



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 05:08 PM BST

PDB ID : 3ILF  
Title : Crystal structure of porphyranase A (PorA) in complex with neo-porphyrerotetraose  
Authors : Hehemann, J.H.; Correc, G.; Barbeyron, T.; Helbert, W.; Michel, G.; Czjzek, M.  
Deposited on : 2009-08-07  
Resolution : 1.80 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

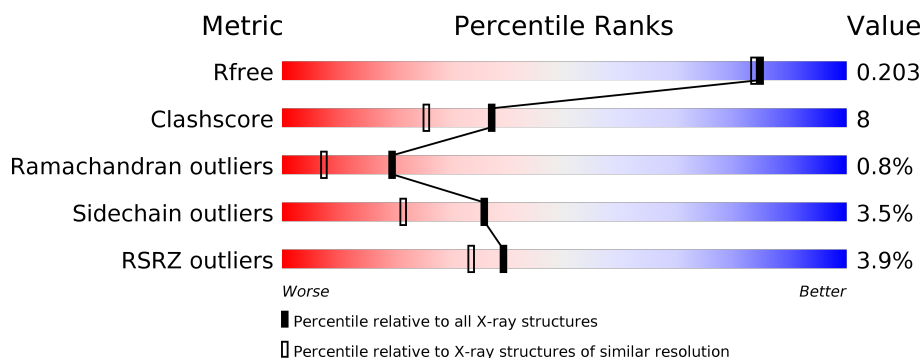
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	268	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• •</div> </div> </div>
2	B	4	<div> <div>75%</div> <div>25%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	L6S	B	4	X	-	-	-
6	ACT	A	282	-	-	X	-

## 2 Entry composition [i](#)

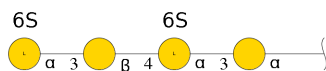
There are 7 unique types of molecules in this entry. The entry contains 2556 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 porphyrinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	8	0
			2159	1386	367	400	6			

- Molecule 2 is an oligosaccharide called 6-O-sulfo-alpha-L-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-6-O-sulfo-alpha-L-galactopyranose-(1-3)-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	O	S	0	0	0
			53	24	27	2			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



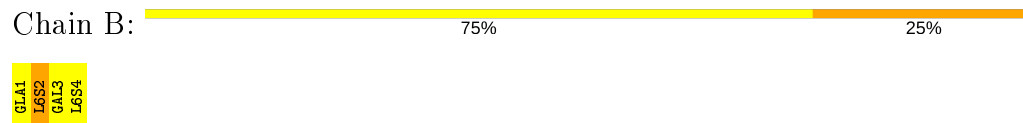
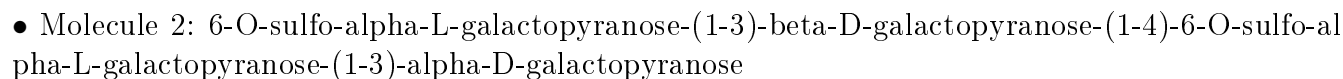
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	324	Total	O	0	0
			324	324		



- Molecule 1: porphyranase A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.09Å 68.38Å 71.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 1.80 18.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.0 (49.34-1.80) 94.1 (18.37-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.93 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.157 , 0.205 0.158 , 0.203	Depositor DCC
$R_{free}$ test set	1381 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2556	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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: MG, L6S, CL, GLA, CA, GAL, ACT

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	1.30	5/2236 (0.2%)	1.07	2/3032 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	GLU	CD-OE2	5.97	1.32	1.25
1	A	192	PHE	CD2-CE2	5.67	1.50	1.39
1	A	169	TYR	CD2-CE2	5.35	1.47	1.39
1	A	208	TYR	CD1-CE1	5.34	1.47	1.39
1	A	34	GLN	CG-CD	5.15	1.62	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	PHE	CB-CG-CD2	-5.38	117.03	120.80
1	A	256	ASP	CB-CG-OD2	-5.09	113.72	118.30

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	2159	0	2063	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	36	1	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	16	0	12	5	0
7	A	324	0	0	6	2
All	All	2556	0	2111	34	2

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 8.

