



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2024 – 12:29 pm GMT

PDB ID : 8PXV  
Title : Targeting extended blood antigens by Akkermansia muciniphila enzymes unveils a missing link for generating universal donor blood  
Authors : Weikum, J.; Jensen, M.; Abou Hachem, M.; Morth, J.P.  
Deposited on : 2023-07-24  
Resolution : 2.50 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

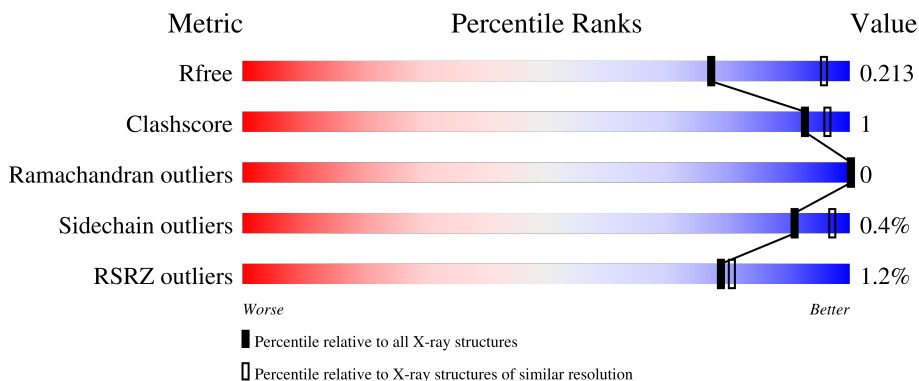
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	655	95%
1	B	655	94%
1	C	655	91% 6%
2	E	2	100%
2	F	2	100%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 30553 atoms, of which 14963 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 Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	646	10102	3230	5019	891	945	17	0	0	0
1	B	634	9963	3188	4955	875	928	17	0	0	0
1	C	632	9932	3178	4942	872	923	17	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B2UN02
A	648	LEU	-	expression tag	UNP B2UN02
A	649	GLU	-	expression tag	UNP B2UN02
A	650	HIS	-	expression tag	UNP B2UN02
A	651	HIS	-	expression tag	UNP B2UN02
A	652	HIS	-	expression tag	UNP B2UN02
A	653	HIS	-	expression tag	UNP B2UN02
A	654	HIS	-	expression tag	UNP B2UN02
A	655	HIS	-	expression tag	UNP B2UN02
B	1	MET	-	initiating methionine	UNP B2UN02
B	648	LEU	-	expression tag	UNP B2UN02
B	649	GLU	-	expression tag	UNP B2UN02
B	650	HIS	-	expression tag	UNP B2UN02
B	651	HIS	-	expression tag	UNP B2UN02
B	652	HIS	-	expression tag	UNP B2UN02
B	653	HIS	-	expression tag	UNP B2UN02
B	654	HIS	-	expression tag	UNP B2UN02
B	655	HIS	-	expression tag	UNP B2UN02
C	1	MET	-	initiating methionine	UNP B2UN02
C	648	LEU	-	expression tag	UNP B2UN02
C	649	GLU	-	expression tag	UNP B2UN02
C	650	HIS	-	expression tag	UNP B2UN02
C	651	HIS	-	expression tag	UNP B2UN02

*Continued on next page...*

Continued from previous page...

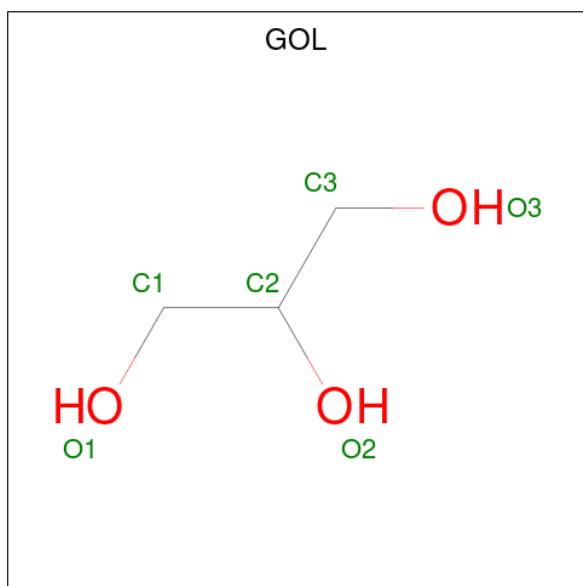
Chain	Residue	Modelled	Actual	Comment	Reference
C	652	HIS	-	expression tag	UNP B2UN02
C	653	HIS	-	expression tag	UNP B2UN02
C	654	HIS	-	expression tag	UNP B2UN02
C	655	HIS	-	expression tag	UNP B2UN02

