



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:44 PM BST

PDB ID : 6V2E  
Title : Crystal structure of the human CLR:RAMP2 extracellular domain heterodimer with bound high-affinity adrenomedullin S45R/K46L/S48G/Q50W variant  
Authors : Booe, J.M.; Pioszak, A.A.  
Deposited on : 2019-11-22  
Resolution : 1.83 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.

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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 : 2.14.2  
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) : 2.14.2

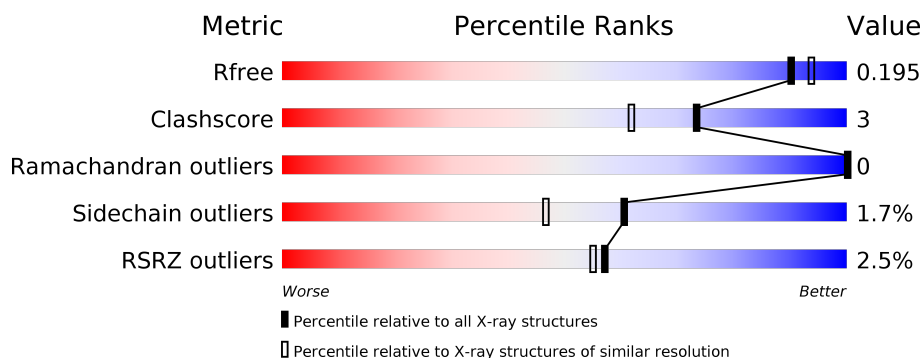
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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  $\leq 5\%$ . 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	591	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
2	B	16	<div> <div>13%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
3	C	2	<div> <div></div> <div>100%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5264 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/maltodextrin-binding periplasmic protein, Receptor activity-modifying protein 2, Calcitonin gene-related peptide type 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	16	0
			4487	2878	735	852	22			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0AEX9
A	369	ASN	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	371	ALA	-	linker	UNP P0AEX9
A	372	ALA	-	linker	UNP P0AEX9
A	373	GLU	-	linker	UNP P0AEX9
A	374	PHE	-	linker	UNP P0AEX9
A	1106	ARG	LEU	engineered mutation	UNP O60895
A	2020	GLY	-	linker	UNP O60895
A	2021	SER	-	linker	UNP O60895
A	2022	ALA	-	linker	UNP O60895
A	2023	GLY	-	linker	UNP O60895
A	2024	SER	-	linker	UNP O60895
A	2025	ALA	-	linker	UNP O60895
A	2026	GLY	-	linker	UNP O60895
A	2027	SER	-	linker	UNP O60895
A	2028	ALA	-	linker	UNP O60895
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

- Molecule 2 is a protein called ADM.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	0	1	0
			142	90	29	23			

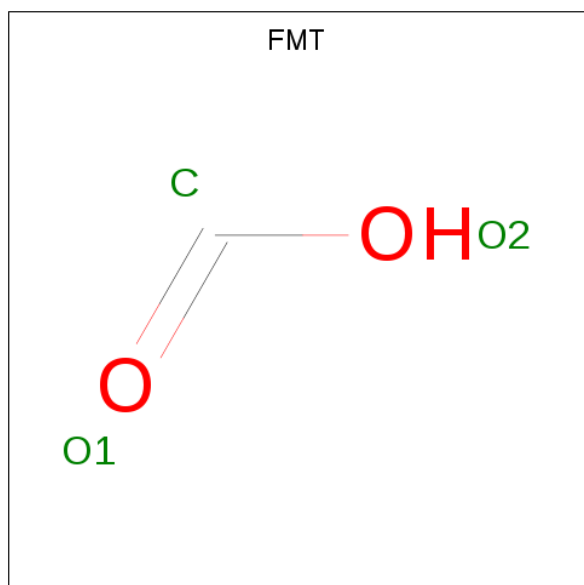
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	45	ARG	SER	engineered mutation	UNP P35318
B	46	LEU	LYS	engineered mutation	UNP P35318
B	48	GLY	SER	engineered mutation	UNP P35318
B	50	TRP	GLN	engineered mutation	UNP P35318

