Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 07:33 pm GMT

PDB ID : 6RV7

Title : Crystal Structure of Glucuronoyl Esterase from Cerrena unicolor inactive S270A variant in complex with the aldouronic acid UXXR

Authors : Ernst, H.A.; Mosbech, C.; Langkilde, A.; Westh, P.; Meyer, A.; Agger, J.W.; Larsen, S.

Deposited on : 2019-05-31

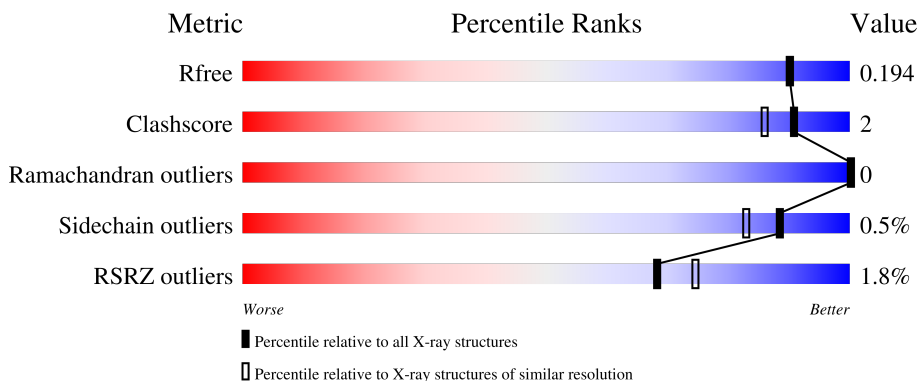Resolution : 1.73 Å(reported)

---

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 1.73 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.

- ▮ Percentile relative to all X-ray structures
- ▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	401	91% · 5%
1	B	401	3% 90% 5% 5%
2	C	4	25% 50% 25%
3	D	2	100%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6451 atoms, of which 61 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 4-O-methyl-glucuronoyl methylesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total 2894	C 1830	N 494	O 555	S 15	0	7	0
1	B	379	Total 2886	C 1824	N 493	O 554	S 15	0	6	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	GLU	-	expression tag	UNP A0A0A7EQR3
A	74	ALA	-	expression tag	UNP A0A0A7EQR3
A	75	GLU	-	expression tag	UNP A0A0A7EQR3
A	76	ALA	-	expression tag	UNP A0A0A7EQR3
A	77	GLU	-	expression tag	UNP A0A0A7EQR3
A	78	PHE	-	expression tag	UNP A0A0A7EQR3
A	270	ALA	SER	engineered mutation	UNP A0A0A7EQR3
A	459	GLU	-	expression tag	UNP A0A0A7EQR3
A	460	ASN	-	expression tag	UNP A0A0A7EQR3
A	461	LEU	-	expression tag	UNP A0A0A7EQR3
A	462	TYR	-	expression tag	UNP A0A0A7EQR3
A	463	PHE	-	expression tag	UNP A0A0A7EQR3
A	464	GLN	-	expression tag	UNP A0A0A7EQR3
A	465	GLY	-	expression tag	UNP A0A0A7EQR3
A	466	VAL	-	expression tag	UNP A0A0A7EQR3
A	467	ASP	-	expression tag	UNP A0A0A7EQR3
A	468	HIS	-	expression tag	UNP A0A0A7EQR3
A	469	HIS	-	expression tag	UNP A0A0A7EQR3
A	470	HIS	-	expression tag	UNP A0A0A7EQR3
A	471	HIS	-	expression tag	UNP A0A0A7EQR3
A	472	HIS	-	expression tag	UNP A0A0A7EQR3
A	473	HIS	-	expression tag	UNP A0A0A7EQR3
B	73	GLU	-	expression tag	UNP A0A0A7EQR3
B	74	ALA	-	expression tag	UNP A0A0A7EQR3
B	75	GLU	-	expression tag	UNP A0A0A7EQR3

