



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 12:20 AM BST

PDB ID : 6EQ1
Title : Structure of the periplasmic binding protein (PBP) MelB (Atu4661) in complex with stachyose from agrobacterium fabrum C58
Authors : Vigouroux, A.; Morera, S.
Deposited on : 2017-10-12
Resolution : 2.10 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 ⓘ 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

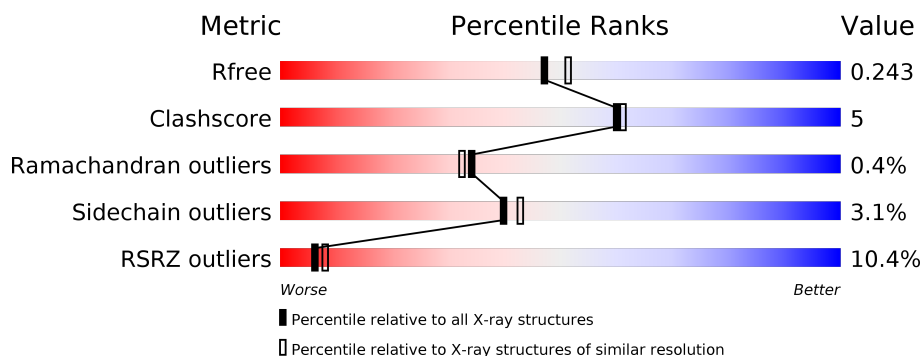
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	683	<div> <div>12%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	B	683	<div> <div>9%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
2	C	4	<div> <div>100%</div> </div>
2	D	4	<div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	B	708	-	-	X	-
5	EDO	B	716	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11000 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.

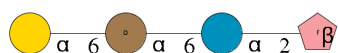
- Molecule 1 is a protein called Periplasmic alpha-galactoside-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	671	Total	C	N	O	S	0	0	0
			5295	3380	899	1000	16			
1	A	669	Total	C	N	O	S	0	0	0
			5277	3370	894	997	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	HIS	-	expression tag	UNP A0A083ZM57
B	679	HIS	-	expression tag	UNP A0A083ZM57
B	680	HIS	-	expression tag	UNP A0A083ZM57
B	681	HIS	-	expression tag	UNP A0A083ZM57
B	682	HIS	-	expression tag	UNP A0A083ZM57
B	683	HIS	-	expression tag	UNP A0A083ZM57
A	678	HIS	-	expression tag	UNP A0A083ZM57
A	679	HIS	-	expression tag	UNP A0A083ZM57
A	680	HIS	-	expression tag	UNP A0A083ZM57
A	681	HIS	-	expression tag	UNP A0A083ZM57
A	682	HIS	-	expression tag	UNP A0A083ZM57
A	683	HIS	-	expression tag	UNP A0A083ZM57

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-alpha-D-idopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-psicofuranose.



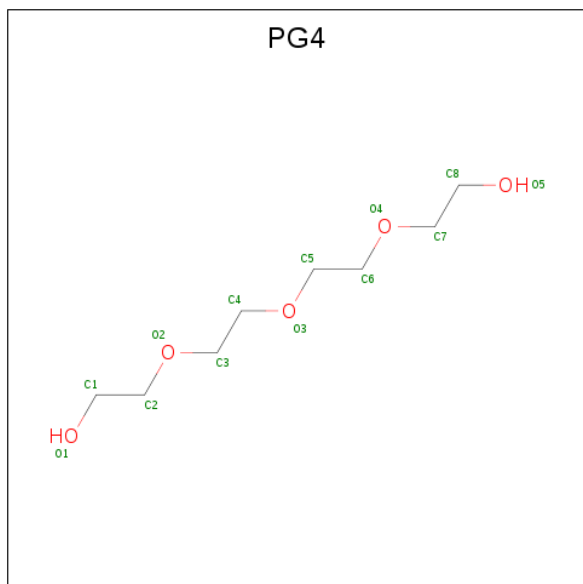
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			

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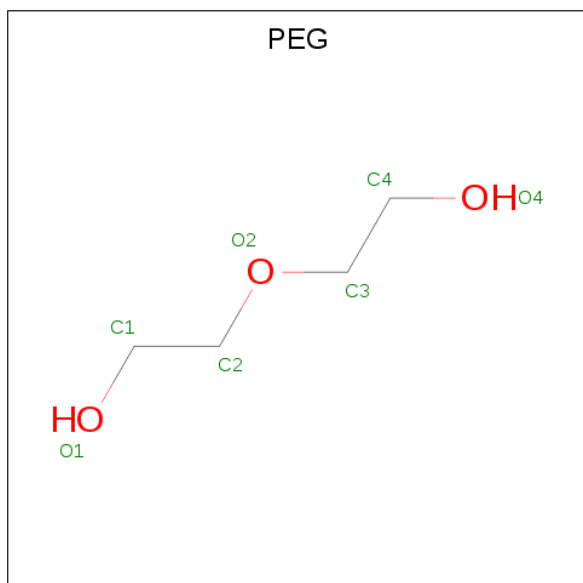
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



