HIS	-	expression tag	UNP A5FBI1
A	7	HIS	-	expression tag	UNP A5FBI1
A	8	HIS	-	expression tag	UNP A5FBI1
A	9	SER	-	expression tag	UNP A5FBI1
A	10	SER	-	expression tag	UNP A5FBI1
A	11	GLY	-	expression tag	UNP A5FBI1
A	12	LEU	-	expression tag	UNP A5FBI1
A	13	VAL	-	expression tag	UNP A5FBI1
A	14	PRO	-	expression tag	UNP A5FBI1
A	15	ARG	-	expression tag	UNP A5FBI1
A	16	GLY	-	expression tag	UNP A5FBI1
A	17	SER	-	expression tag	UNP A5FBI1
A	18	HIS	-	expression tag	UNP A5FBI1
A	19	MET	-	expression tag	UNP A5FBI1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	expression tag	UNP A5FBI1
A	412	ALA	ASP	engineered mutation	UNP A5FBI1
B	-1	MET	-	expression tag	UNP A5FBI1
B	0	GLY	-	expression tag	UNP A5FBI1
B	1	SER	-	expression tag	UNP A5FBI1
B	2	SER	-	expression tag	UNP A5FBI1
B	3	HIS	-	expression tag	UNP A5FBI1
B	4	HIS	-	expression tag	UNP A5FBI1
B	5	HIS	-	expression tag	UNP A5FBI1
B	6	HIS	-	expression tag	UNP A5FBI1
B	7	HIS	-	expression tag	UNP A5FBI1
B	8	HIS	-	expression tag	UNP A5FBI1
B	9	SER	-	expression tag	UNP A5FBI1
B	10	SER	-	expression tag	UNP A5FBI1
B	11	GLY	-	expression tag	UNP A5FBI1
B	12	LEU	-	expression tag	UNP A5FBI1
B	13	VAL	-	expression tag	UNP A5FBI1
B	14	PRO	-	expression tag	UNP A5FBI1
B	15	ARG	-	expression tag	UNP A5FBI1
B	16	GLY	-	expression tag	UNP A5FBI1
B	17	SER	-	expression tag	UNP A5FBI1
B	18	HIS	-	expression tag	UNP A5FBI1
B	19	MET	-	expression tag	UNP A5FBI1
B	20	ALA	-	expression tag	UNP A5FBI1
B	412	ALA	ASP	engineered mutation	UNP A5FBI1
C	-1	MET	-	expression tag	UNP A5FBI1
C	0	GLY	-	expression tag	UNP A5FBI1
C	1	SER	-	expression tag	UNP A5FBI1
C	2	SER	-	expression tag	UNP A5FBI1
C	3	HIS	-	expression tag	UNP A5FBI1
C	4	HIS	-	expression tag	UNP A5FBI1
C	5	HIS	-	expression tag	UNP A5FBI1
C	6	HIS	-	expression tag	UNP A5FBI1
C	7	HIS	-	expression tag	UNP A5FBI1
C	8	HIS	-	expression tag	UNP A5FBI1
C	9	SER	-	expression tag	UNP A5FBI1
C	10	SER	-	expression tag	UNP A5FBI1
C	11	GLY	-	expression tag	UNP A5FBI1
C	12	LEU	-	expression tag	UNP A5FBI1
C	13	VAL	-	expression tag	UNP A5FBI1
C	14	PRO	-	expression tag	UNP A5FBI1
C	15	ARG	-	expression tag	UNP A5FBI1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	GLY	-	expression tag	UNP A5FBI1
C	17	SER	-	expression tag	UNP A5FBI1
C	18	HIS	-	expression tag	UNP A5FBI1
C	19	MET	-	expression tag	UNP A5FBI1
C	20	ALA	-	expression tag	UNP A5FBI1
C	412	ALA	ASP	engineered mutation	UNP A5FBI1
D	-1	MET	-	expression tag	UNP A5FBI1
D	0	GLY	-	expression tag	UNP A5FBI1
D	1	SER	-	expression tag	UNP A5FBI1
D	2	SER	-	expression tag	UNP A5FBI1
D	3	HIS	-	expression tag	UNP A5FBI1
D	4	HIS	-	expression tag	UNP A5FBI1
D	5	HIS	-	expression tag	UNP A5FBI1
D	6	HIS	-	expression tag	UNP A5FBI1
D	7	HIS	-	expression tag	UNP A5FBI1
D	8	HIS	-	expression tag	UNP A5FBI1
D	9	SER	-	expression tag	UNP A5FBI1
D	10	SER	-	expression tag	UNP A5FBI1
D	11	GLY	-	expression tag	UNP A5FBI1
D	12	LEU	-	expression tag	UNP A5FBI1
D	13	VAL	-	expression tag	UNP A5FBI1
D	14	PRO	-	expression tag	UNP A5FBI1
D	15	ARG	-	expression tag	UNP A5FBI1
D	16	GLY	-	expression tag	UNP A5FBI1
D	17	SER	-	expression tag	UNP A5FBI1
D	18	HIS	-	expression tag	UNP A5FBI1
D	19	MET	-	expression tag	UNP A5FBI1
D	20	ALA	-	expression tag	UNP A5FBI1
D	412	ALA	ASP	engineered mutation	UNP A5FBI1

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.



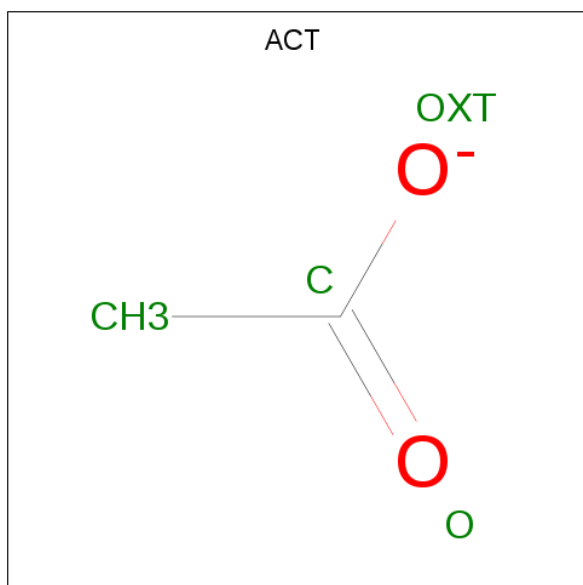
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			34	18	16			
2	F	3	Total	C	O	0	0	0
			34	18	16			

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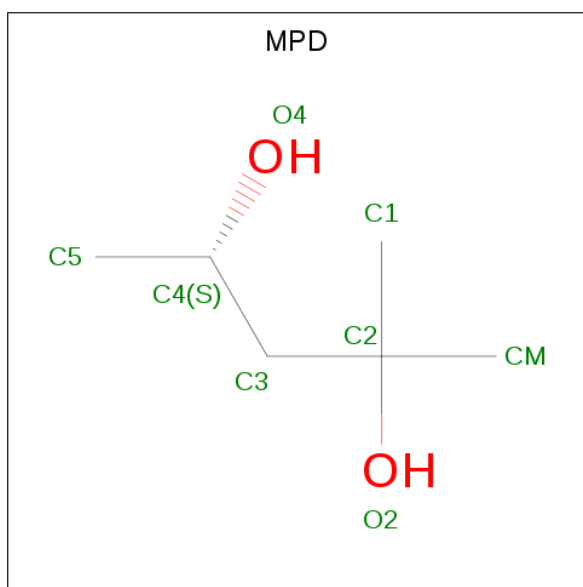
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	3	Total	C	O	0	0	0
			34	18	16			
2	H	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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



