W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 12, 2020 – 12:17 AM GMT

PDB ID	:	6ZAZ
Title	:	Fructo-oligosaccharide transporter BT 1762-63
Authors	:	van den Berg, B.
Deposited on	:	2020-06-06
Resolution	:	2.69 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

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 2.69 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.
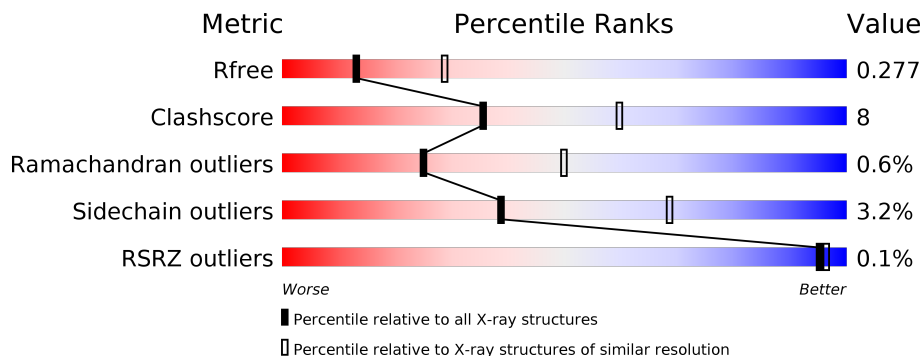
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	580	76% ... 19% ..
2	B	1041	70% ... 17% . 12%
3	C	7	14% 43% 43%
4	D	4	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FRU	C	6	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12118 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 SusD homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	555	4457	2822	740	874	21	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	553	ALA	-	expression tag	UNP Q8A6W4
A	554	ALA	-	expression tag	UNP Q8A6W4
A	555	ALA	-	expression tag	UNP Q8A6W4
A	556	ALA	-	expression tag	UNP Q8A6W4
A	557	HIS	-	expression tag	UNP Q8A6W4
A	558	HIS	-	expression tag	UNP Q8A6W4
A	559	HIS	-	expression tag	UNP Q8A6W4
A	560	HIS	-	expression tag	UNP Q8A6W4
A	561	HIS	-	expression tag	UNP Q8A6W4
A	562	HIS	-	expression tag	UNP Q8A6W4

- Molecule 2 is a protein called SusC homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	921	7243	4571	1241	1410	21	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-[beta-D-fructofuranose-(2-1)]beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.
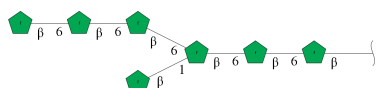
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	7	Total 78	C 42	O 36	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2 -6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.
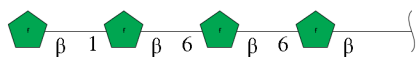
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	D	4	Total 45	C 24	O 21	0	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).

C8E
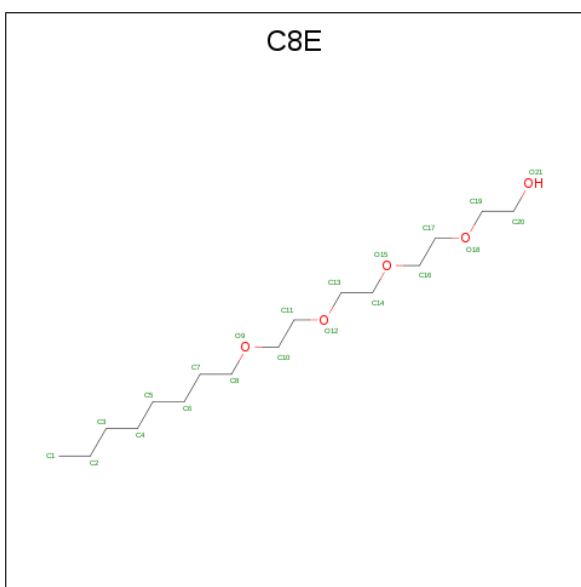
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 16	C 13	O 3	0	0
7	B	1	Total 12	C 10	O 2	0	0
7	B	1	Total 21	C 16	O 5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	113	Total 113	O 113	0	0
8	B	130	Total 130	O 130	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: SusD homolog

- Molecule 2: SusC homolog

M741 K742 E747 G751 T756 A757 F758 G759 L760 T761 Y762 N765 G766 N767 T770 E774 I775 L776 E780 T781 V782 N785 G789 G790 N791 V796 Q804 V805 E846 P857 S858 L867 K870 N871 F872 D873 Q879 V884 V890 K893 S894

F904 G908 T909 R910 A914 W915 S916 P917 T918 I924 D931 R952 Q955 T959 K967 D971 N974 C977 S978 E993 F1016

• Molecule 3: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6
)-[beta-D-fructofuranose-(2-1)]beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fru
ctofuranose

