



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2023 – 12:09 AM EDT

PDB ID : 6D1U  
Title : Crystal structure of the human CLR:RAMP1 extracellular domain heterodimer in complex with adrenomedullin 2/intermedin  
Authors : Pioszak, A.; Roehrkasse, A.  
Deposited on : 2018-04-12  
Resolution : 2.05 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

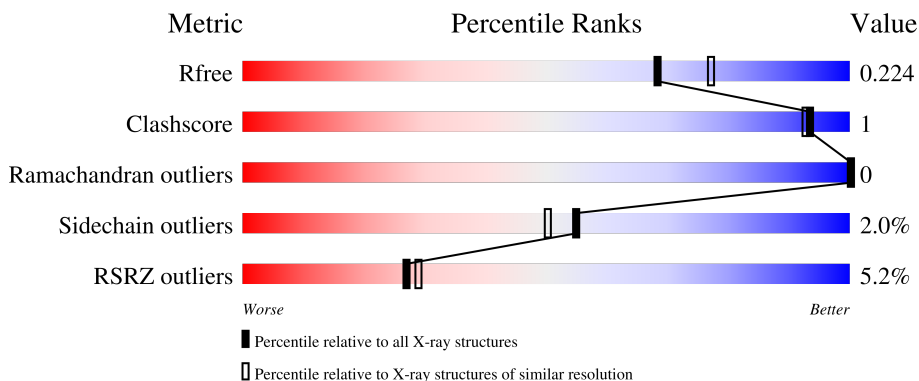
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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.




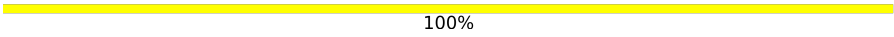

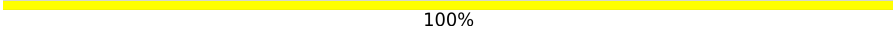
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	593	 89% 7%
1	B	593	 89% 7%
1	C	593	 90% 5%
2	D	20	 60% 10% 30%
2	E	20	 85% 15%

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Mol	Chain	Length	Quality of chain
2	F	20	
3	G	2	
3	H	2	
3	I	2	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 14158 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 Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcitonin gene-related peptide type 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	553	4388	2799	732	833	24	0	3	0
1	B	553	4361	2784	725	829	23	0	0	0
1	C	567	4494	2870	756	846	22	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0AEY0
A	369	ASN	-	linker	UNP P0AEY0
A	370	ALA	-	linker	UNP P0AEY0
A	371	ALA	-	linker	UNP P0AEY0
A	372	ALA	-	linker	UNP P0AEY0
A	373	GLU	-	linker	UNP P0AEY0
A	374	PHE	-	linker	UNP P0AEY0
A	2020	GLY	-	linker	UNP O60894
A	2021	SER	-	linker	UNP O60894
A	2022	ALA	-	linker	UNP O60894
A	2023	GLY	-	linker	UNP O60894
A	2024	SER	-	linker	UNP O60894
A	2025	ALA	-	linker	UNP O60894
A	2026	GLY	-	linker	UNP O60894
A	2027	SER	-	linker	UNP O60894
A	2028	ALA	-	linker	UNP O60894
A	2145	HIS	-	expression tag	UNP Q16602
A	2146	HIS	-	expression tag	UNP Q16602
A	2147	HIS	-	expression tag	UNP Q16602
A	2148	HIS	-	expression tag	UNP Q16602
A	2149	HIS	-	expression tag	UNP Q16602
A	2150	HIS	-	expression tag	UNP Q16602

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P0AEY0
B	369	ASN	-	linker	UNP P0AEY0
B	370	ALA	-	linker	UNP P0AEY0
B	371	ALA	-	linker	UNP P0AEY0
B	372	ALA	-	linker	UNP P0AEY0
B	373	GLU	-	linker	UNP P0AEY0
B	374	PHE	-	linker	UNP P0AEY0
B	2020	GLY	-	linker	UNP O60894
B	2021	SER	-	linker	UNP O60894
B	2022	ALA	-	linker	UNP O60894
B	2023	GLY	-	linker	UNP O60894
B	2024	SER	-	linker	UNP O60894
B	2025	ALA	-	linker	UNP O60894
B	2026	GLY	-	linker	UNP O60894
B	2027	SER	-	linker	UNP O60894
B	2028	ALA	-	linker	UNP O60894
B	2145	HIS	-	expression tag	UNP Q16602
B	2146	HIS	-	expression tag	UNP Q16602
B	2147	HIS	-	expression tag	UNP Q16602
B	2148	HIS	-	expression tag	UNP Q16602
B	2149	HIS	-	expression tag	UNP Q16602
B	2150	HIS	-	expression tag	UNP Q16602
C	1	MET	-	initiating methionine	UNP P0AEY0
C	369	ASN	-	linker	UNP P0AEY0
C	370	ALA	-	linker	UNP P0AEY0
C	371	ALA	-	linker	UNP P0AEY0
C	372	ALA	-	linker	UNP P0AEY0
C	373	GLU	-	linker	UNP P0AEY0
C	1023	PHE	-	linker	UNP P0AEY0
C	2020	GLY	-	linker	UNP O60894
C	2021	SER	-	linker	UNP O60894
C	2022	ALA	-	linker	UNP O60894
C	2023	GLY	-	linker	UNP O60894
C	2024	SER	-	linker	UNP O60894
C	2025	ALA	-	linker	UNP O60894
C	2026	GLY	-	linker	UNP O60894
C	2027	SER	-	linker	UNP O60894
C	2028	ALA	-	linker	UNP O60894
C	2145	HIS	-	expression tag	UNP Q16602
C	2146	HIS	-	expression tag	UNP Q16602
C	2147	HIS	-	expression tag	UNP Q16602
C	2148	HIS	-	expression tag	UNP Q16602