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
2	E	2	45	12	22	11	0	0	0
2	F	2	45	12	22	11	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	9	3	3	3	0	0

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

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

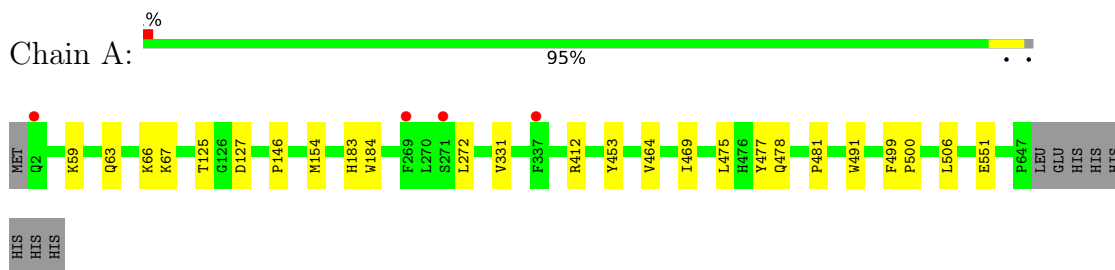
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	165	Total O 165 165	0	0
5	B	142	Total O 142 142	0	0
5	C	149	Total O 149 149	0	0

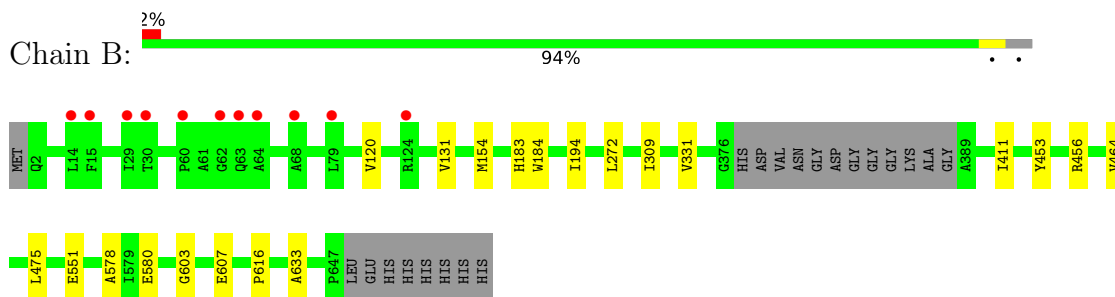
### 3 Residue-property plots [i](#)

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.

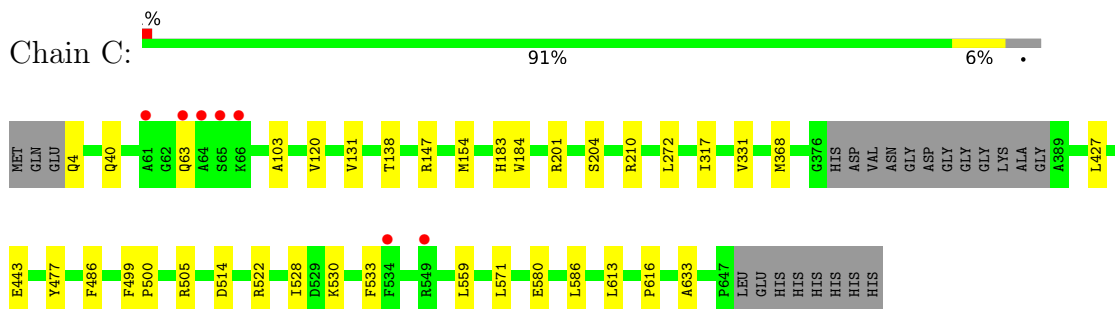
- Molecule 1: Beta-N-acetylhexosaminidase



