



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 19, 2023 – 01:16 AM EDT

PDB ID : 2INV
Title : Crystal structure of Inulin fructotransferase in the presence of di-fructose
Authors : Rhee, S.; Jung, W.S.
Deposited on : 2006-10-09
Resolution : 1.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

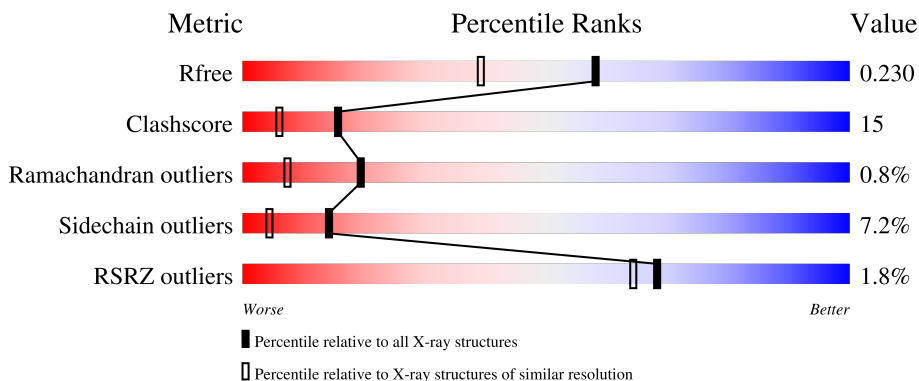
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 $\leq 5\%$. 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	A	410	 67% 26% . .
1	B	410	 67% 27% . .
1	C	410	 69% 26% . .
2	D	2	 50% 50%
2	E	2	 100%

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Mol	Chain	Length	Quality of chain
2	F	2	 50% 50%

2 Entry composition i

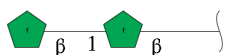
There are 4 unique types of molecules in this entry. The entry contains 9648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Inulin fructotransferase.

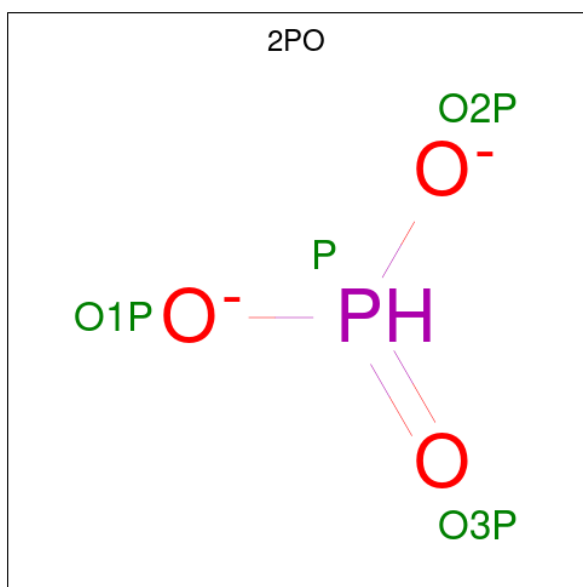
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	399	2982	1859	535	578	6	4	0	0	0
1	B	399	2982	1859	535	578	6	4	0	0	0
1	C	399	2982	1859	535	578	6	4	0	0	0

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	D	2	23	12	11	0	0	0
2	E	2	23	12	11	0	0	0
2	F	2	23	12	11	0	0	0

- Molecule 3 is PHOSPHONATE (three-letter code: 2PO) (formula: HO₃P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 4 3 1	0	0
3	B	1	Total O P 4 3 1	0	0

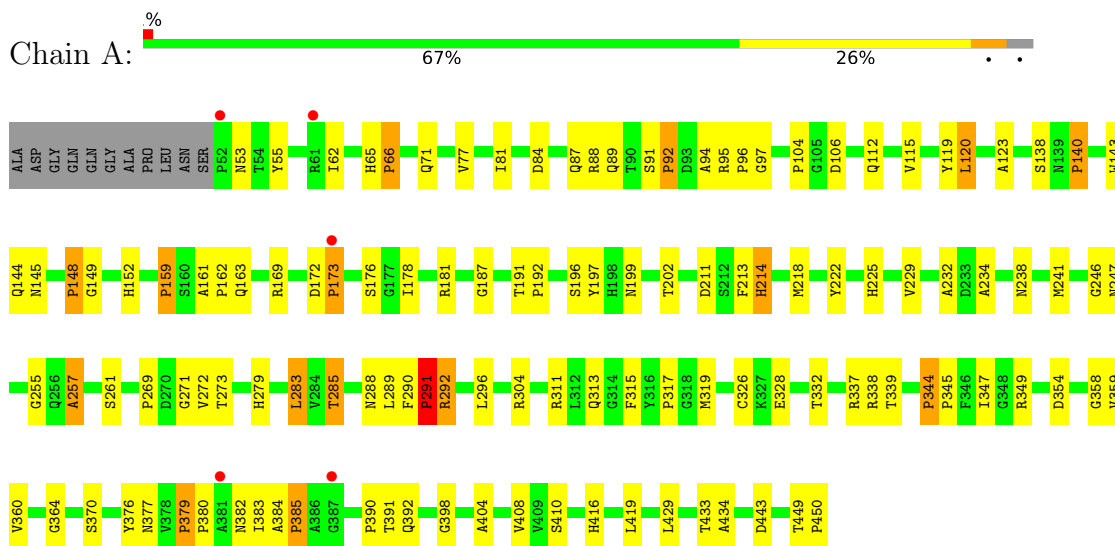
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	203	Total O 203 203	0	0
4	B	210	Total O 210 210	0	0
4	C	212	Total O 212 212	0	0

