



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 08:22 AM BST

PDB ID : 1YY9  
Title : Structure of the extracellular domain of the epidermal growth factor receptor in complex with the Fab fragment of cetuximab/Erbitux/IMC-C225  
Authors : Li, S.; Schmitz, K.R.; Jeffrey, P.D.; Wiltzius, J.J.W.; Kussie, P.; Ferguson, K.M.  
Deposited on : 2005-02-24  
Resolution : 2.60 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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

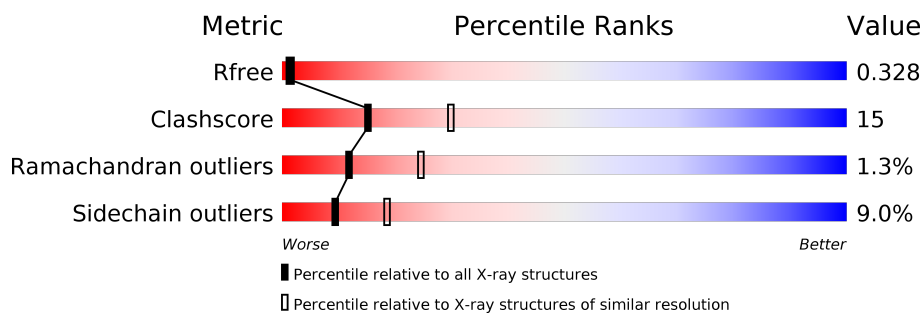
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	624	68% 27% . .
2	C	213	62% 31% 5% .
3	D	221	68% 26% 5%
4	B	9	67% 33%
5	E	2	100%
5	F	2	100%
5	G	2	100%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	G	1	X	-	-	-
5	NAG	G	2	X	-	-	-
6	NAG	A	5041	X	-	-	-
6	NAG	A	625	X	-	-	-
6	NAG	D	881	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8225 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	613	Total	C	N	O	S	0	0	0
			4653	2879	828	886	60			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	LYS	SER	conflict	UNP P00533
A	610	ARG	GLU	conflict	UNP P00533
A	619	HIS	-	expression tag	UNP P00533
A	620	HIS	-	expression tag	UNP P00533
A	621	HIS	-	expression tag	UNP P00533
A	622	HIS	-	expression tag	UNP P00533
A	623	HIS	-	expression tag	UNP P00533
A	624	HIS	-	expression tag	UNP P00533

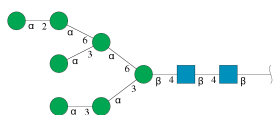
- Molecule 2 is a protein called Cetuximab Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	211	Total	C	N	O	S	0	0	0
			1609	1003	270	332	4			

- Molecule 3 is a protein called Cetuximab Fab Heavy chain.

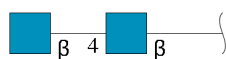
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	220	Total	C	N	O	S	0	0	0
			1648	1046	271	326	5			

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



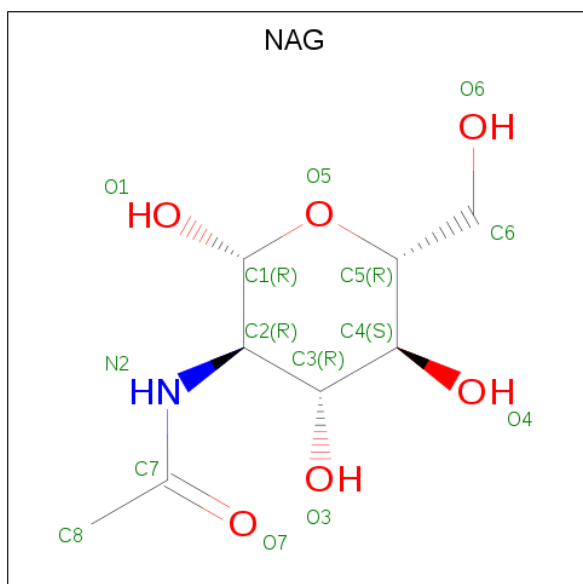
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 5 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
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	35	Total	O	0	0
			35	35		
7	C	6	Total	O	0	0
			6	6		
7	D	15	Total	O	0	0
			15	15		

