

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

#### Aug 30, 2023 - 07:22 AM EDT

PDB ID	:	30XE
Title	:	crystal structure of glycine riboswitch, $Mn2+$ soaked
Authors	:	Huang, L.; Serganov, A.; Patel, D.J.
Deposited on		
Resolution	:	2.90  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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

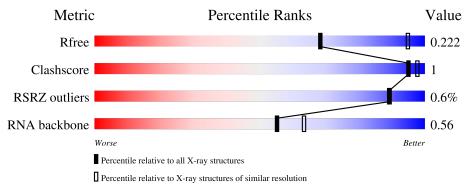
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

#### Overall quality at a glance (i) 1

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

The reported resolution of this entry is 2.90 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.



Matula	Whole archive	Similar resolution
Metric	(# Entries)	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)

RSRZ outliers	127900	1906 (2.90-2.90)	
RNA backbone	3102	1007 (3.16-2.64)	
			'
	• 1		1 • 1,1 •
The table below s	summarises the geometry	etric issues observed across the polymeric	chains and their
fit to the electron	density. The red, or	ange, yellow and green segments of the le	ower bar indicate
the fraction of re	sidues that contain	outliers for $>=3, 2, 1$ and 0 types of g	geometric quality
criteria respective	ly. A grey segment	represents the fraction of residues that a	are not modelled.
The numeric valu	e for each fraction is	s indicated below the corresponding seg	ment, with a dot
representing fracti	ions $<=5\%$ The upper	er red bar (where present) indicates the fr	action of residues

Mol	Chain	Length	Quality of chain		
1	А	88	75%	20%	5%
2	В	88	% <b>78</b> %	16%	6%

that have poor fit to the electron density. The numeric value is given above the bar.

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	MG	В	136	-	-	-	Х



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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	В	141	-	-	-	Х



#### 30XE

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3891 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 RNA chain called domain II of glycine riboswitch.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	88	Total 1906	C 847	N 361	O 608	Р 90	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GDP	-	insertion	GB CP001485.1
А	2	G	-	insertion	GB CP001485.1
A	50	G	С	conflict	GB CP001485.1
А	52	А	U	conflict	GB CP001485.1
А	54	С	U	conflict	GB CP001485.1
А	87	U	-	insertion	GB CP001485.1
А	88	CCC	-	insertion	GB CP001485.1

• Molecule 2 is a RNA chain called domain II of glycine riboswitch.

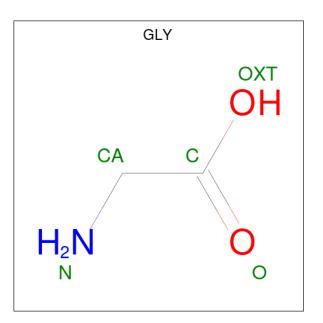
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	88	Total 1901	C 847	N 361	O 604	Р 89	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	1	G	-	insertion	GB CP001485.1
В	2	G	-	insertion	GB CP001485.1
В	50	G	С	conflict	GB CP001485.1
В	52	А	U	conflict	GB CP001485.1
В	54	С	U	conflict	GB CP001485.1
В	87	U	-	insertion	GB CP001485.1
В	88	CCC	-	insertion	GB CP001485.1

• Molecule 3 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 5 & 2 & 1 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 5 & 2 & 1 & 2 \end{array}$	0	0

• Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	19	Total Mn 19 19	0	0
4	В	13	Total Mn 13 13	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	4	Total Mg 4 4	0	0
5	В	6	Total Mg 6 6	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	22	TotalO2222	0	0



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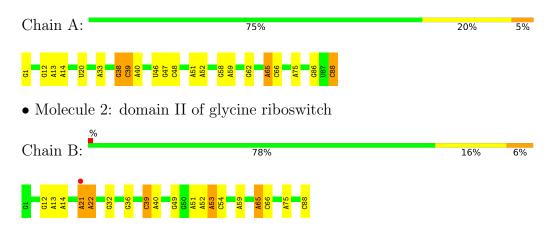
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	10	Total O 10 10	0	0



