



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:54 PM UTC

PDB ID : 4RDL / pdb\_00004rdl  
Title : Crystal structure of Norovirus Boxer P domain in complex with Lewis y tetrasaccharide  
Authors : Hao, N.; Chen, Y.; Xia, M.; Liu, W.; Tan, M.; Jiang, X.; Li, X.  
Deposited on : 2014-09-19  
Resolution : 1.45 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

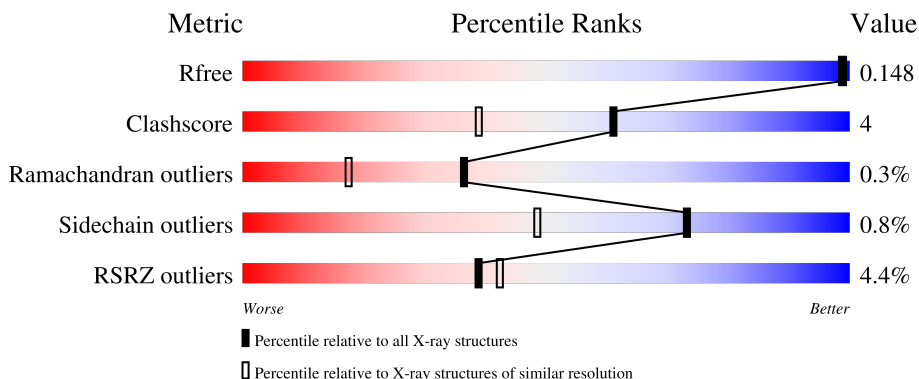
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



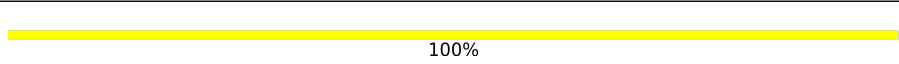
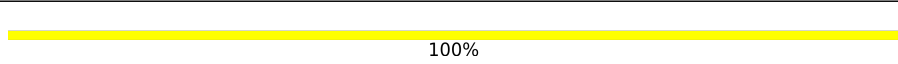
The reported resolution of this entry is 1.45 Å.

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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	308	 5% 88% 8% .
1	B	308	 4% 89% 7% . .
2	C	4	 100%
2	D	4	 100%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5507 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.

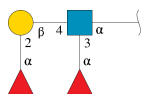
- Molecule 1 is a protein called Capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2295	1461	386	435	13	0	0	0
1	B	297	2295	1461	386	435	13	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLY	-	expression tag	UNP Q8BCA3
A	220	PRO	-	expression tag	UNP Q8BCA3
A	221	LEU	-	expression tag	UNP Q8BCA3
A	222	GLY	-	expression tag	UNP Q8BCA3
A	223	SER	-	expression tag	UNP Q8BCA3
A	224	PRO	-	expression tag	UNP Q8BCA3
A	225	GLU	-	expression tag	UNP Q8BCA3
A	226	PHE	-	expression tag	UNP Q8BCA3
B	219	GLY	-	expression tag	UNP Q8BCA3
B	220	PRO	-	expression tag	UNP Q8BCA3
B	221	LEU	-	expression tag	UNP Q8BCA3
B	222	GLY	-	expression tag	UNP Q8BCA3
B	223	SER	-	expression tag	UNP Q8BCA3
B	224	PRO	-	expression tag	UNP Q8BCA3
B	225	GLU	-	expression tag	UNP Q8BCA3
B	226	PHE	-	expression tag	UNP Q8BCA3

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			46	26	1	19			
2	D	4	Total	C	N	O	0	0	0
			46	26	1	19			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	411	Total	O	0	0
			411	411		
3	B	414	Total	O	0	0
			414	414		



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.39Å 140.39Å 65.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.70 – 1.45 47.70 – 1.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.70-1.45) 100.0 (47.70-1.45)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.72 (at 1.45Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.130 , 0.151 0.126 , 0.148	Depositor DCC
$R_{free}$ test set	6496 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.0	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	5507	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDG, FUC, GAL

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	0.37	0/2362	0.70	0/3231
1	B	0.35	0/2362	0.69	0/3231
All	All	0.36	0/4724	0.69	0/6462

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

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	2295	0	2204	21	0
1	B	2295	0	2204	17	0
2	C	46	0	38	0	0
2	D	46	0	37	0	0
3	A	411	0	0	5	0
3	B	414	0	0	3	0
All	All	5507	0	4483	38	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 4.

