



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2026 – 10:12 AM EDT

PDB ID : 9Z9E / pdb\_00009z9e  
Title : Structure of FabS1CE2\_ER-3c in complex with the extracellular region of EGFR  
Authors : Singer, A.U.; Mallette, E.; Bruce, H.A.; Blazer, L.L.; Adams, J.J.; Suits, M.D.L.; Sidhu, S.S.  
Deposited on : 2025-11-18  
Resolution : 2.40 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](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 Phenix2.0  
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

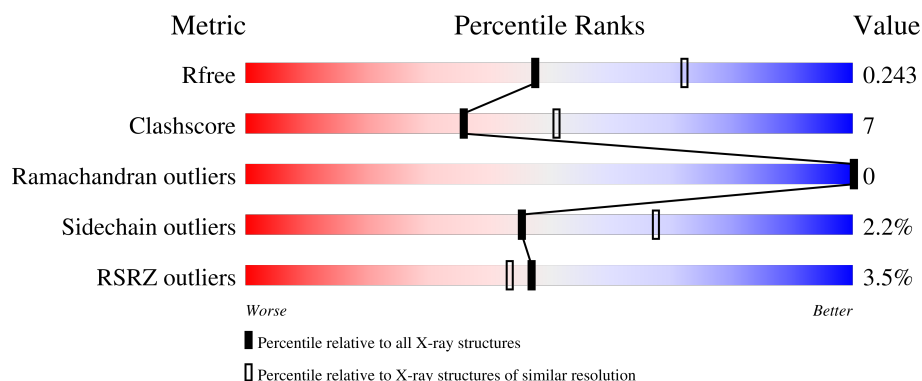
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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	625	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </div> </div>
2	D	231	<div> <div>87%</div> <div>10%</div> <div>.</div> </div>
3	E	212	<div> <div>87%</div> <div>12%</div> </div>
4	B	2	<div> <div>50%</div> <div>50%</div> </div>
4	F	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	2	 50% 50%
5	C	7	 86% 14%

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 8481 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	2	0
			4576	2824	817	877	58			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	622	LEU	-	expression tag	UNP P00533
A	623	VAL	-	expression tag	UNP P00533
A	624	PRO	-	expression tag	UNP P00533
A	625	ARG	-	expression tag	UNP P00533

- Molecule 2 is a protein called heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	226	Total	C	N	O	S	0	4	0
			1730	1097	289	337	7			

- Molecule 3 is a protein called light chain.

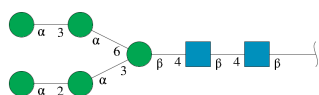
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	212	Total	C	N	O	S	0	1	0
			1642	1026	274	336	6			

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



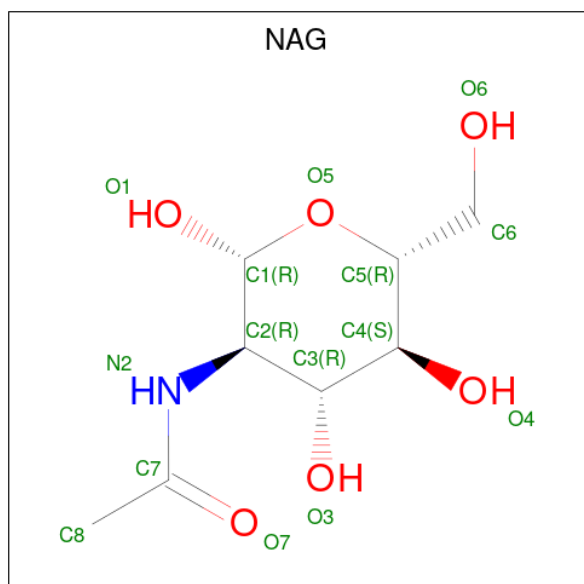
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



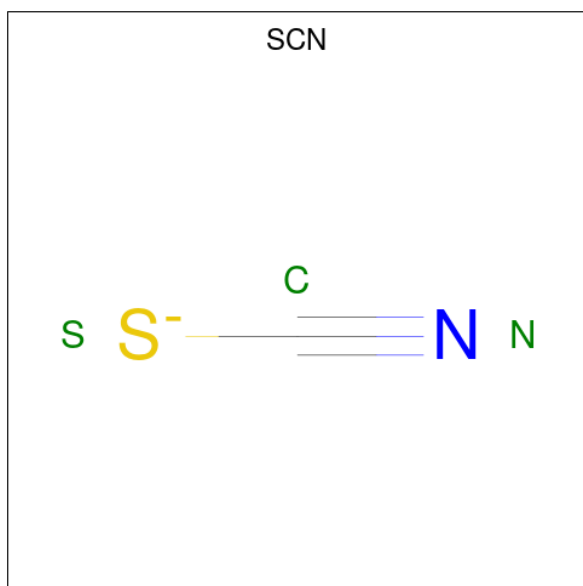
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	S	0	0
			3	1	1	1		
7	D	1	Total	C	N	S	0	0
			3	1	1	1		
7	D	1	Total	C	N	S	0	0
			3	1	1	1		
7	D	1	Total	C	N	S	0	0
			3	1	1	1		
7	E	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	D	4	Total	Cl	0	0
			4	4		
8	E	3	Total	Cl	0	0
			3	3		

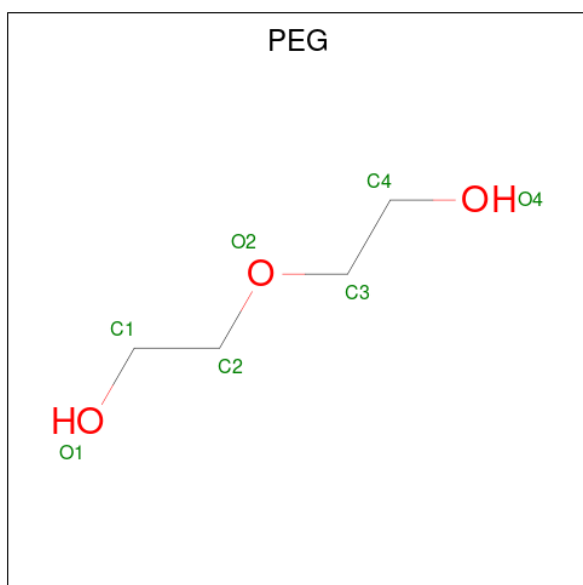
- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	Na	0	0
			2	2		
9	D	2	Total	Na	0	0
			2	2		
9	E	7	Total	Na	0	0
			7	7		

- Molecule 10 is POTASSIUM ION (CCD ID: K) (formula: K).

