



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 08:52 AM BST

PDB ID : 6TSR
Title : Marasmius oreades agglutinin (MOA) activated by manganese (II) and calcium
Authors : Cordara, G.; Manna, D.; Krenzel, U.
Deposited on : 2019-12-21
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 ⓘ 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
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) : 2.13.1

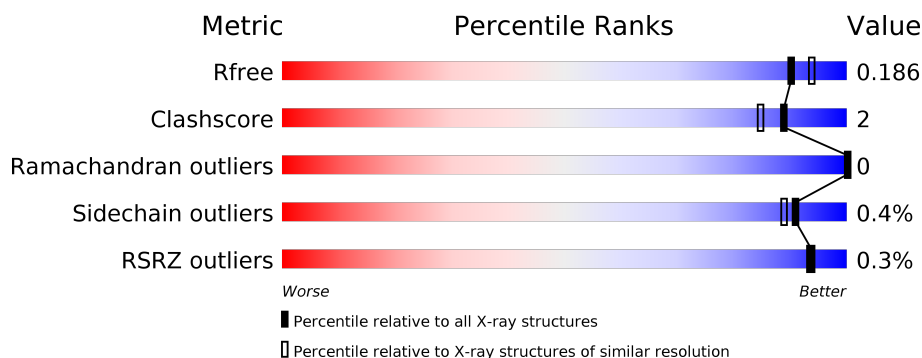
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

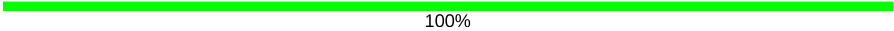
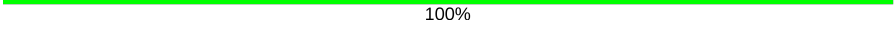

The reported resolution of this entry is 1.85 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 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	AAA	293	 96%
2	A	3	 100%
3	B	3	 100%
3	C	3	 67% 33%

2 Entry composition [i](#)

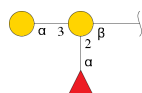
There are 9 unique types of molecules in this entry. The entry contains 2706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

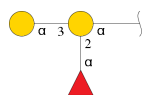
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	292	Total	As	C	N	O	S	0	16	0
			2366	1	1505	397	455	8			

- 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			

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



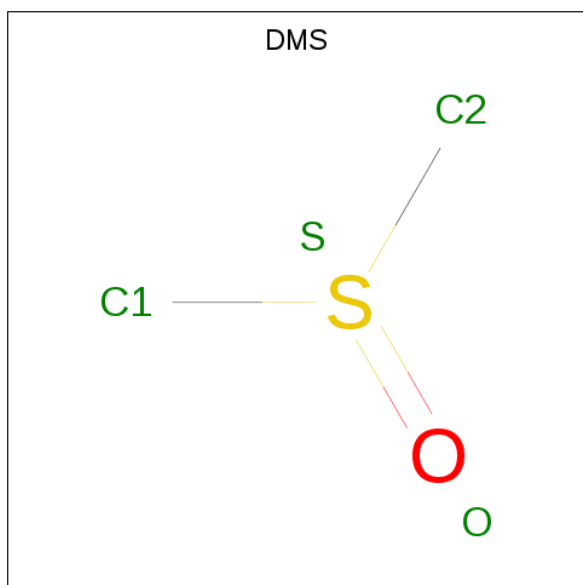
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	B	3	Total	C	O	0	0	0
			33	18	15			
3	C	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- 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
5	AAA	1	Total C O S 4 2 1 1	0	0

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

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

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

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	2	Total Mn 2 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	212	Total O 212 212	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: Agglutinin

Chain AAA:  96%



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

Chain A:  100%



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

Chain B:  100%



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

Chain C:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.57Å 121.57Å 99.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.50 – 1.85 45.01 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.50-1.85) 98.8 (45.01-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.86Å)	Xtriage
Refinement program	REFMAC 7.0.078	Depositor
R, R_{free}	0.152 , 0.175 0.164 , 0.186	Depositor DCC
R_{free} test set	1934 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2706	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CZZ, GLA, CA, MN, EDO, DMS, FUC, NA, 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	0.85	0/2469	0.60	2/3360 (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($^{\circ}$)	Ideal($^{\circ}$)
1	AAA	79[A]	GLU	CA-CB-CG	-7.72	96.42	113.40
1	AAA	79[B]	GLU	CA-CB-CG	-7.72	96.42	113.40