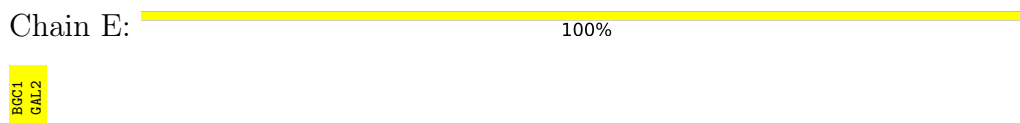
- Molecule 1: Beta-N-acetylhexosaminidase



- Molecule 1: Beta-N-acetylhexosaminidase



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain F:

100%

BGC1  
GAL2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.26Å 170.42Å 171.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.32 – 2.50 60.01 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (54.32-2.50) 95.4 (60.01-2.50)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.178 , 0.212 0.179 , 0.213	Depositor DCC
$R_{free}$ test set	4659 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtrriage
Anisotropy	0.232	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 34.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	30553	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: GOL, BGC, GAL, NA

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	0.26	0/5211	0.52	0/7054
1	B	0.26	0/5134	0.52	0/6950
1	C	0.26	0/5116	0.53	0/6926
All	All	0.26	0/15461	0.53	0/20930

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	5083	5019	5017	14	0
1	B	5008	4955	4953	14	0
1	C	4990	4942	4939	19	0
2	E	23	22	21	0	0
2	F	23	22	21	0	0
3	A	6	3	8	0	0
4	C	1	0	0	0	0
5	A	165	0	0	2	0
5	B	142	0	0	0	0
5	C	149	0	0	0	0
All	All	15590	14963	14959	44	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 1.

The worst 5 of 44 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:B:120:VAL:HG11	1:B:131:VAL:HG21	1.58	0.84
1:B:411:ILE:HG23	1:B:456:ARG:HG3	1.76	0.68
1:A:63:GLN:NE2	5:A:802:HOH:O	2.24	0.66
1:C:120:VAL:HG11	1:C:131:VAL:HG21	1.85	0.58
1:A:272:LEU:HD13	1:A:331:VAL:HG11	1.87	0.57

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	644/655 (98%)	630 (98%)	14 (2%)	0	100	100
1	B	630/655 (96%)	617 (98%)	13 (2%)	0	100	100
1	C	628/655 (96%)	611 (97%)	17 (3%)	0	100	100
All	All	1902/1965 (97%)	1858 (98%)	44 (2%)	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	533/542 (98%)	530 (99%)	3 (1%)	86	95
1	B	527/542 (97%)	526 (100%)	1 (0%)	93	98
1	C	525/542 (97%)	522 (99%)	3 (1%)	86	95
All	All	1585/1626 (98%)	1578 (100%)	7 (0%)	91	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	184	TRP
1	C	63	GLN
1	C	210	ARG
1	C	184	TRP
1	A	184	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	173	GLN

### 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](#)

4 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	BGC	E	1	2	12,12,12	0.20	0	17,17,17	1.79	3 (17%)
2	GAL	E	2	2	11,11,12	0.42	0	15,15,17	1.67	4 (26%)
2	BGC	F	1	2	12,12,12	0.16	0	17,17,17	1.80	6 (35%)
2	GAL	F	2	2	11,11,12	0.43	0	15,15,17	1.63	4 (26%)

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	BGC	E	1	2	-	2/2/22/22	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	1/2/22/22	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	BGC	O4-C4-C3	-3.70	101.79	110.35
2	F	1	BGC	O4-C4-C3	-3.48	102.30	110.35
2	E	1	BGC	C4-C3-C2	-2.69	106.14	110.82
2	E	2	GAL	C1-C2-C3	-2.48	106.62	109.67
2	E	1	BGC	O1-C1-O5	-2.47	102.96	110.38

There are no chirality outliers.