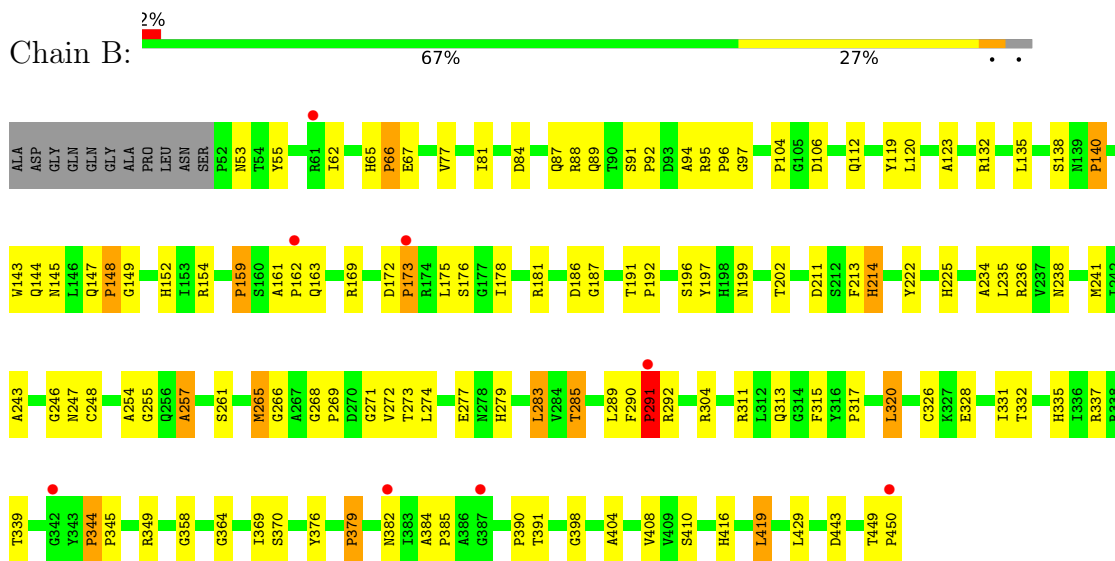
3 Residue-property plots [i](#)