# 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: domain II of glycine riboswitch





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
$\begin{array}{c} \text{Cell constants} \\ \text{a, b, c, } \alpha, \beta, \gamma \end{array}$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor
Resolution (Å)	$\begin{array}{r} 20.00 & - & 2.90 \\ 19.96 & - & 2.90 \end{array}$	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.90) 99.9 (19.96-2.90)	Depositor EDS
R <sub>merge</sub>	0.06	Depositor
$\frac{\mathbf{R}_{sym}}{< I/\sigma(I) > 1}$	(Not available) 2.40 (at 2.88Å)	Depositor Xtriage
Refinement program	REFMAC	Depositor
$R, R_{free}$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor DCC
$R_{free}$ test set	947 reflections $(5.11\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	71.5	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.29 , $62.4$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3891	wwPDB-VP
Average B, all atoms $(Å^2)$	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<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: MG, GDP, CCC, MN

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	Bond lengths		ond angles
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.55	0/2080	1.06	6/3244~(0.2%)
2	В	0.55	0/2106	1.05	4/3285~(0.1%)
All	All	0.55	0/4186	1.05	10/6529~(0.2%)

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	38	G	C3'-C2'-C1'	-7.59	95.42	101.50
1	А	65	А	P-O3'-C3'	6.58	127.59	119.70
1	А	38	G	P-O3'-C3'	6.53	127.53	119.70
2	В	65	А	P-O3'-C3'	6.41	127.39	119.70
1	А	39	С	O4'-C1'-N1	5.71	112.77	108.20
2	В	32	G	O4'-C1'-N9	5.50	112.60	108.20
1	А	62	G	C3'-C2'-C1'	-5.38	97.20	101.50
2	В	53	А	C1'-O4'-C4'	-5.32	105.65	109.90
1	А	48	С	O4'-C1'-N1	5.01	112.20	108.20
2	В	39	С	O4'-C1'-N1	5.00	112.20	108.20

All (10) bond angle outliers are listed below:

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	А	1906	0	953	1	0
2	В	1901	0	953	5	0
3	А	5	0	2	0	0
3	В	5	0	2	2	0
4	А	19	0	0	0	0
4	В	13	0	0	0	0
5	А	4	0	0	0	0
5	В	6	0	0	0	0
6	А	22	0	0	0	0
6	В	10	0	0	1	0
All	All	3891	0	1910	7	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.

All (7) 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)
3:B:89:GLY:OXT	6:B:150:HOH:O	2.14	0.65
2:B:21:A:H4'	2:B:22:A:OP1	1.98	0.63
2:B:22:A:H5"	2:B:75:A:H62	1.69	0.56
2:B:49:G:C2	2:B:52:A:N6	2.83	0.47
2:B:36:G:O6	3:B:89:GLY:HA3	2.16	0.45
2:B:51:A:H2'	2:B:52:A:C8	2.53	0.44
1:A:46:U:H2'	1:A:47:G:C8	2.55	0.41

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

#### 5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

#### 5.3.3 RNA (i)



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	А	86/88~(97%)	16 (18%)	3(3%)
2	В	87/88~(98%)	11 (12%)	4 (4%)
All	All	173/176~(98%)	27 (15%)	7 (4%)

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	А	12 13	G
1	A           B           B           B           B           B           B	13	А
	А	14 20	А
1	А		U
1	А	33	А
1	А	39	С
1	А	39 40	А
	А	51	А
1	А	52	А
	А	58	G
1	А	59	А
	А	65	А
1	А	66	С
1	А	75	А
1	А	86	G
	А	88	CCC
2	В	12	G
2	В	13	А
2	В	88 12 13 14 21	А
$ \begin{array}{c} 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\$	В	21	Type           G           A           U           A           C           A           G           A           G           A           G           A           G           A           G           A           G           CC           A           G           CCCC           G           A           A           A           A           A           A           C           A           C           A           C           A           C           A           C           A           C           A           C           A           C           A           C           A           C           A           C           A           C           A <tr td="">  &lt;</tr>
2	В	22	A
2	B B	39 40	С
2	В	40	А
2	В	53	А
2	В	54	С
2	В	59	А
2	В	66	С

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	А	38	G
1	А	51	А
1	А	65	А
2	В	13	А
2	В	21	А



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Mol	Chain	$\mathbf{Res}$	Type
2	В	53	А
2	В	65	А

