



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2025 – 10:12 am BST

PDB ID : 9G73 / pdb\_00009g73  
Title : Crystal structure of mouse Carboxylesterase 2e (Ces2e)  
Authors : Eisner, H.; Sagmeister, T.; Rammer, L.; Oberer, M.  
Deposited on : 2024-07-19  
Resolution : 2.40 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

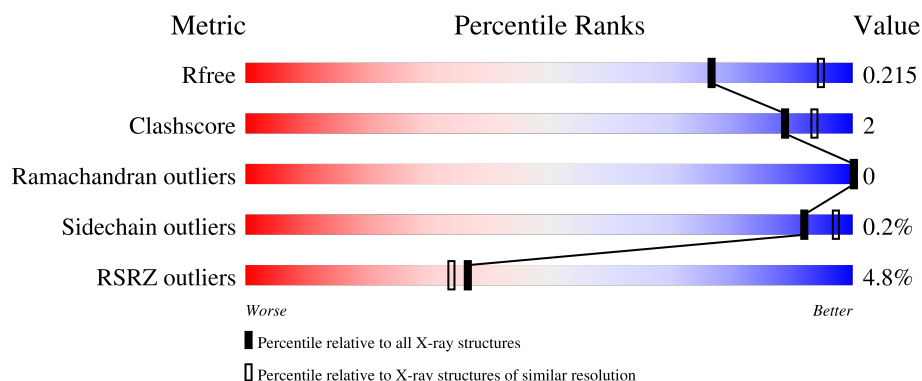
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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  $\geq 3$ , 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	565	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	565	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>8%</div> </div> </div>
2	C	6	<div> <div></div> <div> <div>83%</div> <div>17%</div> </div> </div>
3	D	8	<div> <div></div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17113 atoms, of which 7969 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.

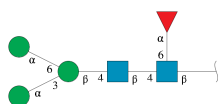
- Molecule 1 is a protein called Pyrethroid hydrolase Ces2e.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	518	Total	C	H	N	O	S	0	4	0
			7991	2612	3908	697	744	30			
1	B	522	Total	C	H	N	O	S	0	4	0
			8045	2628	3931	703	753	30			

There are 12 discrepancies between the modelled and reference sequences:

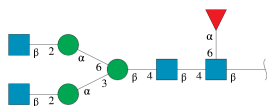
Chain	Residue	Modelled	Actual	Comment	Reference
A	560	HIS	-	expression tag	UNP Q8BK48
A	561	HIS	-	expression tag	UNP Q8BK48
A	562	HIS	-	expression tag	UNP Q8BK48
A	563	HIS	-	expression tag	UNP Q8BK48
A	564	HIS	-	expression tag	UNP Q8BK48
A	565	HIS	-	expression tag	UNP Q8BK48
B	560	HIS	-	expression tag	UNP Q8BK48
B	561	HIS	-	expression tag	UNP Q8BK48
B	562	HIS	-	expression tag	UNP Q8BK48
B	563	HIS	-	expression tag	UNP Q8BK48
B	564	HIS	-	expression tag	UNP Q8BK48
B	565	HIS	-	expression tag	UNP Q8BK48

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	H	N	O	0	0	0
			125	40	54	2	29			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	8	Total	C	H	N	O	0	0	0
			175	56	76	4	39			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	B	2	Total Cl 2 2	0	0

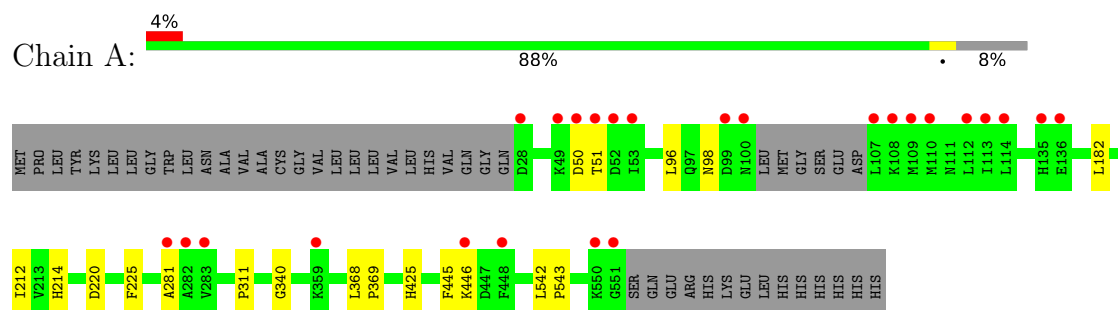
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	368	Total O 368 368	0	0
6	B	330	Total O 330 330	0	0