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

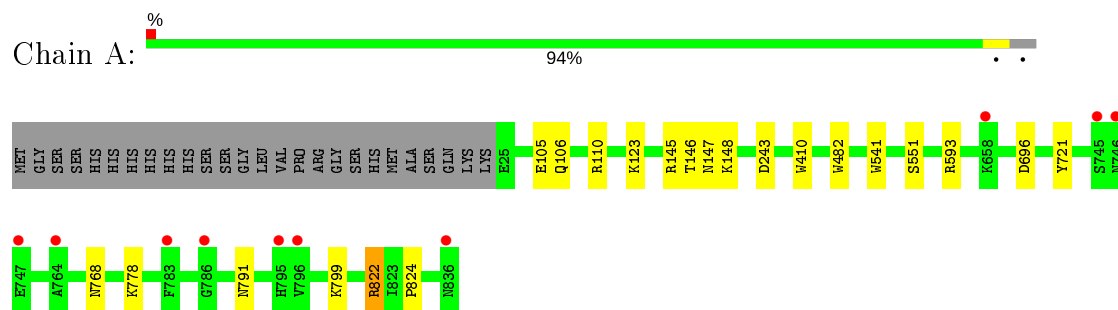
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	918	Total 918	O 918	0	0
5	B	885	Total 885	O 885	0	0
5	C	910	Total 910	O 910	0	0
5	D	908	Total 908	O 908	0	0

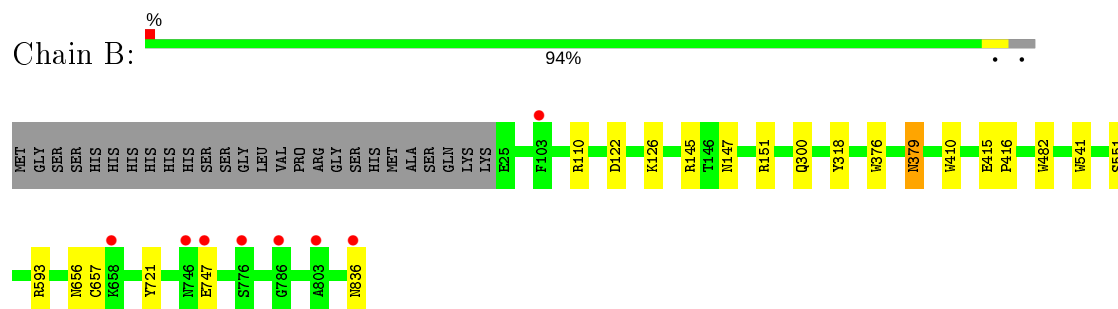
3 Residue-property plots [i](#)

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.

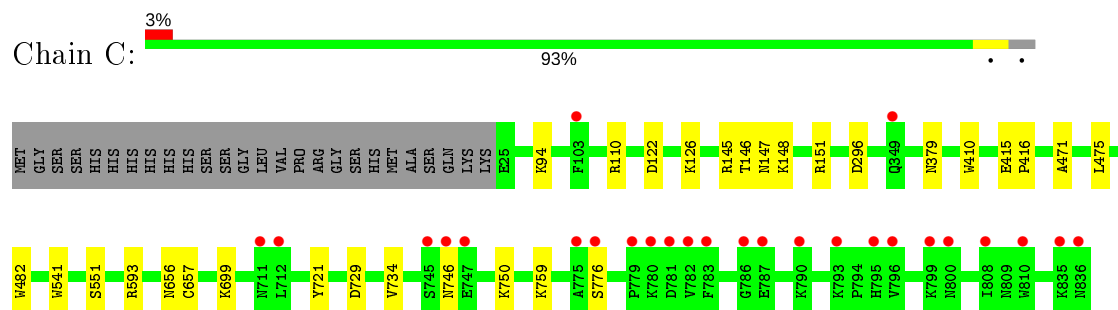
- Molecule 1: Candidate alpha-glycosidase Glycoside hydrolase family 31



- Molecule 1: Candidate alpha-glycosidase Glycoside hydrolase family 31

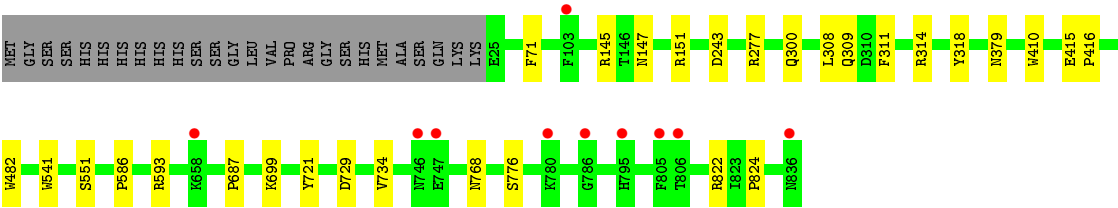


- Molecule 1: Candidate alpha-glycosidase Glycoside hydrolase family 31



- Molecule 1: Candidate alpha-glycosidase Glycoside hydrolase family 31





● Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain E: 100%



● Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain F: 100%



● Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain G: 33% 67%



● Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain H: 33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	102.37Å 112.62Å 114.17Å 111.06° 92.98° 114.54°	Depositor
Resolution (Å)	47.38 – 1.80 47.33 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.38-1.80) 97.0 (47.33-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.150 , 0.174 0.161 , 0.182	Depositor DCC
R_{free} test set	19153 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30205	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, GLC, ACT

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	0.50	0/6764	0.70	2/9152 (0.0%)
1	B	0.50	0/6764	0.70	0/9152
1	C	0.49	0/6764	0.69	0/9152
1	D	0.49	0/6764	0.71	5/9152 (0.1%)
All	All	0.49	0/27056	0.70	7/36608 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	277	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	D	243	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	151	ARG	CG-CD-NE	-5.97	99.27	111.80
1	A	243	ASP	CB-CG-OD1	5.94	123.65	118.30
1	D	822	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	277	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	822	ARG	NE-CZ-NH1	5.67	123.14	120.30

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	6582	0	6344	10	0
1	B	6582	0	6344	11	0
1	C	6582	0	6344	14	0
1	D	6582	0	6344	14	0
2	E	34	0	30	0	0
2	F	34	0	30	0	0
2	G	34	0	30	0	0
2	H	34	0	30	1	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
4	A	16	0	28	0	0
4	B	32	0	56	0	0
4	C	24	0	42	0	0
4	D	32	0	56	5	0
5	A	918	0	0	0	0
5	B	885	0	0	0	0
5	C	910	0	0	0	0
5	D	908	0	0	0	0
All	All	30205	0	25690	47	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 1.