The worst 5 of 38 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:232:PHE:H	1:A:467:ARG:HH22	1.19	0.90
1:B:255:MET:HA	1:B:506:GLN:HG3	1.65	0.78
1:B:506:GLN:HG2	3:B:1027:HOH:O	1.85	0.76
1:B:369:THR:HG21	3:B:1058:HOH:O	1.88	0.72
1:A:317:PHE:HA	1:A:366:HIS:CE1	2.25	0.71

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	295/308 (96%)	286 (97%)	9 (3%)	0	100	100
1	B	295/308 (96%)	284 (96%)	9 (3%)	2 (1%)	18	4
All	All	590/616 (96%)	570 (97%)	18 (3%)	2 (0%)	36	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	504	GLY
1	B	503	GLY

### 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	255/264 (97%)	252 (99%)	3 (1%)	63	32
1	B	255/264 (97%)	254 (100%)	1 (0%)	84	69
All	All	510/528 (97%)	506 (99%)	4 (1%)	73	48

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	THR
1	A	506	GLN
1	A	521	SER
1	B	441	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	415	GLN
1	B	418	GLN
1	B	525	GLN
1	B	474	HIS
1	B	366	HIS

### 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](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NDG	C	1	2	15,15,15	2.49	5 (33%)	21,21,21	0.95	1 (4%)
2	GAL	C	2	2	11,11,12	2.13	4 (36%)	15,15,17	0.67	0
2	FUC	C	3	2	10,10,11	2.11	2 (20%)	14,14,16	0.75	0
2	FUC	C	4	2	10,10,11	2.21	5 (50%)	14,14,16	0.64	0
2	NDG	D	1	2	15,15,15	2.64	9 (60%)	21,21,21	1.54	3 (14%)
2	GAL	D	2	2	11,11,12	2.54	3 (27%)	15,15,17	0.94	0
2	FUC	D	3	2	10,10,11	2.99	5 (50%)	14,14,16	2.44	4 (28%)
2	FUC	D	4	2	10,10,11	2.22	6 (60%)	14,14,16	0.68	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
2	NDG	C	1	2	-	0/6/26/26	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
2	NDG	D	1	2	-	0/6/26/26	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GAL	O5-C1	-6.34	1.33	1.43
2	D	1	NDG	C8-C7	-6.25	1.37	1.50
2	D	3	FUC	C1-C2	-5.69	1.38	1.52
2	D	3	FUC	O5-C1	5.10	1.52	1.43
2	C	1	NDG	C8-C7	-5.00	1.40	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	FUC	C1-C2-C3	5.04	116.99	109.64
2	D	3	FUC	O2-C2-C1	-4.92	97.95	109.22
2	D	3	FUC	O5-C1-C2	-4.19	100.79	110.79
2	D	1	NDG	O5-C1-C2	4.09	113.62	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NDG	C1-C2-N2	-3.27	106.94	110.73