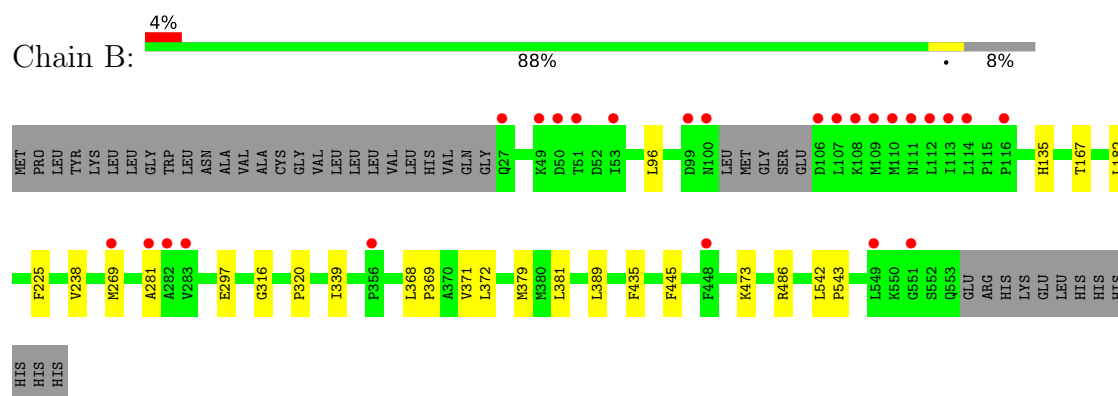
### 3 Residue-property plots [i](#)

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.

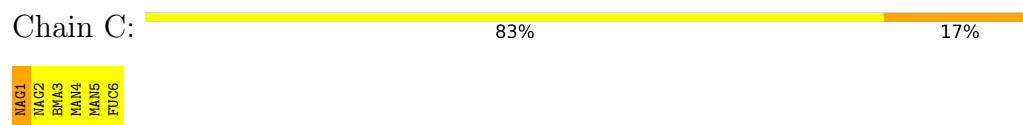
- Molecule 1: Pyrethroid hydrolase Ces2e




- Molecule 1: Pyrethroid hydrolase Ces2e



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1
MAG2
BKA3
MAN4
MAG5
MAG6
MAG7
FUC8

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.93Å 145.24Å 149.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.65 – 2.40 80.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (80.65-2.40) 99.9 (80.65-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.176 , 0.214 0.177 , 0.215	Depositor DCC
$R_{free}$ test set	2718 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.43 % 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 2.3642e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, MAN, BMA, FUC, SO4

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	1.00	1/4211 (0.0%)	1.27	2/5719 (0.0%)
1	B	1.01	0/4242	1.27	2/5761 (0.0%)
All	All	1.00	1/8453 (0.0%)	1.27	4/11480 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	GLY	C-O	5.56	1.29	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	225	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	225	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	238	VAL	CA-C-O	-5.01	115.74	120.95

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	4083	3908	3990	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4114	3931	4015	17	0
2	C	71	54	61	1	0
3	D	99	76	85	0	0
4	A	35	0	0	0	0
4	B	40	0	0	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	368	0	0	6	0
6	B	330	0	0	8	0
All	All	9144	7969	8151	29	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.