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: Inulin fructotransferase

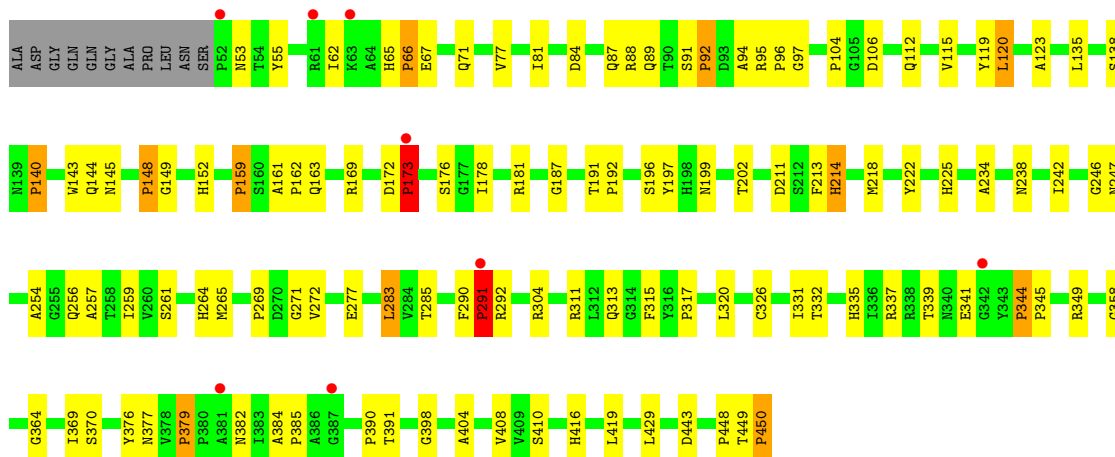


- Molecule 1: Inulin fructotransferase



- Molecule 1: Inulin fructotransferase





- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose

Chain D: 50% 50%

FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose

Chain E: 100%

FRU1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose

Chain F: 50% 50%

FRU1
FRU2

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.17Å 91.90Å 92.92Å 90.00° 124.82° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 46.45 – 1.80	Depositor EDS
% Data completeness (in resolution range)	82.4 (50.00-1.80) 98.1 (46.45-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 1.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.227 0.210 , 0.230	Depositor DCC
R_{free} test set	10154 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.012 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.013 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.019 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.019 for $-h+k-l, -l, -k$ 0.005 for $-h-k-l, l, k$ 0.019 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.005 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.487 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.487 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.013 for $-h-2^*l, -k, l$	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9648	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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: FRU, 2PO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	4/3042 (0.1%)	1.05	9/4143 (0.2%)
1	B	0.52	2/3042 (0.1%)	1.07	11/4143 (0.3%)
1	C	0.49	1/3042 (0.0%)	1.07	10/4143 (0.2%)
All	All	0.52	7/9126 (0.1%)	1.06	30/12429 (0.2%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	PRO	C-N	11.36	1.60	1.34
1	B	291	PRO	C-N	10.70	1.58	1.34
1	C	291	PRO	C-N	9.93	1.56	1.34
1	B	285	THR	CB-OG1	7.35	1.57	1.43
1	A	285	THR	CB-OG1	7.27	1.57	1.43

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	PRO	O-C-N	-29.27	75.86	122.70
1	C	291	PRO	O-C-N	-28.55	77.02	122.70
1	A	291	PRO	O-C-N	-28.07	77.78	122.70
1	C	172	ASP	C-N-CD	-20.71	75.03	120.60
1	B	172	ASP	C-N-CD	-20.41	75.70	120.60

There are no chirality outliers.

There are no planarity outliers.

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	A	2982	0	2905	105	0
1	B	2982	0	2905	102	0
1	C	2982	0	2905	99	0
2	D	23	0	21	3	0
2	E	23	0	21	4	0
2	F	23	0	21	3	0
3	A	4	0	1	0	0
3	B	4	0	1	0	0
4	A	203	0	0	1	0
4	B	210	0	0	0	0
4	C	212	0	0	2	0
All	All	9648	0	8780	261	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 15.

The worst 5 of 261 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:MSE:HE3	1:B:273:THR:HG22	1.32	1.10
1:A:319:MSE:HE1	1:A:338:ARG:HB2	1.39	1.01
1:C:291:PRO:HB2	2:F:2:FRU:O6	1.67	0.93
1:A:291:PRO:HB2	2:D:2:FRU:O6	1.70	0.90
1:B:291:PRO:HB2	2:E:2:FRU:O6	1.73	0.89

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	A	397/410 (97%)	369 (93%)	25 (6%)	3 (1%)	19	7
1	B	397/410 (97%)	369 (93%)	25 (6%)	3 (1%)	19	7
1	C	397/410 (97%)	368 (93%)	26 (6%)	3 (1%)	19	7
All	All	1191/1230 (97%)	1106 (93%)	76 (6%)	9 (1%)	19	7

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	173	PRO
1	A	199	ASN
1	B	199	ASN
1	C	199	ASN
1	B	257	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/325 (99%)	299 (93%)	23 (7%)	14	5
1	B	322/325 (99%)	298 (92%)	24 (8%)	13	4
1	C	322/325 (99%)	299 (93%)	23 (7%)	14	5
All	All	966/975 (99%)	896 (93%)	70 (7%)	14	4

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	256	GLN
1	C	291	PRO
1	C	379	PRO
1	B	67	GLU
1	B	66	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	152	HIS
1	C	377	ASN
1	C	214	HIS
1	C	264	HIS
1	C	425	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FRU	D	1	2	11,12,12	3.94	3 (27%)	10,18,18	2.43	3 (30%)
2	FRU	D	2	2	11,11,12	1.13	1 (9%)	15,15,18	2.49	4 (26%)
2	FRU	E	1	2	11,12,12	3.35	3 (27%)	10,18,18	2.88	4 (40%)
2	FRU	E	2	2	11,11,12	1.13	1 (9%)	15,15,18	2.49	4 (26%)
2	FRU	F	1	2	11,12,12	3.15	3 (27%)	10,18,18	1.98	3 (30%)
2	FRU	F	2	2	11,11,12	1.13	1 (9%)	15,15,18	2.49	4 (26%)

