



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 01:24 PM UTC

PDB ID : 8FRD / pdb_00008frd
Title : Mouse acidic mammalian chitinase, catalytic domain in complex with N,N'-diacetylchitobiose at pH 5.25
Authors : Diaz, R.E.; Fraser, J.S.
Deposited on : 2023-01-06
Resolution : 1.68 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

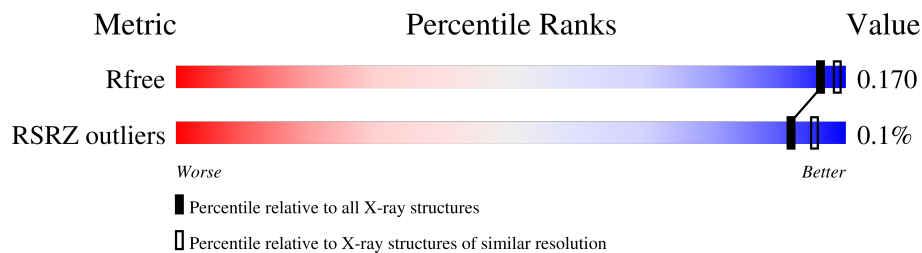
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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}	180053	1054 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 12796 atoms, of which 5863 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 Acidic mammalian chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	369	5896	1945	2866	495	577	13	0	11	0
1	B	369	5818	1924	2829	486	566	13	0	6	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	HIS	-	expression tag	UNP Q91XA9
A	393	HIS	-	expression tag	UNP Q91XA9
A	394	HIS	-	expression tag	UNP Q91XA9
A	395	HIS	-	expression tag	UNP Q91XA9
A	396	HIS	-	expression tag	UNP Q91XA9
A	397	HIS	-	expression tag	UNP Q91XA9
B	392	HIS	-	expression tag	UNP Q91XA9
B	393	HIS	-	expression tag	UNP Q91XA9
B	394	HIS	-	expression tag	UNP Q91XA9
B	395	HIS	-	expression tag	UNP Q91XA9
B	396	HIS	-	expression tag	UNP Q91XA9
B	397	HIS	-	expression tag	UNP Q91XA9

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	2	114	32	56	4	22	0	2	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	D	2	Total	C	H	N	O	0	2	0
			57	16	28	2	11			
2	E	2	Total	C	H	N	O	0	2	0
			57	16	28	2	11			
2	F	2	Total	C	H	N	O	0	2	0
			57	16	28	2	11			
2	G	2	Total	C	H	N	O	0	2	0
			57	16	28	2	11			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	354	Total	O	0	0
			354	354		
4	B	384	Total	O	0	0
			384	384		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.75Å 92.45Å 104.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.67 – 1.68 58.67 – 1.68	Depositor EDS
% Data completeness (in resolution range)	98.5 (58.67-1.68) 98.7 (58.67-1.68)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 1.68Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.139 , 0.168 0.141 , 0.170	Depositor DCC
R_{free} test set	3886 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtrriage
Anisotropy	0.070	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12796	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5090e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

12 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	NAG	C	1[A]	2	15,15,15	1.93	5 (33%)	21,21,21	1.02	0
2	NAG	C	1[C]	2	15,15,15	2.75	7 (46%)	21,21,21	2.23	4 (19%)
2	NAG	C	2[A]	2	14,14,15	2.41	5 (35%)	17,19,21	1.18	1 (5%)
2	NAG	C	2[C]	2	14,14,15	2.06	4 (28%)	17,19,21	0.83	0
2	NAG	D	1[B]	2	15,15,15	1.53	3 (20%)	21,21,21	0.91	0
2	NAG	D	2[B]	2	14,14,15	1.33	1 (7%)	17,19,21	1.06	2 (11%)
2	NAG	E	1[D]	2	15,15,15	2.08	7 (46%)	21,21,21	0.98	0
2	NAG	E	2[D]	2	14,14,15	2.93	5 (35%)	17,19,21	2.09	2 (11%)
2	NAG	F	1[C]	2	15,15,15	2.15	5 (33%)	21,21,21	2.07	4 (19%)
2	NAG	F	2[C]	2	14,14,15	1.64	1 (7%)	17,19,21	1.06	0
2	NAG	G	1[B]	2	15,15,15	1.71	3 (20%)	21,21,21	0.99	0
2	NAG	G	2[B]	2	14,14,15	1.42	1 (7%)	17,19,21	1.09	1 (5%)

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	NAG	C	1[A]	2	-	0/6/26/26	0/1/1/1
2	NAG	C	1[C]	2	-	1/6/26/26	0/1/1/1
2	NAG	C	2[A]	2	-	2/6/23/26	0/1/1/1
2	NAG	C	2[C]	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1[B]	2	-	0/6/26/26	0/1/1/1
2	NAG	D	2[B]	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1[D]	2	-	0/6/26/26	0/1/1/1
2	NAG	E	2[D]	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1[C]	2	-	1/6/26/26	0/1/1/1
2	NAG	F	2[C]	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1[B]	2	-	0/6/26/26	0/1/1/1
2	NAG	G	2[B]	2	-	0/6/23/26	0/1/1/1

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2[D]	NAG	C1-C2	8.83	1.64	1.52
2	C	1[C]	NAG	C1-C2	7.22	1.61	1.52
2	C	2[A]	NAG	C1-C2	5.68	1.60	1.52
2	F	1[C]	NAG	C1-C2	5.12	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2[C]	NAG	C1-C2	4.74	1.58	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1[C]	NAG	O5-C1-C2	8.40	117.95	109.52
2	F	1[C]	NAG	O5-C1-C2	7.37	116.92	109.52
2	E	2[D]	NAG	C1-O5-C5	7.12	121.73	112.19
2	G	2[B]	NAG	C1-O5-C5	3.42	116.78	112.19
2	F	1[C]	NAG	C1-O5-C5	3.39	120.21	113.65

There are no chirality outliers.