All (29) 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:A:425:HIS:ND1	6:A:702:HOH:O	2.16	0.78
1:B:473:LYS:HG2	6:B:988:HOH:O	1.86	0.74
1:B:269:MET:SD	6:B:984:HOH:O	2.46	0.74
1:A:220:ASP:OD2	6:A:701:HOH:O	2.13	0.66
1:A:281:ALA:HB2	2:C:1:NAG:H81	1.83	0.60
1:B:96:LEU:HD12	1:B:182:LEU:HD11	1.91	0.53
1:B:281:ALA:HA	6:B:706:HOH:O	2.09	0.52
1:B:379[A]:MET:HE3	1:B:381:LEU:HD12	1.91	0.52
1:A:446:LYS:HD3	6:A:1004:HOH:O	2.11	0.49
1:B:379[A]:MET:HE3	1:B:381:LEU:CD1	2.43	0.48
1:A:542:LEU:HB3	1:A:543:PRO:HD3	1.96	0.48
1:A:96:LEU:HD12	1:A:182:LEU:HD11	1.97	0.47
1:B:135[A]:HIS:CD2	4:B:601:SO4:O4	2.68	0.47
1:B:167:THR:HG22	6:B:874:HOH:O	2.17	0.45
1:A:51:THR:HB	6:A:786:HOH:O	2.19	0.43
1:B:368:LEU:HB3	1:B:369:PRO:HD3	2.01	0.43
1:B:379[A]:MET:CE	1:B:389:LEU:HD11	2.49	0.42
1:B:372:LEU:HG	6:B:938:HOH:O	2.19	0.42
1:B:486:ARG:HD2	6:B:985:HOH:O	2.20	0.42
1:B:542:LEU:HB3	1:B:543:PRO:HD3	2.02	0.41
1:B:339:ILE:O	1:B:435:PHE:HA	2.20	0.41
1:A:311:PRO:HG2	6:A:764:HOH:O	2.21	0.41
1:A:368:LEU:HB3	1:A:369:PRO:HD3	2.03	0.41
1:B:297:GLU:HB3	6:B:704:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:VAL:HG12	6:B:938:HOH:O	2.20	0.41
1:A:212:ILE:HD12	1:A:212:ILE:HA	1.95	0.40
1:B:316:GLY:HA2	1:B:320:PRO:HA	2.03	0.40
1:A:98:ASN:HB3	6:A:840:HOH:O	2.21	0.40

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	518/565 (92%)	501 (97%)	17 (3%)	0	100	100
1	B	522/565 (92%)	503 (96%)	19 (4%)	0	100	100
All	All	1040/1130 (92%)	1004 (96%)	36 (4%)	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	A	446/483 (92%)	445 (100%)	1 (0%)	92	97
1	B	450/483 (93%)	449 (100%)	1 (0%)	92	97
All	All	896/966 (93%)	894 (100%)	2 (0%)	92	97

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

Mol	Chain	Res	Type
1	A	445	PHE
1	B	445	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	244	GLN
1	A	422	GLN
1	B	98	ASN
1	B	139	ASN
1	B	271	HIS
1	B	422	GLN
1	B	547	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](#)

14 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	1,2	14,14,15	0.38	0	17,19,21	1.09	2 (11%)
2	NAG	C	2	2	14,14,15	0.67	0	17,19,21	1.07	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BMA	C	3	2	11,11,12	0.46	0	15,15,17	1.31	2 (13%)
2	MAN	C	4	2	11,11,12	0.42	0	15,15,17	1.56	1 (6%)
2	MAN	C	5	2	11,11,12	0.46	0	15,15,17	1.44	1 (6%)
2	FUC	C	6	2	10,10,11	0.56	0	14,14,16	0.97	1 (7%)
3	NAG	D	1	1,3	14,14,15	0.73	0	17,19,21	0.94	1 (5%)
3	NAG	D	2	3	14,14,15	0.59	0	17,19,21	1.14	2 (11%)
3	BMA	D	3	3	11,11,12	0.30	0	15,15,17	0.95	1 (6%)
3	MAN	D	4	3	11,11,12	0.50	0	15,15,17	1.47	2 (13%)
3	NAG	D	5	3	14,14,15	0.60	0	17,19,21	1.59	1 (5%)
3	MAN	D	6	3	11,11,12	0.70	0	15,15,17	1.32	2 (13%)
3	NAG	D	7	3	14,14,15	0.49	0	17,19,21	1.50	2 (11%)
3	FUC	D	8	3	10,10,11	0.41	0	14,14,16	0.79	1 (7%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	0/1/1/1
2	FUC	C	6	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	NAG	D	5	3	-	0/6/23/26	0/1/1/1
3	MAN	D	6	3	-	1/2/19/22	0/1/1/1
3	NAG	D	7	3	-	0/6/23/26	0/1/1/1
3	FUC	D	8	3	-	-	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	NAG	C1-O5-C5	5.16	119.19	112.19
2	C	5	MAN	C1-O5-C5	5.02	118.99	112.19
3	D	7	NAG	C1-O5-C5	4.93	118.88	112.19
2	C	4	MAN	C1-O5-C5	4.65	118.50	112.19
3	D	4	MAN	C1-O5-C5	4.39	118.14	112.19
2	C	3	BMA	C1-O5-C5	3.07	116.35	112.19
2	C	3	BMA	O5-C1-C2	2.91	115.26	110.77
2	C	1	NAG	C1-O5-C5	2.54	115.63	112.19
2	C	6	FUC	O5-C1-C2	2.54	114.69	110.77
3	D	7	NAG	O5-C1-C2	2.51	115.25	111.29
3	D	4	MAN	O5-C5-C6	2.43	111.01	107.20
3	D	6	MAN	O2-C2-C3	2.42	115.00	110.14
2	C	1	NAG	C8-C7-N2	-2.36	112.11	116.10
3	D	6	MAN	C1-O5-C5	2.30	115.31	112.19
3	D	2	NAG	C1-C2-N2	2.27	114.36	110.49
3	D	8	FUC	O5-C1-C2	2.25	114.25	110.77
3	D	2	NAG	O5-C5-C4	-2.24	105.39	110.83
2	C	2	NAG	C1-O5-C5	2.16	115.12	112.19
3	D	3	BMA	C1-O5-C5	2.14	115.10	112.19
2	C	2	NAG	O5-C1-C2	2.09	114.58	111.29
3	D	1	NAG	C3-C4-C5	2.07	113.92	110.24

