



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 07:40 AM BST

PDB ID : 1BFN  
Title : BETA-AMYLASE/BETA-CYCLODEXTRIN COMPLEX  
Authors : Adachi, M.; Mikami, B.; Katsube, T.; Utsumi, S.  
Deposited on : 1998-05-22  
Resolution : 2.07 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 : 2.13.1  
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) : 2.13.1

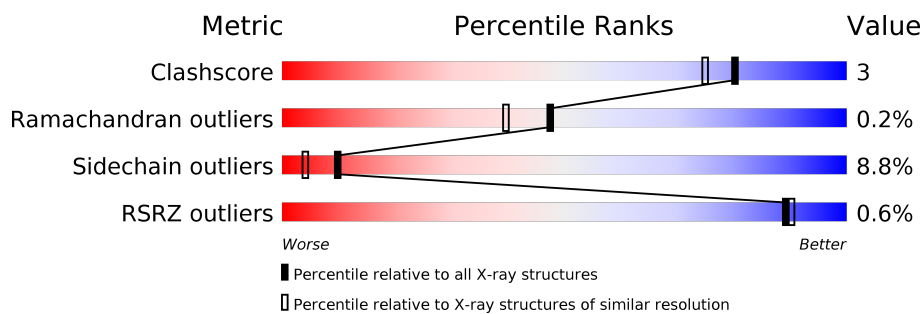
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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))
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 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	495	<div> <div></div> <div>80%</div> <div>16%</div> <div>..</div> </div>
2	B	7	<div> <div>100%</div> </div>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4315 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.

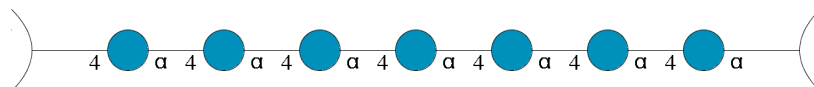
- Molecule 1 is a protein called BETA-AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	3915	2510	660	728	17	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	LEU	PHE	cloning artifact	UNP P10538
A	202	GLY	ARG	variant	UNP P10538
A	399	ARG	LYS	variant	UNP P10538

- Molecule 2 is an oligosaccharide called Cycloheptakis-(1-4)-(alpha-D-glucopyranose).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	7	77	42	35	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

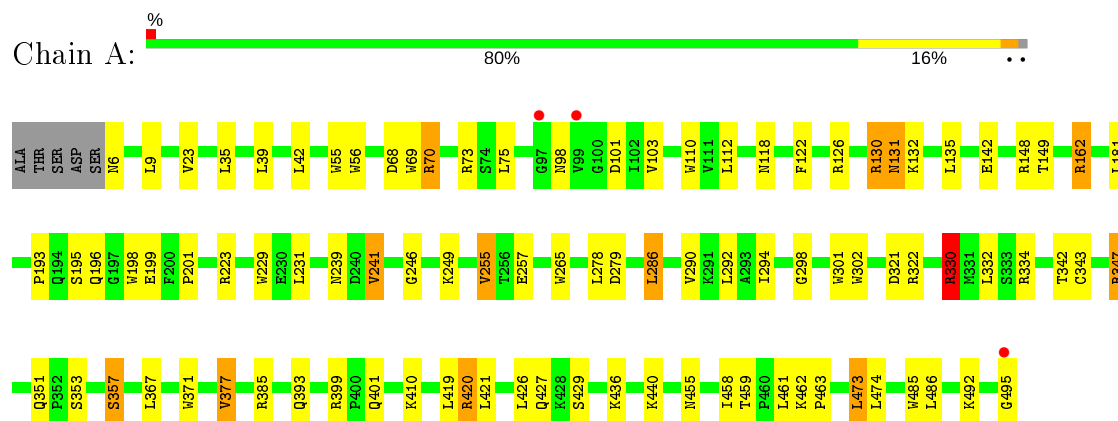
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		

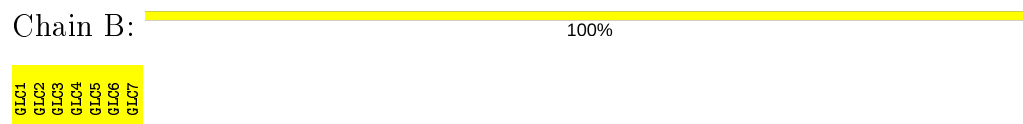
### 3 Residue-property plots [i](#)