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

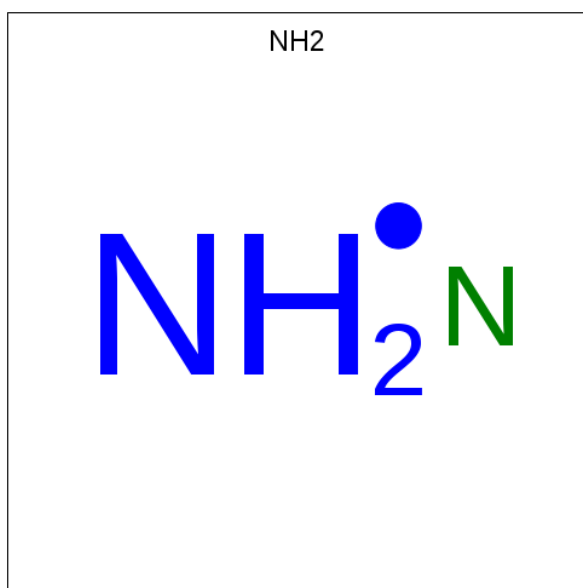
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

- Molecule 5 is AMINO GROUP (three-letter code: NH2) (formula: H<sub>2</sub>N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total N 1 1	0	0

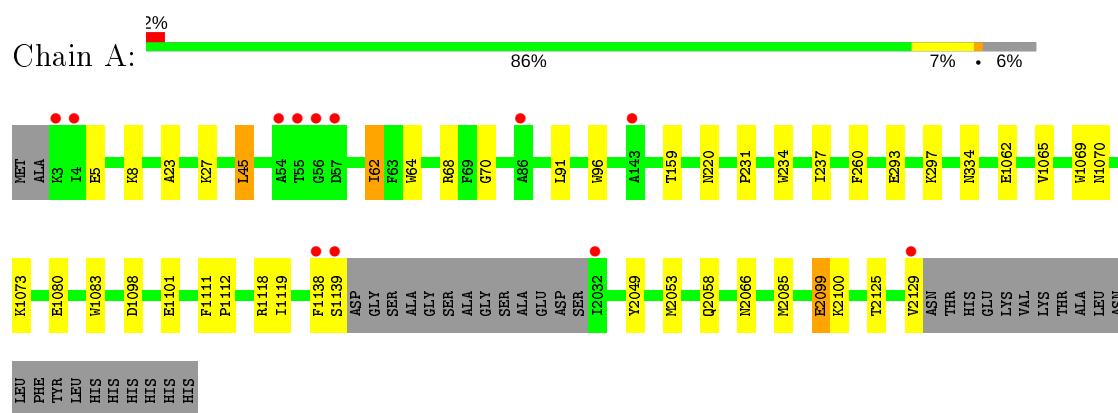
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	581	Total O 581 581	0	0
6	B	21	Total O 21 21	0	0

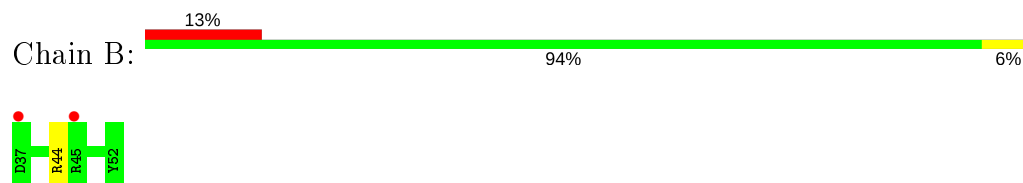
### 3 Residue-property plots [i](#)

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.

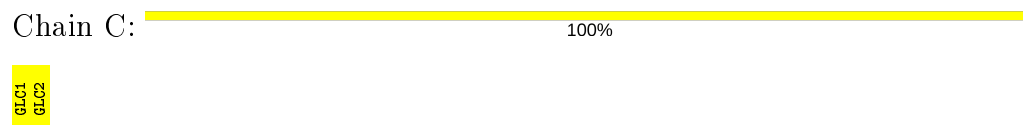
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Receptor activity-modifying protein 2, Calcitonin gene-related peptide type 1 receptor



- Molecule 2: ADM



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.02Å 84.99Å 123.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.97 – 1.83 36.94 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.97-1.83) 99.5 (36.94-1.83)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.157 , 0.190 0.167 , 0.195	Depositor DCC
$R_{free}$ test set	3235 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: FMT, GLC, NH2

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	0.72	2/4649 (0.0%)	0.80	0/6312
2	B	0.58	0/146	0.84	0/197
All	All	0.71	2/4795 (0.0%)	0.80	0/6509

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2099	GLU	CD-OE2	-5.26	1.19	1.25
1	A	1062	GLU	CD-OE1	5.20	1.31	1.25

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	4487	0	4363	30	0
2	B	142	0	139	0	0
3	C	23	0	21	0	0
4	A	9	0	3	1	0
5	B	1	0	0	0	0
6	A	581	0	0	8	0
6	B	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5264	0	4526	30	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 3.

