wwPDB X-ray Structure Validation Summary Report (i)

Jan 13, 2024 – 10:46 pm GMT

PDB ID	:	6TSN
Title	:	Marasmius oreades agglutinin (MOA), papain back.swap W208Q-Q276W variant
Authors	:	Cordara, G.; Manna, D.; Krengel, U.
Deposited on	:	2019-12-20
Resolution	:	1.60 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:

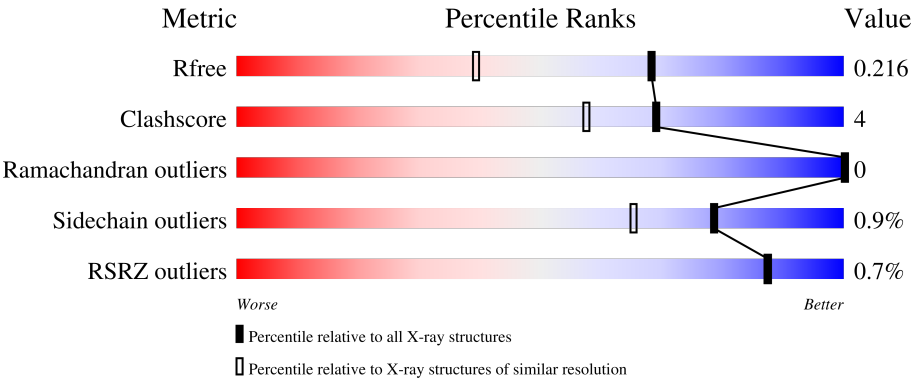
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	AAA	293	% 92% 8%
2	A	3	33% 67%
2	B	3	33% 33% 33%
3	C	3	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 2710 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.

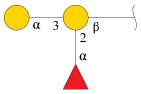
- Molecule 1 is a protein called Agglutinin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	292	Total	As	C	N	O	S	0	19	0
			2403	2	1525	401	466	9			

There are 2 discrepancies between the modelled and reference sequences:

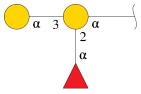
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	208	GLN	TRP	engineered mutation	UNP Q8X123
AAA	276	TRP	GLN	engineered mutation	UNP Q8X123

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose.



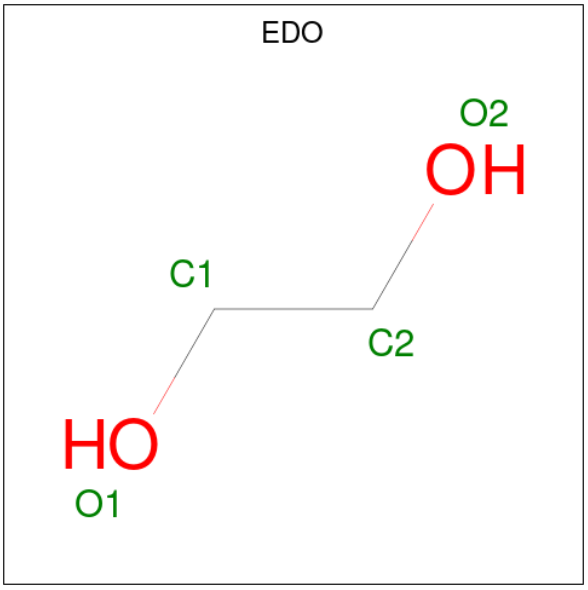
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	3	Total	C	O		0	0	0
			33	18	15				
2	B	3	Total	C	O		0	0	0
			33	18	15				

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]alpha-D-galactopyranose.



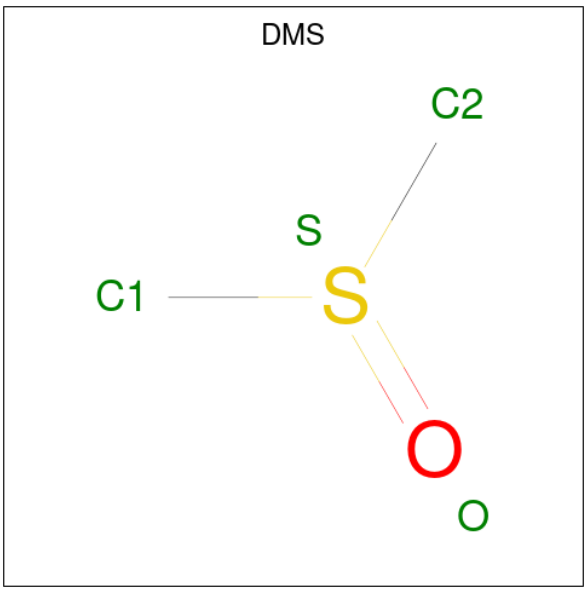
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	3	Total C O 33 18 15	0	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	2	Total Ca 2 2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total Na 1 1	0	0

- Molecule 8 is water.