All (34) 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:18:ALA:HB2	7:A:449:HOH:O	1.60	1.00
1:A:240[B]:THR:HG23	1:A:241[B]:ALA:N	1.83	0.93
1:A:266:TRP:HE1	6:A:285:ACT:H2	1.33	0.91
1:A:259:LYS:HZ3	6:A:282:ACT:H3	1.39	0.84
1:A:259:LYS:NZ	6:A:282:ACT:H3	1.91	0.84
1:A:240[B]:THR:HG23	1:A:242[B]:GLY:N	1.97	0.79
1:A:240[B]:THR:HG22	1:A:243:VAL:N	2.01	0.75
1:A:240[B]:THR:O	1:A:241[B]:ALA:C	2.28	0.71
1:A:240[B]:THR:HG23	1:A:242[B]:GLY:H	1.55	0.70
1:A:245:ASN:HB2	7:A:567:HOH:O	1.91	0.69
1:A:28:LYS:N	1:A:28:LYS:HE2	2.08	0.69
1:A:240[B]:THR:HG23	1:A:241[B]:ALA:CA	2.22	0.68
1:A:240[B]:THR:CG2	1:A:242[B]:GLY:H	2.06	0.68
1:A:273:VAL:O	1:A:274:ASP:HB2	1.94	0.67
1:A:42:ASN:ND2	7:A:421:HOH:O	2.27	0.67
1:A:240[B]:THR:CG2	1:A:242[B]:GLY:N	2.59	0.64
1:A:56:TRP:CE2	2:B:2:L6S:H4	2.39	0.57
1:A:259:LYS:NZ	6:A:282:ACT:CH3	2.66	0.56
1:A:239:ALA:O	1:A:240[A]:THR:HB	2.12	0.50
1:A:19:GLN:HE21	1:A:19:GLN:HA	1.78	0.49
1:A:83[B]:ARG:NH1	7:A:376:HOH:O	2.33	0.49
1:A:240[B]:THR:HG23	1:A:241[B]:ALA:HB3	1.95	0.47
1:A:240[B]:THR:HG22	1:A:242[B]:GLY:C	2.35	0.46
1:A:240[B]:THR:HG23	1:A:241[B]:ALA:CB	2.46	0.46
1:A:83[B]:ARG:HD2	1:A:99:ASP:OD1	2.16	0.46
1:A:83[B]:ARG:CD	1:A:99:ASP:OD1	2.65	0.44
1:A:259:LYS:HZ2	6:A:282:ACT:CH3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240[B]:THR:HG23	1:A:241[B]:ALA:C	2.38	0.44
1:A:50:TYR:O	1:A:103:ALA:HA	2.20	0.42
1:A:133:ARG:HG3	1:A:139:SER:HB3	2.02	0.42
1:A:245:ASN:HA	7:A:6:HOH:O	2.19	0.41
1:A:94:LYS:HD3	7:A:439:HOH:O	2.21	0.41
1:A:151:LYS:HA	1:A:151:LYS:HD3	1.96	0.41
1:A:19:GLN:NE2	1:A:19:GLN:HA	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:565:HOH:O	7:A:567:HOH:O[2_554]	1.74	0.46
7:A:558:HOH:O	7:A:561:HOH:O[4_555]	2.17	0.03

## 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	263/268 (98%)	247 (94%)	13 (5%)	3 (1%)	14 4

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241[A]	ALA
1	A	241[B]	ALA
1	A	243	VAL

### 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	232/234 (99%)	223 (96%)	9 (4%)	32	17

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	28	LYS
1	A	157	ASP
1	A	162	TYR
1	A	165	ASN
1	A	212	LYS
1	A	252[A]	GLU
1	A	252[B]	GLU
1	A	274	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	42	ASN
1	A	165	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 ⓘ

