



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:10 AM UTC

PDB ID : 7R55 / pdb_00007r55
Title : B-trefoil lectin from *Salpingoeca rosetta* in complex with Gb3
Authors : Notova, S.; Varrot, A.
Deposited on : 2022-02-10
Resolution : 1.84 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

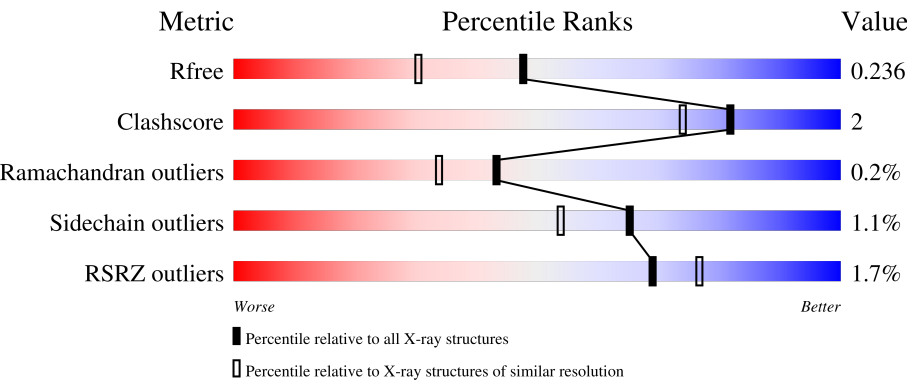
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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.



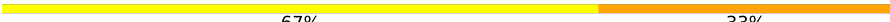
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
2	C	3	
2	D	3	
2	E	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	3	 67% 33%

2 Entry composition [i](#)

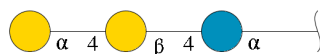
There are 4 unique types of molecules in this entry. The entry contains 10902 atoms, of which 5083 are hydrogens and 0 are deuteriums.

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 Sarol-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	324	Total	C	H	N	O	S	120	9	0
			5023	1593	2480	454	488	8			
1	B	325	Total	C	H	N	O	S	119	6	0
			4996	1586	2469	448	485	8			

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	H	O	11	0	0
			66	18	32	16			
2	D	3	Total	C	H	O	11	0	0
			66	18	32	16			
2	E	3	Total	C	H	O	11	0	0
			66	18	32	16			
2	F	3	Total	C	H	O	11	0	0
			66	18	32	16			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	1	0
			10	2	6	2		

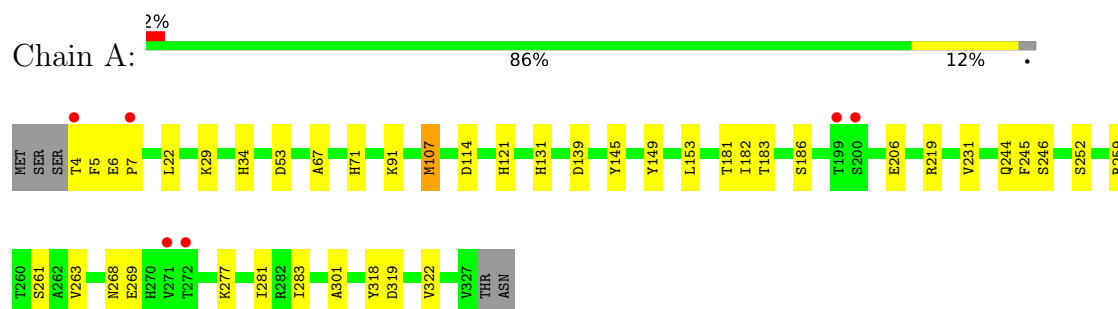
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	331	Total	O	0	2
			333	333		
4	B	273	Total	O	0	3
			276	276		

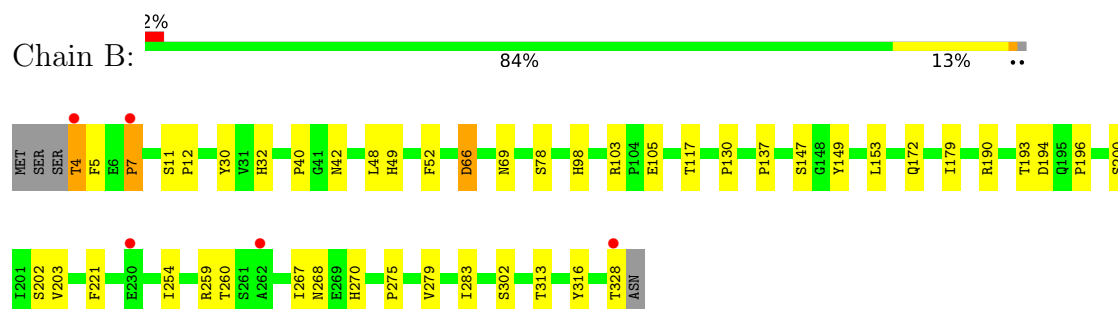
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

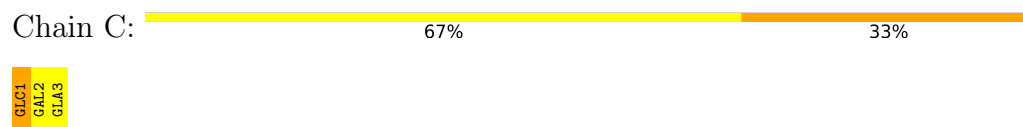
- Molecule 1: Sarol-1



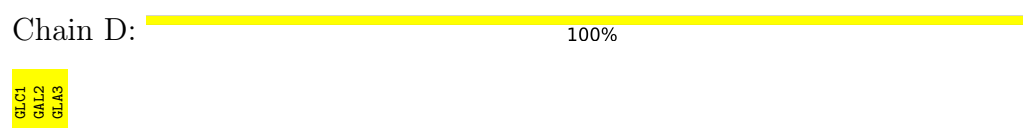
- Molecule 1: Sarol-1



- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranos e



- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranos e



- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranos e

Chain E:  100%

GLC1
GAL2
GLA3

- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain F:  67%  33%

GLC1
GAL2
GLA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.34Å 59.00Å 210.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.18 – 1.84 45.18 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.18-1.84) 99.6 (45.18-1.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.184 , 0.240 0.181 , 0.236	Depositor DCC
R_{free} test set	2982 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10902	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1221e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, EDO, GLA, GAL

