



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:40 AM UTC

PDB ID : 5GUB / pdb_00005gub
Title : Crystal structure of solute-binding protein complexed with sulfate group-free unsaturated chondroitin disaccharide
Authors : Oiki, S.; Mikami, B.; Murata, K.; Hashimoto, W.
Deposited on : 2016-08-26
Resolution : 1.78 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	:	4-5-2 with Phenix2.0
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

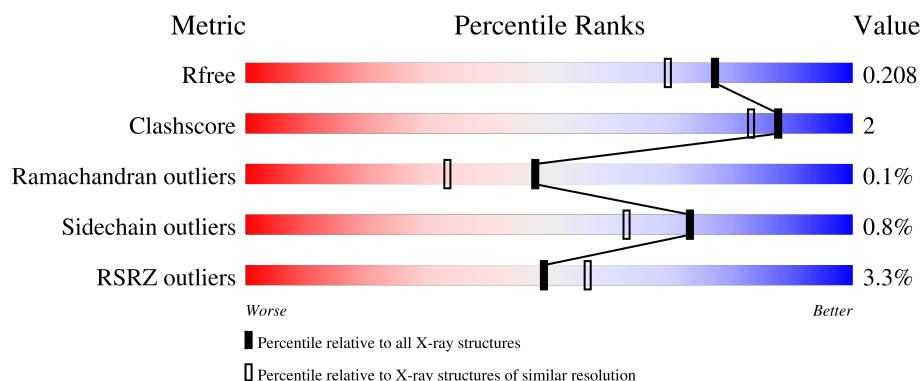
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	483	2% 93% 5%
1	B	483	3% 94%
1	C	483	5% 91% 7%
2	D	2	100%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12783 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 Extracellular solute-binding protein family 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	1	0
			3844	2476	634	728	6			
1	B	471	Total	C	N	O	S	0	1	0
			3821	2459	631	725	6			
1	C	473	Total	C	N	O	S	0	1	0
			3833	2467	633	727	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	expression tag	UNP D1AWE0
B	18	MET	-	expression tag	UNP D1AWE0
C	18	MET	-	expression tag	UNP D1AWE0

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose.

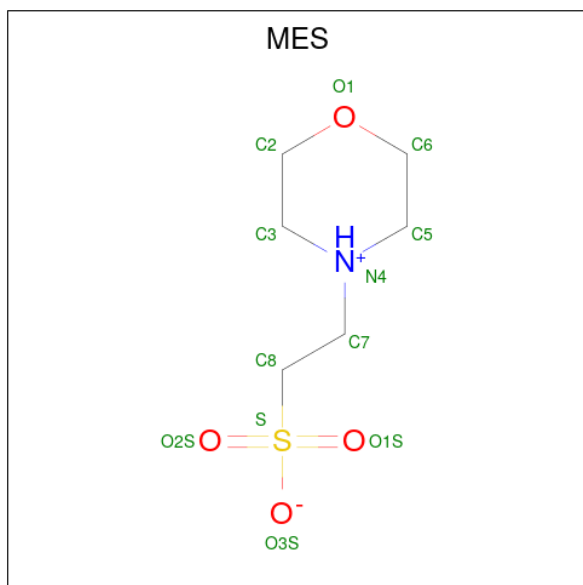


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	E	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	F	2	Total	C	N	O	0	0	0
			26	14	1	11			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	2	1		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	394	Total	O	0	1
			395	395		
6	B	425	Total	O	0	0
			425	425		
6	C	333	Total	O	0	0
			333	333		

- Molecule 1: Extracellular solute-binding protein family 1



- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose

Chain E:  50% 50%

NGA1
GCD2

- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose

Chain F:  50% 50%

NGA1
GCD2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.91Å 112.21Å 166.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.57 – 1.78 41.57 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.57-1.78) 99.7 (41.57-1.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.174 , 0.208 0.176 , 0.208	Depositor DCC
R_{free} test set	6984 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12783	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: EDO, GCD, NGA, MES, CA

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	0.44	0/3939	0.70	2/5331 (0.0%)
1	B	0.44	0/3914	0.70	0/5297
1	C	0.43	0/3927	0.73	2/5315 (0.0%)
All	All	0.43	0/11780	0.71	4/15943 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	443	GLU	CA-C-N	5.53	128.25	120.28
1	C	443	GLU	C-N-CA	5.53	128.25	120.28
1	A	435	LEU	CA-C-N	-5.30	114.50	119.85
1	A	435	LEU	C-N-CA	-5.30	114.50	119.85

There are no chirality outliers.