All (30) 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:2085[A]:MET:CE	1:A:2100:LYS:HD2	1.99	0.91
1:A:2085[A]:MET:HE3	1:A:2100:LYS:HD2	1.54	0.88
1:A:2085[A]:MET:HE3	1:A:2100:LYS:CD	2.12	0.79
1:A:1118:ARG:CZ	6:A:2323:HOH:O	2.36	0.73
1:A:1098:ASP:OD2	6:A:2301:HOH:O	2.14	0.65
1:A:45:LEU:CD1	1:A:62:ILE:HD11	2.28	0.63
1:A:1101[B]:GLU:HG2	1:A:1111:PHE:CG	2.34	0.63
1:A:1073[A]:LYS:HE2	6:A:2789:HOH:O	2.03	0.59
1:A:2066[A]:ASN:ND2	6:A:2309:HOH:O	2.36	0.57
1:A:159[A]:THR:HG23	6:A:2381:HOH:O	2.09	0.53
1:A:2085[A]:MET:HE3	1:A:2100:LYS:CG	2.40	0.52
1:A:231:PRO:HA	1:A:234:TRP:CE2	2.44	0.52
1:A:1065:VAL:HG13	1:A:1119:ILE:HG13	1.91	0.52
1:A:1080:GLU:HA	1:A:1083:TRP:CE2	2.46	0.51
1:A:2099:GLU:C	1:A:2100:LYS:HD3	2.33	0.49
1:A:1070:ASN:ND2	4:A:2203:FMT:O1	2.46	0.49
1:A:1101[B]:GLU:OE1	6:A:2302:HOH:O	2.20	0.47
1:A:1069:TRP:NE1	1:A:1073[A]:LYS:HD2	2.29	0.46
1:A:220:ASN:HD21	1:A:237:ILE:HG12	1.81	0.46
1:A:64:TRP:CD1	1:A:68:ARG:HG3	2.51	0.46
1:A:1101[A]:GLU:HG3	6:A:2499:HOH:O	2.16	0.44
1:A:2049:TYR:HA	1:A:2053:MET:HB2	2.00	0.44
1:A:1065:VAL:CG1	1:A:1119:ILE:HG13	2.47	0.44
1:A:2125:THR:O	1:A:2129:VAL:HG13	2.20	0.41
1:A:23:ALA:O	1:A:27[B]:LYS:HG2	2.20	0.41
1:A:1118:ARG:NE	6:A:2323:HOH:O	2.48	0.41
1:A:5:GLU:OE1	1:A:8:LYS:HD3	2.21	0.41
1:A:91:LEU:HD12	1:A:96:TRP:CZ2	2.56	0.41
1:A:70:GLY:HA3	1:A:334:ASN:O	2.20	0.40
1:A:293:GLU:O	1:A:297:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	567/591 (96%)	558 (98%)	9 (2%)	0	100	100
2	B	15/16 (94%)	15 (100%)	0	0	100	100
All	All	582/607 (96%)	573 (98%)	9 (2%)	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	477/489 (98%)	470 (98%)	7 (2%)	65	52
2	B	14/13 (108%)	13 (93%)	1 (7%)	14	3
All	All	491/502 (98%)	483 (98%)	8 (2%)	60	49

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	62	ILE
1	A	260	PHE
1	A	1112	PRO
1	A	1138	PHE
1	A	1139	SER
1	A	2058	GLN
2	B	44	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	220	ASN
1	A	1130	ASN
1	A	2118	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 ⓘ

2 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	C	1	3	12,12,12	0.63	0	17,17,17	1.03	1 (5%)
3	GLC	C	2	3	11,11,12	0.59	0	15,15,17	1.15	2 (13%)

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	C	1	3	-	0/2/22/22	0/1/1/1
3	GLC	C	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	GLC	O5-C1-C2	2.60	114.92	110.28
3	C	2	GLC	C1-O5-C5	2.50	115.58	112.19
3	C	2	GLC	C6-C5-C4	-2.05	108.19	113.00