All (47) 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:145:ARG:HE	1:B:147:ASN:HD21	1.26	0.81
1:C:145:ARG:HE	1:C:147:ASN:HD21	1.28	0.81
1:A:110:ARG:HH21	1:B:379:ASN:HD21	1.30	0.79
1:D:145:ARG:HE	1:D:147:ASN:HD21	1.33	0.76
1:A:145:ARG:HE	1:A:147:ASN:HD21	1.34	0.75
1:B:110:ARG:HH21	1:C:379:ASN:HD21	1.40	0.70
1:C:110:ARG:HH21	1:D:379:ASN:HD21	1.39	0.67
1:C:145:ARG:HE	1:C:147:ASN:ND2	2.00	0.59
4:D:907:MPD:HO4	2:H:3:GLC:HO6	1.49	0.59
1:D:314:ARG:NH2	4:D:907:MPD:H31	2.20	0.56
1:B:593:ARG:HD3	1:B:721:TYR:CZ	2.42	0.53
1:A:145:ARG:HE	1:A:147:ASN:ND2	2.06	0.53
1:C:145:ARG:NE	1:C:147:ASN:HD21	2.03	0.53
1:C:146:THR:CG2	1:C:148:LYS:HE2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLU:HG2	1:A:106:GLN:OE1	2.10	0.52
1:A:593:ARG:HD3	1:A:721:TYR:CZ	2.46	0.51
1:D:593:ARG:HD3	1:D:721:TYR:CZ	2.46	0.51
1:D:145:ARG:HE	1:D:147:ASN:ND2	2.04	0.50
1:B:747:GLU:HA	1:B:836:ASN:HD22	1.75	0.50
1:A:799:LYS:O	1:A:822:ARG:NH2	2.44	0.49
1:D:145:ARG:NE	1:D:147:ASN:HD21	2.07	0.49
1:A:778:LYS:NZ	1:A:791:ASN:HD21	2.12	0.48
1:A:145:ARG:NE	1:A:147:ASN:HD21	2.08	0.48
1:B:122:ASP:OD2	1:B:126:LYS:HE3	2.13	0.48
1:C:122:ASP:OD2	1:C:126:LYS:HE3	2.14	0.48
1:C:593:ARG:HD3	1:C:721:TYR:CZ	2.49	0.47
1:B:145:ARG:HE	1:B:147:ASN:ND2	2.03	0.47
1:A:146:THR:CG2	1:A:148:LYS:HE2	2.46	0.45
1:C:729:ASP:HB3	1:C:734:VAL:HB	1.99	0.45
1:C:656:ASN:OD1	1:C:657:CYS:N	2.50	0.44
1:D:729:ASP:HB3	1:D:734:VAL:HB	1.99	0.44
1:D:308:LEU:HG	4:D:907:MPD:HM3	2.01	0.43
1:D:415:GLU:N	1:D:416:PRO:HA	2.34	0.43
1:D:586:PRO:HB2	1:D:687:PRO:HB2	2.00	0.42
1:B:656:ASN:OD1	1:B:657:CYS:N	2.52	0.42
1:D:768:ASN:HD22	1:D:824:PRO:HA	1.85	0.42
1:C:94:LYS:NZ	4:D:907:MPD:H51	2.35	0.42
1:D:300:GLN:NE2	1:D:318:TYR:OH	2.53	0.41
1:A:768:ASN:HD22	1:A:824:PRO:HA	1.85	0.41
1:B:415:GLU:N	1:B:416:PRO:HA	2.35	0.41
1:B:300:GLN:NE2	1:B:318:TYR:OH	2.51	0.41
1:B:145:ARG:NE	1:B:147:ASN:HD21	2.05	0.41
1:C:415:GLU:N	1:C:416:PRO:HA	2.36	0.41
1:C:471:ALA:CB	1:C:475:LEU:HD13	2.51	0.41
1:C:734:VAL:HA	1:C:759:LYS:O	2.21	0.40
1:D:309:GLN:HG3	1:D:311:PHE:CE1	2.57	0.40
1:D:71:PHE:CD2	4:D:906:MPD:HM1	2.56	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	810/838 (97%)	789 (97%)	20 (2%)	1 (0%)	51	36
1	B	810/838 (97%)	792 (98%)	17 (2%)	1 (0%)	51	36
1	C	810/838 (97%)	788 (97%)	20 (2%)	2 (0%)	47	33
1	D	810/838 (97%)	790 (98%)	19 (2%)	1 (0%)	51	36
All	All	3240/3352 (97%)	3159 (98%)	76 (2%)	5 (0%)	47	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	SER
1	B	551	SER
1	C	551	SER
1	C	746	ASN
1	D	551	SER

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	702/724 (97%)	697 (99%)	5 (1%)	84	81
1	B	702/724 (97%)	696 (99%)	6 (1%)	78	75
1	C	702/724 (97%)	694 (99%)	8 (1%)	73	68
1	D	702/724 (97%)	697 (99%)	5 (1%)	84	81
All	All	2808/2896 (97%)	2784 (99%)	24 (1%)	78	75

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
1	A	410	TRP
1	A	482	TRP
1	A	541	TRP
1	A	696	ASP
1	B	151	ARG
1	B	376	TRP
1	B	379	ASN
1	B	410	TRP
1	B	482	TRP
1	B	541	TRP
1	C	151	ARG
1	C	296	ASP
1	C	410	TRP
1	C	482	TRP
1	C	541	TRP
1	C	699	LYS
1	C	750	LYS
1	C	776	SER
1	D	410	TRP
1	D	482	TRP
1	D	541	TRP
1	D	699	LYS
1	D	776	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	125	GLN
1	A	147	ASN
1	A	242	ASN
1	A	250	ASN
1	A	300	GLN
1	A	379	ASN
1	A	501	ASN
1	A	655	ASN
1	A	768	ASN
1	A	791	ASN
1	A	829	ASN
1	B	112	ASN

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Mol	Chain	Res	Type
1	B	125	GLN
1	B	147	ASN
1	B	250	ASN
1	B	300	GLN
1	B	379	ASN
1	B	655	ASN
1	B	768	ASN
1	B	791	ASN
1	B	829	ASN
1	B	836	ASN
1	C	112	ASN
1	C	125	GLN
1	C	147	ASN
1	C	250	ASN
1	C	300	GLN
1	C	379	ASN
1	C	501	ASN
1	C	655	ASN
1	C	688	GLN
1	C	768	ASN
1	C	791	ASN
1	C	829	ASN
1	D	47	ASN
1	D	112	ASN
1	D	125	GLN
1	D	147	ASN
1	D	250	ASN
1	D	300	GLN
1	D	379	ASN
1	D	655	ASN
1	D	768	ASN
1	D	829	ASN