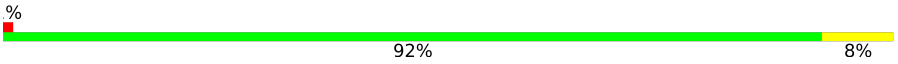
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	197	Total O 197 197	0	0

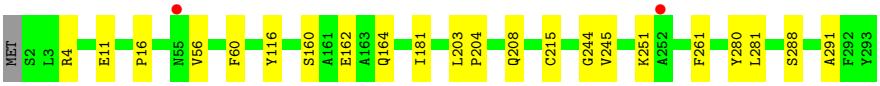
3 Residue-property plots (i)

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: Agglutinin

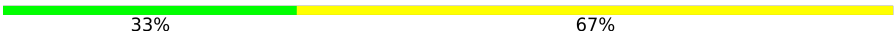
Chain AAA:





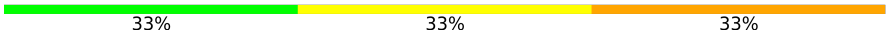
• Molecule 2: alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain A:



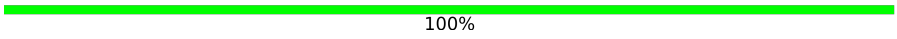
• Molecule 2: alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain B:



• Molecule 3: alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]alpha-D-galactopyranose

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	121.61Å 121.61Å 100.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 1.60 46.60 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (46.60-1.60) 96.6 (46.60-1.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 1.60Å)	Xtriage
Refinement program	REFMAC 7.0.078	Depositor
R, R_{free}	0.185 , 0.209 0.197 , 0.216	Depositor DCC
R_{free} test set	2756 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2710	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: NA, CZZ, EDO, CA, FUC, DMS, 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	AAA	0.86	0/2488	0.60	2/3386 (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	AAA	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	288[A]	SER	CA-CB-OG	-7.05	92.17	111.20
1	AAA	288[B]	SER	CA-CB-OG	-7.05	92.17	111.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	60	PHE	Peptide

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	AAA	2403	0	2233	17	0
2	A	33	0	30	0	0
2	B	33	0	30	1	0
3	C	33	0	30	0	0
4	AAA	4	0	6	0	0
5	AAA	4	0	6	0	0
6	AAA	2	0	0	0	0
7	AAA	1	0	0	0	0
8	AAA	197	0	0	5	0
All	All	2710	0	2335	18	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 18 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:AAA:4[B]:ARG:NH1	1:AAA:162[B]:GLU:OE2	1.88	1.05
1:AAA:11[B]:GLU:OE1	8:AAA:402:HOH:O	1.85	0.92
1:AAA:11[B]:GLU:HG2	8:AAA:402:HOH:O	1.76	0.83
1:AAA:280:TYR:C	1:AAA:281[A]:LEU:HD22	2.24	0.57
1:AAA:11[B]:GLU:CG	8:AAA:402:HOH:O	2.43	0.56

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	AAA	307/293 (105%)	297 (97%)	10 (3%)	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	AAA	250/233 (107%)	248 (99%)	2 (1%)	81 70

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	208	GLN
1	AAA	251	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CZZ	AAA	215[B]	-	3,7,8	0.96	0	0,7,9	-	-
1	CZZ	AAA	215[A]	-	3,7,8	1.36	1 (33%)	0,7,9	-	-

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
1	CZZ	AAA	215[B]	-	-	0/0/6/8	-
1	CZZ	AAA	215[A]	-	-	0/0/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	215[A]	CZZ	CB-CA	2.25	1.58	1.53

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.