Chain C: 14%   43%   43%

FRU1 FRU2 FRU3 FRU4 FRU5 FRU6 FRU7
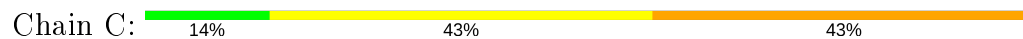
• Molecule 4: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6
)-beta-D-fructofuranose

Chain D: 50%   50%

FRU1 FRU2 FRU3 FRU4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.57Å 237.84Å 170.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.83 – 2.69 118.92 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.0 (106.83-2.69) 99.2 (118.92-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.58 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.208 , 0.275 0.211 , 0.277	Depositor DCC
R_{free} test set	3313 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.6	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12118	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, C8E, FRU, CL

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	0.41	0/4563	0.60	0/6192
2	B	0.44	0/7416	0.63	0/10053
All	All	0.43	0/11979	0.62	0/16245

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
2	B	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
2	B	470	ASN	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	A	4457	0	4226	70	0
2	B	7243	0	6929	119	0
3	C	78	0	72	3	0
4	D	45	0	42	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	49	0	75	2	0
8	A	113	0	0	3	0
8	B	130	0	0	2	0
All	All	12118	0	11344	188	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 8.

The worst 5 of 188 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)
2:B:599:TRP:CE2	2:B:601:ILE:HD13	2.02	0.93
2:B:227:SER:HB3	2:B:993:GLU:HB3	1.49	0.93
2:B:599:TRP:NE1	2:B:601:ILE:HD11	1.92	0.83
1:A:502:LYS:HD3	1:A:526:GLU:HB3	1.65	0.78
1:A:102:ASN:HD21	1:A:130:ARG:HH11	1.34	0.75

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	553/580 (95%)	526 (95%)	24 (4%)	3 (0%)	29	54
2	B	919/1041 (88%)	859 (94%)	54 (6%)	6 (1%)	22	46
All	All	1472/1621 (91%)	1385 (94%)	78 (5%)	9 (1%)	25	50

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	499	GLY
2	B	464	GLN
2	B	790	GLY
1	A	142	LYS
1	A	422	ASN

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	473/495 (96%)	460 (97%)	13 (3%)	44	74
2	B	766/869 (88%)	739 (96%)	27 (4%)	36	65
All	All	1239/1364 (91%)	1199 (97%)	40 (3%)	39	68

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	321	SER
2	B	500	LYS
2	B	780	GLU
2	B	453	ASN
2	B	501	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	442	ASN
2	B	455	GLN
2	B	765	ASN
2	B	366	ASN
2	B	744	GLN

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)

11 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
3	FRU	C	1	3	11,12,12	0.78	1 (9%)	10,18,18	1.55	2 (20%)
3	FRU	C	2	3	11,11,12	0.39	0	15,15,18	1.17	2 (13%)
3	FRU	C	3	3	11,11,12	0.59	0	15,15,18	1.03	0
3	FRU	C	4	3	11,11,12	0.38	0	15,15,18	0.77	0
3	FRU	C	5	3	11,11,12	0.43	0	15,15,18	1.18	1 (6%)
3	FRU	C	6	3	11,11,12	0.67	0	15,15,18	1.13	1 (6%)
3	FRU	C	7	3	11,11,12	0.44	0	15,15,18	0.85	0
4	FRU	D	1	4	11,12,12	0.73	0	10,18,18	1.21	1 (10%)
4	FRU	D	2	4	11,11,12	0.40	0	15,15,18	1.01	2 (13%)
4	FRU	D	3	4	11,11,12	0.42	0	15,15,18	0.90	0
4	FRU	D	4	4	11,11,12	0.34	0	15,15,18	0.72	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
3	FRU	C	1	3	-	2/5/24/24	0/1/1/1
3	FRU	C	2	3	-	0/4/20/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FRU	C	3	3	-	4/4/20/24	0/1/1/1
3	FRU	C	4	3	-	0/4/20/24	0/1/1/1
3	FRU	C	5	3	-	4/4/20/24	0/1/1/1
3	FRU	C	6	3	-	2/4/20/24	0/1/1/1
3	FRU	C	7	3	-	2/4/20/24	0/1/1/1
4	FRU	D	1	4	-	5/5/24/24	0/1/1/1
4	FRU	D	2	4	-	4/4/20/24	0/1/1/1
4	FRU	D	3	4	-	0/4/20/24	0/1/1/1
4	FRU	D	4	4	-	2/4/20/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FRU	O2-C2	2.06	1.44	1.40

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	FRU	O6-C6-C5	-3.83	98.14	111.29
3	C	6	FRU	O3-C3-C2	2.84	119.27	111.05
3	C	2	FRU	O5-C2-C1	2.84	115.35	109.21
4	D	2	FRU	O5-C5-C6	2.23	114.04	109.21
3	C	1	FRU	O5-C5-C4	2.15	110.83	105.49

