

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 9, 2020 – 01:57 AM BST

PDB ID : 2X97

Title: Crystal structure of AnCE-RXP407 complex

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 $Deposited \ on \quad : \quad 2010 \hbox{--} 03 \hbox{--} 14$ 

Resolution : 1.85 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) 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 buster-report : 1.1.7 (2018)

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)

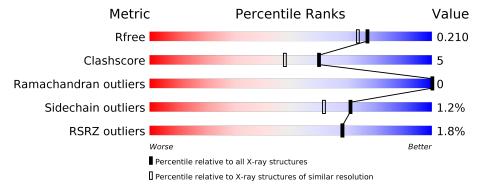
Validation Pipeline (wwPDB-VP) : 2.13.1

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{aligned}  ext{Similar resolution} \ (\# ext{Entries},  ext{resolution range}( ext{Å})) \end{aligned}$
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 >=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 <=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	598	86%	13%						
2	В	6	100%							

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
5	NAG	A	1622	-	-	-	X



## 2 Entry composition (i)

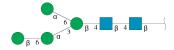
There are 6 unique types of molecules in this entry. The entry contains 5756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ANGIOTENSIN CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	598	Total	С	N	О	S	0	9	0
1	A	J90	4883	3124	806	933	20	U	2	

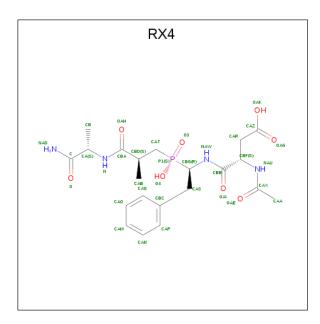
• Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose e-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	6	Total C N O 72 40 2 30	0	0	0

• Molecule 3 is N 2 -acetyl-N- $\{(1R)-1-[(S)-[(2S)-3-\{[(2S)-1-amino-1-oxopropan-2-yl]amino}\}-2-methyl-3-oxopropyl](hydroxy)phosphoryl]-2-phenylethyl}-L-alpha-asparagine (three-letter code: RX4) (formula: <math>C_{21}H_{31}N_4O_8P$ ).



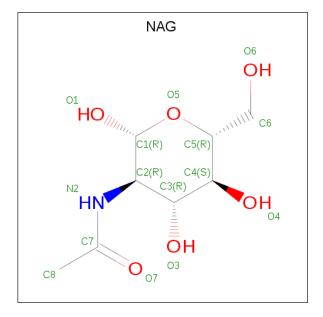


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	Α	1	Total	С	Ν	О	Р	0	0
) o	A	1	34	21	4	8	1	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

 $\bullet$  Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $\rm C_8H_{15}NO_6).$ 





$\mathbf{Mol}$	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf
5	A	1	Total 14		_	O 5	0	0
5	A	1	Total 14	C 8	N 1	O 5	0	0

### $\bullet\,$ Molecule 6 is water.

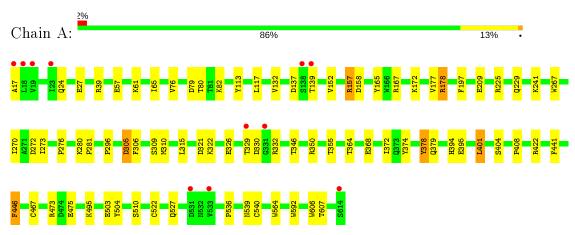
$\mathbf{M}$	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
(	3	A	738	Total O 738 738	0	0



## 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: ANGIOTENSIN CONVERTING ENZYME



 $\bullet \ \, Molecule \ 2: \ beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-ace$ 