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	ALA	-	expression tag	UNP A0A0A7EQR3
B	77	GLU	-	expression tag	UNP A0A0A7EQR3
B	78	PHE	-	expression tag	UNP A0A0A7EQR3
B	270	ALA	SER	engineered mutation	UNP A0A0A7EQR3
B	459	GLU	-	expression tag	UNP A0A0A7EQR3
B	460	ASN	-	expression tag	UNP A0A0A7EQR3
B	461	LEU	-	expression tag	UNP A0A0A7EQR3
B	462	TYR	-	expression tag	UNP A0A0A7EQR3
B	463	PHE	-	expression tag	UNP A0A0A7EQR3
B	464	GLN	-	expression tag	UNP A0A0A7EQR3
B	465	GLY	-	expression tag	UNP A0A0A7EQR3
B	466	VAL	-	expression tag	UNP A0A0A7EQR3
B	467	ASP	-	expression tag	UNP A0A0A7EQR3
B	468	HIS	-	expression tag	UNP A0A0A7EQR3
B	469	HIS	-	expression tag	UNP A0A0A7EQR3
B	470	HIS	-	expression tag	UNP A0A0A7EQR3
B	471	HIS	-	expression tag	UNP A0A0A7EQR3
B	472	HIS	-	expression tag	UNP A0A0A7EQR3
B	473	HIS	-	expression tag	UNP A0A0A7EQR3

- Molecule 2 is an oligosaccharide called 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-Xylitol.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
2	C	4	78	22	37	19	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
3	D	2	37	10	18	9	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
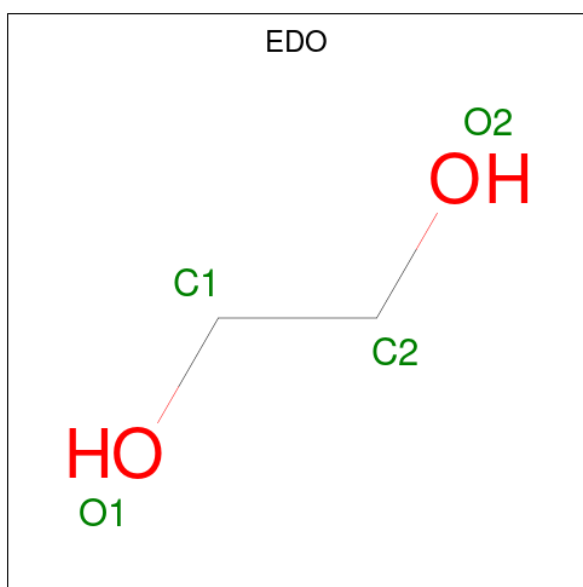
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is water.

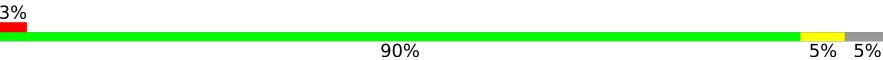| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	288	Total	O	0	0
			288	288		
6	B	230	Total	O	0	0
			230	230		

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.
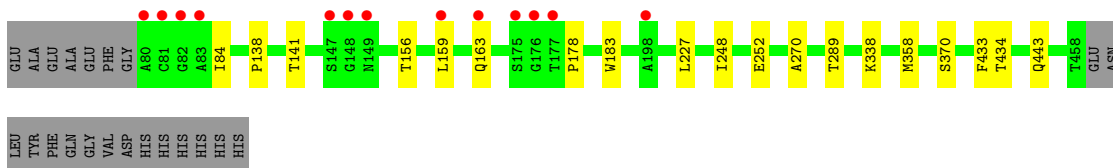
• Molecule 1: 4-O-methyl-glucuronoyl methylesterase

Chain A:

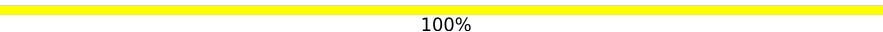

• Molecule 1: 4-O-methyl-glucuronoyl methylesterase

Chain B:

• Molecule 2: 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-Xylitol

Chain C:

• Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.78Å 84.78Å 260.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 1.73 49.33 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.33-1.73) 99.8 (49.33-1.73)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 1.73Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.166 , 0.194 0.166 , 0.194	Depositor DCC
R_{free} test set	4947 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6451	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: XYP, NAG, GCV, EDO, XYL

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	0.36	0/2993	0.55	0/4097
1	B	0.34	0/2982	0.54	0/4082
All	All	0.35	0/5975	0.55	0/8179

There are no bond length outliers.