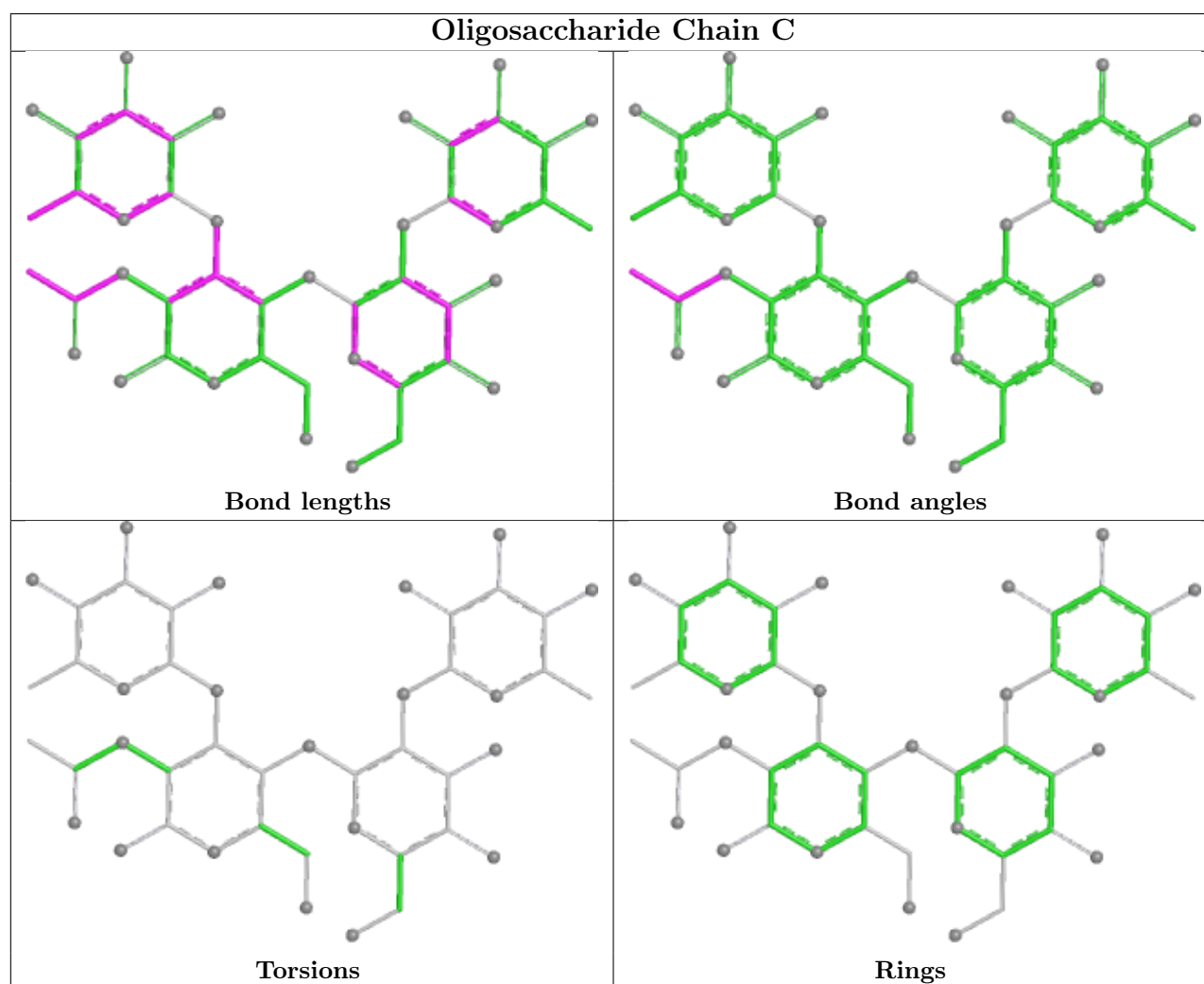
There are no chirality outliers.

