wwPDB X-ray Structure Validation Summary Report (i)

Nov 9, 2026 – 06:18 pm GMT

PDB ID	:	9I2J / pdb_00009i2j
Title	:	Branching Sucrase BRS-B in complex with Sucrose
Authors	:	Cioci, G.; Benkoulouche, M.; Claverie, M.; Remaud-Simeon, M.; Moulis, C.; Guieysse, D.
Deposited on	:	2025-01-20
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

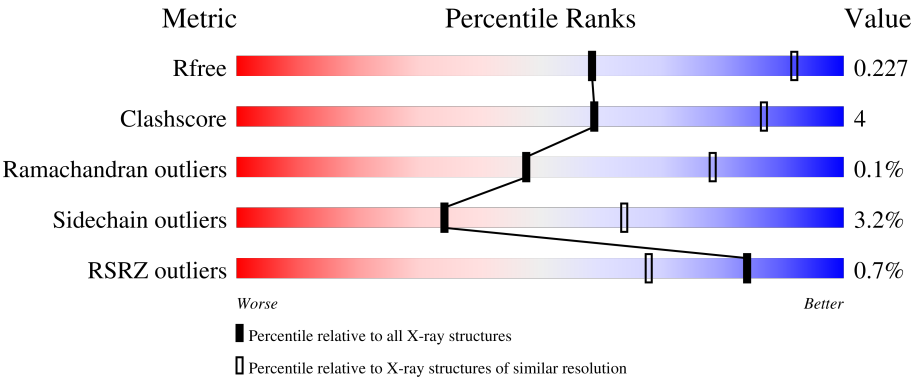
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	1183	% 85% 11%
1	B	1183	86% 10%
2	C	9	33% 67%
2	E	9	44% 56%
3	D	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	F	3	67% 33%
5	G	2	50% 50%
5	H	2	50% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18647 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 dextransucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1153	Total	C	N	O	S	0	0	0
			9062	5690	1533	1815	24			
1	B	1155	Total	C	N	O	S	0	0	0
			9099	5709	1545	1821	24			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	MET	-	initiating methionine	UNP A0A5A5U0V5
A	152	ALA	-	expression tag	UNP A0A5A5U0V5
A	153	SER	-	expression tag	UNP A0A5A5U0V5
A	709	GLN	GLU	conflict	UNP A0A5A5U0V5
A	768	SER	PHE	conflict	UNP A0A5A5U0V5
A	1103	THR	ALA	conflict	UNP A0A5A5U0V5
A	1314	LYS	-	expression tag	UNP A0A5A5U0V5
A	1315	GLY	-	expression tag	UNP A0A5A5U0V5
A	1316	GLY	-	expression tag	UNP A0A5A5U0V5
A	1317	ARG	-	expression tag	UNP A0A5A5U0V5
A	1318	ALA	-	expression tag	UNP A0A5A5U0V5
A	1319	ASP	-	expression tag	UNP A0A5A5U0V5
A	1320	PRO	-	expression tag	UNP A0A5A5U0V5
A	1321	ALA	-	expression tag	UNP A0A5A5U0V5
A	1322	PHE	-	expression tag	UNP A0A5A5U0V5
A	1323	LEU	-	expression tag	UNP A0A5A5U0V5
A	1324	TYR	-	expression tag	UNP A0A5A5U0V5
A	1325	LYS	-	expression tag	UNP A0A5A5U0V5
A	1326	VAL	-	expression tag	UNP A0A5A5U0V5
A	1327	VAL	-	expression tag	UNP A0A5A5U0V5
A	1328	HIS	-	expression tag	UNP A0A5A5U0V5
A	1329	HIS	-	expression tag	UNP A0A5A5U0V5
A	1330	HIS	-	expression tag	UNP A0A5A5U0V5
A	1331	HIS	-	expression tag	UNP A0A5A5U0V5
A	1332	HIS	-	expression tag	UNP A0A5A5U0V5

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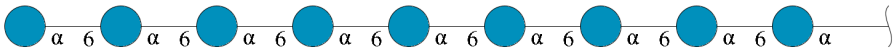
Chain	Residue	Modelled	Actual	Comment	Reference
A	1333	HIS	-	expression tag	UNP A0A5A5U0V5
B	151	MET	-	initiating methionine	UNP A0A5A5U0V5
B	152	ALA	-	expression tag	UNP A0A5A5U0V5
B	153	SER	-	expression tag	UNP A0A5A5U0V5
B	709	GLN	GLU	conflict	UNP A0A5A5U0V5
B	768	SER	PHE	conflict	UNP A0A5A5U0V5
B	1103	THR	ALA	conflict	UNP A0A5A5U0V5
B	1314	LYS	-	expression tag	UNP A0A5A5U0V5
B	1315	GLY	-	expression tag	UNP A0A5A5U0V5
B	1316	GLY	-	expression tag	UNP A0A5A5U0V5
B	1317	ARG	-	expression tag	UNP A0A5A5U0V5
B	1318	ALA	-	expression tag	UNP A0A5A5U0V5
B	1319	ASP	-	expression tag	UNP A0A5A5U0V5
B	1320	PRO	-	expression tag	UNP A0A5A5U0V5
B	1321	ALA	-	expression tag	UNP A0A5A5U0V5
B	1322	PHE	-	expression tag	UNP A0A5A5U0V5
B	1323	LEU	-	expression tag	UNP A0A5A5U0V5
B	1324	TYR	-	expression tag	UNP A0A5A5U0V5
B	1325	LYS	-	expression tag	UNP A0A5A5U0V5
B	1326	VAL	-	expression tag	UNP A0A5A5U0V5
B	1327	VAL	-	expression tag	UNP A0A5A5U0V5
B	1328	HIS	-	expression tag	UNP A0A5A5U0V5
B	1329	HIS	-	expression tag	UNP A0A5A5U0V5
B	1330	HIS	-	expression tag	UNP A0A5A5U0V5
B	1331	HIS	-	expression tag	UNP A0A5A5U0V5
B	1332	HIS	-	expression tag	UNP A0A5A5U0V5
B	1333	HIS	-	expression tag	UNP A0A5A5U0V5

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



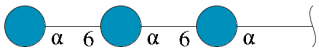
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	9	Total C O 99 54 45	0	0	0
2	E	9	Total C O 99 54 45	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.



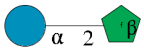
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	F	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

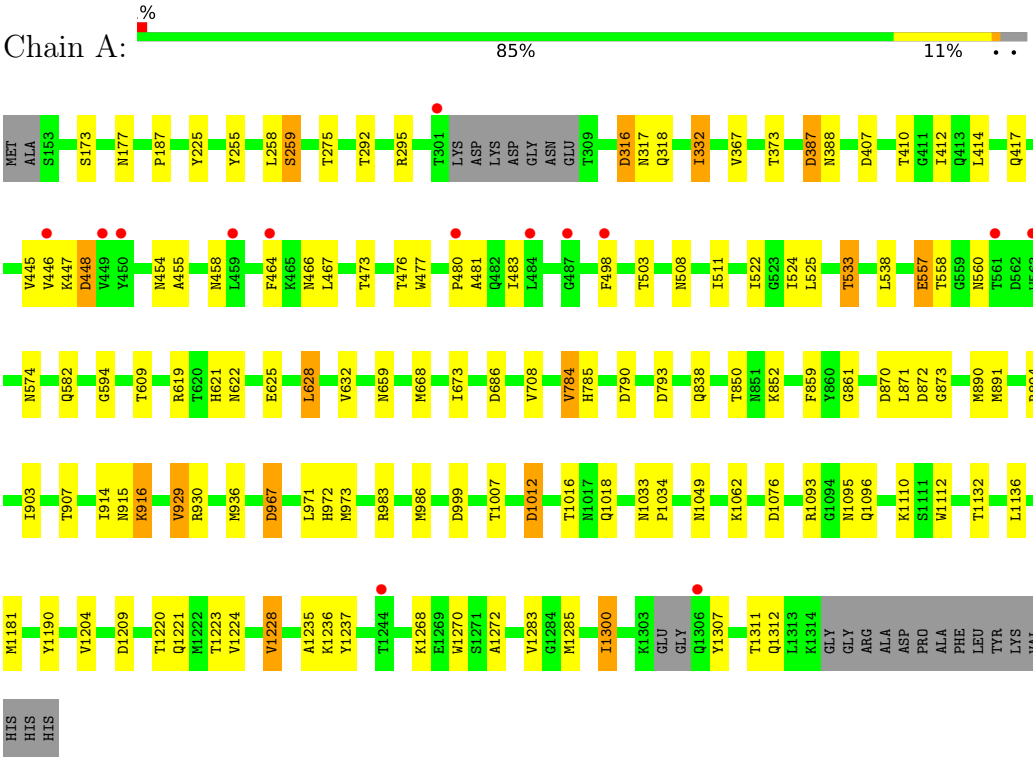
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	67	Total O 67 67	0	0
7	B	118	Total O 118 118	0	0

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.