There are no bond angle outliers.

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	2894	0	2792	9	0
1	B	2886	0	2783	12	0
2	C	41	37	20	1	0
3	D	19	18	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	4	6	6	0	0
6	A	288	0	0	1	0
6	B	230	0	0	3	0
All	All	6390	61	5627	20	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 2.

All (20) 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:138:PRO:HD2	1:B:159:LEU:HA	1.75	0.69
1:A:250:ALA:HA	1:A:253:MET:HE2	1.85	0.58
1:B:443:GLN:NE2	6:B:601:HOH:O	2.40	0.55
1:B:248:ILE:O	1:B:252:GLU:HG3	2.09	0.52
1:B:270:ALA:HB1	2:C:4:GCV:C6	2.43	0.48
1:B:178:PRO:HB3	1:B:183:TRP:NE1	2.28	0.48
1:B:84:ILE:HA	6:B:643:HOH:O	2.14	0.47
1:B:434[B]:THR:HG21	6:B:781:HOH:O	2.13	0.47
1:A:255:PRO:HD2	6:A:812:HOH:O	2.14	0.46
1:A:178:PRO:HB3	1:A:183:TRP:NE1	2.31	0.45
1:B:289:THR:O	1:B:358[B]:MET:HG2	2.16	0.45
1:A:178:PRO:HB3	1:A:183:TRP:CE2	2.53	0.43
1:A:429:THR:HG21	1:B:338:LYS:NZ	2.34	0.42
1:A:304:LEU:CD2	1:A:449:TRP:CD2	3.03	0.42
1:B:141:THR:OG1	1:B:156:THR:HB	2.19	0.42
1:A:141:THR:OG1	1:A:156:THR:HB	2.20	0.41
1:A:144:PHE:HB2	1:A:254:THR:HG21	2.01	0.41
1:B:227:LEU:HD23	1:B:227:LEU:HA	1.96	0.41
1:A:385:TRP:CD2	1:A:394:HIS:HB2	2.56	0.41
1:B:163:GLN:HG3	1:B:163:GLN:O	2.21	0.41

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	384/401 (96%)	369 (96%)	15 (4%)	0	100	100
1	B	383/401 (96%)	369 (96%)	14 (4%)	0	100	100

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	767/802 (96%)	738 (96%)	29 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	309/320 (97%)	308 (100%)	1 (0%)	92 89
1	B	308/320 (96%)	306 (99%)	2 (1%)	86 79
All	All	617/640 (96%)	614 (100%)	3 (0%)	88 83

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	SER
1	B	370	SER
1	B	433	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	443	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

6 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	XYL	C	1	2	9,9,9	0.74	0	11,11,11	0.70	0
2	XYP	C	2	2	9,9,10	1.92	3 (33%)	10,12,14	1.18	1 (10%)
2	XYP	C	3	2	9,9,10	1.85	3 (33%)	10,12,14	1.34	2 (20%)
2	GCV	C	4	2	13,13,14	1.79	2 (15%)	14,18,20	1.35	2 (14%)
3	XYP	D	1	3	10,10,10	1.89	4 (40%)	14,14,14	0.94	0
3	XYP	D	2	3	9,9,10	3.19	7 (77%)	10,12,14	1.31	2 (20%)