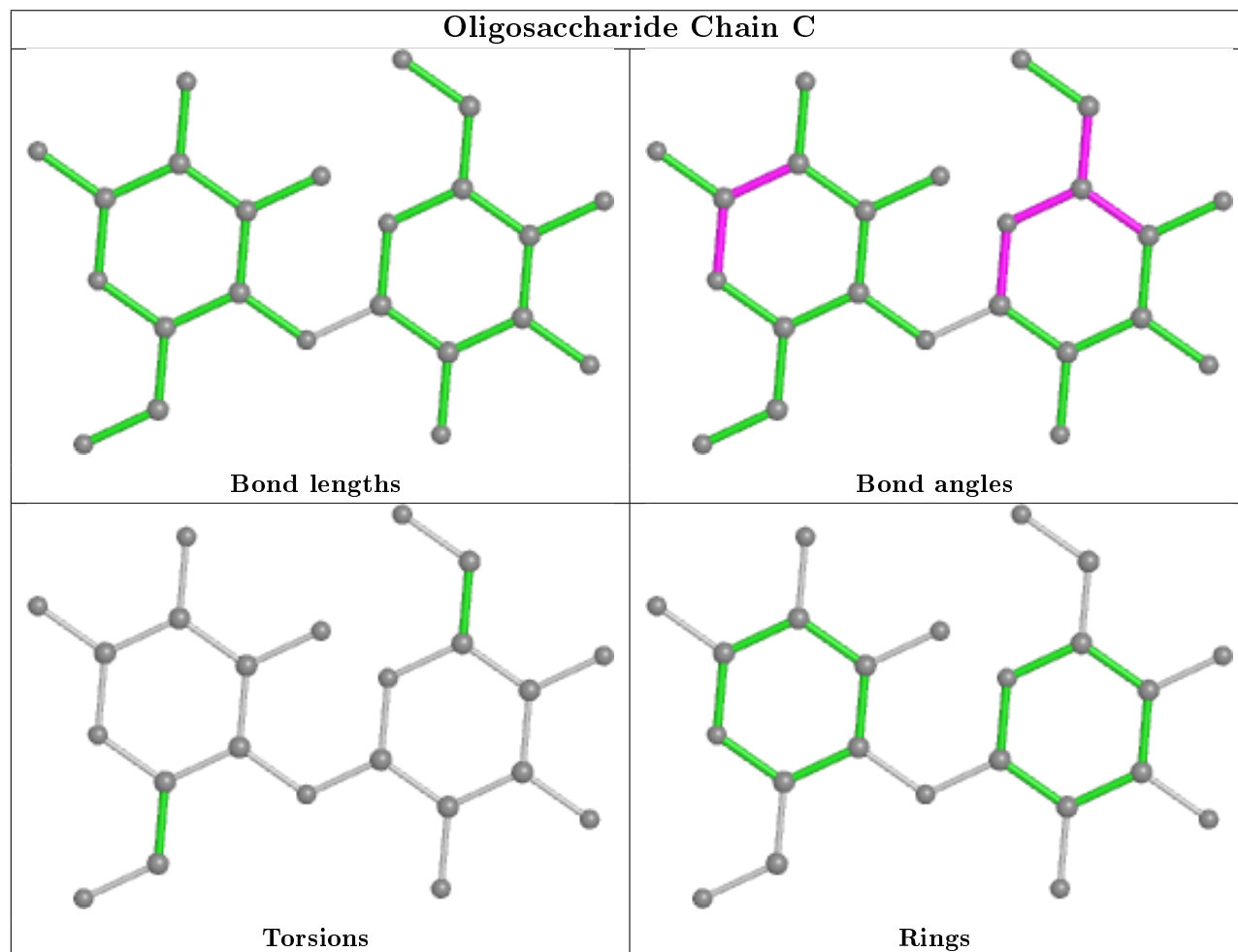
There are no chirality outliers.

There are no torsion outliers.

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, 1 is modelled with single atom - leaving 3 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	FMT	A	2203	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	2202	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	2204	-	0,2,2	0.00	-	0,1,1	0.00	-

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	A	2203	FMT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	555/591 (93%)	-0.23	12 (2%) 62 60	16, 28, 51, 77	0
2	B	16/16 (100%)	0.19	2 (12%) 3 3	18, 27, 46, 58	0
All	All	571/607 (94%)	-0.22	14 (2%) 57 55	16, 28, 51, 77	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2032	ILE	5.6
1	A	1139	SER	4.4
1	A	2129	VAL	4.1
1	A	54	ALA	4.0
1	A	3	LYS	3.9
2	B	37	ASP	3.4
1	A	57	ASP	3.1
1	A	55	THR	2.8
1	A	56	GLY	2.6
1	A	1138	PHE	2.4
2	B	45[A]	ARG	2.2
1	A	143	ALA	2.2
1	A	86	ALA	2.1
1	A	4	ILE	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.