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-AMYLASE



#### • Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.03Å 86.03Å 144.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.07 66.25 – 2.07	Depositor EDS
% Data completeness (in resolution range)	80.7 (10.00-2.07) 89.4 (66.25-2.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.34 (at 2.07Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.158 , 0.211 0.162 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: GLC, SO4

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	0.78	0/4021	1.49	70/5463 (1.3%)

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ARG	NE-CZ-NH1	15.14	127.87	120.30
1	A	385	ARG	NE-CZ-NH1	13.87	127.24	120.30
1	A	385	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	A	330	ARG	NE-CZ-NH2	-11.97	114.31	120.30
1	A	330	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	A	419	LEU	CA-C-N	-10.64	93.78	117.20
1	A	162	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	70	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	A	419	LEU	O-C-N	8.39	136.13	122.70
1	A	265	TRP	CD1-CG-CD2	8.38	113.00	106.30
1	A	322	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	A	371	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	A	229	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	A	130	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	130	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	485	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	A	110	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	A	56	TRP	CD1-CG-CD2	7.66	112.42	106.30
1	A	55	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	A	371	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	A	198	TRP	CD1-CG-CD2	7.53	112.32	106.30
1	A	485	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	A	55	TRP	CE2-CD2-CG	-7.42	101.37	107.30
1	A	229	TRP	CE2-CD2-CG	-7.36	101.41	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A	198	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A	347	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	126	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	265	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	302	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	69	TRP	CE2-CD2-CG	-6.88	101.79	107.30
1	A	110	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	148	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	485	TRP	CB-CG-CD1	-6.64	118.37	127.00
1	A	334	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	301	TRP	CE2-CD2-CG	-6.54	102.07	107.30
1	A	69	TRP	CD1-CG-CD2	6.52	111.51	106.30
1	A	420	ARG	CA-CB-CG	-6.47	99.16	113.40
1	A	101	ASP	CA-C-N	-6.46	103.00	117.20
1	A	334	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	495	GLY	N-CA-C	6.24	128.69	113.10
1	A	302	TRP	CD1-CG-CD2	6.13	111.21	106.30
1	A	162	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	265	TRP	CG-CD1-NE1	-5.92	104.19	110.10
1	A	322	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	301	TRP	CD1-CG-CD2	5.82	110.95	106.30
1	A	485	TRP	CG-CD2-CE3	5.81	139.13	133.90
1	A	420	ARG	N-CA-C	5.81	126.69	111.00
1	A	420	ARG	CA-C-N	-5.80	104.43	117.20
1	A	357	SER	N-CA-CB	-5.76	101.86	110.50
1	A	223	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	255	VAL	N-CA-CB	-5.69	98.97	111.50
1	A	321	ASP	CB-CG-OD1	5.68	123.42	118.30
1	A	73	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	241	VAL	N-CA-CB	-5.55	99.29	111.50
1	A	229	TRP	CG-CD2-CE3	5.54	138.88	133.90
1	A	302	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	A	301	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	A	419	LEU	C-N-CA	5.47	135.37	121.70
1	A	302	TRP	CB-CG-CD1	-5.33	120.07	127.00
1	A	399	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	229	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	A	241	VAL	CB-CA-C	5.17	121.23	111.40
1	A	257	GLU	CA-CB-CG	5.13	124.68	113.40
1	A	371	TRP	CG-CD2-CE3	5.12	138.50	133.90
1	A	301	TRP	CB-CG-CD1	-5.11	120.36	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	A	377	VAL	CG1-CB-CG2	-5.06	102.81	110.90
1	A	343	CYS	CA-CB-SG	-5.04	104.93	114.00
1	A	420	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	3915	0	3814	21	0
2	B	77	0	63	0	0
3	A	5	0	0	0	0
4	A	318	0	0	0	0
All	All	4315	0	3877	21	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 (21) 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:199:GLU:H	1:A:239:ASN:HD21	1.40	0.69
1:A:347:ARG:HH11	1:A:393:GLN:NE2	2.01	0.58
1:A:367:LEU:HD22	1:A:377:VAL:HG11	1.86	0.56
1:A:193:PRO:HG2	1:A:196:GLN:HB2	1.89	0.55
1:A:68:ASP:OD1	1:A:70:ARG:HD3	2.06	0.54
1:A:246:GLY:HA2	1:A:249:LYS:HE3	1.89	0.54
1:A:330:ARG:HG2	1:A:473:LEU:HD12	1.91	0.52
1:A:351:GLN:HG3	1:A:357:SER:OG	2.10	0.52
1:A:294:ILE:HG12	1:A:332:LEU:HD21	2.00	0.44
1:A:131:ASN:HD22	1:A:132:LYS:N	2.15	0.44
1:A:367:LEU:HD22	1:A:377:VAL:CG1	2.48	0.44
1:A:199:GLU:H	1:A:239:ASN:ND2	2.10	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLN:HE22	1:A:410:LYS:HE3	1.83	0.42
1:A:122:PHE:HB3	1:A:131:ASN:O	2.19	0.42
1:A:199:GLU:N	1:A:239:ASN:HD21	2.12	0.42
1:A:142:GLU:O	1:A:149:THR:HA	2.19	0.42
1:A:298:GLY:H	1:A:342:THR:CG2	2.33	0.41
1:A:436:LYS:O	1:A:440:LYS:HG2	2.21	0.41
1:A:98:ASN:ND2	1:A:195:SER:HB3	2.36	0.41
1:A:286:LEU:HD21	1:A:463:PRO:HD3	2.01	0.40
1:A:458:ILE:HG22	1:A:459:THR:O	2.21	0.40