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2149	HIS	-	expression tag	UNP Q16602
C	2150	HIS	-	expression tag	UNP Q16602

- Molecule 2 is a protein called ADM2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	14	Total	C	N	O	0	0	1
			96	58	16	22			
2	E	17	Total	C	N	O	0	0	1
			120	71	23	26			
2	F	14	Total	C	N	O	0	0	1
			96	58	16	22			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	G	2	Total	C	O	0	0	0
			23	12	11			
3	H	2	Total	C	O	0	0	0
			23	12	11			
3	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	C	3	Total	Na	0	0
			3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	293	Total	O	0	0
			293	293		
5	B	104	Total	O	0	0
			104	104		

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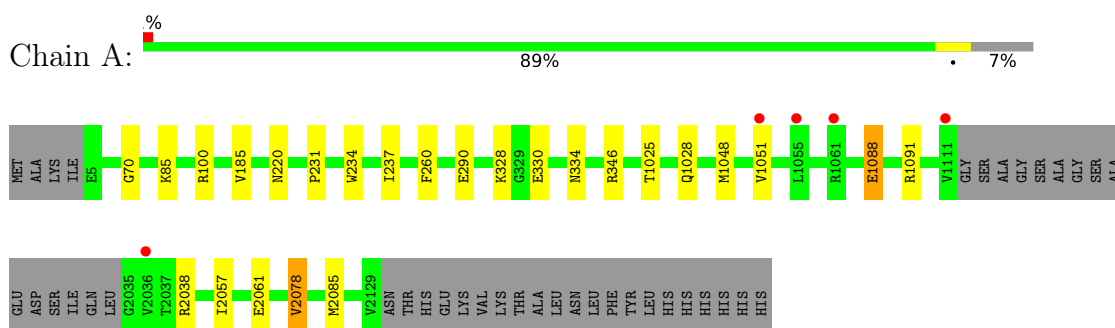
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	C	117	Total 117	O 117	0	0
5	D	8	Total 8	O 8	0	0
5	E	5	Total 5	O 5	0	0
5	F	3	Total 3	O 3	0	0

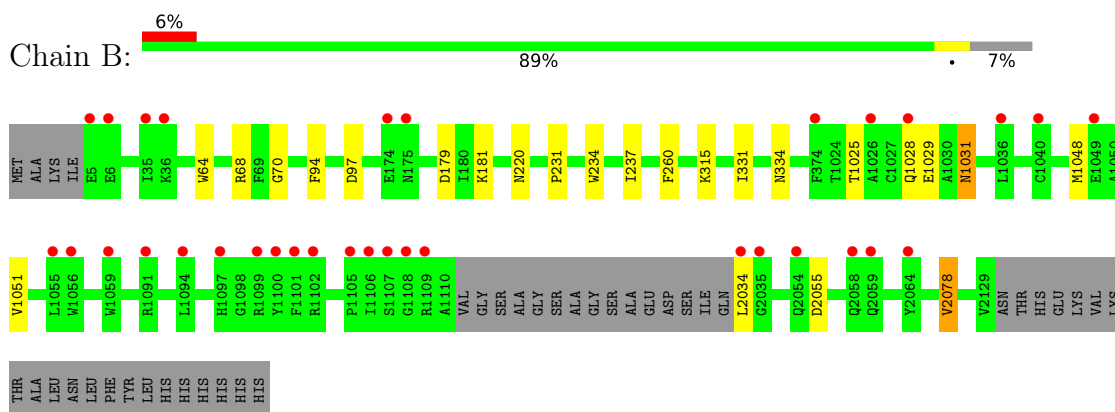
### 3 Residue-property plots [i](#)

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.