5.5 Carbohydrates (i)

9 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	GAL	A	1	2	12,12,12	1.09	1 (8%)	17,17,17	0.55	0
2	FUC	A	2	2	10,10,11	0.89	0	14,14,16	0.54	0
2	GLA	A	3	2	11,11,12	1.02	1 (9%)	15,15,17	0.62	0
2	GAL	B	1	2	12,12,12	0.96	1 (8%)	17,17,17	0.59	0
2	FUC	B	2	2	10,10,11	0.54	0	14,14,16	0.62	0
2	GLA	B	3	2	11,11,12	0.61	0	15,15,17	0.71	0
3	GLA	C	1	3	12,12,12	0.89	0	17,17,17	0.59	0
3	FUC	C	2	3	10,10,11	0.97	0	14,14,16	0.70	0
3	GLA	C	3	3	11,11,12	0.78	0	15,15,17	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	GAL	A	1	2	-	2/2/22/22	0/1/1/1
2	FUC	A	2	2	-	-	0/1/1/1
2	GLA	A	3	2	-	0/2/19/22	0/1/1/1
2	GAL	B	1	2	-	2/2/22/22	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1
2	GLA	B	3	2	-	0/2/19/22	0/1/1/1
3	GLA	C	1	3	-	2/2/22/22	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
3	GLA	C	3	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	GAL	O3-C3	3.07	1.50	1.43
2	A	3	GLA	C1-C2	2.10	1.57	1.52
2	B	1	GAL	O1-C1	2.05	1.46	1.39

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	GLA	C4-C5-C6-O6
3	C	1	GLA	O5-C5-C6-O6
2	B	1	GAL	C4-C5-C6-O6
2	B	1	GAL	O5-C5-C6-O6
2	A	1	GAL	C4-C5-C6-O6

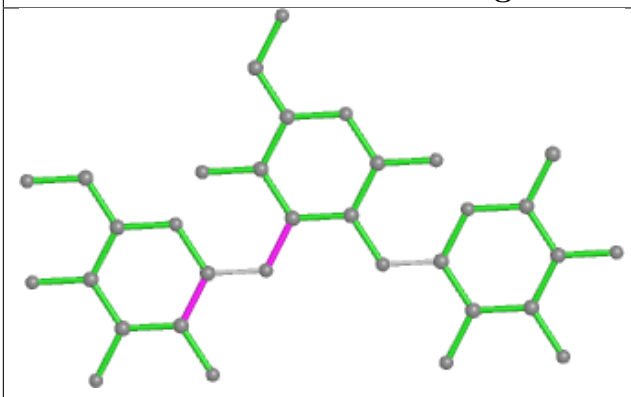
There are no ring outliers.

2 monomers are involved in 1 short contact:

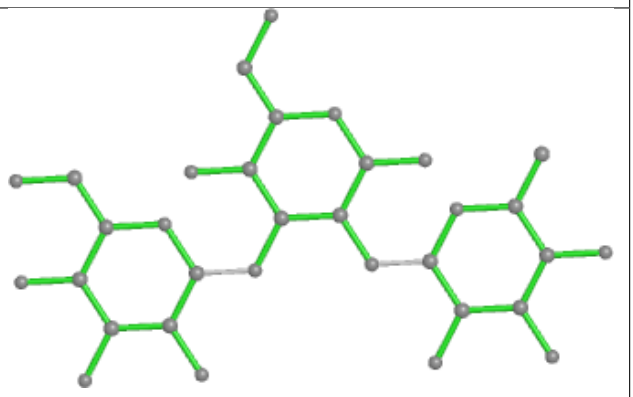
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	FUC	1	0
2	B	1	GAL	1	0