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	488/495 (99%)	475 (97%)	12 (2%)	1 (0%)	47 39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	ARG

### 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	420/424 (99%)	383 (91%)	37 (9%)	10 4

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	9	LEU
1	A	23	VAL
1	A	35	LEU
1	A	39	LEU
1	A	42	LEU
1	A	75	LEU
1	A	103	VAL
1	A	112	LEU
1	A	118	ASN
1	A	130	ARG
1	A	131	ASN
1	A	135	LEU
1	A	162	ARG
1	A	181	LEU
1	A	201	PRO
1	A	231	LEU
1	A	241	VAL
1	A	255	VAL
1	A	278	LEU
1	A	279	ASP
1	A	286	LEU
1	A	290	VAL
1	A	292	LEU
1	A	330	ARG
1	A	353	SER
1	A	421	LEU
1	A	426	LEU
1	A	427	GLN
1	A	429	SER
1	A	455	ASN
1	A	461	LEU
1	A	462	LYS
1	A	473	LEU
1	A	474	LEU
1	A	486	LEU
1	A	492	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	98	ASN
1	A	118	ASN
1	A	131	ASN
1	A	196	GLN
1	A	207	GLN
1	A	239	ASN
1	A	268	ASN
1	A	340	ASN
1	A	393	GLN
1	A	401	GLN
1	A	456	HIS

### 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 ⓘ

7 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	GLC	B	1	2	11,11,12	1.04	0	15,15,17	1.12	1 (6%)
2	GLC	B	2	2	11,11,12	0.67	0	15,15,17	1.23	1 (6%)
2	GLC	B	3	2	11,11,12	0.88	0	15,15,17	1.05	1 (6%)
2	GLC	B	4	2	11,11,12	0.76	0	15,15,17	0.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	B	5	2	11,11,12	0.62	0	15,15,17	1.10	1 (6%)
2	GLC	B	6	2	11,11,12	1.00	0	15,15,17	1.05	2 (13%)
2	GLC	B	7	2	11,11,12	1.15	1 (9%)	15,15,17	1.33	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
2	GLC	B	1	2	-	0/2/19/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1
2	GLC	B	3	2	-	0/2/19/22	0/1/1/1
2	GLC	B	4	2	-	1/2/19/22	0/1/1/1
2	GLC	B	5	2	-	0/2/19/22	0/1/1/1
2	GLC	B	6	2	-	0/2/19/22	0/1/1/1
2	GLC	B	7	2	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	GLC	C2-C3	2.30	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GLC	C1-O5-C5	3.92	117.50	112.19
2	B	7	GLC	C1-O5-C5	3.75	117.28	112.19
2	B	5	GLC	C1-O5-C5	3.14	116.44	112.19
2	B	6	GLC	O4-C4-C3	-2.59	104.36	110.35
2	B	4	GLC	C1-O5-C5	2.51	115.59	112.19
2	B	1	GLC	O4-C4-C3	-2.24	105.18	110.35
2	B	3	GLC	C3-C4-C5	2.17	114.11	110.24
2	B	7	GLC	C3-C4-C5	-2.14	106.42	110.24
2	B	6	GLC	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