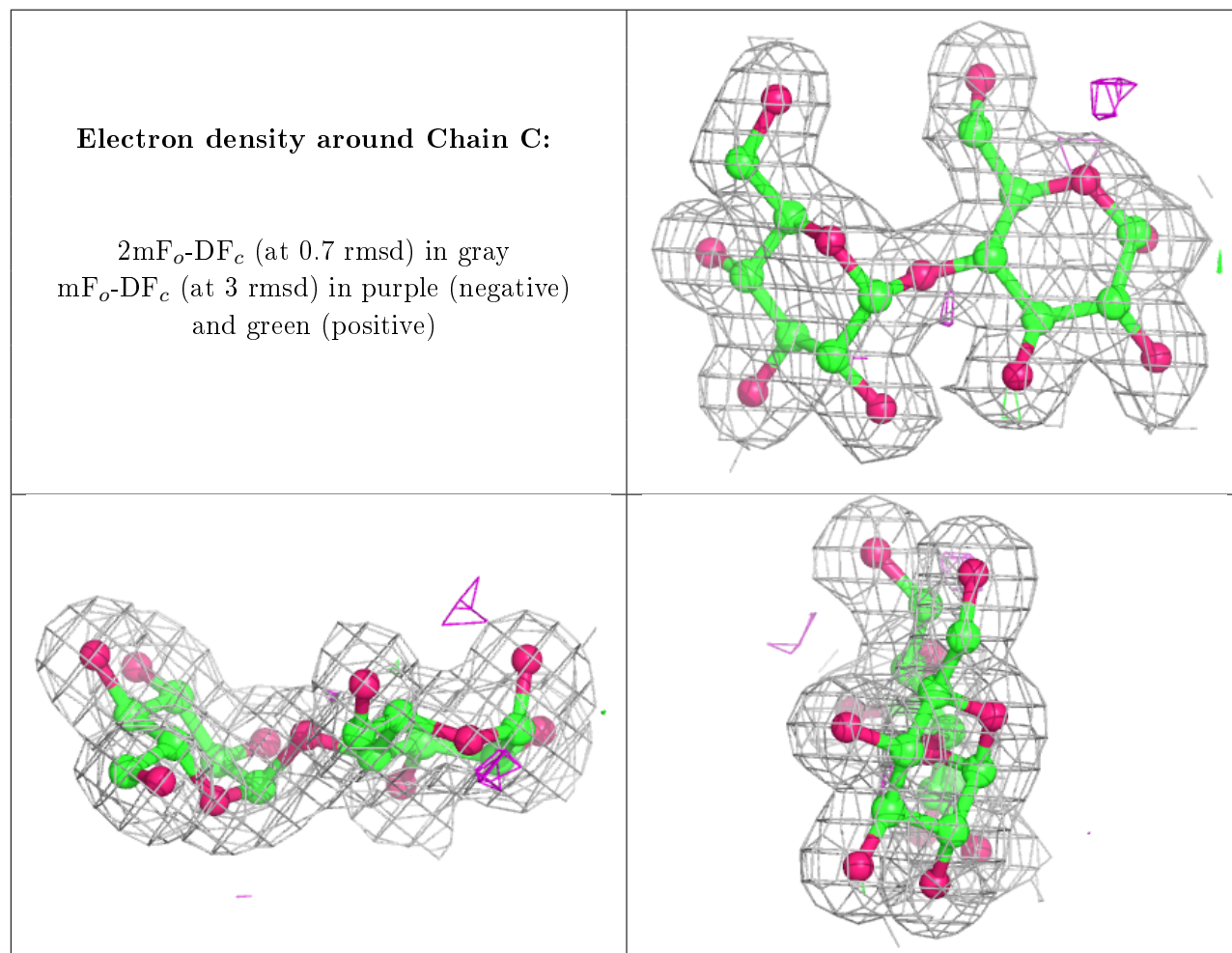
### 6.3 Carbohydrates [i](#)

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	GLC	C	1	12/12	0.97	0.12	18,19,24,24	0
3	GLC	C	2	11/12	0.99	0.15	17,18,19,19	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 ⓘ

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	FMT	A	2203	3/3	0.90	0.23	46,46,48,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FMT	A	2204	3/3	0.91	0.11	36,36,39,42	0
4	FMT	A	2202	3/3	0.94	0.14	32,32,37,44	0
5	NH2	B	101	1/1	0.99	0.12	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.