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	1.34	16/2605 (0.6%)	1.38	10/3549 (0.3%)
1	B	1.36	10/2589 (0.4%)	1.41	10/3533 (0.3%)
All	All	1.35	26/5194 (0.5%)	1.39	20/7082 (0.3%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	ILE	C-O	7.37	1.32	1.24
1	A	319	ASP	C-O	7.22	1.32	1.23
1	A	318	TYR	C-O	7.00	1.33	1.24
1	B	283	ILE	C-O	6.76	1.31	1.24
1	A	245	PHE	C-O	6.74	1.32	1.24
1	A	231	VAL	C-O	6.54	1.30	1.23
1	A	7	PRO	C-O	6.39	1.32	1.24
1	A	131	HIS	CE1-NE2	6.09	1.38	1.32
1	B	279	VAL	C-O	6.02	1.30	1.23
1	B	316	TYR	C-O	5.94	1.30	1.23
1	A	283	ILE	C-O	5.93	1.30	1.24
1	A	107	MET	C-O	5.89	1.30	1.23
1	A	145	TYR	C-O	-5.74	1.16	1.23
1	A	206	GLU	C-O	5.70	1.30	1.24
1	A	301	ALA	C-O	-5.69	1.17	1.24
1	B	117	THR	C-O	5.62	1.30	1.24
1	A	22	LEU	C-O	5.58	1.30	1.24
1	B	130	PRO	C-O	-5.43	1.17	1.23
1	B	98	HIS	CE1-NE2	5.35	1.37	1.32
1	B	49	HIS	CE1-NE2	5.20	1.37	1.32
1	B	147	SER	C-O	5.19	1.30	1.23
1	B	302	SER	C-O	5.15	1.30	1.24
1	A	34	HIS	CE1-NE2	5.14	1.37	1.32
1	B	202	SER	C-O	5.12	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	GLU	N-CA	5.07	1.51	1.46
1	A	71	HIS	CE1-NE2	5.02	1.37	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	THR	CA-CB-OG1	-7.04	99.04	109.60
1	B	4	THR	CA-CB-OG1	-6.82	99.37	109.60
1	A	53	ASP	CA-CB-CG	-6.62	105.98	112.60
1	A	114	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	67	ALA	CA-C-N	5.96	128.27	120.28
1	A	67	ALA	C-N-CA	5.96	128.27	120.28
1	B	32	HIS	CA-CB-CG	5.74	119.54	113.80
1	A	319	ASP	N-CA-C	-5.63	100.16	108.99
1	B	5	PHE	CA-C-O	-5.42	114.57	120.81
1	B	66	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	69	ASN	CA-CB-CG	-5.38	107.22	112.60
1	B	196	PRO	N-CA-C	-5.36	102.77	111.14
1	A	268	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	183	THR	CA-C-O	-5.19	114.72	120.38
1	B	194	ASP	CB-CA-C	-5.17	101.82	110.56
1	A	5	PHE	CA-C-O	-5.09	114.89	120.69
1	A	206	GLU	CA-C-N	5.07	127.07	120.28
1	A	206	GLU	C-N-CA	5.07	127.07	120.28
1	B	268	ASN	CA-CB-CG	-5.03	107.57	112.60
1	B	275	PRO	CB-CA-C	5.02	117.94	111.46

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	2543	2480	2424	11	1
1	B	2527	2469	2415	14	1
2	C	34	32	30	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	34	32	30	0	0
2	E	34	32	30	0	0
2	F	34	32	30	1	0
3	B	4	6	6	0	0
4	A	333	0	0	1	0
4	B	276	0	0	4	0
All	All	5819	5083	4965	25	1

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 2.

All (25) 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:269:GLU:HG3	1:A:322:VAL:HG11	1.64	0.77
1:B:203[A]:VAL:HG22	1:B:267:ILE:HB	1.72	0.71
1:B:221:PHE:CD2	1:B:254[B]:ILE:HD11	2.29	0.68
1:B:105:GLU:OE2	4:B:501:HOH:O	2.12	0.68
1:A:29:LYS:HE3	1:A:139:ASP:OD1	1.95	0.67
1:A:219:ARG:O	1:A:252[A]:SER:OG	2.23	0.57
1:B:48:LEU:HD12	1:B:137:PRO:HG2	1.92	0.52
1:B:42:ASN:HD22	2:F:1:GLC:H3	1.77	0.50
1:B:66:ASP:HA	4:B:503:HOH:O	2.11	0.50
1:B:12:PRO:HG2	4:B:618:HOH:O	2.12	0.48
1:B:7:PRO:O	1:B:11:SER:HB3	2.13	0.48
1:A:149:TYR:HA	1:A:153:LEU:HD12	1.96	0.47
1:B:190:ARG:NH2	4:B:518:HOH:O	2.47	0.47
1:B:259:ARG:O	1:B:260:THR:C	2.61	0.44
1:A:107:MET:O	1:A:121:HIS:HA	2.19	0.43
1:B:149:TYR:HA	1:B:153:LEU:HD12	2.01	0.43
1:A:186:SER:HB3	1:A:281:ILE:HG12	2.00	0.43
1:B:40:PRO:HD2	1:B:78:SER:HB3	2.00	0.42
1:B:200:SER:HB3	1:B:270:HIS:CD2	2.55	0.42
1:A:244:GLN:HB3	1:A:259:ARG:HD3	2.01	0.42
1:A:261:SER:OG	1:A:263:VAL:HG22	2.20	0.42
1:A:91:LYS:NZ	2:C:1:GLC:O2	2.46	0.41
1:A:4:THR:N	4:A:420:HOH:O	2.54	0.41
1:B:30:TYR:CE1	1:B:52:PHE:HB2	2.56	0.41
1:A:277:LYS:HA	1:A:277:LYS:HD3	1.96	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:THR:HG1	1:B:179:ILE:H[1_565]	1.33	0.27