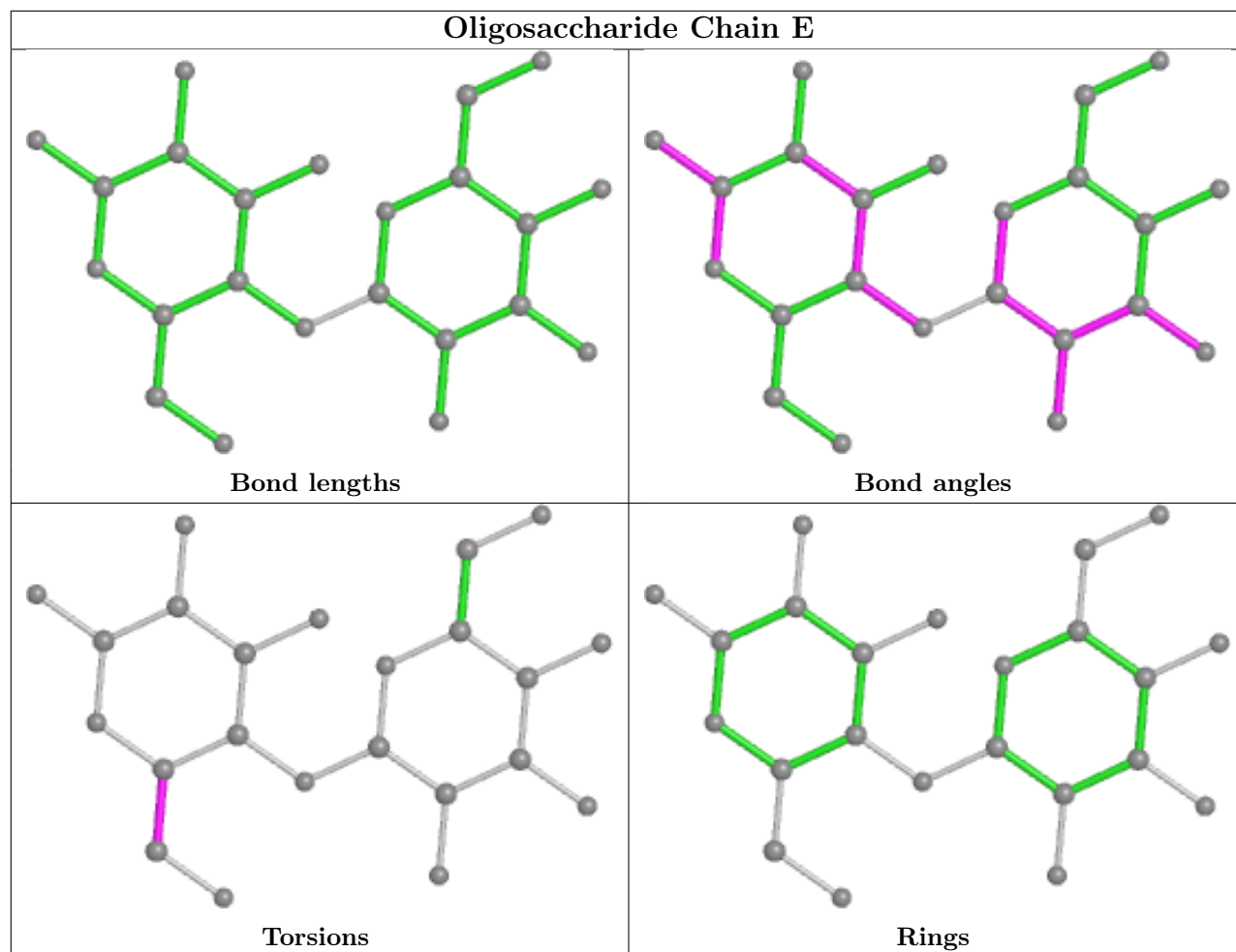
All (3) torsion outliers are listed below:

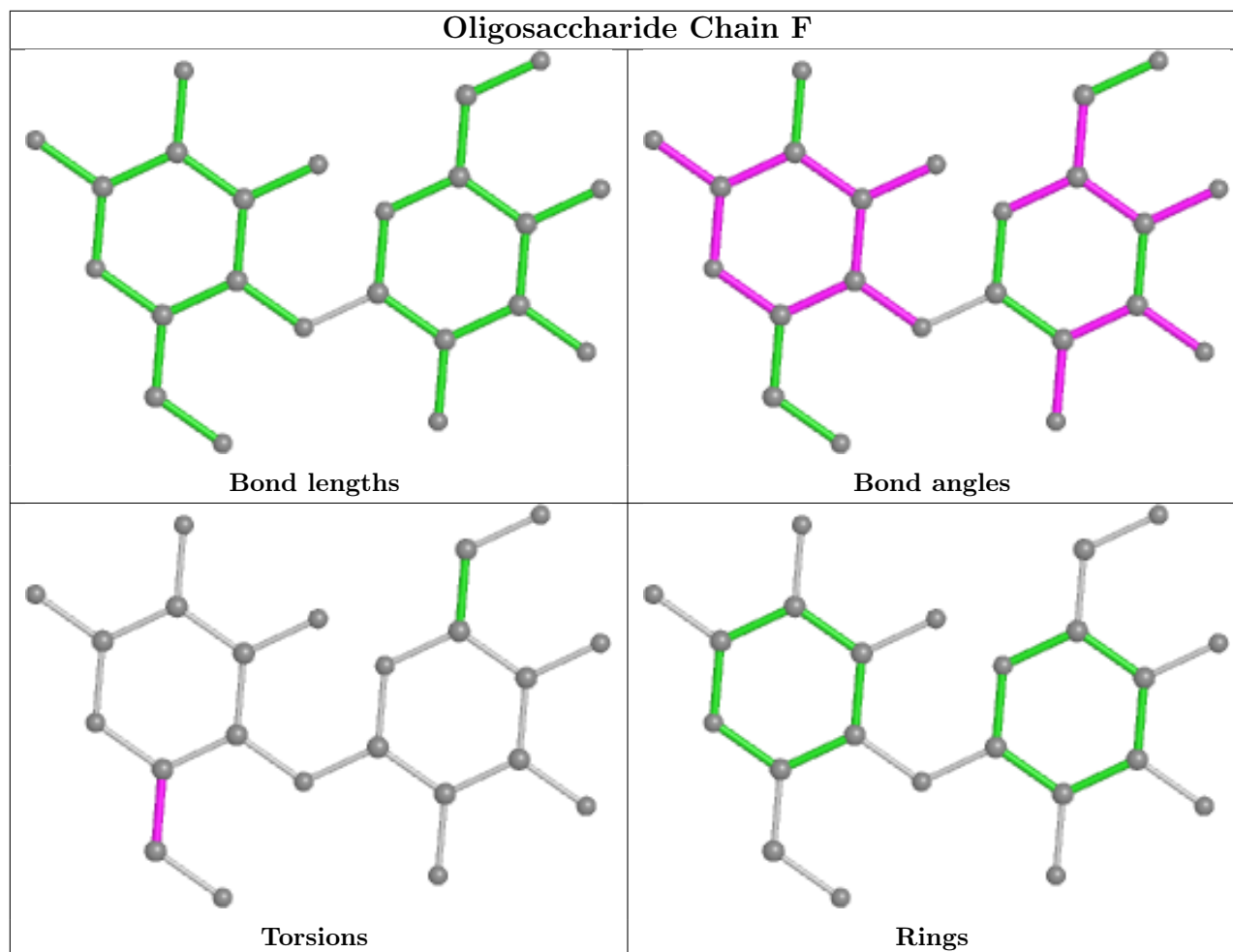
Mol	Chain	Res	Type	Atoms
2	E	1	BGC	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	F	1	BGC	O5-C5-C6-O6

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
3	GOL	A	701	-	5,5,5	0.94	0	5,5,5	0.98	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
3	GOL	A	701	-	-	0/4/4/4	-

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 [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	646/655 (98%)	0.07	4 (0%) 89 90	35, 49, 71, 102	0
1	B	634/655 (96%)	0.08	11 (1%) 70 72	34, 48, 83, 142	0
1	C	632/655 (96%)	0.05	7 (1%) 80 82	34, 47, 77, 137	0
All	All	1912/1965 (97%)	0.07	22 (1%) 79 80	34, 48, 78, 142	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	ALA	6.9
1	B	64	ALA	6.6
1	C	65	SER	6.2
1	B	62	GLY	4.0
1	C	534	PHE	3.7