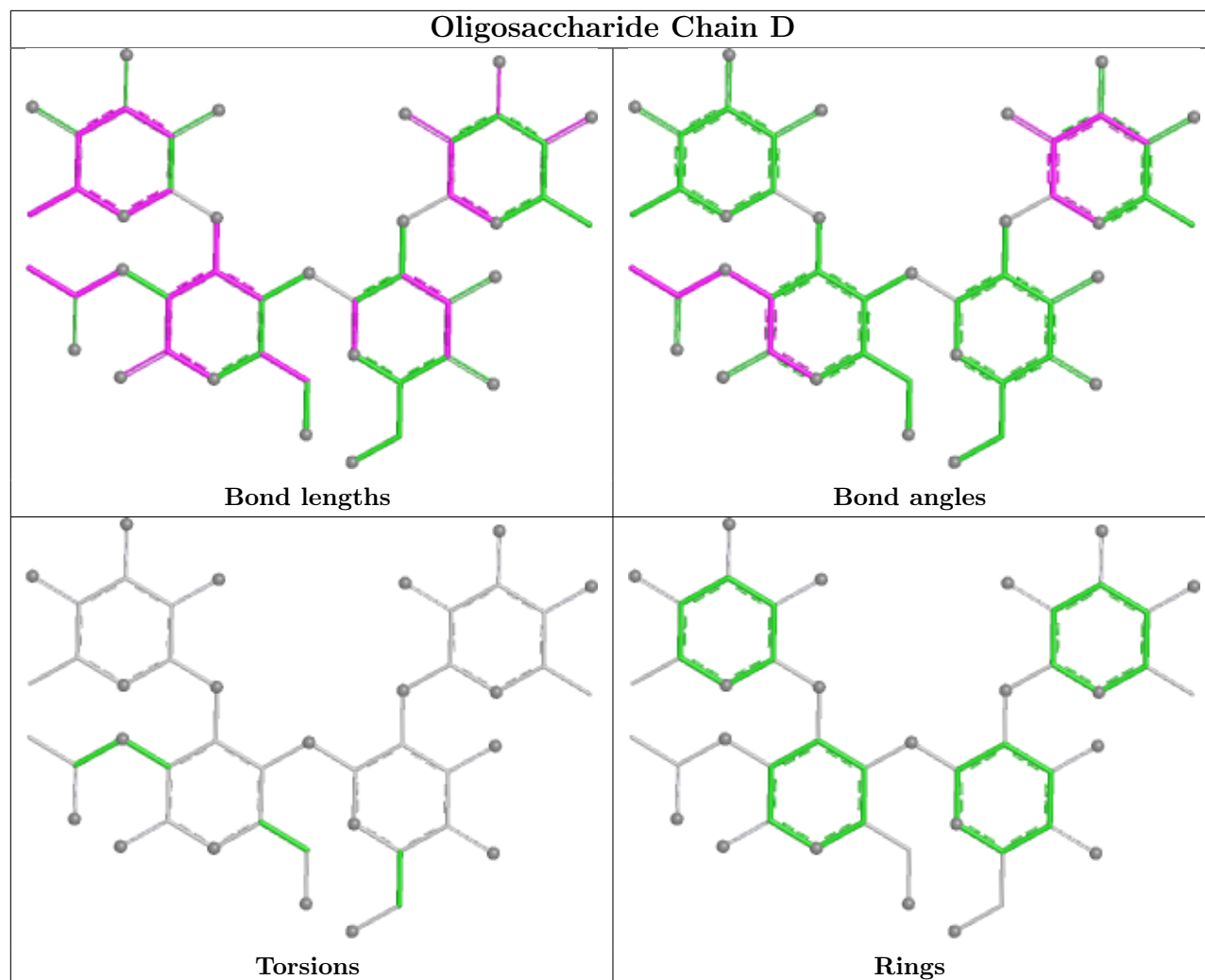
There are no torsion outliers.

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](#)

There are no ligands in this entry.

## 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	297/308 (96%)	-0.30	15 (5%) 33 35	9, 14, 34, 57	0
1	B	297/308 (96%)	-0.31	11 (3%) 45 48	9, 16, 35, 58	0
All	All	594/616 (96%)	-0.30	26 (4%) 39 42	9, 15, 35, 58	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	GLY	9.9
1	A	504	GLY	9.3
1	A	316	ALA	6.5
1	A	505	PRO	6.4
1	B	503	GLY	5.8