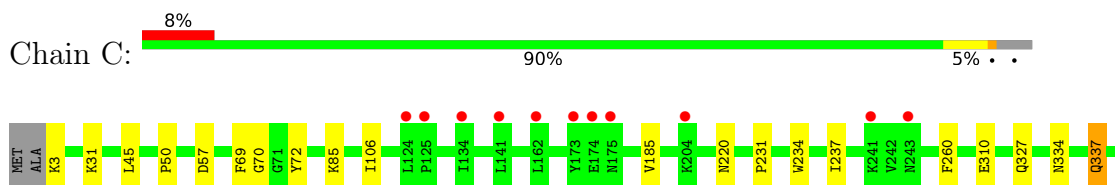
- Molecule 1: Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcitonin gene-related peptide type 1 receptor



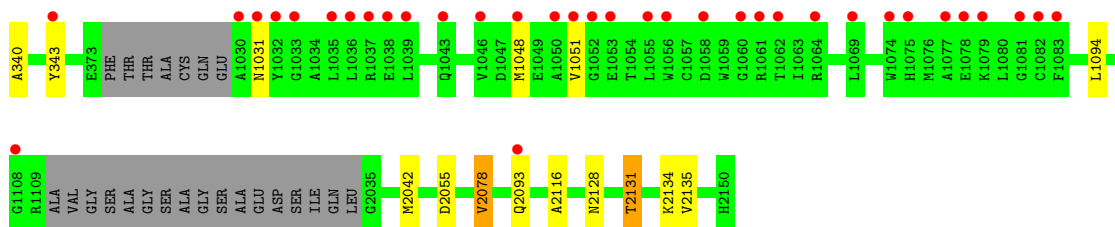
- Molecule 1: Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcitonin gene-related peptide type 1 receptor



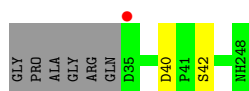
- Molecule 1: Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcitonin gene-related peptide type 1 receptor



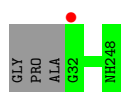
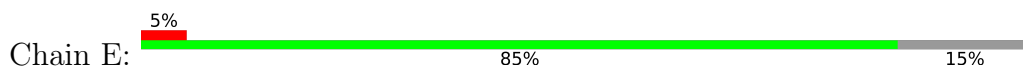




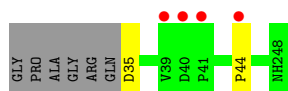
- Molecule 2: ADM2



- Molecule 2: ADM2



- Molecule 2: ADM2



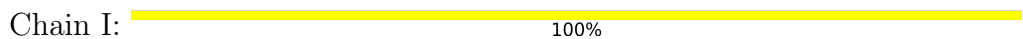
- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.29Å 106.04Å 136.91Å 90.00° 122.53° 90.00°	Depositor
Resolution (Å)	45.64 – 2.05 45.63 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.64-2.05) 97.7 (45.63-2.04)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.194 , 0.223 0.200 , 0.224	Depositor DCC
$R_{free}$ test set	6618 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.3	Xtrriage
Anisotropy	0.566	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: NH2, NA, GLC

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	0.70	1/4500 (0.0%)	0.77	4/6112 (0.1%)
1	B	0.62	0/4473	0.74	3/6077 (0.0%)
1	C	0.65	0/4613	0.76	2/6264 (0.0%)
2	D	0.72	0/99	0.65	0/137
2	E	0.80	0/123	0.87	0/168
2	F	0.56	0/99	0.67	0/137
All	All	0.66	1/13907 (0.0%)	0.76	9/18895 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1088	GLU	CD-OE1	-6.09	1.19	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2078	VAL	CB-CA-C	-7.78	96.62	111.40
1	A	2078	VAL	CB-CA-C	-7.37	97.40	111.40
1	A	346	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	2055	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	2078	VAL	CG1-CB-CG2	6.12	120.70	110.90

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	4388	0	4222	8	0
1	B	4361	0	4197	10	0
1	C	4494	0	4320	17	0
2	D	96	0	78	1	0
2	E	120	0	102	0	0
2	F	96	0	78	3	0
3	G	23	0	21	0	0
3	H	23	0	21	0	0
3	I	23	0	21	0	0
4	A	1	0	0	0	0
4	C	3	0	0	0	0
5	A	293	0	0	2	0
5	B	104	0	0	0	1
5	C	117	0	0	0	1
5	D	8	0	0	0	0
5	E	5	0	0	0	0
5	F	3	0	0	0	0
All	All	14158	0	13060	36	1

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 1.

The worst 5 of 36 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:C:337:GLN:NE2	1:C:337:GLN:H	1.87	0.73
1:C:337:GLN:H	1:C:337:GLN:HE21	1.48	0.59
1:C:2093:GLN:N	2:F:35:ASP:O	2.35	0.59
1:B:1029:GLU:HB3	1:B:1031:ASN:HD22	1.68	0.58
1:A:290:GLU:HG2	5:A:2552:HOH:O	2.04	0.57

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2330:HOH:O	5:C:2328:HOH:O[2_556]	2.11	0.09

## 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	552/593 (93%)	547 (99%)	5 (1%)	0	100	100
1	B	549/593 (93%)	545 (99%)	4 (1%)	0	100	100
1	C	561/593 (95%)	555 (99%)	6 (1%)	0	100	100
2	D	12/20 (60%)	12 (100%)	0	0	100	100
2	E	15/20 (75%)	15 (100%)	0	0	100	100
2	F	12/20 (60%)	12 (100%)	0	0	100	100
All	All	1701/1839 (92%)	1686 (99%)	15 (1%)	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	455/484 (94%)	445 (98%)	10 (2%)	52	46
1	B	452/484 (93%)	447 (99%)	5 (1%)	73	73
1	C	466/484 (96%)	452 (97%)	14 (3%)	41	34
2	D	12/15 (80%)	12 (100%)	0	100	100
2	E	14/15 (93%)	14 (100%)	0	100	100
2	F	12/15 (80%)	12 (100%)	0	100	100
All	All	1411/1497 (94%)	1382 (98%)	29 (2%)	55	48

