



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2026 – 08:17 PM JST

PDB ID : 22HK / pdb\_000022hk  
Title : Beta-1,2-glucan-binding protein complexed with cyclic beta-1,2-glucononadec  
aose  
Authors : Hirayama, R.; Nakajima, M.  
Deposited on : 2026-01-11  
Resolution : 1.27 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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

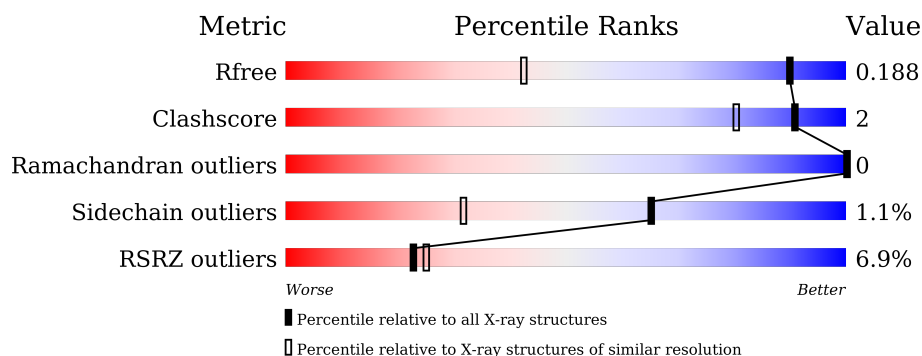
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.27 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	2836 (1.30-1.26)
Clashscore	190562	2911 (1.30-1.26)
Ramachandran outliers	187476	2841 (1.30-1.26)
Sidechain outliers	187428	2840 (1.30-1.26)
RSRZ outliers	180081	2832 (1.30-1.26)

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	474	
2	C	19	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4103 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.

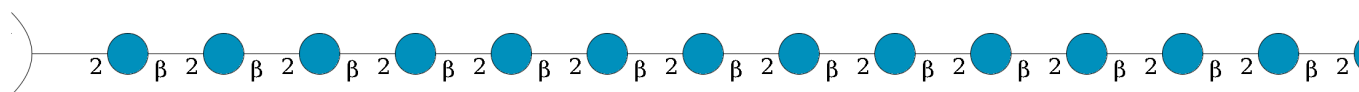
- Molecule 1 is a protein called Extracellular solute-binding protein family 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	9	0
			3454	2215	569	650	20			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP A9WCS2
A	487	LEU	-	expression tag	UNP A9WCS2
A	488	GLU	-	expression tag	UNP A9WCS2
A	489	HIS	-	expression tag	UNP A9WCS2
A	490	HIS	-	expression tag	UNP A9WCS2
A	491	HIS	-	expression tag	UNP A9WCS2
A	492	HIS	-	expression tag	UNP A9WCS2
A	493	HIS	-	expression tag	UNP A9WCS2
A	494	HIS	-	expression tag	UNP A9WCS2

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



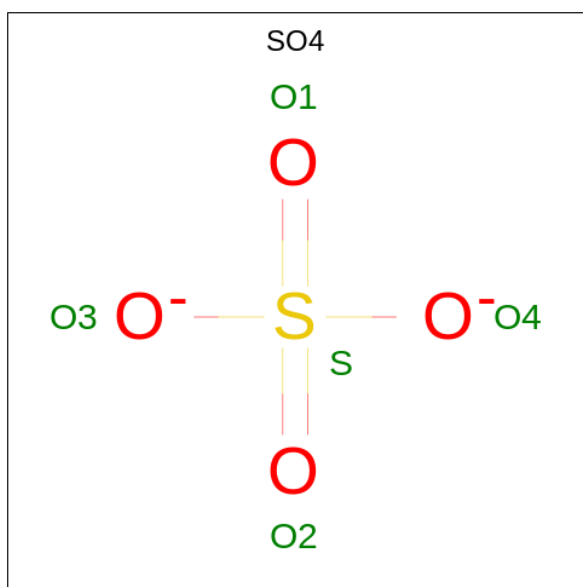
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	19	Total	C	O	0	0	0
			209	114	95			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	412	Total	O	0	0
			412	412		