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 ⓘ

12 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	GLC	E	1	2	12,12,12	0.57	0	17,17,17	0.80	1 (5%)
2	GLC	E	2	2	11,11,12	0.37	0	15,15,17	1.08	2 (13%)
2	GLC	E	3	2	11,11,12	0.33	0	15,15,17	0.92	1 (6%)
2	GLC	F	1	2	12,12,12	0.73	1 (8%)	17,17,17	0.78	0
2	GLC	F	2	2	11,11,12	0.50	0	15,15,17	1.08	1 (6%)
2	GLC	F	3	2	11,11,12	0.43	0	15,15,17	0.82	1 (6%)
2	GLC	G	1	2	12,12,12	0.61	0	17,17,17	0.53	0
2	GLC	G	2	2	11,11,12	0.34	0	15,15,17	1.05	1 (6%)
2	GLC	G	3	2	11,11,12	0.26	0	15,15,17	1.09	1 (6%)
2	GLC	H	1	2	12,12,12	0.56	0	17,17,17	0.74	0
2	GLC	H	2	2	11,11,12	0.29	0	15,15,17	1.05	1 (6%)
2	GLC	H	3	2	11,11,12	0.35	0	15,15,17	0.97	1 (6%)

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	GLC	E	1	2	-	2/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	2/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	3	2	-	0/2/19/22	0/1/1/1
2	GLC	G	1	2	-	2/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	H	1	2	-	2/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	GLC	O1-C1	2.00	1.46	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	GLC	C1-O5-C5	2.91	116.13	112.19
2	G	3	GLC	C1-O5-C5	2.87	116.08	112.19
2	F	2	GLC	C1-C2-C3	2.40	112.62	109.67
2	G	2	GLC	C1-C2-C3	2.32	112.52	109.67
2	E	2	GLC	C1-C2-C3	2.30	112.49	109.67
2	H	2	GLC	C1-C2-C3	2.28	112.47	109.67
2	E	3	GLC	C1-O5-C5	2.28	115.28	112.19
2	H	3	GLC	C1-O5-C5	2.04	114.95	112.19
2	E	1	GLC	C4-C3-C2	-2.01	107.32	110.82
2	F	3	GLC	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

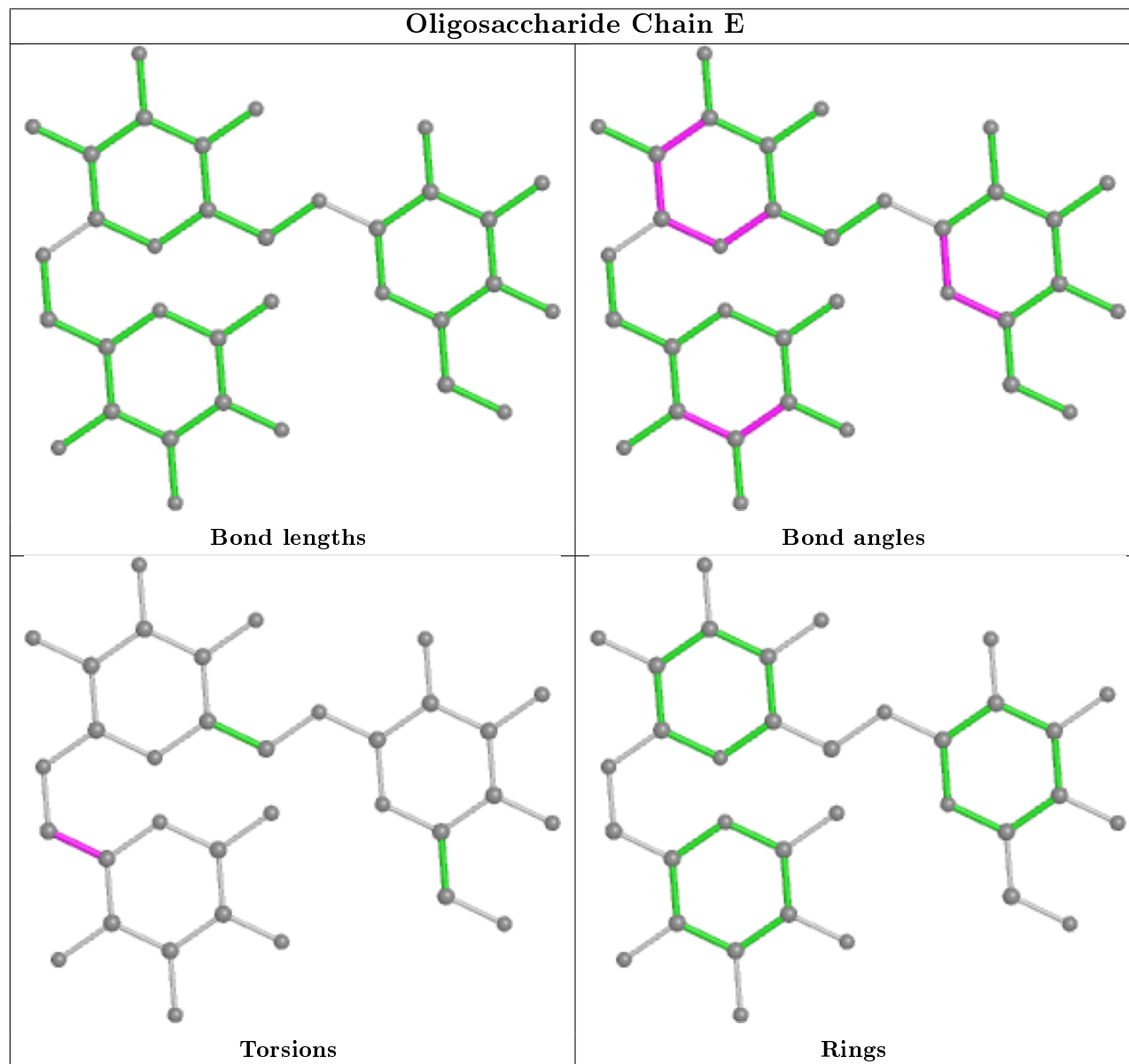
Mol	Chain	Res	Type	Atoms
2	F	1	GLC	O5-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	G	1	GLC	C4-C5-C6-O6
2	H	1	GLC	C4-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6