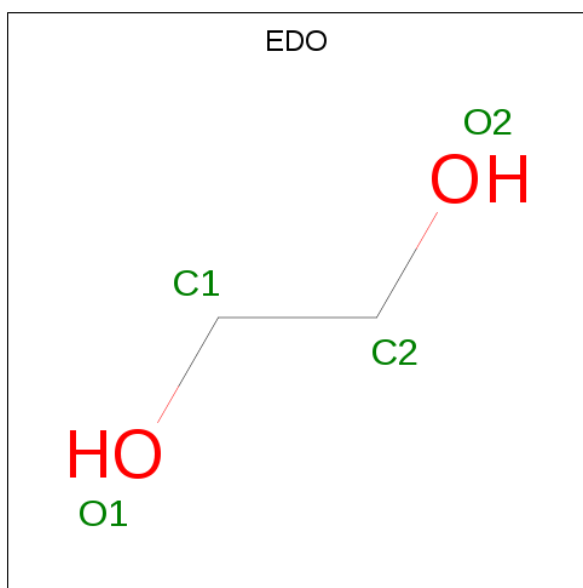
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	5	Total 5	Ca 5	0	0
6	A	4	Total 4	Ca 4	0	0

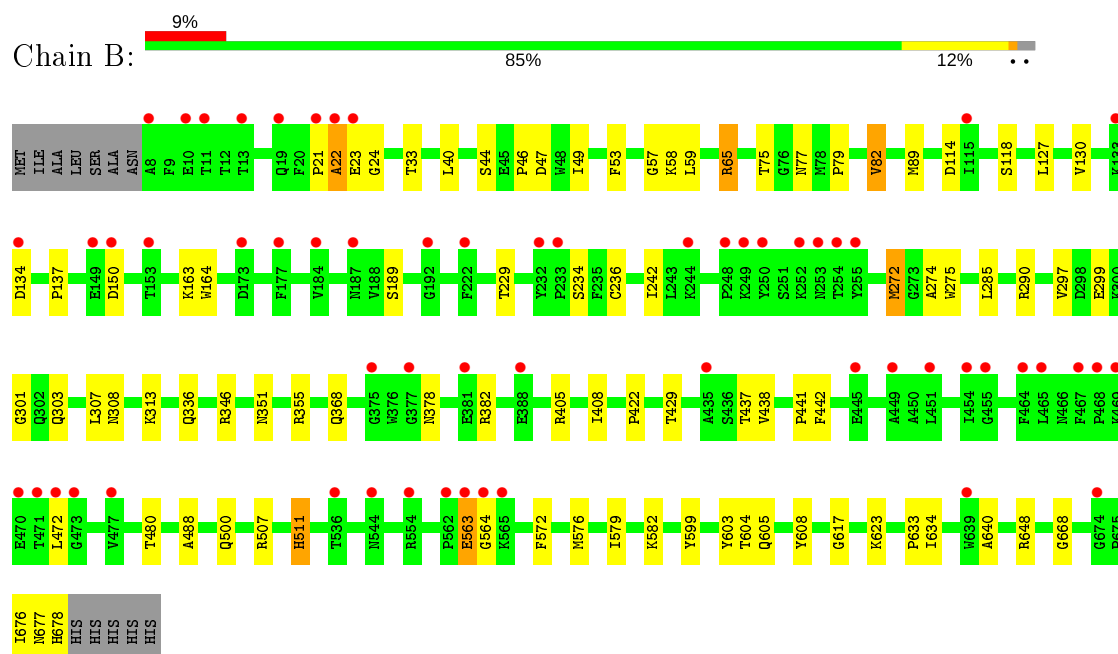
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	145	Total 145	O 145	0	0
7	A	63	Total 63	O 63	0	0