There are no chirality outliers.

All (11) torsion outliers are listed below:

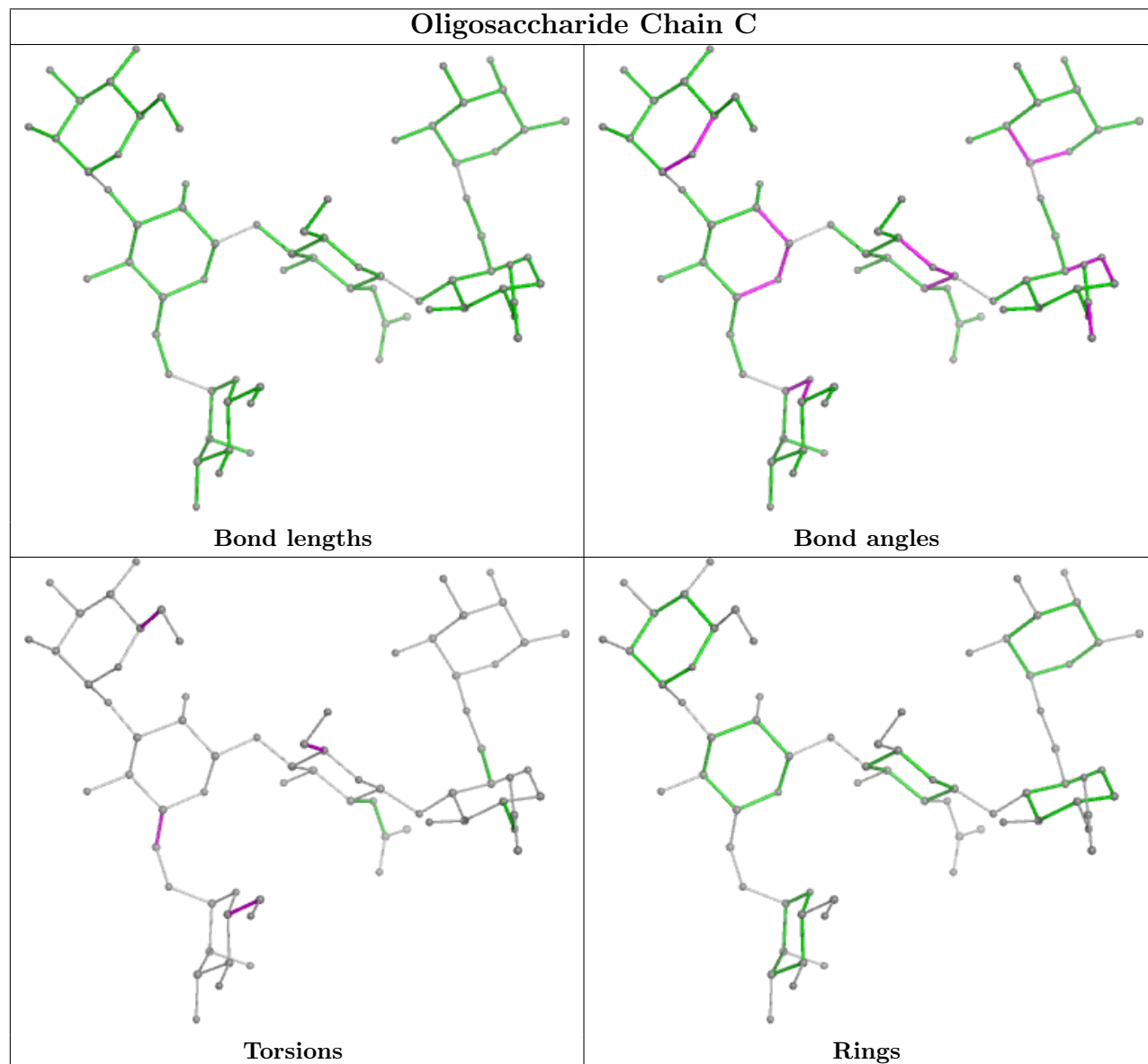
Mol	Chain	Res	Type	Atoms
3	D	4	MAN	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