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

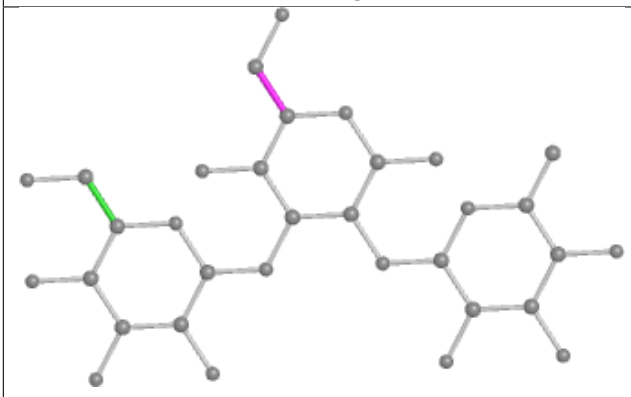
Oligosaccharide Chain A



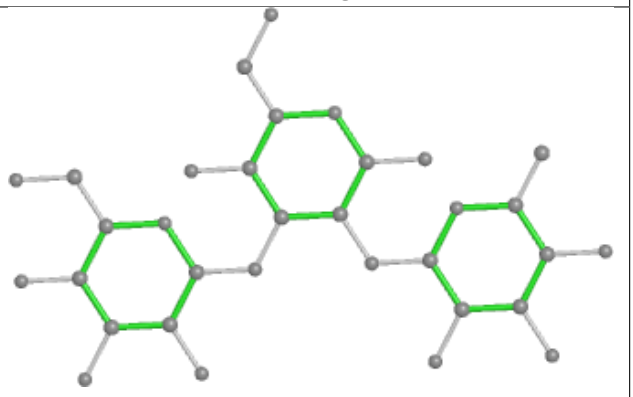
Bond lengths



Bond angles

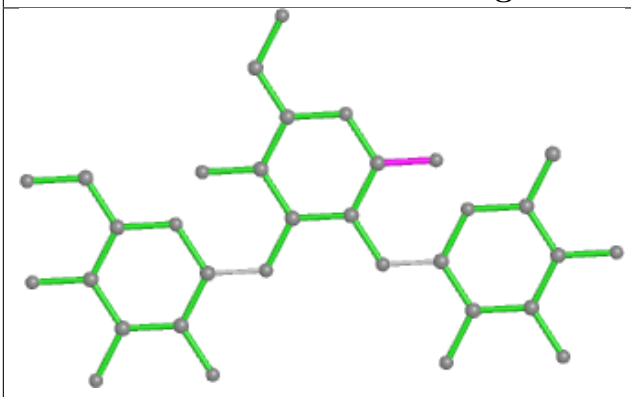


Torsions

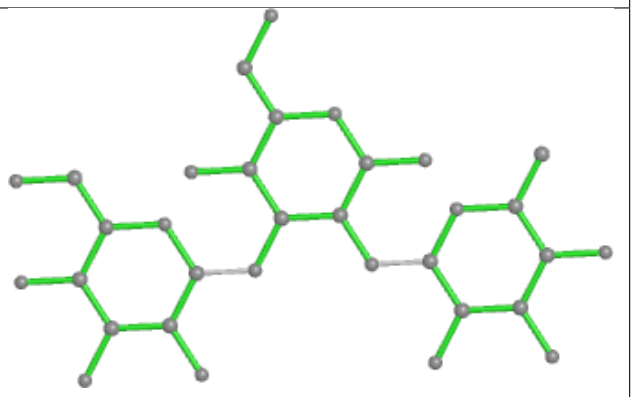


Rings

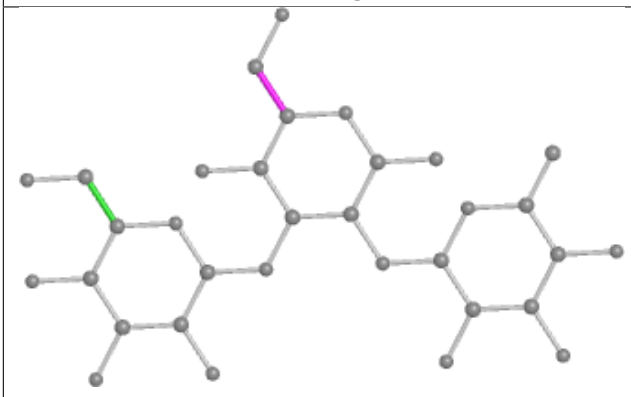
Oligosaccharide Chain B



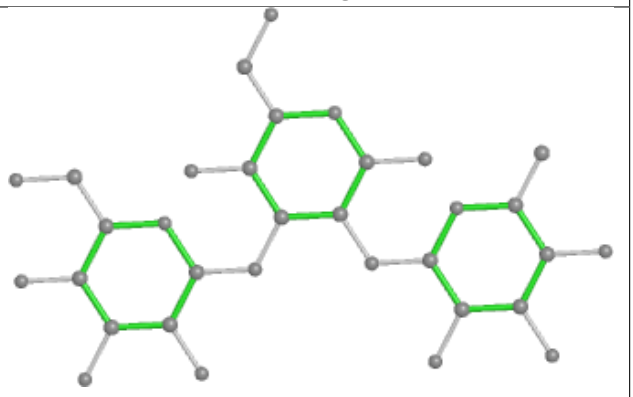
Bond lengths



Bond angles

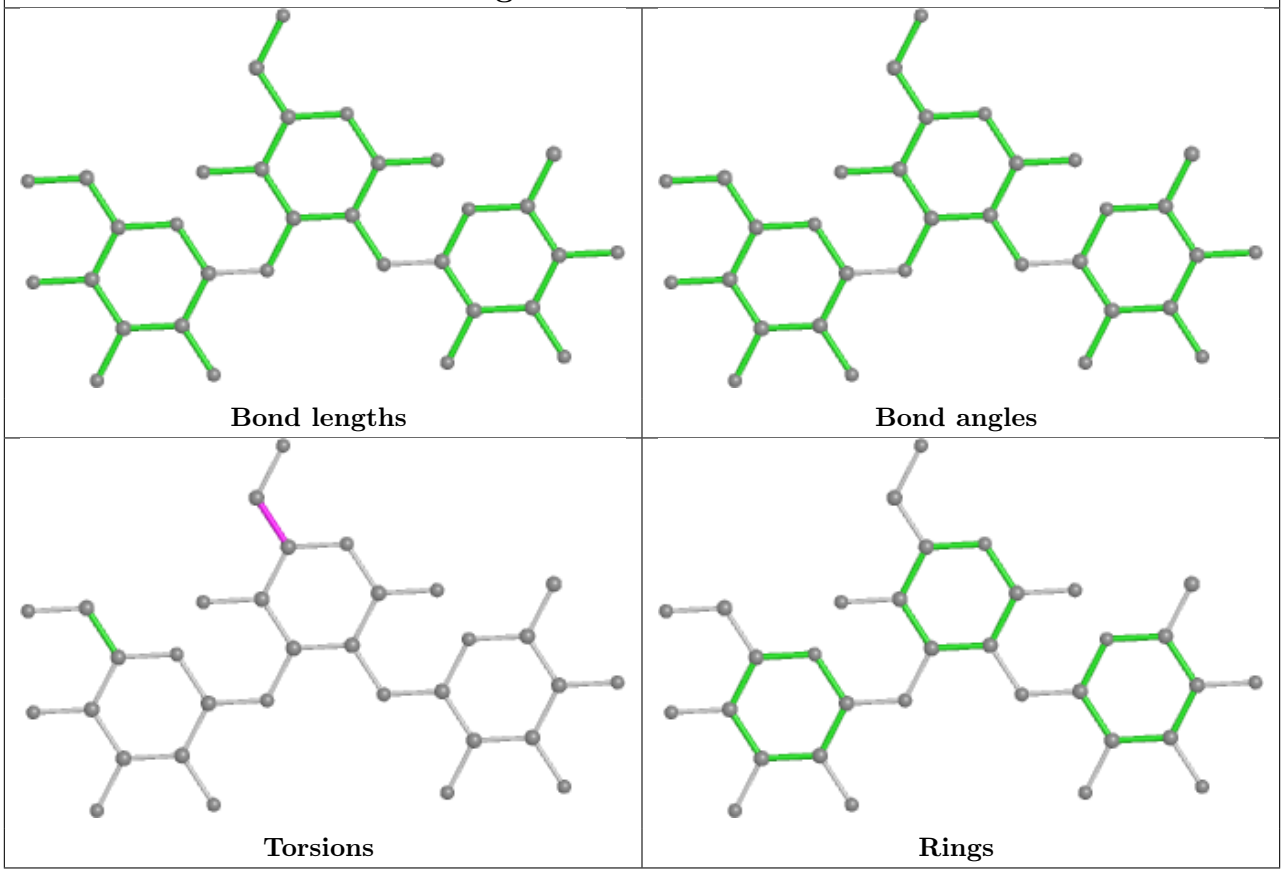


Torsions



Rings

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	EDO	AAA	301	-	3,3,3	0.39	0	2,2,2	0.20	0
5	DMS	AAA	302	-	3,3,3	0.26	0	3,3,3	0.15	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
4	EDO	AAA	301	-	-	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, 95^{th} 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	AAA	291/293 (99%)	-0.65	2 (0%)	87	87	13, 18, 28, 53	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	55[A]	ASN	3.0
1	AAA	252	ALA	2.0