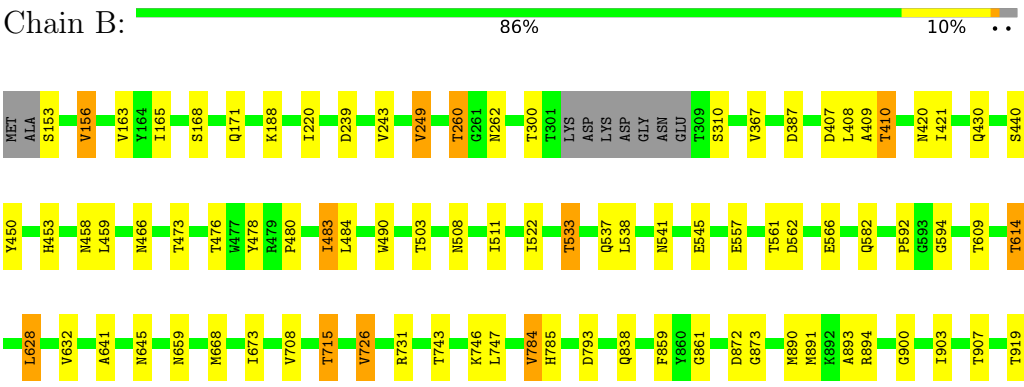
• Molecule 1: dextransucrase

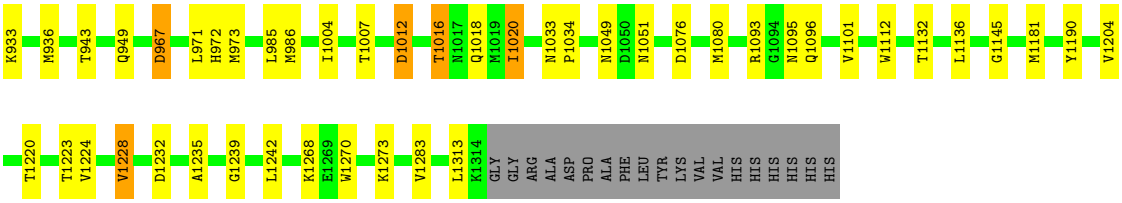
Chain A:



• Molecule 1: dextransucrase

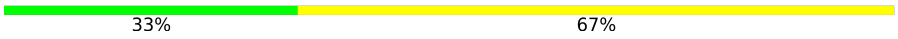
Chain B:





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

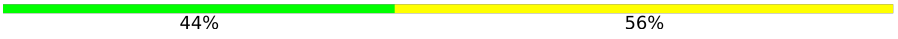
Chain C:

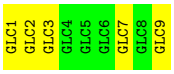




• Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain E:





• Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

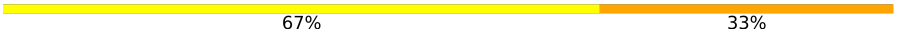
Chain D:





• Molecule 4: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain F:





• Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain G:





• Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain H:




GTC1
FRU2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	255.13Å 255.13Å 344.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.26 – 3.10 48.26 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.26-3.10) 98.5 (48.26-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.193 , 0.225 0.196 , 0.227	Depositor DCC
R_{free} test set	3803 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18647	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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: GLC, FRU, CA

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	0.49	0/9249	0.97	11/12551 (0.1%)
1	B	0.48	0/9289	0.96	11/12604 (0.1%)
All	All	0.48	0/18538	0.96	22/25155 (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.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	533	THR	CA-CB-OG1	-7.08	98.97	109.60
1	B	533	THR	CA-CB-OG1	-6.95	99.18	109.60
1	A	1132	THR	CA-CB-OG1	-6.48	99.88	109.60
1	A	387	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	498	PHE	CA-CB-CG	5.89	119.69	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	594	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	594	GLY	Peptide
1	B	731	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	9062	0	8637	83	0
1	B	9099	0	8683	77	0
2	C	99	0	82	0	0
2	E	99	0	82	0	0
3	D	22	0	19	1	0
4	F	33	0	28	1	0
5	G	23	0	21	1	0
5	H	23	0	21	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	67	0	0	2	0
7	B	118	0	0	2	0
All	All	18647	0	17573	160	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.

The worst 5 of 160 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:557:GLU:HG3	1:B:557:GLU:CB	1.99	0.93
1:A:850:THR:O	1:A:930:ARG:HD2	1.72	0.87
1:A:870:ASP:OD1	1:A:871:LEU:N	2.25	0.70
1:B:746:LYS:C	1:B:747:LEU:HD12	2.17	0.69
1:B:621:HIS:HA	1:B:625:GLU:HG3	1.75	0.69

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	1147/1183 (97%)	1090 (95%)	56 (5%)	1 (0%)	48 78
1	B	1151/1183 (97%)	1094 (95%)	56 (5%)	1 (0%)	48 78
All	All	2298/2366 (97%)	2184 (95%)	112 (5%)	2 (0%)	48 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1300	ILE
1	B	592	PRO

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	975/1007 (97%)	948 (97%)	27 (3%)	38 66
1	B	982/1007 (98%)	947 (96%)	35 (4%)	31 62
All	All	1957/2014 (97%)	1895 (97%)	62 (3%)	34 64

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	168	SER
1	B	1051	ASN
1	B	458	ASN
1	B	1049	ASN

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Mol	Chain	Res	Type
1	B	1220	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	430	GLN
1	B	939	GLN
1	B	560	ASN
1	B	622	ASN
1	B	1070	HIS

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)