There are no planarity outliers.

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	A	3844	0	3798	14	0
1	B	3821	0	3776	12	0
1	C	3833	0	3789	19	0
2	D	26	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	26	0	19	2	0
2	F	26	0	19	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	12	0	13	0	0
4	B	12	0	12	0	0
4	C	12	0	12	1	0
5	A	3	0	2	0	0
5	B	12	0	14	2	0
6	A	395	0	0	4	0
6	B	425	0	0	6	0
6	C	333	0	0	4	0
All	All	12783	0	11473	46	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 2.

The worst 5 of 46 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:393:ARG:HH22	2:E:1:NGA:H82	1.41	0.85
1:C:131:ASP:OD1	6:C:701:HOH:O	2.07	0.72
1:C:228:GLU:OE1	6:C:702:HOH:O	2.10	0.68
1:C:444:LYS:HE3	1:C:495:ILE:HG12	1.77	0.66
1:B:36:HIS:NE2	2:E:1:NGA:H83	2.15	0.62

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	473/483 (98%)	467 (99%)	6 (1%)	0	100	100
1	B	470/483 (97%)	463 (98%)	7 (2%)	0	100	100
1	C	472/483 (98%)	463 (98%)	8 (2%)	1 (0%)	43	29
All	All	1415/1449 (98%)	1393 (98%)	21 (2%)	1 (0%)	48	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	443	GLU

5.3.2 Protein sidechains ⓘ

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	409/416 (98%)	408 (100%)	1 (0%)	87	83
1	B	407/416 (98%)	403 (99%)	4 (1%)	68	55
1	C	408/416 (98%)	403 (99%)	5 (1%)	63	49
All	All	1224/1248 (98%)	1214 (99%)	10 (1%)	73	63

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	442	LYS
1	C	446	LYS
1	C	494	GLN
1	B	409	TYR
1	B	496	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	150	ASN
1	C	405	GLN

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Mol	Chain	Res	Type
1	B	70	GLN
1	B	150	ASN
1	B	155	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	NGA	D	1	2	15,15,15	0.44	0	21,21,21	0.73	0
2	GCD	D	2	2	10,11,12	1.99	1 (10%)	12,15,17	1.22	2 (16%)
2	NGA	E	1	2	15,15,15	0.62	0	21,21,21	0.96	1 (4%)
2	GCD	E	2	2	10,11,12	1.93	1 (10%)	12,15,17	1.40	2 (16%)
2	NGA	F	1	2	15,15,15	0.40	0	21,21,21	0.77	0
2	GCD	F	2	2	10,11,12	2.27	3 (30%)	12,15,17	1.07	2 (16%)

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	NGA	D	1	2	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GCD	D	2	2	-	0/4/17/20	0/1/1/1
2	NGA	E	1	2	-	2/6/26/26	0/1/1/1
2	GCD	E	2	2	-	0/4/17/20	0/1/1/1
2	NGA	F	1	2	-	0/6/26/26	0/1/1/1
2	GCD	F	2	2	-	0/4/17/20	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	GCD	O5-C5	6.13	1.45	1.37
2	D	2	GCD	O5-C5	5.33	1.44	1.37
2	E	2	GCD	O5-C5	5.10	1.44	1.37
2	F	2	GCD	O5-C1	-2.21	1.41	1.45
2	F	2	GCD	O6B-C6	-2.01	1.25	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GCD	O5-C5-C4	-3.10	122.09	124.94
2	E	2	GCD	O6B-C6-C5	2.97	120.80	114.06
2	E	2	GCD	O5-C5-C4	-2.63	122.52	124.94
2	E	1	NGA	O3-C3-C2	-2.15	105.31	109.58
2	F	2	GCD	O5-C5-C4	-2.13	122.98	124.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