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

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, 95^{th} 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
1	CZZ	AAA	215[A]	8/9	0.96	0.07	15,16,29,33	5
1	CZZ	AAA	215[B]	8/9	0.96	0.07	15,17,35,36	5

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, 95^{th} 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	FUC	B	2	10/11	0.90	0.21	30,37,41,45	0
3	FUC	C	2	10/11	0.93	0.08	23,32,35,36	0
2	GLA	B	3	11/12	0.94	0.11	22,25,27,28	0

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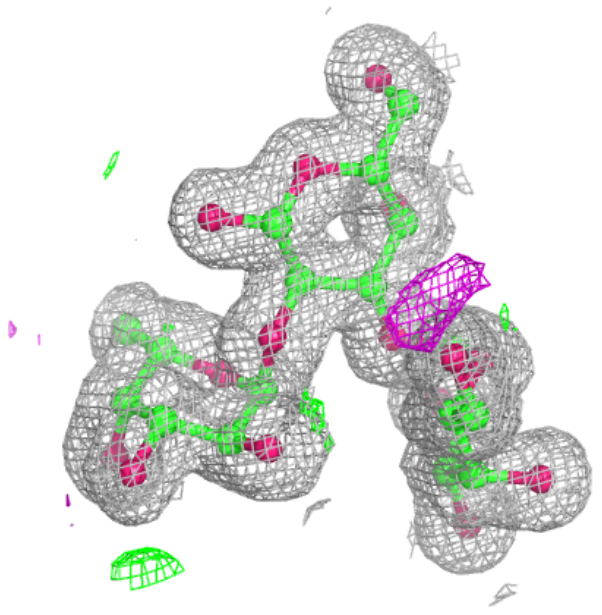
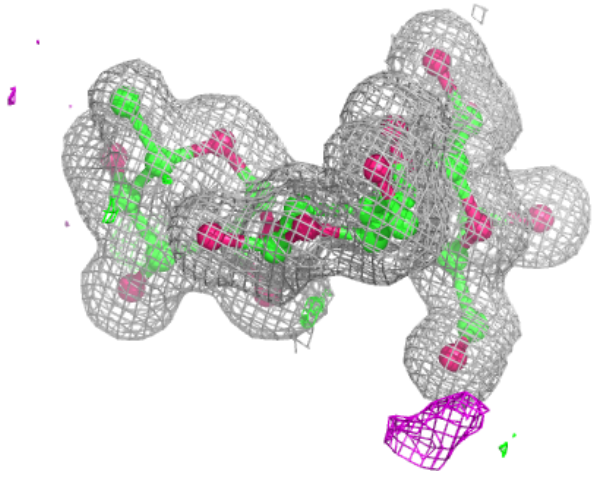
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	B	1	12/12	0.94	0.09	17,23,29,36	0
3	GLA	C	3	11/12	0.96	0.06	17,19,23,23	0
2	FUC	A	2	10/11	0.97	0.07	14,16,17,18	0
3	GLA	C	1	12/12	0.97	0.05	15,17,18,21	0
2	GAL	A	1	12/12	0.98	0.06	12,13,13,16	0
2	GLA	A	3	11/12	0.98	0.05	11,12,13,13	0

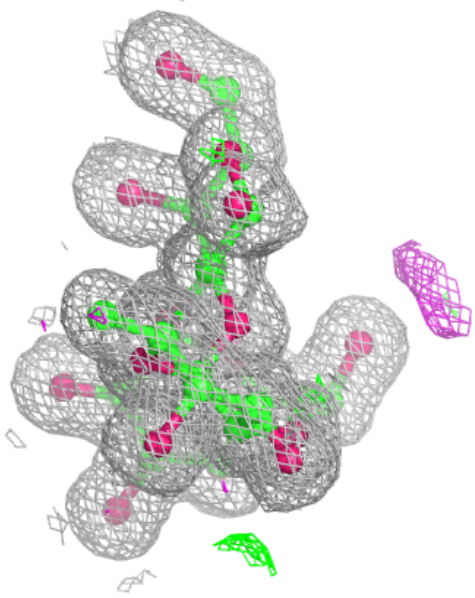
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