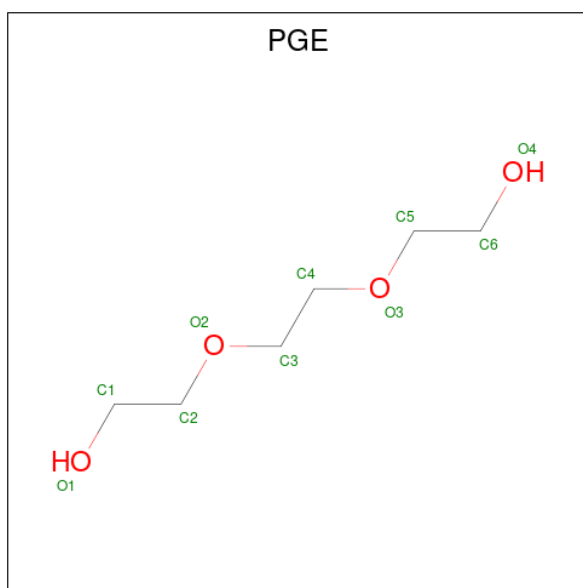
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	K	0	0
			1	1		
10	D	1	Total	K	0	0
			1	1		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



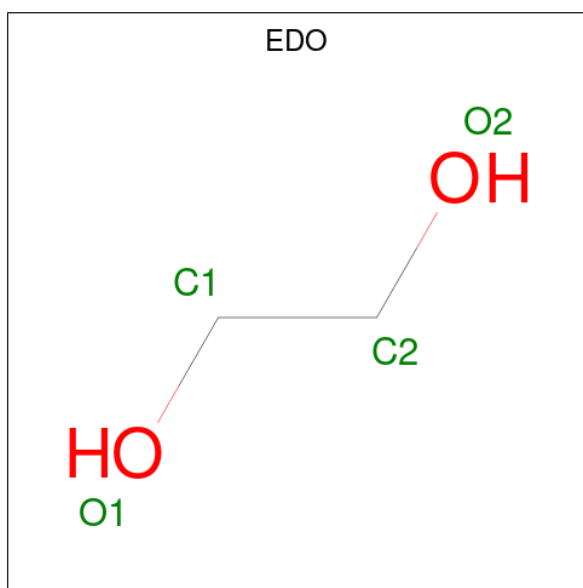
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	C	O	0	0
			7	4	3		
11	D	1	Total	C	O	0	0
			7	4	3		
11	E	1	Total	C	O	0	0
			7	4	3		
11	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	C	O	0	0
			4	2	2		
13	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	93	Total	O	0	0
			93	93		
14	D	81	Total	O	0	0
			81	81		
14	E	77	Total	O	0	1
			78	78		

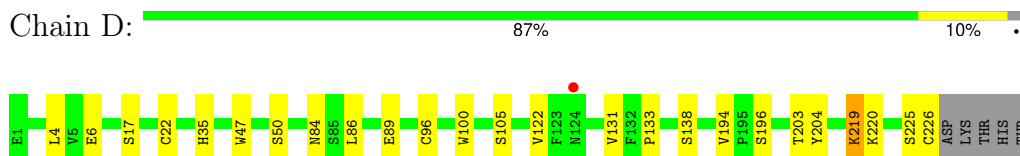
### 3 Residue-property plots [i](#)

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.

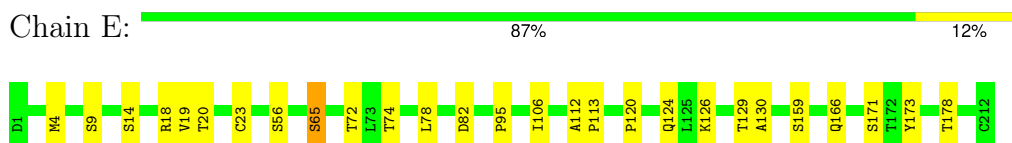
- Molecule 1: Epidermal growth factor receptor



- Molecule 2: heavy chain



- Molecule 3: light chain



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  50% 50%


MAG1  
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%


MAG1  
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

MAG1  
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  86% 14%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.06Å 72.12Å 126.21Å 90.00° 101.65° 90.00°	Depositor
Resolution (Å)	43.11 – 2.40 43.11 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (43.11-2.40) 95.0 (43.11-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.195 , 0.243 0.195 , 0.243	Depositor DCC
$R_{free}$ test set	3286 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: MAN, CL, EDO, PGE, PEG, BMA, NAG, K, NA, SCN

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	0.35	0/4664	0.58	0/6323
2	D	0.46	0/1779	0.64	0/2429
3	E	0.43	0/1678	0.63	0/2280
All	All	0.39	0/8121	0.60	0/11032

There are no bond length outliers.

There are no bond angle outliers.

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	4576	0	4315	77	0
2	D	1730	0	1655	17	0
3	E	1642	0	1587	22	0
4	B	28	0	25	0	0
4	F	28	0	25	2	0
4	G	28	0	25	1	0
5	C	83	0	70	1	0
6	A	28	0	26	1	0
7	A	3	0	0	0	0
7	D	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	3	0	0	0	0
8	A	1	0	0	0	0
8	D	4	0	0	0	0
8	E	3	0	0	0	0
9	A	2	0	0	0	0
9	D	2	0	0	0	0
9	E	7	0	0	0	0
10	A	1	0	0	0	0
10	D	1	0	0	0	0
11	D	14	0	20	1	0
11	E	14	0	20	4	0
12	D	10	0	14	4	0
13	E	12	0	18	4	0
14	A	93	0	0	3	0
14	D	81	0	0	0	0
14	E	78	0	0	2	0
All	All	8481	0	7800	117	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 7.