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2078	VAL
1	C	2131	THR
1	C	85	LYS
1	C	2042	MET
1	C	45	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	327	GLN
1	C	2045	GLN
1	C	1045	GLN
1	C	2058	GLN
1	B	102	ASN

### 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](#)

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	$\# Z  > 2$
3	GLC	G	1	3	12,12,12	0.66	0	17,17,17	1.81	4 (23%)
3	GLC	G	2	3	11,11,12	0.99	0	15,15,17	1.22	2 (13%)
3	GLC	H	1	3	12,12,12	0.67	0	17,17,17	0.96	0
3	GLC	H	2	3	11,11,12	0.80	0	15,15,17	1.37	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLC	I	1	3	12,12,12	0.67	0	17,17,17	1.56	2 (11%)
3	GLC	I	2	3	11,11,12	0.52	0	15,15,17	1.00	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	G	1	3	-	0/2/22/22	0/1/1/1
3	GLC	G	2	3	-	0/2/19/22	0/1/1/1
3	GLC	H	1	3	-	2/2/22/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
3	GLC	I	1	3	-	0/2/22/22	0/1/1/1
3	GLC	I	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	GLC	O5-C1-C2	4.60	118.49	110.28
3	I	1	GLC	O5-C1-C2	4.08	117.56	110.28
3	G	1	GLC	C1-O5-C5	3.13	119.57	113.66
3	H	2	GLC	C1-O5-C5	3.11	116.41	112.19
3	G	1	GLC	O3-C3-C2	-2.73	104.04	110.35

There are no chirality outliers.

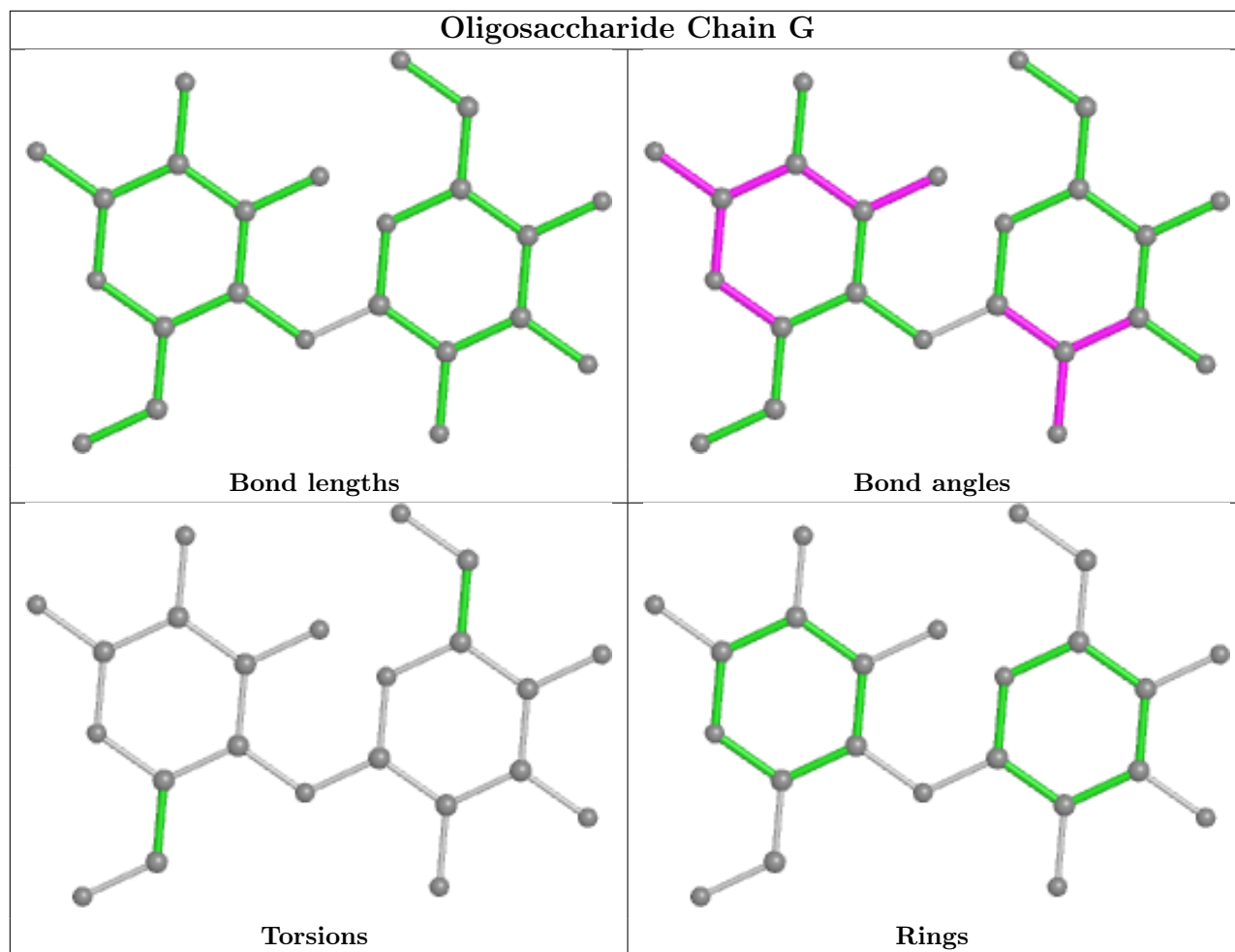
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	GLC	C4-C5-C6-O6
3	H	1	GLC	O5-C5-C6-O6