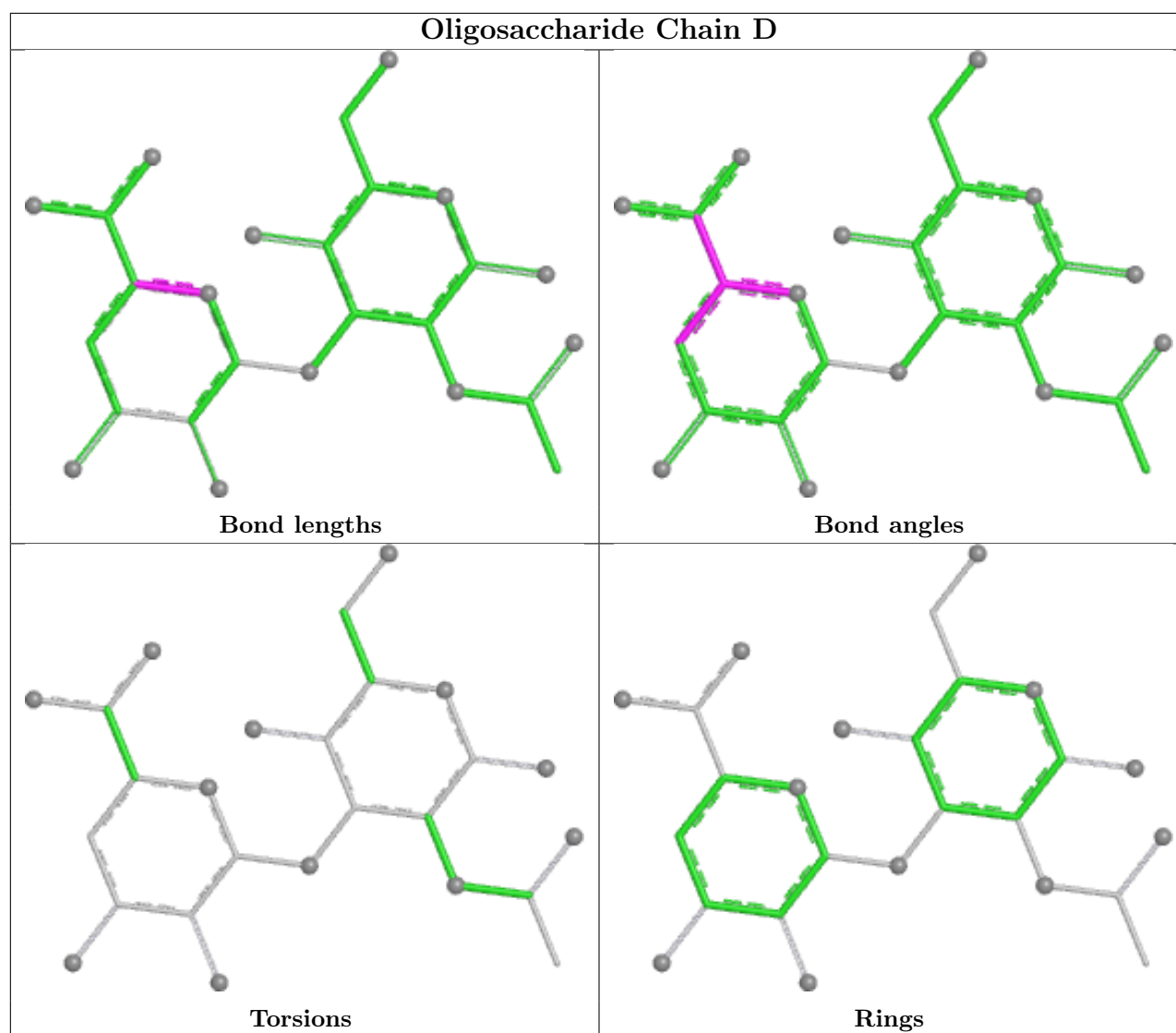
Mol	Chain	Res	Type	Atoms
2	E	1	NGA	C8-C7-N2-C2
2	E	1	NGA	O7-C7-N2-C2

There are no ring outliers.

