

Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 - 04:14 pm GMT

PDB ID	:	6 TSQ
Title	:	Marasmius oreades agglutinin (MOA) activated by manganese (II)
Authors	:	Cordara, G.; Manna, D.; Krengel, U.
Deposited on		
Resolution	:	1.85 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 (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 (1)) were used in the production of this report:

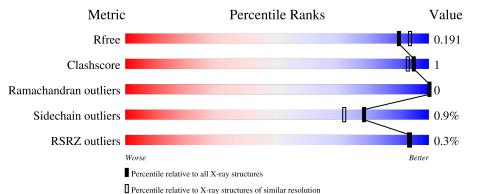
MolProbity		4 02b-467
·		
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.85 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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		96%	•
2	А	3	33%	67%	
3	В	3		100%	
3	С	3		100%	



6TSQ

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 2728 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			Atom	ıs			ZeroOcc	AltConf	Trace
1	AAA	292	Total 2385	As 1	C 1522	N 397	0 456	S 9	0	17	0

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



Mol	Chain	Residues	At	\mathbf{oms}		ZeroOcc	AltConf	Trace
2	А	3	Total 33	C 18	O 15	0	0	0

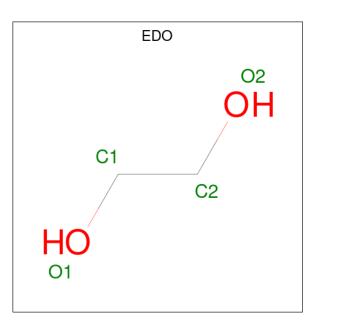
• Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranos e-(1-3)]alpha-D-galactopyranose.



Mol	Chain	Residues	Atom	5	ZeroOcc	AltConf	Trace
3	В	3	TotalC3318		0	0	0
3	С	3	Total C 33 18	O 15	0	0	0

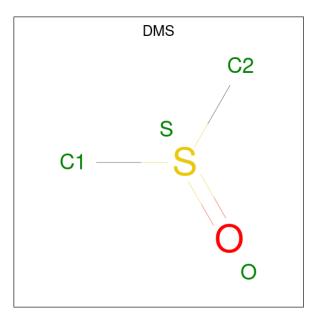
• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	AAA	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	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 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	S 1	0	0

• Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).



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

• Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	3	Total Mn 3 3	0	0

• Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	1	Total 1	Ca 1	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	226	Total O 226 226	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:	96% •	
MET 82 N55 760 7164 R169 R169	1203 1204 1215 1216 1216 1216 1216 1218 1204	
• Molecule 2: • e	lpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]beta-D-galacto	pyranos
Chain A:	33% 67%	
GAL1 FUC2 GLA3		
• Molecule 3: a e	lpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]alpha-D-galacto	pyranos
Chain B:	100%	
GLA1 FUC2 GLA3		
• Molecule 3: a e	lpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]alpha-D-galacto	pyranos
Chain C:	100%	
GLA1 FUC2 GLA3		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants	120.95Å 120.95Å 99.48Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.30 - 1.85	Depositor
Resolution (A)	44.93 - 1.85	EDS
% Data completeness	93.1 (46.30-1.85)	Depositor
(in resolution range)	93.2 (44.93-1.85)	EDS
R _{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.49 (at 1.86 \text{\AA})$	Xtriage
Refinement program	REFMAC 7.0.078	Depositor
D D.	0.156 , 0.182	Depositor
R, R_{free}	0.168 , 0.191	DCC
R_{free} test set	1728 reflections (5.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	19.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 40.2	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	2728	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 3.90% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: CZZ, NA, CA, FUC, GAL, DMS, GLA, EDO, MN

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).

Mal	Mol Chain Bond lengths		Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	AAA	0.79	0/2481	0.57	0/3376

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.

There are no bond angle outliers.

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 (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	AAA	2385	0	2249	5	0
2	А	33	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	33	0	30	0	0
3	С	33	0	30	0	0
4	AAA	8	0	11	0	0
5	AAA	4	0	6	0	0
6	AAA	2	0	0	0	0
7	AAA	3	0	0	0	0
8	AAA	1	0	0	1	0
9	AAA	226	0	0	1	0
All	All	2728	0	2356	6	0

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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 1.