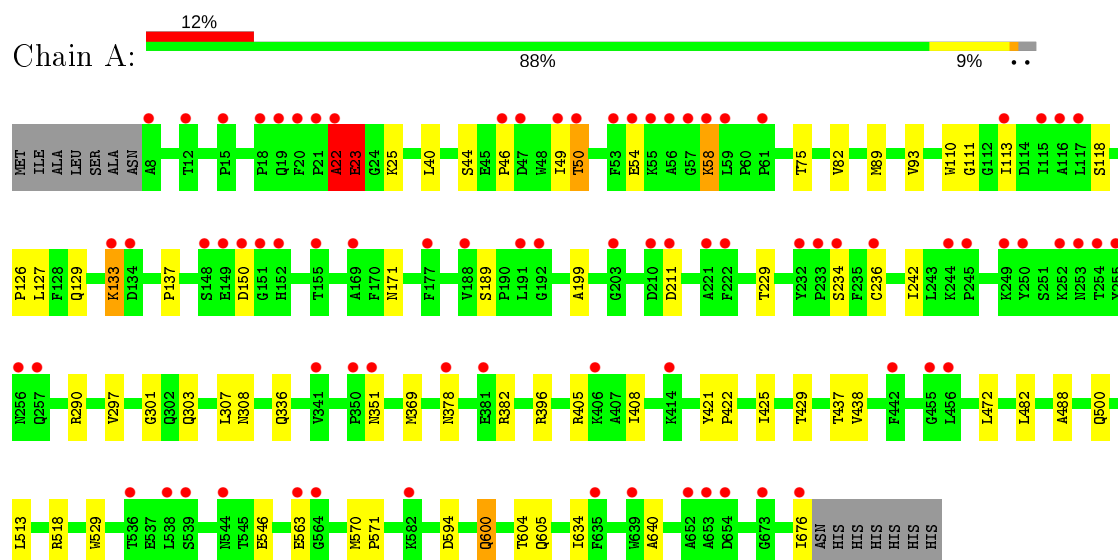
3 Residue-property plots

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: Periplasmic alpha-galactoside-binding protein



- Molecule 1: Periplasmic alpha-galactoside-binding protein




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

Chain C:  100%

TTV1
GLC2
ZCD3
GLA4

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

Chain D:  100%

TTV1
GLC2
ZCD3
GLA4

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.18Å 73.98Å 171.45Å 90.00° 92.45° 90.00°	Depositor
Resolution (Å)	46.61 – 2.10 46.61 – 2.10	Depositor EDS
% Data completeness (in resolution range)	73.4 (46.61-2.10) 73.3 (46.61-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.191 , 0.225 0.204 , 0.243	Depositor DCC
R_{free} test set	2849 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11000	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZCD, GLA, CA, GLC, EDO, TTV, PG4, PEG

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	0.47	0/5429	0.68	1/7387 (0.0%)
1	B	0.54	1/5448 (0.0%)	0.71	1/7413 (0.0%)
All	All	0.51	1/10877 (0.0%)	0.69	2/14800 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	MET	SD-CE	-6.46	1.41	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ALA	C-N-CA	6.07	136.87	121.70
1	B	130	VAL	C-N-CA	5.33	135.01	121.70

There are no chirality outliers.

There are no planarity outliers.

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	5277	0	5100	36	0
1	B	5295	0	5114	60	1
2	C	45	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	45	0	19	0	0
3	B	13	0	18	1	0
4	A	7	0	10	1	0
4	B	49	0	70	10	0
5	A	4	0	6	0	0
5	B	48	0	72	5	0
6	A	4	0	0	0	0
6	B	5	0	0	0	0
7	A	63	0	0	1	0
7	B	145	0	0	0	0
All	All	11000	0	10428	96	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 5.

The worst 5 of 96 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:633:PRO:HA	4:B:707:PEG:H11	1.50	0.93
1:B:405:ARG:H	5:B:716:EDO:H21	1.45	0.81
1:B:164:TRP:HA	1:B:272:MET:CE	2.11	0.81
1:B:33:THR:HA	4:B:708:PEG:H32	1.68	0.75
1:B:668:GLY:HA2	1:B:676:ILE:HD12	1.69	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLY:O	1:B:57:GLY:O[2_556]	2.13	0.07

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	667/683 (98%)	635 (95%)	29 (4%)	3 (0%)	34	32
1	B	669/683 (98%)	632 (94%)	34 (5%)	3 (0%)	34	32
All	All	1336/1366 (98%)	1267 (95%)	63 (5%)	6 (0%)	34	32

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	B	21	PRO
1	B	22	ALA
1	B	58	LYS
1	A	22	ALA

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	556/568 (98%)	540 (97%)	16 (3%)	42	46
1	B	558/568 (98%)	539 (97%)	19 (3%)	37	39
All	All	1114/1136 (98%)	1079 (97%)	35 (3%)	40	43

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	500	GLN
1	A	23	GLU
1	A	594	ASP
1	B	507	ARG
1	B	511	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	466	ASN

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Mol	Chain	Res	Type
1	A	77	ASN
1	A	336	GLN
1	B	368	GLN
1	A	339	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 ⓘ