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	FRU	O1-C1-C2-C3
4	D	1	FRU	O1-C1-C2-O2
3	C	7	FRU	O1-C1-C2-C3
3	C	7	FRU	O1-C1-C2-O5
3	C	5	FRU	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 3 short contacts:

| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	FRU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	6	FRU	1	0
3	C	7	FRU	2	0
3	C	3	FRU	1	0
3	C	5	FRU	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 C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings
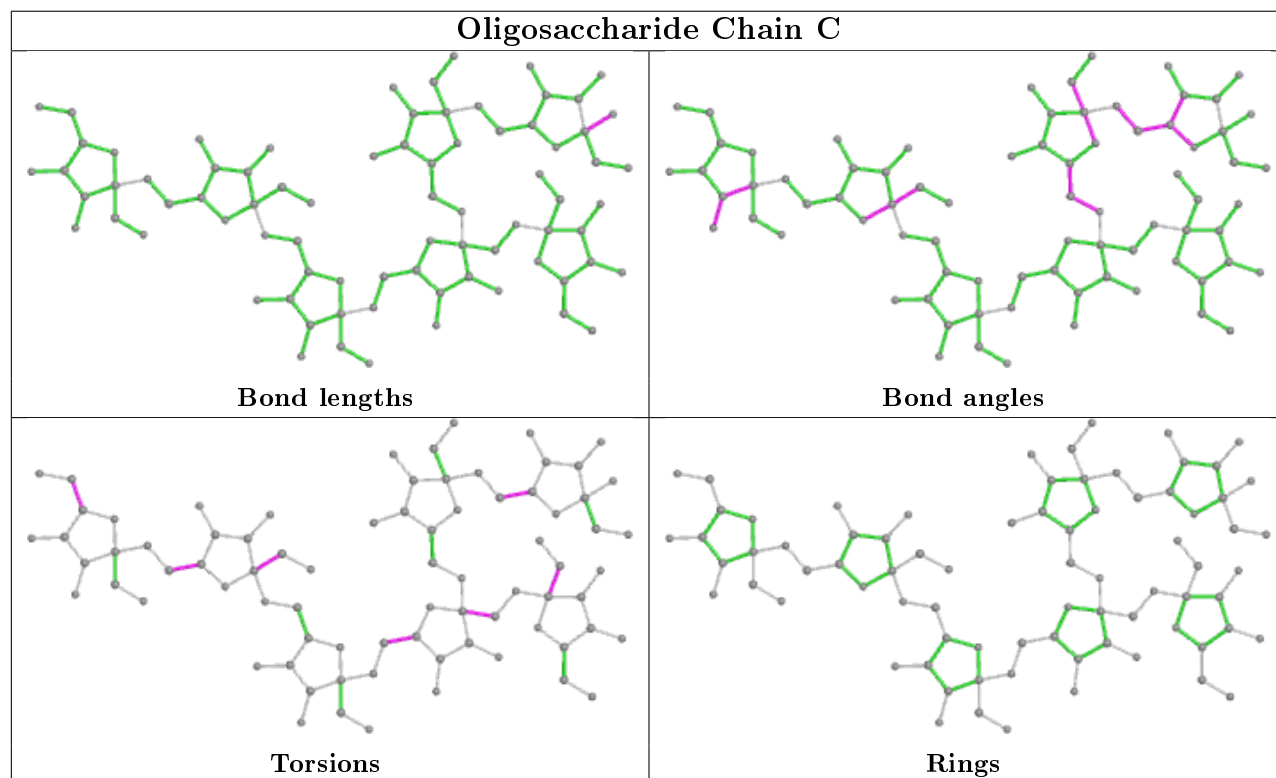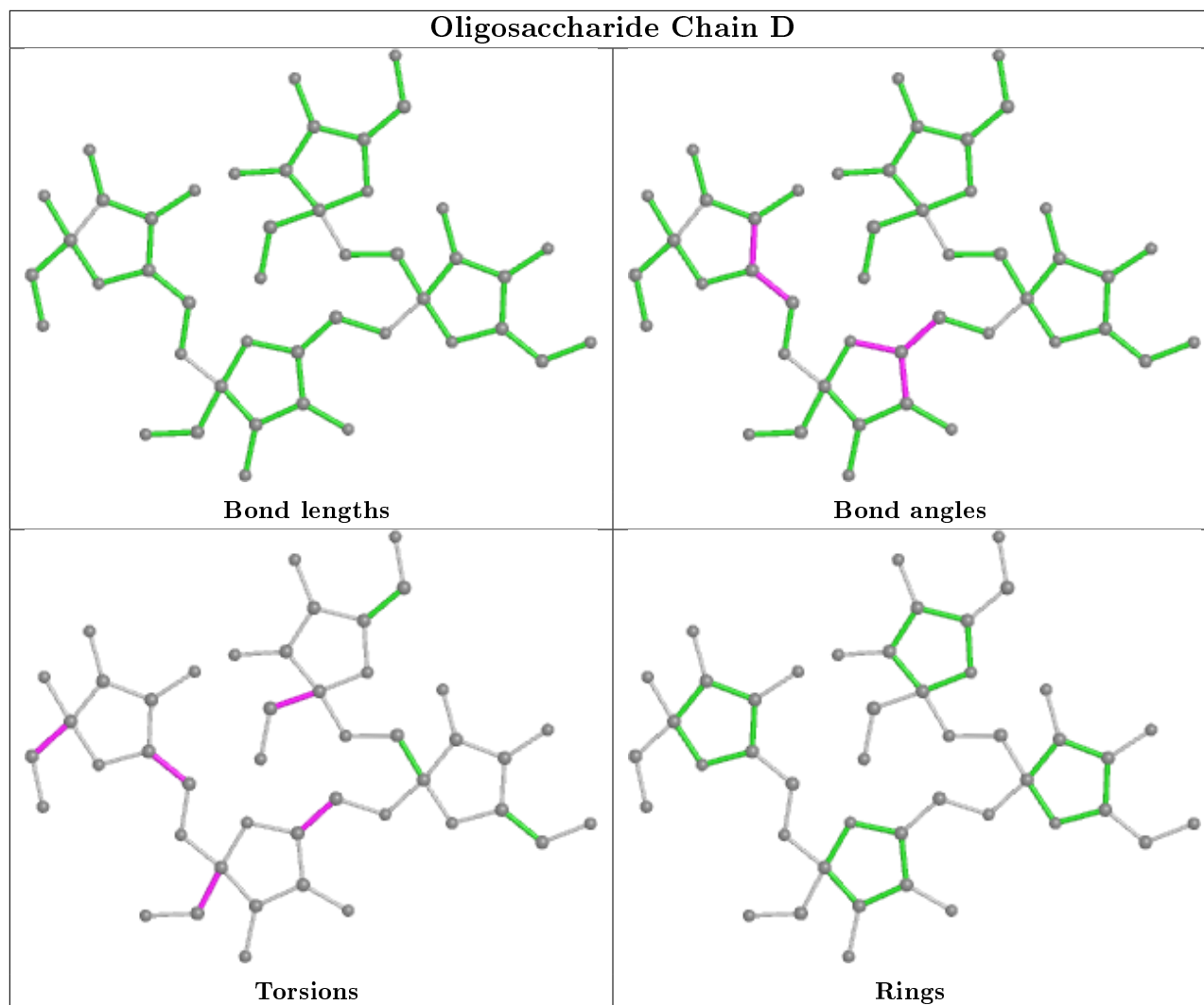
5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
7	C8E	B	1103	-	20,20,20	0.45	0	19,19,19	0.47	0
7	C8E	B	1102	-	11,11,20	0.42	0	10,10,19	0.39	0
7	C8E	B	1101	-	15,15,20	0.45	0	14,14,19	0.24	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
7	C8E	B	1103	-	-	9/18/18/18	-
7	C8E	B	1102	-	-	1/9/9/18	-
7	C8E	B	1101	-	-	8/13/13/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1103	C8E	C7-C8-O9-C10
7	B	1103	C8E	O15-C16-C17-O18
7	B	1101	C8E	O12-C13-C14-O15
7	B	1101	C8E	C3-C4-C5-C6
7	B	1101	C8E	O9-C10-C11-O12