All (6) 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)
8:AAA:308:CA:CA	9:AAA:415:HOH:O	1.75	0.64
1:AAA:203:LEU:N	1:AAA:204:PRO:CD	2.68	0.56
1:AAA:164[B]:GLN:CD	1:AAA:181:ILE:HD11	2.33	0.49
1:AAA:244:GLY:HA3	1:AAA:261:PHE:CE1	2.47	0.49
1:AAA:169[B]:ARG:HD2	1:AAA:268:ALA:O	2.15	0.47
1:AAA:169[B]:ARG:O	1:AAA:169[B]:ARG:HG3	2.17	0.43

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	5
1	AAA	306/293~(104%)	292~(95%)	14 (5%)	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 side chain 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	249/233~(107%)	247~(99%)	2(1%)	81 76

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

Mol	Chain	Res	Type
1	AAA	2	SER
1	AAA	216	ASP

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)

1 non-standard protein/DNA/RNA residue 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).

Mal	Type	Chain	Dog	Link	B	ond leng	$_{ m gths}$	В	ond ang	gles
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CZZ	AAA	215	1	3,7,8	1.33	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	1	-	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	CZZ	CB-CA	2.08	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	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	GAL	А	1	2	$12,\!12,\!12$	0.69	0	$17,\!17,\!17$	0.52	0
2	FUC	А	2	2	10, 10, 11	0.96	1 (10%)	$14,\!14,\!16$	0.53	0
2	GLA	А	3	2	11,11,12	1.13	1 (9%)	$15,\!15,\!17$	0.71	0
3	GLA	В	1	3	12,12,12	0.69	0	17,17,17	0.66	0
3	FUC	В	2	3	10,10,11	0.47	0	$14,\!14,\!16$	0.68	0
3	GLA	В	3	3	$11,\!11,\!12$	0.53	0	$15,\!15,\!17$	0.57	0
3	GLA	С	1	3	12,12,12	0.86	0	$17,\!17,\!17$	0.65	0
3	FUC	С	2	3	10,10,11	0.71	0	$14,\!14,\!16$	0.73	0
3	GLA	С	3	3	$11,\!11,\!12$	0.58	0	$15,\!15,\!17$	0.53	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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	А	1	2	-	2/2/22/22	0/1/1/1
2	FUC	А	2	2	-	-	0/1/1/1
2	GLA	А	3	2	-	0/2/19/22	0/1/1/1
3	GLA	В	1	3	-	2/2/22/22	0/1/1/1
3	FUC	В	2	3	-	-	0/1/1/1
3	GLA	В	3	3	-	0/2/19/22	0/1/1/1
3	GLA	С	1	3	-	2/2/22/22	0/1/1/1
3	FUC	С	2	3	-	-	0/1/1/1
3	GLA	С	3	3	-	0/2/19/22	0/1/1/1

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	А	2	FUC	O5-C1	-2.30	1.40	1.43
2	А	3	GLA	O6-C6	2.10	1.51	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

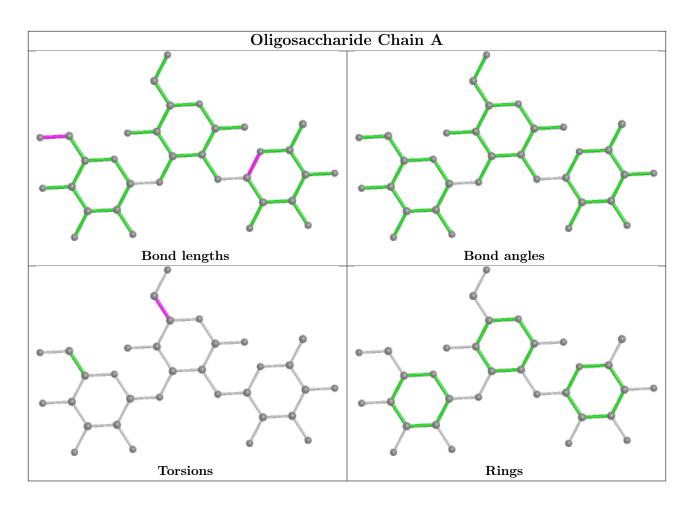
Mol	Chain	Res	Type	Atoms
3	С	1	GLA	C4-C5-C6-O6
3	В	1	GLA	C4-C5-C6-O6
2	А	1	GAL	C4-C5-C6-O6
3	С	1	GLA	O5-C5-C6-O6
3	В	1	GLA	O5-C5-C6-O6
2	А	1	GAL	O5-C5-C6-O6

There are no ring outliers.