The worst 5 of 117 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:327:ILE:HD11	1:A:345:LEU:HD22	1.52	0.90
1:A:390:ARG:HD3	1:A:394:HIS:CE1	2.11	0.85
1:A:384:GLN:HG2	1:A:417:VAL:HG23	1.59	0.84
1:A:509:ARG:HH11	1:A:509:ARG:HG2	1.42	0.82
1:A:387:PRO:HB2	1:A:390:ARG:HG3	1.68	0.74

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	598/625 (96%)	561 (94%)	37 (6%)	0	100	100
2	D	228/231 (99%)	222 (97%)	6 (3%)	0	100	100
3	E	211/212 (100%)	204 (97%)	7 (3%)	0	100	100
All	All	1037/1068 (97%)	987 (95%)	50 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	507/546 (93%)	495 (98%)	12 (2%)	43	65
2	D	190/192 (99%)	184 (97%)	6 (3%)	34	56
3	E	188/187 (100%)	185 (98%)	3 (2%)	55	76
All	All	885/925 (96%)	864 (98%)	21 (2%)	45	65

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	86	LEU
2	D	219	LYS
3	E	65	SER
3	E	9	SER
2	D	196	SER

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

Mol	Chain	Res	Type
3	E	37	GLN
3	E	79	GLN
2	D	3	GLN

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Mol	Chain	Res	Type
2	D	13	GLN
2	D	39	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 ⓘ

13 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	$\# Z  > 2$
4	NAG	B	1	4,1	14,14,15	0.50	0	17,19,21	0.80	0
4	NAG	B	2	4	14,14,15	0.39	0	17,19,21	0.84	1 (5%)
5	NAG	C	1	5,1	14,14,15	0.59	1 (7%)	17,19,21	0.53	0
5	NAG	C	2	5	14,14,15	0.93	1 (7%)	17,19,21	0.60	0
5	BMA	C	3	5	11,11,12	0.93	1 (9%)	15,15,17	1.09	1 (6%)
5	MAN	C	4	5	11,11,12	1.14	0	15,15,17	1.19	2 (13%)
5	MAN	C	5	5	11,11,12	1.52	4 (36%)	15,15,17	1.31	2 (13%)
5	MAN	C	6	5	11,11,12	0.83	0	15,15,17	1.27	1 (6%)
5	MAN	C	7	5	11,11,12	1.74	3 (27%)	15,15,17	1.12	1 (6%)
4	NAG	F	1	4,1	14,14,15	1.35	1 (7%)	17,19,21	0.73	0
4	NAG	F	2	4	14,14,15	1.02	2 (14%)	17,19,21	1.08	1 (5%)
4	NAG	G	1	4,1	14,14,15	0.36	0	17,19,21	0.73	1 (5%)
4	NAG	G	2	4	14,14,15	0.31	0	17,19,21	0.69	1 (5%)



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	4/6/23/26	0/1/1/1
5	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	0/2/19/22	0/1/1/1
5	MAN	C	5	5	-	1/2/19/22	0/1/1/1
5	MAN	C	6	5	-	1/2/19/22	0/1/1/1
5	MAN	C	7	5	-	2/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	-4.74	1.35	1.43
5	C	7	MAN	C2-C3	3.93	1.58	1.52
5	C	2	NAG	O5-C1	-3.17	1.38	1.43
5	C	7	MAN	O5-C5	2.89	1.49	1.43
4	F	2	NAG	O5-C1	2.79	1.48	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2	NAG	C1-O5-C5	3.94	117.47	112.19
5	C	6	MAN	C1-O5-C5	3.64	117.06	112.19
5	C	3	BMA	C1-O5-C5	3.08	116.31	112.19
5	C	4	MAN	O2-C2-C3	-2.76	104.43	110.15
4	G	2	NAG	C1-O5-C5	2.55	115.60	112.19

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2	NAG	O5-C5-C6-O6

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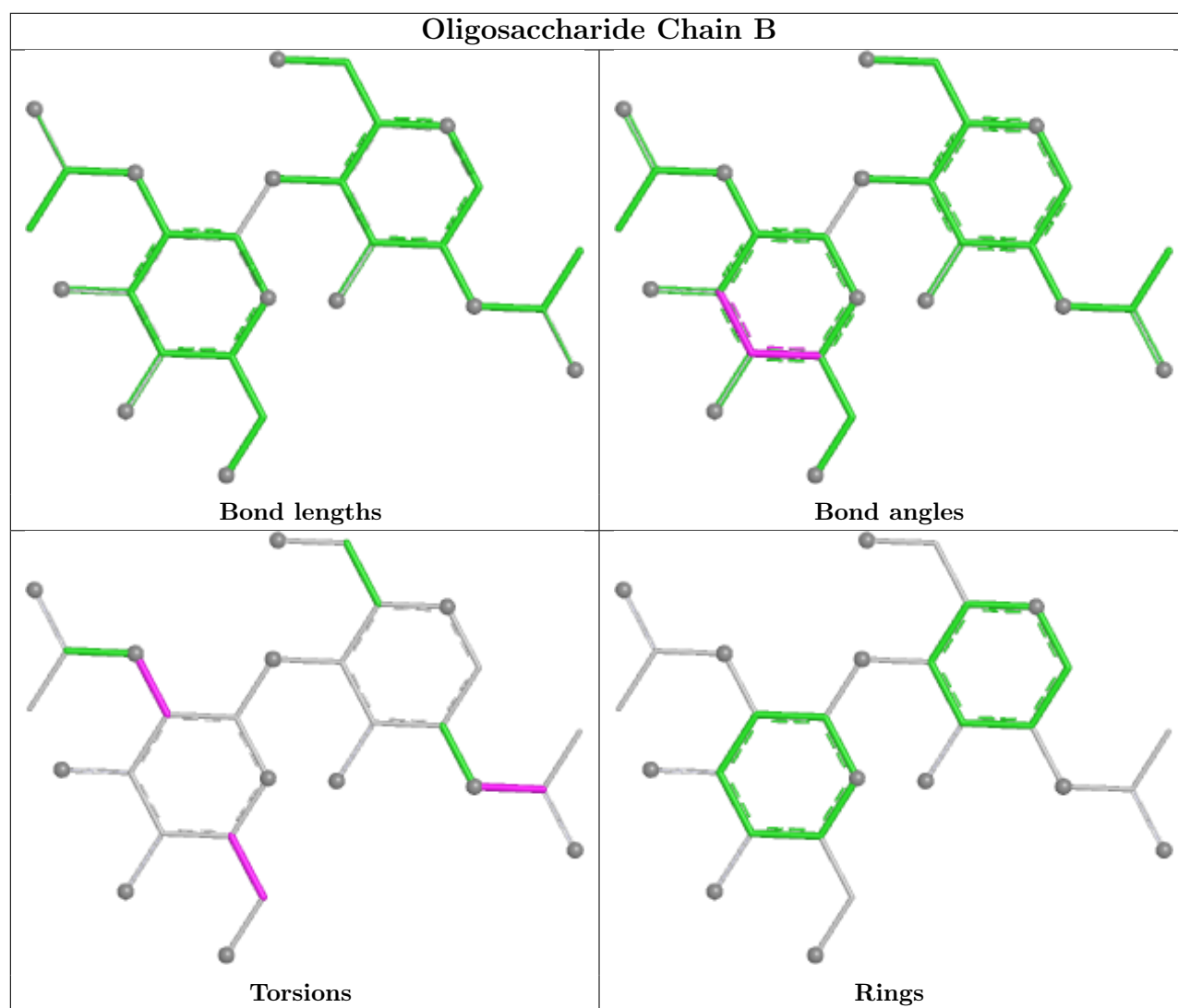
Mol	Chain	Res	Type	Atoms
5	C	7	MAN	O5-C5-C6-O6
5	C	7	MAN	C4-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
4	B	1	NAG	C8-C7-N2-C2