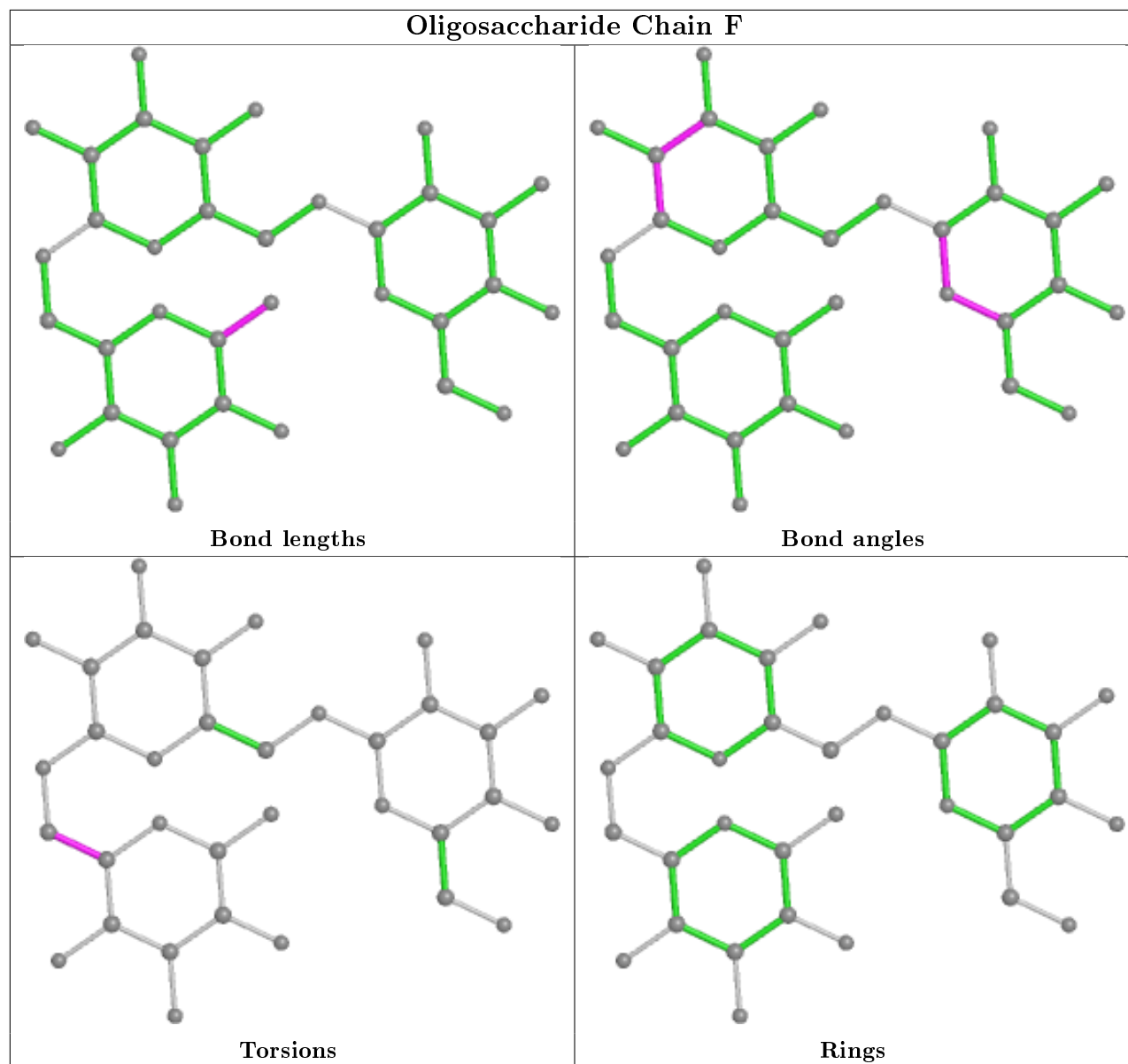
There are no ring outliers.

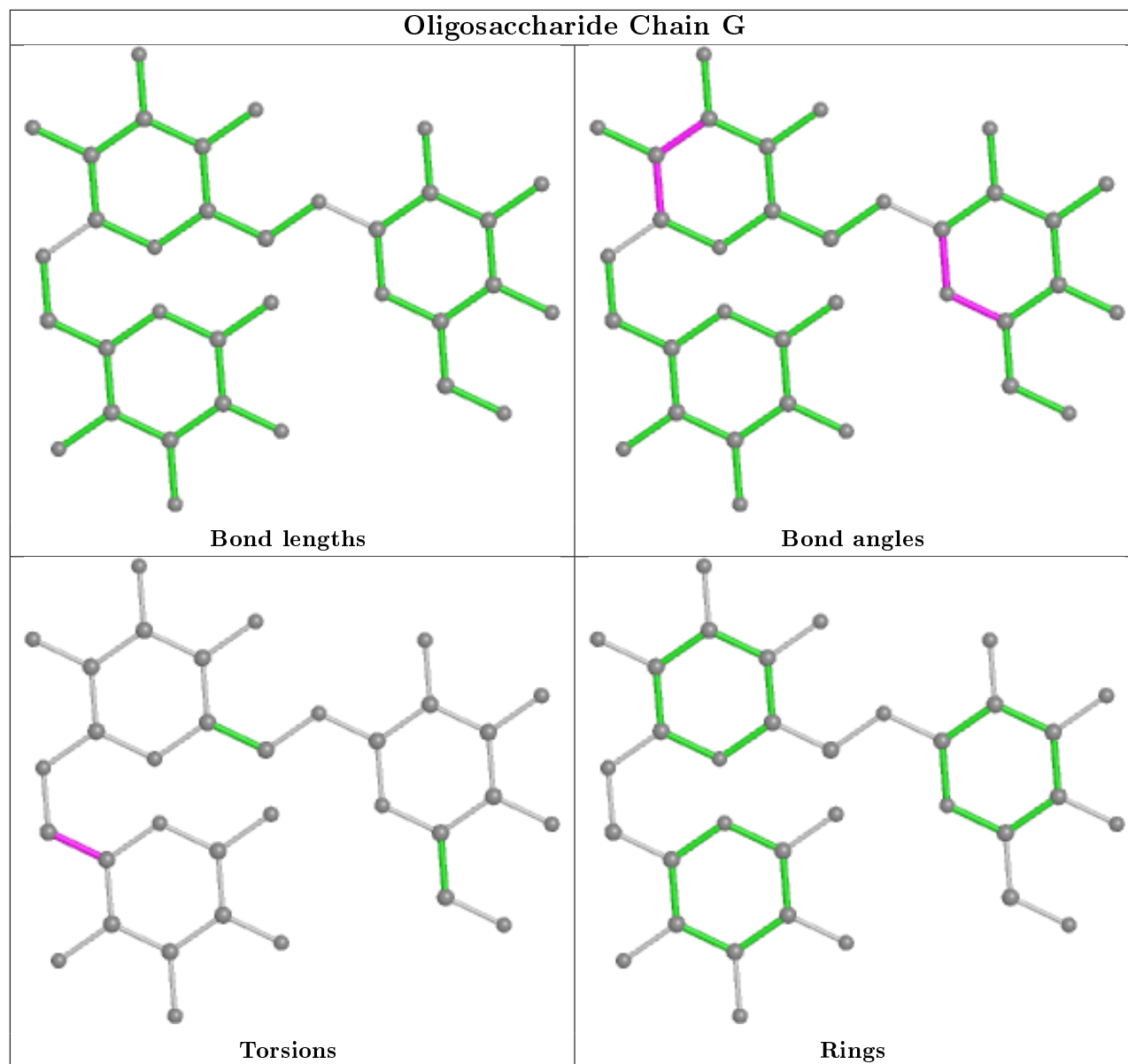
1 monomer is involved in 1 short contact:

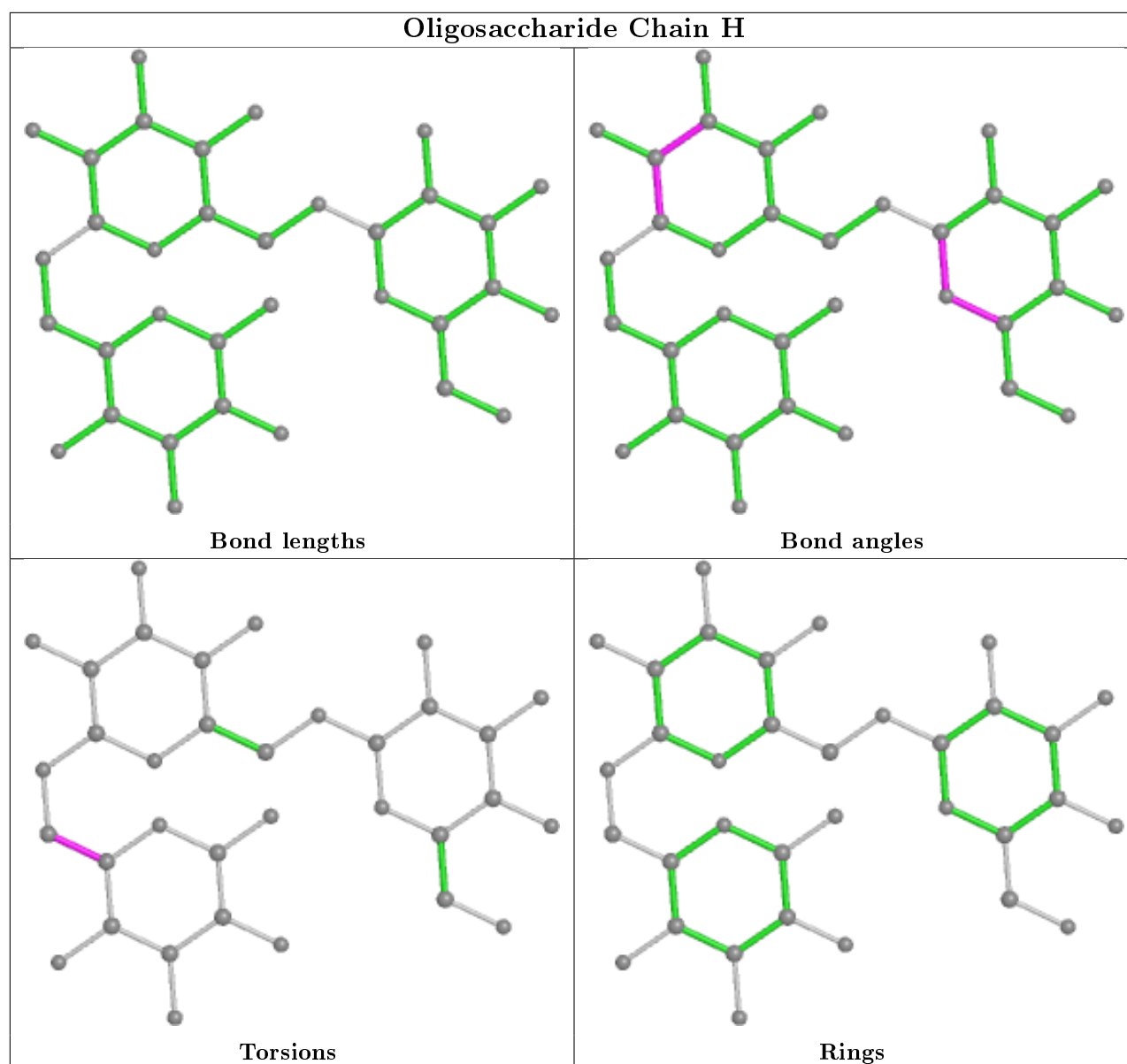
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	3	GLC	1	0

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 [i](#)

17 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
4	MPD	B	906	-	7,7,7	0.35	0	9,10,10	0.45	0
4	MPD	D	905	-	7,7,7	0.22	0	9,10,10	0.39	0
4	MPD	B	908	-	7,7,7	0.36	0	9,10,10	0.28	0
4	MPD	D	907	-	7,7,7	0.31	0	9,10,10	0.83	0
4	MPD	C	905	-	7,7,7	0.28	0	9,10,10	0.32	0
4	MPD	A	905	-	7,7,7	0.26	0	9,10,10	0.39	0
4	MPD	D	908	-	7,7,7	0.38	0	9,10,10	0.56	0
4	MPD	B	905	-	7,7,7	0.33	0	9,10,10	0.36	0
4	MPD	C	906	-	7,7,7	0.27	0	9,10,10	0.28	0
3	ACT	B	904	-	1,3,3	1.16	0	0,3,3	0.00	-
3	ACT	A	904	-	1,3,3	1.29	0	0,3,3	0.00	-
4	MPD	A	906	-	7,7,7	0.24	0	9,10,10	0.44	0
4	MPD	B	907	-	7,7,7	0.43	0	9,10,10	0.76	0
4	MPD	D	906	-	7,7,7	0.32	0	9,10,10	0.55	0
3	ACT	D	904	-	1,3,3	1.37	0	0,3,3	0.00	-
4	MPD	C	907	-	7,7,7	0.29	0	9,10,10	0.66	0
3	ACT	C	904	-	1,3,3	0.52	0	0,3,3	0.00	-

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
4	MPD	B	906	-	-	0/5/5/5	-
4	MPD	D	905	-	-	0/5/5/5	-
4	MPD	B	908	-	-	0/5/5/5	-
4	MPD	C	905	-	-	0/5/5/5	-
4	MPD	D	908	-	-	0/5/5/5	-
4	MPD	A	905	-	-	0/5/5/5	-
4	MPD	B	905	-	-	0/5/5/5	-
4	MPD	C	906	-	-	0/5/5/5	-
4	MPD	A	906	-	-	1/5/5/5	-
4	MPD	B	907	-	-	1/5/5/5	-
4	MPD	D	907	-	-	2/5/5/5	-
4	MPD	C	907	-	-	4/5/5/5	-
4	MPD	D	906	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	907	MPD	C2-C3-C4-O4
4	C	907	MPD	C2-C3-C4-O4
4	C	907	MPD	C2-C3-C4-C5
4	C	907	MPD	O2-C2-C3-C4
4	B	907	MPD	C1-C2-C3-C4
4	C	907	MPD	CM-C2-C3-C4
4	D	907	MPD	O2-C2-C3-C4
4	A	906	MPD	O2-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	907	MPD	4	0
4	D	906	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	812/838 (96%)	-0.44	10 (1%) 79 76	10, 17, 44, 73	0
1	B	812/838 (96%)	-0.36	8 (0%) 82 80	12, 19, 39, 78	0
1	C	812/838 (96%)	-0.38	26 (3%) 47 41	11, 18, 48, 88	0
1	D	812/838 (96%)	-0.37	10 (1%) 79 76	11, 17, 42, 71	0
All	All	3248/3352 (96%)	-0.39	54 (1%) 70 66	10, 18, 43, 88	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	747	GLU	4.8
1	B	747	GLU	4.7
1	C	746	ASN	4.7
1	C	836	ASN	4.4
1	C	712	LEU	4.3
1	C	747	GLU	4.1
1	D	836	ASN	3.9
1	C	745	SER	3.8
1	D	658	LYS	3.8
1	A	786	GLY	3.8
1	C	783	PHE	3.8
1	C	795	HIS	3.7
1	A	746	ASN	3.7
1	A	836	ASN	3.5
1	A	747	GLU	3.3
1	D	786	GLY	3.1
1	B	746	ASN	3.1
1	C	786	GLY	3.1
1	A	795	HIS	3.0
1	A	783	PHE	3.0
1	C	780	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	795	HIS	3.0
1	A	745	SER	3.0
1	C	790	LYS	3.0
1	C	776	SER	2.9
1	D	780	LYS	2.9
1	B	786	GLY	2.9
1	B	836	ASN	2.8
1	C	711	ASN	2.8
1	D	103	PHE	2.8
1	C	799	LYS	2.7
1	A	764	ALA	2.7
1	C	103	PHE	2.7
1	C	796	VAL	2.6
1	B	103	PHE	2.4
1	D	746	ASN	2.4
1	C	810	TRP	2.4
1	C	782	VAL	2.4
1	C	793	LYS	2.3
1	B	803	ALA	2.3
1	C	775	ALA	2.3
1	C	800	ASN	2.2
1	C	808	ILE	2.2
1	C	349	GLN	2.2
1	A	658	LYS	2.1
1	B	776	SER	2.1
1	B	658	LYS	2.1
1	C	781	ASP	2.1
1	D	806	THR	2.1
1	C	835	LYS	2.1
1	C	779	PRO	2.1
1	D	805	PHE	2.1
1	A	796	VAL	2.1
1	C	787	GLU	2.0