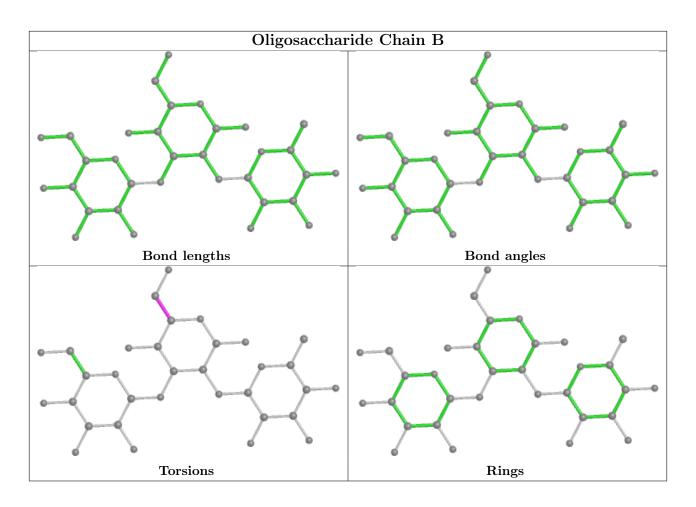
No monomer is involved in short contacts.

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

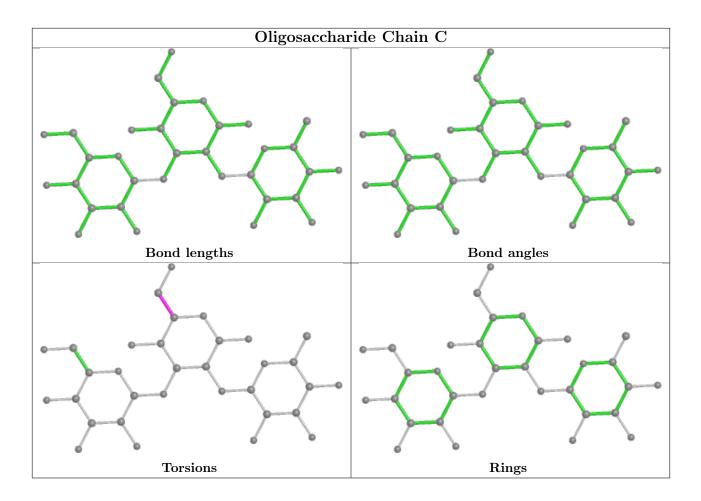












5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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).

Mal	Mol Type Chain Res Link		Tinle	B	ond leng	gths	Bond angles			
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
5	DMS	AAA	303	-	3,3,3	0.76	0	3,3,3	0.13	0
4	EDO	AAA	301	-	3,3,3	0.24	0	2,2,2	0.17	0
4	EDO	AAA	302	7	3,3,3	0.29	0	$2,\!2,\!2$	0.17	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	-
4	EDO	AAA	302	7	-	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, 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%)	-0.63	1 (0%) 94 93	12, 18, 27, 43	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	55[A]	ASN	3.1

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
1	CZZ	AAA	215	8/9	0.95	0.07	$14,\!16,\!27,\!31$	3

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, 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	GLA	В	1	12/12	0.94	0.11	17,19,25,30	0
3	FUC	В	2	10/11	0.94	0.12	24,28,30,33	10
3	FUC	С	2	10/11	0.95	0.08	$25,\!32,\!38,\!38$	0
2	FUC	А	2	10/11	0.96	0.07	14,16,18,18	0
3	GLA	В	3	11/12	0.97	0.10	20,22,23,24	0