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1103	C8E	1	0
7	B	1102	C8E	1	0
7	B	1101	C8E	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand C8E B 1103

Ligand C8E B 1102

Ligand C8E B 1101
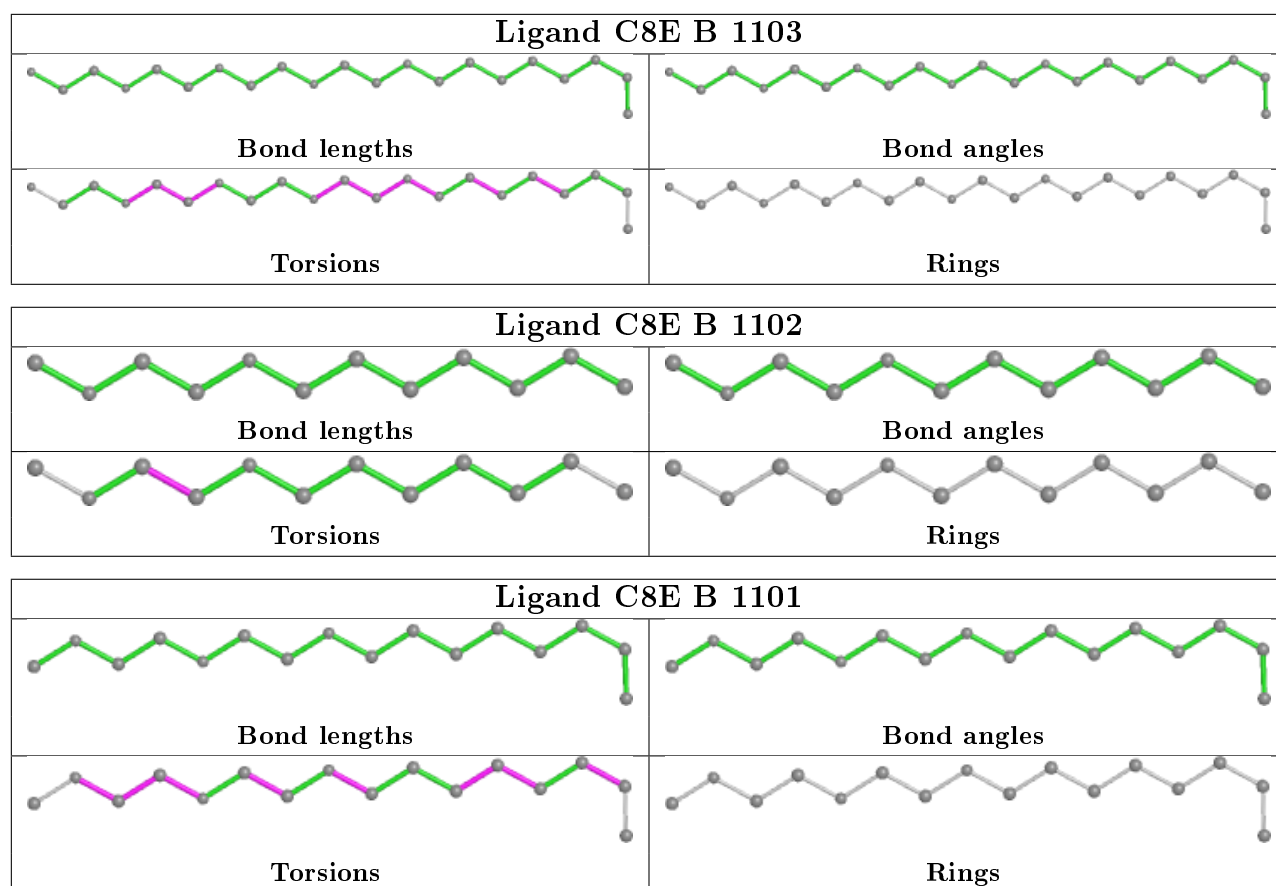
5.7 Other polymers (i)

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	555/580 (95%)	0.02	1 (0%)	95	96	26, 46, 74, 110	0
2	B	921/1041 (88%)	-0.10	0	100	100	20, 45, 89, 129	0
All	All	1476/1621 (91%)	-0.06	1 (0%)	95	96	20, 46, 83, 129	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	CYS	2.3