27 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	C	1	2	11,11,12	0.88	1 (9%)	15,15,17	1.98	2 (13%)
2	GLC	C	2	2	11,11,12	0.46	0	15,15,17	1.14	2 (13%)
2	GLC	C	3	2	11,11,12	0.43	0	15,15,17	0.63	0
2	GLC	C	4	2	11,11,12	0.37	0	15,15,17	1.03	1 (6%)
2	GLC	C	5	2	11,11,12	0.52	0	15,15,17	0.84	0
2	GLC	C	6	2	11,11,12	0.49	0	15,15,17	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	C	7	2	11,11,12	0.39	0	15,15,17	1.05	1 (6%)
2	GLC	C	8	2	11,11,12	0.34	0	15,15,17	0.74	0
2	GLC	C	9	2	11,11,12	0.41	0	15,15,17	1.31	2 (13%)
3	GLC	D	1	3	11,11,12	0.42	0	15,15,17	0.84	1 (6%)
3	GLC	D	2	3	11,11,12	0.37	0	15,15,17	1.03	1 (6%)
2	GLC	E	1	2	11,11,12	0.65	0	15,15,17	1.72	2 (13%)
2	GLC	E	2	2	11,11,12	0.47	0	15,15,17	1.04	1 (6%)
2	GLC	E	3	2	11,11,12	0.33	0	15,15,17	0.75	1 (6%)
2	GLC	E	4	2	11,11,12	0.27	0	15,15,17	0.54	0
2	GLC	E	5	2	11,11,12	0.48	0	15,15,17	0.71	0
2	GLC	E	6	2	11,11,12	0.49	0	15,15,17	0.55	0
2	GLC	E	7	2	11,11,12	0.44	0	15,15,17	0.90	1 (6%)
2	GLC	E	8	2	11,11,12	0.36	0	15,15,17	0.96	0
2	GLC	E	9	2	11,11,12	0.70	0	15,15,17	1.14	1 (6%)
4	GLC	F	1	4	11,11,12	0.60	0	15,15,17	0.95	1 (6%)
4	GLC	F	2	4	11,11,12	0.80	0	15,15,17	1.08	2 (13%)
4	GLC	F	3	4	11,11,12	0.87	1 (9%)	15,15,17	1.67	2 (13%)
5	GLC	G	1	5	11,11,12	0.86	1 (9%)	15,15,17	1.28	1 (6%)
5	FRU	G	2	5	11,12,12	0.57	0	10,18,18	0.52	0
5	GLC	H	1	5	11,11,12	0.65	0	15,15,17	1.16	2 (13%)
5	FRU	H	2	5	11,12,12	0.51	0	10,18,18	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	2/2/19/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
2	GLC	C	7	2	-	0/2/19/22	0/1/1/1
2	GLC	C	8	2	-	0/2/19/22	0/1/1/1
2	GLC	C	9	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/19/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	1	2	-	0/2/19/22	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	E	4	2	-	0/2/19/22	0/1/1/1
2	GLC	E	5	2	-	0/2/19/22	0/1/1/1
2	GLC	E	6	2	-	0/2/19/22	0/1/1/1
2	GLC	E	7	2	-	0/2/19/22	0/1/1/1
2	GLC	E	8	2	-	0/2/19/22	0/1/1/1
2	GLC	E	9	2	-	0/2/19/22	0/1/1/1
4	GLC	F	1	4	-	0/2/19/22	0/1/1/1
4	GLC	F	2	4	-	1/2/19/22	0/1/1/1
4	GLC	F	3	4	-	2/2/19/22	0/1/1/1
5	GLC	G	1	5	-	0/2/19/22	0/1/1/1
5	FRU	G	2	5	-	5/5/24/24	0/1/1/1
5	GLC	H	1	5	-	2/2/19/22	0/1/1/1
5	FRU	H	2	5	-	2/5/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	GLC	O5-C5	2.40	1.48	1.43
2	C	1	GLC	C2-C3	2.37	1.56	1.52
5	G	1	GLC	C2-C3	-2.30	1.49	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	GLC	C1-C2-C3	6.51	117.66	109.67
2	E	1	GLC	C1-C2-C3	5.50	116.42	109.67
4	F	3	GLC	C1-O5-C5	4.58	118.39	112.19
5	G	1	GLC	C1-O5-C5	3.55	117.00	112.19
2	C	7	GLC	C1-C2-C3	3.11	113.49	109.67

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	2	FRU	O1-C1-C2-C3
5	G	2	FRU	O1-C1-C2-O2
5	G	2	FRU	O1-C1-C2-O5
5	G	2	FRU	O5-C5-C6-O6

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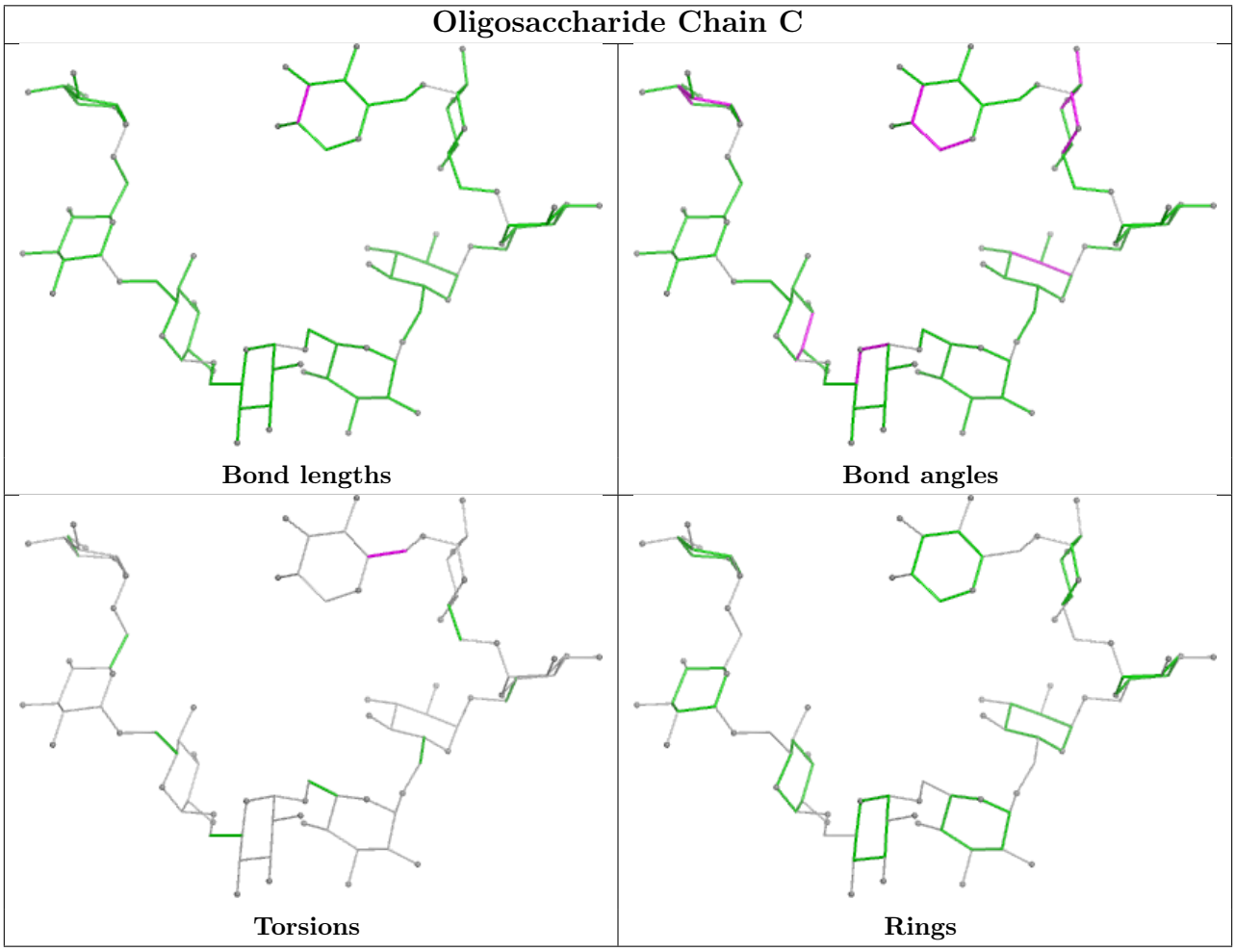
Mol	Chain	Res	Type	Atoms
2	C	1	GLC	O5-C5-C6-O6

There are no ring outliers.

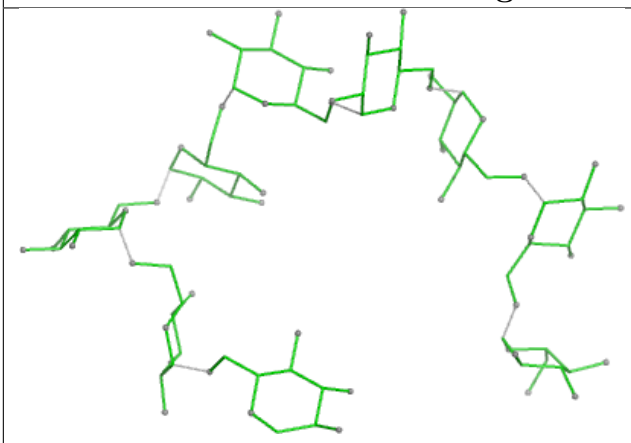
4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	FRU	1	0
5	G	1	GLC	1	0
3	D	2	GLC	1	0
4	F	1	GLC	1	0