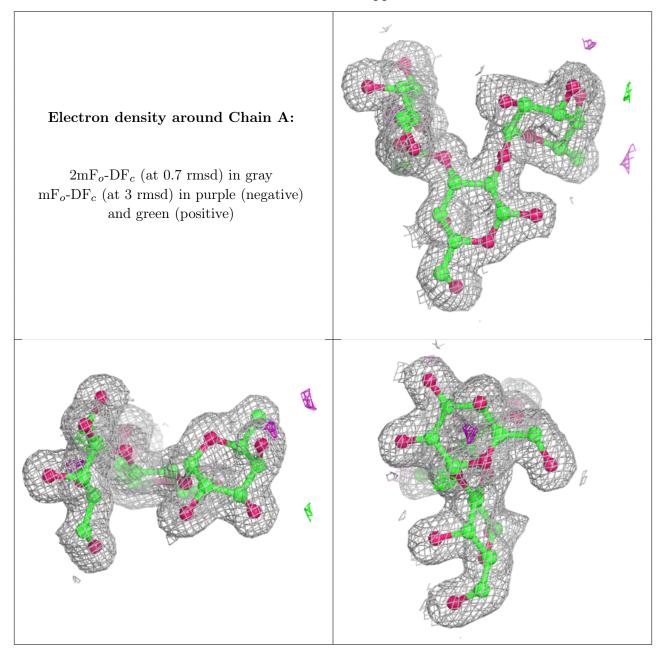
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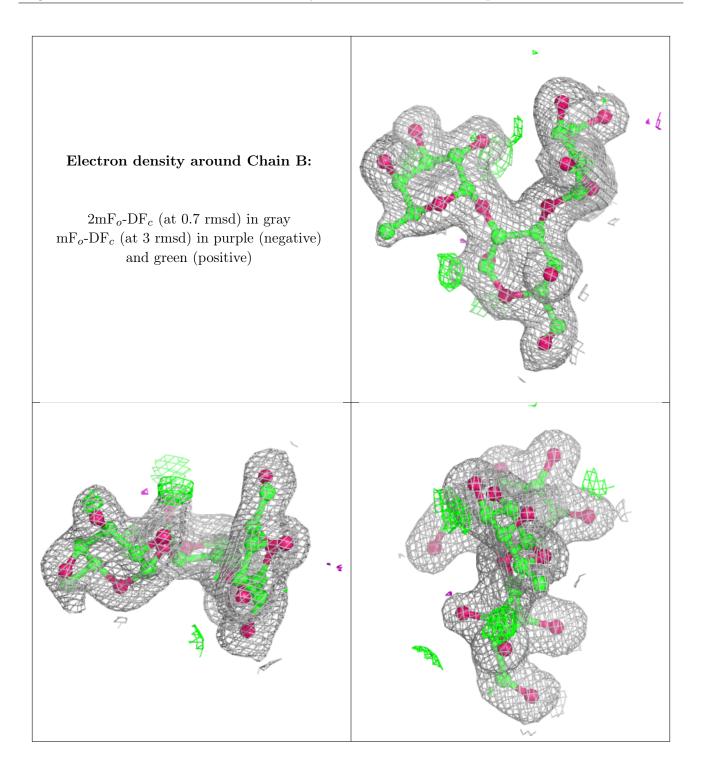
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	$Q{<}0.9$	
3	GLA	С	1	12/12	0.97	0.06	$14,\!15,\!19,\!20$	0	
2	GLA	А	3	11/12	0.97	0.07	11,12,13,14	0	
3	GLA	С	3	11/12	0.97	0.06	$15,\!17,\!18,\!19$	0	
2	GAL	А	1	12/12	0.98	0.07	11,13,16,18	0	