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.
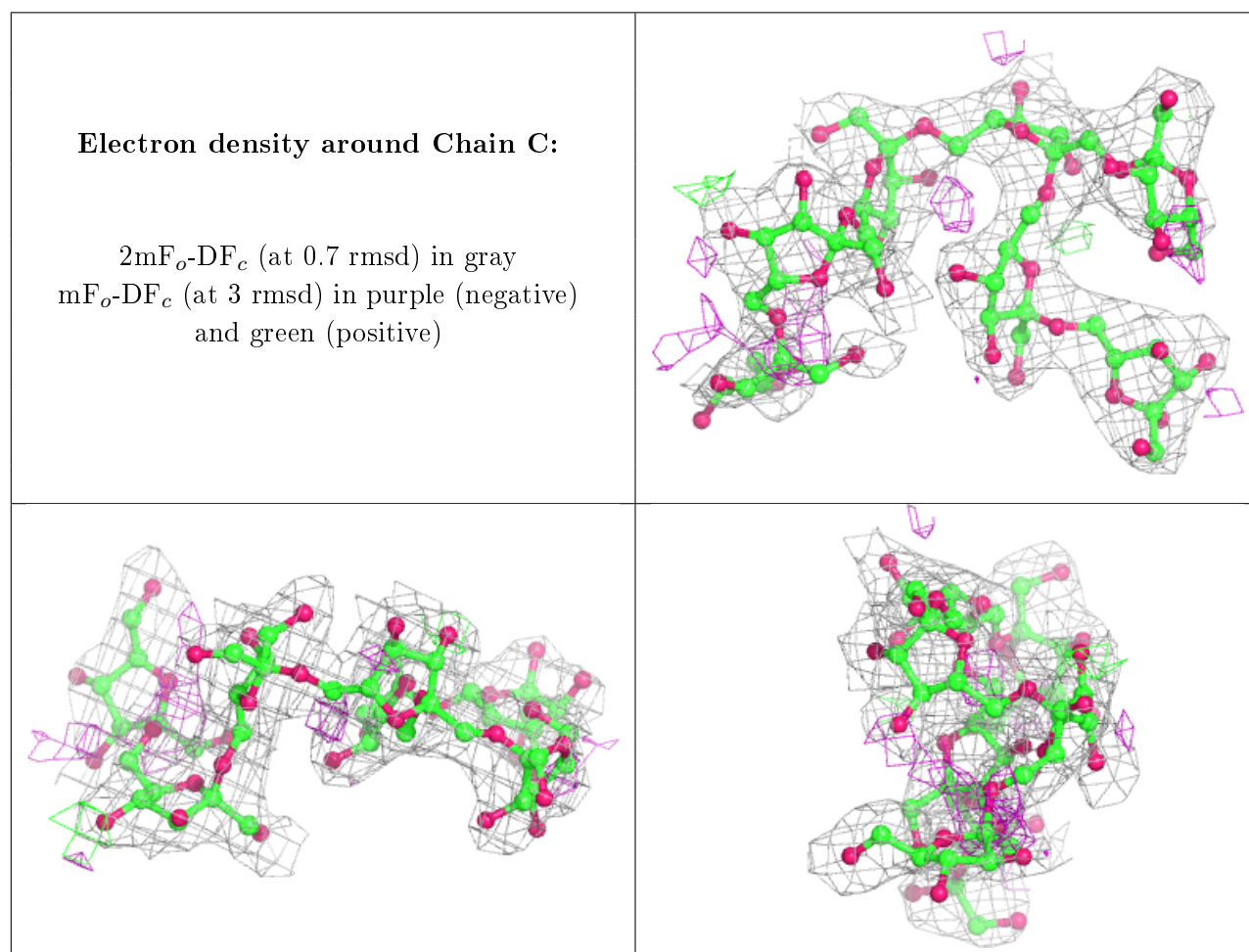
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FRU	C	6	11/12	0.57	0.44	63,82,92,104	0
4	FRU	D	4	11/12	0.85	0.42	70,104,113,116	0
3	FRU	C	7	11/12	0.86	0.32	53,80,114,114	0
4	FRU	D	1	12/12	0.89	0.33	60,84,90,96	0
4	FRU	D	3	11/12	0.90	0.32	80,91,101,107	0
4	FRU	D	2	11/12	0.92	0.25	50,76,85,91	0