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	XYL	C	1	2	-	4/12/12/12	-
2	XYP	C	2	2	-	-	0/1/1/1
2	XYP	C	3	2	-	-	0/1/1/1
2	GCV	C	4	2	-	2/6/23/26	0/1/1/1
3	XYP	D	1	3	-	-	0/1/1/1
3	XYP	D	2	3	-	-	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	XYP	C4-C3	-6.15	1.43	1.52
2	C	4	GCV	O5-C1	4.16	1.50	1.43
2	C	2	XYP	O5-C1	3.74	1.50	1.42
3	D	2	XYP	O5-C1	3.72	1.50	1.42
2	C	3	XYP	O5-C1	3.69	1.50	1.42
2	C	4	GCV	O5-C5	3.60	1.50	1.43
3	D	1	XYP	C4-C3	-3.24	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	XYP	O3-C3	3.08	1.50	1.43
3	D	1	XYP	O5-C1	3.07	1.47	1.43
2	C	2	XYP	O5-C5	3.02	1.48	1.42
3	D	2	XYP	C1-C2	2.87	1.58	1.52
3	D	2	XYP	O4-C4	2.84	1.49	1.43
3	D	2	XYP	O5-C5	2.78	1.48	1.42
2	C	3	XYP	O5-C5	2.67	1.48	1.42
3	D	1	XYP	O5-C5	2.63	1.47	1.43
2	C	3	XYP	C2-C3	-2.55	1.48	1.52
3	D	2	XYP	C2-C3	-2.42	1.48	1.52
2	C	2	XYP	C2-C3	-2.35	1.49	1.52
3	D	1	XYP	O3-C3	2.06	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	GCV	O3-C3-C2	-3.09	104.08	109.99
3	D	2	XYP	C5-C4-C3	2.77	113.07	109.67
2	C	3	XYP	C4-C3-C2	2.72	114.15	110.92
2	C	2	XYP	C1-C2-C3	2.61	112.88	109.67
2	C	4	GCV	O2-C2-C1	-2.25	104.55	109.15
2	C	3	XYP	O3-C3-C4	-2.06	106.05	109.99
3	D	2	XYP	C4-C3-C2	2.00	113.30	110.92