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	2366	0	2213	9	0
2	A	33	0	30	0	0
3	B	33	0	30	0	0
3	C	33	0	30	0	0
4	AAA	16	0	23	0	0
5	AAA	8	0	12	0	0
6	AAA	1	0	0	0	0
7	AAA	2	0	0	0	0
8	AAA	2	0	0	0	0
9	AAA	212	0	0	0	1
All	All	2706	0	2338	9	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (9) 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:77:SER:OG	1:AAA:79[A]:GLU:CG	2.18	0.92
1:AAA:77:SER:OG	1:AAA:79[A]:GLU:HG3	1.92	0.68
1:AAA:77:SER:OG	1:AAA:79[A]:GLU:HG2	2.00	0.61
1:AAA:77:SER:OG	1:AAA:79[A]:GLU:CD	2.44	0.56
1:AAA:203:LEU:N	1:AAA:204:PRO:CD	2.69	0.54
1:AAA:244:GLY:HA3	1:AAA:261:PHE:CE1	2.46	0.51
1:AAA:77:SER:OG	1:AAA:79[A]:GLU:OE1	2.30	0.49
1:AAA:169[B]:ARG:HD2	1:AAA:268:ALA:O	2.18	0.44
1:AAA:144:GLU:O	1:AAA:150[B]:LYS:NZ	2.49	0.43

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)
9:AAA:499:HOH:O	9:AAA:499:HOH:O[10_555]	2.18	0.02

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	305/293 (104%)	295 (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	248/233 (106%)	246 (99%)	2 (1%)	81	76

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

Mol	Chain	Res	Type
1	AAA	79[A]	GLU
1	AAA	79[B]	GLU

Some 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CZZ	AAA	215	1	3,7,8	1.51	1 (33%)	0,7,9	0.00	-

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	2.48	1.59	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

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	0.73	0	17,17,17	0.60	0
2	FUC	A	2	2	10,10,11	0.75	0	14,14,16	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLA	A	3	2	11,11,12	0.88	0	15,15,17	0.72	0
3	GLA	B	1	3	12,12,12	0.70	0	17,17,17	0.65	0
3	FUC	B	2	3	10,10,11	0.60	0	14,14,16	0.64	0
3	GLA	B	3	3	11,11,12	0.83	0	15,15,17	0.54	0
3	GLA	C	1	3	12,12,12	0.60	0	17,17,17	0.67	0
3	FUC	C	2	3	10,10,11	1.05	1 (10%)	14,14,16	0.69	0
3	GLA	C	3	3	11,11,12	0.61	0	15,15,17	0.59	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	-	1/2/22/22	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
3	GLA	B	1	3	-	2/2/22/22	0/1/1/1
3	FUC	B	2	3	-	-	0/1/1/1
3	GLA	B	3	3	-	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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	FUC	O5-C1	-2.81	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

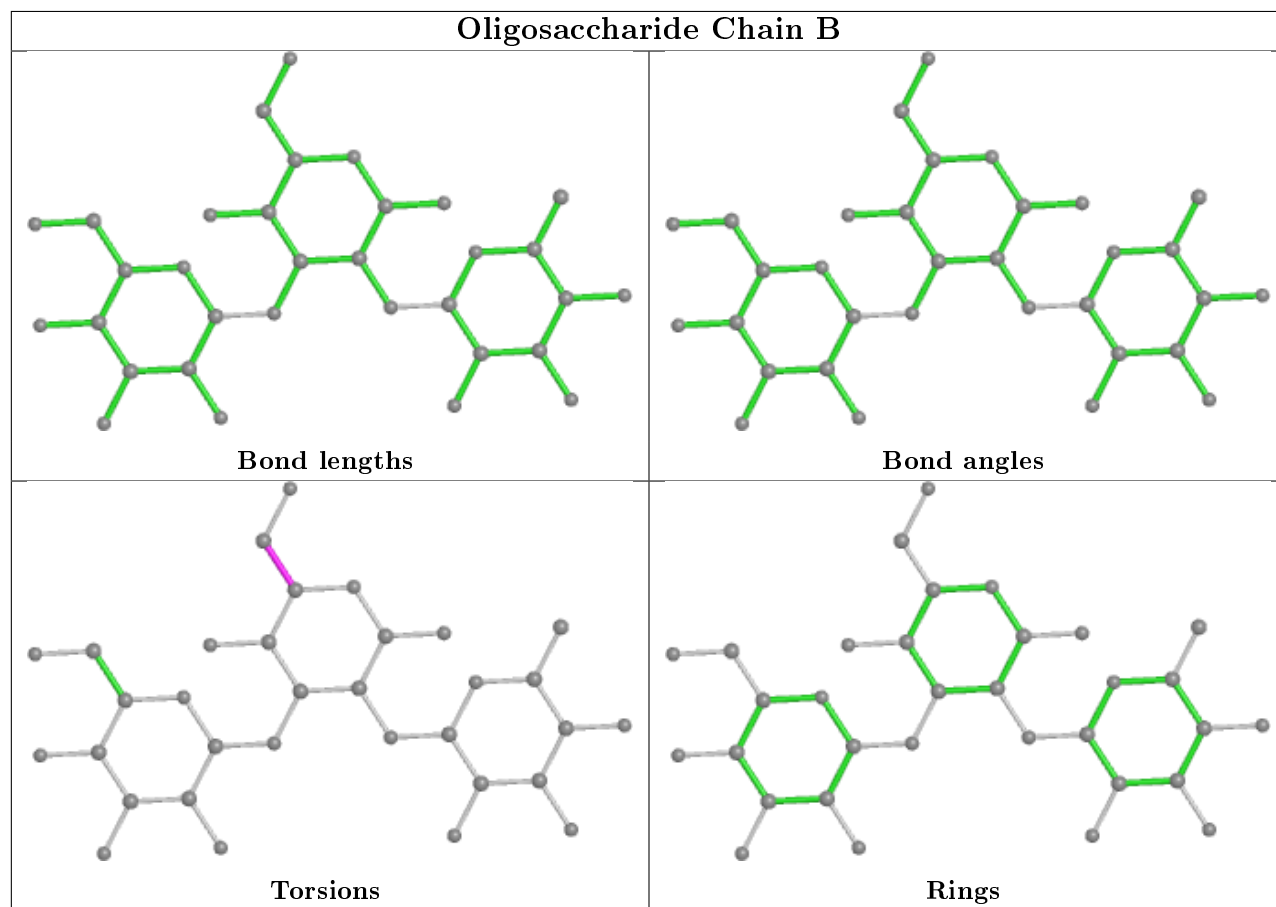
All (5) torsion outliers are listed below:

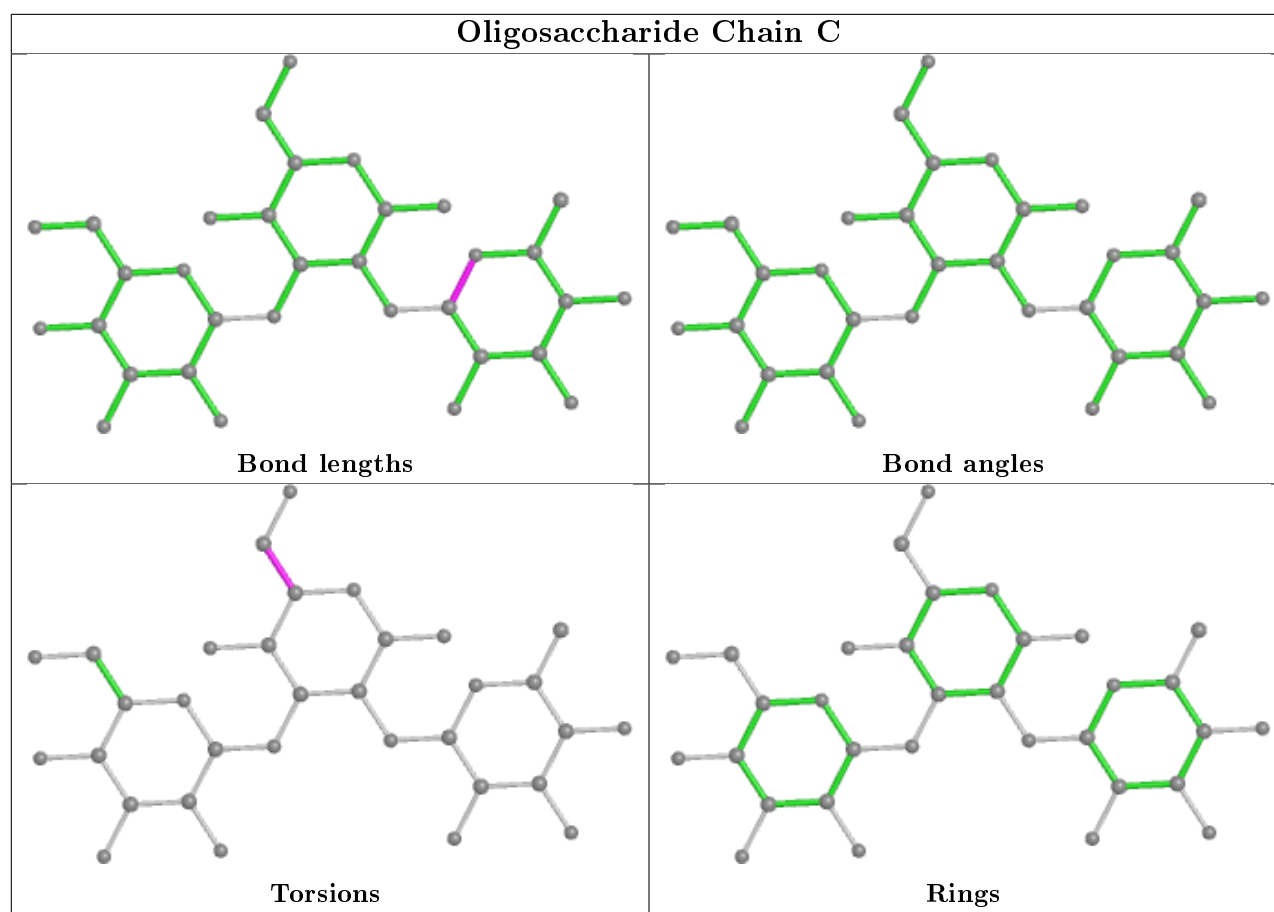
Mol	Chain	Res	Type	Atoms
3	B	1	GLA	C4-C5-C6-O6
3	C	1	GLA	C4-C5-C6-O6
3	B	1	GLA	O5-C5-C6-O6
3	C	1	GLA	O5-C5-C6-O6
2	A	1	GAL	C4-C5-C6-O6