3	FRU	C	1	12/12	0.93	0.21	66,76,79,80	0
3	FRU	C	5	11/12	0.96	0.20	31,37,47,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	FRU	C	2	11/12	0.97	0.17	35,46,63,63	0
3	FRU	C	3	11/12	0.97	0.18	32,40,53,53	0
3	FRU	C	4	11/12	0.99	0.17	22,29,38,42	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.
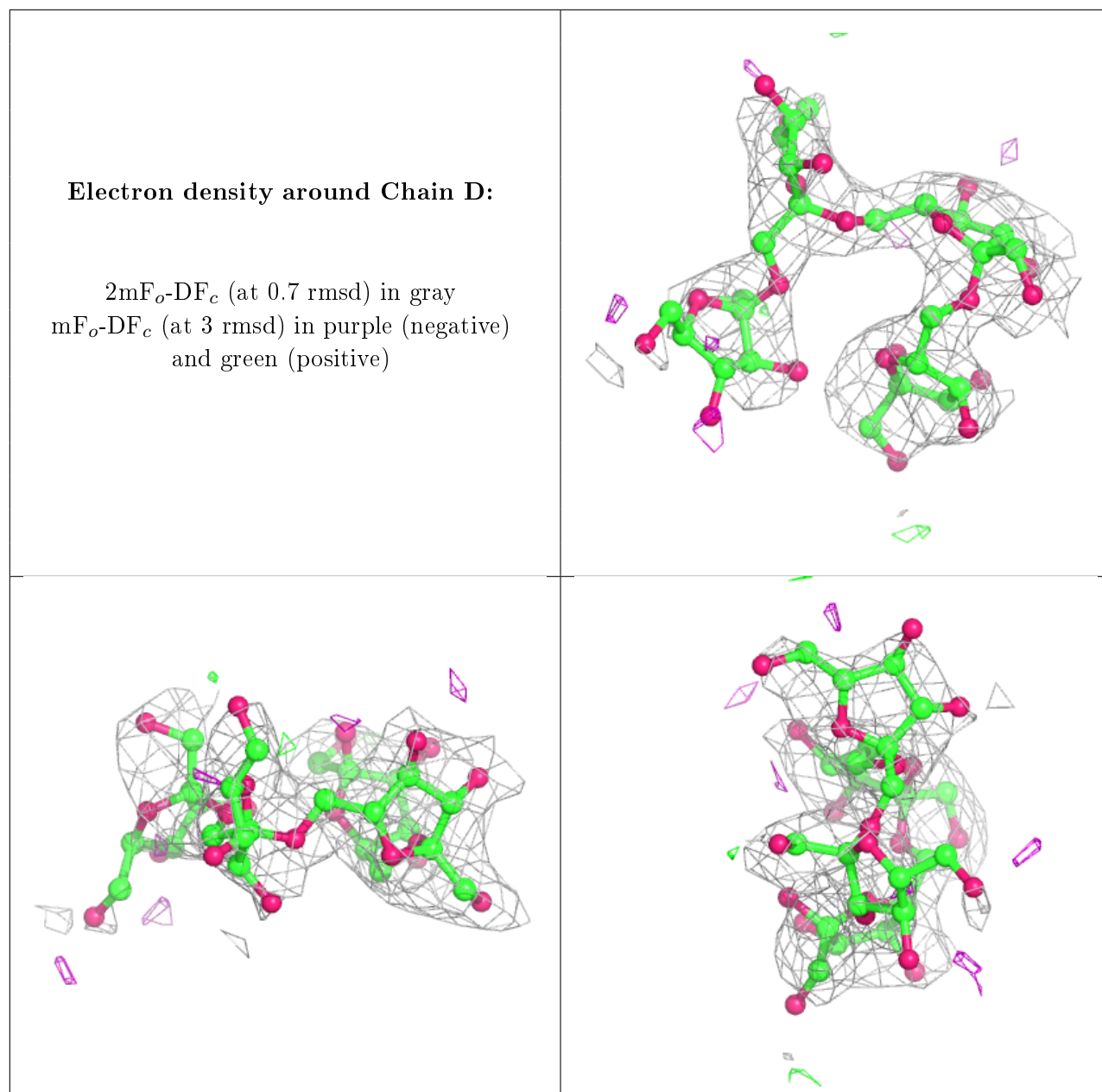
Electron density around Chain C:

$2mF_o$-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 D:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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, 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
7	C8E	B	1103	21/21	0.90	0.39	25,59,72,75	0
7	C8E	B	1101	16/21	0.92	0.22	33,57,84,87	0
5	CL	A	601	1/1	0.93	0.14	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	C8E	B	1102	12/21	0.94	0.21	39,42,63,66	0
6	MG	A	602	1/1	0.95	0.23	29,29,29,29	0
6	MG	B	1104	1/1	0.96	0.15	28,28,28,28	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.
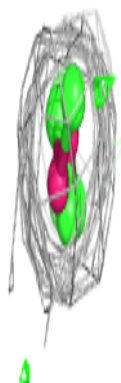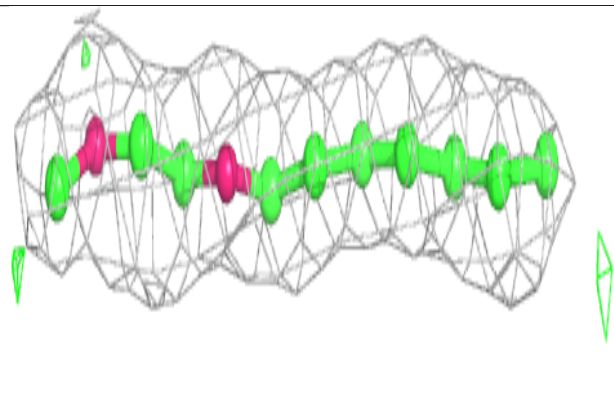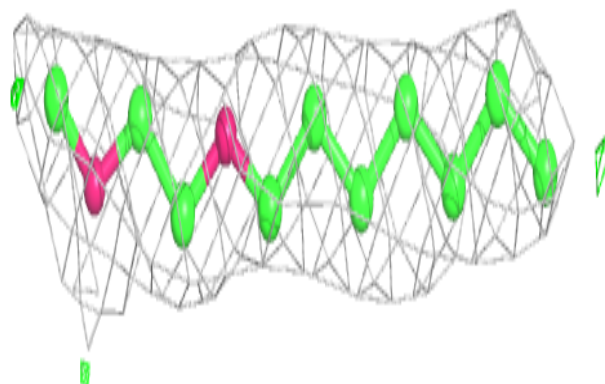