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

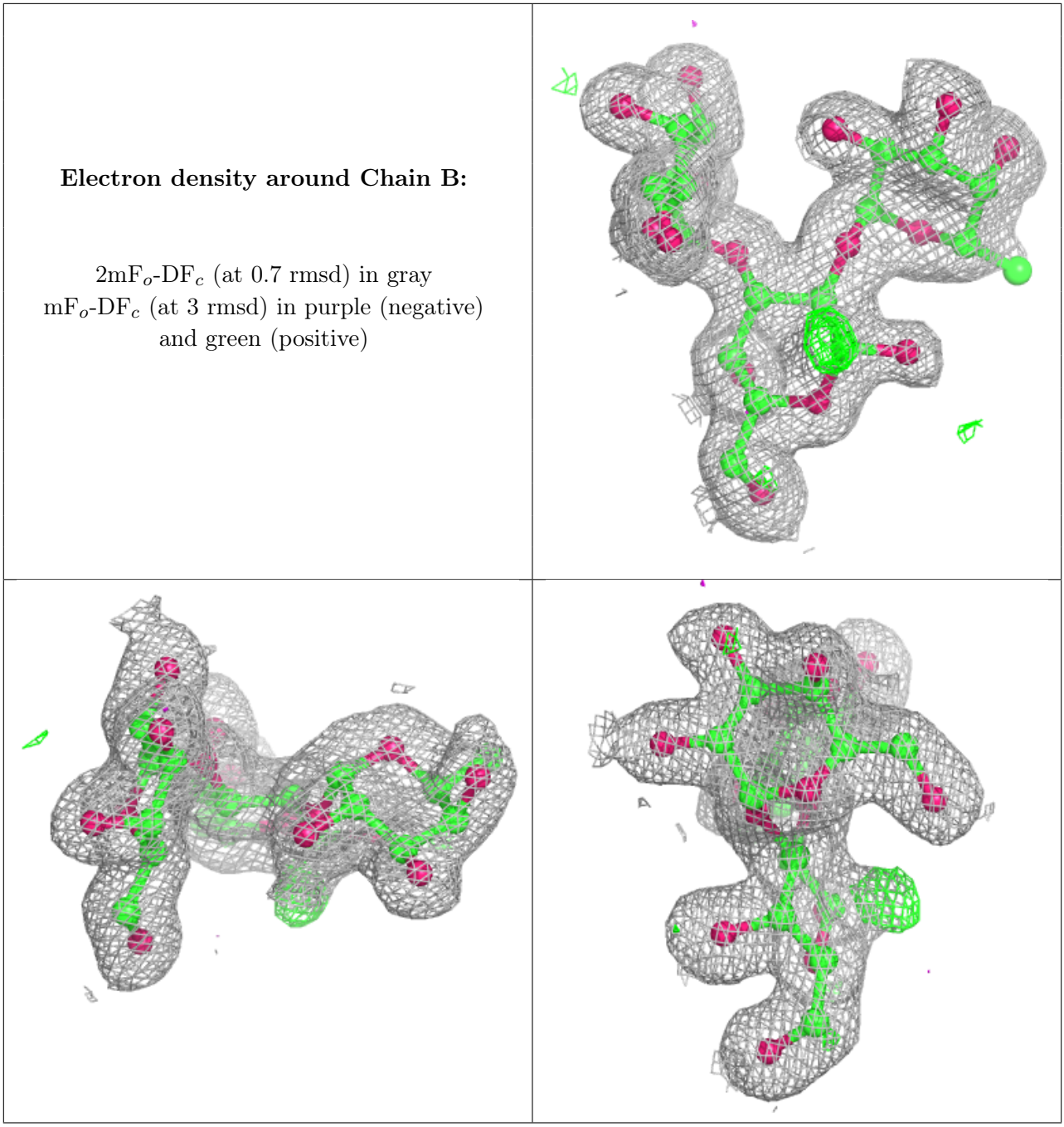






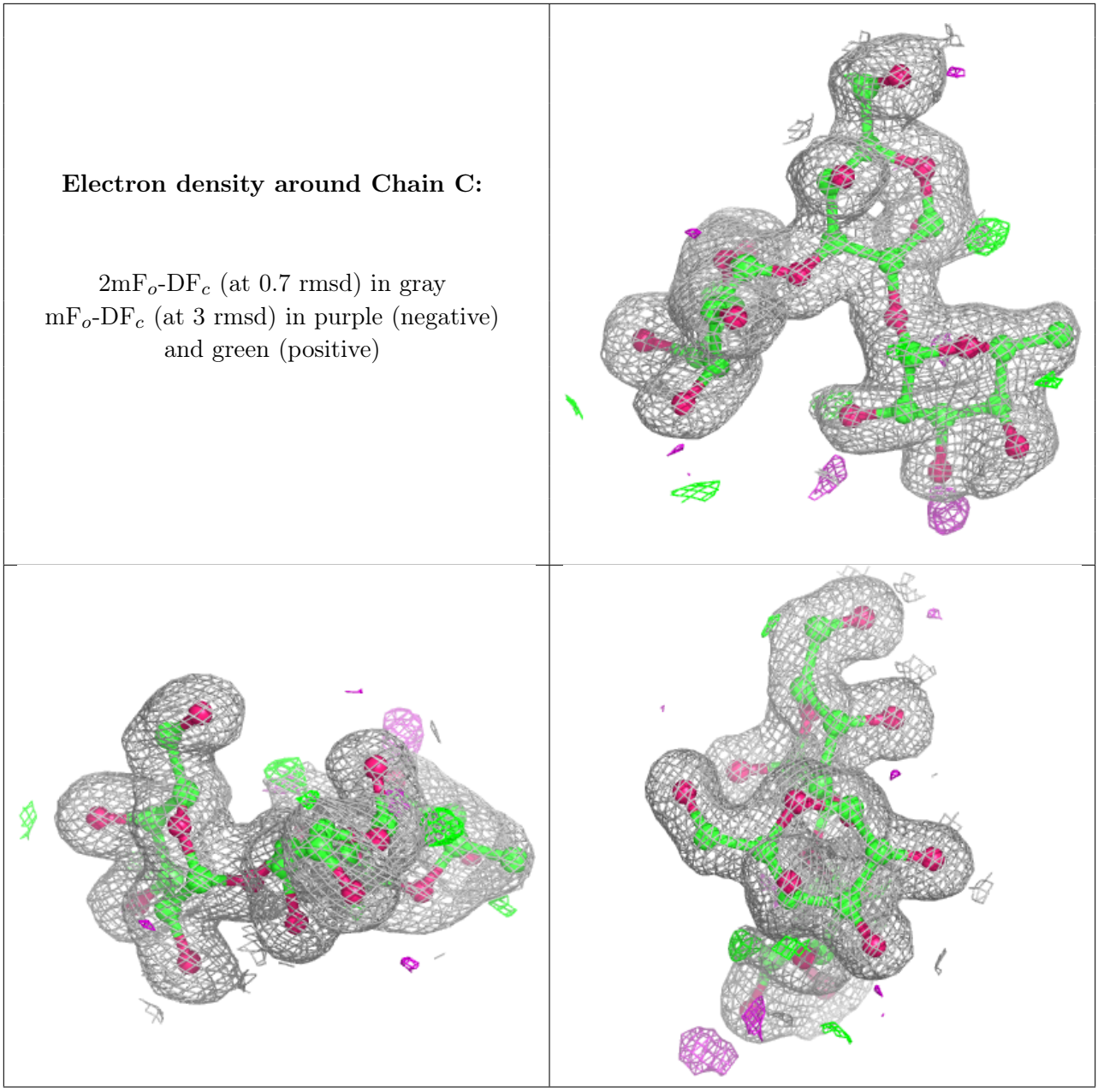
Electron density around Chain B:

$2mF_o$-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 C:

$2mF_o$-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, 95^{th} 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
7	NA	AAA	305	1/1	0.95	0.14	31,31,31,31	1
4	EDO	AAA	301	4/4	0.96	0.06	26,27,27,29	0
6	CA	AAA	304	1/1	0.99	0.05	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	AAA	302	4/4	0.99	0.05	19,20,21,25	1
6	CA	AAA	303	1/1	1.00	0.05	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.