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	GCV	C3-C4-O4-C7
2	C	1	XYL	O2-C2-C3-C4
2	C	1	XYL	C1-C2-C3-C4
2	C	1	XYL	C1-C2-C3-O3
2	C	1	XYL	O2-C2-C3-O3
2	C	4	GCV	C5-C4-O4-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	GCV	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.
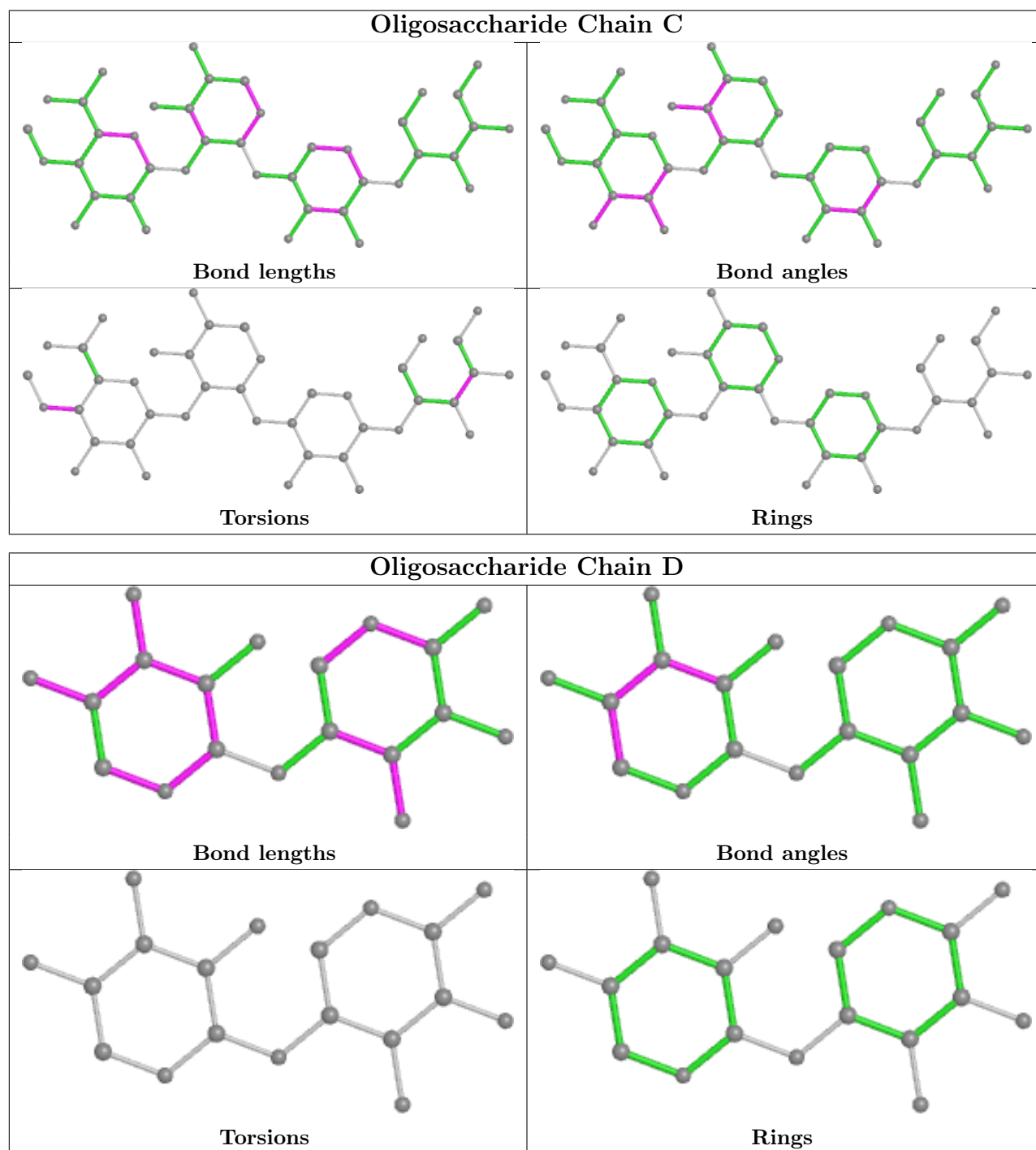
5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	EDO	A	502	-	3,3,3	0.55	0	2,2,2	0.33	0
4	NAG	A	501	1	14,14,15	0.26	0	17,19,21	0.60	0
4	NAG	B	501	1	14,14,15	0.19	0	17,19,21	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
5	EDO	A	502	-	-	0/1/1/1	-
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	B	501	1	-	0/6/23/26	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 ⓘ

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(Å²)	Q<0.9
1	A	379/401 (94%)	-0.40	1 (0%)	94	95	14, 19, 34, 54	0
1	B	379/401 (94%)	-0.10	13 (3%)	45	51	14, 22, 42, 81	0
All	All	758/802 (94%)	-0.25	14 (1%)	68	74	14, 20, 40, 81	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	SER	4.2
1	B	177	THR	3.8
1	B	159	LEU	3.6
1	B	147	SER	3.6
1	B	176	GLY	3.5
1	B	149	ASN	3.4
1	B	198	ALA	3.4
1	B	148	GLY	3.4
1	B	163	GLN	3.0
1	B	80	ALA	2.8
1	B	82	GLY	2.3
1	B	83	ALA	2.2
1	A	80	ALA	2.2
1	B	81	CYS	2.1