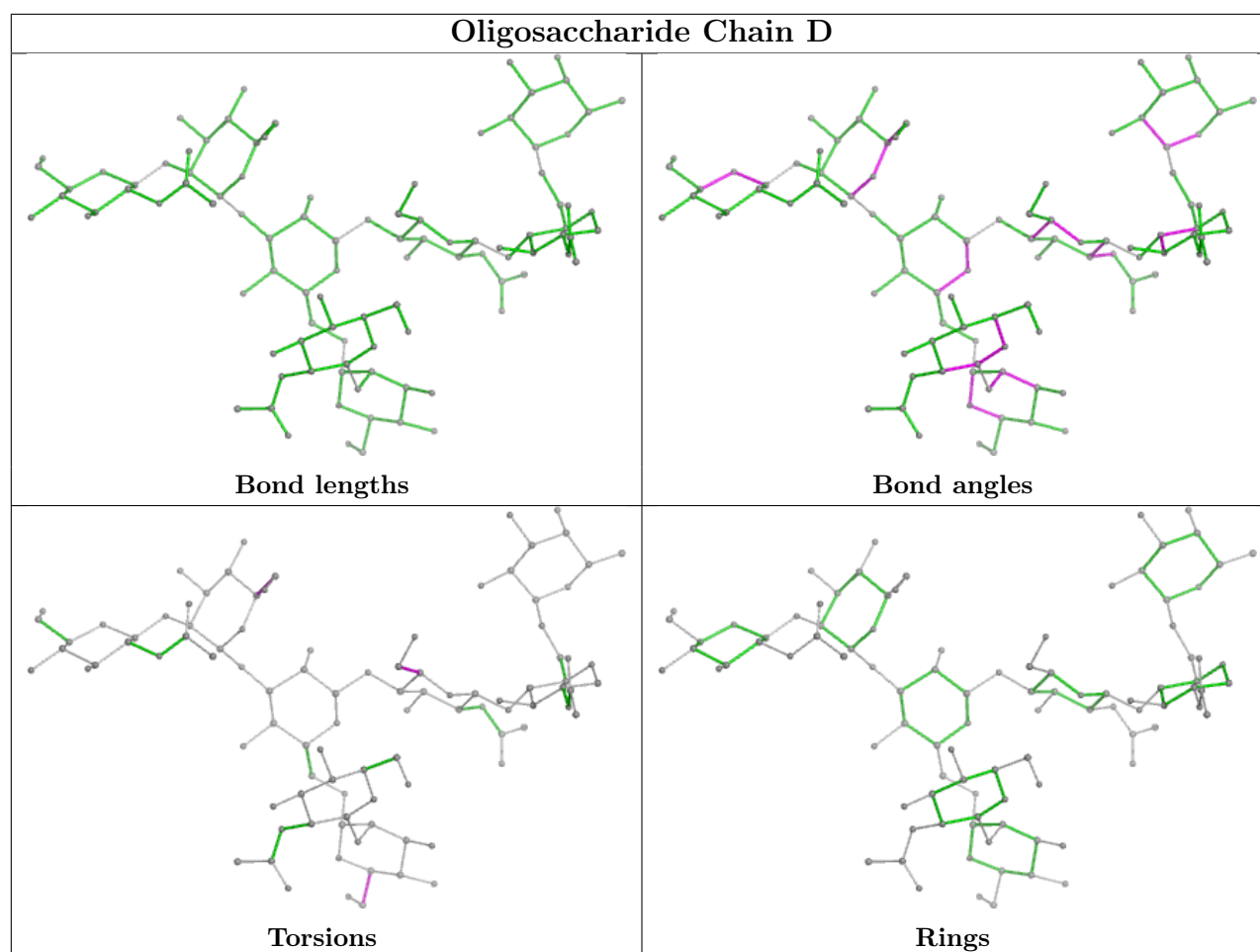
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	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.





## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	$\# Z  > 2$
4	SO4	B	605	-	4,4,4	0.37	0	6,6,6	0.09	0
4	SO4	B	607	-	4,4,4	0.35	0	6,6,6	0.13	0
4	SO4	A	604	-	4,4,4	0.41	0	6,6,6	0.12	0
4	SO4	A	601	-	4,4,4	0.44	0	6,6,6	0.18	0
4	SO4	A	606	-	4,4,4	0.39	0	6,6,6	0.10	0
4	SO4	A	602	-	4,4,4	0.35	0	6,6,6	0.20	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	A	607	-	4,4,4	0.33	0	6,6,6	0.10	0
4	SO4	B	603	-	4,4,4	0.32	0	6,6,6	0.14	0
4	SO4	B	604	-	4,4,4	0.37	0	6,6,6	0.10	0
4	SO4	A	605	-	4,4,4	0.32	0	6,6,6	0.16	0
4	SO4	B	608	-	4,4,4	0.37	0	6,6,6	0.20	0
4	SO4	A	603	-	4,4,4	0.37	0	6,6,6	0.07	0
4	SO4	B	601	-	4,4,4	0.44	0	6,6,6	0.14	0
4	SO4	B	606	-	4,4,4	0.41	0	6,6,6	0.07	0
4	SO4	B	602	-	4,4,4	0.43	0	6,6,6	0.17	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	SO4	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

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	518/565 (91%)	-0.36	25 (4%)	36 34	14, 32, 80, 123	4 (0%)
1	B	522/565 (92%)	-0.35	25 (4%)	36 34	14, 32, 84, 134	4 (0%)
All	All	1040/1130 (92%)	-0.36	50 (4%)	36 34	14, 32, 82, 134	8 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	ALA	5.6
1	A	107	LEU	5.5
1	B	100	ASN	4.7
1	B	283	VAL	4.7
1	B	282	ALA	4.2
1	B	107	LEU	4.1
1	A	448	PHE	4.0
1	A	53	ILE	3.9
1	A	110	MET	3.7
1	B	448	PHE	3.6
1	B	114	LEU	3.4
1	A	113	ILE	3.2
1	B	113	ILE	3.2
1	A	551	GLY	3.1
1	A	283	VAL	3.1
1	A	281	ALA	3.1
1	B	51	THR	3.0
1	A	108	LYS	2.9
1	A	100	ASN	2.9
1	A	51	THR	2.9
1	B	549	LEU	2.9
1	B	53	ILE	2.9
1	A	28	ASP	2.8
1	B	551	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	112	LEU	2.7
1	B	110	MET	2.7
1	A	52	ASP	2.7
1	B	111	ASN	2.7
1	A	109	MET	2.6
1	B	108	LYS	2.6
1	A	446	LYS	2.6
1	B	49	LYS	2.6
1	A	50	ASP	2.5
1	B	116	PRO	2.4
1	B	109	MET	2.4
1	A	49	LYS	2.4
1	B	269	MET	2.4
1	A	550	LYS	2.3
1	B	50	ASP	2.3
1	B	99	ASP	2.2
1	B	27	GLN	2.2
1	A	135[A]	HIS	2.2
1	B	356	PRO	2.2
1	A	112	LEU	2.2
1	A	359	LYS	2.1
1	A	114	LEU	2.1
1	B	106	ASP	2.1
1	A	282	ALA	2.0
1	A	136[A]	GLU	2.0
1	A	99	ASP	2.0

## 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, 95<sup>th</sup> 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.