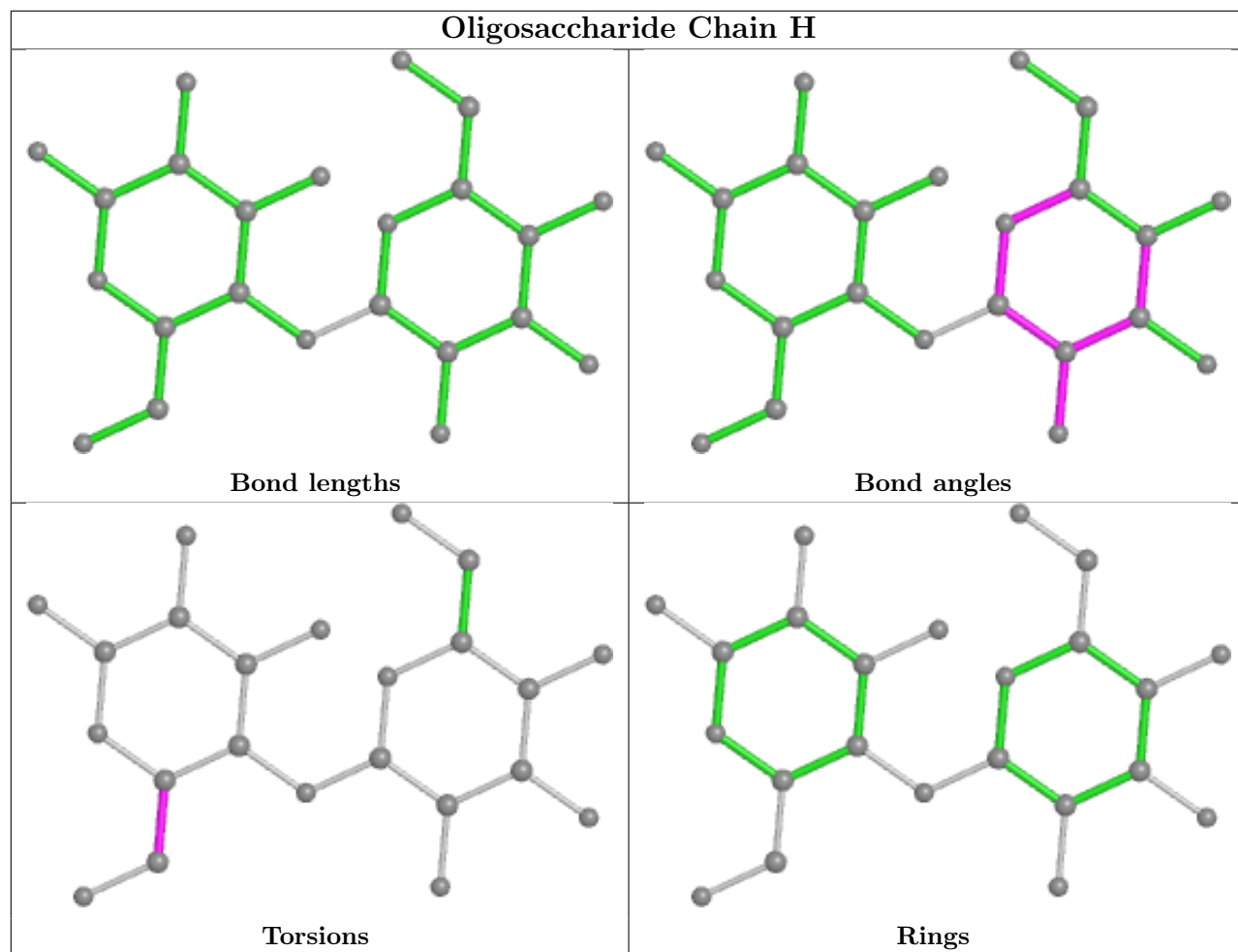
There are no ring outliers.