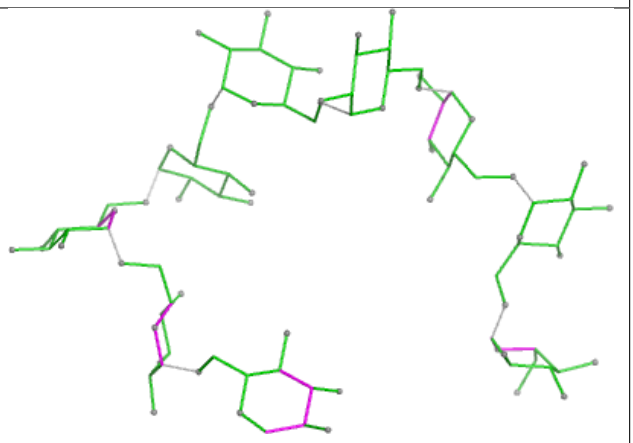
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



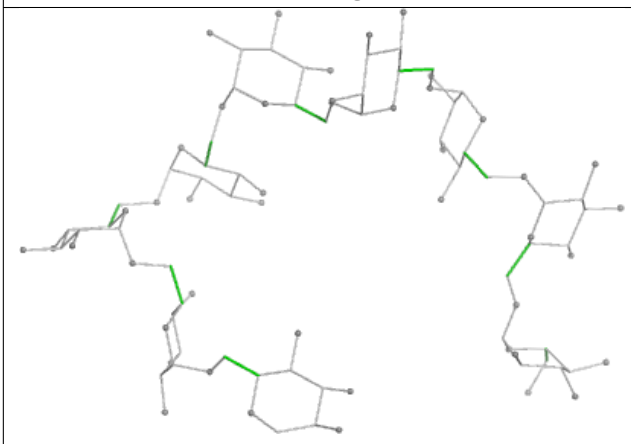
Oligosaccharide Chain E



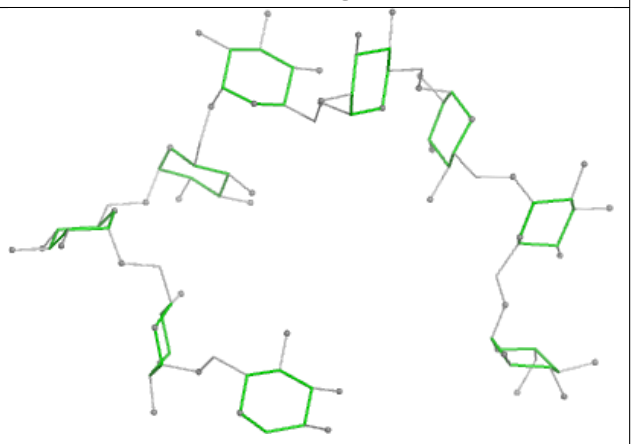
Bond lengths



Bond angles

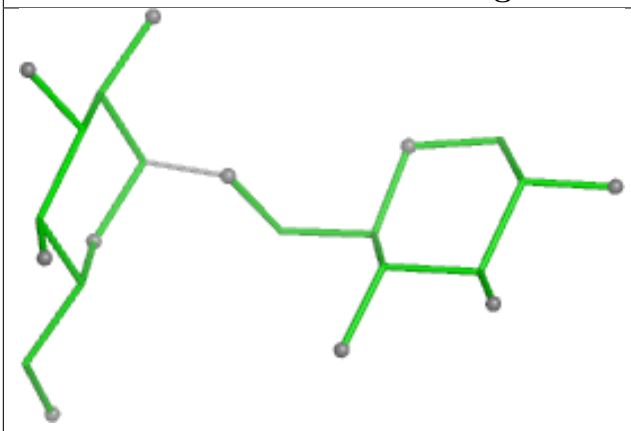


Torsions

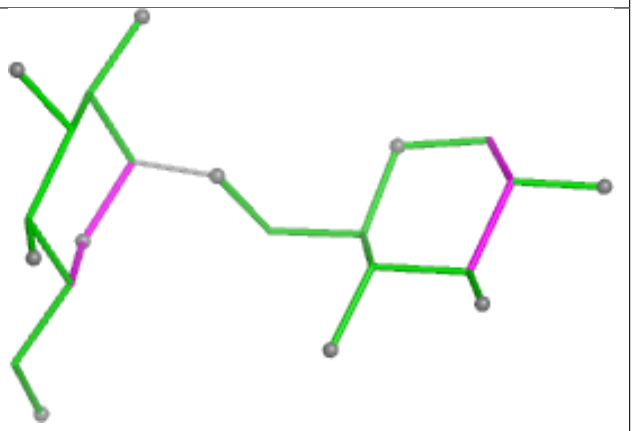


Rings

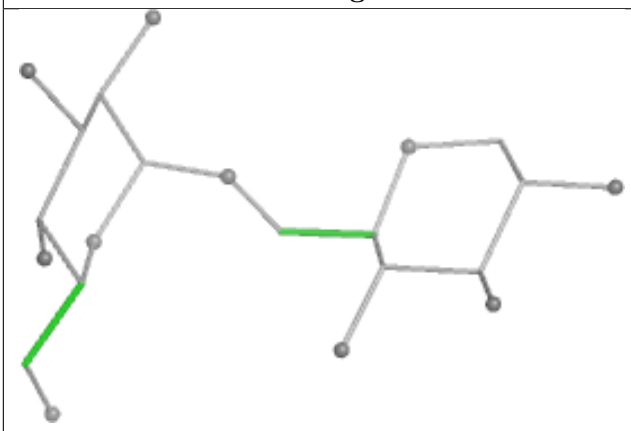
Oligosaccharide Chain D



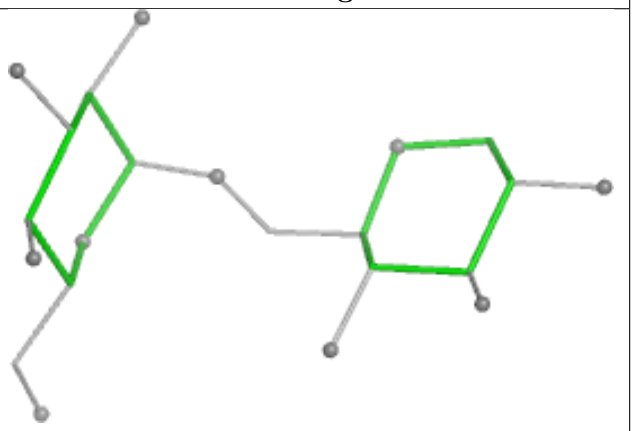
Bond lengths



Bond angles

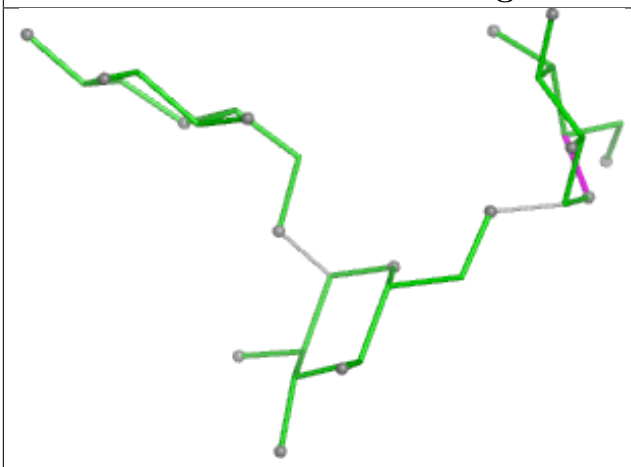


Torsions

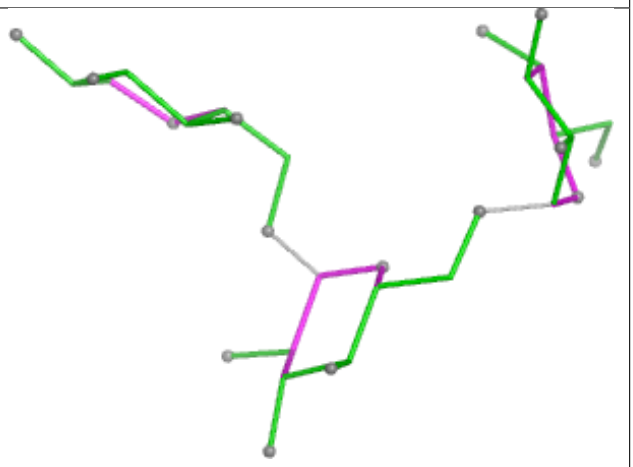


Rings

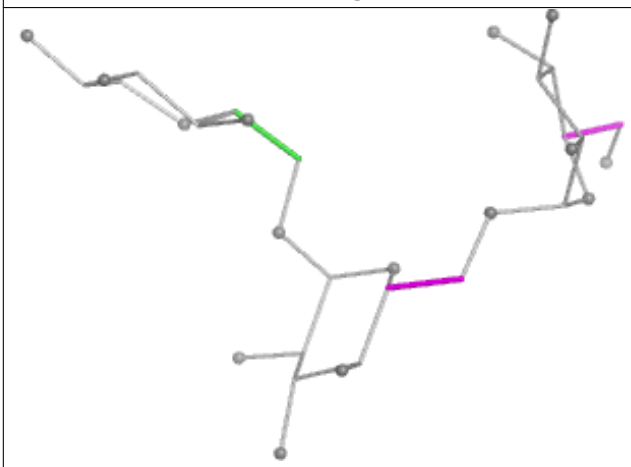
Oligosaccharide Chain F



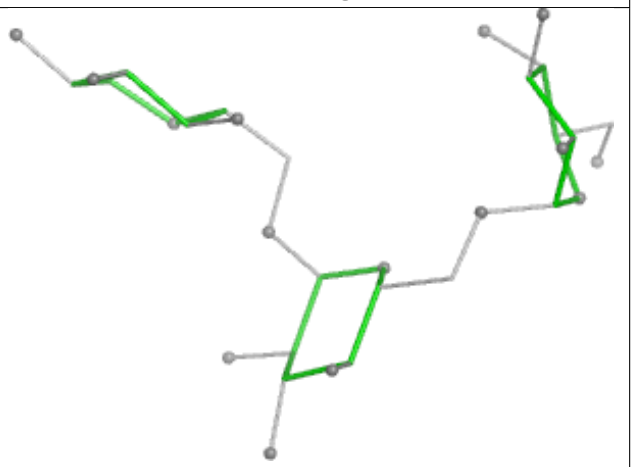
Bond lengths



Bond angles

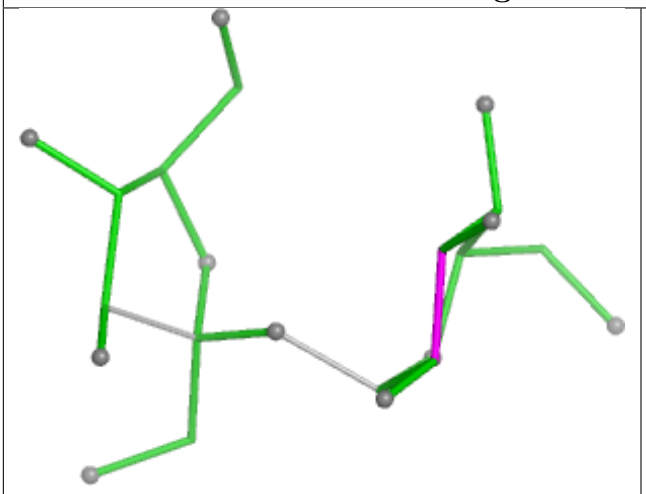


Torsions

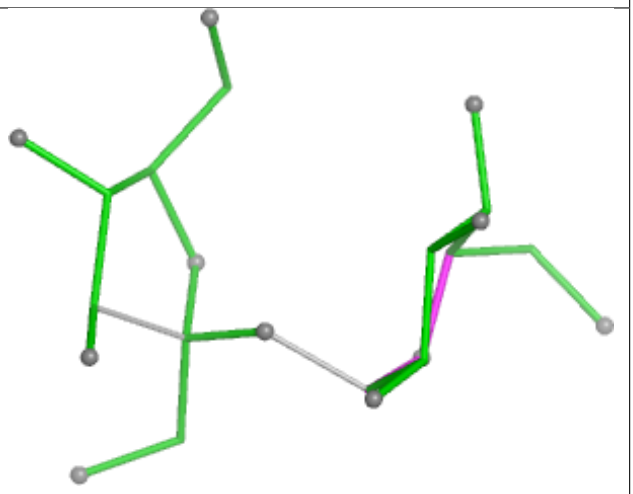


Rings

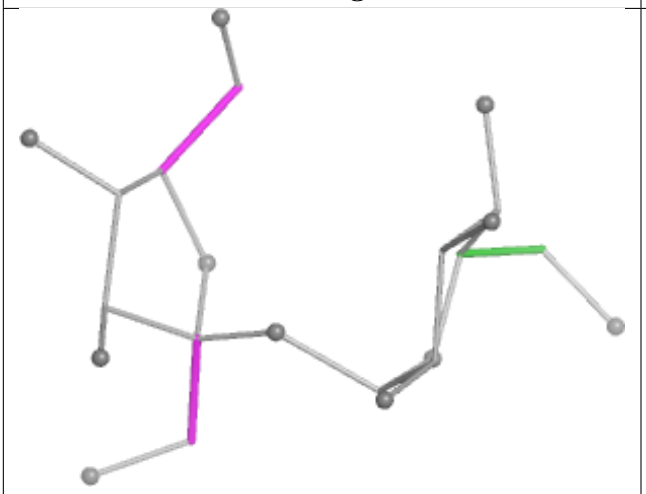
Oligosaccharide Chain G