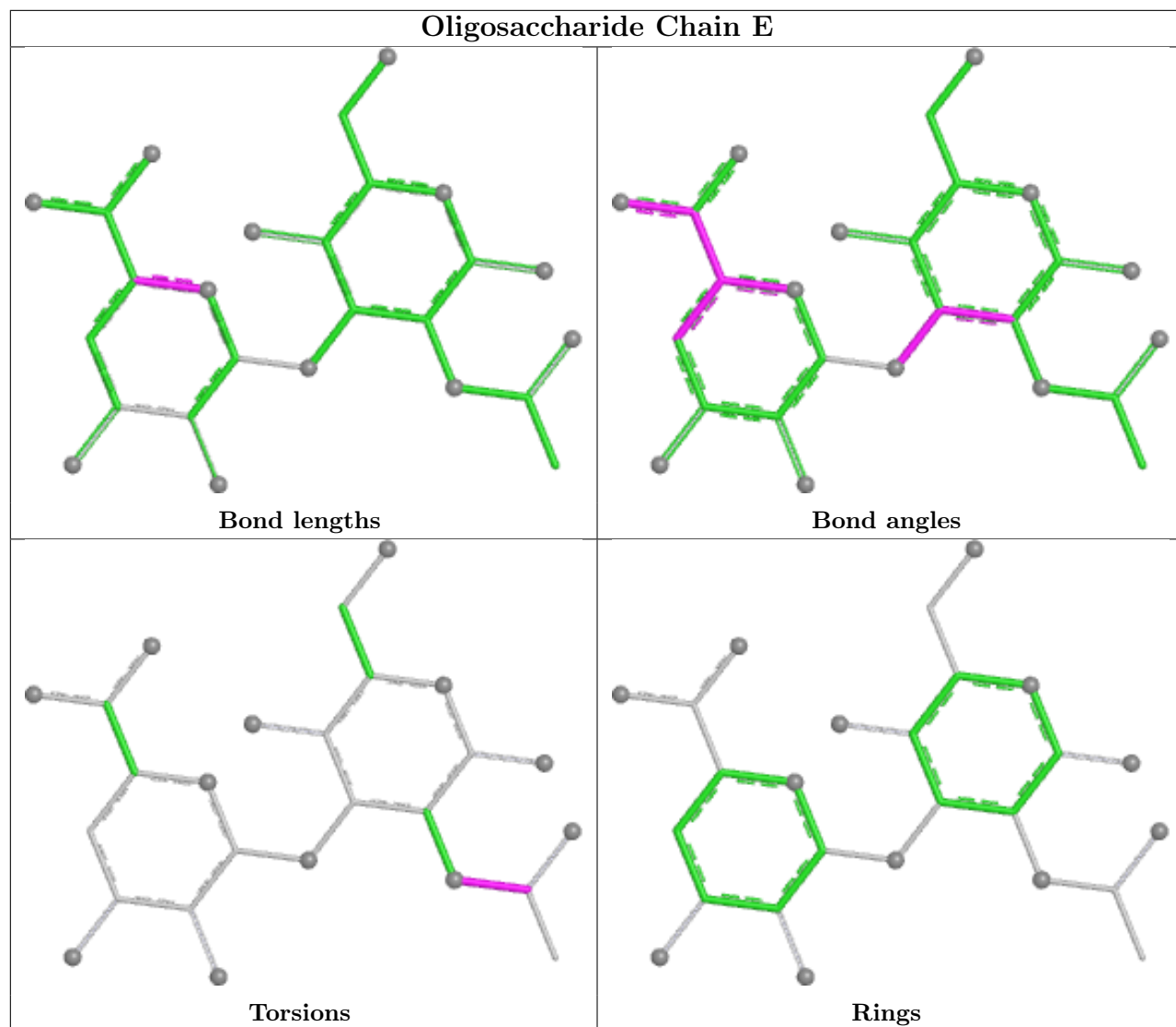
2 monomers are involved in 3 short contacts:

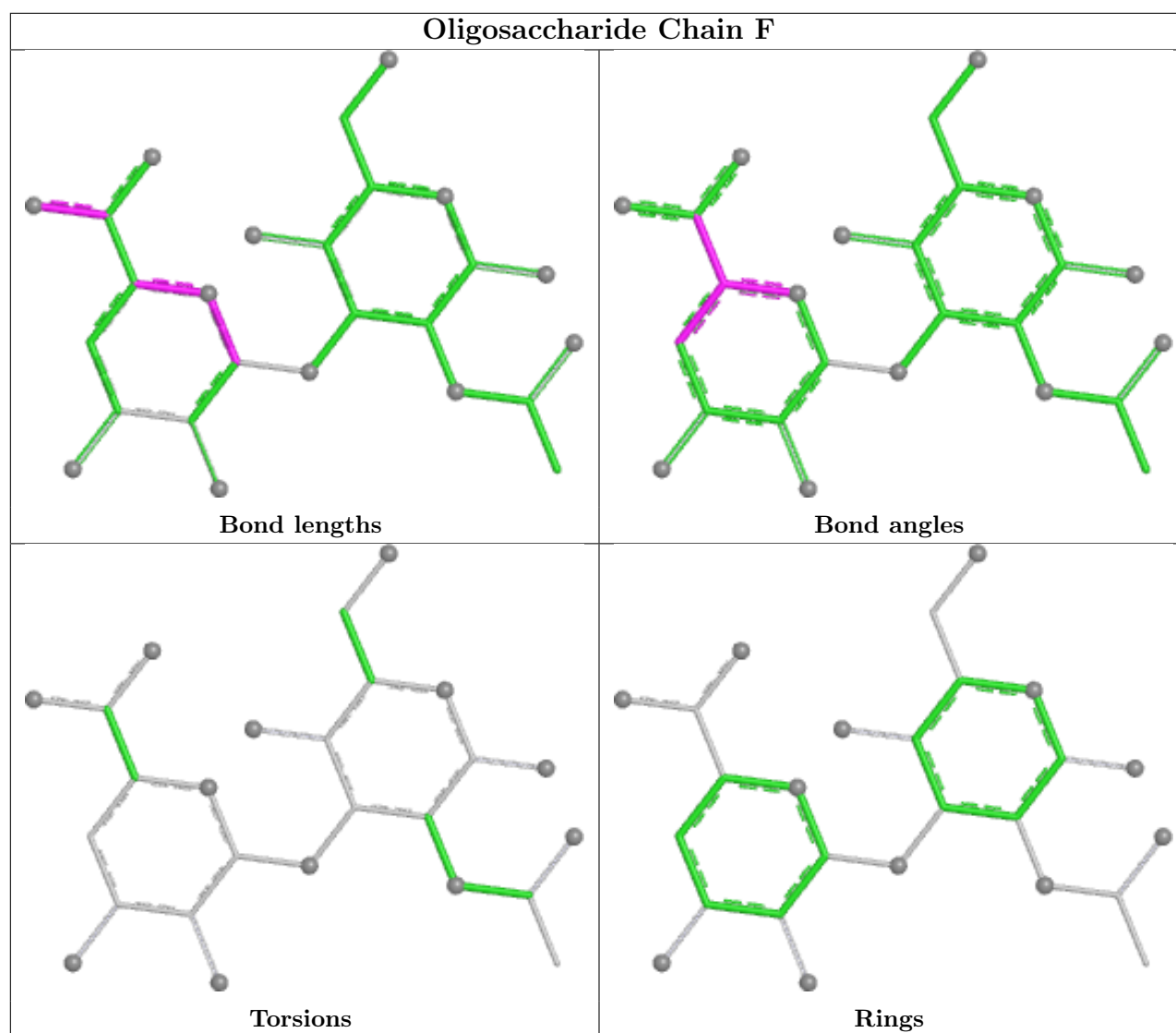
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NGA	2	0
2	D	1	NGA	1	0

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 E





5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	EDO	B	607	-	3,3,3	0.91	0	2,2,2	0.51	0
5	EDO	A	605	-	2,2,3	0.57	0	1,1,2	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	B	604	-	12,12,12	2.31	1 (8%)	15,16,16	2.21	7 (46%)
4	MES	C	604	-	12,12,12	2.19	1 (8%)	15,16,16	1.97	2 (13%)
5	EDO	B	606	-	3,3,3	0.98	0	2,2,2	0.89	0
4	MES	A	604	-	12,12,12	1.88	1 (8%)	15,16,16	1.42	2 (13%)
5	EDO	B	605	-	3,3,3	1.21	0	2,2,2	0.45	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
5	EDO	B	607	-	-	0/1/1/1	-
5	EDO	B	606	-	-	1/1/1/1	-
4	MES	B	604	-	-	4/6/14/14	0/1/1/1
4	MES	C	604	-	-	0/6/14/14	0/1/1/1
4	MES	A	604	-	-	0/6/14/14	0/1/1/1
5	EDO	B	605	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	604	MES	C8-S	-7.75	1.66	1.77
4	C	604	MES	C8-S	-7.23	1.67	1.77
4	A	604	MES	C8-S	-6.21	1.68	1.77