## 5.4 Non-standard residues in protein, DNA, RNA chains (i)

3 non-standard protein/DNA/RNA residues 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	Tuno	Chain	Res	Link	Bond lengths			B	ond ang	les
NIOI	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CCC	А	88	1	$20,\!25,\!26$	2.69	4 (20%)	28,38,41	1.58	6 (21%)
1	GDP	А	1	4,1	24,30,30	1.18	2 (8%)	30,47,47	1.52	7 (23%)
2	CCC	В	88	2	20,25,26	2.69	4 (20%)	28,38,41	1.48	6 (21%)

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
1	CCC	А	88	1	-	0/7/35/36	0/3/3/3
1	GDP	А	1	4,1	-	4/12/32/32	0/3/3/3
2	CCC	В	88	2	-	0/7/35/36	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	88	CCC	C5-C4	-7.08	1.26	1.42
1	А	88	CCC	C5-C4	-7.05	1.26	1.42
1	А	88	CCC	C6-C5	-6.47	1.19	1.35
2	В	88	CCC	C6-C5	-6.47	1.19	1.35
2	В	88	CCC	C6-N1	-6.25	1.22	1.38
1	А	88	CCC	C6-N1	-6.23	1.22	1.38
1	А	1	GDP	C5-C6	-3.85	1.39	1.47



	Chain	-	10	Ζ	Observed(Å)	Ideal(Å)	
1	A	88	CCC	C2-N1	-2.70	1.34	1.40
2	В	88	CCC	C2-N1	-2.63	1.34	1.40
1	А	1	GDP	C2-N3	2.30	1.38	1.33

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All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	В	88	CCC	O3'-C3'-C2'	3.66	111.79	105.08
1	А	88	CCC	O3'-C3'-C2'	3.58	111.65	105.08
1	А	1	GDP	PA-O3A-PB	-3.53	120.70	132.83
1	А	88	CCC	O2'-C2'-C3'	3.40	111.31	105.08
1	А	1	GDP	C5-C6-N1	3.29	119.76	113.95
2	В	88	CCC	C6-C5-C4	3.07	122.45	117.50
1	А	88	CCC	C6-C5-C4	3.07	122.45	117.50
2	В	88	CCC	O2'-C2'-C3'	2.96	110.50	105.08
1	А	1	GDP	C8-N7-C5	2.95	108.61	102.99
1	А	1	GDP	C2-N1-C6	-2.83	119.89	125.10
1	А	88	CCC	02'-PC-01C	-2.46	109.26	115.76
1	А	88	CCC	C4-N3-C2	-2.43	116.33	120.25
2	В	88	CCC	C4-N3-C2	-2.34	116.47	120.25
2	В	88	CCC	02'-PC-01C	-2.24	109.85	115.76
2	В	88	CCC	O3'-PC-O1C	-2.24	109.86	115.76
1	А	1	GDP	O6-C6-C5	-2.17	120.13	124.37
1	А	88	CCC	O3'-PC-O1C	-2.16	110.06	115.76
1	А	1	GDP	C2'-C3'-C4'	2.07	106.66	102.64
1	А	1	GDP	C3'-C2'-C1'	-2.02	97.94	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	1	GDP	C5'-O5'-PA-O1A
1	А	1	GDP	O4'-C4'-C5'-O5'
1	А	1	GDP	C3'-C4'-C5'-O5'
1	А	1	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.



### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 42 are monoatomic - leaving 2 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	Trune	Chain	Dec	Link	Bond lengths			B	Bond ang	gles
IVIOI	Type	Chain	$\operatorname{Res}$		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	GLY	А	89	-	4,4,4	1.13	1 (25%)	3,4,4	1.60	1 (33%)
3	GLY	В	89	-	4,4,4	1.17	1 (25%)	3,4,4	1.56	1 (33%)

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	GLY	А	89	-	-	0/2/2/2	-
3	GLY	В	89	-	-	0/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	В	89	GLY	OXT-C	-2.21	1.23	1.30
3	А	89	GLY	OXT-C	-2.14	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	89	GLY	OXT-C-O	-2.16	117.92	123.30
3	В	89	GLY	OXT-C-O	-2.10	118.08	123.30

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	89	GLY	2	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,  $95^{th}$  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.