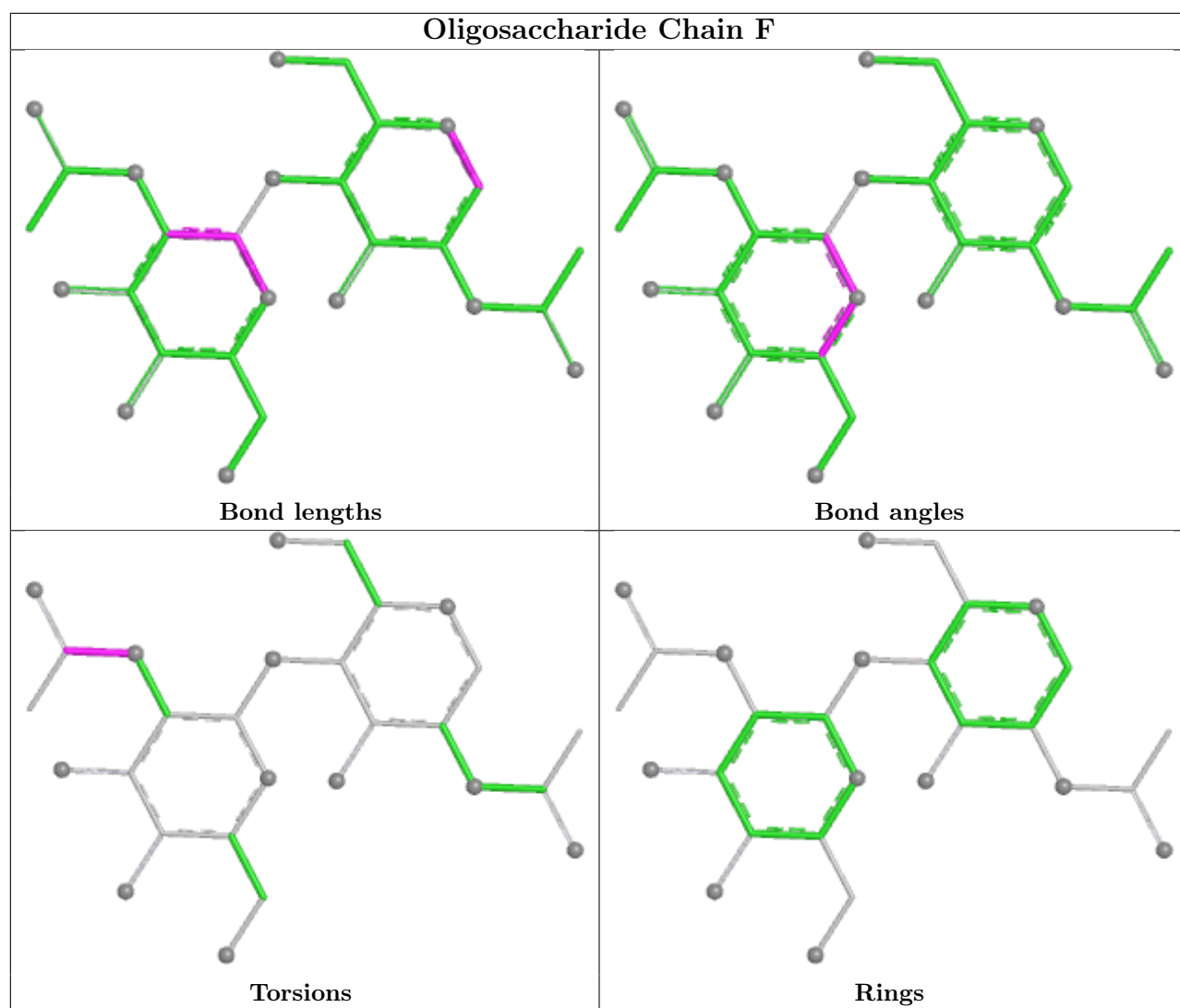
There are no ring outliers.