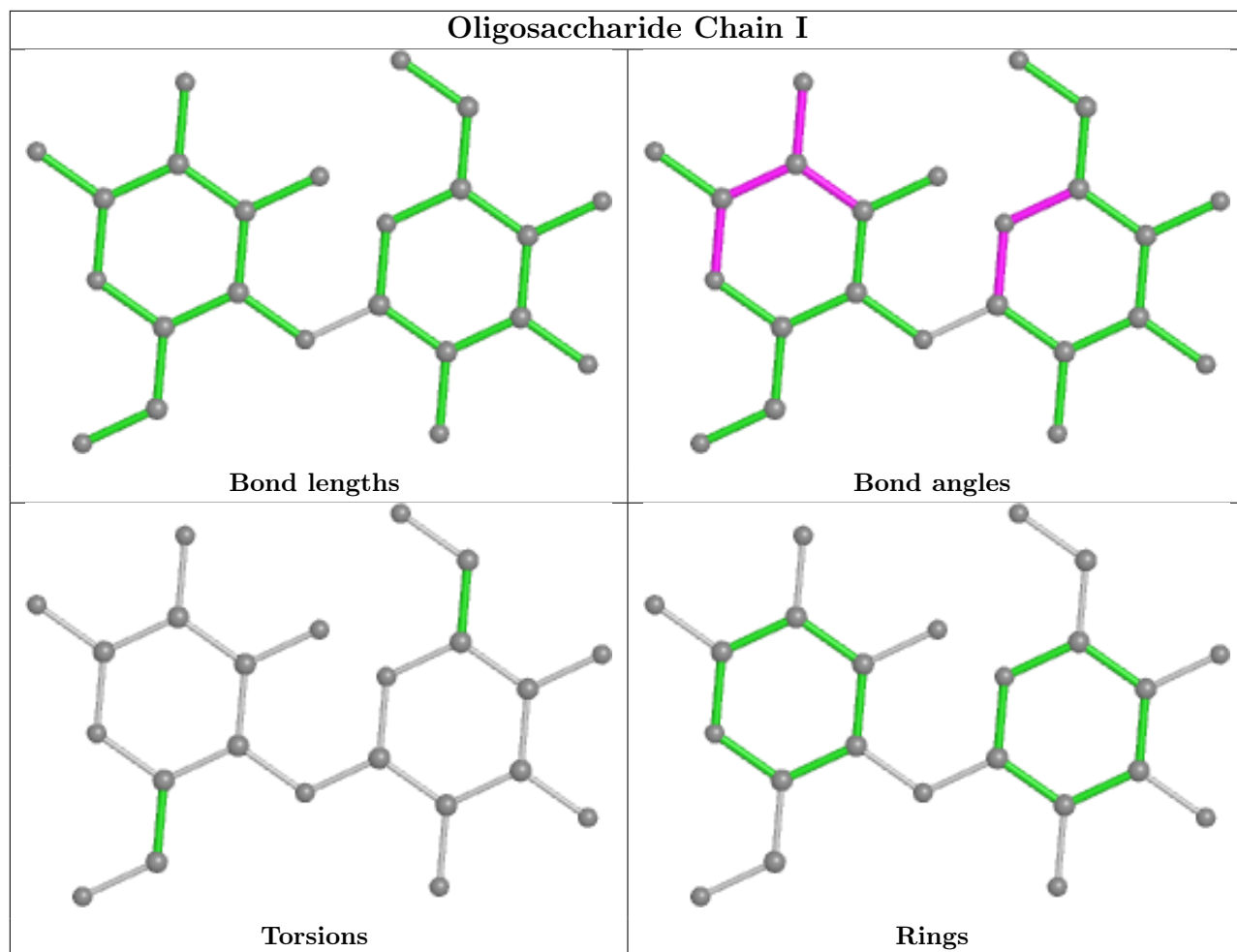
No monomer is involved in short contacts.

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	553/593 (93%)	-0.10	5 (0%) 84 86	34, 53, 84, 104	0
1	B	553/593 (93%)	0.14	33 (5%) 21 23	45, 70, 107, 138	0
1	C	567/593 (95%)	0.45	46 (8%) 12 12	37, 71, 114, 149	0
2	D	13/20 (65%)	0.53	1 (7%) 13 14	51, 68, 103, 119	0
2	E	16/20 (80%)	-0.17	1 (6%) 20 21	54, 61, 78, 78	0
2	F	13/20 (65%)	1.57	4 (30%) 0 0	73, 99, 108, 108	0
All	All	1715/1839 (93%)	0.17	90 (5%) 27 29	34, 65, 106, 149	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1082	CYS	8.1
1	C	1083	PHE	6.6
1	C	1039	LEU	6.6
1	C	1051	VAL	6.5
1	C	1038	GLU	5.7