### 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.

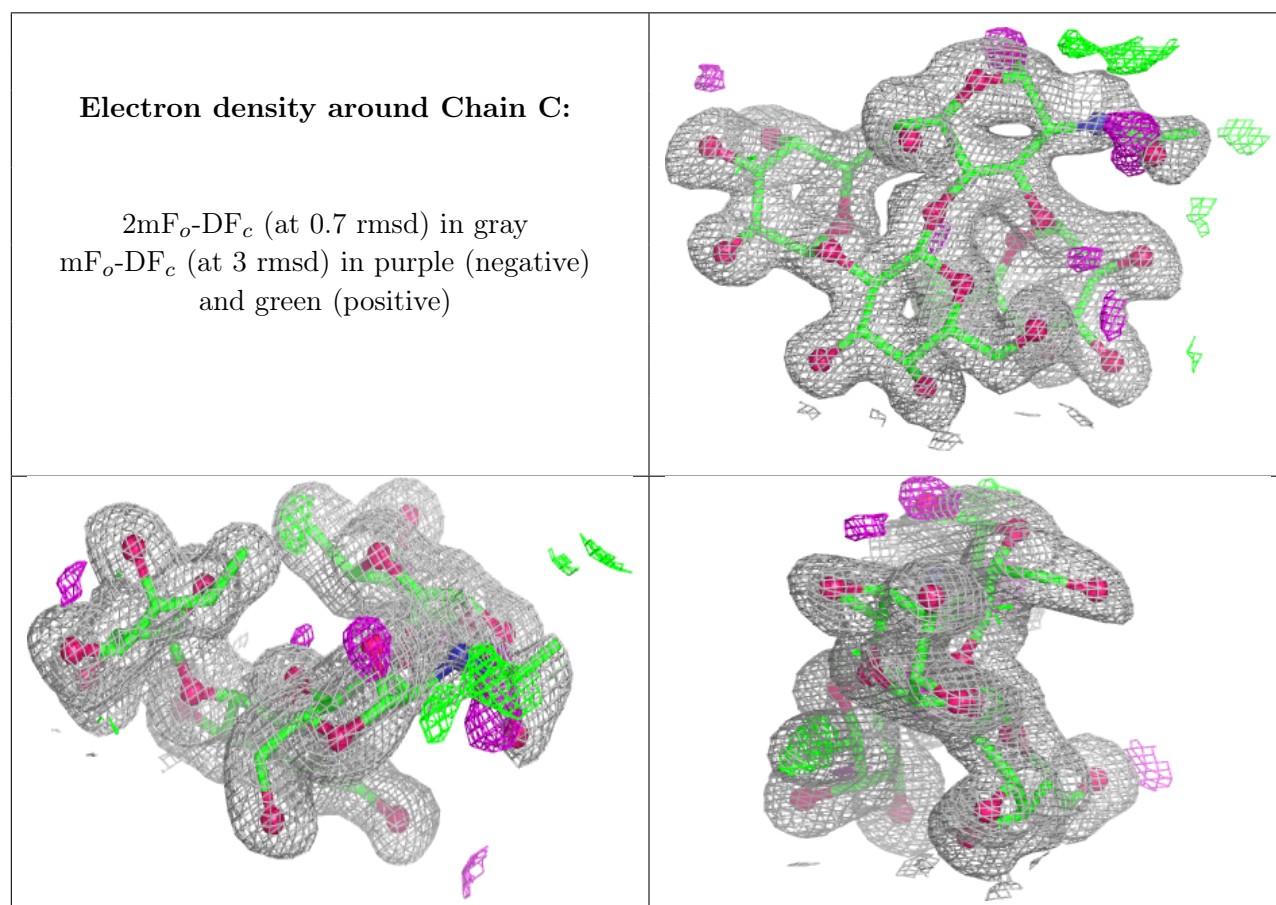
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FUC	D	3	10/11	0.76	0.19	23,27,30,33	0
2	NDG	C	1	15/15	0.88	0.13	26,38,50,52	0
2	FUC	C	4	10/11	0.93	0.08	24,25,27,27	0
2	NDG	D	1	15/15	0.96	0.08	21,29,36,37	0
2	GAL	D	2	11/12	0.96	0.06	17,19,22,25	0