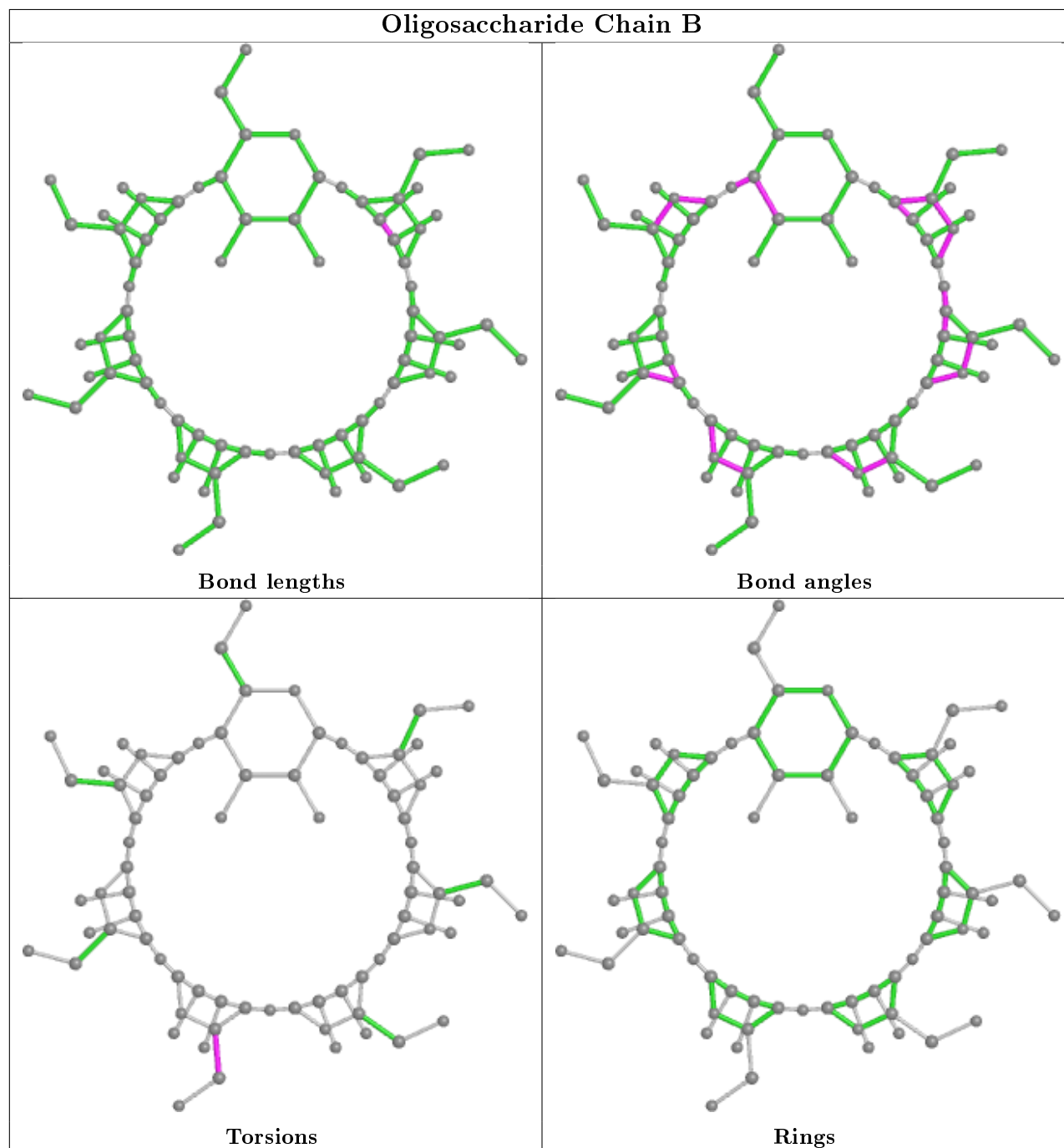
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	GLC	C4-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 ⓘ

1 ligand is 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	SO4	A	503	-	4,4,4	0.46	0	6,6,6	0.56	0

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	490/495 (98%)	-0.74	3 (0%) 89 90	11, 18, 36, 67	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	GLY	3.8
1	A	99	VAL	3.3
1	A	97	GLY	2.1

