

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

#### Mar 5, 2024 – 12:31 PM EST

PDB ID : 2ZUW

Title: Crystal structure of Galacto-N-biose/Lacto-N-biose I phosphorylase in

complex with GlcNAc and sulfate

Authors: Hidaka, M.; Nishimoto, M.; Kitaoka, M.; Wakagi, T.; Shoun, H.; Fushinobu,

S.

Deposited on : 2008-10-28

Resolution : 2.11 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 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 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

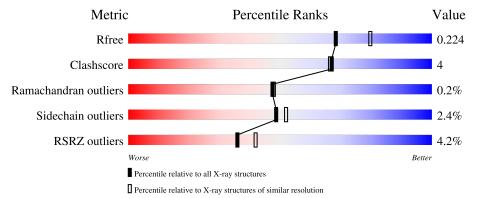
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.11 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 >=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	759	91%	6% ••
1	В	759	6% 87%	8% • •
1	С	759	92%	6% •
1	D	759	7% 81%	11% • 6%



# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25782 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 Lacto-N-biose phosphorylase.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace	
1	Λ	745	Total C N O S	0	0	0	
1	A	740	5926 3782 995 1133 16	0	0		
1	В	734	Total C N O S	0	0	0	
1	Ъ	194	5833 3723 983 1111 16	U		U	
1	С	710	748	Total C N O S	0	0	0
1		140	5950 3795 1000 1139 16	0	U	U	
1	D	713	Total C N O S	0	0	0	
1	ע	110	5686 3635 957 1078 16		U	U	

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	LEU	-	expression tag	UNP Q5NU17
A	753	GLU	-	expression tag	UNP Q5NU17
A	754	HIS	-	expression tag	UNP Q5NU17
A	755	HIS	-	expression tag	UNP Q5NU17
A	756	HIS	-	expression tag	UNP Q5NU17
A	757	HIS	-	expression tag	UNP Q5NU17
A	758	HIS	-	expression tag	UNP Q5NU17
A	759	HIS	-	expression tag	UNP Q5NU17
В	752	LEU	-	expression tag	UNP Q5NU17
В	753	GLU	-	expression tag	UNP Q5NU17
В	754	HIS	-	expression tag	UNP Q5NU17
В	755	HIS	_	expression tag	UNP Q5NU17
В	756	HIS	-	expression tag	UNP Q5NU17
В	757	HIS	_	expression tag	UNP Q5NU17
В	758	HIS	-	expression tag	UNP Q5NU17
В	759	HIS	-	expression tag	UNP Q5NU17
С	752	LEU	-	expression tag	UNP Q5NU17
С	753	GLU	-	expression tag	UNP Q5NU17
С	754	HIS	-	expression tag	UNP Q5NU17
С	755	HIS	-	expression tag	UNP Q5NU17
С	756	HIS	-	expression tag	UNP Q5NU17

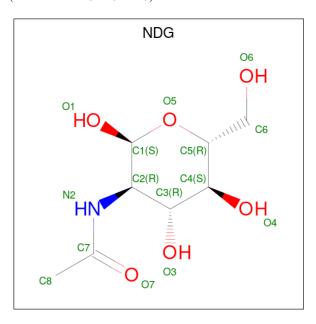
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Chain	Residue	Modelled	Actual	Comment	Reference
С	757	HIS	-	expression tag	UNP Q5NU17
С	758	HIS	-	expression tag	UNP Q5NU17
С	759	HIS	-	expression tag	UNP Q5NU17
D	752	LEU	-	expression tag	UNP Q5NU17
D	753	GLU	-	expression tag	UNP Q5NU17
D	754	HIS	-	expression tag	UNP Q5NU17
D	755	HIS	-	expression tag	UNP Q5NU17
D	756	HIS	-	expression tag	UNP Q5NU17
D	757	HIS	-	expression tag	UNP Q5NU17
D	758	HIS	-	expression tag	UNP Q5NU17
D	759	HIS	-	expression tag	UNP Q5NU17