- Molecule 1: Extracellular solute-binding protein family 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.49Å 83.20Å 94.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.28 – 1.27 47.28 – 1.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.28-1.27) 100.0 (47.28-1.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 1.27Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.165 , 0.181 0.175 , 0.188	Depositor DCC
$R_{free}$ test set	7517 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 33.0	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	4103	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: SO4, BGC, GOL

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	0.86	0/3547	1.15	5/4827 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	203	PHE	CA-CB-CG	8.64	122.44	113.80
1	A	187	ASN	OD1-CG-ND2	5.50	128.10	122.60
1	A	113	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	226	ASP	CA-CB-CG	5.42	118.03	112.60
1	A	480	GLU	CB-CG-CD	5.27	121.56	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	ARG	Sidechain
1	A	179[A]	GLN	Mainchain
1	A	179[B]	GLN	Mainchain
1	A	478[A]	ARG	Sidechain



## 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	3454	0	3294	12	0
2	C	209	0	171	0	0
3	A	18	0	24	0	0
4	A	10	0	0	0	0
5	A	412	0	0	3	0
All	All	4103	0	3489	12	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 2.

The worst 5 of 12 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:335[B]:MET:SD	5:A:975:HOH:O	2.53	0.67
1:A:168:TYR:HB3	1:A:485:LEU:HD11	1.81	0.61
1:A:65:GLN:HE21	1:A:65:GLN:N	1.99	0.61
1:A:162:LEU:HD22	1:A:335[B]:MET:HG2	1.88	0.55
1:A:168:TYR:HB3	1:A:485:LEU:CD1	2.41	0.50

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	430/474 (91%)	416 (97%)	14 (3%)	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	359/389 (92%)	353 (98%)	6 (2%)	53 17

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312[B]	GLN
1	A	333[A]	ILE
1	A	333[B]	ILE
1	A	203	PHE
1	A	65	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	472	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](#)

19 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	C	1	2	11,11,12	0.30	0	15,15,17	0.56	0
2	BGC	C	10	2	11,11,12	0.37	0	15,15,17	0.74	0
2	BGC	C	11	2	11,11,12	0.37	0	15,15,17	0.65	0
2	BGC	C	12	2	11,11,12	0.34	0	15,15,17	0.52	0
2	BGC	C	13	2	11,11,12	0.27	0	15,15,17	0.51	0
2	BGC	C	14	2	11,11,12	0.36	0	15,15,17	0.65	0
2	BGC	C	15	2	11,11,12	0.25	0	15,15,17	0.57	0
2	BGC	C	16	2	11,11,12	0.39	0	15,15,17	0.95	1 (6%)
2	BGC	C	17	2	11,11,12	0.20	0	15,15,17	0.60	0
2	BGC	C	18	2	11,11,12	0.27	0	15,15,17	0.51	0
2	BGC	C	19	2	11,11,12	0.30	0	15,15,17	0.98	1 (6%)
2	BGC	C	2	2	11,11,12	0.30	0	15,15,17	0.60	0
2	BGC	C	3	2	11,11,12	0.35	0	15,15,17	0.63	0
2	BGC	C	4	2	11,11,12	0.27	0	15,15,17	0.62	0
2	BGC	C	5	2	11,11,12	0.35	0	15,15,17	0.52	0
2	BGC	C	6	2	11,11,12	0.24	0	15,15,17	1.02	1 (6%)
2	BGC	C	7	2	11,11,12	0.33	0	15,15,17	0.65	0
2	BGC	C	8	2	11,11,12	0.34	0	15,15,17	0.49	0
2	BGC	C	9	2	11,11,12	0.30	0	15,15,17	0.98	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
2	BGC	C	1	2	-	0/2/19/22	0/1/1/1
2	BGC	C	10	2	-	0/2/19/22	0/1/1/1
2	BGC	C	11	2	-	0/2/19/22	0/1/1/1
2	BGC	C	12	2	-	0/2/19/22	0/1/1/1
2	BGC	C	13	2	-	0/2/19/22	0/1/1/1
2	BGC	C	14	2	-	0/2/19/22	0/1/1/1
2	BGC	C	15	2	-	0/2/19/22	0/1/1/1
2	BGC	C	16	2	-	0/2/19/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	17	2	-	0/2/19/22	0/1/1/1
2	BGC	C	18	2	-	0/2/19/22	0/1/1/1
2	BGC	C	19	2	-	0/2/19/22	0/1/1/1
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	C	6	2	-	0/2/19/22	0/1/1/1
2	BGC	C	7	2	-	0/2/19/22	0/1/1/1
2	BGC	C	8	2	-	0/2/19/22	0/1/1/1
2	BGC	C	9	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	19	BGC	C1-C2-C3	3.30	113.72	109.67
2	C	9	BGC	C1-C2-C3	3.09	113.47	109.67
2	C	6	BGC	C1-C2-C3	2.67	112.94	109.67
2	C	16	BGC	C1-C2-C3	2.13	112.29	109.67