### 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](#)

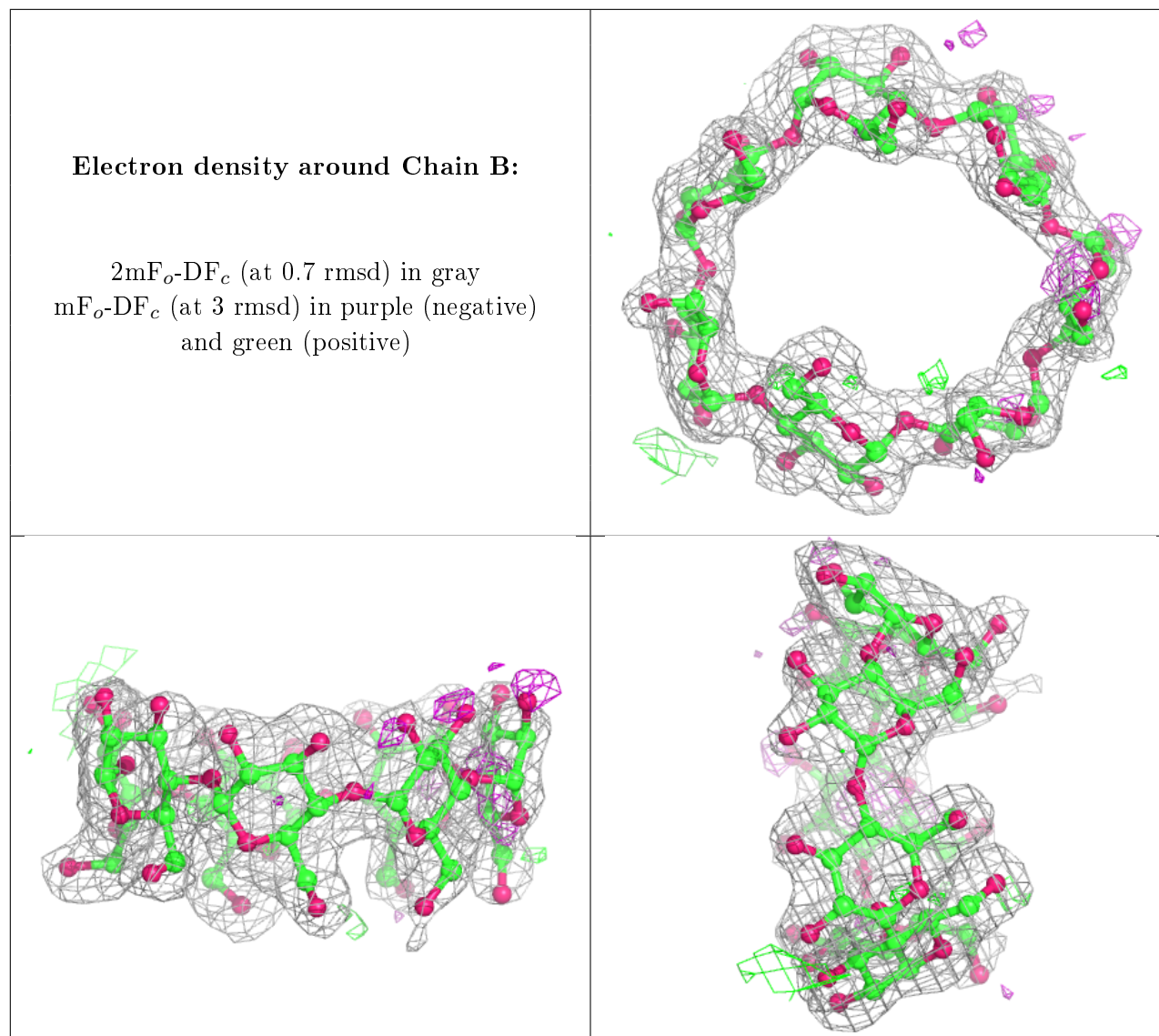
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	GLC	B	3	11/12	0.84	0.26	46,53,58,58	0
2	GLC	B	1	11/12	0.90	0.11	42,47,51,54	0
2	GLC	B	2	11/12	0.91	0.17	49,52,55,59	0
2	GLC	B	7	11/12	0.91	0.18	47,50,52,52	0
2	GLC	B	4	11/12	0.93	0.17	37,46,49,53	0
2	GLC	B	6	11/12	0.94	0.11	32,35,41,44	0
2	GLC	B	5	11/12	0.96	0.07	25,27,29,29	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-



charide. 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( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	503	5/5	0.94	0.11	52,52,55,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.