Chain B: 100%



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants	173.09Å 173.09Å 101.90Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	31.62 - 1.85	Depositor
	30.19 - 1.85	EDS
% Data completeness	93.3 (31.62-1.85)	Depositor
(in resolution range)	73.8 (30.19-1.85)	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.57 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
$R, R_{free}$	0.172 , $0.201$	Depositor
·	0.182 , 0.210	DCC
$R_{free}$ test set	3564  reflections  (4.99%)	wwPDB-VP
Wilson B-factor $(\mathring{A}^2)$	26.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38, 46.8	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	$\begin{array}{c} 0.017 \; \text{for} \; -2/3*\text{h-}1/3*\text{k-}4/3*\text{l}, -1/3*\text{h-}2/3*\text{k} + \\ \; 4/3*\text{l}, -1/3*\text{h+}1/3*\text{k} + 1/3*\text{l} \\ 0.018 \; \text{for} \; -\text{h}, 1/3*\text{h-}1/3*\text{k-}4/3*\text{l}, -1/3*\text{h-}2/3*\text{k} \\ \; +1/3*\text{l} \\ 0.011 \; \text{for} \; -1/3*\text{h+}1/3*\text{k} + 4/3*\text{l}, -\text{k}, 2/3*\text{h+}1/3*\text{k} \\ \; 3*\text{k+}1/3*\text{l} \\ 0.014 \; \text{for} \; -\text{h}, 2/3*\text{h+}1/3*\text{k} + 4/3*\text{l}, 1/3*\text{h+}2/3 \\ \; & \text{k-}1/3*\text{l} \\ 0.028 \; \text{for} \; -1/3*\text{h-}2/3*\text{k} + 4/3*\text{l}, -2/3*\text{h-}1/3*\text{k} - \\ \; 4/3*\text{l}, 1/3*\text{h-}1/3*\text{k-}1/3*\text{l} \\ 0.026 \; \text{for} \; 1/3*\text{h+}2/3*\text{k-}4/3*\text{l}, -\text{k}, -2/3*\text{h-}1/3* \\ \; & \text{k-}1/3*\text{l} \\ 0.116 \; \text{for} \; \text{h}, -\text{h-k}, -\text{l} \end{array}$	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.86% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: MAN, ZN, BMA, NAG, RX4

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	Bo	nd lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	1.34	21/5015~(0.4%)	1.02	$13/6796 \ (0.2\%)$	

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
1	A	24	GLN	CB-CG	-9.89	1.25	1.52
1	A	467	CYS	CB-SG	9.24	1.98	1.82
1	A	157	ARG	CZ-NH1	7.68	1.43	1.33
1	A	346	THR	CB-OG1	6.54	1.56	1.43
1	A	27	GLU	CG-CD	6.05	1.61	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
1	Α	157	ARG	NE-CZ-NH2	-14.65	112.98	120.30
1	A	157	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	177	VAL	CG1-CB-CG2	7.83	123.42	110.90
1	A	167	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	39	ARG	NE-CZ-NH1	7.29	123.95	120.30

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	4883	0	4677	45	0
2	В	72	0	61	0	0
3	A	34	0	29	1	0
4	A	1	0	0	0	0
5	A	28	0	26	0	0
6	A	738	0	0	6	0
All	All	5756	0	4793	45	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 5.

The worst 5 of 45 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{l}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:A:322:LYS:HB2	1:A:350:ARG:HD3	1.34	1.08
1:A:322:LYS:CB	1:A:350:ARG:HD3	1.86	1.06
1:A:270:ILE:HB	1:A:273:ILE:HD11	1.40	1.01
1:A:178:ARG:NH1	6:A:2267:HOH:O	2.03	0.87
1:A:322:LYS:HB3	1:A:350:ARG:HD3	1.67	0.77

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	ed Favoured Allowed		Outliers	Perce	Percentiles	
1	A	598/598 (100%)	586 (98%)	12 (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	521/520 (100%)	515 (99%)	6 (1%)	71 62	2.

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

Mol	Chain	${f Res}$	$\mathbf{Type}$
1	A	394	HIS
1	A	540	CYS
1	A	446	PHE
1	A	378	TYR
1	A	503	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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)

6 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	Trino	Chain	Res	Link	Во	nd leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	В	1	1,2	14,14,15	0.89	0	17,19,21	1.42	2 (11%)
2	NAG	В	2	2	14,14,15	0.80	0	17,19,21	2.01	5 (29%)
2	BMA	В	3	2	11,11,12	0.57	0	15,15,17	1.36	1 (6%)
2	MAN	В	4	2	11,11,12	0.80	0	15,15,17	1.19	1 (6%)
2	BMA	В	5	2	11,11,12	0.91	0	15,15,17	2.71	7 (46%)
2	MAN	В	6	2	11,11,12	1.54	2 (18%)	15,15,17	2.83	9 (60%)

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	NAG	В	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	3/6/23/26	0/1/1/1
2	BMA	В	3	2	-	2/2/19/22	0/1/1/1
2	MAN	В	4	2	-	2/2/19/22	0/1/1/1
2	BMA	В	5	2	-	2/2/19/22	1/1/1/1
2	MAN	В	6	2	-	2/2/19/22	0/1/1/1

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	В	6	MAN	C2-C3	3.54	1.57	1.52
2	В	6	MAN	C1-C2	2.72	1.58	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	В	6	MAN	C1-C2-C3	5.52	116.46	109.67
2	В	5	BMA	O3-C3-C4	5.19	122.34	110.35
2	В	6	MAN	O5-C5-C6	5.05	115.11	107.20
2	В	5	BMA	O2-C2-C3	-4.60	100.92	110.14
2	В	5	BMA	C2-C3-C4	-4.34	103.38	110.89

There are no chirality outliers.