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

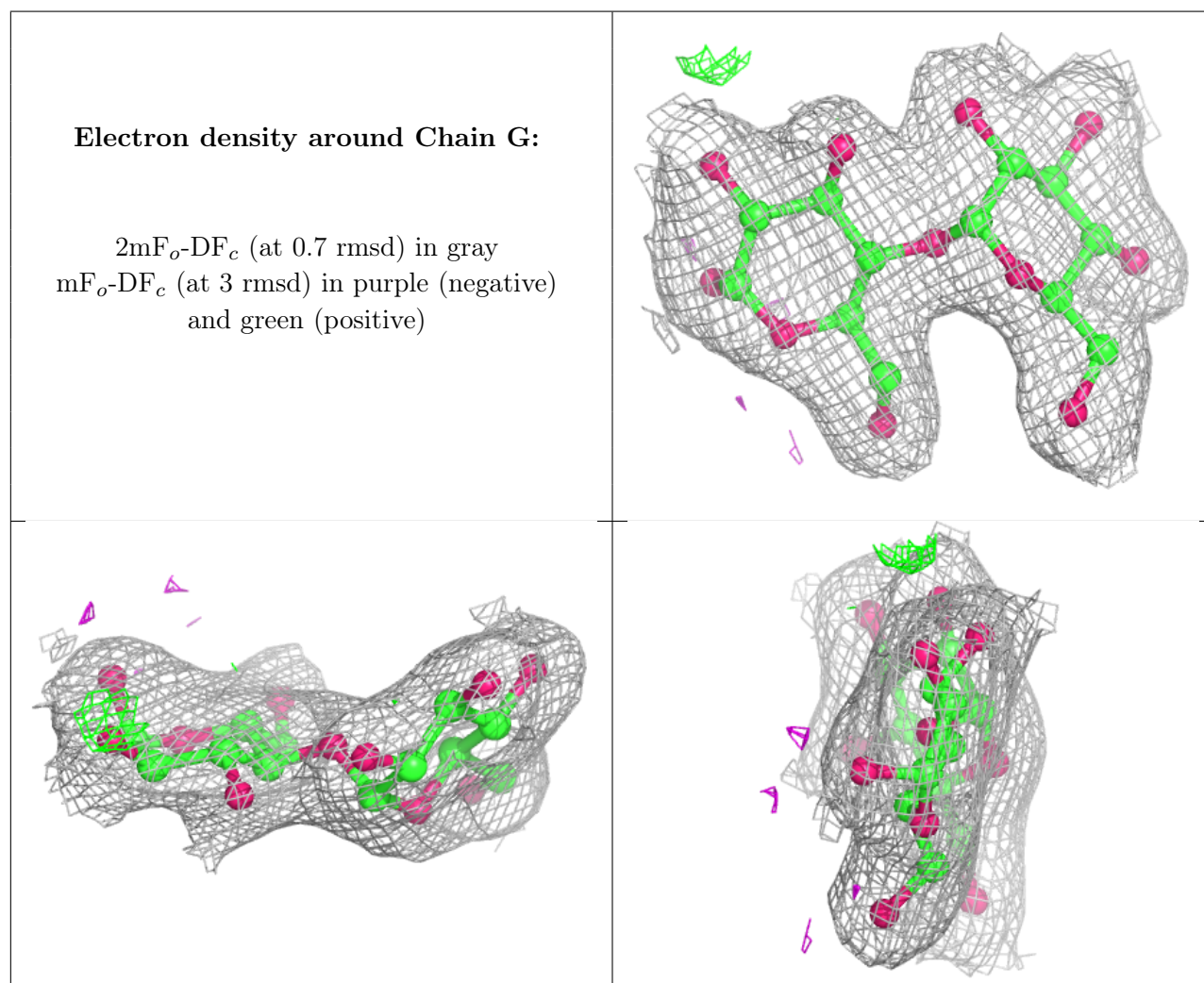
There are no non-standard protein/DNA/RNA residues in this entry.

### 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.

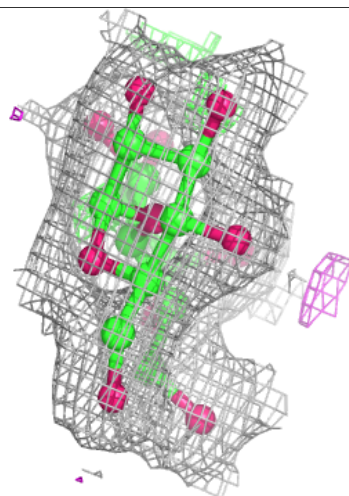
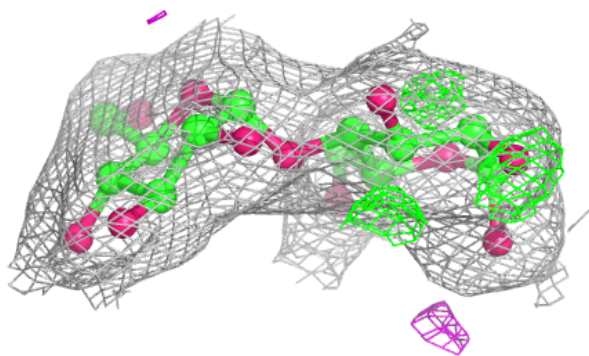
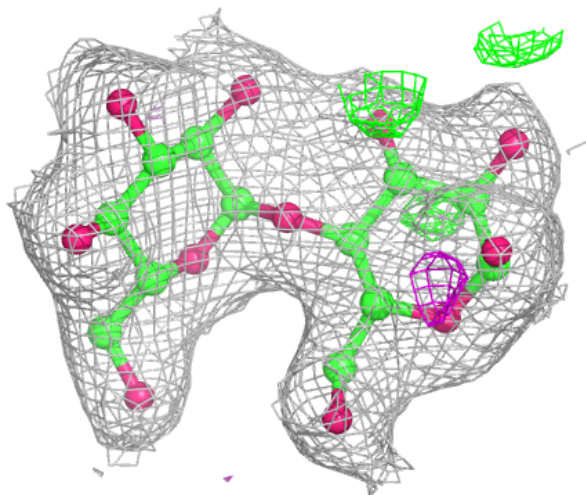
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GLC	H	1	12/12	0.97	0.10	49,53,55,55	0
3	GLC	I	2	11/12	0.97	0.13	50,53,54,55	0
3	GLC	H	2	11/12	0.98	0.11	44,47,49,49	0
3	GLC	I	1	12/12	0.98	0.13	52,54,57,59	0
3	GLC	G	1	12/12	0.98	0.11	40,45,51,52	0
3	GLC	G	2	11/12	0.99	0.14	36,38,40,41	0