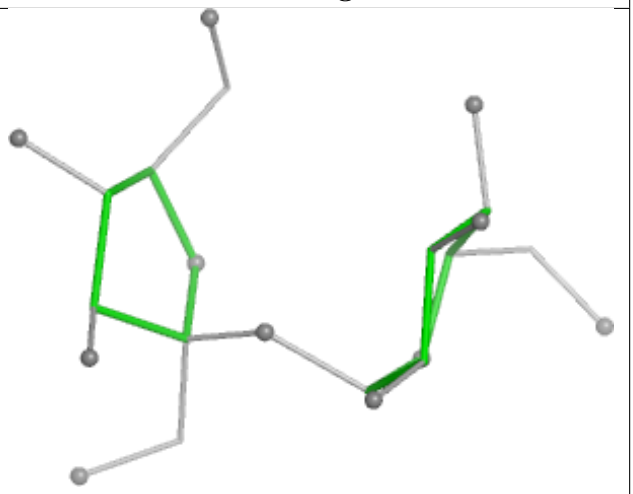
Bond lengths



Bond angles

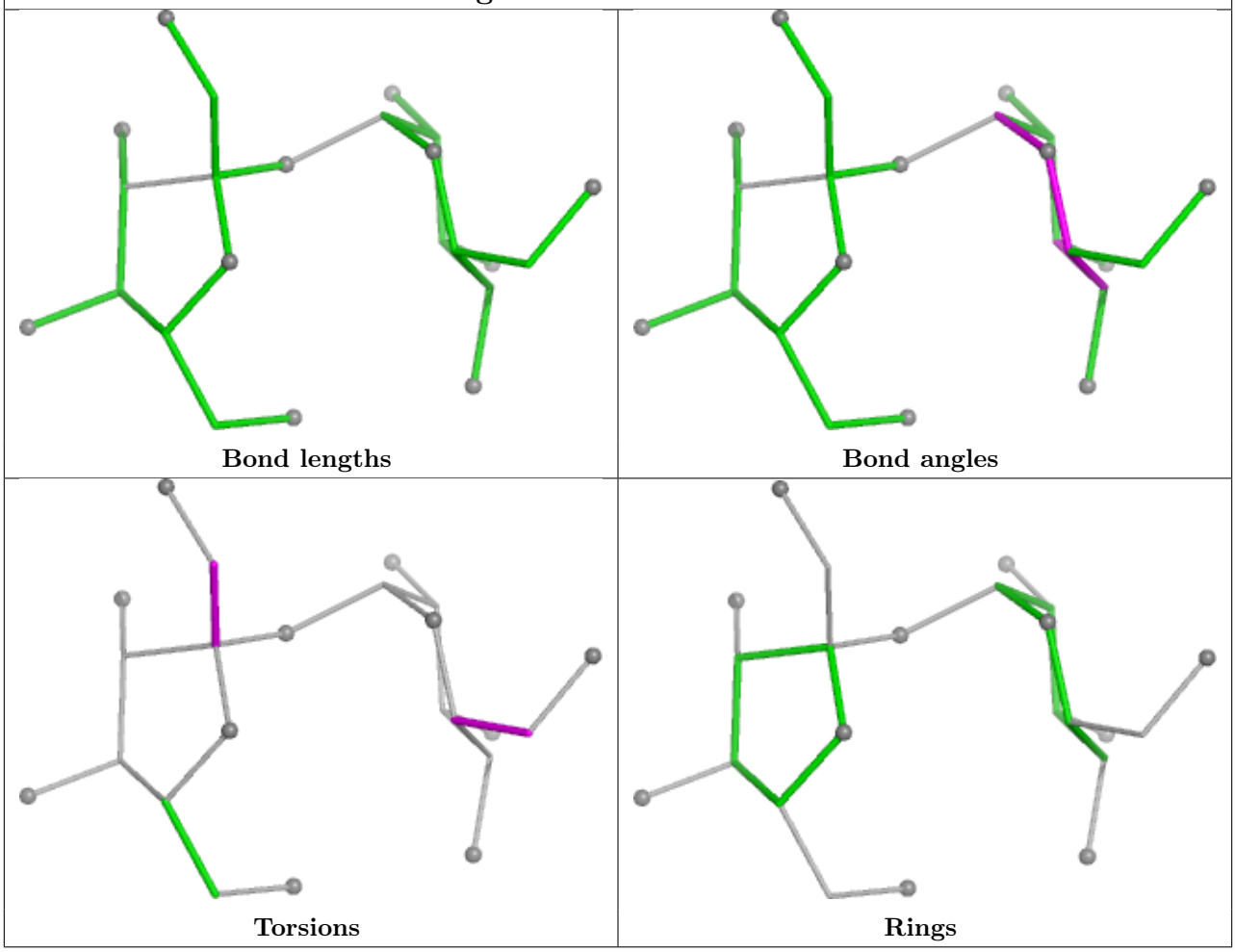


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1153/1183 (97%)	-0.10	14 (1%)	76	58	43, 66, 116, 184	0
1	B	1155/1183 (97%)	-0.30	2 (0%)	91	83	32, 59, 92, 139	0
All	All	2308/2366 (97%)	-0.20	16 (0%)	84	68	32, 63, 107, 184	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1306	GLN	3.3
1	A	449	VAL	3.0
1	A	446	VAL	3.0
1	A	561	THR	2.7
1	A	450	TYR	2.5

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(Å^2)	Q<0.9
4	GLC	F	3	11/12	0.57	0.17	112,137,151,156	0
3	GLC	D	1	11/12	0.69	0.13	110,125,133,137	0
3	GLC	D	2	11/12	0.72	0.15	101,119,133,133	0
2	GLC	E	1	11/12	0.79	0.13	58,86,91,97	0
2	GLC	C	1	11/12	0.86	0.13	63,89,93,98	0

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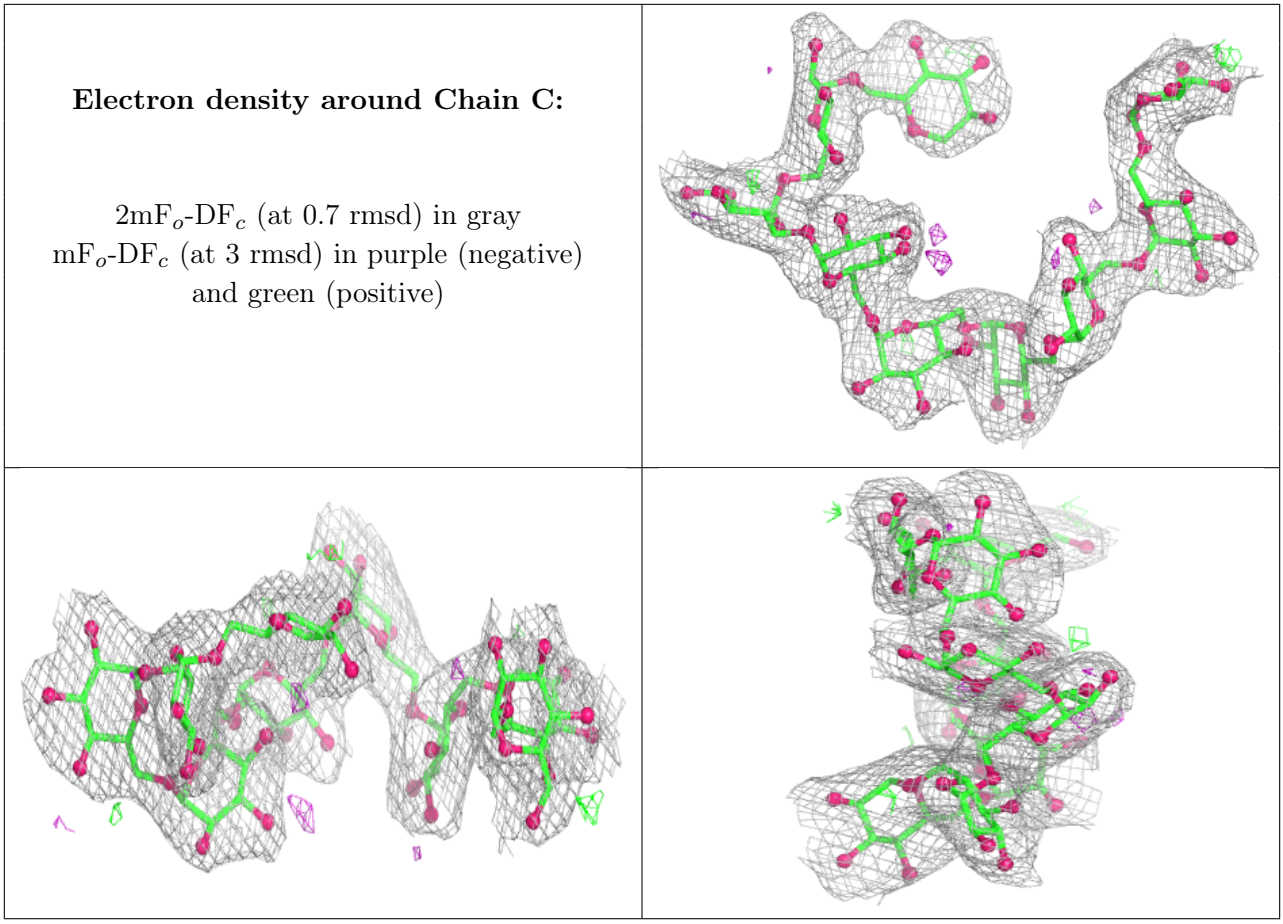
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	C	9	11/12	0.86	0.09	66,74,79,82	0