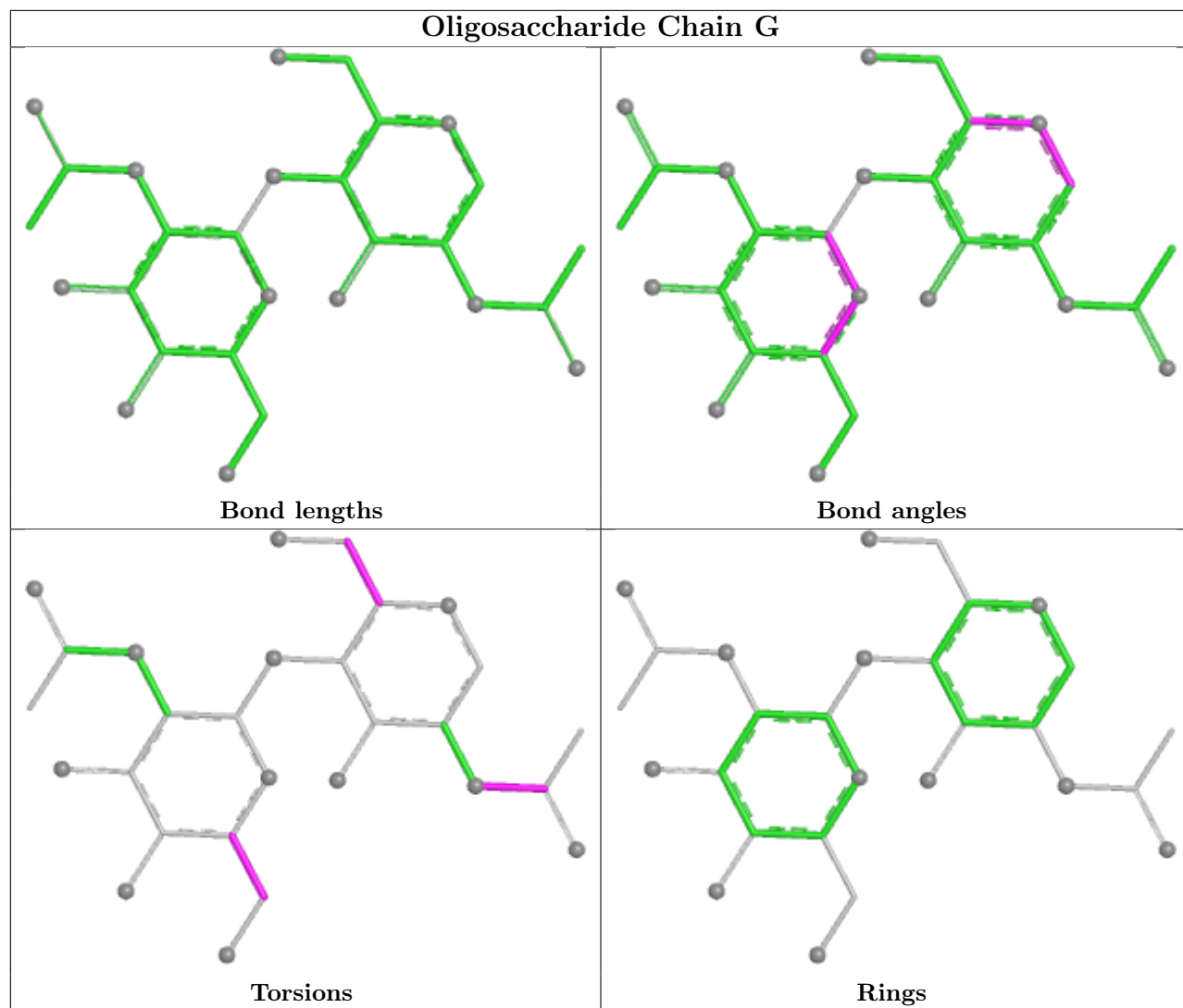
4 monomers are involved in 4 short contacts:

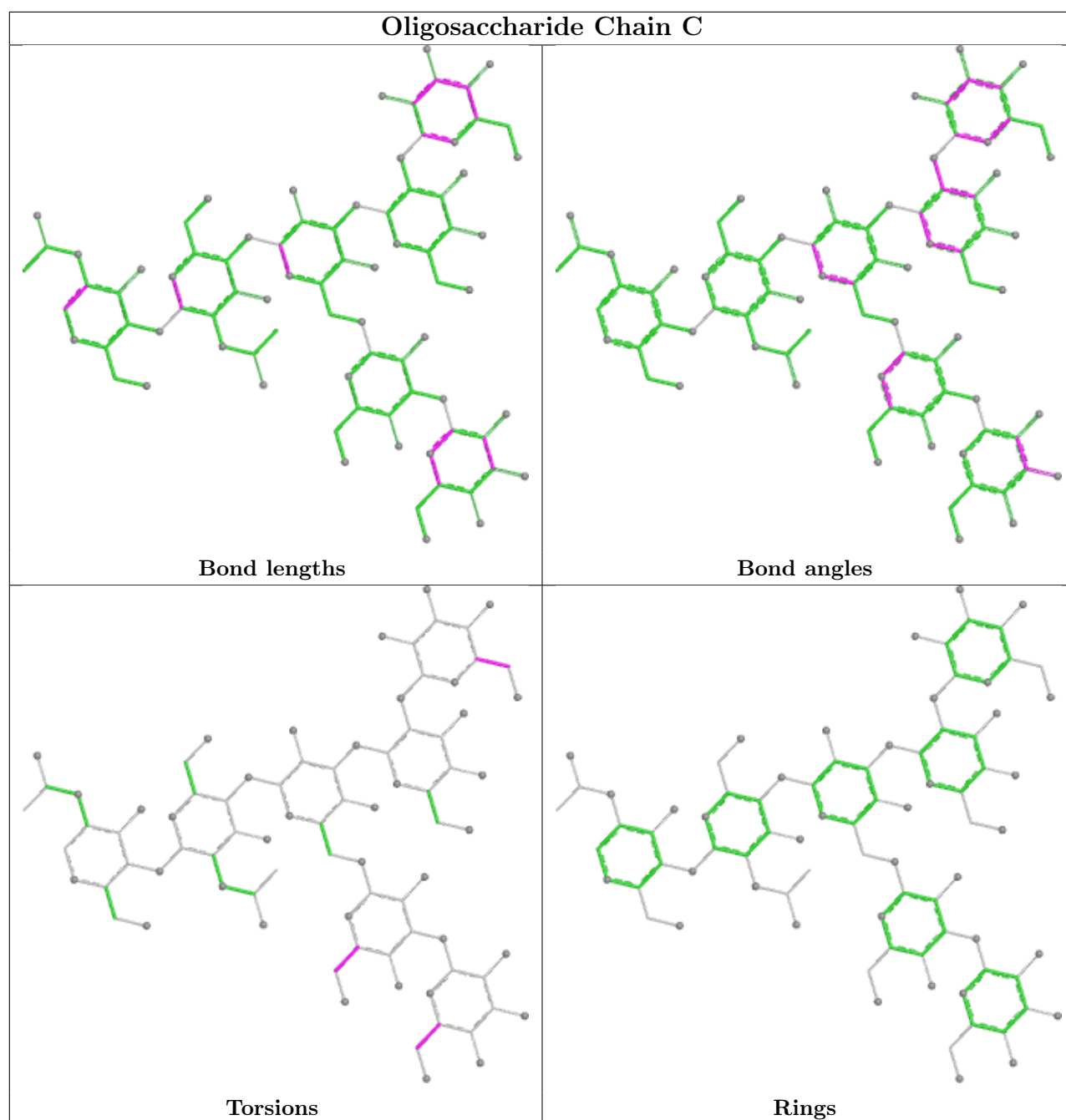
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	2	0
4	F	2	NAG	2	0
4	G	1	NAG	1	0
5	C	1	NAG	1	0