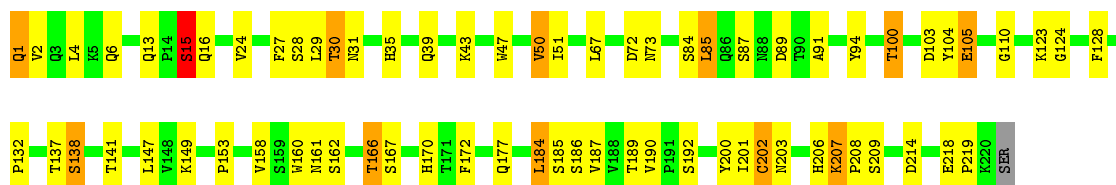


- Molecule 1: Epidermal Growth Factor Receptor

H597	P488	T327	P241	M134	LEU
P598	E489	K336	P241	E2	
P607	G490	K336	L243	I138	C7
G608	C491	N337	L243	S146	
L609	H492	C338	L244	L149	T10
R610	E495	T339	L245		
G611			Y246		
T614	D498	D844			L17
GLY	D498	L345			G18
ASN	H346	H346			T19
LVS	V505				F20
PRO	S506	V350			E21
HVS	R507				D22
HIS	G508	K372			H23
HIS	R509				
HIS		E376			F31
HIS	V512	T377			N32
HIS	D513	T378			
HIS	C514	G379			E35
HIS	C515				V36
HIS	K516	R390			V37
	L517	T391			
	L518				E42
					I43
	E521	E397			T44
	P522	R403			Y45
					V46
	V526	K407			
					Q59
	E530	S418			
	H535	S423			V72
	P536				E73
	E537	S433			R74
	C538	D434			
	L539				L80
					Q81
	T546	G441			
	C547				R84
	E547	I451			
	D553	K454			Y89
					E90
	I556	G458			N91
	A559	T459			
		S460			L98
	I562	G461			S99
		G462			K105
	V568	K463			T106
	G569	T464			
	T570	K465			M113
					R114
	V575	K474			N115
					L116
	N580	T478			Q117
	Y586	H483			R125
		A484			F126
		L485			S127
	C593	G486			N128
		S487			E522

G200	A111	D1
L201		I2
S202	S114	L3
	V115	
F209	F116	Q6
M210	I117	
R211		L11
GLY	D122	
ALA	E123	G16
	Q124	
	L125	V19
		S20
	T129	F21
	A130	S22
	S131	
	V132	I29
	F133	G30
	C134	T31
	L135	M32
	L136	
	M137	R39
	N138	T40
	F139	
	Y140	L47
	P141	I48
		K49
	K149	Y50
	V150	I55
	D151	
	M152	I58
	Q155	R61
	M158	S67
	D167	T72
	S168	
	K169	N76
	D170	S77
	S171	V78
		E79
	S174	S80
	L175	E81
	S176	D82
	L179	Y87
	S182	Q90
		N91
	Y186	N92
	E187	
	Y192	T96
	A193	T97
	C194	
	E195	L104
	V196	E105
	T197	L106
	H198	K107
	D199	

Chain D:  68% 26% 5%



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

Chain B: 67% 33%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.82Å 70.86Å 147.12Å 90.00° 102.48° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 30.06 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.00-2.60) 98.3 (30.06-2.61)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.239 , 0.289 0.291 , 0.328	Depositor DCC
$R_{free}$ test set	2352 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: BMA, NAG, MAN

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	0.66	0/4745	0.76	0/6426
2	C	0.65	0/1643	0.79	0/2237
3	D	0.68	0/1692	0.76	0/2316
All	All	0.66	0/8080	0.77	0/10979

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	4653	0	4451	120	0
2	C	1609	0	1535	58	0
3	D	1648	0	1584	65	0
4	B	105	0	88	5	0
5	E	28	0	25	0	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0
6	A	56	0	52	1	0
6	D	14	0	13	0	0
7	A	35	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	6	0	0	0	0
7	D	15	0	0	0	0
All	All	8225	0	7798	239	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 239 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)
4:B:6:MAN:C6	4:B:6:MAN:O6	1.92	1.18
1:A:10:THR:HG22	1:A:42:GLU:OE1	1.56	1.05
1:A:157:GLN:HB3	1:A:159:HIS:NE2	1.80	0.96
2:C:136:LEU:HD21	2:C:196:VAL:HG21	1.48	0.95
1:A:44:THR:HG23	1:A:45:TYR:CD1	2.08	0.87

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	611/624 (98%)	543 (89%)	60 (10%)	8 (1%)	12	24
2	C	209/213 (98%)	189 (90%)	17 (8%)	3 (1%)	11	22
3	D	218/221 (99%)	200 (92%)	16 (7%)	2 (1%)	17	35
All	All	1038/1058 (98%)	932 (90%)	93 (9%)	13 (1%)	12	24