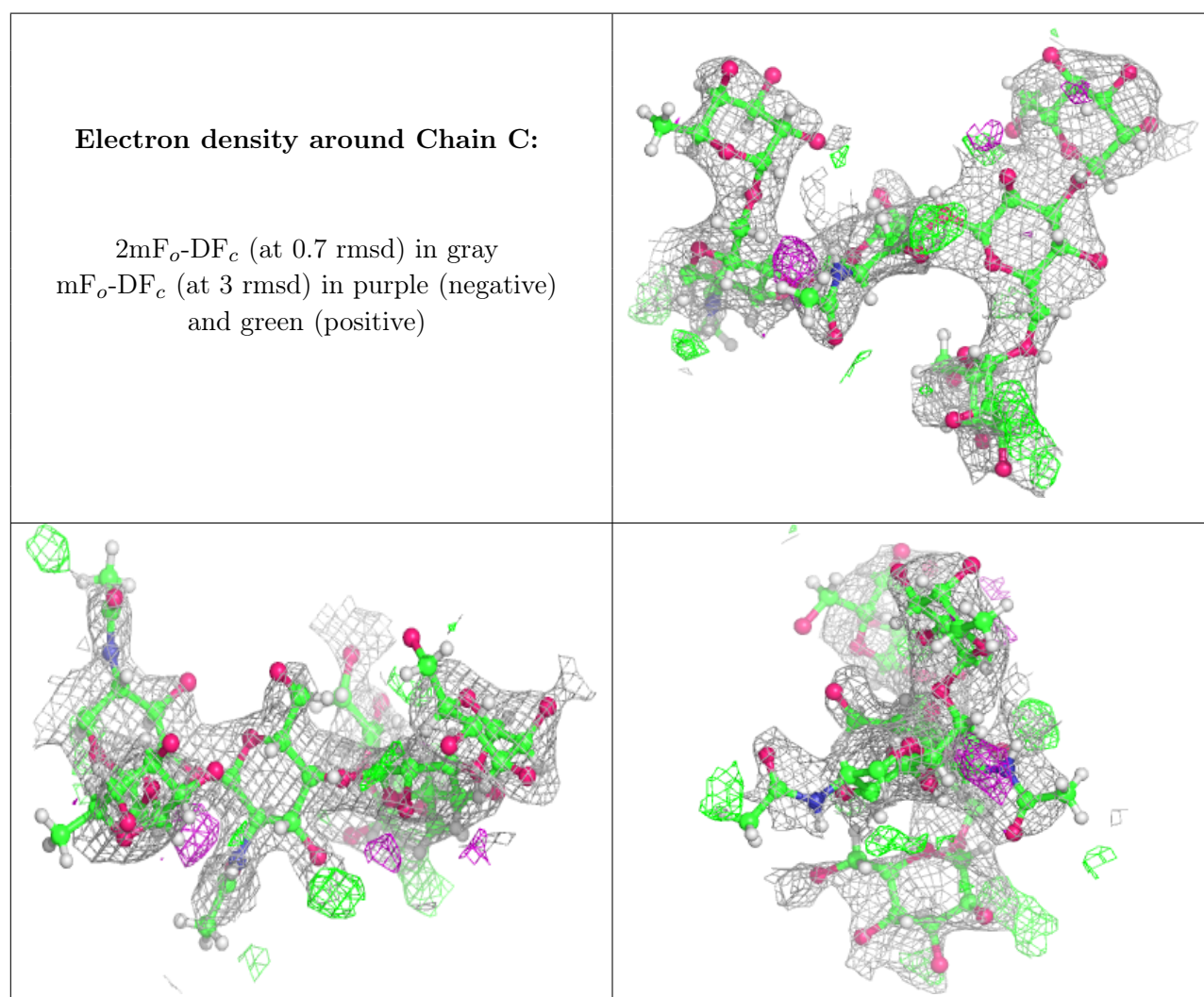
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	D	5	14/15	0.39	0.23	118,137,146,147	0
3	NAG	D	7	14/15	0.54	0.19	105,130,139,141	0