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 36 ligands modelled in this entry, 21 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
11	PEG	D	305	-	6,6,6	0.27	0	5,5,5	0.04	0
6	NAG	A	701	1	14,14,15	0.65	0	17,19,21	0.61	0
7	SCN	D	304	-	1,2,2	0.63	0	0,1,1	-	-
7	SCN	D	302	-	1,2,2	1.10	0	0,1,1	-	-
13	EDO	E	305	-	3,3,3	0.69	0	2,2,2	0.24	0
6	NAG	A	702	1	14,14,15	0.42	0	17,19,21	0.49	0
11	PEG	E	303	-	6,6,6	0.40	0	5,5,5	0.31	0
11	PEG	E	302	-	6,6,6	0.34	0	5,5,5	0.14	0
11	PEG	D	301	-	6,6,6	0.28	0	5,5,5	0.13	0
13	EDO	E	301	9	3,3,3	0.42	0	2,2,2	0.24	0
13	EDO	E	306	-	3,3,3	0.67	0	2,2,2	0.33	0
7	SCN	E	304	-	1,2,2	0.90	0	0,1,1	-	-
7	SCN	D	306	-	1,2,2	0.49	0	0,1,1	-	-
7	SCN	A	703	-	1,2,2	0.87	0	0,1,1	-	-
12	PGE	D	303	-	9,9,9	0.55	0	8,8,8	0.54	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
6	NAG	A	701	1	-	1/6/23/26	0/1/1/1
13	EDO	E	305	-	-	1/1/1/1	-
6	NAG	A	702	1	-	4/6/23/26	0/1/1/1
11	PEG	E	303	-	-	2/4/4/4	-
11	PEG	E	302	-	-	2/4/4/4	-
11	PEG	D	301	-	-	2/4/4/4	-
13	EDO	E	301	9	-	0/1/1/1	-
13	EDO	E	306	-	-	1/1/1/1	-
11	PEG	D	305	-	-	2/4/4/4	-
12	PGE	D	303	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	303	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
6	A	702	NAG	C8-C7-N2-C2
6	A	702	NAG	O7-C7-N2-C2
11	D	301	PEG	O1-C1-C2-O2
11	E	302	PEG	O2-C3-C4-O4

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	305	EDO	3	0
6	A	702	NAG	1	0
11	E	303	PEG	3	0
11	E	302	PEG	1	0
11	D	301	PEG	1	0
13	E	301	EDO	1	0
12	D	303	PGE	4	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, 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	604/625 (96%)	0.38	35 (5%) 29 25	29, 68, 114, 159	2 (0%)
2	D	226/231 (97%)	-0.41	1 (0%) 88 86	18, 37, 62, 114	4 (1%)
3	E	212/212 (100%)	-0.34	0 100 100	26, 44, 61, 115	1 (0%)
All	All	1042/1068 (97%)	0.06	36 (3%) 47 43	18, 53, 108, 159	7 (0%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	MET	5.0
1	A	308	PRO	4.9
1	A	578	GLU	4.6
1	A	310	ARG	4.4
1	A	543	MET	4.2

### 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.

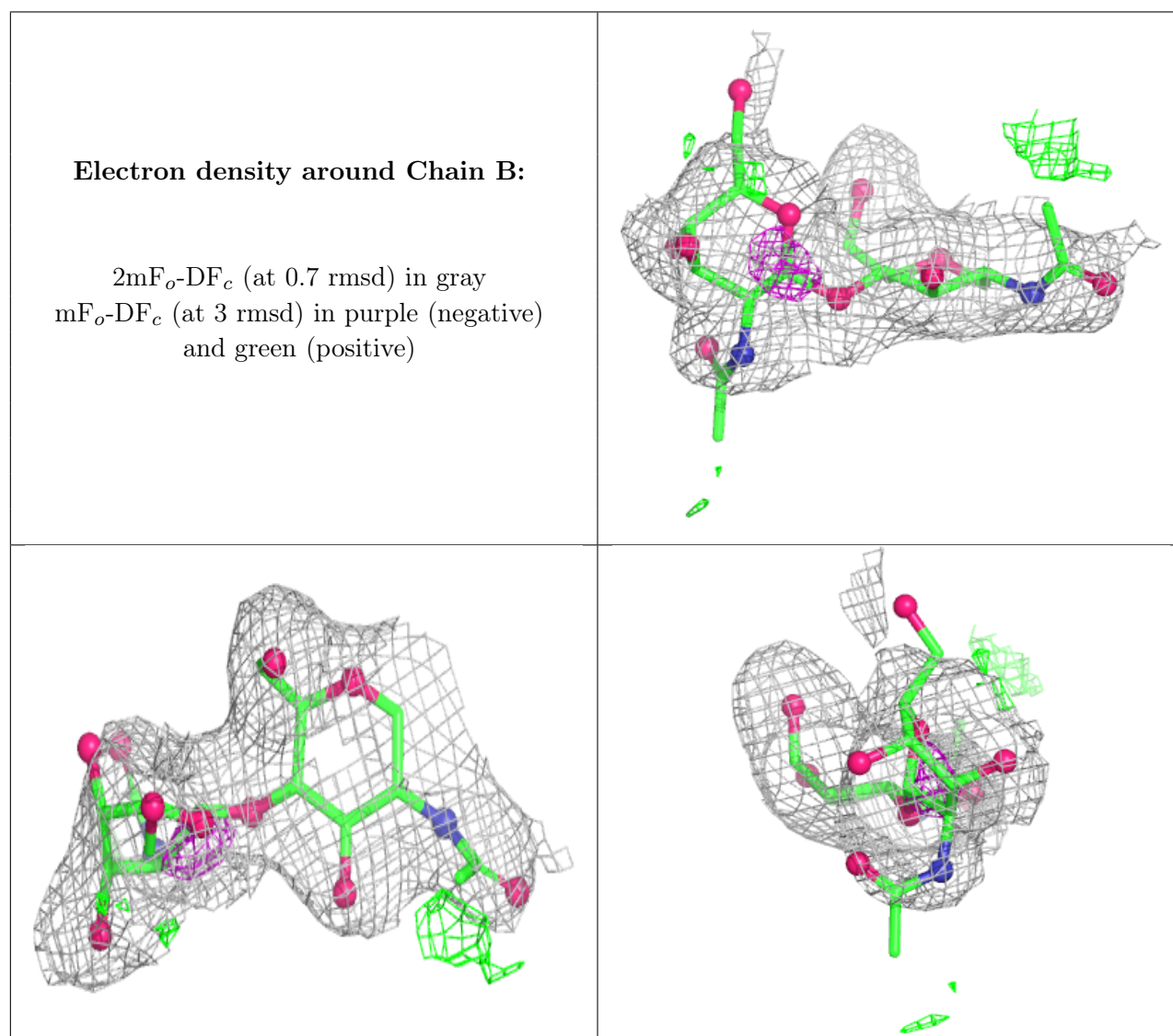
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	B	1	14/15	-	-	65,72,83,88	0
4	NAG	B	2	14/15	-	-	88,94,97,102	0
4	NAG	F	2	14/15	0.33	0.19	88,97,104,105	0