8 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	TTV	C	1	2	11,12,12	2.70	4 (36%)	10,18,18	1.11	0
2	GLC	C	2	2	11,11,12	1.40	3 (27%)	15,15,17	1.96	3 (20%)
2	ZCD	C	3	2	11,11,12	1.53	3 (27%)	15,15,17	1.90	3 (20%)
2	GLA	C	4	2	11,11,12	1.54	1 (9%)	15,15,17	1.28	2 (13%)
2	TTV	D	1	2	11,12,12	2.12	3 (27%)	10,18,18	1.75	2 (20%)
2	GLC	D	2	2	11,11,12	1.00	0	15,15,17	1.06	1 (6%)
2	ZCD	D	3	2	11,11,12	1.36	1 (9%)	15,15,17	1.58	3 (20%)
2	GLA	D	4	2	11,11,12	1.09	1 (9%)	15,15,17	1.20	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	TTV	C	1	2	-	3/5/24/24	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	ZCD	C	3	2	-	1/2/19/22	0/1/1/1
2	GLA	C	4	2	-	0/2/19/22	0/1/1/1
2	TTV	D	1	2	-	1/5/24/24	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	ZCD	D	3	2	-	1/2/19/22	0/1/1/1
2	GLA	D	4	2	-	0/2/19/22	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	TTV	O2-C2	6.39	1.51	1.40
2	D	1	TTV	O2-C2	4.56	1.48	1.40
2	D	1	TTV	O5-C2	4.18	1.49	1.43
2	C	4	GLA	O5-C1	3.98	1.50	1.43
2	C	1	TTV	O5-C2	3.89	1.49	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	ZCD	C1-C2-C3	5.50	116.42	109.67
2	C	2	GLC	O5-C5-C6	-5.12	99.17	107.20
2	D	3	ZCD	C1-C2-C3	4.59	115.31	109.67
2	C	2	GLC	C1-C2-C3	3.85	114.39	109.67
2	D	1	TTV	O2-C2-O5	3.83	116.91	109.50

There are no chirality outliers.