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	331/329 (101%)	324 (98%)	7 (2%)	0	100	100
1	B	329/329 (100%)	317 (96%)	11 (3%)	1 (0%)	36	25
All	All	660/658 (100%)	641 (97%)	18 (3%)	1 (0%)	43	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	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	276/289 (96%)	275 (100%)	1 (0%)	84	78
1	B	275/289 (95%)	270 (98%)	5 (2%)	51	35
All	All	551/578 (95%)	545 (99%)	6 (1%)	65	54

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	SER
1	B	4	THR
1	B	103	ARG
1	B	172	GLN
1	B	193	THR
1	B	328	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	B	42	ASN
1	B	195	GLN
1	B	270	HIS
1	B	280	GLN

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	C	1	2	12,12,12	0.74	0	17,17,17	1.13	2 (11%)
2	GAL	C	2	2	11,11,12	0.83	1 (9%)	15,15,17	1.56	2 (13%)
2	GLA	C	3	2	11,11,12	1.18	2 (18%)	15,15,17	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	D	1	2	12,12,12	1.61	4 (33%)	17,17,17	3.05	10 (58%)
2	GAL	D	2	2	11,11,12	1.05	1 (9%)	15,15,17	1.81	3 (20%)
2	GLA	D	3	2	11,11,12	0.96	0	15,15,17	1.47	2 (13%)
2	GLC	E	1	2	12,12,12	1.24	2 (16%)	17,17,17	1.61	4 (23%)
2	GAL	E	2	2	11,11,12	0.91	1 (9%)	15,15,17	1.55	3 (20%)
2	GLA	E	3	2	11,11,12	1.11	1 (9%)	15,15,17	0.95	0
2	GLC	F	1	2	12,12,12	1.52	4 (33%)	17,17,17	3.05	11 (64%)
2	GAL	F	2	2	11,11,12	1.20	1 (9%)	15,15,17	2.14	9 (60%)
2	GLA	F	3	2	11,11,12	1.03	1 (9%)	15,15,17	1.48	2 (13%)

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	-	2/2/22/22	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	GLA	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GAL	D	2	2	-	1/2/19/22	0/1/1/1
2	GLA	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	1	2	-	2/2/22/22	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	GLA	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	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	GLA	F	3	2	-	0/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	GLC	O1-C1	3.12	1.49	1.39
2	F	2	GAL	O5-C5	2.52	1.48	1.43
2	F	1	GLC	O4-C4	2.47	1.49	1.43
2	E	1	GLC	O5-C1	2.36	1.48	1.42
2	C	3	GLA	C2-C3	2.34	1.56	1.52
2	D	1	GLC	O4-C4	2.32	1.48	1.43
2	F	1	GLC	O1-C1	2.25	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	GLC	C1-C2	-2.23	1.47	1.52
2	E	1	GLC	C3-C2	2.20	1.58	1.52
2	F	1	GLC	C4-C5	-2.19	1.48	1.53
2	C	2	GAL	O2-C2	-2.17	1.38	1.43
2	E	3	GLA	C2-C3	-2.14	1.49	1.52
2	D	2	GAL	O5-C5	2.13	1.47	1.43
2	F	1	GLC	C3-C2	2.10	1.57	1.52
2	C	3	GLA	O5-C5	-2.10	1.39	1.43
2	D	1	GLC	O2-C2	2.06	1.48	1.43
2	F	3	GLA	O5-C5	2.04	1.47	1.43
2	E	2	GAL	O5-C5	2.03	1.47	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	GLC	O3-C3-C2	-6.77	94.42	110.38
2	D	1	GLC	O2-C2-C1	-5.73	96.01	109.25
2	D	1	GLC	O5-C5-C4	5.19	119.05	109.70
2	F	1	GLC	O4-C4-C3	4.65	121.34	110.38
2	D	1	GLC	O5-C1-C2	4.65	118.48	110.30
2	F	1	GLC	C3-C4-C5	-4.49	102.09	110.23
2	F	3	GLA	C1-O5-C5	-4.19	106.57	112.19
2	F	1	GLC	O5-C1-C2	-4.15	103.01	110.30
2	D	1	GLC	O1-C1-C2	-4.12	97.01	108.98
2	C	2	GAL	O6-C6-C5	-4.07	97.47	111.33
2	E	2	GAL	O6-C6-C5	-3.70	98.74	111.33
2	D	2	GAL	C1-O5-C5	-3.61	107.35	112.19
2	F	1	GLC	O6-C6-C5	-3.44	99.62	111.33
2	F	2	GAL	O2-C2-C1	-3.37	101.51	109.22
2	D	1	GLC	O3-C3-C2	-3.34	102.51	110.38
2	F	1	GLC	O2-C2-C3	3.15	117.79	110.38
2	D	3	GLA	C3-C4-C5	-3.14	104.53	110.23
2	F	2	GAL	O4-C4-C3	3.03	117.51	110.38
2	D	1	GLC	O6-C6-C5	-2.98	101.19	111.33
2	F	1	GLC	C1-O5-C5	2.90	119.27	113.65
2	D	1	GLC	C4-C3-C2	-2.89	105.76	110.83
2	C	1	GLC	O3-C3-C2	-2.82	103.73	110.38
2	E	1	GLC	C6-C5-C4	2.82	119.93	113.02
2	F	2	GAL	C3-C4-C5	-2.80	105.16	110.23
2	C	2	GAL	O4-C4-C5	-2.70	102.67	109.32
2	F	1	GLC	O5-C5-C6	2.69	113.10	106.44
2	F	2	GAL	C1-O5-C5	-2.66	108.62	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GAL	C3-C4-C5	-2.52	105.66	110.23
2	E	1	GLC	O2-C2-C1	-2.51	103.45	109.25
2	F	3	GLA	O4-C4-C5	2.48	115.43	109.32
2	F	2	GAL	C1-C2-C3	2.45	113.22	109.64
2	D	1	GLC	O1-C1-O5	2.42	117.60	110.41
2	F	2	GAL	O6-C6-C5	-2.36	103.28	111.33
2	D	1	GLC	O4-C4-C3	2.35	115.91	110.38
2	F	2	GAL	C6-C5-C4	-2.32	107.32	113.02
2	E	1	GLC	O5-C1-C2	2.25	114.25	110.30
2	E	2	GAL	O4-C4-C3	2.19	115.54	110.38
2	F	2	GAL	O3-C3-C4	-2.17	105.26	110.38
2	E	2	GAL	O4-C4-C5	-2.15	104.02	109.32
2	C	1	GLC	O6-C6-C5	-2.14	104.05	111.33
2	F	1	GLC	O2-C2-C1	-2.13	104.33	109.25
2	D	1	GLC	O2-C2-C3	2.09	115.31	110.38
2	D	2	GAL	C1-C2-C3	2.06	112.65	109.64
2	F	2	GAL	O3-C3-C2	2.04	114.22	110.05
2	F	1	GLC	O5-C5-C4	2.04	113.37	109.70
2	F	1	GLC	O1-C1-O5	2.03	116.44	110.41
2	E	1	GLC	C1-O5-C5	-2.01	109.77	113.65
2	D	3	GLA	O5-C5-C6	-2.00	103.77	107.66