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	FRU	D	1	2	-	0/5/24/24	0/1/1/1
2	FRU	D	2	2	-	1/4/20/24	0/1/1/1
2	FRU	E	1	2	-	2/5/24/24	0/1/1/1
2	FRU	E	2	2	-	1/4/20/24	0/1/1/1
2	FRU	F	1	2	-	0/5/24/24	0/1/1/1
2	FRU	F	2	2	-	1/4/20/24	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	FRU	O1-C1	-8.79	1.13	1.42
2	D	1	FRU	O1-C1	-8.79	1.13	1.42
2	E	1	FRU	O1-C1	-8.79	1.13	1.42
2	D	1	FRU	O6-C6	-8.29	1.07	1.42
2	E	1	FRU	O6-C6	-4.30	1.24	1.42

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	FRU	O6-C6-C5	7.77	137.96	111.29
2	E	2	FRU	O3-C3-C2	7.51	132.75	111.05
2	D	2	FRU	O3-C3-C2	7.50	132.75	111.05
2	F	2	FRU	O3-C3-C2	7.50	132.73	111.05
2	D	1	FRU	O6-C6-C5	6.18	132.49	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	FRU	C4-C5-C6-O6
2	E	1	FRU	O5-C5-C6-O6
2	D	2	FRU	C4-C5-C6-O6
2	E	2	FRU	C4-C5-C6-O6
2	F	2	FRU	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 10 short contacts:

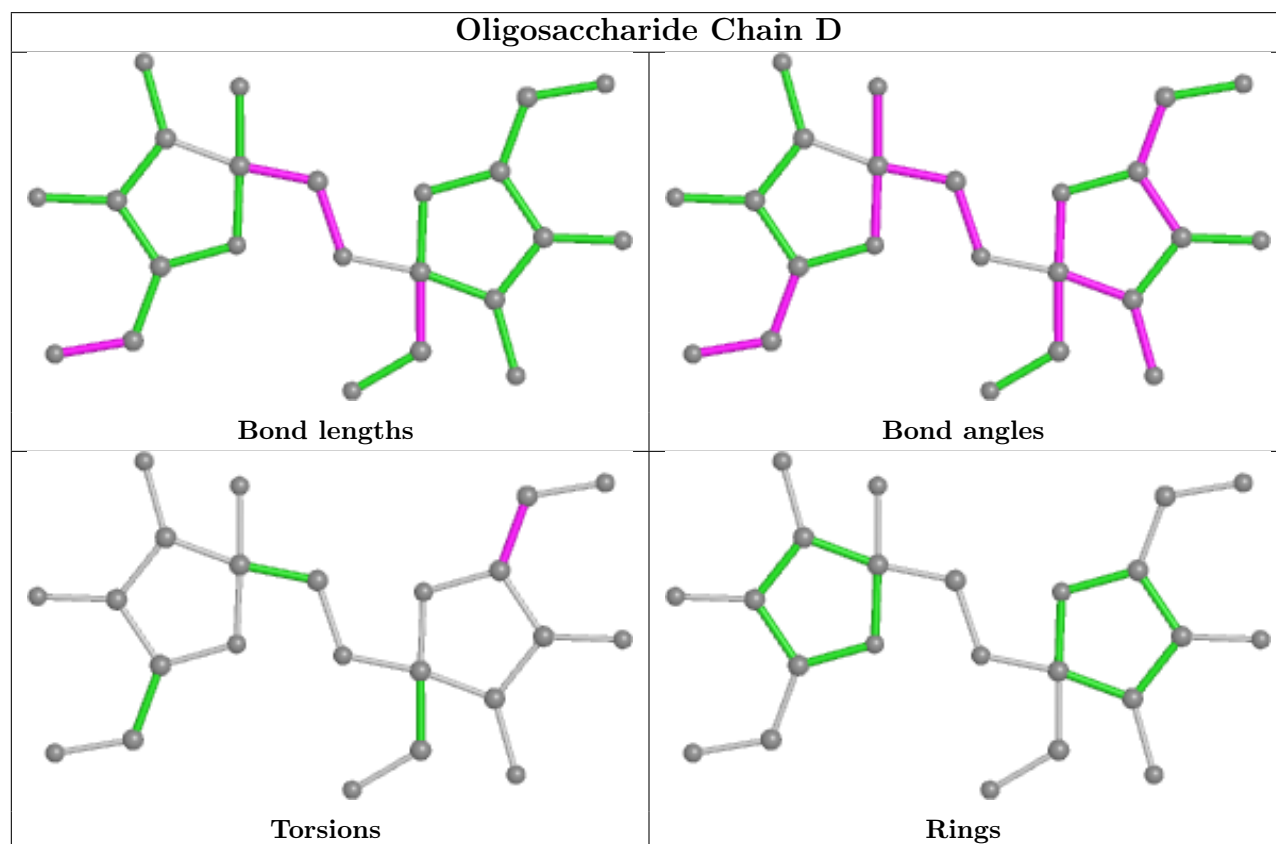
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	FRU	4	0