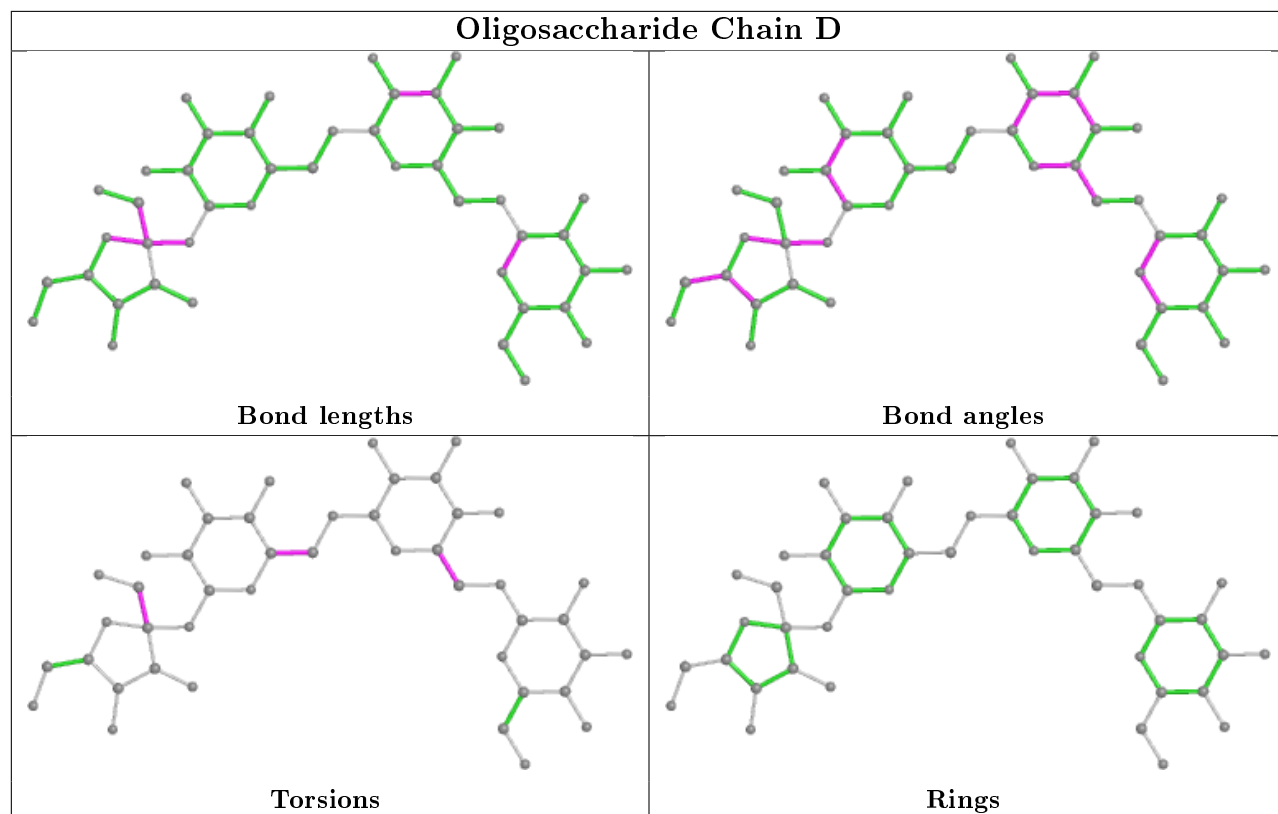
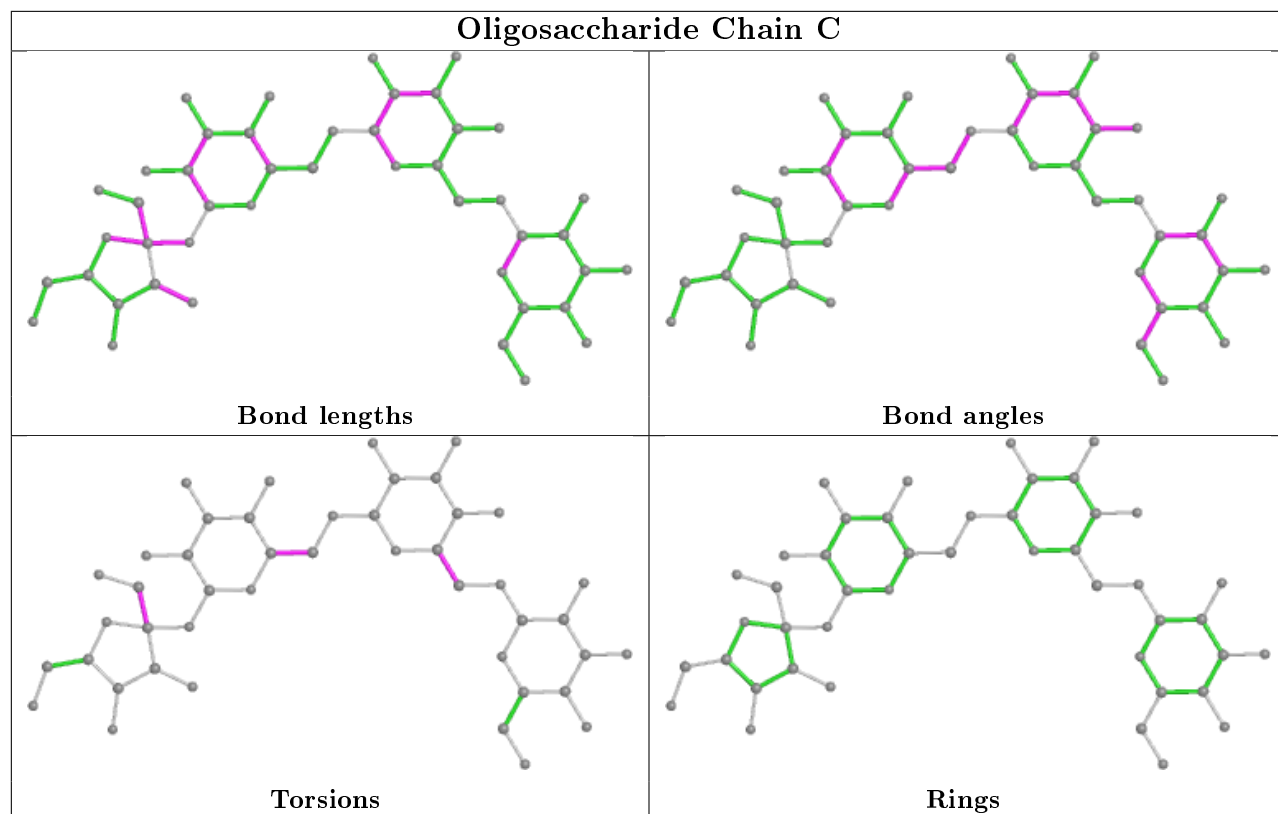
5 of 10 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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