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	GLC	O5-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	D	2	GAL	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

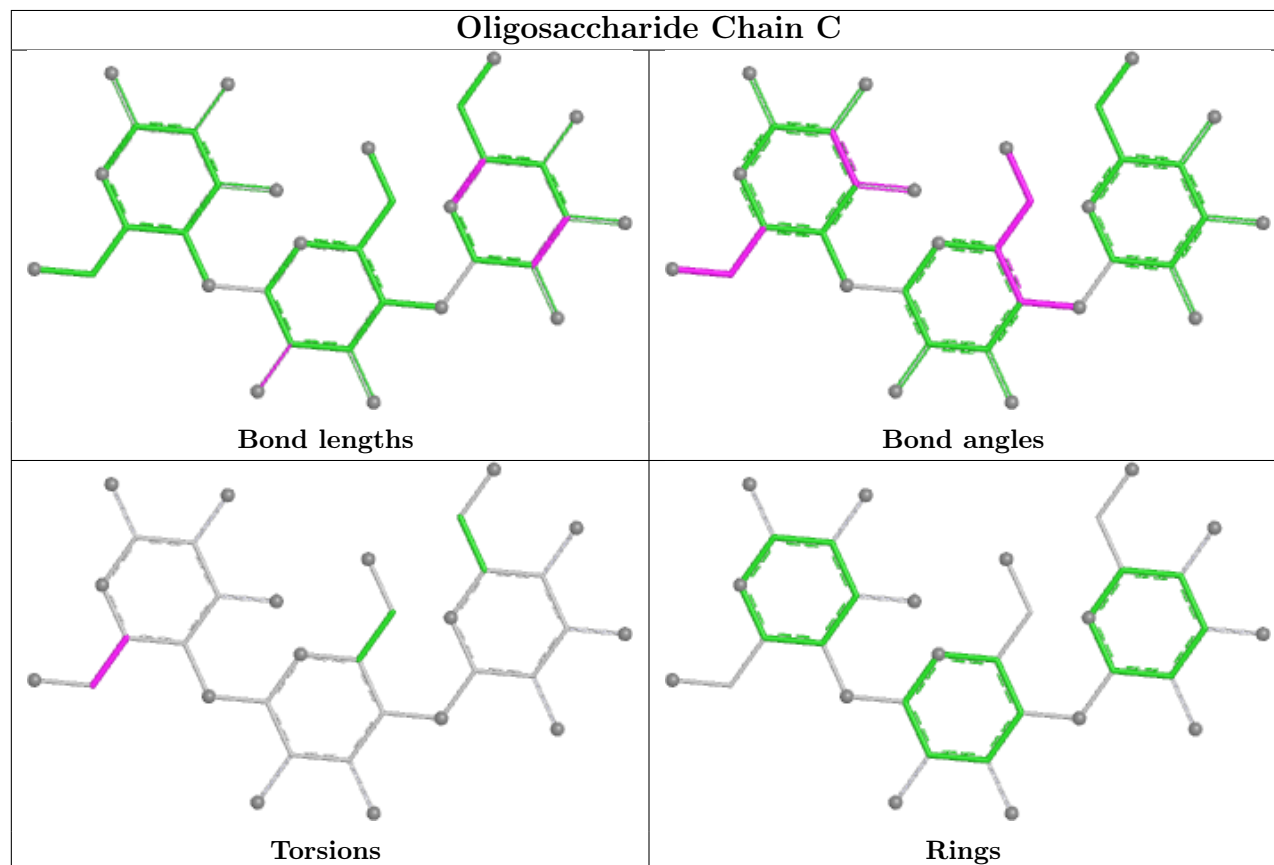
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	1	0

Continued on next page...