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 [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	DMS	AAA	305	-	3,3,3	0.59	0	3,3,3	0.14	0
4	EDO	AAA	304	8,7	3,3,3	0.14	0	2,2,2	0.16	0
5	DMS	AAA	306	-	3,3,3	0.31	0	3,3,3	0.10	0
4	EDO	AAA	301	-	3,3,3	0.52	0	2,2,2	0.17	0
4	EDO	AAA	302	-	3,3,3	0.40	0	2,2,2	0.14	0
4	EDO	AAA	303	-	3,3,3	0.48	0	2,2,2	0.12	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	302	-	-	0/1/1/1	-
4	EDO	AAA	301	-	-	0/1/1/1	-
4	EDO	AAA	304	8,7	-	0/1/1/1	-
4	EDO	AAA	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	303	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	291/293 (99%)	-0.63	1 (0%) 94 93	14, 18, 28, 53	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	55[A]	ASN	2.2

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, 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
1	CZZ	AAA	215	8/9	0.96	0.08	14,16,28,32	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, 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	GLA	B	1	12/12	0.93	0.12	18,23,28,36	0
3	FUC	C	2	10/11	0.94	0.11	25,34,39,41	0
3	FUC	B	2	10/11	0.94	0.21	32,37,40,44	0
3	GLA	C	1	12/12	0.96	0.07	16,17,20,21	0
3	GLA	C	3	11/12	0.96	0.06	17,18,21,21	0