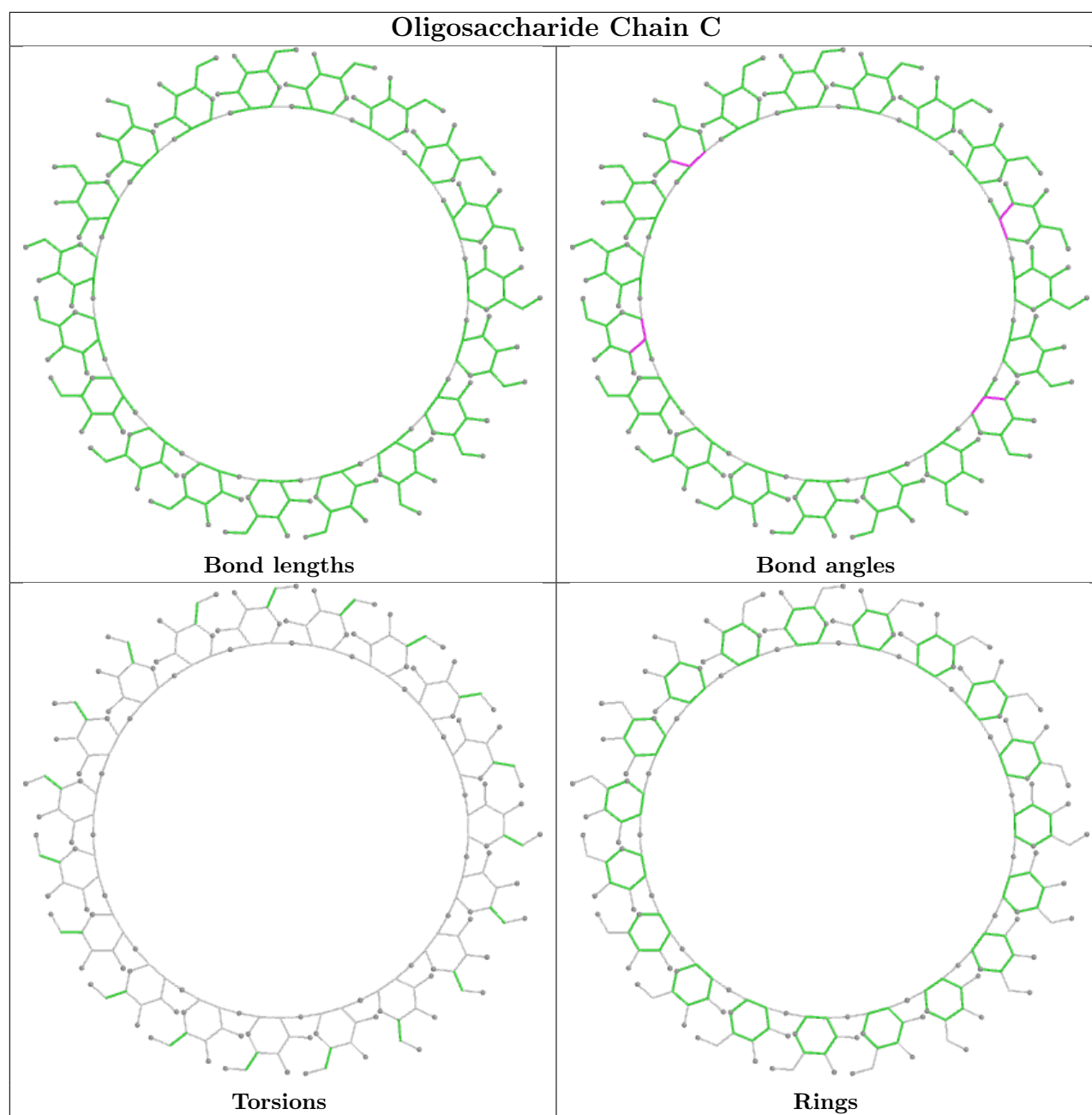
There are no chirality outliers.