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	GLY

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Mol	Chain	Res	Type
2	C	187	GLU
3	D	138	SER
1	A	507	ARG
2	C	77	SER

### 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	520/545 (95%)	479 (92%)	41 (8%)	12	24
2	C	184/188 (98%)	163 (89%)	21 (11%)	5	10
3	D	186/191 (97%)	168 (90%)	18 (10%)	8	15
All	All	890/924 (96%)	810 (91%)	80 (9%)	9	18

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	ILE
2	C	29	ILE
3	D	184	LEU
1	A	562	ILE
1	A	610	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	580	ASN
2	C	92	ASN
3	D	203	ASN
2	C	6	GLN
2	C	137	ASN

### 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 ⓘ

15 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	1,4	14,14,15	0.56	0	17,19,21	1.63	4 (23%)
4	NAG	B	2	4	14,14,15	0.65	0	17,19,21	1.51	1 (5%)
4	BMA	B	3	4	11,11,12	0.75	0	15,15,17	1.58	3 (20%)
4	MAN	B	4	4	11,11,12	0.91	0	15,15,17	1.66	5 (33%)
4	MAN	B	5	4	11,11,12	0.97	1 (9%)	15,15,17	2.46	4 (26%)
4	MAN	B	6	4	11,11,12	3.72	2 (18%)	15,15,17	2.13	3 (20%)
4	MAN	B	7	4	11,11,12	0.63	0	15,15,17	1.21	1 (6%)
4	MAN	B	8	4	11,11,12	1.50	2 (18%)	15,15,17	2.39	6 (40%)
4	MAN	B	9	4	11,11,12	1.53	2 (18%)	15,15,17	1.34	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.50	0	17,19,21	1.64	4 (23%)
5	NAG	E	2	5	14,14,15	0.57	0	17,19,21	1.21	1 (5%)
5	NAG	F	1	1,5	14,14,15	0.73	0	17,19,21	1.36	1 (5%)
5	NAG	F	2	5	14,14,15	0.52	0	17,19,21	1.44	1 (5%)
5	NAG	G	1	1,5	14,14,15	0.82	1 (7%)	17,19,21	1.19	2 (11%)
5	NAG	G	2	5	14,14,15	0.49	0	17,19,21	1.44	3 (17%)

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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	BMA	B	3	4	-	2/2/19/22	0/1/1/1
4	MAN	B	4	4	-	2/2/19/22	0/1/1/1
4	MAN	B	5	4	-	2/2/19/22	0/1/1/1
4	MAN	B	6	4	-	2/2/19/22	1/1/1/1
4	MAN	B	7	4	-	0/2/19/22	0/1/1/1
4	MAN	B	8	4	-	1/2/19/22	0/1/1/1
4	MAN	B	9	4	-	0/2/19/22	1/1/1/1
5	NAG	E	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	NAG	G	1	1,5	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	G	2	5	1/1/5/7	4/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	6	MAN	O6-C6	11.80	1.92	1.42
4	B	8	MAN	O5-C1	3.16	1.48	1.43
4	B	6	MAN	C6-C5	2.97	1.61	1.51
4	B	5	MAN	O6-C6	2.80	1.54	1.42
4	B	9	MAN	O5-C5	2.67	1.48	1.43

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	6	MAN	C1-O5-C5	5.94	120.24	112.19
4	B	5	MAN	C1-O5-C5	5.86	120.13	112.19
4	B	8	MAN	O3-C3-C4	5.50	123.08	110.35
4	B	5	MAN	O2-C2-C1	5.07	119.52	109.15
4	B	6	MAN	O6-C6-C5	-4.39	96.23	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	1	NAG	C1
5	G	2	NAG	C1