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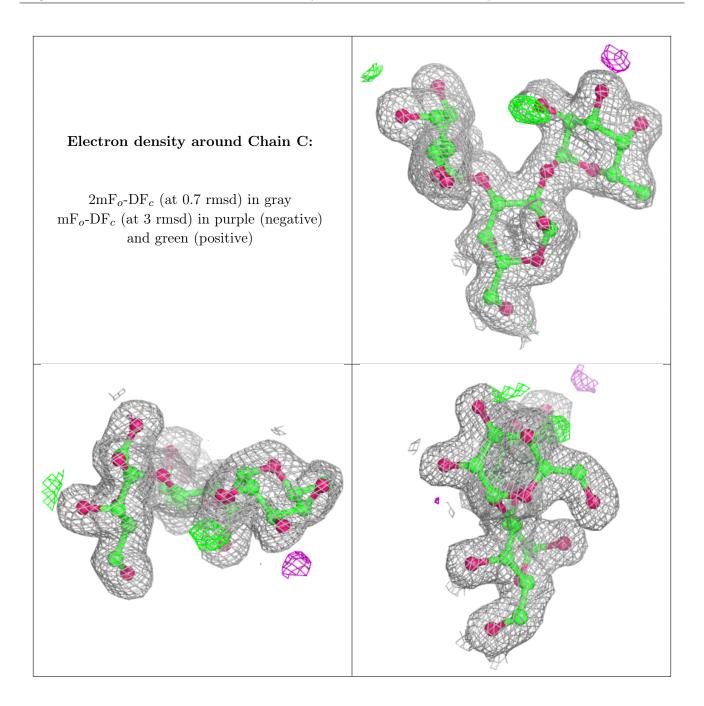
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.











6.4 Ligands (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, 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
6	NA	AAA	305	1/1	0.90	0.14	44,44,44,44	0
4	EDO	AAA	302	4/4	0.92	0.12	27,31,31,32	0
4	EDO	AAA	301	4/4	0.95	0.09	23,25,25,29	0

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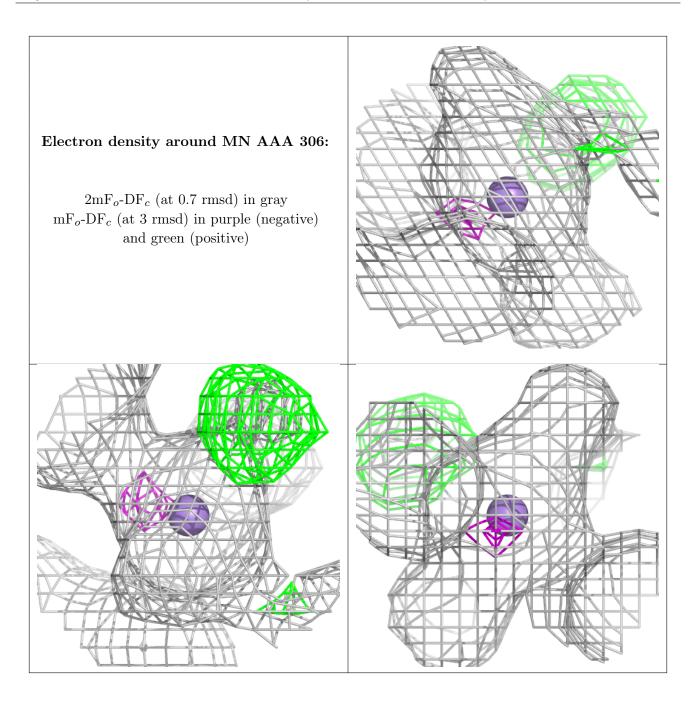


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q < 0.9
6	NA	AAA	304	1/1	0.97	0.08	32,32,32,32	1
7	MN	AAA	306	1/1	0.97	0.12	27,27,27,27	1
5	DMS	AAA	303	4/4	0.98	0.09	20,23,24,26	3
7	MN	AAA	307	1/1	1.00	0.08	18,18,18,18	0
7	MN	AAA	309	1/1	1.00	0.05	16, 16, 16, 16	1
8	CA	AAA	308	1/1	1.00	0.07	$7,\!7,\!7,\!7$	1