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

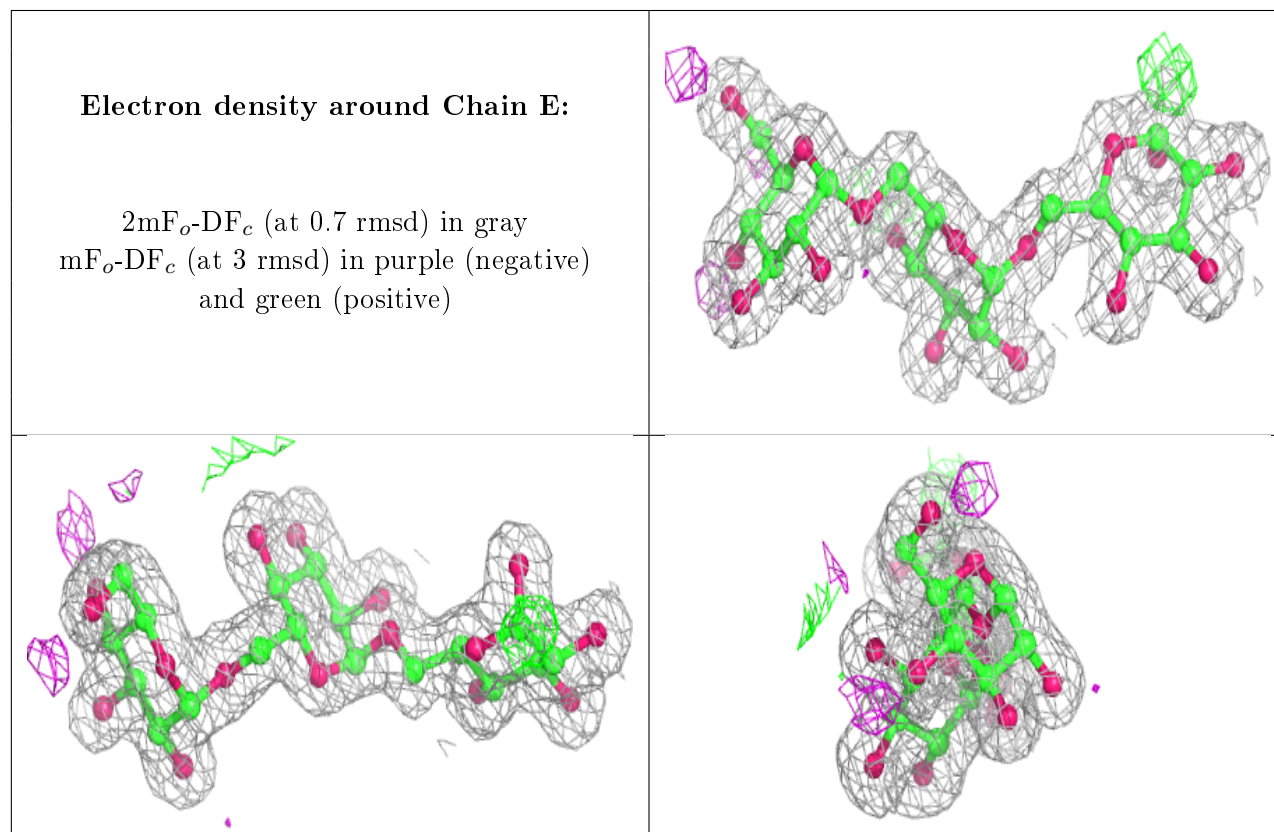
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

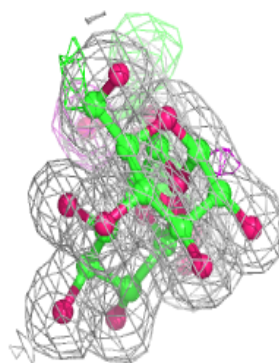
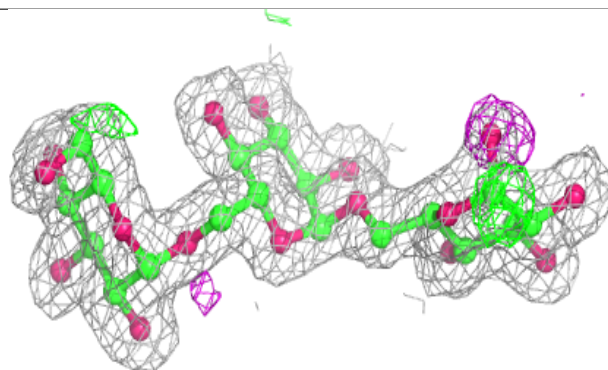
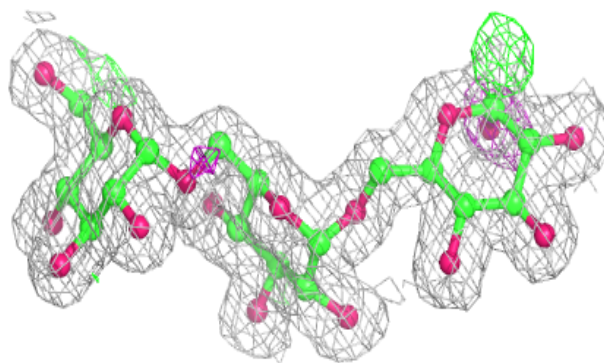
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	F	1	12/12	0.95	0.14	13,14,16,20	0
2	GLC	E	3	11/12	0.96	0.07	18,20,22,22	0
2	GLC	H	3	11/12	0.96	0.08	18,19,21,22	0
2	GLC	F	3	11/12	0.96	0.07	17,19,21,21	0
2	GLC	G	3	11/12	0.96	0.08	21,24,27,30	0
2	GLC	G	2	11/12	0.97	0.09	15,17,19,20	0
2	GLC	E	1	12/12	0.98	0.11	11,12,13,14	0
2	GLC	G	1	12/12	0.98	0.10	12,13,14,16	0
2	GLC	H	2	11/12	0.98	0.08	13,15,17,18	0
2	GLC	F	2	11/12	0.98	0.07	13,14,15,16	0
2	GLC	E	2	11/12	0.98	0.07	13,15,16,18	0
2	GLC	H	1	12/12	0.99	0.09	11,11,12,12	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.