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
4	B	5	MAN	O5-C5-C6-O6

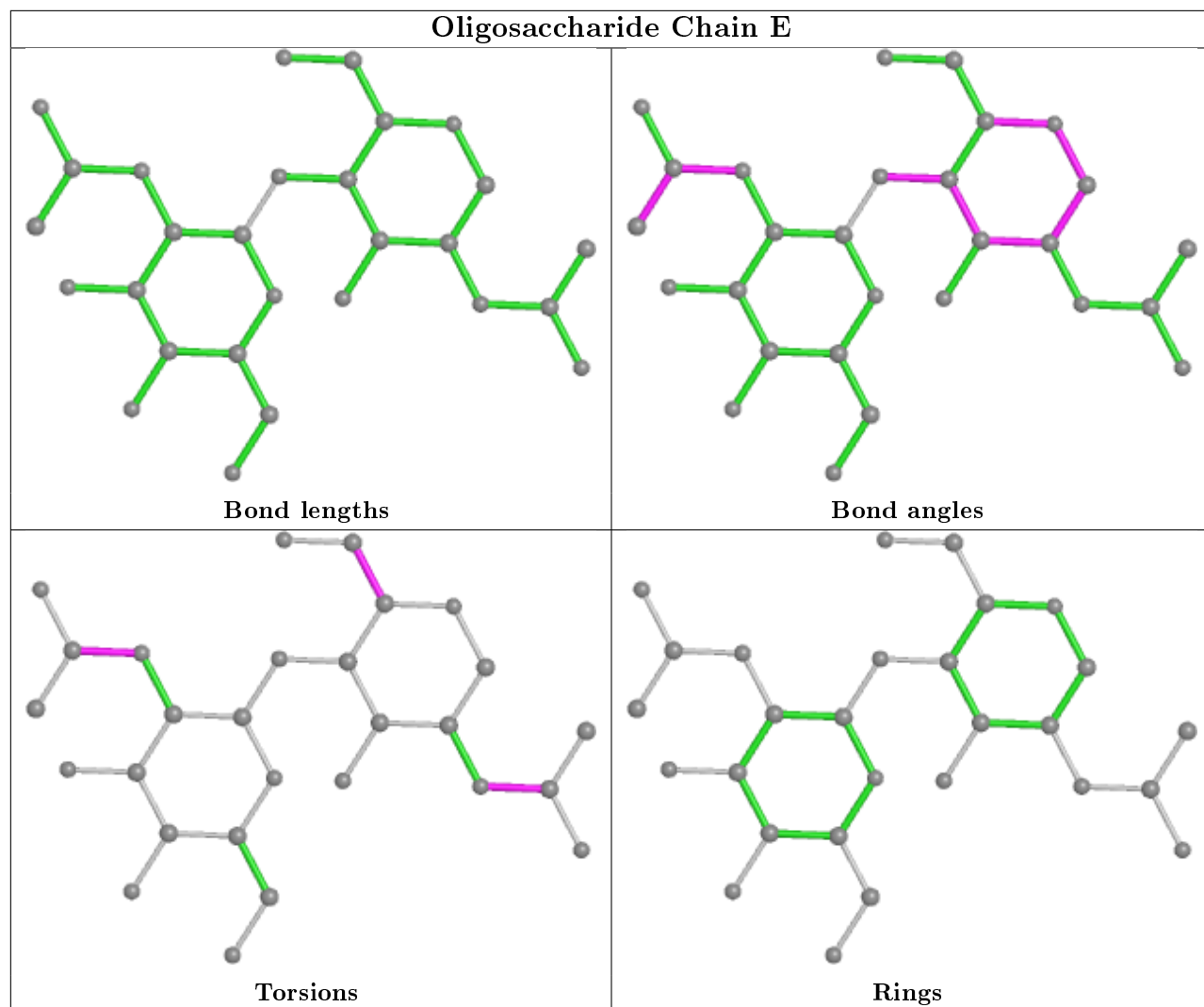
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	9	MAN	C1-C2-C3-C4-C5-O5
4	B	6	MAN	C1-C2-C3-C4-C5-O5