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

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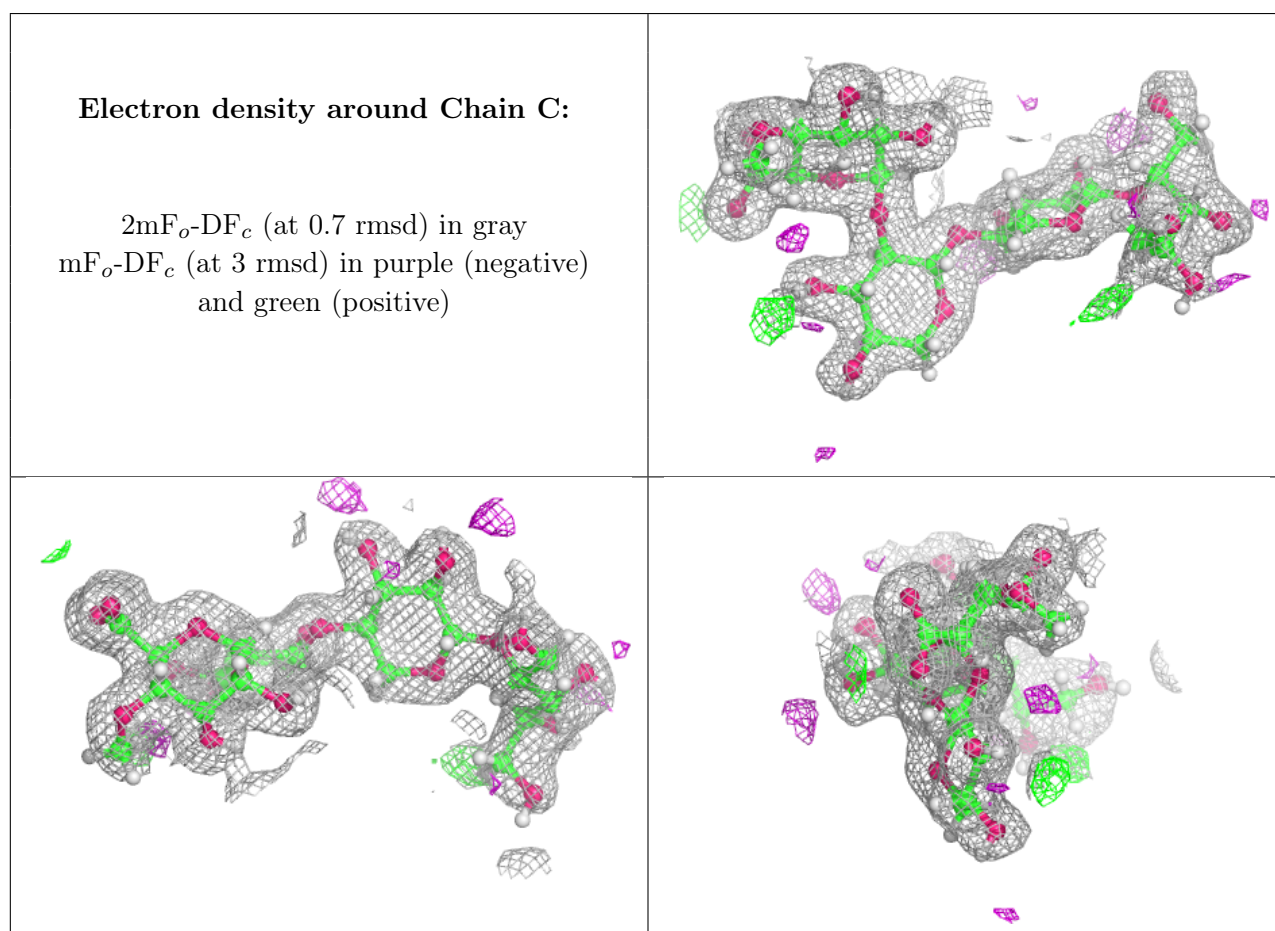
6.3   Carbohydrates ⓘ