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	GLA	B	1	2	12,12,12	1.05	0	17,17,17	3.26	6 (35%)
2	L6S	B	2	2	15,15,16	1.10	3 (20%)	20,22,24	3.30	8 (40%)
2	GAL	B	3	2	11,11,12	1.43	1 (9%)	15,15,17	3.01	6 (40%)
2	L6S	B	4	2	15,15,16	1.95	2 (13%)	20,22,24	5.23	11 (55%)

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	GLA	B	1	2	-	0/2/22/22	0/1/1/1
2	L6S	B	2	2	-	0/6/23/26	0/1/1/1
2	GAL	B	3	2	-	0/2/19/22	0/1/1/1
2	L6S	B	4	2	1/1/5/6	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	L6S	C2-C3	-5.23	1.44	1.52
2	B	4	L6S	O5-C1	4.39	1.50	1.43
2	B	3	GAL	O3-C3	3.62	1.51	1.43
2	B	2	L6S	O5-C1	-2.57	1.39	1.43
2	B	2	L6S	C1-C2	-2.33	1.46	1.52
2	B	2	L6S	O4-C4	2.02	1.47	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	L6S	C1-C2-C3	-16.91	88.88	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLA	C1-C2-C3	-8.84	91.97	110.31
2	B	2	L6S	O4-C4-C3	-8.70	90.24	110.35
2	B	4	L6S	C1-O5-C5	-8.56	100.60	112.19
2	B	3	GAL	O3-C3-C4	8.39	129.74	110.35
2	B	4	L6S	O2-C2-C3	-6.95	96.22	110.14
2	B	2	L6S	C1-O5-C5	-6.56	103.30	112.19
2	B	4	L6S	O4-C4-C5	-6.42	93.36	109.30
2	B	2	L6S	C1-C2-C3	-6.22	102.02	109.67
2	B	4	L6S	O4-C4-C3	5.95	124.11	110.35
2	B	1	GLA	O5-C1-C2	5.55	120.19	110.28
2	B	1	GLA	O3-C3-C4	-4.91	99.00	110.35
2	B	3	GAL	O3-C3-C2	-4.80	100.80	109.99
2	B	1	GLA	C1-O5-C5	-4.35	105.45	113.66
2	B	2	L6S	C2-C3-C4	4.26	118.26	110.89
2	B	4	L6S	C3-C4-C5	4.25	117.82	110.24
2	B	3	GAL	C1-O5-C5	-3.57	107.36	112.19
2	B	1	GLA	O1-C1-C2	3.53	118.98	109.03
2	B	4	L6S	O5-C5-C4	-3.37	102.62	110.83
2	B	2	L6S	O2-C2-C1	3.30	115.91	109.15
2	B	4	L6S	O5-C5-C6	3.27	114.86	107.61
2	B	3	GAL	C3-C4-C5	-2.80	105.24	110.24
2	B	3	GAL	O5-C5-C6	2.67	111.39	107.20
2	B	4	L6S	C2-C3-C4	2.52	115.26	110.89
2	B	4	L6S	O6-S1-O2S	2.49	114.41	106.88
2	B	2	L6S	O5-C5-C6	2.30	112.69	107.61
2	B	4	L6S	O6-C6-C5	2.29	111.90	107.62
2	B	3	GAL	C1-C2-C3	-2.27	106.88	109.67
2	B	2	L6S	C6-C5-C4	-2.23	107.44	112.09
2	B	1	GLA	C3-C4-C5	-2.02	106.64	110.24
2	B	2	L6S	O5-C1-C2	2.01	113.88	110.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	4	L6S	C1

All (2) torsion outliers are listed below:

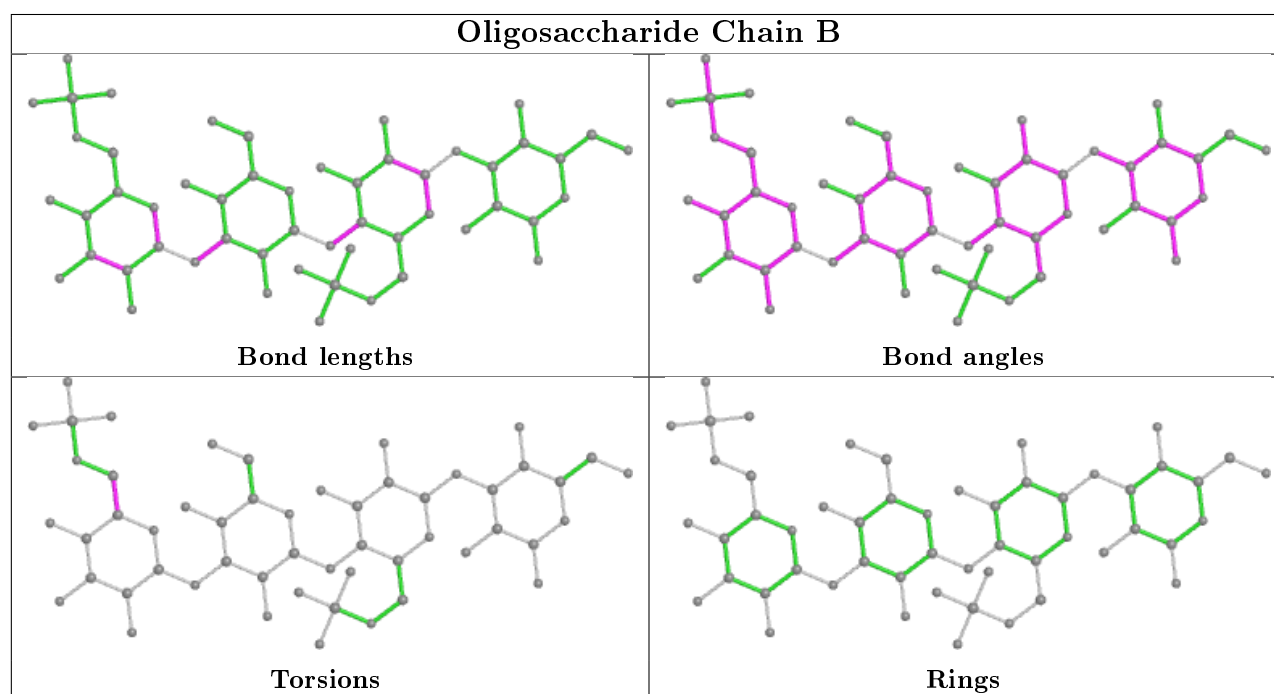
Mol	Chain	Res	Type	Atoms
2	B	4	L6S	C4-C5-C6-O6
2	B	4	L6S	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	L6S	1	0

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z  > 2$
6	ACT	A	282	-	1,3,3	0.38	0	0,3,3	0.00	-
6	ACT	A	285	-	1,3,3	3.63	1 (100%)	0,3,3	0.00	-
6	ACT	A	284	-	1,3,3	1.88	0	0,3,3	0.00	-
6	ACT	A	283	-	1,3,3	1.64	0	0,3,3	0.00	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	285	ACT	CH3-C	3.63	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	282	ACT	4	0
6	A	285	ACT	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	257/268 (95%)	-0.37	10 (3%) 39 33	4, 9, 23, 39	5 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	ALA	11.0
1	A	242[A]	GLY	8.5
1	A	241[A]	ALA	8.3
1	A	18	ALA	6.4
1	A	240[A]	THR	6.3
1	A	156	ASP	2.4
1	A	153	ASN	2.3
1	A	152	GLU	2.3
1	A	243	VAL	2.3
1	A	19	GLN	2.2

### 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	L6S	B	4	15/16	0.79	0.23	33,39,57,58	0
2	GAL	B	3	11/12	0.93	0.10	10,13,20,26	0