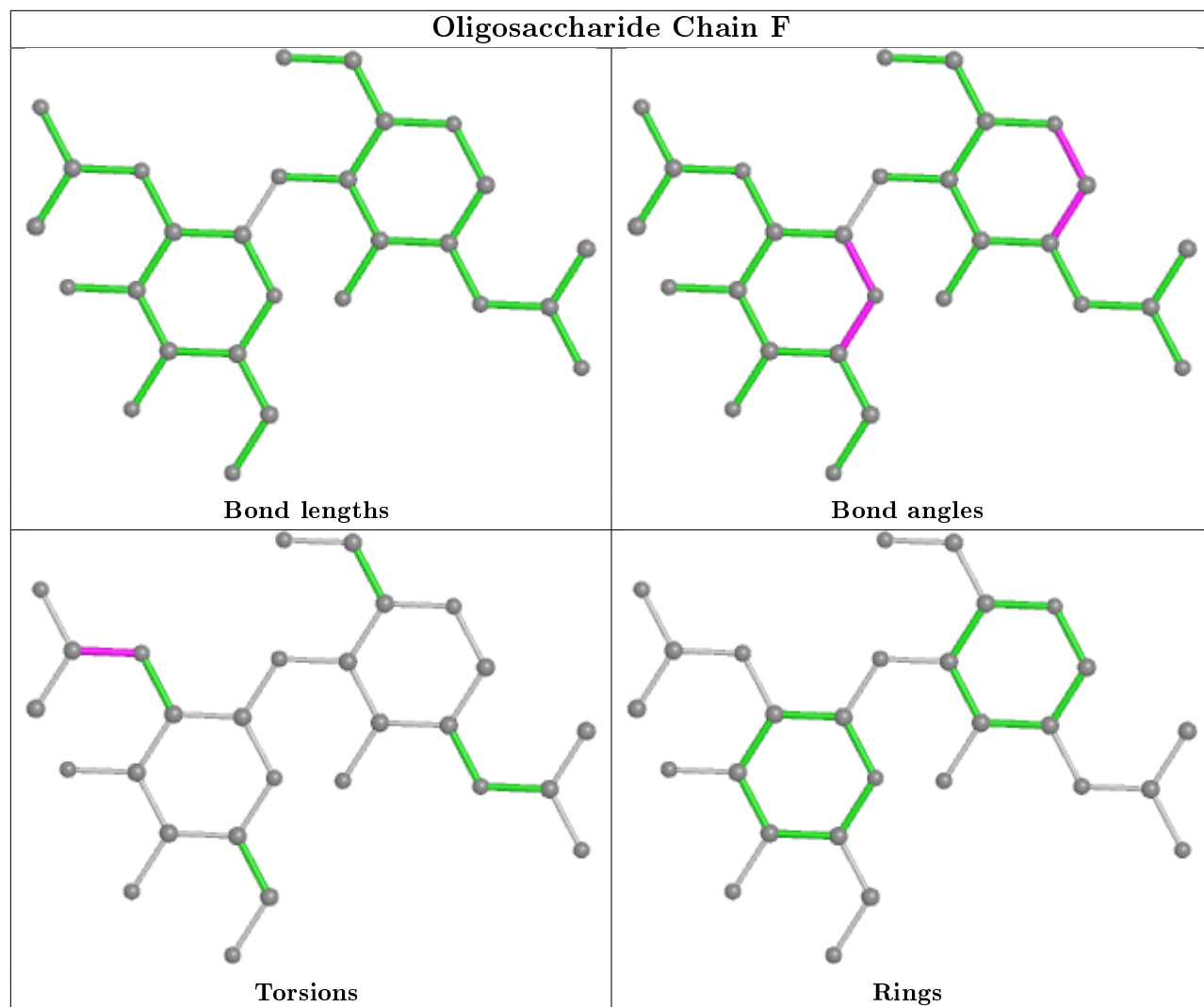
3 monomers are involved in 5 short contacts:

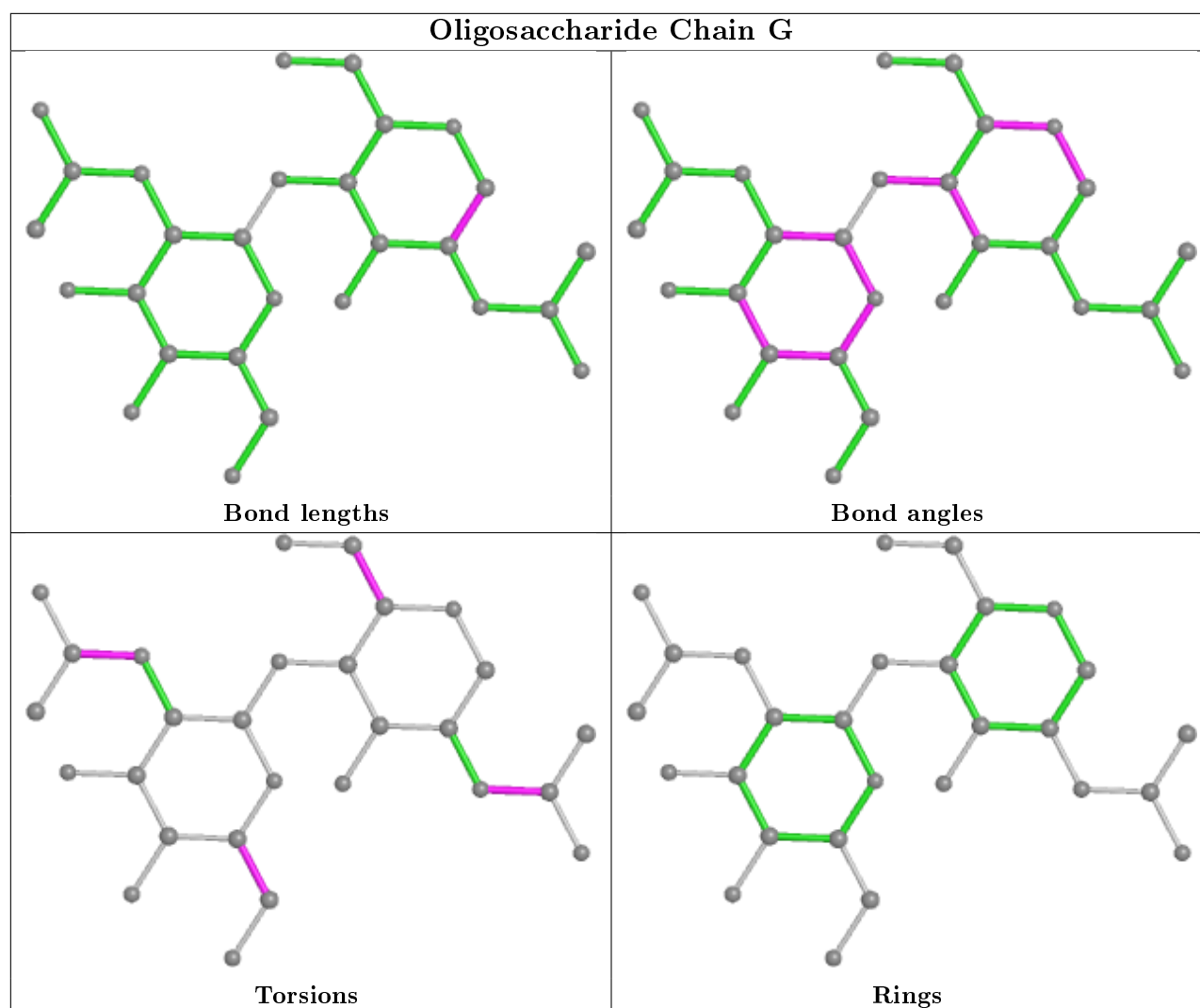
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4	MAN	3	0
4	B	6	MAN	2	0
4	B	5	MAN	3	0

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









## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NAG	D	881	3	14,14,15	0.61	0	17,19,21	1.70	3 (17%)
6	NAG	A	5041	1	14,14,15	0.87	1 (7%)	17,19,21	1.43	2 (11%)
6	NAG	A	625	1	14,14,15	0.98	1 (7%)	17,19,21	1.75	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	3891	1	14,14,15	0.74	0	17,19,21	1.51	4 (23%)
6	NAG	A	5441	1	14,14,15	0.70	0	17,19,21	1.54	3 (17%)

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	D	881	3	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	A	5041	1	1/1/5/7	6/6/23/26	0/1/1/1
6	NAG	A	625	1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	A	3891	1	-	3/6/23/26	0/1/1/1
6	NAG	A	5441	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	625	NAG	C1-C2	2.80	1.56	1.52
6	A	5041	NAG	C1-C2	2.25	1.55	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	881	NAG	C1-O5-C5	4.70	118.56	112.19
6	A	5441	NAG	C1-O5-C5	4.13	117.79	112.19
6	A	3891	NAG	C2-N2-C7	4.10	128.74	122.90
6	A	625	NAG	O5-C1-C2	-3.66	105.51	111.29
6	D	881	NAG	C2-N2-C7	3.43	127.79	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	881	NAG	C1
6	A	5041	NAG	C1
6	A	625	NAG	C1

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	881	NAG	C3-C2-N2-C7
6	D	881	NAG	C8-C7-N2-C2
6	D	881	NAG	O7-C7-N2-C2
6	A	5041	NAG	C8-C7-N2-C2
6	A	5041	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	3891	NAG	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