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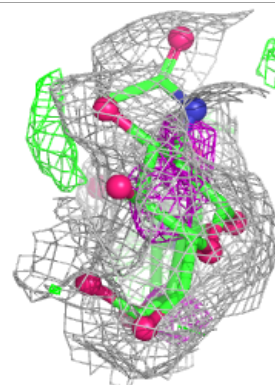
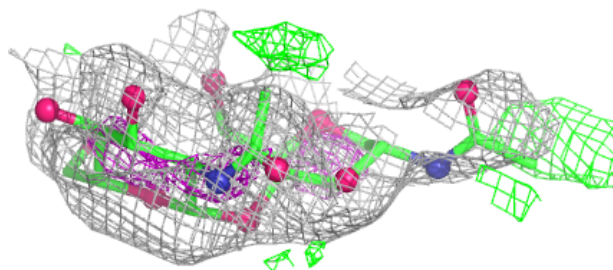
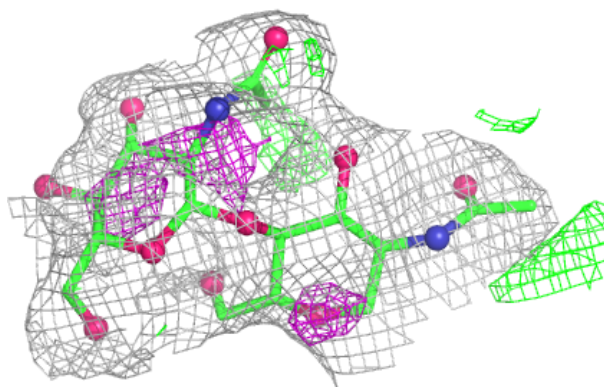
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	F	1	14/15	0.58	0.18	91,101,105,105	0
4	NAG	G	1	14/15	0.65	0.15	84,90,97,100	0
4	NAG	G	2	14/15	0.72	0.14	74,99,109,114	0
5	NAG	C	1	14/15	-	-	32,41,46,48	0
5	NAG	C	2	14/15	-	-	41,44,54,58	0
5	BMA	C	3	11/12	-	-	44,52,58,63	0
5	MAN	C	4	11/12	-	-	45,51,54,59	0
5	MAN	C	5	11/12	-	-	62,67,74,77	0
5	MAN	C	6	11/12	-	-	70,73,78,83	0
5	MAN	C	7	11/12	-	-	74,80,86,87	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.

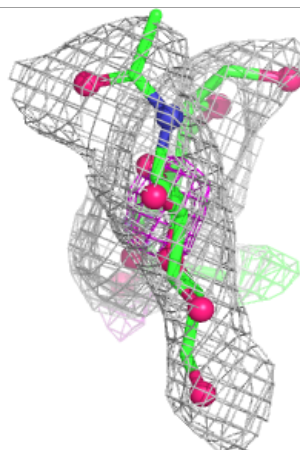
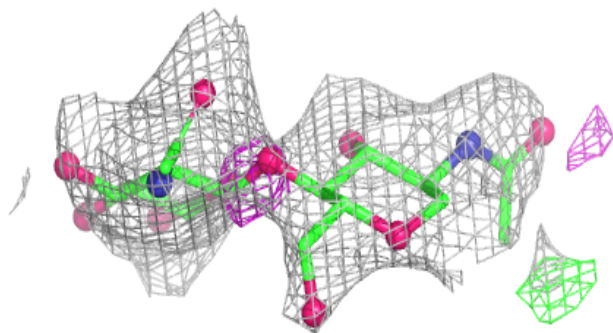
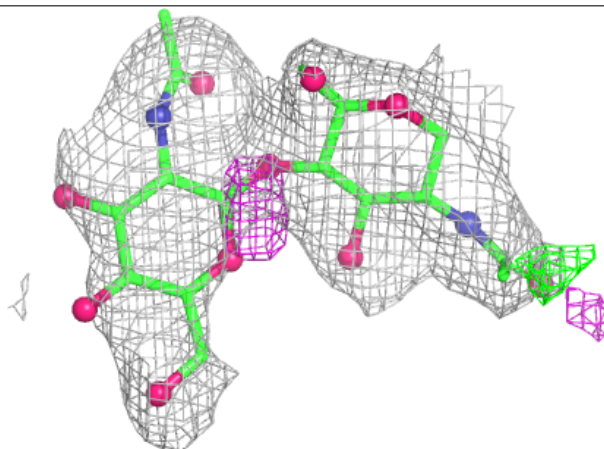