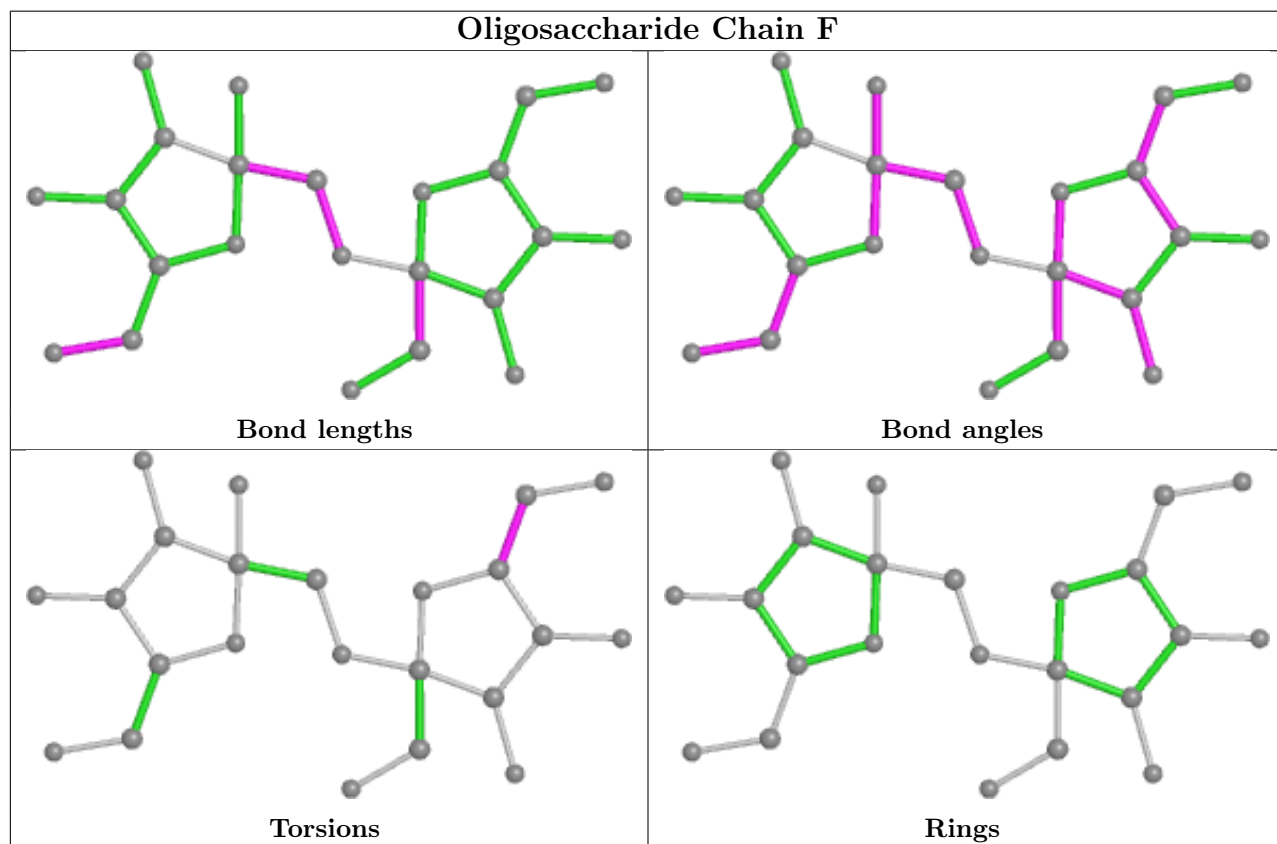
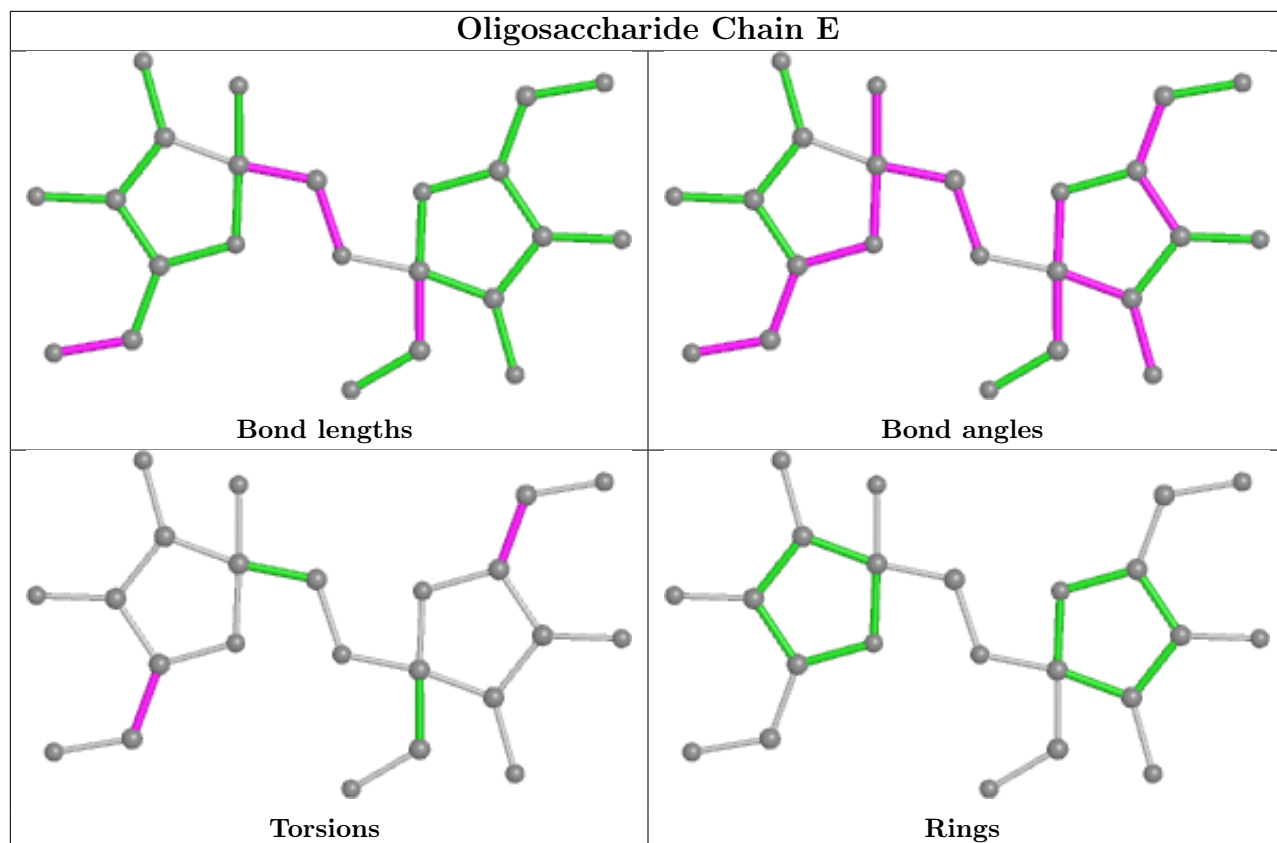
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	FRU	1	0
2	F	2	FRU	3	0
2	D	2	FRU	3	0