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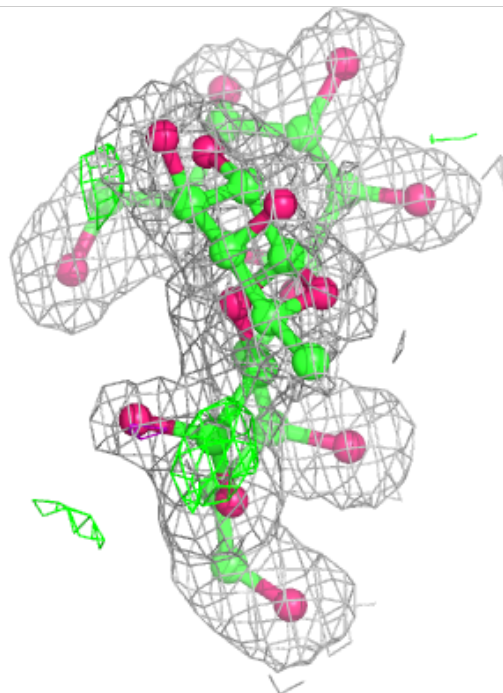
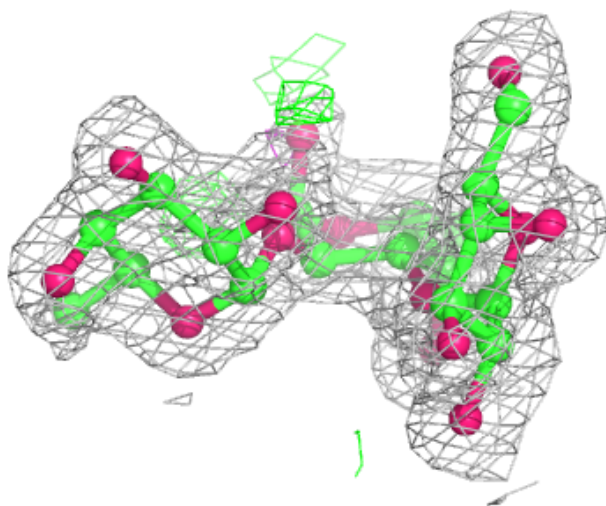
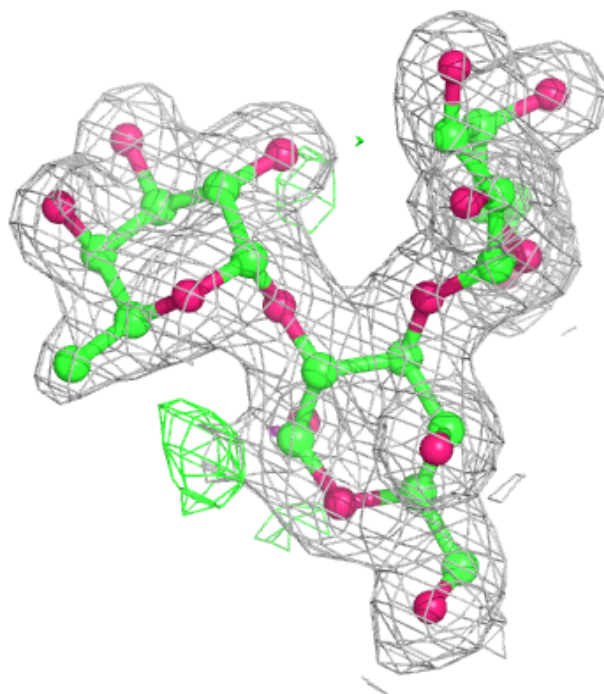
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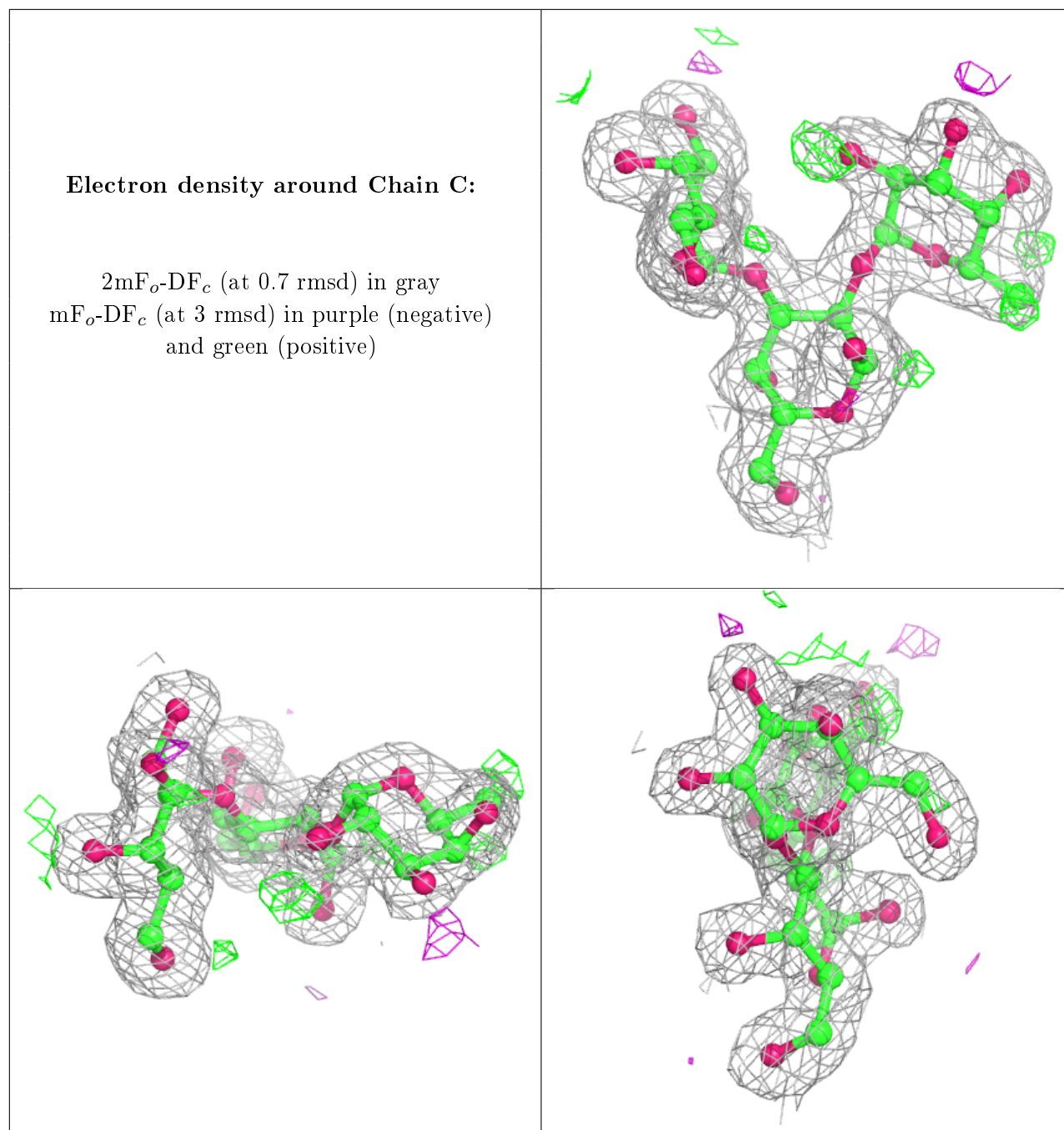
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLA	A	3	11/12	0.97	0.07	12,13,14,14	0
2	GAL	A	1	12/12	0.97	0.07	13,14,17,18	0
3	GLA	B	3	11/12	0.97	0.14	22,24,25,27	0
2	FUC	A	2	10/11	0.97	0.07	16,19,20,21	0