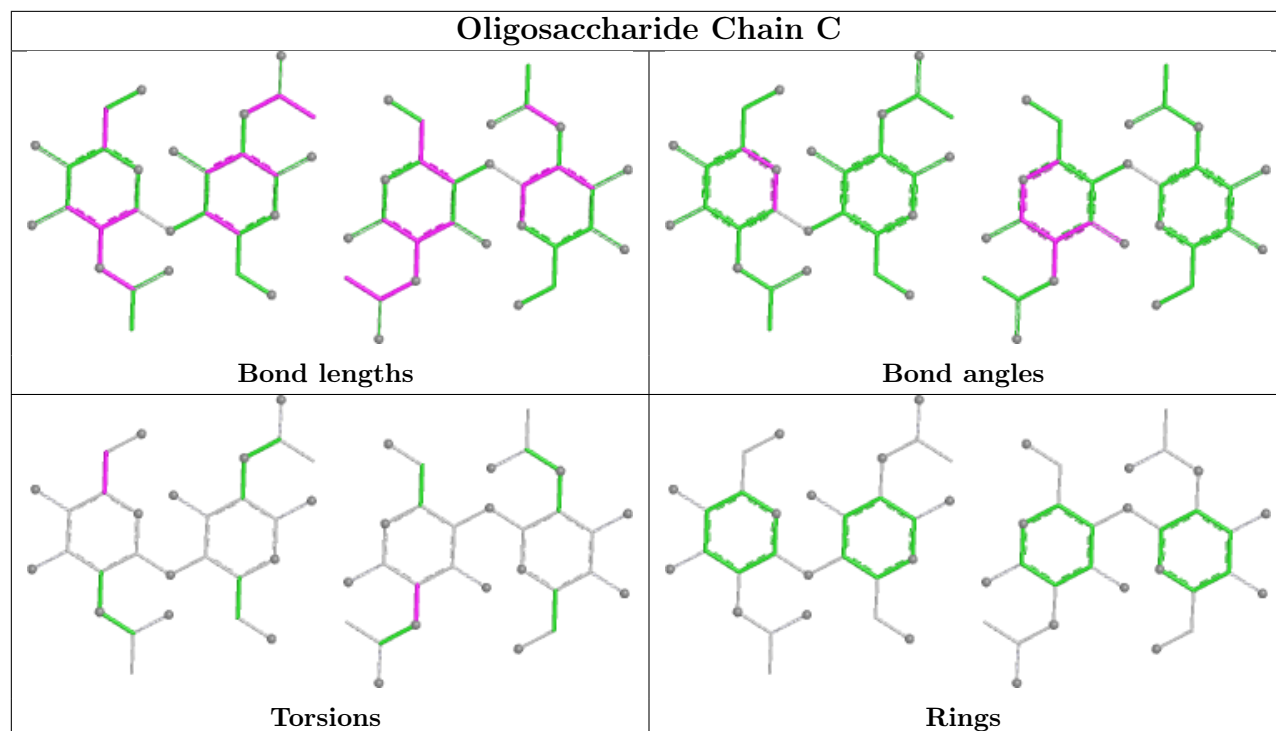
All (5) torsion outliers are listed below:

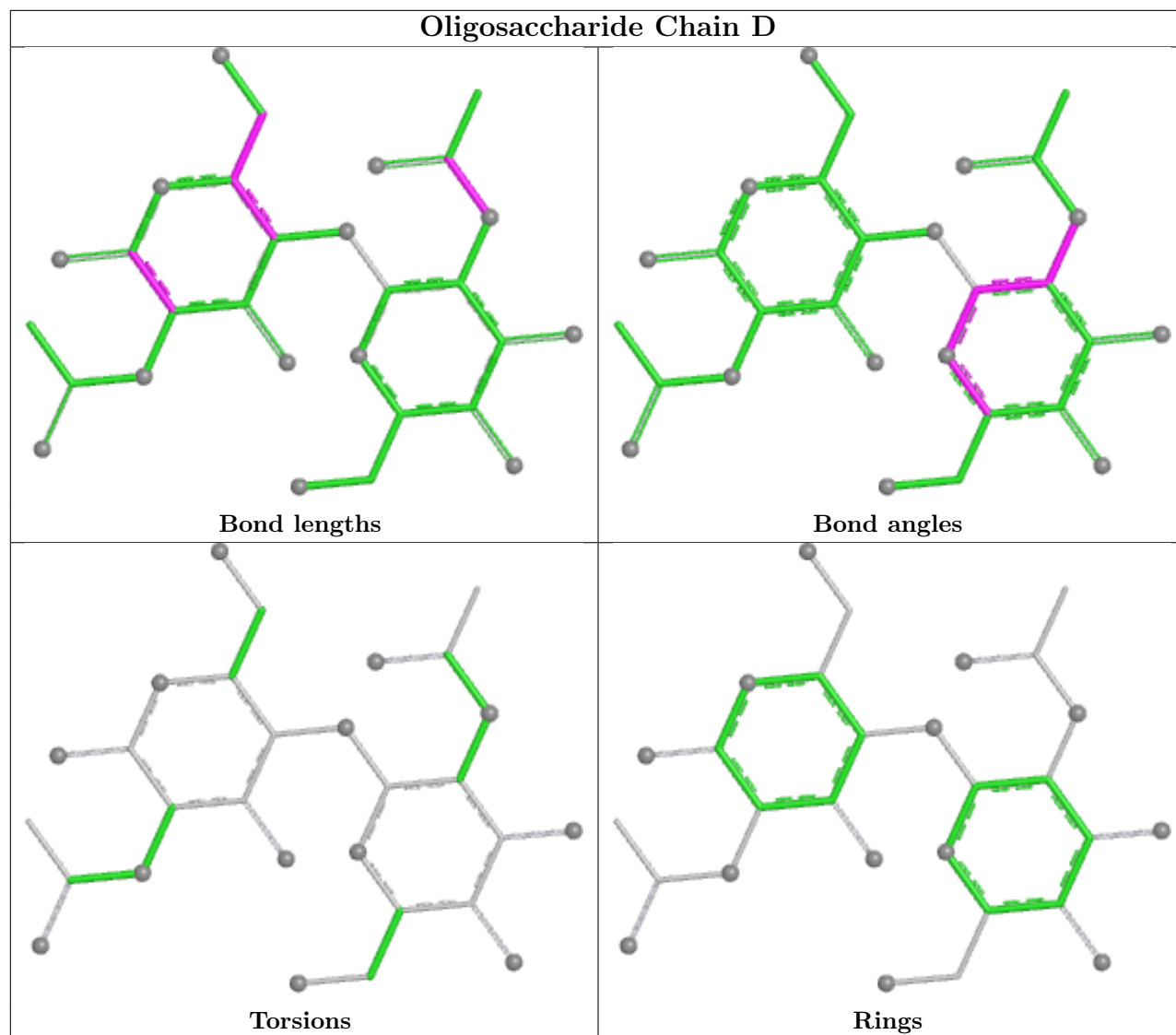
Mol	Chain	Res	Type	Atoms
2	C	1[C]	NAG	C1-C2-N2-C7
2	E	2[D]	NAG	C1-C2-N2-C7
2	F	1[C]	NAG	C1-C2-N2-C7
2	C	2[A]	NAG	O5-C5-C6-O6
2	C	2[A]	NAG	C4-C5-C6-O6

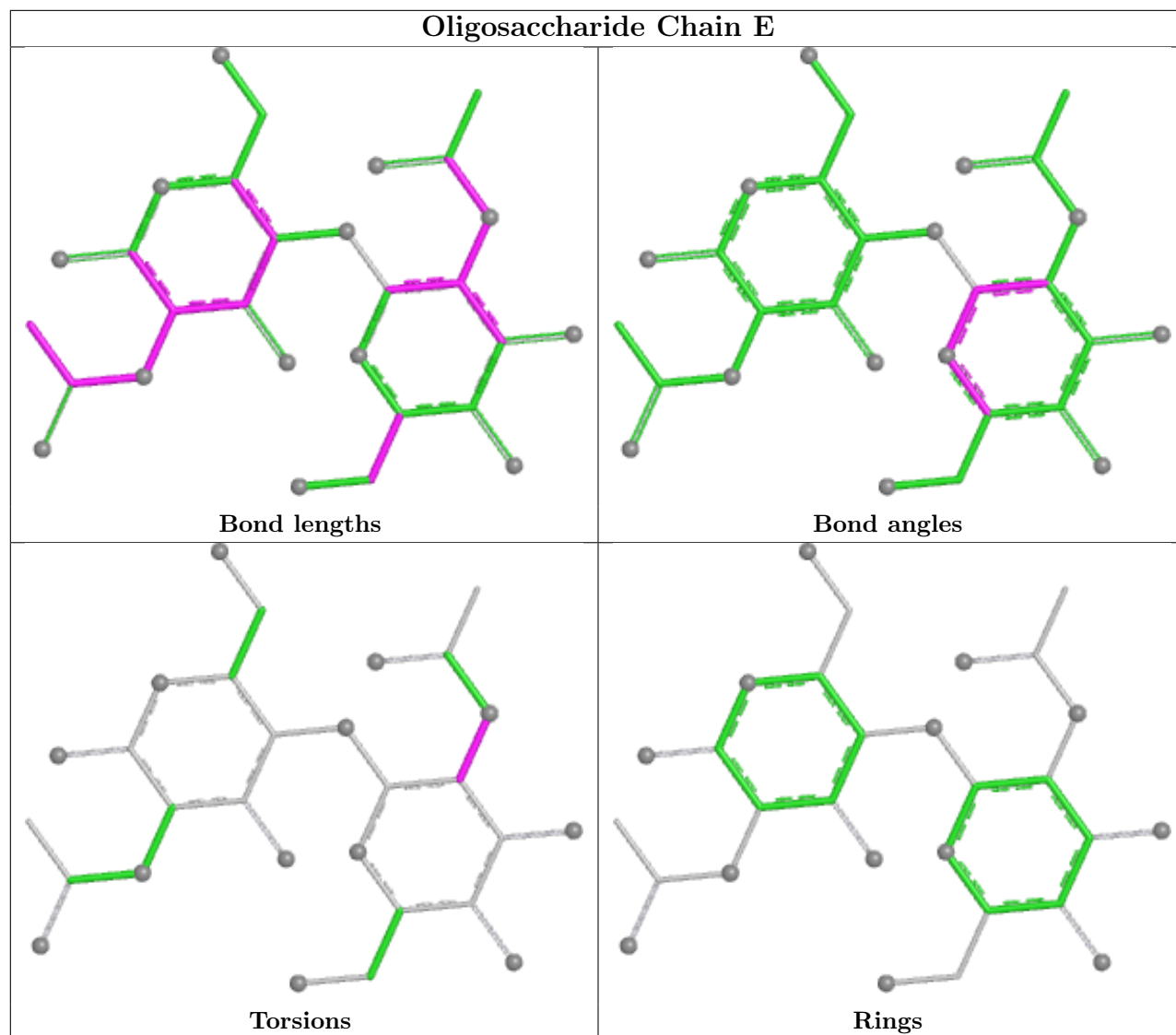
There are no ring outliers.