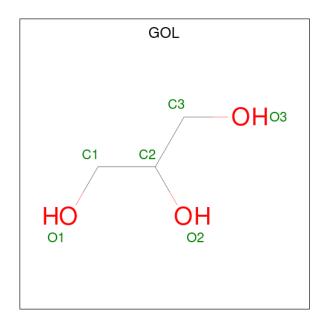
• Molecule 2 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 15 8 1 6	0	0
2	В	1	Total C N O 15 8 1 6	0	0
2	С	1	Total C N O 15 8 1 6	0	0
2	D	1	Total C N O 15 8 1 6	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

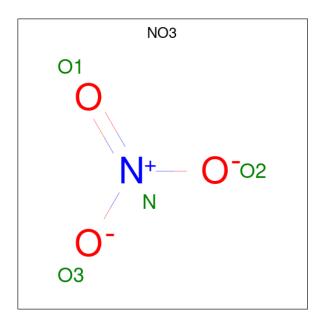




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	В	1	Total C O 6 3 3	0	0
3	С	1	Total C O 6 3 3	0	0
3	С	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

 $\bullet$  Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO3).



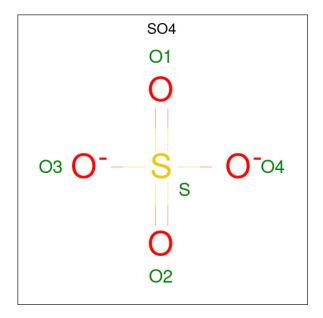


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total 4	N 1	O 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Mg 1 1	0	0

 $\bullet$  Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $\mathrm{O_4S}).$ 





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

### • Molecule 7 is water.

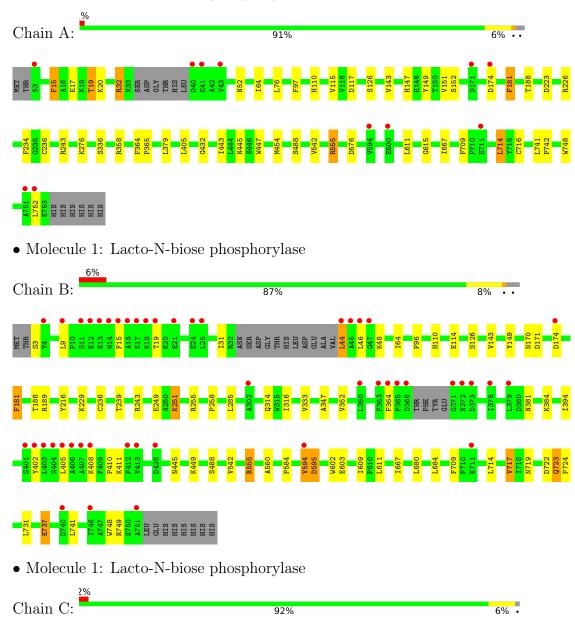
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	627	Total O 627 627	0	0
7	В	533	Total O 533 533	2	0
7	С	601	Total O 601 601	1	0
7	D	520	Total O 520 520	0	0



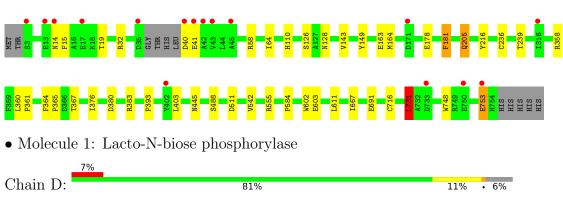
# 3 Residue-property plots (i)

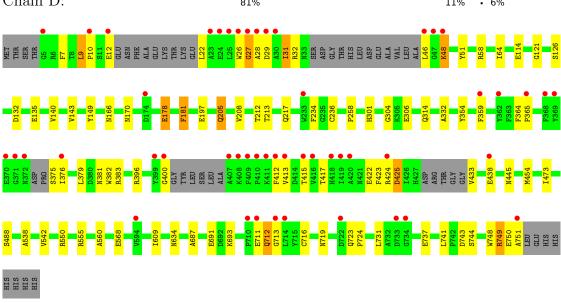
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Lacto-N-biose phosphorylase











# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	67.91Å 112.04Å 118.66Å	Donositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$105.21^{\circ}$ $90.43^{\circ}$ $107.32^{\circ}$	Depositor
Resolution (Å)	41.07 - 2.11	Depositor
Resolution (A)	40.88 - 2.11	EDS
% Data completeness	97.4 (41.07-2.11)	Depositor
(in resolution range)	97.3 (40.88-2.11)	EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.66 (at 2.12Å)	Xtriage
Refinement program	REFMAC	Depositor
D D	0.169 , 0.225	Depositor
$R, R_{free}$	0.169 , $0.224$	DCC
$R_{free}$ test set	8997 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.37\;,51.2$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	25782	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.53% 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: SO4, NO3, NDG, GOL, MG

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		
MIOI		RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	0.65	0/6093	0.66	1/8299 (0.0%)	
1	В	0.58	0/5997	0.62	0/8166	
1	С	0.63	1/6118 (0.0%)	0.65	1/8333 (0.0%)	
1	D	0.63	1/5846~(0.0%)	0.65	0/7958	
All	All	0.62	$2/24054 \ (0.0\%)$	0.64	$2/32756 \ (0.0\%)$	

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

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	Ideal(Å)
1	D	236	CYS	CB-SG	-7.78	1.69	1.82
1	С	236	CYS	CB-SG	-6.72	1.70	1.82

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

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	С	731	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	223	ASP	CB-CG-OD1	5.10	122.89	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	5926	0	5615	30	0
1	В	5833	0	5536	52	0
1	С	5950	0	5631	32	0
1	D	5686	0	5386	64	0
2	A	15	0	12	0	0
2	В	15	0	12	0	0
2	С	15	0	12	0	0
2	D	15	0	12	0	0
3	A	6	0	8	1	0
3	В	6	0	8	2	0
3	С	12	0	16	0	0
3	D	12	0	16	1	0
4	A	4	0	0	0	0
5	В	1	0	0	0	0
6	D	5	0	0	0	0
7	A	627	0	0	7	0
7	В	533	0	0	12	0
7	С	601	0	0	7	0
7	D	520	0	0	11	0
All	All	25782	0	22264	177	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 4.

The worst 5 of 177 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & & & & & & & & & & & & & & & & & & &$	Clash overlap (Å)
1:D:359:PHE:HD1	7:D:831:HOH:O	1.37	1.04
1:B:251:LYS:HE2	7:B:961:HOH:O	1.58	1.00
1:C:691:GLU:HG2	7:C:964:HOH:O	1.67	0.93
1:D:412:PHE:HA	1:D:415:THR:HG22	1.52	0.92
1:D:121:GLY:O	3:D:4010:GOL:H12	1.69	0.91

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	Perce	entiles
1	A	741/759 (98%)	711 (96%)	30 (4%)	0	100	100
1	В	728/759 (96%)	694 (95%)	32 (4%)	2 (0%)	41	40
1	C	744/759 (98%)	718 (96%)	25 (3%)	1 (0%)	51	53
1	D	701/759~(92%)	663 (95%)	34 (5%)	4 (1%)	25	20
All	All	$2914/3036 \ (96\%)$	2786 (96%)	121 (4%)	7 (0%)	47	48

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	594	VAL
1	D	27	GLY
1	D	712	GLN
1	В	595	ASP
1	С	41	GLU

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	621/634~(98%)	604 (97%)	17 (3%)	44 47	
1	В	611/634~(96%)	597 (98%)	14 (2%)	50 53	
1	С	624/634~(98%)	615 (99%)	9 (1%)	67 72	
1	D	596/634~(94%)	578 (97%)	18 (3%)	41 43	
All	All	$2452/2536\ (97\%)$	2394 (98%)	58 (2%)	49 52	

5 of 58 residues with a non-rotameric sidechain are listed below:

Mo	ol	Chain	Res	Type
1		В	723	GLN
1		D	712	GLN
1		С	358	ARG

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Mol	Chain	Res	Type
1	D	609	ILE
1	D	376	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	720	ASN
1	D	170	ASN
1	D	720	ASN
1	D	381	ASN
1	D	166	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)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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 Chair	rpe Chain Res Link		B	Bond lengths			Bond angles			
		Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
	2	NDG	A	4001	-	15,15,15	0.59	0	21,21,21	1.07	1 (4%)