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](#)

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
3	GOL	A	503	-	5,5,5	0.20	0	5,5,5	0.23	0
3	GOL	A	501	-	5,5,5	0.22	0	5,5,5	0.33	0
4	SO4	A	504	-	4,4,4	0.37	0	6,6,6	0.32	0
4	SO4	A	505	-	4,4,4	0.36	0	6,6,6	0.19	0
3	GOL	A	502	-	5,5,5	0.10	0	5,5,5	0.52	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	502	-	-	3/4/4/4	-
3	GOL	A	501	-	-	0/4/4/4	-
3	GOL	A	503	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-C3
3	A	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O1-C1-C2-O2

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	423/474 (89%)	0.39	29 (6%) 23 25	7, 17, 30, 52	9 (2%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	VAL	5.0
1	A	434	GLY	4.1
1	A	160	GLU	3.3
1	A	435	ILE	3.3
1	A	487	LEU	3.2

### 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	C	1	11/12	-	-	13,15,19,23	0
2	BGC	C	2	11/12	-	-	12,15,19,21	0
2	BGC	C	3	11/12	-	-	10,11,11,12	0
2	BGC	C	4	11/12	-	-	11,12,13,14	0
2	BGC	C	5	11/12	-	-	11,12,12,12	0
2	BGC	C	6	11/12	-	-	12,13,14,14	0
2	BGC	C	7	11/12	-	-	13,16,19,21	0