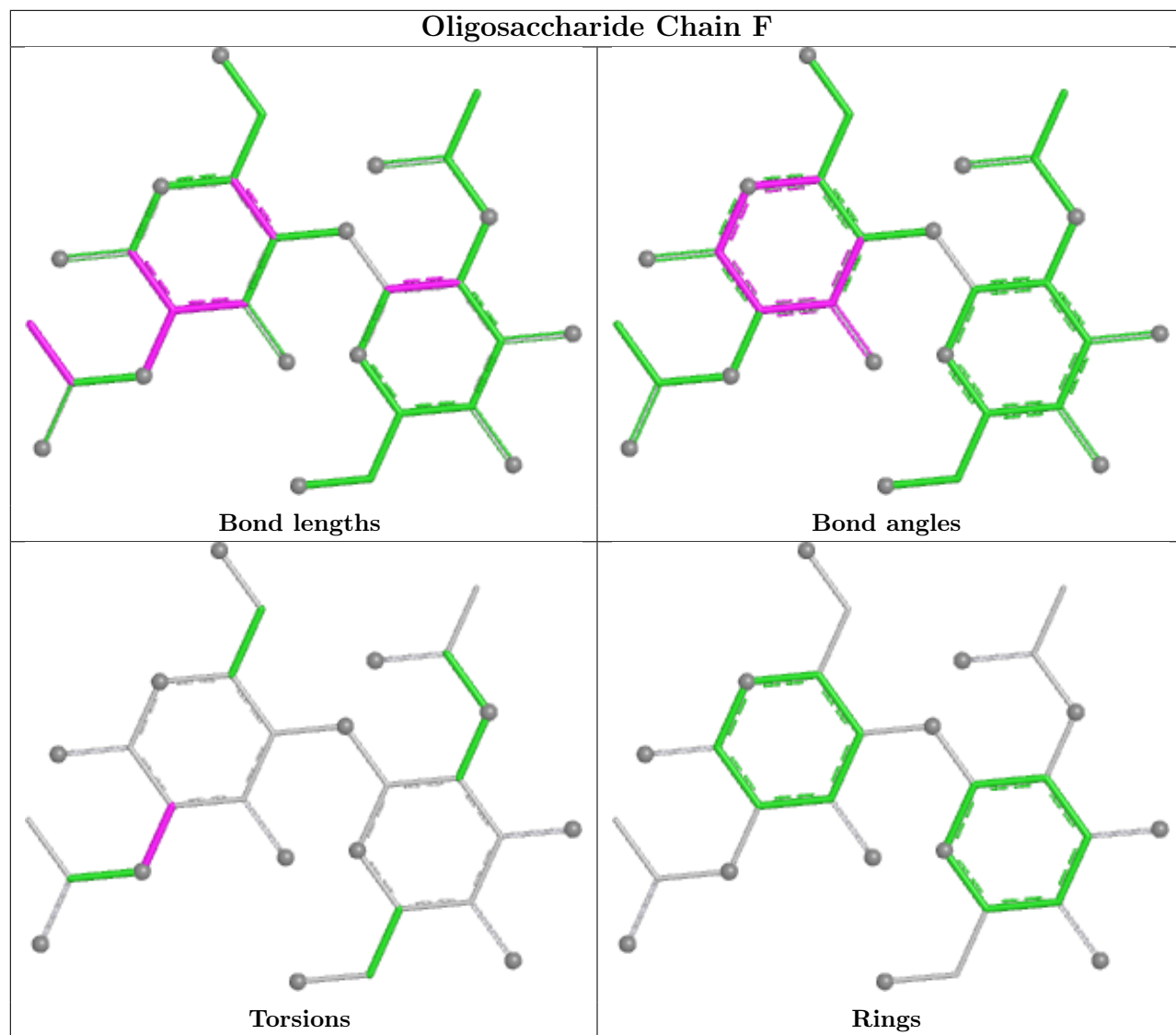
No monomer is involved in short contacts.