5 of 11 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	В	6	MAN	O5-C5-C6-O6
2	В	5	BMA	O5-C5-C6-O6
2	В	3	BMA	O5-C5-C6-O6
2	В	4	MAN	C4-C5-C6-O6
2	В	5	BMA	C4-C5-C6-O6

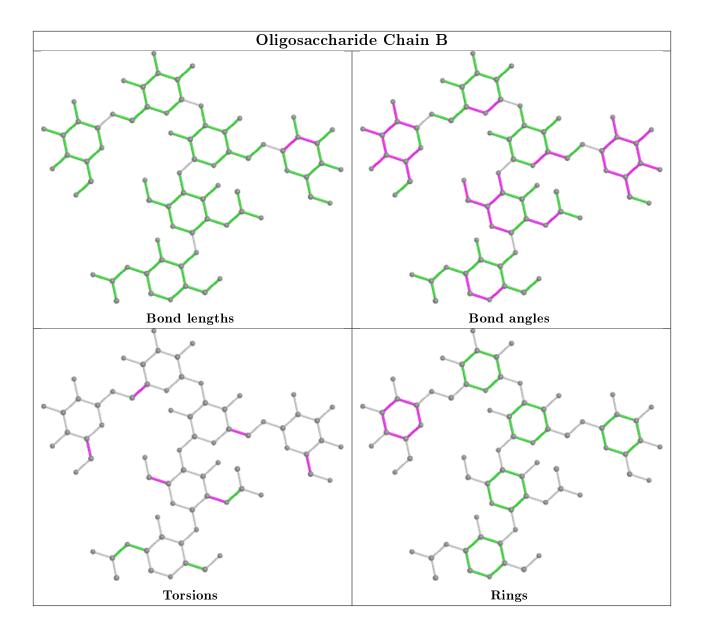
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	5	BMA	C1-C2-C3-C4-C5-O5

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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).

Mal	Type	Chain	Res	Link	Bond lengths			Bond angles		
WIOI			ites		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	RX4	A	1615	4	28,34,34	1.50	7 (25%)	34,47,47	1.61	8 (23%)



Mol	l Type	Chain	Res	Link	Bond lengths			Bond angles		
MIOI			nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1622	1	14,14,15	0.66	0	17,19,21	1.65	3 (17%)
5	NAG	A	1623	1	14,14,15	0.58	0	17,19,21	0.70	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	RX4	A	1615	4	-	2/36/43/43	0/1/1/1
5	NAG	A	1622	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1623	1	_	2/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
3	A	1615	RX4	CA-N	2.80	1.51	1.45
3	A	1615	RX4	CAA-CAX	2.70	1.56	1.50
3	A	1615	RX4	CAB-CBD	2.57	1.61	1.52
3	A	1615	RX4	CAS-CBG	2.45	1.58	1.54
3	A	1615	RX4	CBF-NAU	2.42	1.51	1.45

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	A	1615	RX4	CAM-CAN-CAP	-3.84	114.34	120.19
3	A	1615	RX4	CAB-CBD-CBA	-3.54	103.71	109.42
3	A	1615	RX4	CBC-CAS-CBG	-3.48	105.69	113.38
5	A	1622	NAG	C4-C3-C2	-3.26	106.25	111.02
5	A	1622	NAG	C1-O5-C5	3.22	116.55	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	${f Atoms}$
5	A	1623	NAG	O5-C5-C6-O6
5	A	1623	NAG	C4-C5-C6-O6
3	A	1615	RX4	OAH-CBA-CBD-CAT
3	A	1615	RX4	N-CBA-CBD-CAT