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	604	MES	C5-N4-C3	5.37	120.41	108.84
4	B	604	MES	C5-N4-C3	5.01	119.64	108.84
4	A	604	MES	C5-N4-C3	3.75	116.91	108.84
4	B	604	MES	C7-N4-C5	2.85	118.84	111.24
4	A	604	MES	O2S-S-C8	2.83	111.00	106.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	604	MES	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
4	B	604	MES	C7-C8-S-O3S
4	B	604	MES	C7-C8-S-O1S
4	B	604	MES	C7-C8-S-O2S
5	B	606	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	604	MES	1	0
5	B	606	EDO	1	0
5	B	605	EDO	1	0

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	474/483 (98%)	-0.20	9 (1%) 66 74	5, 14, 28, 53	1 (0%)
1	B	471/483 (97%)	-0.24	15 (3%) 50 57	5, 13, 28, 58	1 (0%)
1	C	473/483 (97%)	0.15	23 (4%) 35 41	5, 16, 40, 60	1 (0%)
All	All	1418/1449 (97%)	-0.10	47 (3%) 49 56	5, 14, 32, 60	3 (0%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	PRO	7.1
1	C	437	ILE	5.9
1	C	442	LYS	4.7
1	C	438	LEU	4.7
1	B	438	LEU	4.5

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	NGA	E	1	15/15	0.95	0.07	4,9,18,20	0
2	NGA	F	1	15/15	0.95	0.06	7,10,17,17	0
2	NGA	D	1	15/15	0.96	0.06	7,9,14,14	0

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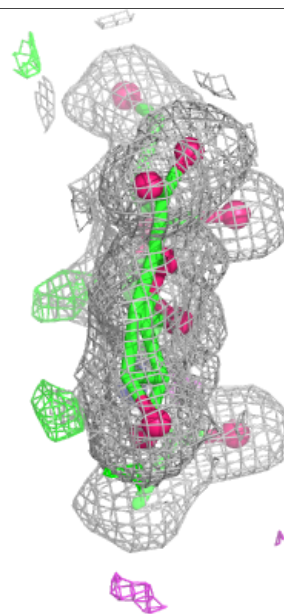
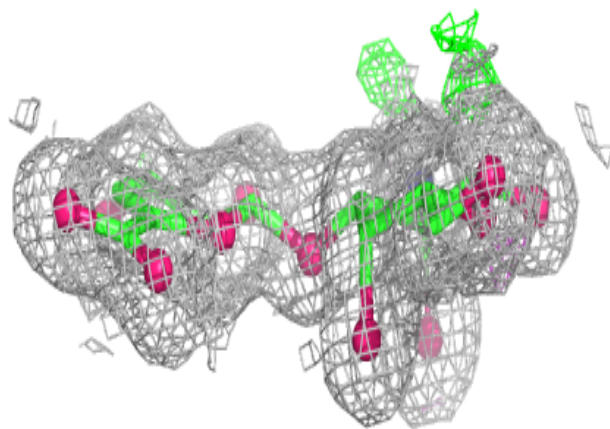
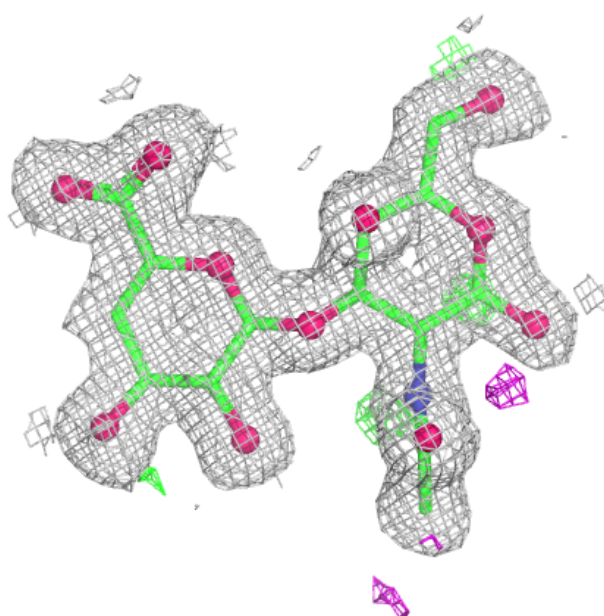
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GCD	F	2	11/12	0.97	0.05	10,11,13,14	0
2	GCD	D	2	11/12	0.98	0.04	6,8,9,9	0
2	GCD	E	2	11/12	0.98	0.04	5,7,8,8	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.