Of 31 ligands modelled in this entry, 9 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	710	-	3,3,3	0.81	0	2,2,2	0.20	0
4	PEG	B	708	6	6,6,6	0.31	0	5,5,5	0.38	0
4	PEG	B	702	-	6,6,6	0.17	0	5,5,5	0.13	0
5	EDO	B	711	-	3,3,3	0.56	0	2,2,2	0.40	0
5	EDO	B	709	-	3,3,3	0.68	0	2,2,2	0.14	0
4	PEG	A	701	-	6,6,6	0.09	0	5,5,5	0.10	0
4	PEG	B	703	-	6,6,6	0.20	0	5,5,5	0.14	0
4	PEG	B	706	-	6,6,6	0.17	0	5,5,5	0.11	0
4	PEG	B	704	-	6,6,6	0.12	0	5,5,5	0.10	0
4	PEG	B	705	-	6,6,6	0.31	0	5,5,5	0.18	0
5	EDO	B	719	-	3,3,3	0.50	0	2,2,2	0.22	0
5	EDO	B	713	-	3,3,3	0.61	0	2,2,2	0.24	0
3	PG4	B	701	-	12,12,12	0.91	0	11,11,11	0.61	0
5	EDO	B	715	-	3,3,3	0.69	0	2,2,2	0.27	0
5	EDO	B	718	-	3,3,3	0.72	0	2,2,2	0.04	0
5	EDO	B	717	-	3,3,3	0.53	0	2,2,2	0.39	0
5	EDO	B	714	6	3,3,3	0.56	0	2,2,2	0.25	0
4	PEG	B	707	-	6,6,6	0.41	0	5,5,5	0.51	0
5	EDO	B	720	-	3,3,3	0.67	0	2,2,2	0.39	0
5	EDO	A	702	-	3,3,3	0.65	0	2,2,2	0.20	0
5	EDO	B	716	-	3,3,3	0.49	0	2,2,2	0.26	0
5	EDO	B	712	-	3,3,3	0.86	0	2,2,2	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	710	-	-	0/1/1/1	-
4	PEG	B	708	6	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	B	702	-	-	0/4/4/4	-
5	EDO	B	711	-	-	1/1/1/1	-
5	EDO	B	709	-	-	0/1/1/1	-
4	PEG	A	701	-	-	1/4/4/4	-
4	PEG	B	703	-	-	1/4/4/4	-
4	PEG	B	706	-	-	0/4/4/4	-
4	PEG	B	704	-	-	0/4/4/4	-
4	PEG	B	705	-	-	1/4/4/4	-
5	EDO	B	719	-	-	0/1/1/1	-
5	EDO	B	713	-	-	1/1/1/1	-
3	PG4	B	701	-	-	7/10/10/10	-
5	EDO	B	715	-	-	0/1/1/1	-
5	EDO	B	718	-	-	0/1/1/1	-
5	EDO	B	717	-	-	0/1/1/1	-
5	EDO	B	714	6	-	0/1/1/1	-
4	PEG	B	707	-	-	4/4/4/4	-
5	EDO	B	720	-	-	1/1/1/1	-
5	EDO	A	702	-	-	1/1/1/1	-
5	EDO	B	716	-	-	0/1/1/1	-
5	EDO	B	712	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	708	PEG	O1-C1-C2-O2
3	B	701	PG4	O3-C5-C6-O4
3	B	701	PG4	C4-C3-O2-C2
3	B	701	PG4	O2-C3-C4-O3
3	B	701	PG4	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	708	PEG	5	0
4	B	702	PEG	1	0
4	A	701	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	706	PEG	1	0
3	B	701	PG4	1	0
5	B	714	EDO	1	0
4	B	707	PEG	3	0
5	B	716	EDO	4	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 [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	669/683 (97%)	0.74	80 (11%) 4 5	31, 64, 107, 145	0
1	B	671/683 (98%)	0.48	59 (8%) 10 12	15, 56, 104, 150	0
All	All	1340/1366 (98%)	0.61	139 (10%) 6 8	15, 61, 107, 150	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ALA	10.9
1	A	22	ALA	10.8
1	A	21	PRO	9.2
1	B	22	ALA	7.3
1	B	468	PRO	5.9