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 B:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	AAA	304	4/4	0.93	0.12	33,37,37,44	0

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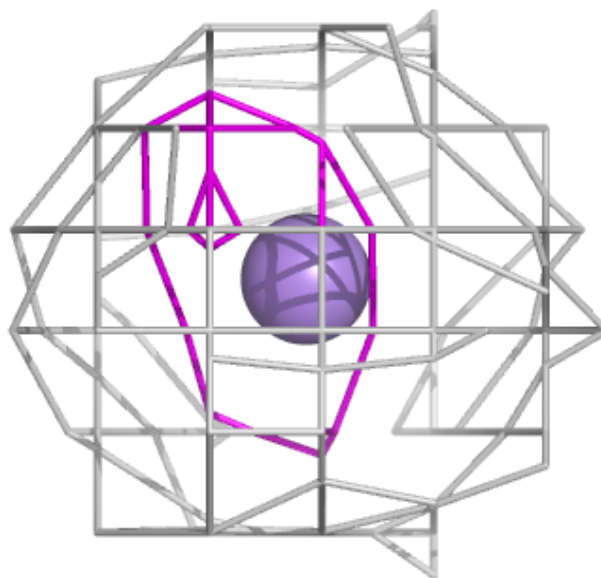
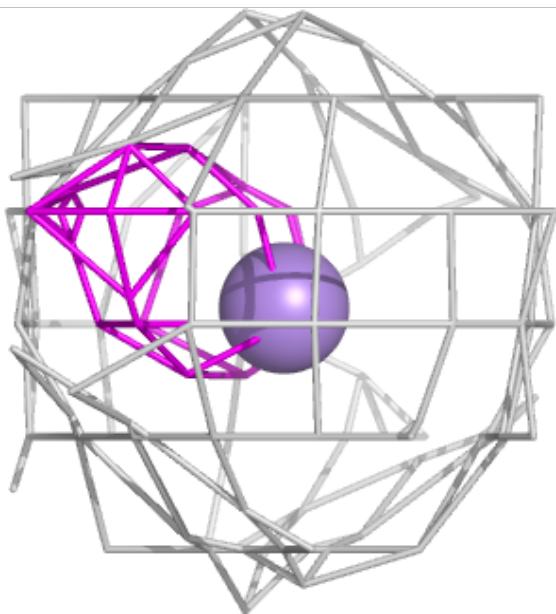
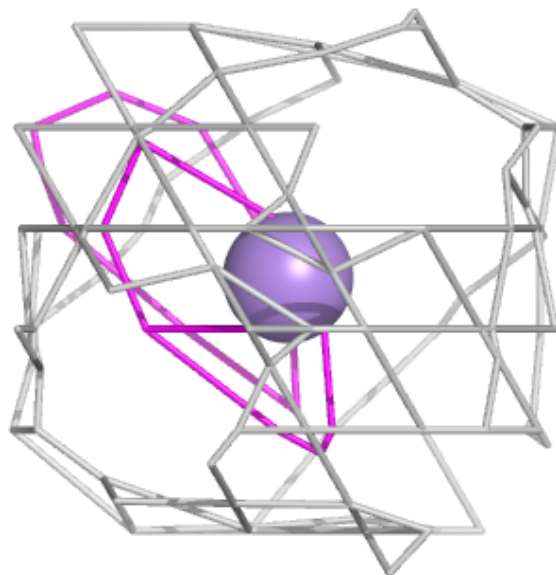
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NA	AAA	307	1/1	0.95	0.08	40,40,40,40	0
5	DMS	AAA	306	4/4	0.95	0.12	25,30,31,38	1
4	EDO	AAA	302	4/4	0.96	0.07	20,25,28,28	0
4	EDO	AAA	303	4/4	0.97	0.11	31,36,36,39	0
4	EDO	AAA	301	4/4	0.98	0.08	23,23,24,24	0
5	DMS	AAA	305	4/4	0.99	0.10	21,22,22,25	3
8	MN	AAA	311	1/1	0.99	0.03	19,19,19,19	1
7	CA	AAA	309	1/1	1.00	0.03	17,17,17,17	1
8	MN	AAA	310	1/1	1.00	0.08	25,25,25,25	1
7	CA	AAA	308	1/1	1.00	0.03	14,14,14,14	0

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.