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,
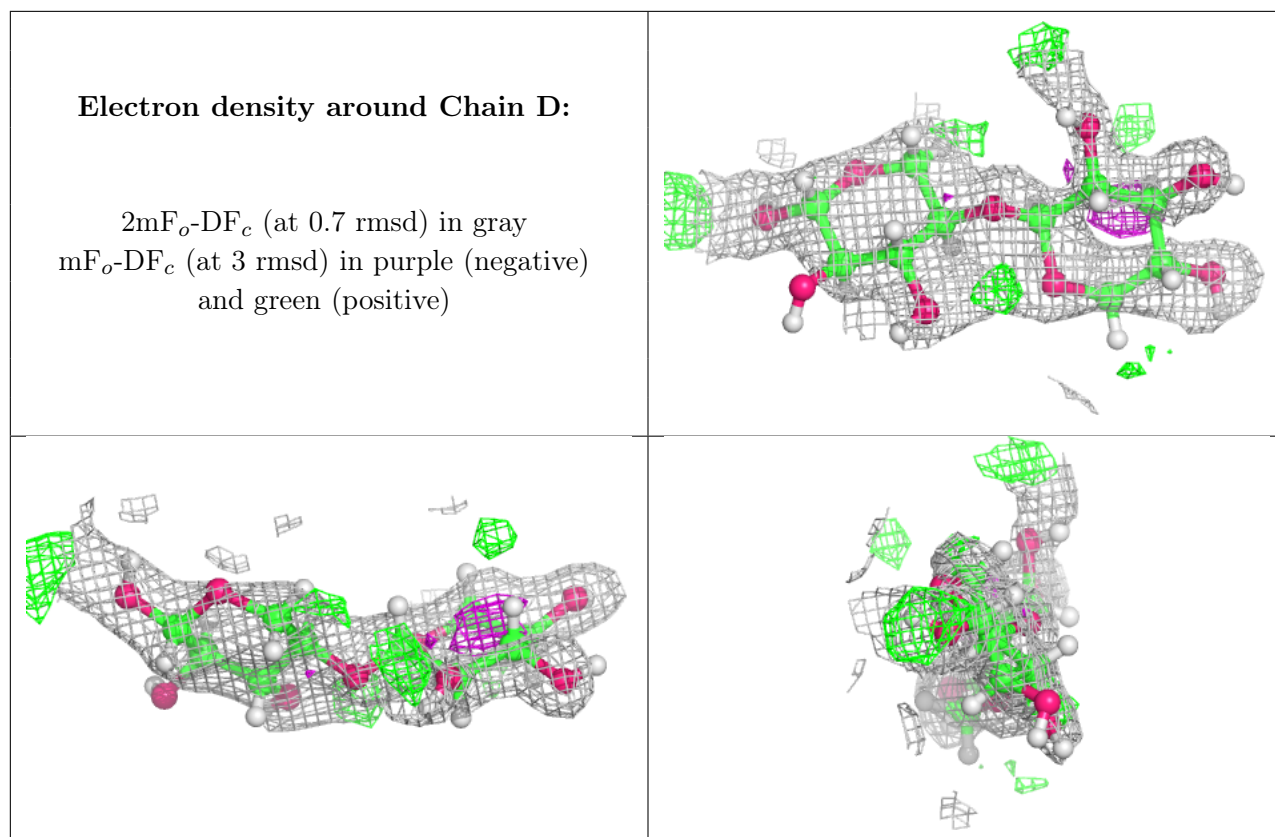
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	XYP	D	2	9/10	0.75	0.24	34,42,51,54	18
3	XYP	D	1	10/10	0.83	0.20	35,42,54,61	19
2	XYL	C	1	10/10	0.93	0.17	29,50,65,67	0
2	XYP	C	3	9/10	0.96	0.10	18,28,37,38	0
2	XYP	C	2	9/10	0.97	0.12	23,28,37,42	0
2	GCV	C	4	13/14	0.98	0.06	18,22,29,29	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:

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

Electron density around Chain D:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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(Å²)	Q<0.9
5	EDO	A	502	4/4	0.95	0.07	20,34,42,42	0
4	NAG	B	501	14/15	0.96	0.11	21,24,27,29	0
4	NAG	A	501	14/15	0.97	0.06	19,24,27,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.