Electron density around C8E B 1103:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
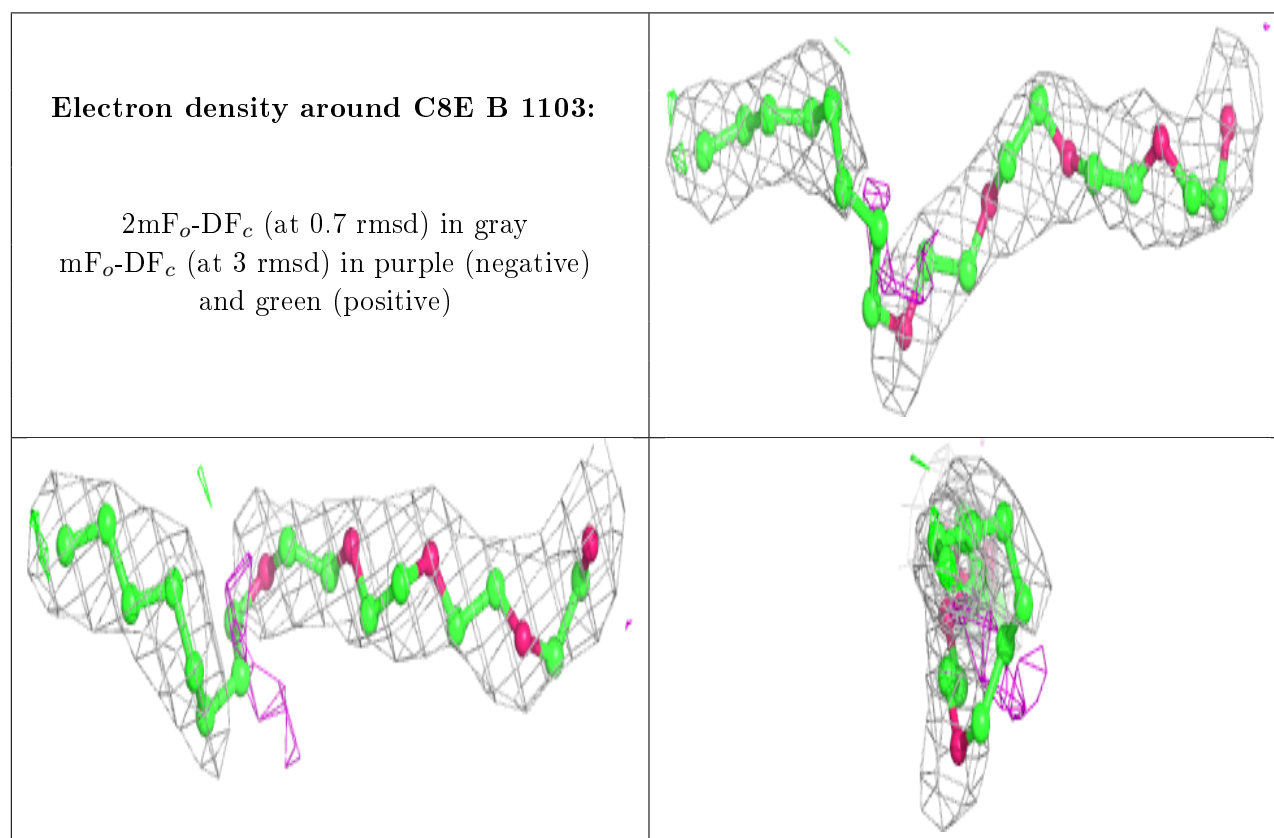
Electron density around C8E B 1101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
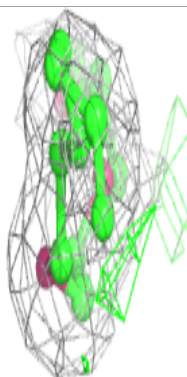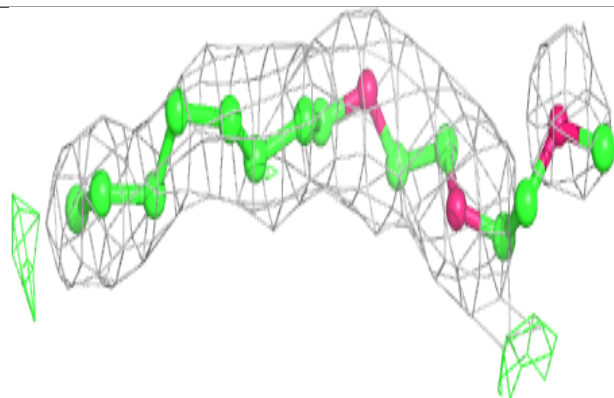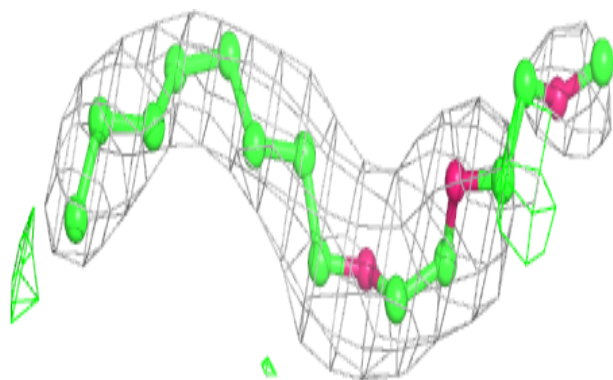
Electron density around C8E B 1102:

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.