4	GLC	F	1	11/12	0.87	0.12	80,99,109,115	0
4	GLC	F	2	11/12	0.89	0.12	66,76,100,123	0
2	GLC	E	9	11/12	0.90	0.14	68,77,84,86	0
2	GLC	E	5	11/12	0.92	0.08	51,64,66,69	0
5	FRU	G	2	12/12	0.92	0.11	56,63,70,72	0
5	GLC	H	1	11/12	0.93	0.08	46,58,62,62	0
2	GLC	C	4	11/12	0.94	0.07	45,47,49,51	0
2	GLC	C	5	11/12	0.95	0.07	51,56,58,62	0
2	GLC	C	7	11/12	0.95	0.07	48,50,53,54	0
2	GLC	E	2	11/12	0.95	0.07	45,46,50,51	0
5	FRU	H	2	12/12	0.95	0.08	48,55,59,64	0
2	GLC	C	2	11/12	0.96	0.06	47,49,52,54	0
2	GLC	E	7	11/12	0.96	0.06	42,47,51,57	0
5	GLC	G	1	11/12	0.96	0.08	53,58,61,63	0
2	GLC	C	3	11/12	0.97	0.06	43,47,51,52	0
2	GLC	E	8	11/12	0.97	0.06	42,46,57,64	0
2	GLC	C	8	11/12	0.97	0.06	47,53,59,65	0
2	GLC	E	3	11/12	0.97	0.06	41,46,50,51	0
2	GLC	E	4	11/12	0.97	0.06	42,46,52,58	0
2	GLC	C	6	11/12	0.97	0.06	47,48,51,51	0
2	GLC	E	6	11/12	0.98	0.05	46,49,50,52	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.