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





5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	2PO	B	1001	-	0,3,3	-	-	0,3,3	-	-
3	2PO	A	1002	-	0,3,3	-	-	0,3,3	-	-

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, 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	395/410 (96%)	0.03	5 (1%) 77 74	10, 14, 25, 30	0
1	B	395/410 (96%)	0.02	8 (2%) 65 61	10, 14, 25, 30	0
1	C	395/410 (96%)	0.02	8 (2%) 65 61	10, 14, 25, 30	0
All	All	1185/1230 (96%)	0.02	21 (1%) 68 64	10, 14, 25, 30	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	342	GLY	3.8
1	C	173	PRO	3.1
1	C	342	GLY	3.0
1	C	291	PRO	3.0
1	B	450	PRO	2.9

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

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

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.

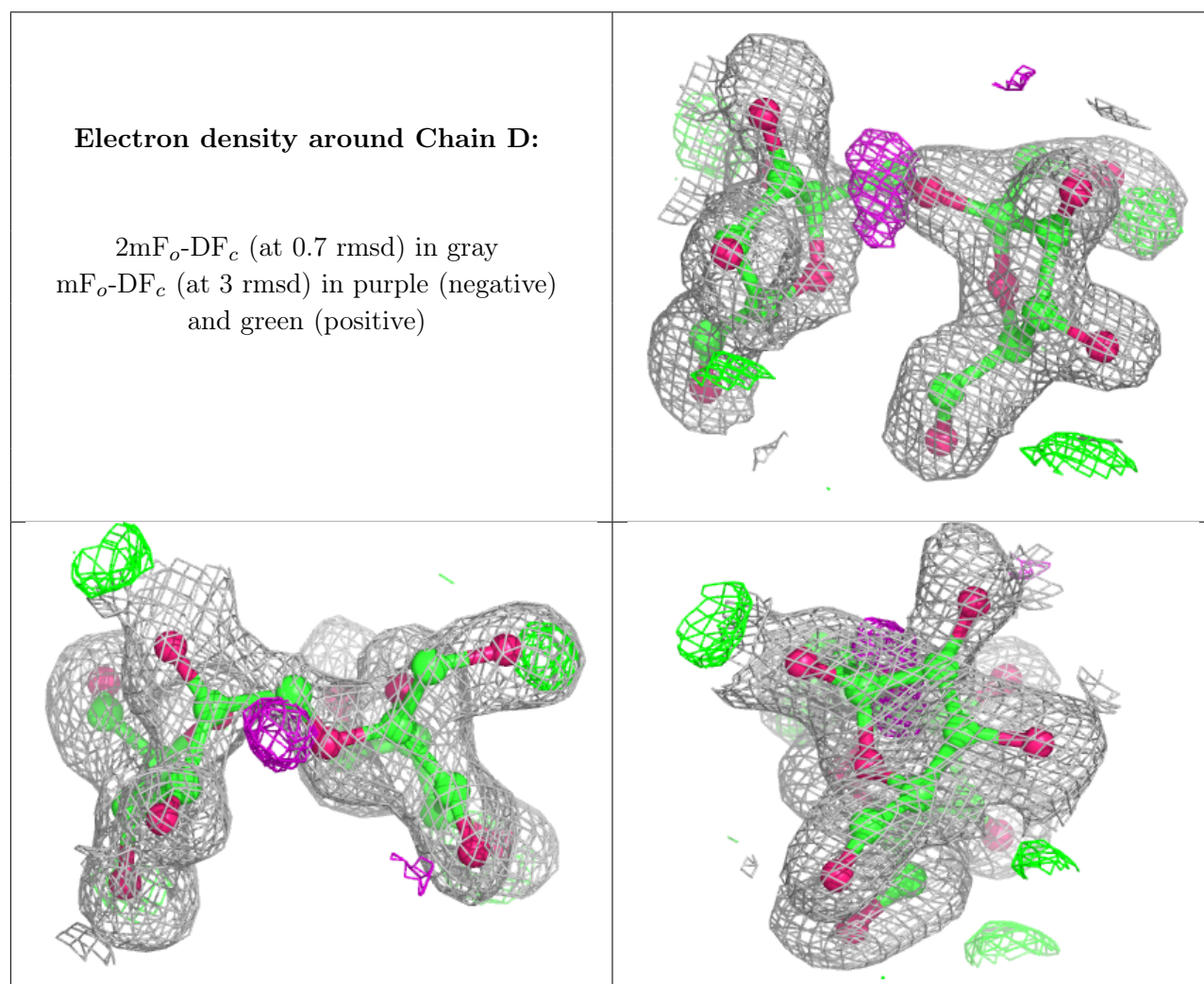
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FRU	D	1	12/12	0.72	0.20	27,29,30,32	0
2	FRU	E	1	12/12	0.78	0.16	28,29,30,32	0
2	FRU	F	1	12/12	0.80	0.17	26,29,30,31	0

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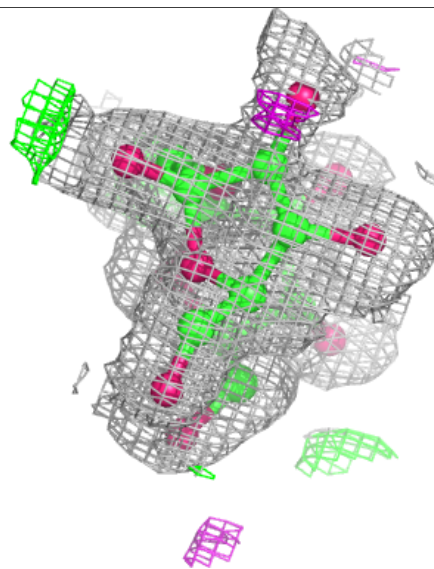
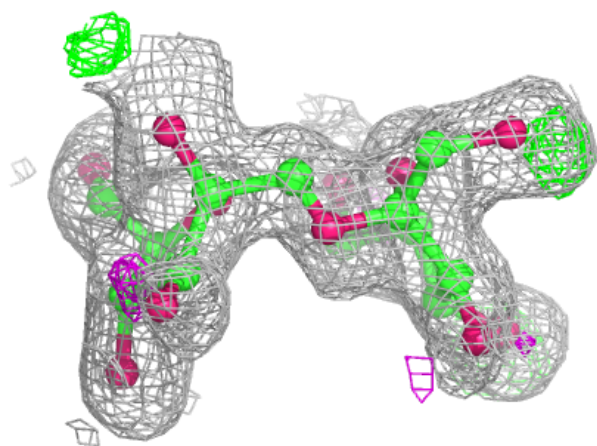
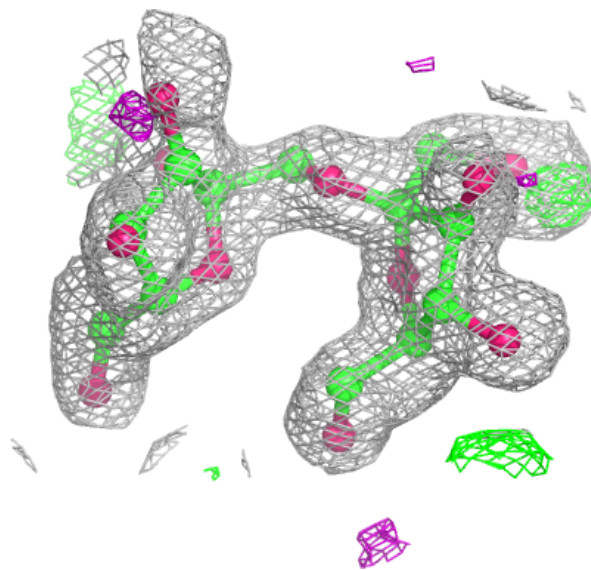
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FRU	F	2	11/12	0.80	0.14	22,24,25,25	0
2	FRU	E	2	11/12	0.83	0.14	24,25,26,26	0
2	FRU	D	2	11/12	0.86	0.14	22,23,25,25	0