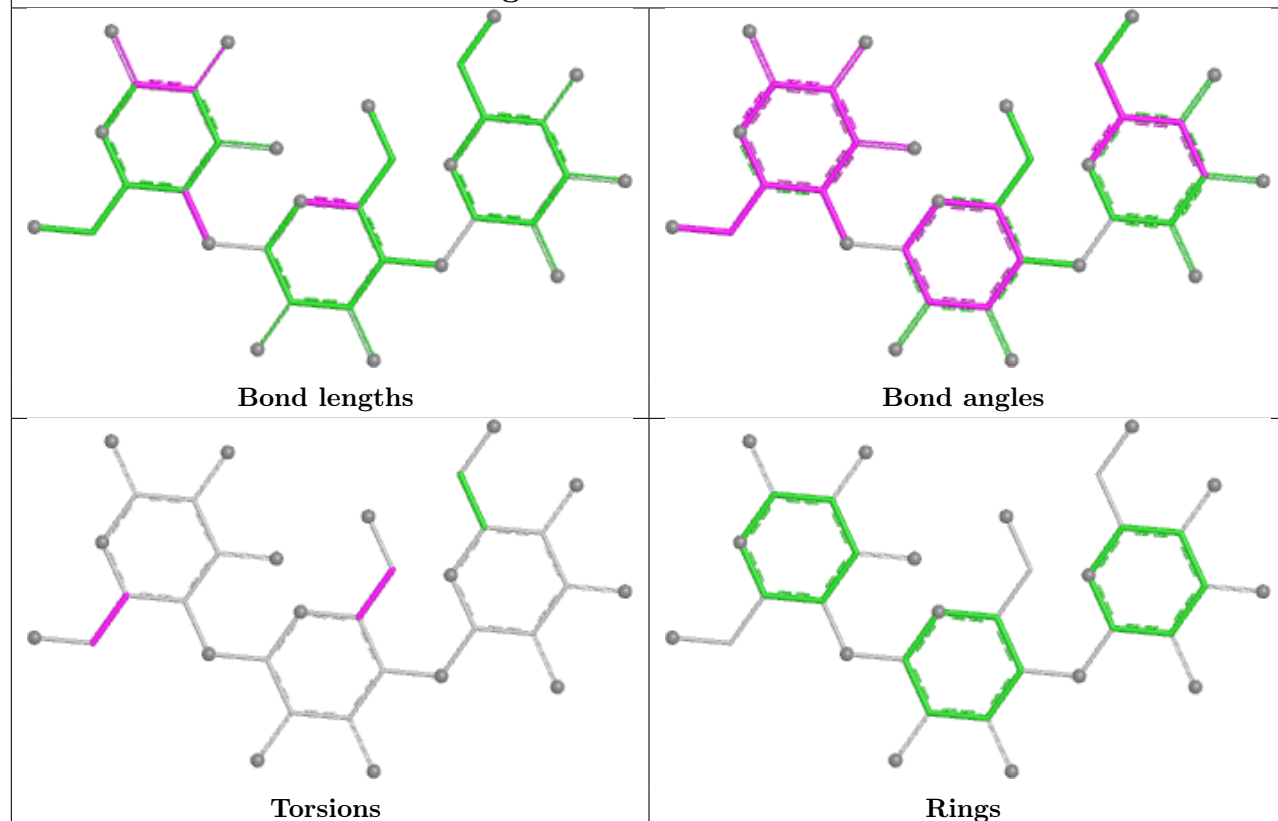
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	GLC	1	0

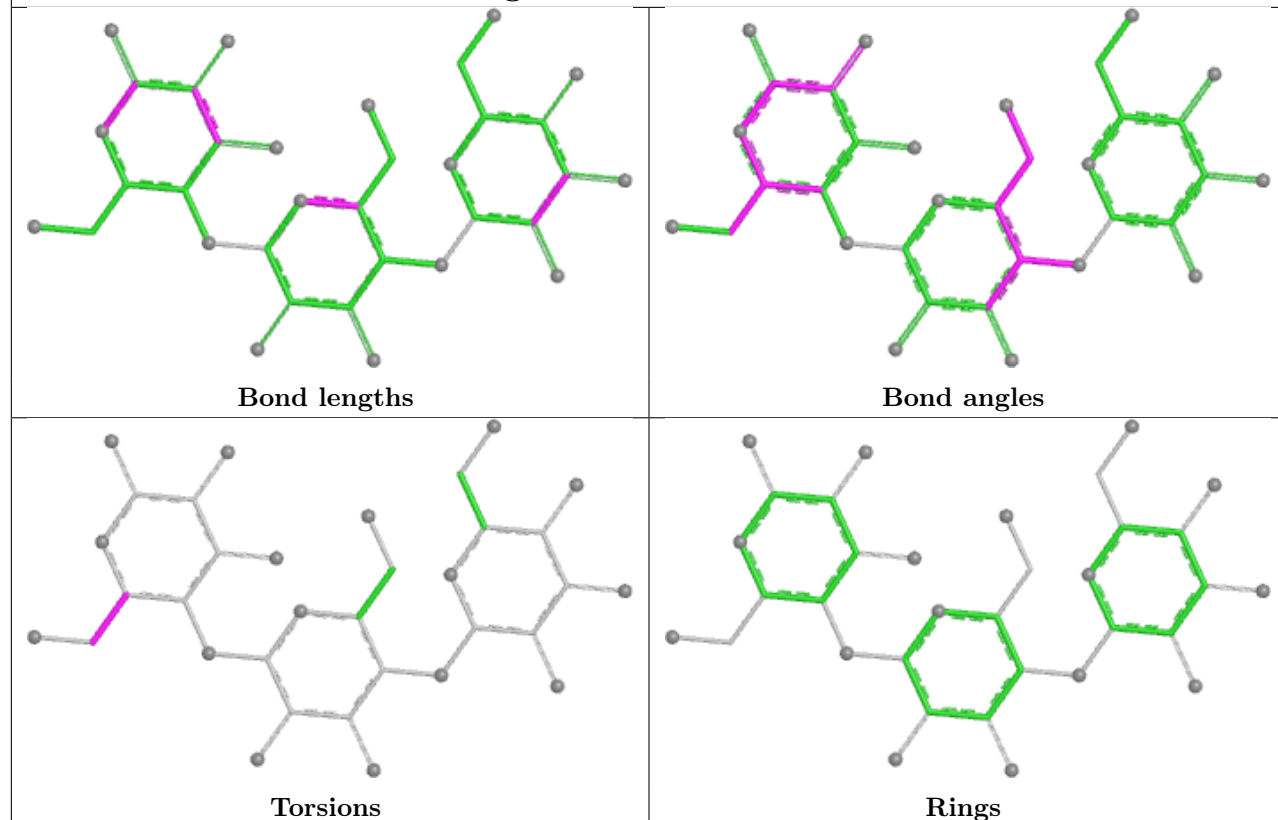
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