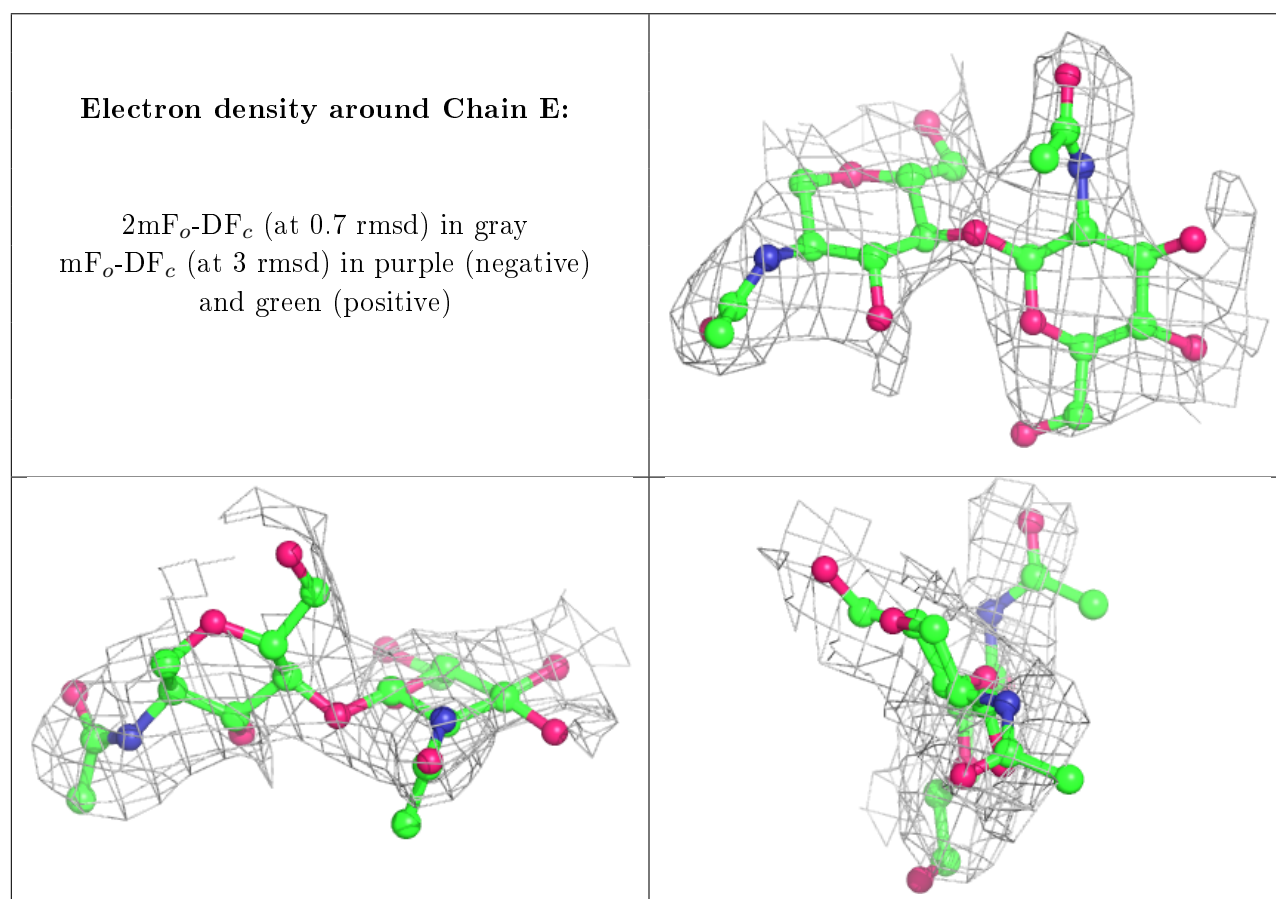
### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

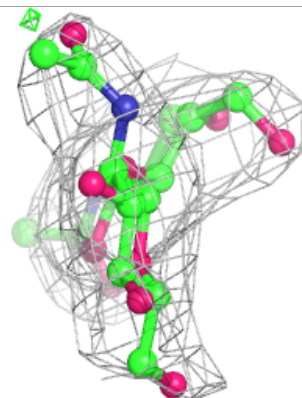
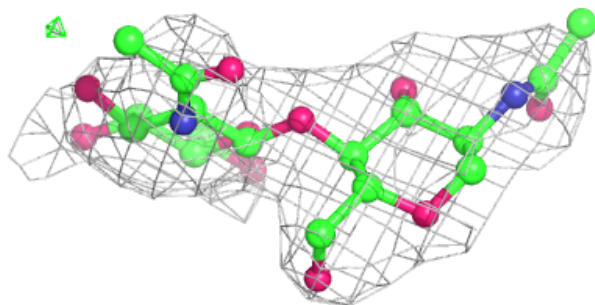
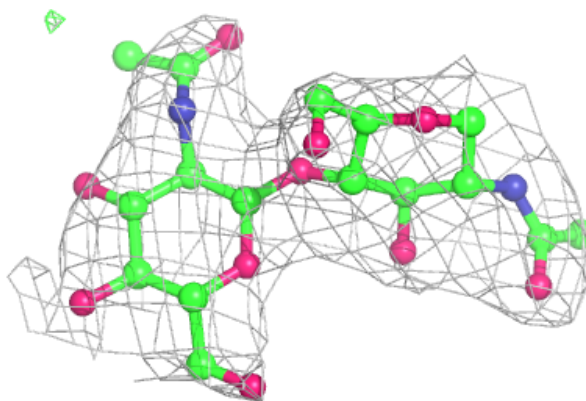
Unable to reproduce the depositors R factor - this section is therefore empty.