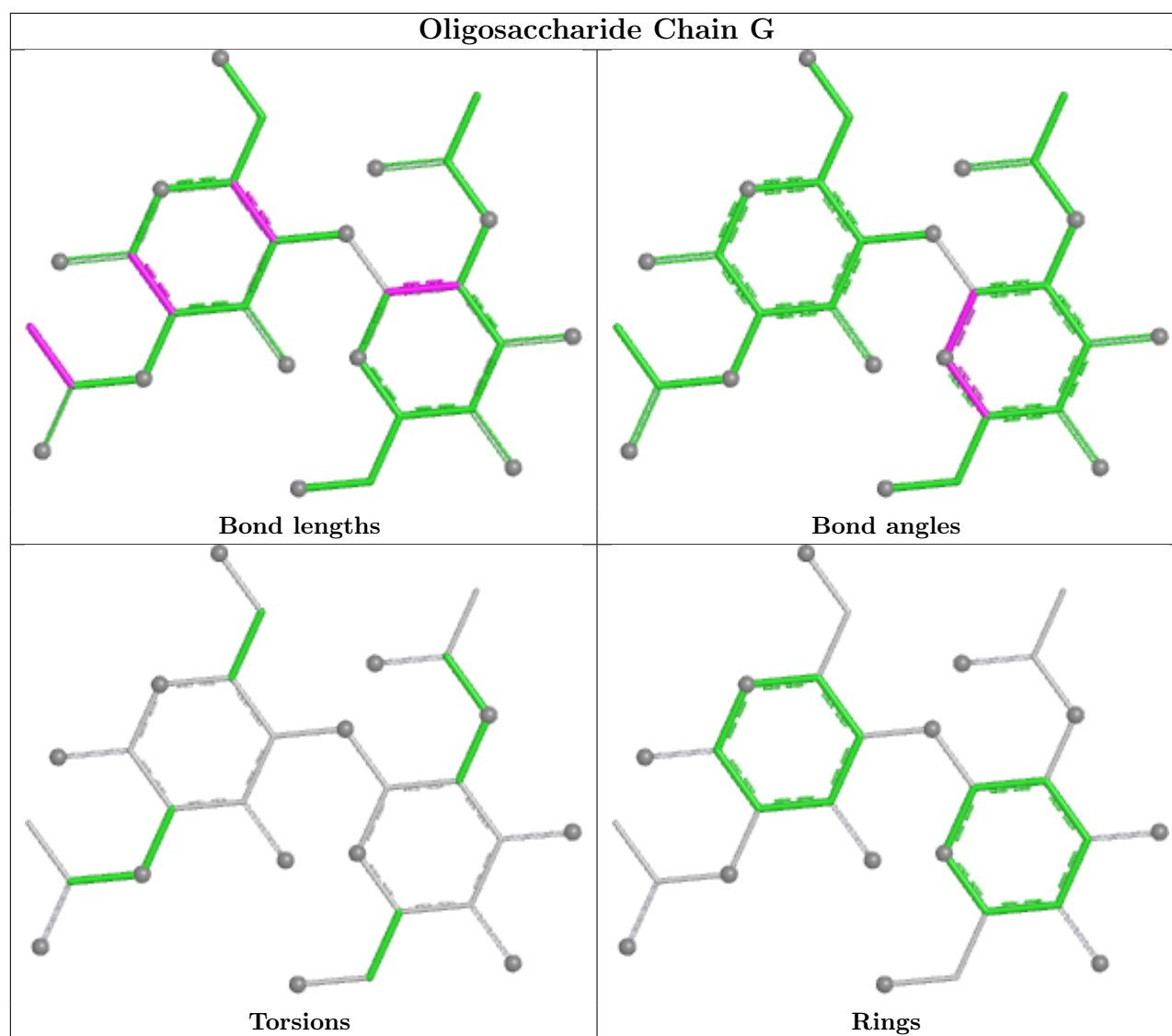
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











4.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	369/397 (92%)	-0.45	1 (0%) 90 95	5, 12, 27, 64	11 (2%)
1	B	369/397 (92%)	-0.50	0 100 100	4, 12, 26, 43	6 (1%)
All	All	738/794 (92%)	-0.48	1 (0%) 92 95	4, 12, 26, 64	17 (2%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	LYS	2.8