Mol	Chain	Analysed	<rsrz> <math>#</math>RSRZ&gt;2</rsrz>		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	86/88~(97%)	-0.39	0 100 100	55, 68, 100, 113	0
2	В	87/88~(98%)	-0.19	1 (1%) 80 80	52, 68, 101, 105	0
All	All	173/176~(98%)	-0.29	1 (0%) 89 89	52, 68, 102, 113	0

All (1) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
2	В	21	А	2.6

## 6.2 Non-standard residues in protein, DNA, RNA chains (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	$B-factors(Å^2)$	Q<0.9
1	GDP	А	1	28/28	0.87	0.21	112,115,120,121	0
2	CCC	В	88	23/24	0.93	0.20	98,101,105,106	0
1	CCC	А	88	23/24	0.94	0.17	120,123,129,132	0

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 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,



3OXE	Ð

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
4	MN	А	101	1/1	0.61	0.29	116,116,116,116	0
4	MN	А	109	1/1	0.69	0.19	135,135,135,135	0
5	MG	В	136	1/1	0.70	0.65	91,91,91,91	0
4	MN	А	115	1/1	0.73	0.34	124,124,124,124	0
5	MG	В	138	1/1	0.73	0.17	105,105,105,105	0
5	MG	В	141	1/1	0.76	1.27	100,100,100,100	0
4	MN	В	130	1/1	0.79	0.10	$153,\!153,\!153,\!153$	0
5	MG	В	140	1/1	0.82	1.74	101,101,101,101	0
5	MG	А	135	1/1	0.83	0.28	74,74,74,74	0
4	MN	А	108	1/1	0.84	0.09	160,160,160,160	0
4	MN	А	117	1/1	0.85	0.44	106,106,106,106	0
4	MN	А	114	1/1	0.86	0.28	118,118,118,118	0
4	MN	А	103	1/1	0.86	0.40	108,108,108,108	0
4	MN	В	122	1/1	0.86	0.37	97,97,97,97	0
3	GLY	В	89	5/5	0.87	0.28	63,63,63,64	0
5	MG	А	133	1/1	0.88	0.14	110,110,110,110	0
4	MN	В	124	1/1	0.88	0.29	129,129,129,129	0
4	MN	А	113	1/1	0.88	0.30	116,116,116,116	0
4	MN	В	129	1/1	0.89	0.32	83,83,83,83	0
4	MN	В	118	1/1	0.89	0.21	$153,\!153,\!153,\!153$	0
4	MN	А	131	1/1	0.89	0.47	$151,\!151,\!151,\!151,\!151$	0
4	MN	А	105	1/1	0.89	0.33	111,111,111,111	0
4	MN	А	112	1/1	0.90	0.07	149,149,149,149	0
5	MG	А	142	1/1	0.90	0.74	$70,\!70,\!70,\!70$	0
4	MN	А	132	1/1	0.91	0.47	146,146,146,146	0
4	MN	А	110	1/1	0.92	0.29	123,123,123,123	0
4	MN	В	123	1/1	0.92	0.37	$116,\!116,\!116,\!116$	0
5	MG	В	134	1/1	0.93	0.12	$95,\!95,\!95,\!95$	0
5	MG	В	139	1/1	0.94	1.15	$107,\!107,\!107,\!107$	0
4	MN	В	120	1/1	0.94	0.36	104,104,104,104	0
3	GLY	А	89	5/5	0.94	0.26	69,69,70,71	0
4	MN	А	111	1/1	0.95	0.19	125, 125, 125, 125	0
4	MN	А	104	1/1	0.96	0.29	104,104,104,104	0
4	MN	А	116	1/1	0.96	0.48	124,124,124,124	0
4	MN	В	125	1/1	0.97	0.25	112,112,112,112	0
4	MN	В	127	1/1	0.97	0.34	104,104,104,104	0
4	MN	В	121	1/1	0.97	0.27	104,104,104,104	0
4	MN	А	102	1/1	0.97	0.17	88,88,88,88	0
4	MN	В	119	1/1	0.97	0.05	143,143,143,143	0
4	MN	А	106	1/1	0.97	0.31	118,118,118,118	0
5	MG	А	137	1/1	0.97	1.03	106,106,106,106	0

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	$B-factors(Å^2)$	Q < 0.9
4	MN	В	126	1/1	0.98	0.51	103,103,103,103	0
4	MN	А	107	1/1	0.98	0.20	112,112,112,112	0
4	MN	В	128	1/1	0.99	0.55	100,100,100,100	0

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# 6.5 Other polymers (i)

There are no such residues in this entry.