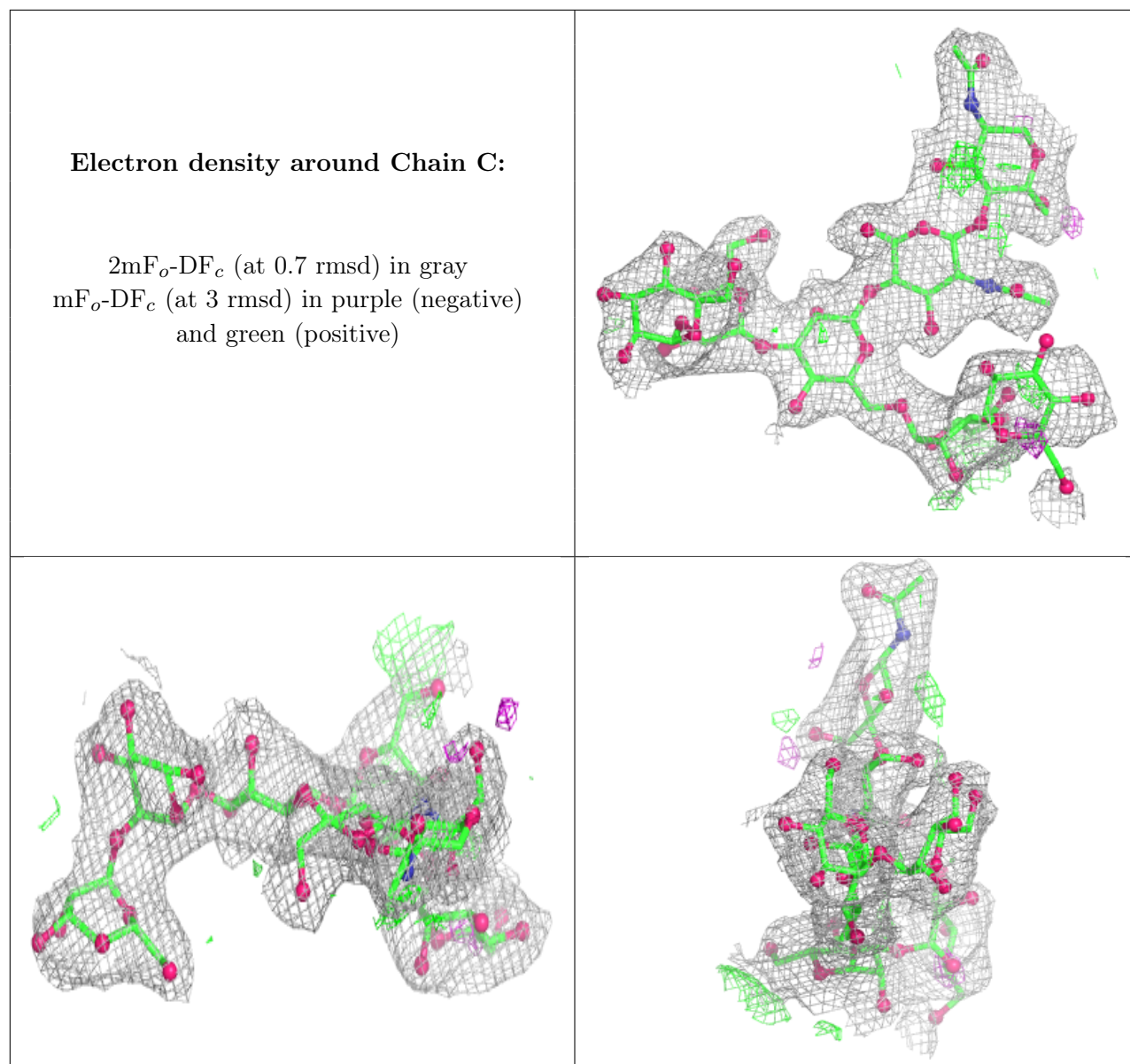
**Electron density around Chain F:**

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

**Electron density around Chain G:**

$2mF_o-DF_c$  (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, 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
6	NAG	A	701	14/15	0.44	0.17	82,91,94,94	0
6	NAG	A	702	14/15	0.51	0.19	79,84,87,90	0
11	PEG	D	305	7/7	0.78	0.19	58,64,71,72	0
11	PEG	E	303	7/7	0.81	0.25	48,52,66,70	0
12	PGE	D	303	10/10	0.81	0.18	37,42,50,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NA	E	315	1/1	0.82	0.22	54,54,54,54	0
9	NA	E	311	1/1	0.84	0.25	66,66,66,66	0
10	K	A	707	1/1	0.84	0.13	86,86,86,86	0
11	PEG	D	301	7/7	0.84	0.26	49,51,57,70	0
8	CL	E	308	1/1	0.85	0.16	73,73,73,73	0
7	SCN	D	306	3/3	0.87	0.21	48,48,49,77	0
7	SCN	A	703	3/3	0.88	0.16	33,33,39,65	0
7	SCN	D	302	3/3	0.90	0.17	47,47,55,78	0
9	NA	E	314	1/1	0.90	0.16	63,63,63,63	0
7	SCN	D	304	3/3	0.90	0.16	53,53,57,94	0
8	CL	E	309	1/1	0.90	0.16	80,80,80,80	0
13	EDO	E	306	4/4	0.90	0.20	44,52,53,58	0
11	PEG	E	302	7/7	0.91	0.25	54,56,59,61	0
9	NA	E	310	1/1	0.91	0.09	50,50,50,50	0
9	NA	A	705	1/1	0.93	0.15	51,51,51,51	0
8	CL	A	704	1/1	0.93	0.15	63,63,63,63	0
13	EDO	E	301	4/4	0.94	0.14	36,38,47,50	0
13	EDO	E	305	4/4	0.94	0.13	48,52,57,58	0
9	NA	D	311	1/1	0.94	0.10	50,50,50,50	0
8	CL	D	307	1/1	0.95	0.14	60,60,60,60	0
8	CL	D	309	1/1	0.95	0.21	54,54,54,54	0
9	NA	E	316	1/1	0.95	0.13	46,46,46,46	0
8	CL	E	307	1/1	0.95	0.07	65,65,65,65	0
9	NA	D	312	1/1	0.96	0.19	54,54,54,54	0
9	NA	A	706	1/1	0.96	0.10	61,61,61,61	0
7	SCN	E	304	3/3	0.96	0.15	49,49,54,57	0
9	NA	E	312	1/1	0.96	0.06	48,48,48,48	0
10	K	D	313	1/1	0.97	0.07	69,69,69,69	0
8	CL	D	308	1/1	0.97	0.07	77,77,77,77	0
9	NA	E	313	1/1	0.97	0.14	38,38,38,38	0
8	CL	D	310	1/1	0.98	0.05	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.