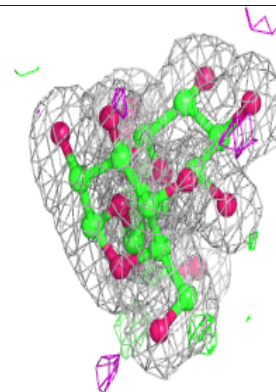
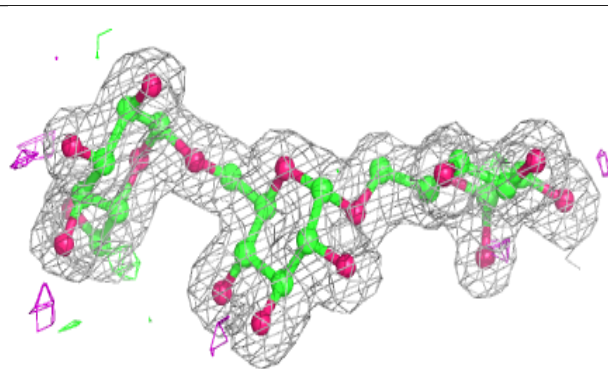
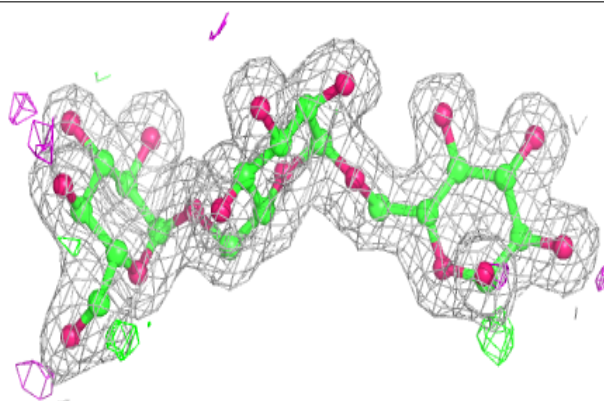


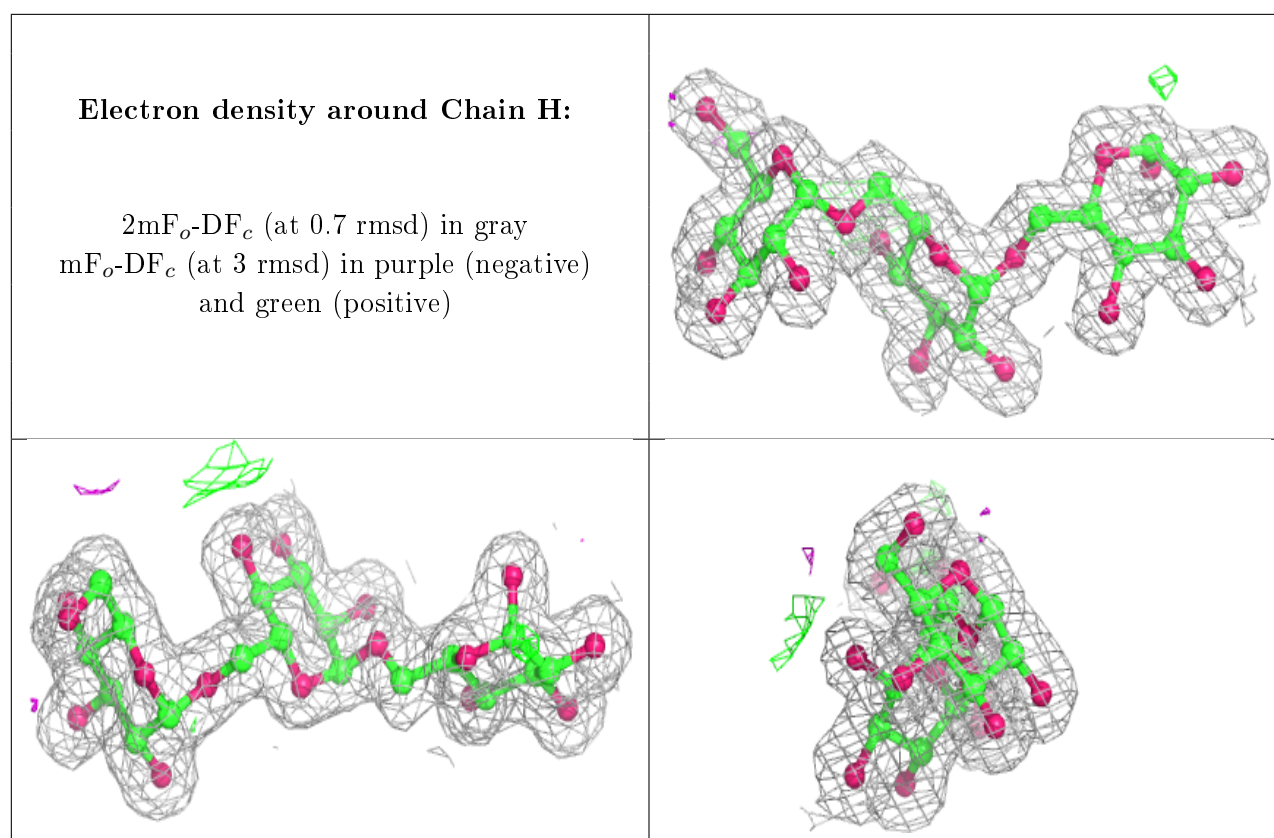
Electron density around Chain F:

$2mF_o-DF_c$ (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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MPD	C	906	8/8	0.72	0.27	68,74,78,82	0
4	MPD	D	907	8/8	0.79	0.26	48,49,50,51	0
4	MPD	B	905	8/8	0.80	0.19	40,41,43,47	0
4	MPD	B	908	8/8	0.81	0.21	48,51,53,54	0
4	MPD	B	906	8/8	0.82	0.31	61,64,66,69	0
4	MPD	C	907	8/8	0.84	0.20	49,50,53,54	0
4	MPD	D	908	8/8	0.84	0.17	44,46,48,50	0
4	MPD	D	906	8/8	0.85	0.25	51,55,59,61	0
4	MPD	A	906	8/8	0.89	0.14	35,38,40,43	0
4	MPD	D	905	8/8	0.92	0.12	27,28,29,31	0
4	MPD	C	905	8/8	0.92	0.13	34,34,35,37	0
4	MPD	B	907	8/8	0.92	0.12	35,36,40,42	0
4	MPD	A	905	8/8	0.94	0.10	29,29,30,31	0
3	ACT	C	904	4/4	0.97	0.09	16,16,17,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACT	B	904	4/4	0.98	0.13	19,20,20,20	0
3	ACT	D	904	4/4	0.98	0.07	16,16,16,17	0
3	ACT	A	904	4/4	0.99	0.09	15,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.