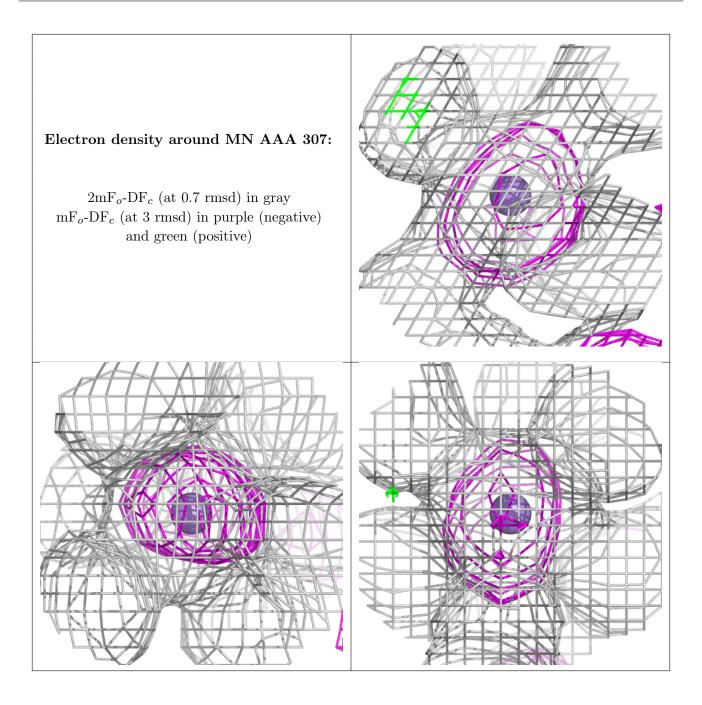
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The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

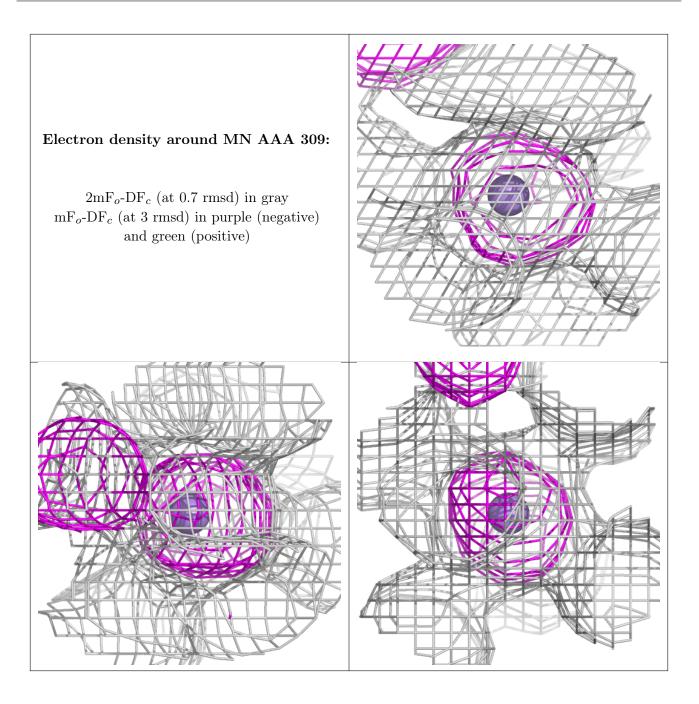




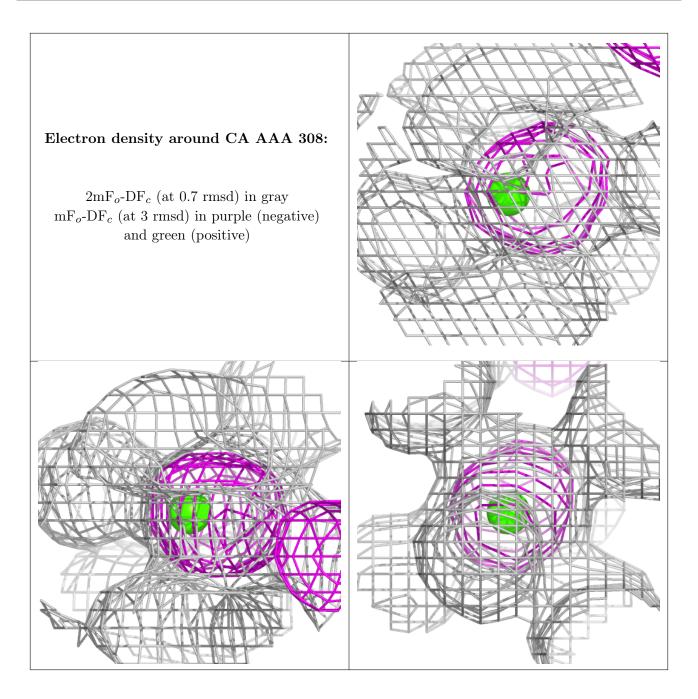












6.5 Other polymers (i)

There are no such residues in this entry.