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

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

5.3 Carbohydrates [i](#)

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

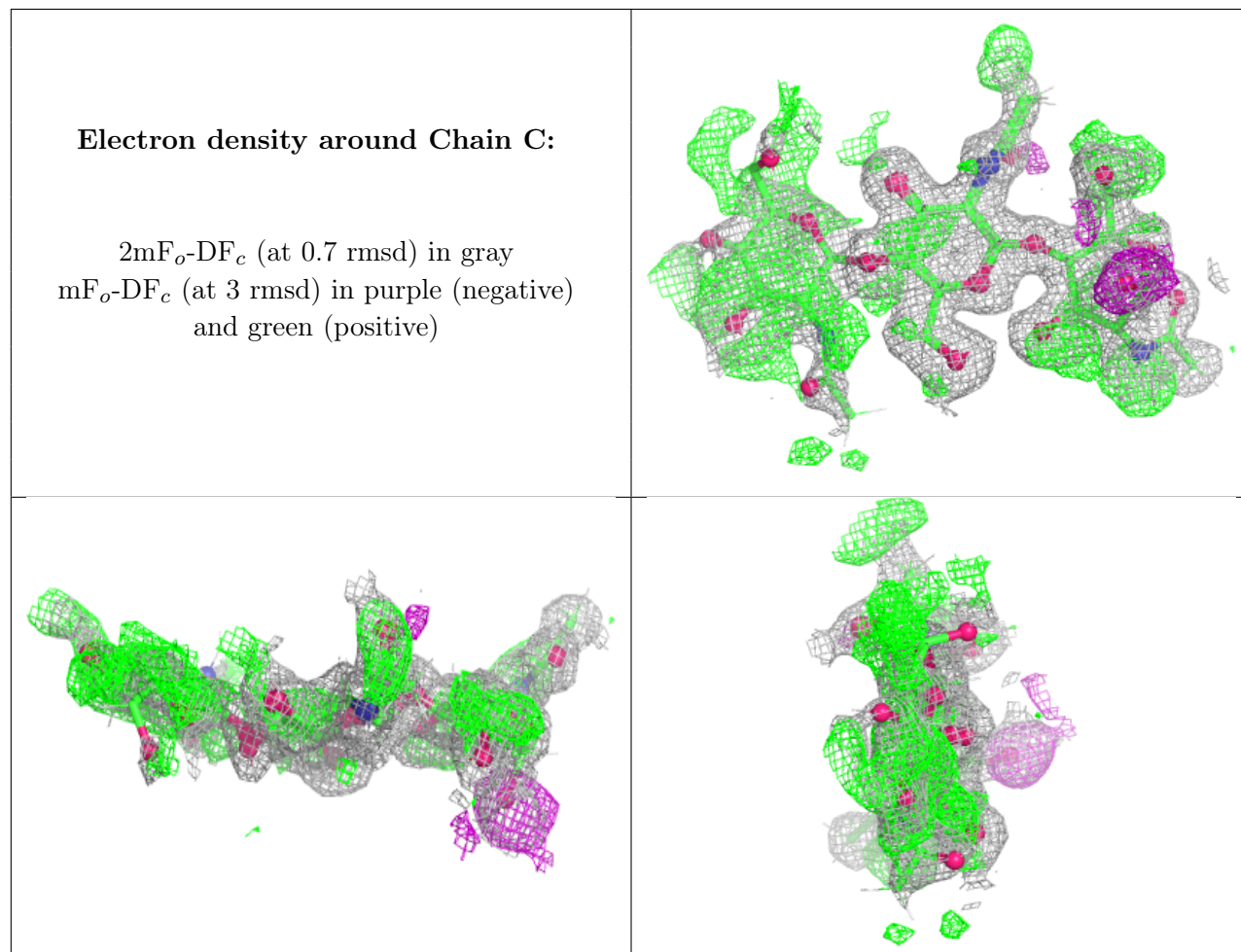
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2[D]	14/15	0.40	0.24	8,12,16,22	28
2	NAG	C	2[C]	14/15	0.66	0.29	10,16,22,26	28
2	NAG	C	2[A]	14/15	0.66	0.29	11,20,29,32	28
2	NAG	E	1[D]	15/15	0.72	0.15	12,19,28,28	29
2	NAG	C	1[A]	15/15	0.87	0.13	10,16,22,23	29
2	NAG	C	1[C]	15/15	0.87	0.13	8,12,17,21	29
2	NAG	D	2[B]	14/15	0.89	0.10	11,19,28,28	0
2	NAG	D	1[B]	15/15	0.90	0.08	13,20,26,34	0