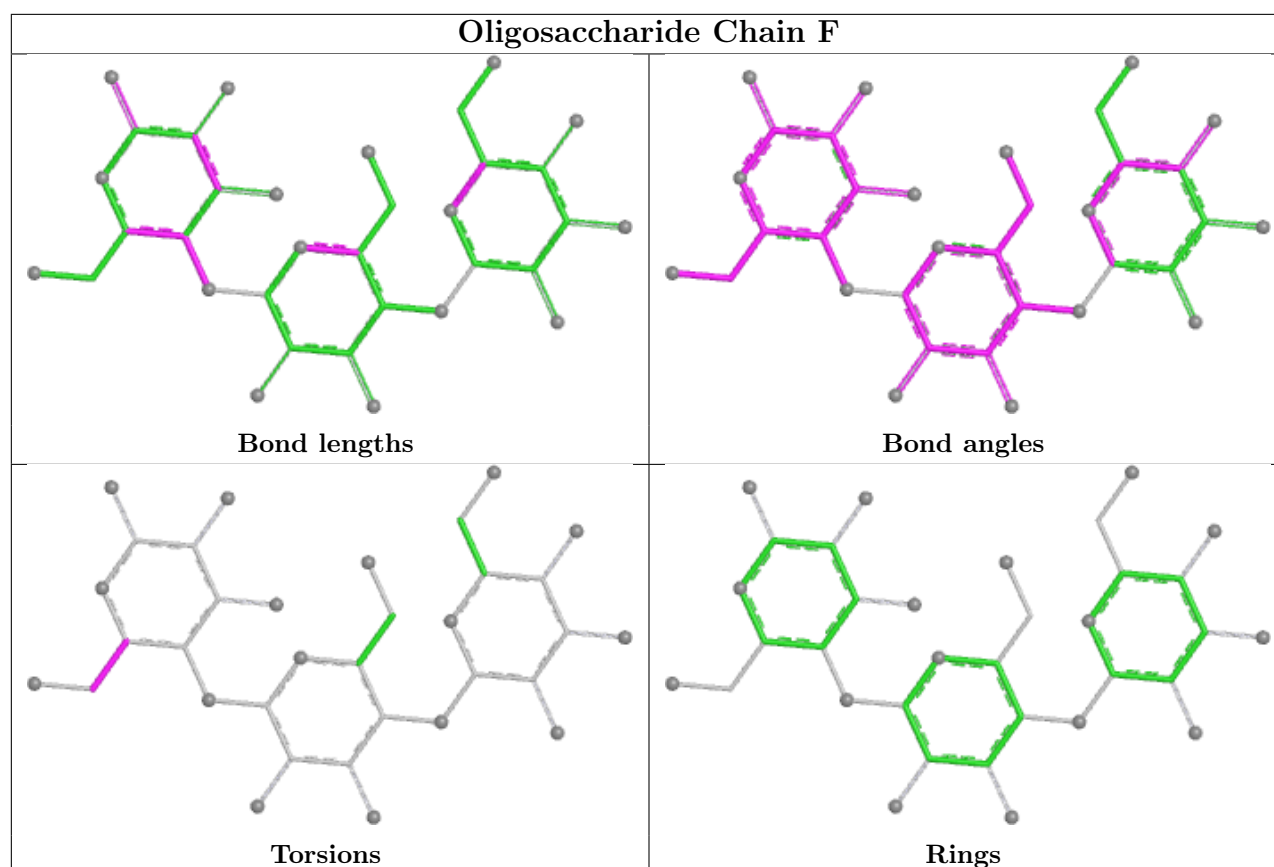


Oligosaccharide Chain D



Oligosaccharide Chain E





5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	EDO	B	401	-	3,3,3	1.13	0	2,2,2	0.49	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
3	EDO	B	401	-	-	0/1/1/1	-

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	324/329 (98%)	-0.26	6 (1%) 66 73	11, 25, 46, 56	9 (2%)
1	B	325/329 (98%)	-0.18	5 (1%) 72 79	12, 28, 48, 65	6 (1%)
All	All	649/658 (98%)	-0.22	11 (1%) 69 77	11, 26, 47, 65	15 (2%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	328	THR	4.1
1	A	272	THR	4.0
1	A	199	THR	3.3
1	A	200	SER	3.1
1	B	4	THR	3.1
1	A	271	VAL	3.0
1	A	7	PRO	2.7
1	B	7	PRO	2.5
1	A	4	THR	2.5
1	B	230[A]	GLU	2.1
1	B	262	ALA	2.1