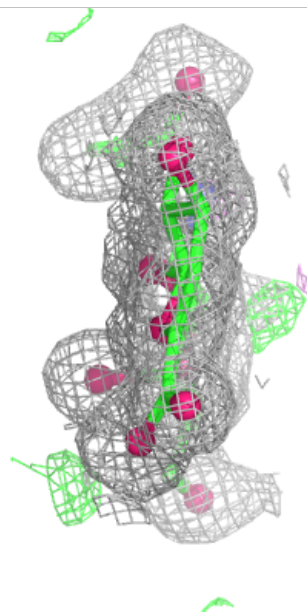
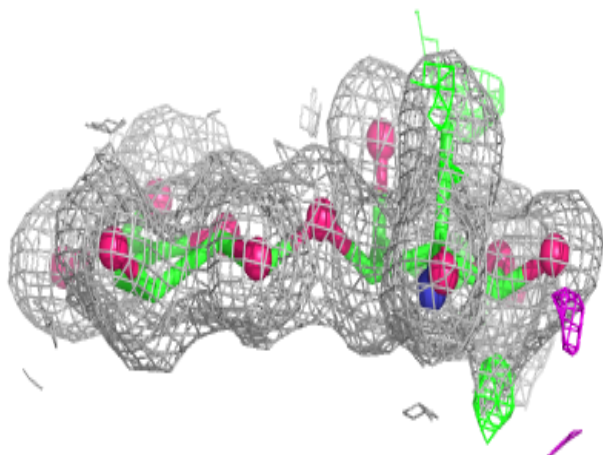
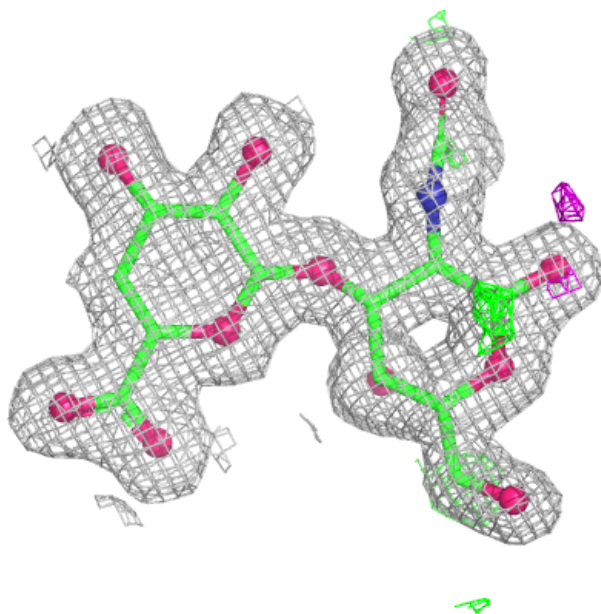
Electron density around Chain D:

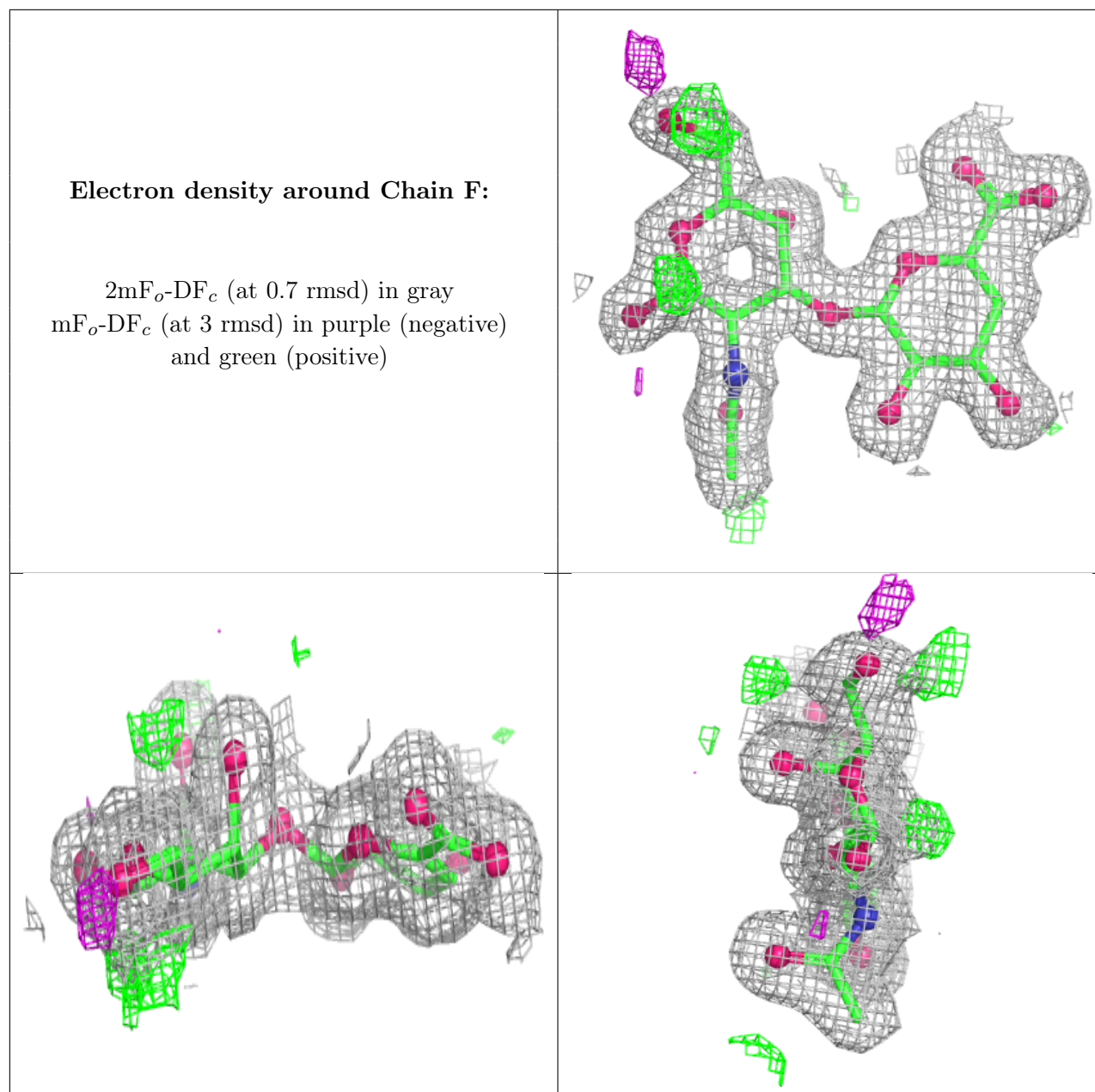
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
5	EDO	B	606	4/4	0.73	0.29	20,20,20,20	0
4	MES	B	604	12/12	0.78	0.22	27,34,37,41	9
5	EDO	A	605	3/4	0.81	0.12	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MES	C	604	12/12	0.88	0.13	15,23,26,28	0
5	EDO	B	607	4/4	0.91	0.09	20,20,20,20	0
5	EDO	B	605	4/4	0.97	0.08	20,20,20,20	0
4	MES	A	604	12/12	0.97	0.06	12,15,18,18	0
3	CA	C	601	1/1	0.97	0.05	19,19,19,19	0
3	CA	A	601	1/1	0.99	0.03	14,14,14,14	0
3	CA	B	601	1/1	0.99	0.03	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.