### 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(Å <sup>2</sup> )	Q<0.9
2	BGC	F	1	12/12	0.81	0.25	41,61,73,81	0
2	GAL	F	2	11/12	0.90	0.19	42,53,62,64	0
2	BGC	E	1	12/12	0.94	0.14	41,50,59,68	0

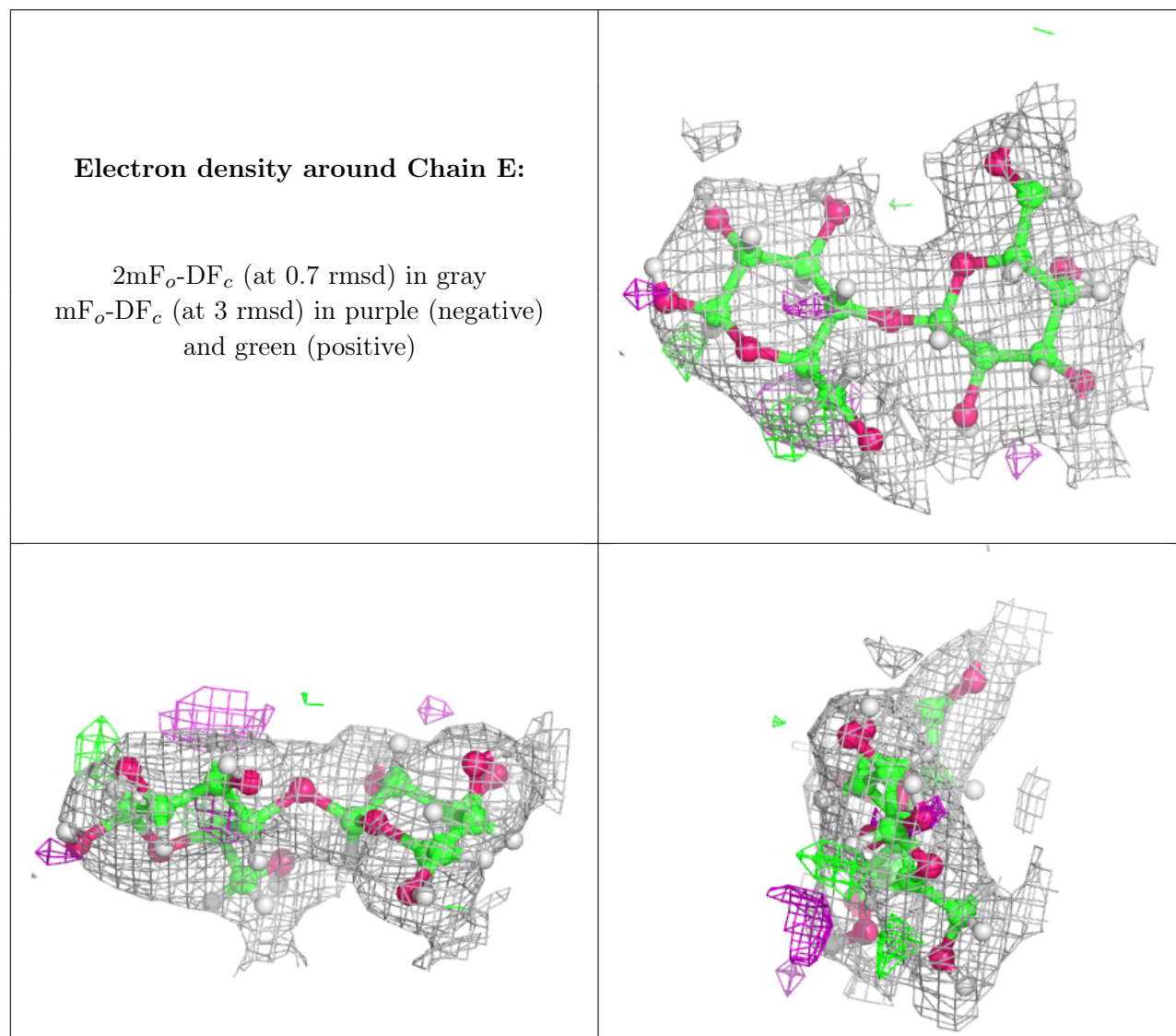
*Continued on next page...*

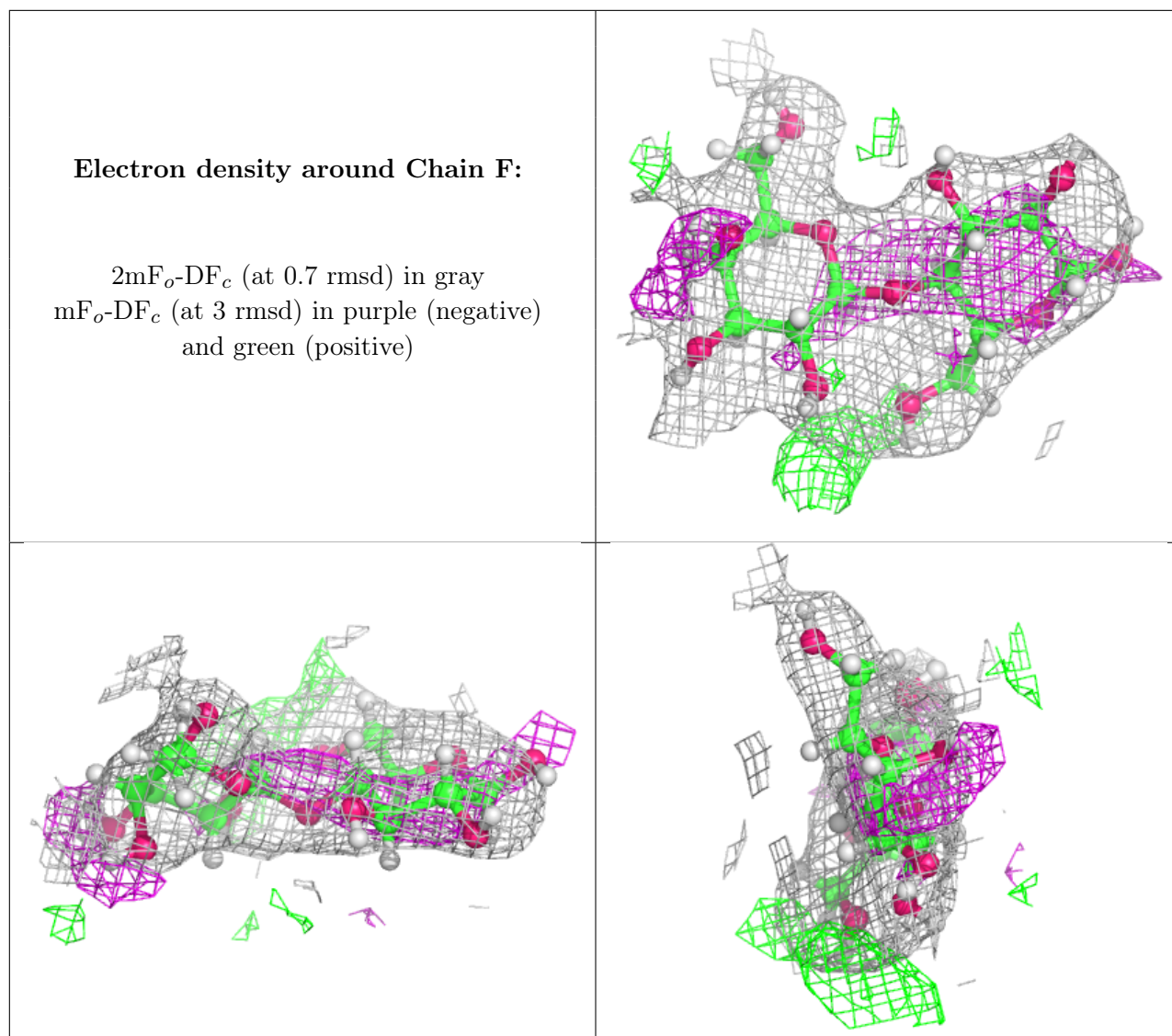


Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GAL	E	2	11/12	0.98	0.14	33,42,50,55	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](#)

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	C	701	1/1	0.84	0.25	55,55,55,55	0
3	GOL	A	701	6/6	0.86	0.25	44,53,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.