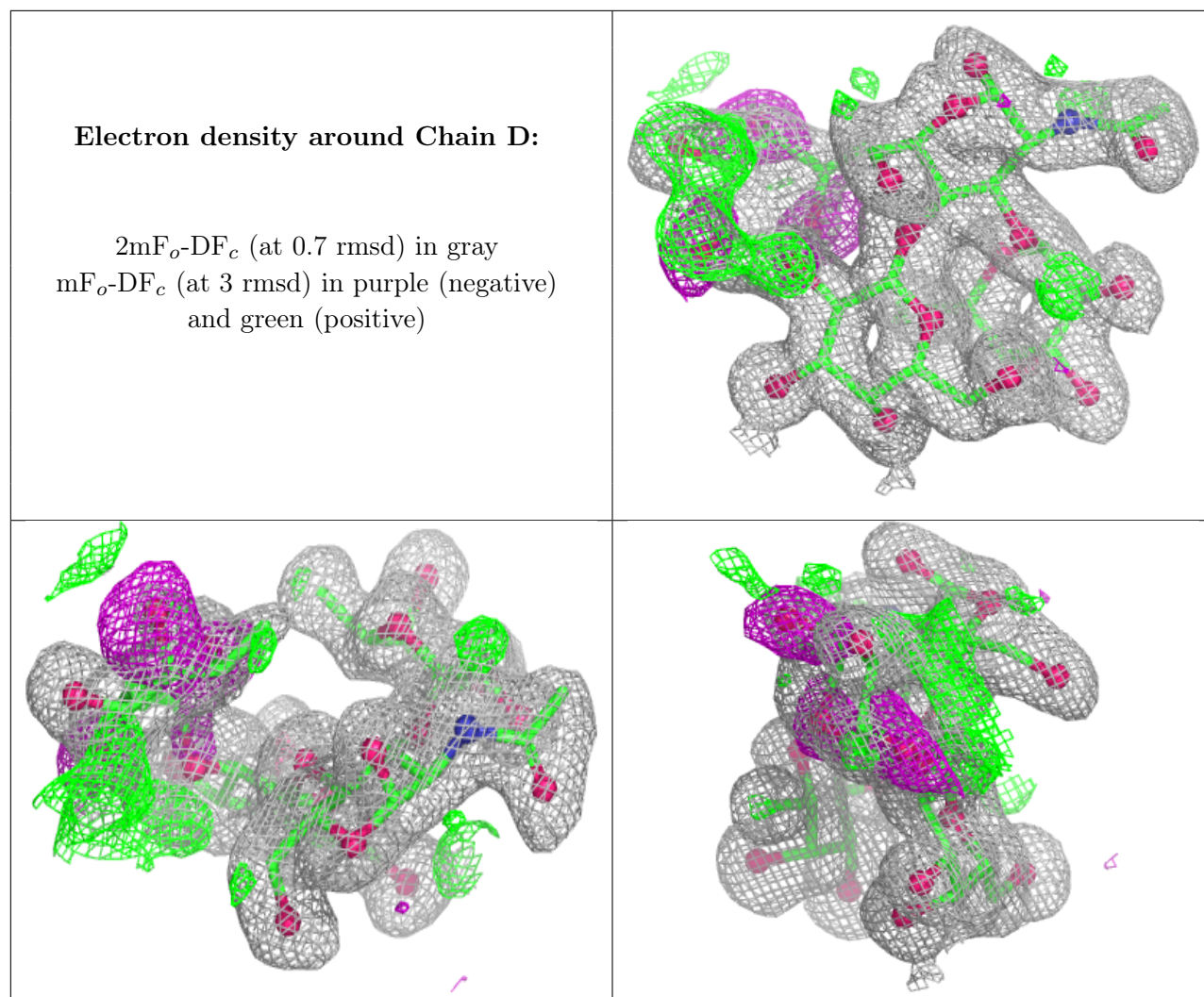
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FUC	C	3	10/11	0.96	0.07	22,23,25,25	0
2	FUC	D	4	10/11	0.96	0.06	19,20,22,24	0
2	GAL	C	2	11/12	0.97	0.05	18,20,25,26	0

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.