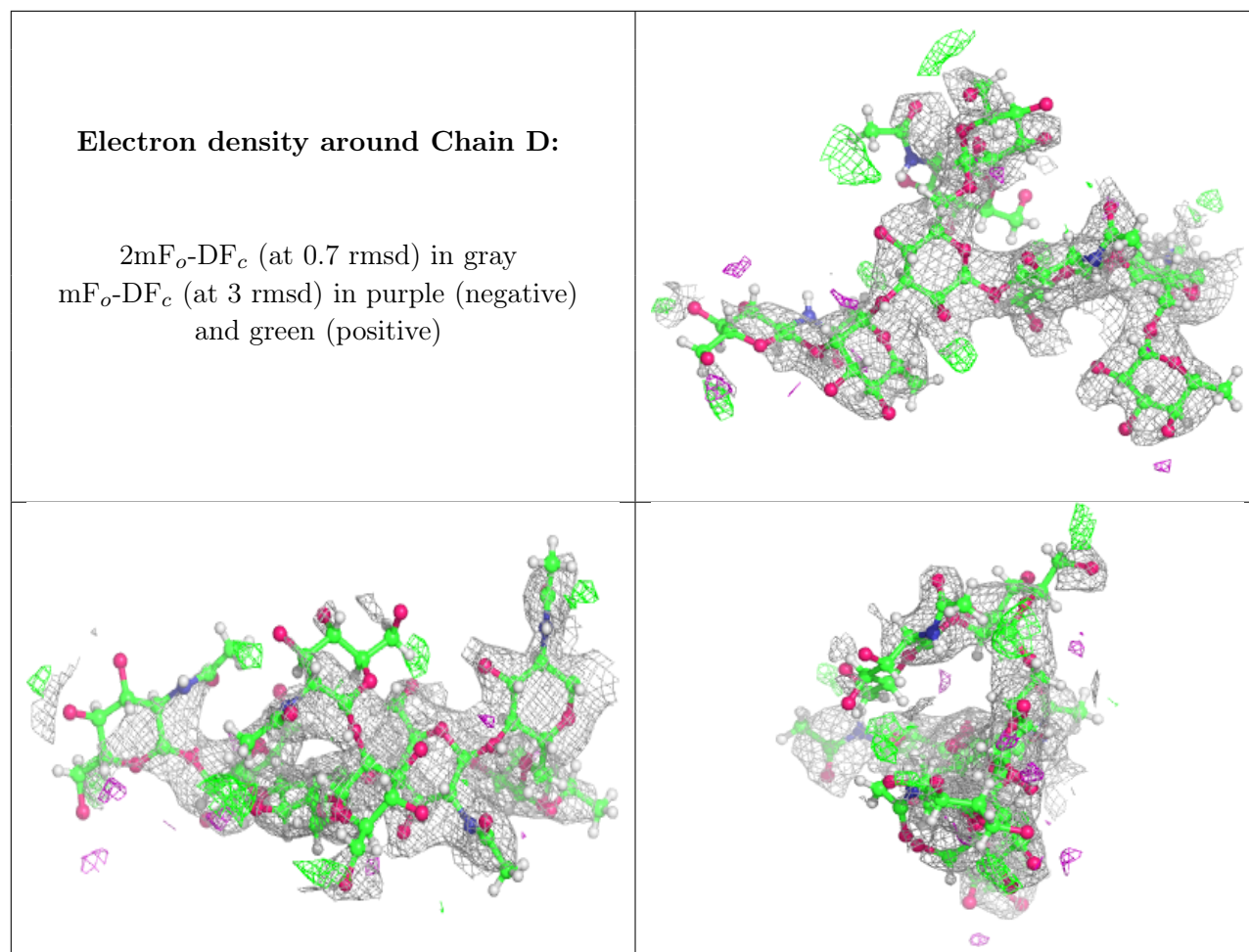
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	C	5	11/12	0.60	0.20	100,112,119,122	0
3	MAN	D	6	11/12	0.72	0.19	75,104,112,114	0
2	NAG	C	2	14/15	0.77	0.16	73,83,88,91	0
2	MAN	C	4	11/12	0.79	0.12	72,86,94,97	0
3	MAN	D	4	11/12	0.81	0.15	77,81,92,92	0
2	FUC	C	6	10/11	0.81	0.16	88,95,98,105	0
2	NAG	C	1	14/15	0.83	0.15	74,85,91,91	0
3	FUC	D	8	10/11	0.84	0.17	85,91,95,104	0
3	BMA	D	3	11/12	0.85	0.12	70,75,81,82	0
2	BMA	C	3	11/12	0.87	0.13	75,82,94,97	0
3	NAG	D	1	14/15	0.87	0.12	62,72,74,76	0
3	NAG	D	2	14/15	0.88	0.11	51,65,68,69	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.





## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	605	5/5	0.85	0.14	61,63,70,76	5
4	SO4	A	607	5/5	0.90	0.12	53,67,68,71	5
4	SO4	A	606	5/5	0.91	0.14	58,68,71,71	5
4	SO4	B	604	5/5	0.91	0.09	67,67,72,73	5
4	SO4	B	608	5/5	0.91	0.13	53,55,57,60	5
4	SO4	B	607	5/5	0.92	0.09	57,58,60,61	5
4	SO4	B	603	5/5	0.92	0.11	53,55,59,65	5
4	SO4	A	604	5/5	0.93	0.10	62,63,65,72	5
4	SO4	A	602	5/5	0.94	0.09	42,45,46,46	5
4	SO4	B	602	5/5	0.94	0.10	47,51,53,57	5
4	SO4	A	601	5/5	0.94	0.09	51,52,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	603	5/5	0.95	0.07	56,59,63,64	5
4	SO4	B	605	5/5	0.95	0.10	42,45,47,50	5
4	SO4	B	606	5/5	0.96	0.06	53,55,58,61	5
4	SO4	B	601	5/5	0.97	0.06	40,40,44,49	0
5	CL	A	609	1/1	0.98	0.05	38,38,38,38	1
5	CL	A	608	1/1	0.99	0.02	26,26,26,26	0
5	CL	B	609	1/1	0.99	0.02	37,37,37,37	0
5	CL	B	610	1/1	1.00	0.04	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.