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

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

6.3 Carbohydrates [i](#)

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

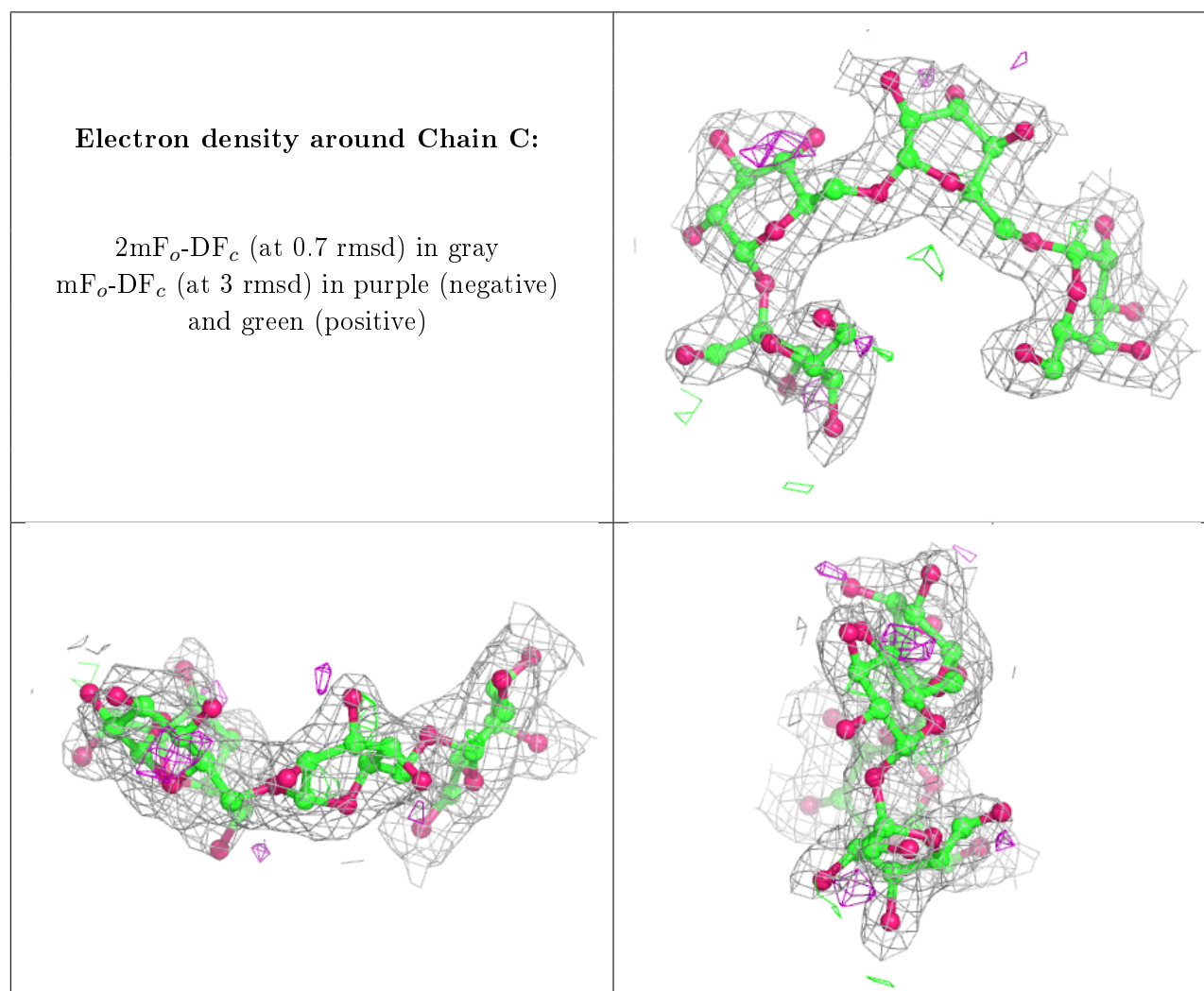
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TTV	C	1	12/12	0.80	0.27	59,64,65,65	0
2	TTV	D	1	12/12	0.80	0.35	75,78,80,81	0
2	GLC	C	2	11/12	0.84	0.29	45,62,65,66	0
2	GLC	D	2	11/12	0.92	0.26	63,70,72,73	0
2	ZCD	C	3	11/12	0.94	0.21	29,41,47,52	0