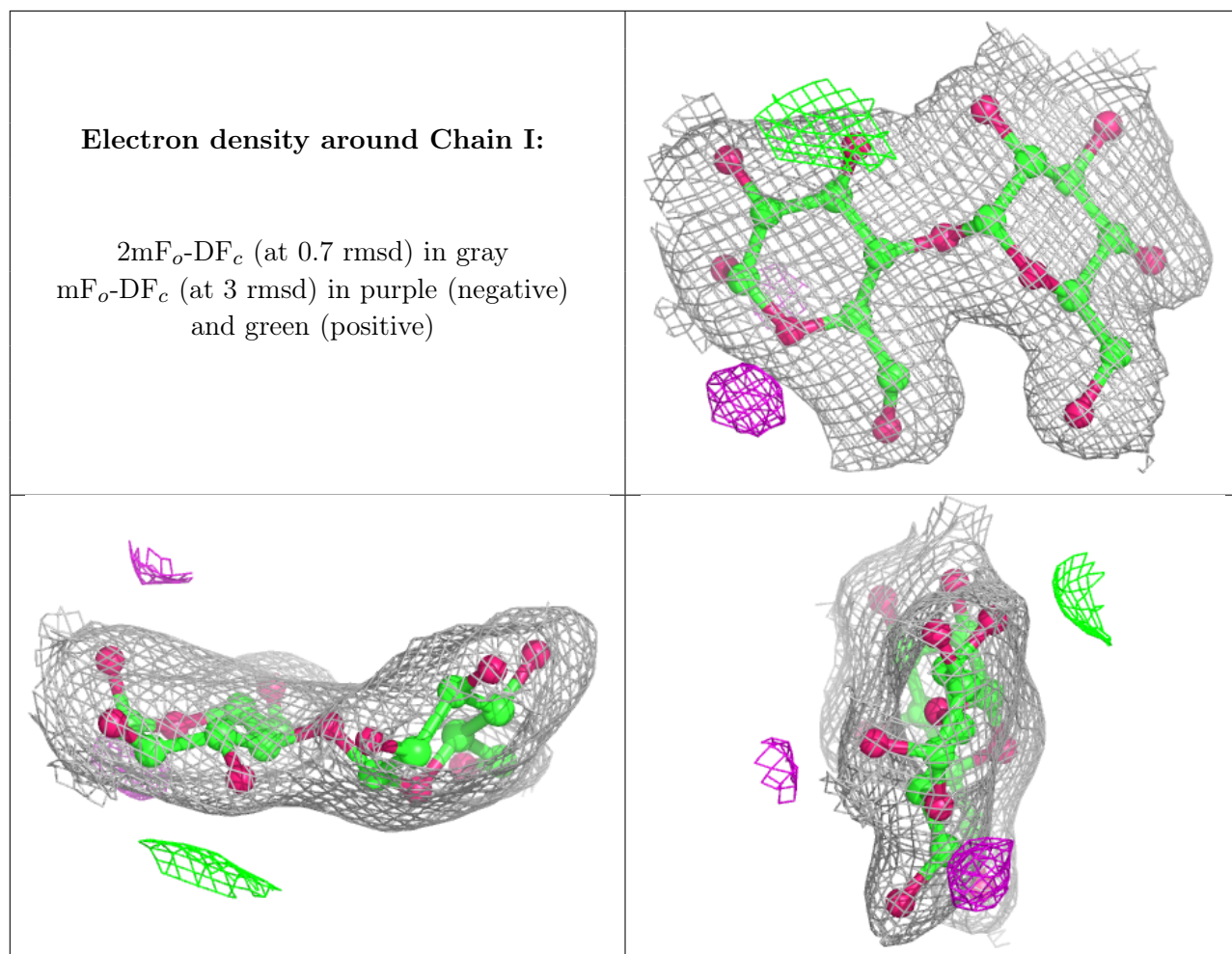
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain H:**

$2mF_o-DF_c$  (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
4	NA	A	2202	1/1	0.88	0.19	61,61,61,61	0
4	NA	C	2203	1/1	0.91	0.07	52,52,52,52	0
4	NA	C	2204	1/1	0.92	0.08	60,60,60,60	0
4	NA	C	2202	1/1	0.99	0.10	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.