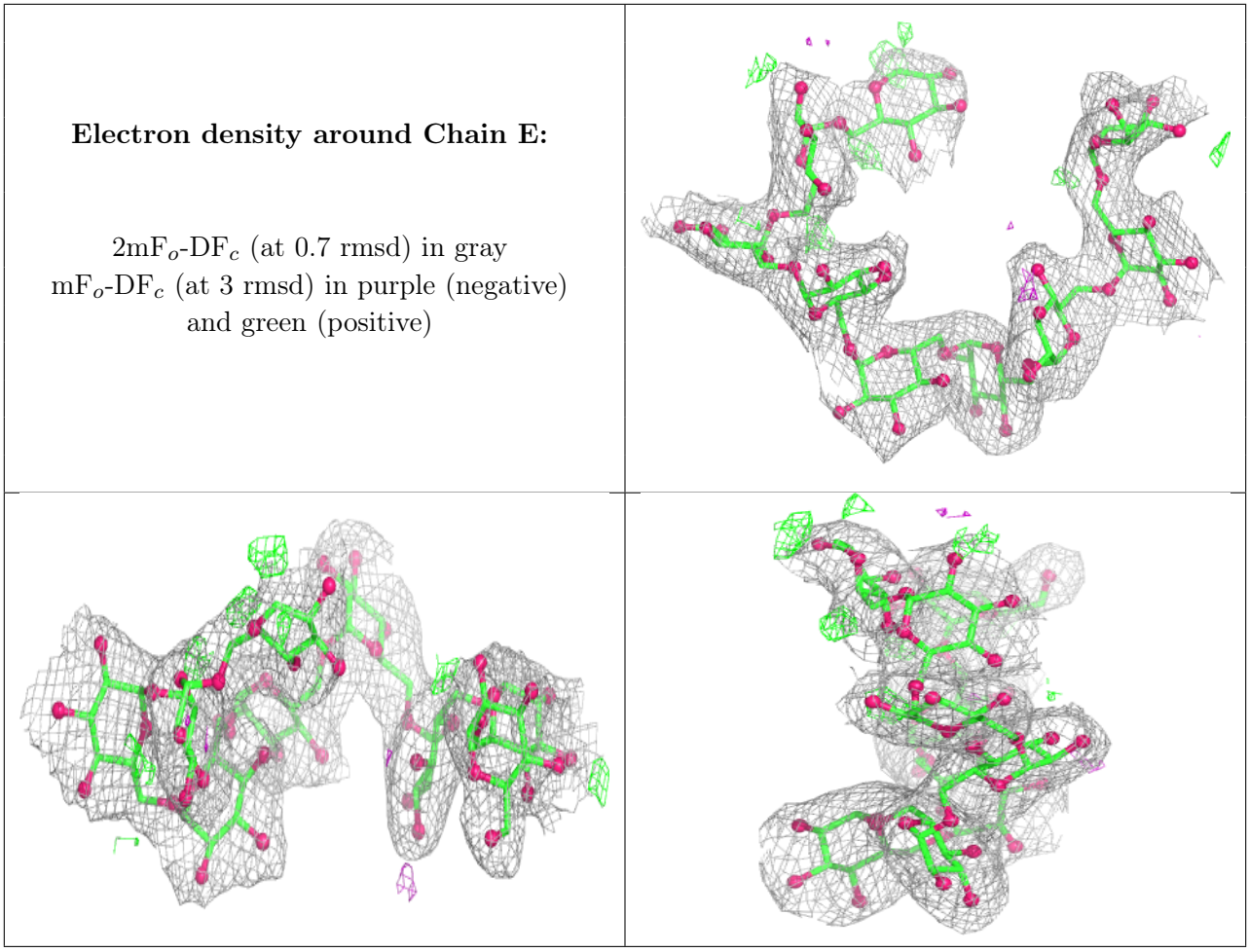
Electron density around Chain C:

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



Electron density around Chain E:

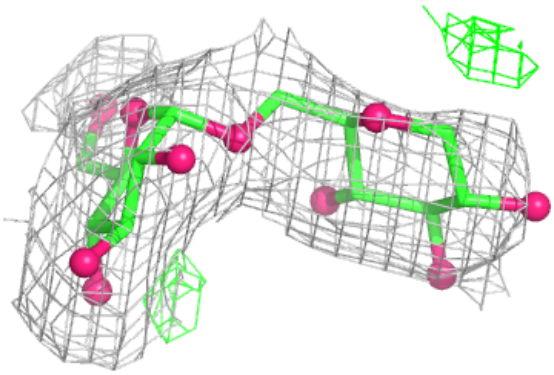
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

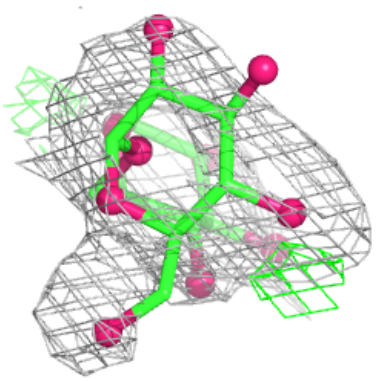


Electron density around Chain D:

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

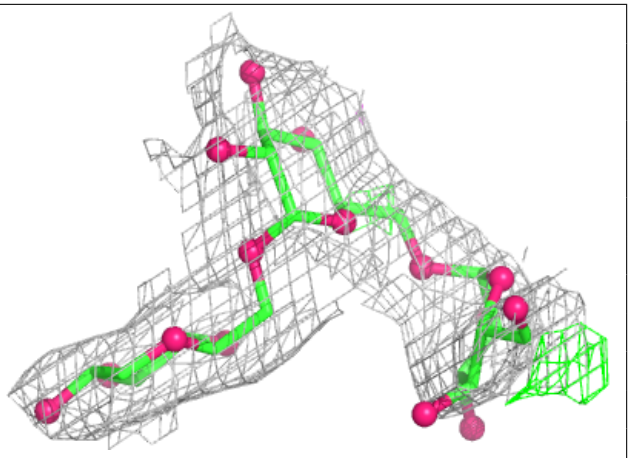


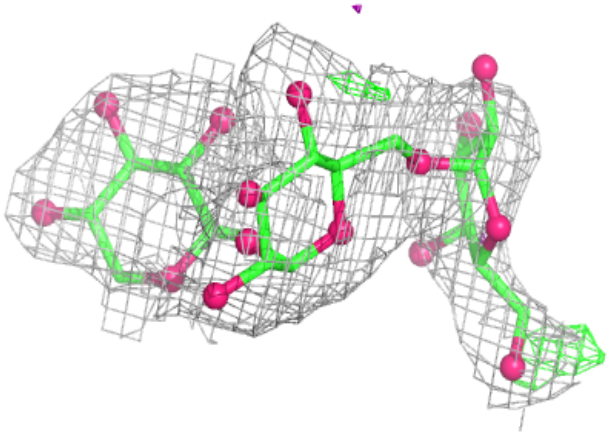


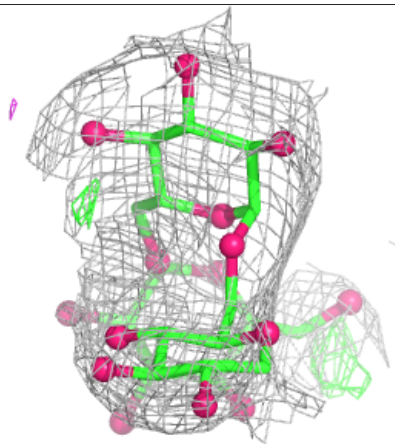


Electron density around Chain F:

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

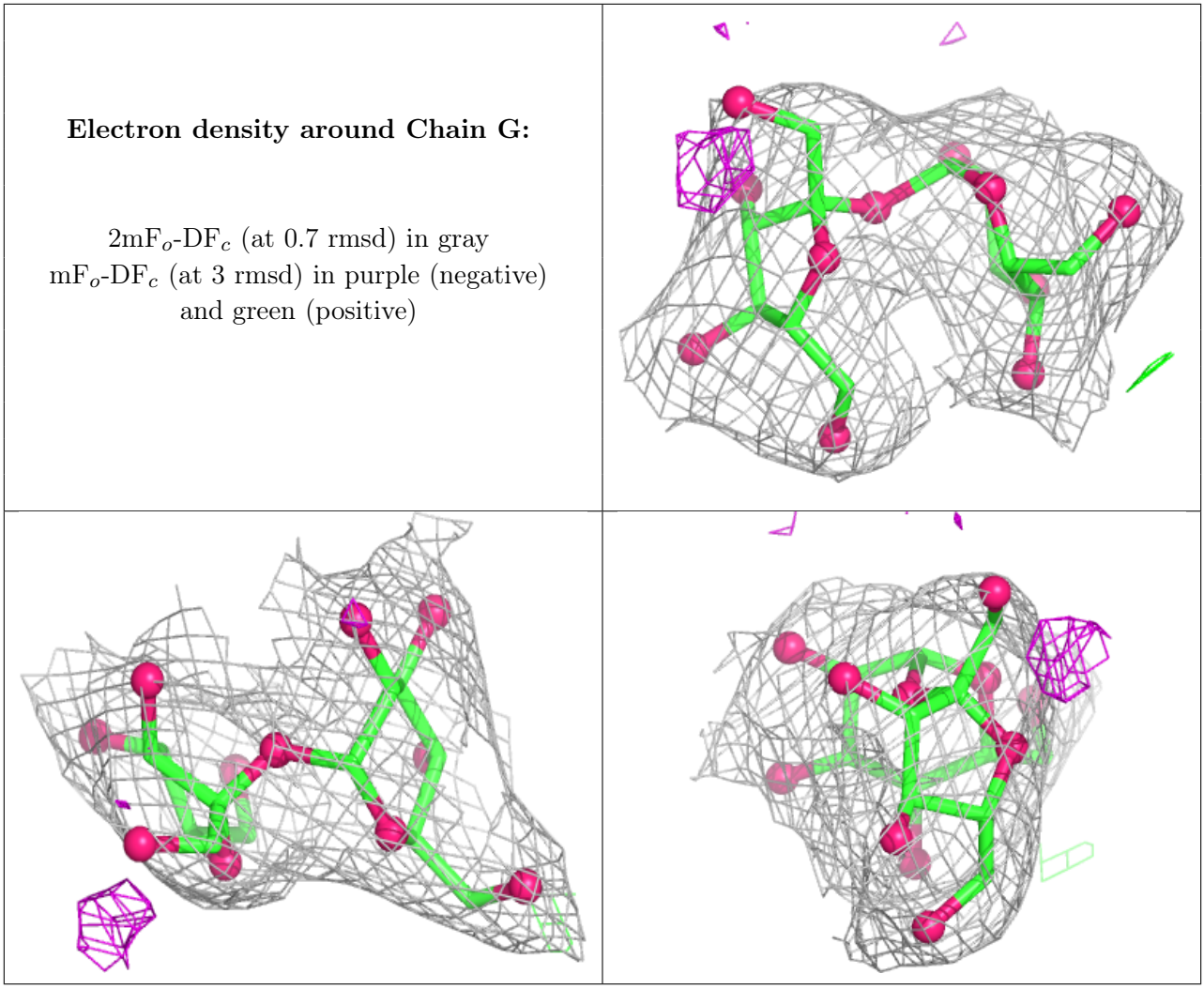






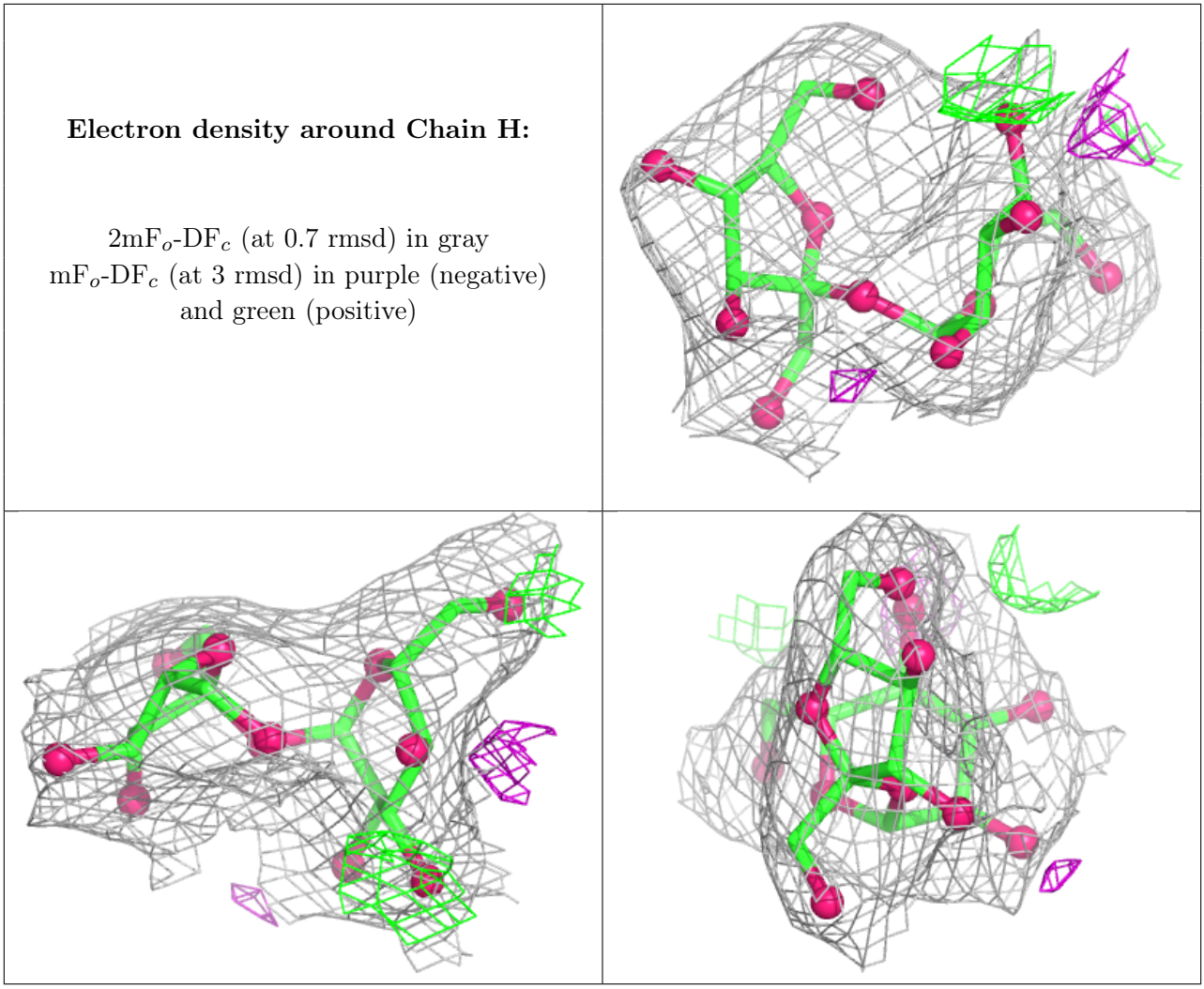
Electron density around Chain G:

$2mF_o$-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, 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
6	CA	B	1401	1/1	0.98	0.04	46,46,46,46	0
6	CA	A	1401	1/1	0.99	0.02	48,48,48,48	0

6.5 Other polymers

There are no such residues in this entry.