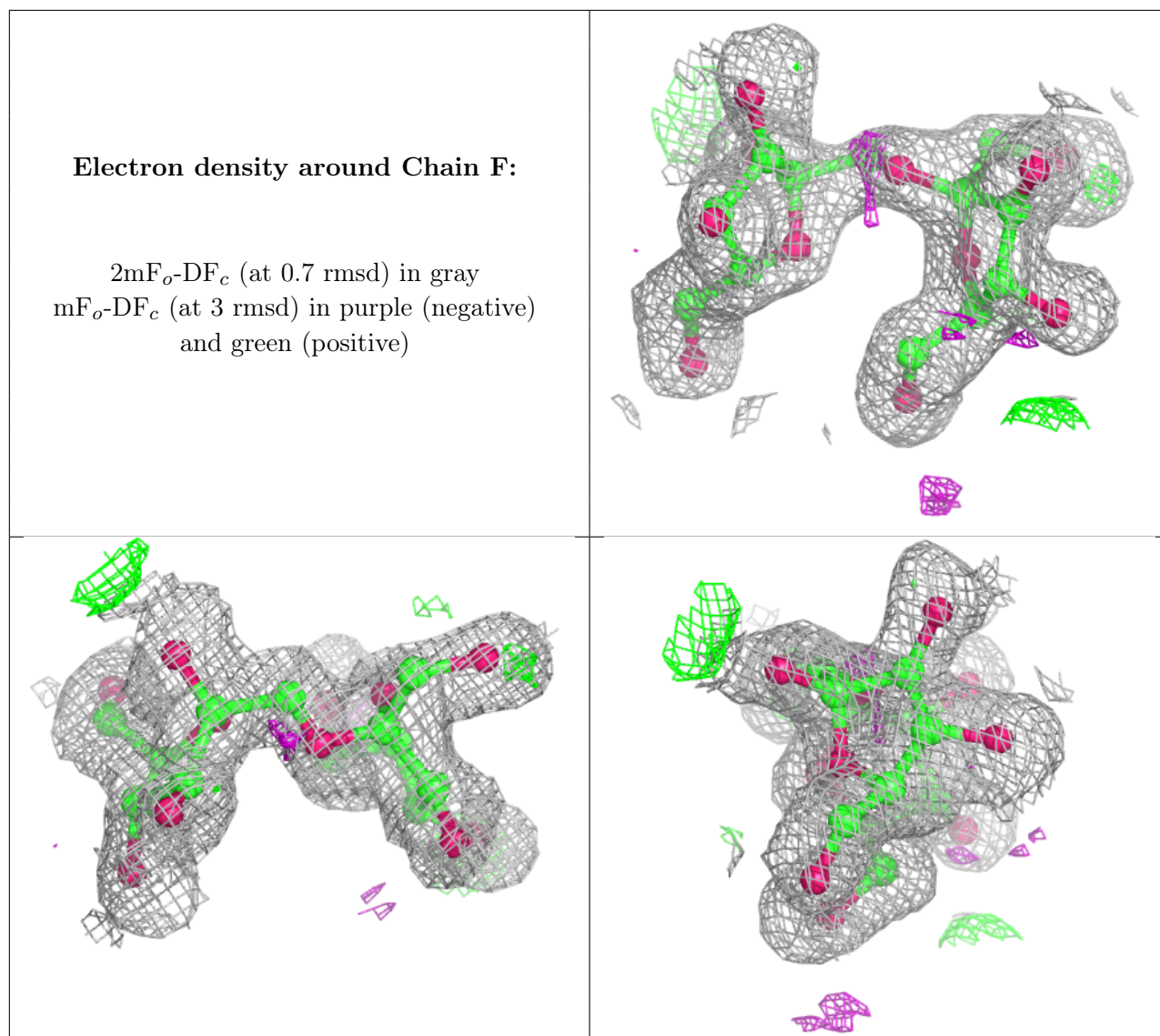
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain E:

$2mF_o-DF_c$ (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
3	2PO	A	1002	4/4	0.85	0.13	45,45,46,47	0
3	2PO	B	1001	4/4	0.86	0.16	33,33,33,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.