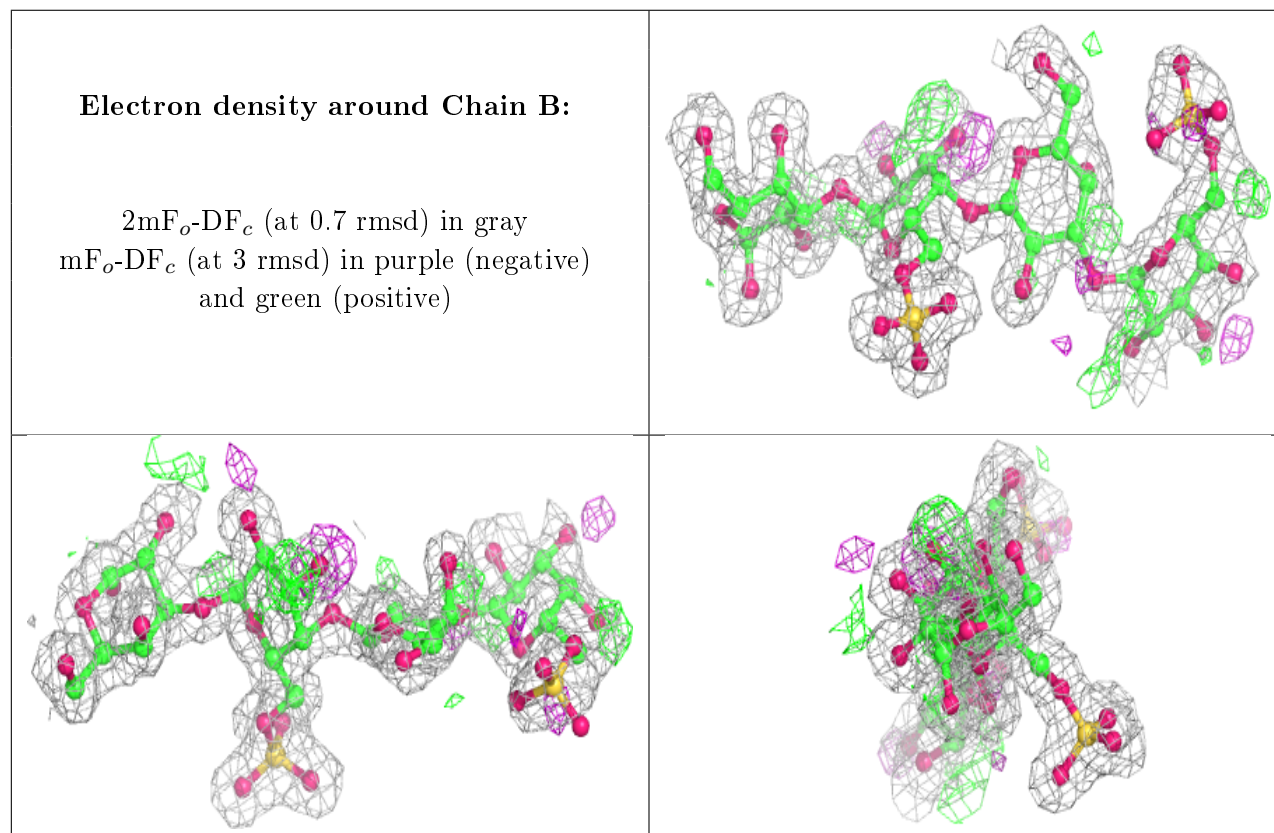
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	L6S	B	2	15/16	0.96	0.08	4,6,9,10	0
2	GLA	B	1	12/12	0.97	0.06	2,5,10,14	0

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( $\text{\AA}^2$ )	Q<0.9
6	ACT	A	284	4/4	0.58	0.24	62,62,63,63	0
6	ACT	A	285	4/4	0.80	0.16	28,31,31,31	0
6	ACT	A	282	4/4	0.90	0.13	29,29,31,32	0
6	ACT	A	283	4/4	0.96	0.15	23,25,25,26	0
4	MG	A	279	1/1	0.99	0.24	7,7,7,7	0
5	CL	A	280	1/1	0.99	0.17	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	A	278	1/1	1.00	0.03	8,8,8,8	0
5	CL	A	281	1/1	1.00	0.03	8,8,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.