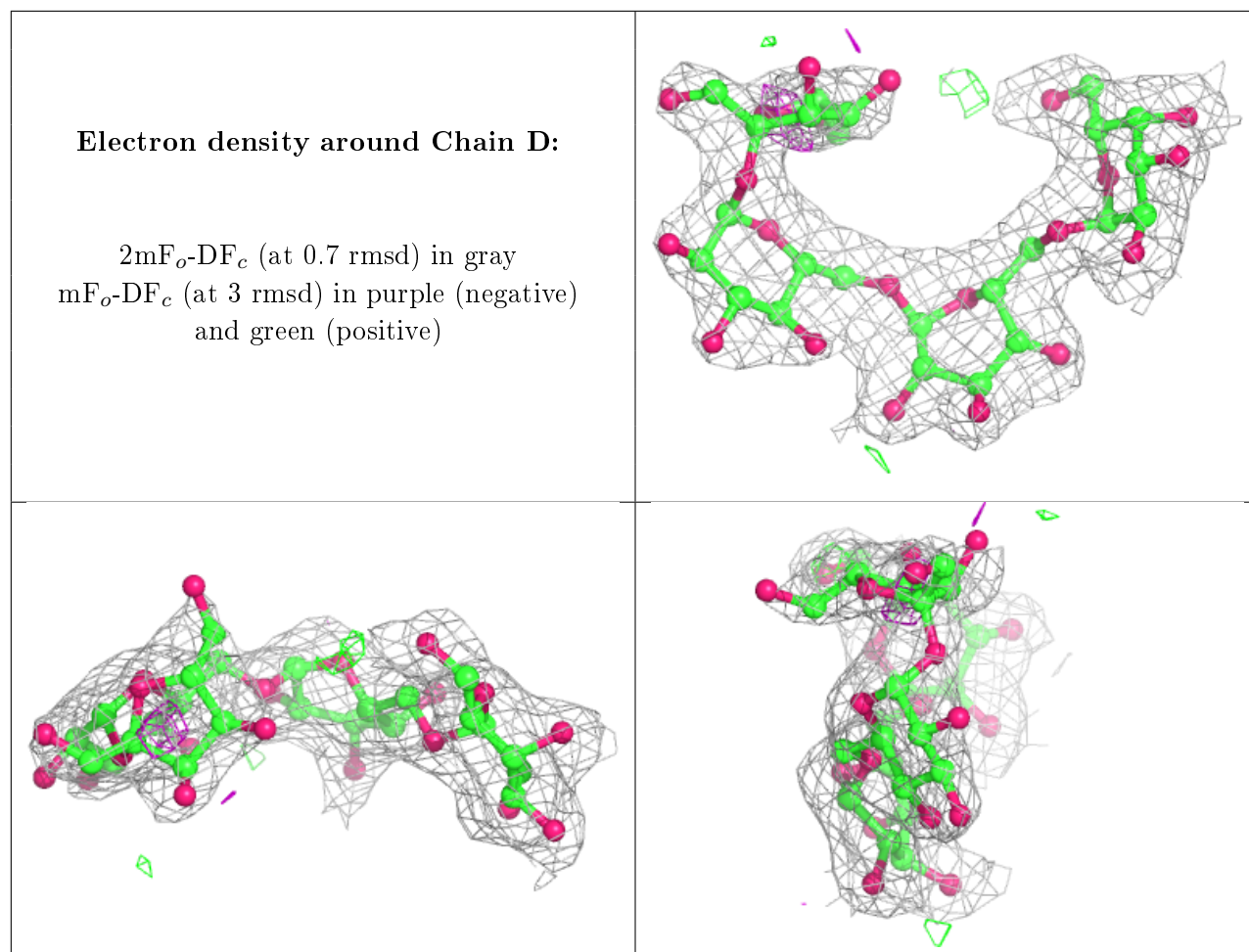
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZCD	D	3	11/12	0.96	0.18	39,47,53,55	0
2	GLA	D	4	11/12	0.97	0.21	34,37,39,39	0
2	GLA	C	4	11/12	0.98	0.20	19,21,23,25	0

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.





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
5	EDO	B	718	4/4	0.66	0.35	73,76,77,77	0
5	EDO	B	712	4/4	0.68	0.21	51,52,52,54	0
4	PEG	B	705	7/7	0.72	0.34	50,59,64,66	0
4	PEG	B	707	7/7	0.76	0.25	40,45,49,49	0
5	EDO	B	709	4/4	0.79	0.23	60,61,61,61	0
5	EDO	A	702	4/4	0.80	0.22	73,74,75,76	0
6	CA	B	721	1/1	0.82	0.09	92,92,92,92	0
4	PEG	B	706	7/7	0.82	0.15	60,63,72,74	0
5	EDO	B	720	4/4	0.83	0.18	53,54,54,55	0
5	EDO	B	716	4/4	0.84	0.41	36,37,43,50	0
6	CA	A	704	1/1	0.85	0.14	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CA	B	724	1/1	0.85	0.08	83,83,83,83	0
4	PEG	B	708	7/7	0.86	0.28	26,33,42,48	0
4	PEG	B	703	7/7	0.86	0.12	61,62,64,64	0
5	EDO	B	717	4/4	0.86	0.17	57,58,59,59	0
5	EDO	B	710	4/4	0.89	0.18	40,41,42,43	0
5	EDO	B	713	4/4	0.89	0.15	67,68,68,69	0
3	PG4	B	701	13/13	0.89	0.16	40,44,47,52	0
4	PEG	B	704	7/7	0.90	0.15	51,53,56,56	0
6	CA	B	725	1/1	0.91	0.15	84,84,84,84	0
5	EDO	B	714	4/4	0.91	0.13	45,46,46,46	0
4	PEG	A	701	7/7	0.92	0.18	66,69,72,74	0
5	EDO	B	719	4/4	0.92	0.11	33,33,35,38	0
5	EDO	B	715	4/4	0.92	0.12	41,41,42,42	0
6	CA	A	705	1/1	0.92	0.07	81,81,81,81	0
5	EDO	B	711	4/4	0.93	0.14	54,54,55,56	0
6	CA	A	706	1/1	0.94	0.14	93,93,93,93	0
4	PEG	B	702	7/7	0.96	0.11	29,33,42,48	0
6	CA	A	703	1/1	0.98	0.03	55,55,55,55	0
6	CA	B	722	1/1	0.98	0.06	49,49,49,49	0
6	CA	B	723	1/1	0.99	0.07	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.