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

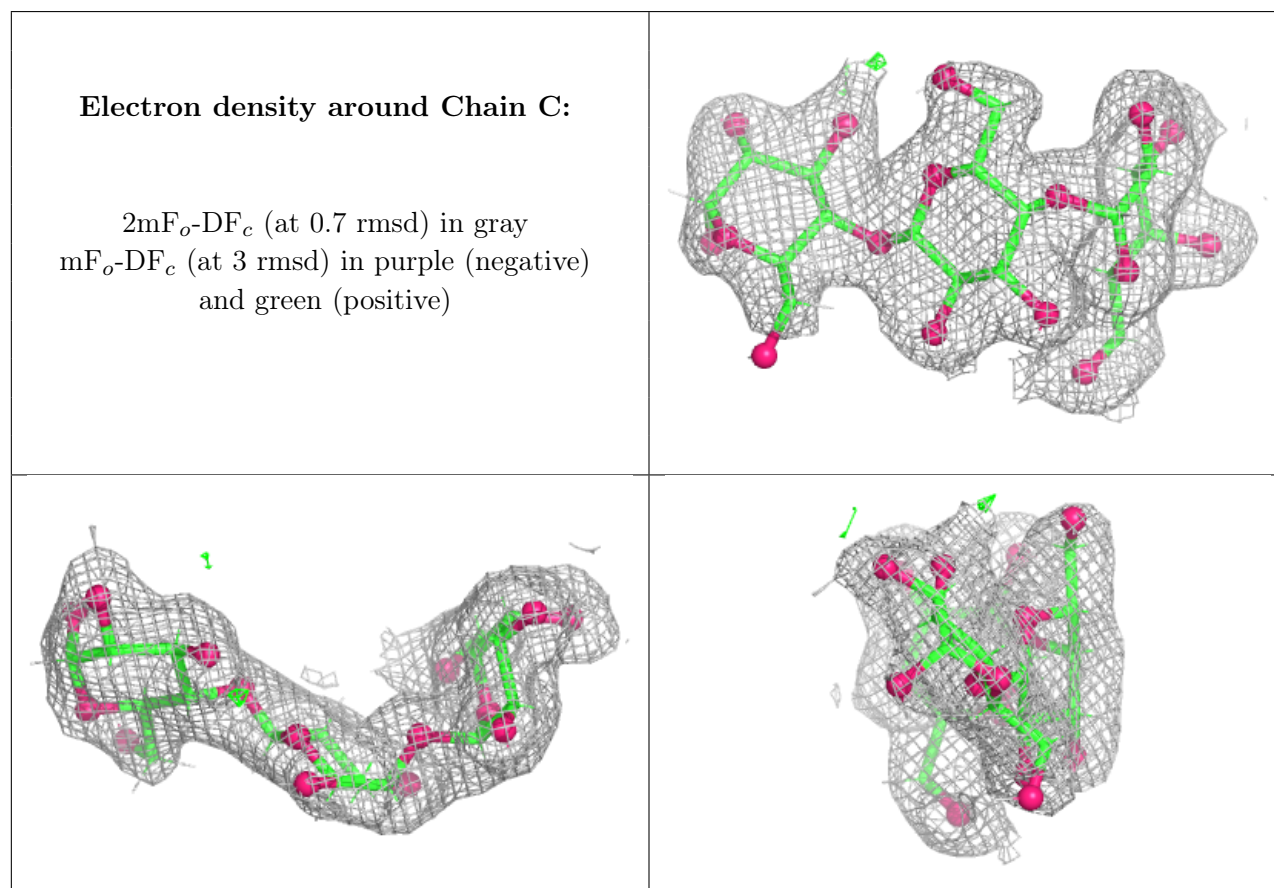
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

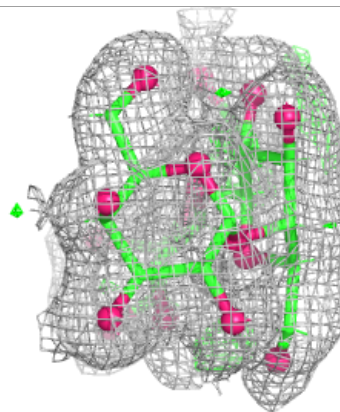
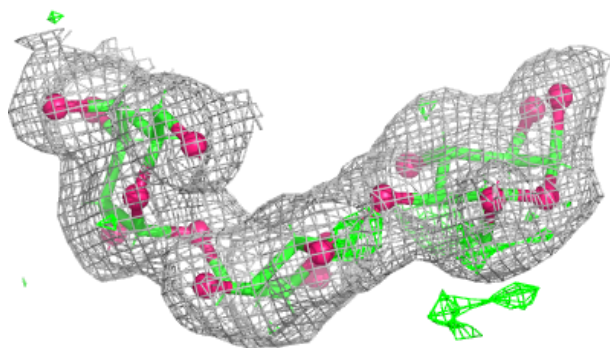
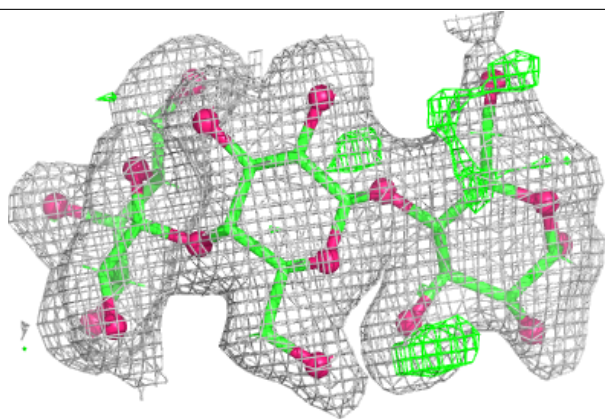
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	D	1	12/12	0.86	0.11	30,42,50,53	4
2	GLC	F	1	12/12	0.86	0.12	30,45,57,60	4
2	GLC	E	1	12/12	0.88	0.10	30,44,54,62	4
2	GLC	C	1	12/12	0.92	0.09	30,42,51,62	4
2	GAL	E	2	11/12	0.95	0.06	23,29,31,35	3
2	GAL	C	2	11/12	0.95	0.07	22,31,41,54	3
2	GAL	D	2	11/12	0.96	0.06	24,28,34,42	3
2	GAL	F	2	11/12	0.96	0.07	22,28,33,39	3
2	GLA	D	3	11/12	0.97	0.04	22,26,30,31	4
2	GLA	C	3	11/12	0.98	0.05	19,23,30,30	4
2	GLA	F	3	11/12	0.98	0.04	20,23,30,30	4
2	GLA	E	3	11/12	0.99	0.03	18,22,30,30	4

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.