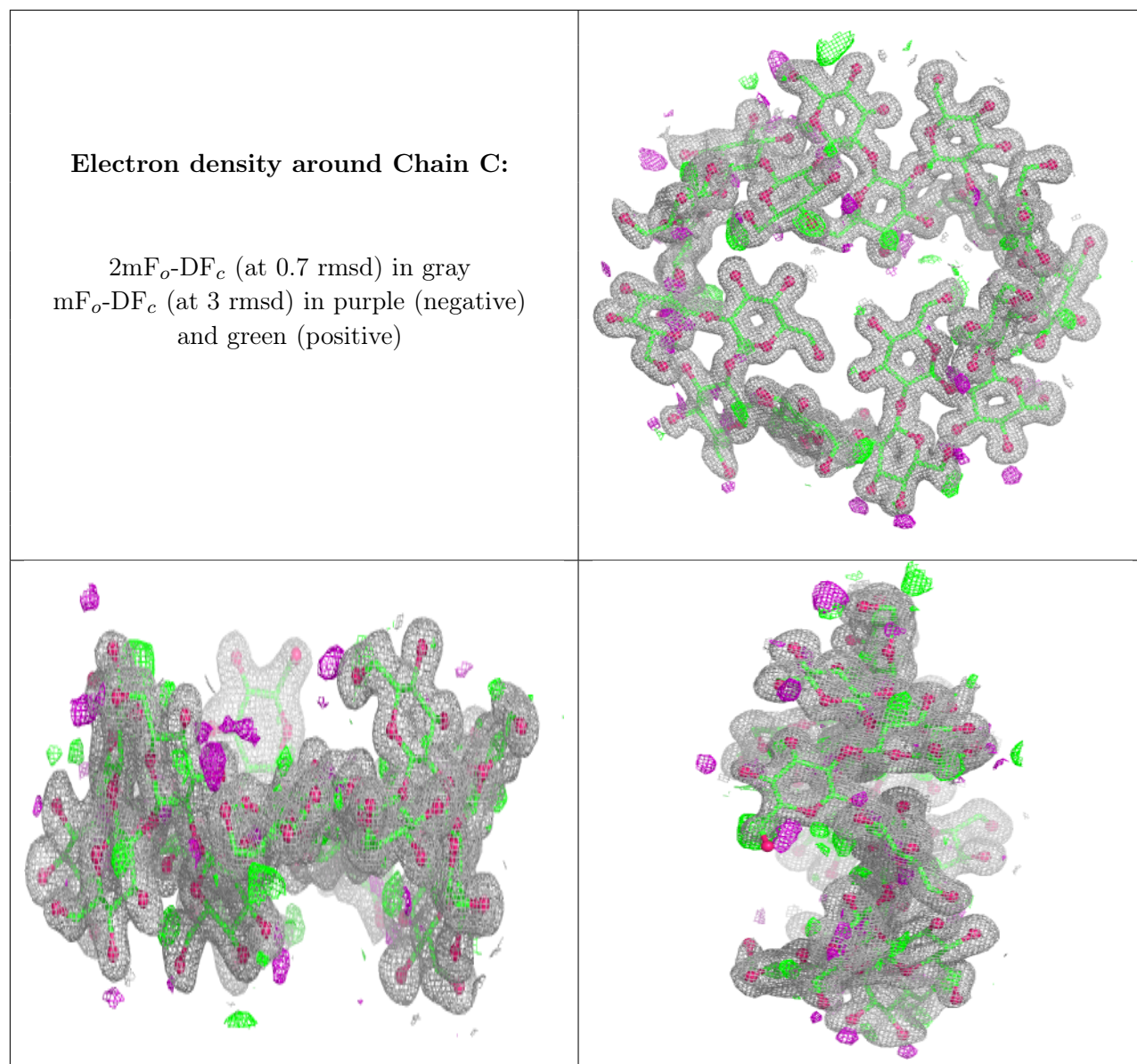
*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	C	8	11/12	-	-	14,15,18,19	0
2	BGC	C	9	11/12	-	-	19,20,22,23	0
2	BGC	C	10	11/12	-	-	22,27,35,37	0
2	BGC	C	11	11/12	-	-	25,32,36,45	0
2	BGC	C	12	11/12	-	-	23,25,29,39	0
2	BGC	C	13	11/12	-	-	23,29,35,42	0
2	BGC	C	14	11/12	-	-	21,22,23,23	0
2	BGC	C	15	11/12	-	-	23,26,32,33	0
2	BGC	C	16	11/12	-	-	25,32,43,62	0
2	BGC	C	17	11/12	-	-	21,28,36,43	0
2	BGC	C	18	11/12	-	-	18,20,23,25	0
2	BGC	C	19	11/12	-	-	16,20,23,28	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
3	GOL	A	502	6/6	0.66	0.20	36,38,43,45	0
3	GOL	A	503	6/6	0.89	0.12	25,30,35,37	0
4	SO4	A	504	5/5	0.91	0.11	29,32,38,41	5
4	SO4	A	505	5/5	0.92	0.11	30,31,41,42	5
3	GOL	A	501	6/6	0.95	0.09	18,19,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.