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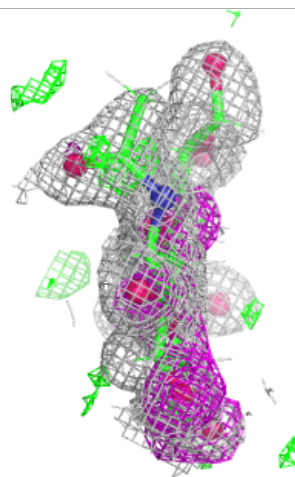
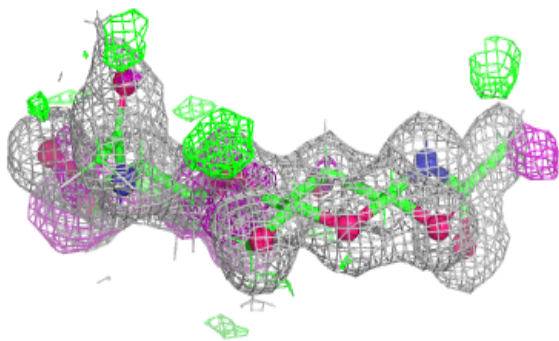
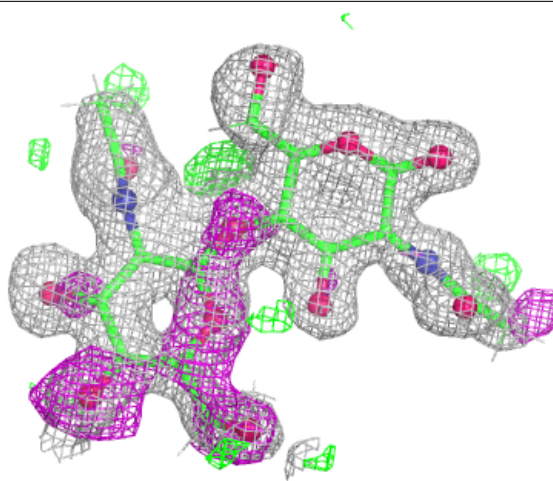
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	G	2[B]	14/15	0.90	0.09	11,17,26,26	0
2	NAG	F	1[C]	15/15	0.92	0.08	7,11,17,25	0
2	NAG	G	1[B]	15/15	0.93	0.08	13,21,29,31	0
2	NAG	F	2[C]	14/15	0.96	0.06	5,10,12,15	0

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.



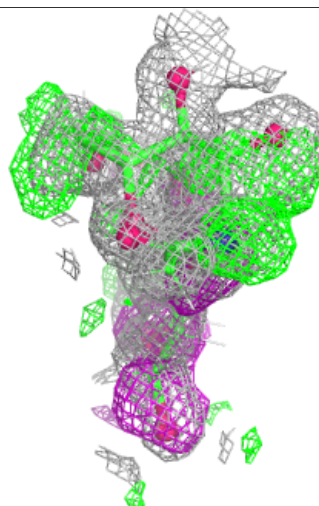
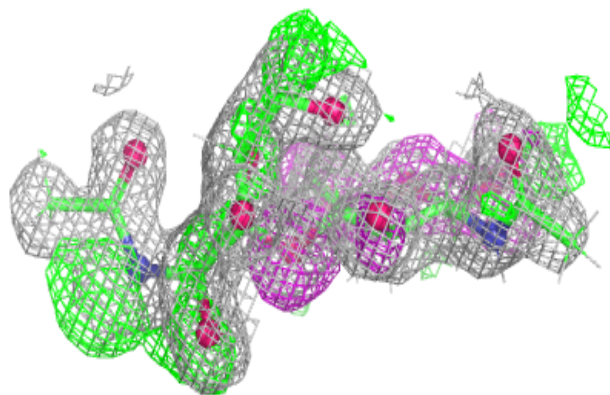
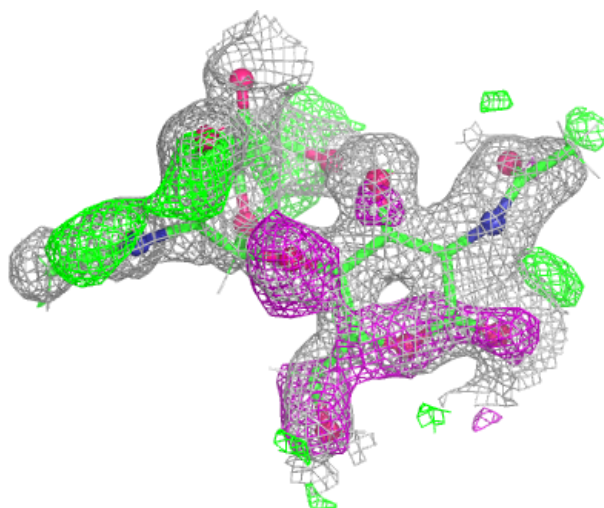
Electron density around Chain D:

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



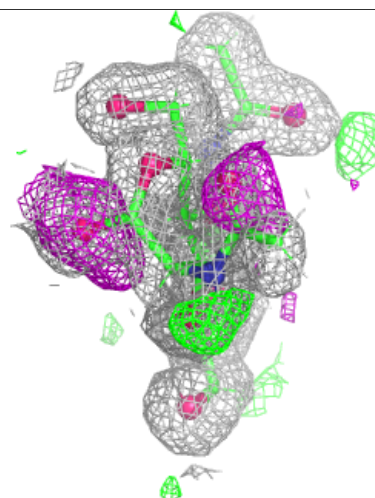
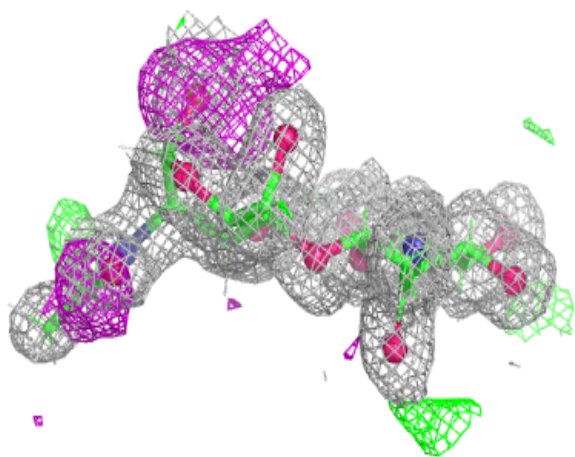
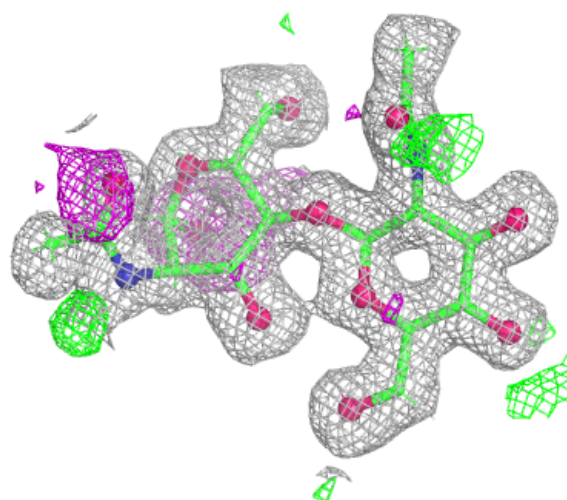
Electron density around Chain E:

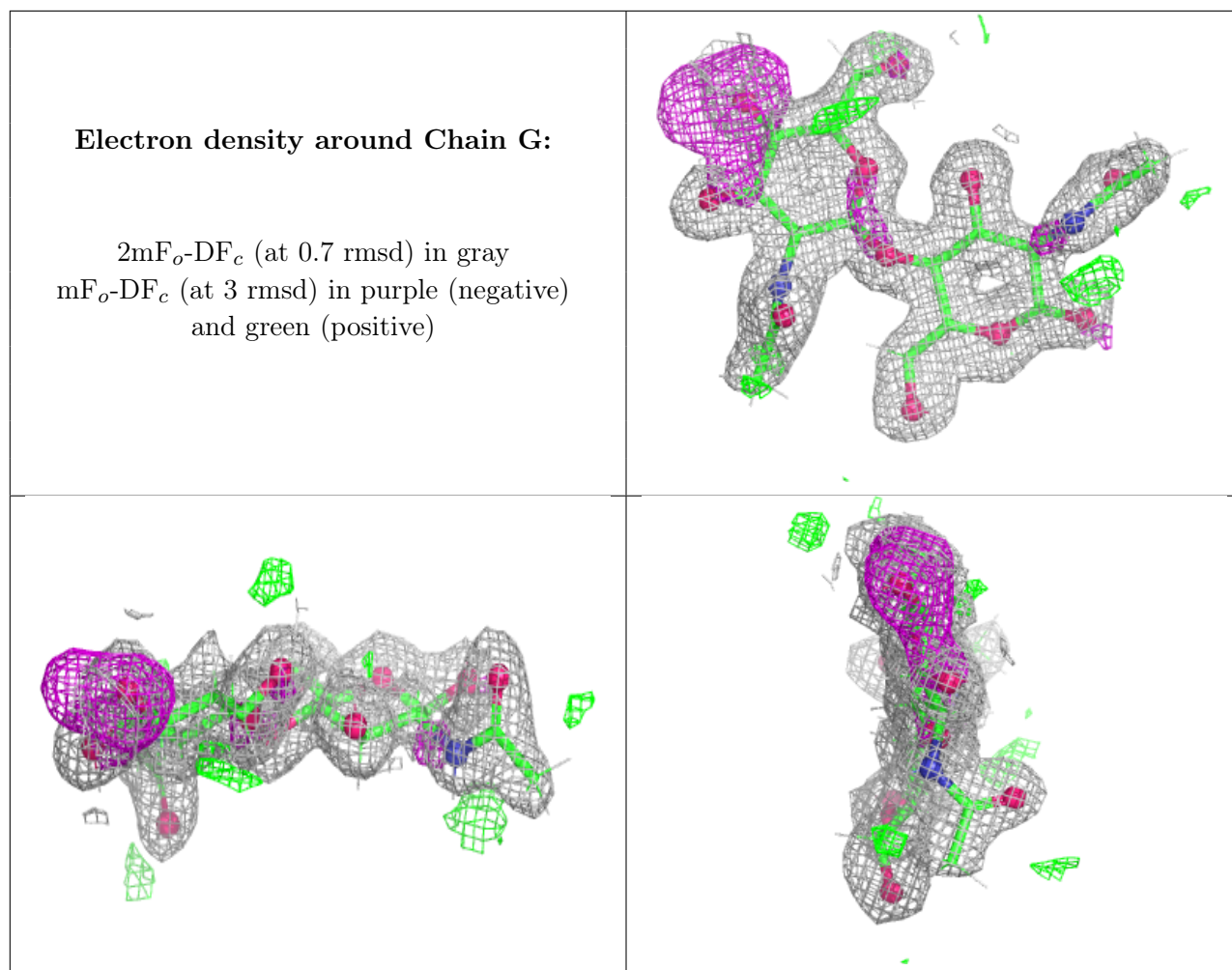
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

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





5.4 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(Å ²)	Q<0.9
3	MG	A	401	1/1	0.96	0.06	22,22,22,22	1
3	MG	B	401	1/1	0.97	0.04	19,19,19,19	1

5.5 Other polymers [i](#)

There are no such residues in this entry.