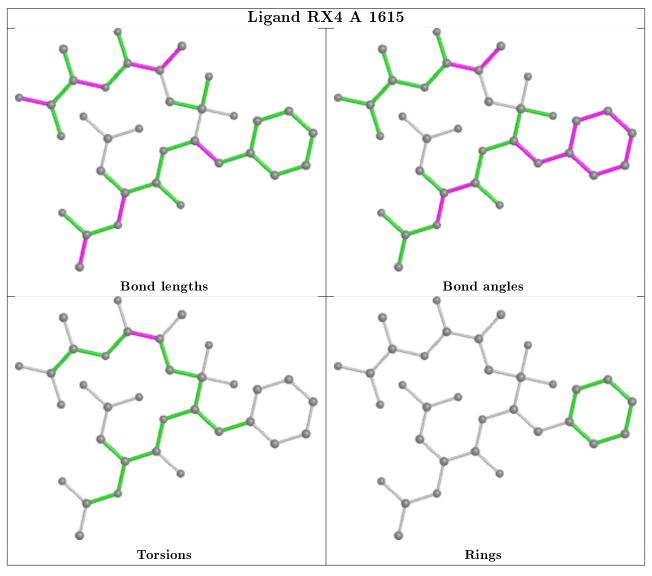
There are no ring outliers.



1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1615	RX4	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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,  $95^{th}$  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.

Mo	Chain	Analysed	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q < 0.9
1	A	598/598 (100%)	-0.53	11 (1%) 68 68	16, 25, 40, 52	7 (1%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	VAL	3.8
1	A	139	THR	3.7
1	A	329	THR	3.3
1	A	19	VAL	3.1
1	A	18	LEU	2.8

#### 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)

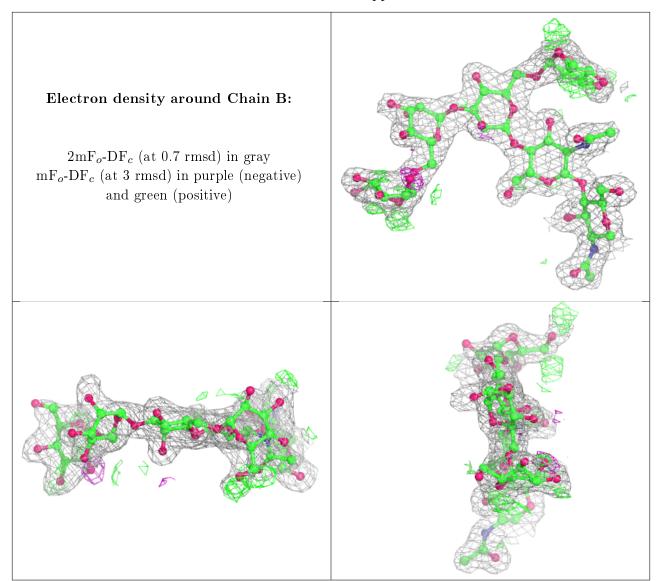
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	MAN	В	6	11/12	0.84	0.32	64,68,70,71	0
2	BMA	В	5	11/12	0.87	0.14	52,57,66,68	0
2	MAN	В	4	11/12	0.94	0.15	43,45,49,51	0
2	BMA	В	3	11/12	0.97	0.12	38,43,53,58	0
2	NAG	В	1	14/15	0.98	0.06	22,26,29,30	0
2	NAG	В	2	14/15	0.99	0.10	24,29,37,40	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.



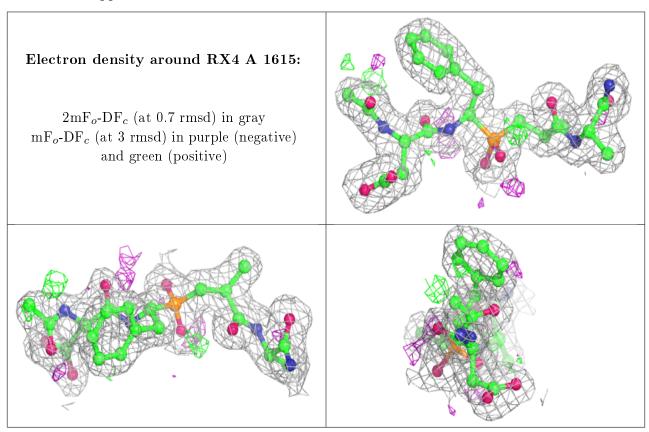
### 6.4 Ligands (i)

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,  $95^{th}$  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	${f Res}$	Atoms	RSCC	RSR	$oxed{f B-factors({ m \AA}^2)}$	$\mathbf{Q}{<}0.9$
5	NAG	A	1622	14/15	0.73	0.55	39,42,46,46	14
5	NAG	A	1623	14/15	0.81	0.43	44,45,45,45	14
3	RX4	A	1615	34/34	0.99	0.08	17,23,36,38	0
4	ZN	A	1616	1/1	1.00	0.07	22,22,22,22	0



The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



#### 6.5 Other polymers (i)

There are no such residues in this entry.