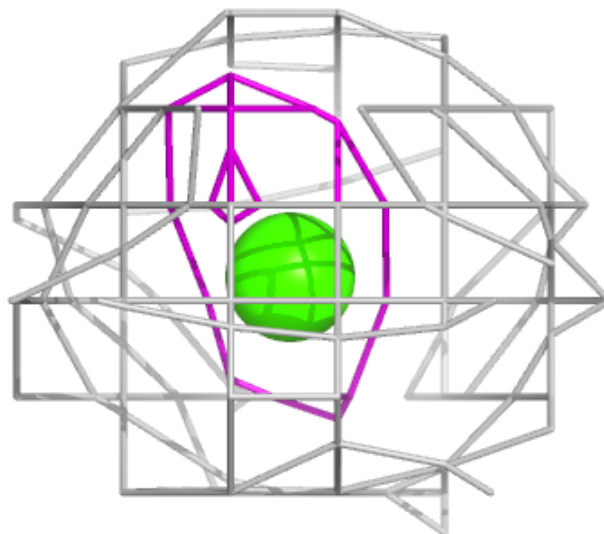
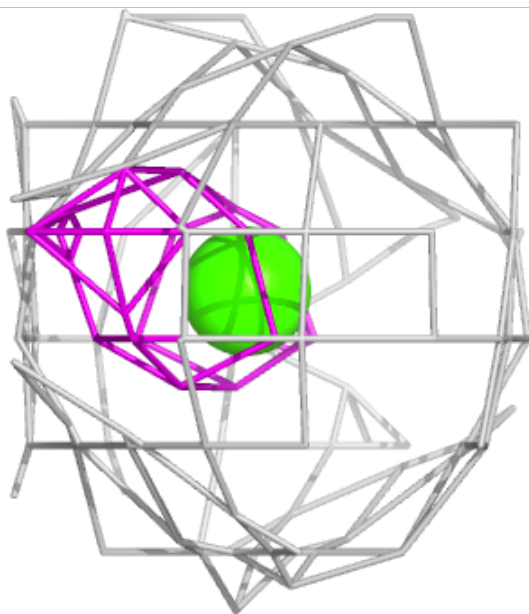
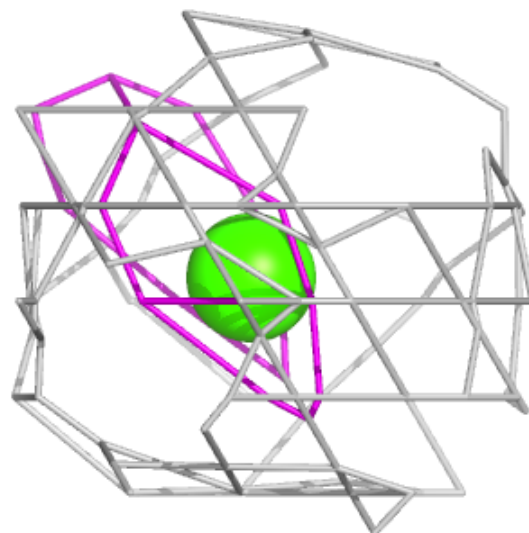
Electron density around MN AAA 311:

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



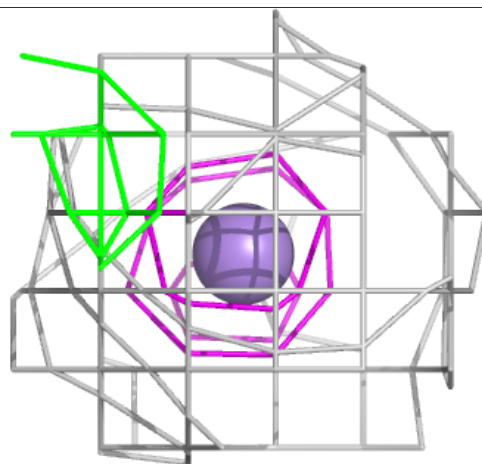
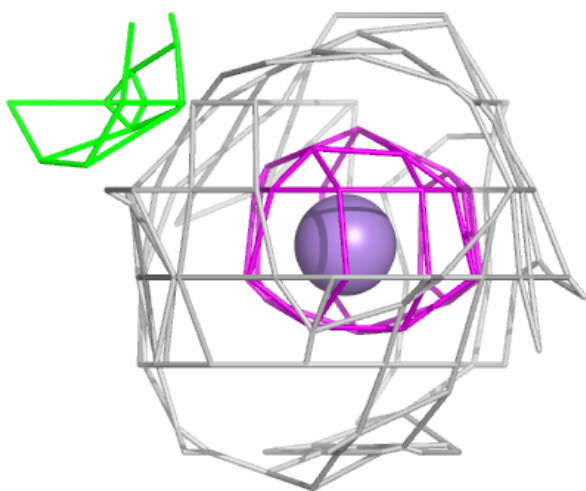
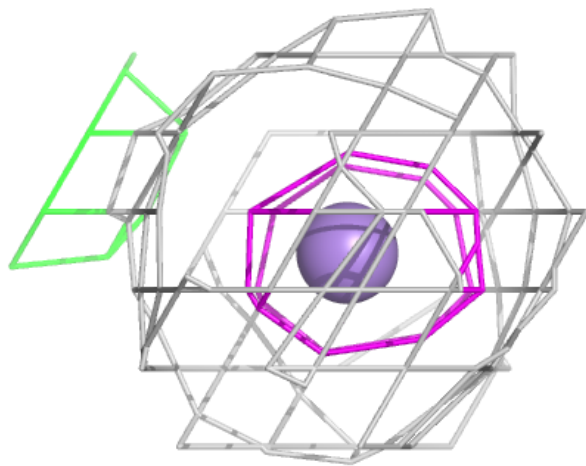
Electron density around CA AAA 309:

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



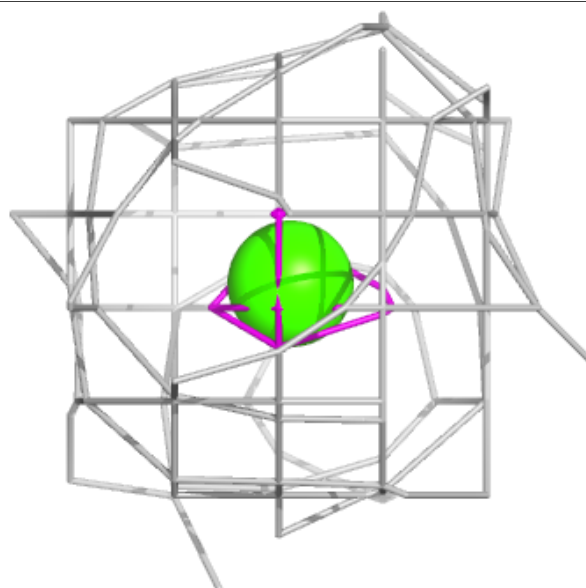
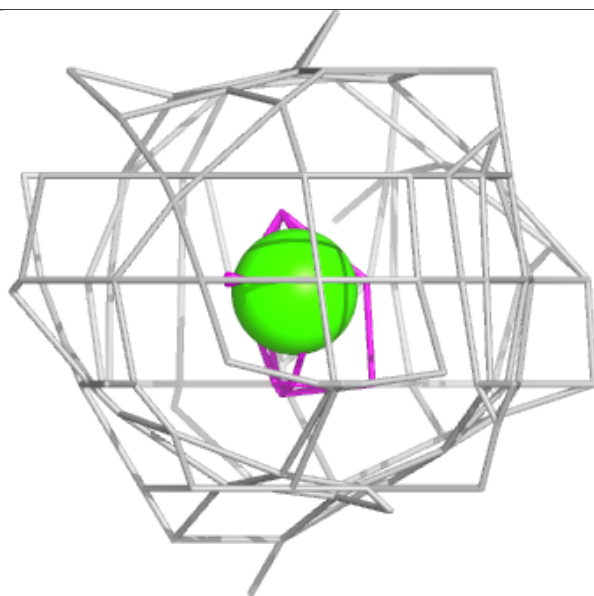
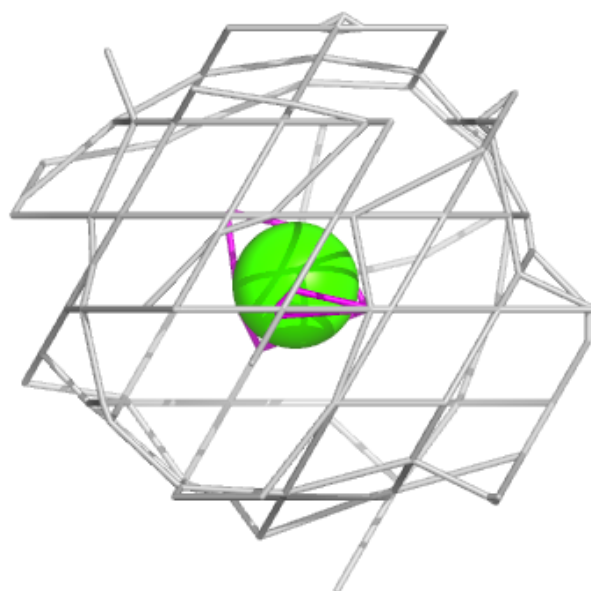
Electron density around MN AAA 310:

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



Electron density around CA AAA 308:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.