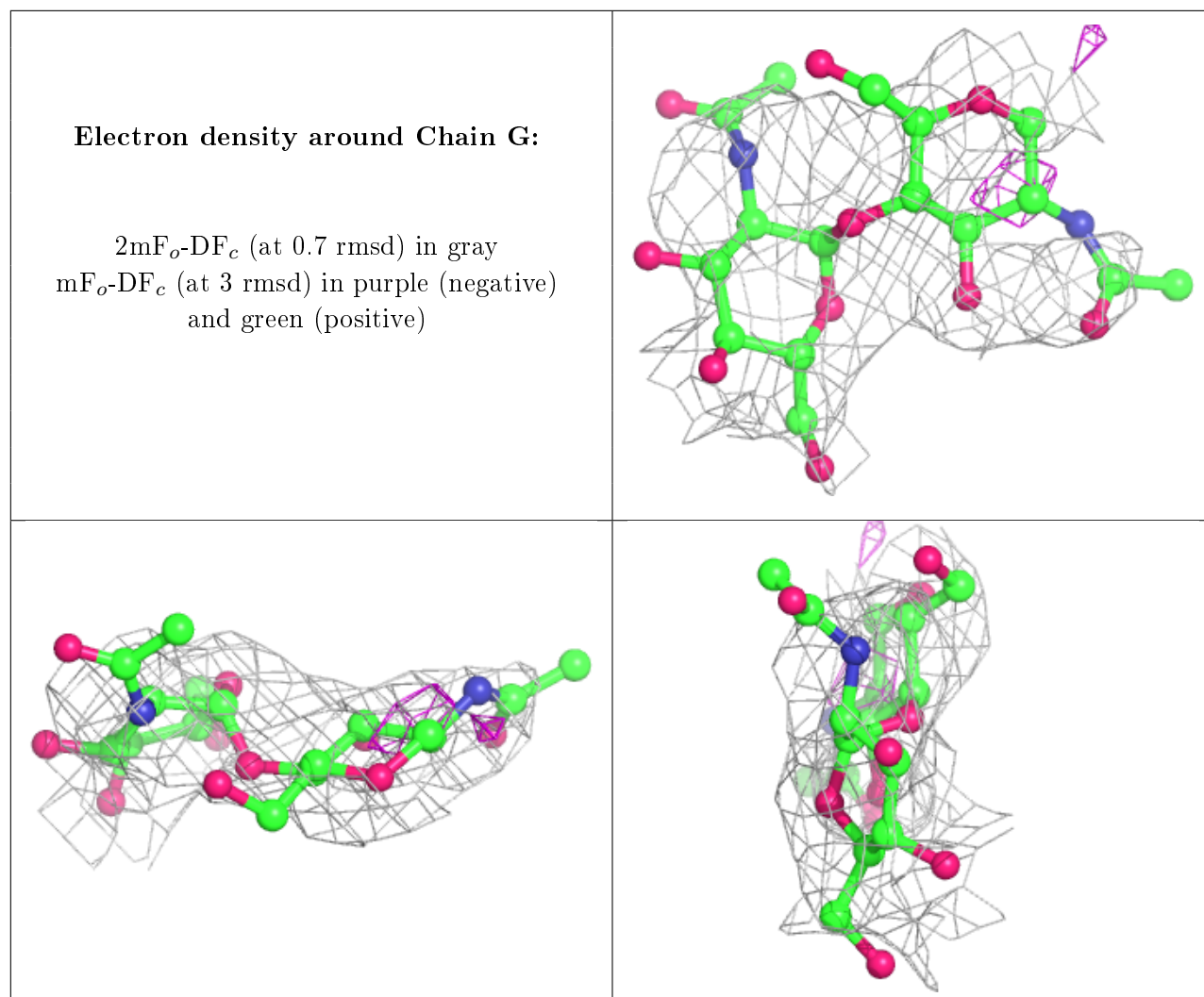
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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)





## 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.