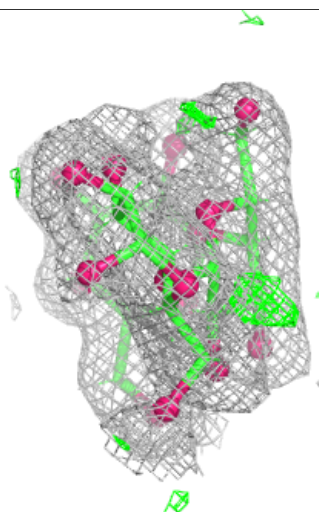
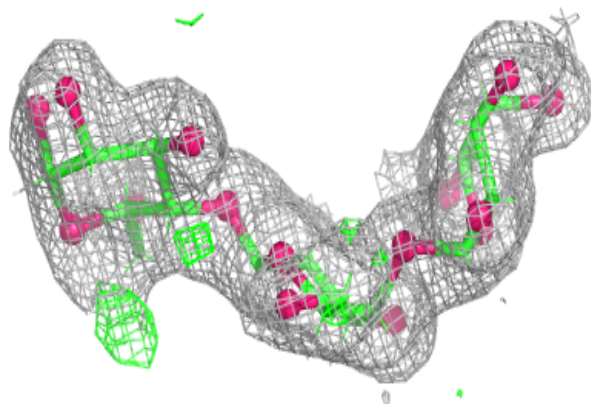
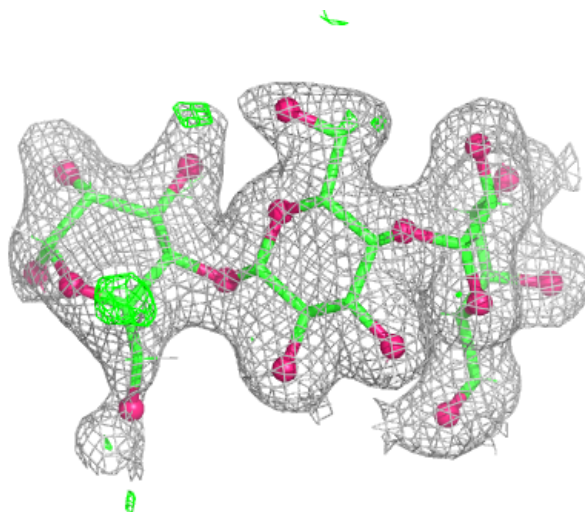
Electron density around Chain D:

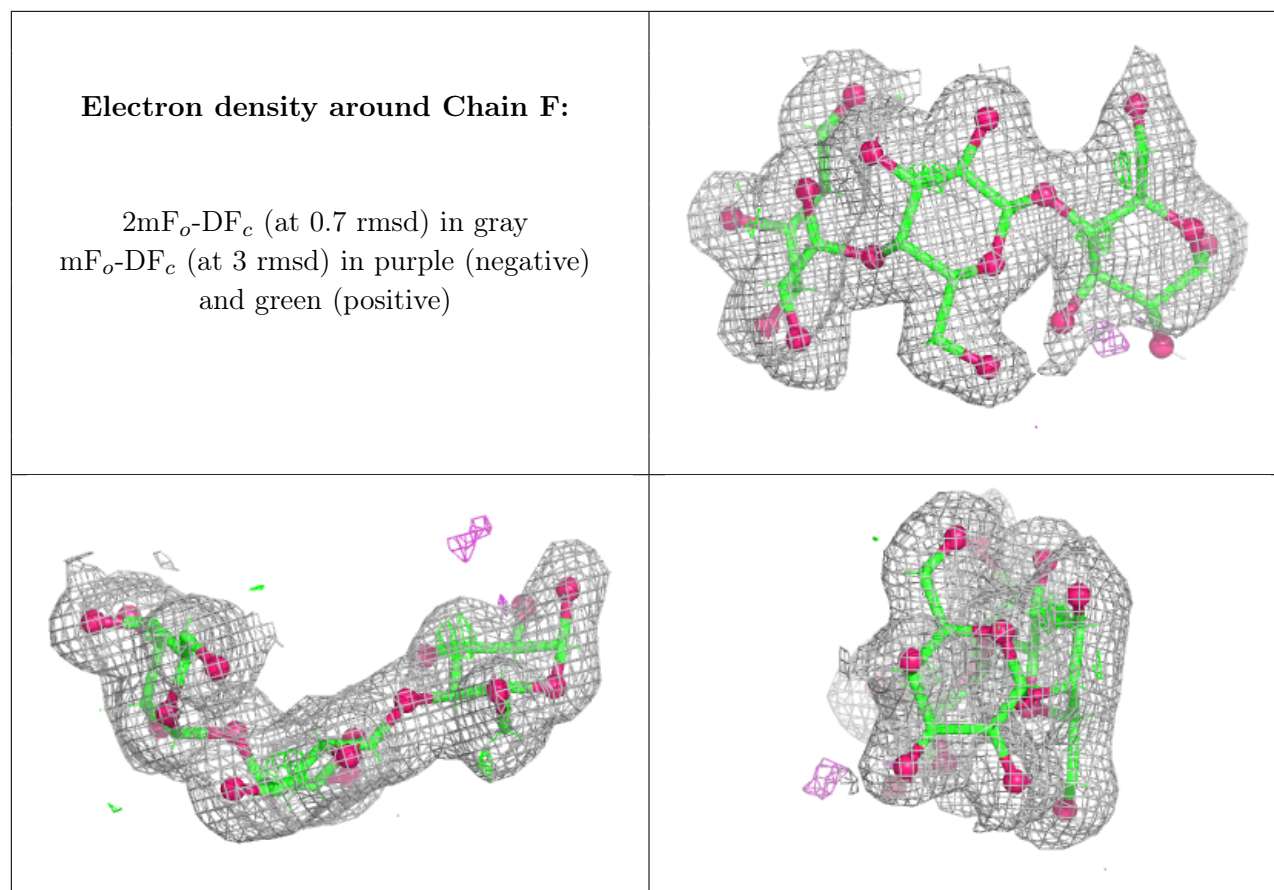
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
3	EDO	B	401	4/4	0.93	0.09	28,30,31,37	1

6.5 Other polymers [i](#)

There are no such residues in this entry.