Mol	Trino	Chain	Res	Link	В	ond leng	$_{ m gths}$	В	ond ang	les		
MIOI	Type	Chain	rtes	nes	nes	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	D	4011	-	4,4,4	0.17	0	6,6,6	0.21	0		
2	NDG	В	4002	-	15,15,15	0.63	0	21,21,21	1.27	2 (9%)		
3	GOL	С	4008	-	5,5,5	0.31	0	5,5,5	0.53	0		
3	GOL	D	4010	-	5,5,5	0.38	0	5,5,5	0.54	0		
3	GOL	В	4006	-	5,5,5	0.29	0	5,5,5	0.76	0		
3	GOL	С	4007	_	5,5,5	0.26	0	5,5,5	0.66	0		
3	GOL	A	4005	_	5,5,5	0.33	0	5,5,5	0.75	0		
2	NDG	С	4003	-	15,15,15	0.62	0	21,21,21	1.04	1 (4%)		
4	NO3	A	4012	-	1,3,3	3.78	1 (100%)	0,3,3	-	_		
3	GOL	D	4009	-	5,5,5	0.29	0	5,5,5	0.81	0		
2	NDG	D	4004	-	15,15,15	0.64	0	21,21,21	1.27	3 (14%)		

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	NDG	A	4001	-	-	0/6/26/26	0/1/1/1
2	NDG	В	4002	-	-	0/6/26/26	0/1/1/1
3	GOL	С	4008	-	-	4/4/4/4	-
3	GOL	D	4010	-	-	2/4/4/4	-
3	GOL	В	4006	-	-	2/4/4/4	-
3	GOL	С	4007	-	=	0/4/4/4	-
3	GOL	A	4005	-	-	2/4/4/4	-
2	NDG	С	4003	-	-	0/6/26/26	0/1/1/1
3	GOL	D	4009	-	-	0/4/4/4	-
2	NDG	D	4004	-	-	0/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$Ideal(\AA)$
4	A	4012	NO3	O1-N	3.78	1.41	1.24

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

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	4002	NDG	C1-C2-N2	-4.54	105.47	110.73
2	A	4001	NDG	C1-C2-N2	-3.58	106.59	110.73
2	D	4004	NDG	C1-C2-N2	-3.54	106.62	110.73

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Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	С	4003	NDG	C1-C2-N2	-3.51	106.66	110.73
2	D	4004	NDG	O5-C1-C2	2.45	111.98	109.52

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4005	GOL	O1-C1-C2-C3
3	В	4006	GOL	C1-C2-C3-O3
3	С	4008	GOL	O1-C1-C2-C3
3	В	4006	GOL	O2-C2-C3-O3
3	С	4008	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4010	GOL	1	0
3	В	4006	GOL	2	0
3	A	4005	GOL	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,  $95^{th}$  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></rsrz>	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	745/759 (98%)	-0.27	11 (1%) 73 77	12, 21, 35, 66	0
1	В	734/759 (96%)	0.08	46 (6%) 20 24	13, 24, 55, 69	0
1	С	748/759 (98%)	-0.25	16 (2%) 63 68	11, 21, 38, 64	0
1	D	713/759 (93%)	0.09	50 (7%) 16 20	12, 23, 53, 64	0
All	All	2940/3036 (96%)	-0.09	123 (4%) 36 42	11, 22, 49, 69	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	406	ALA	7.5
1	D	24	GLU	6.1
1	D	25	LEU	6.0
1	D	371	GLY	5.9
1	В	594	VAL	5.8

## 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)

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, 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
4	NO3	A	4012	4/4	0.81	0.16	41,41,42,43	0
3	GOL	D	4010	6/6	0.86	0.18	50,51,52,52	0
3	GOL	D	4009	6/6	0.88	0.18	26,30,31,36	0
3	GOL	В	4006	6/6	0.89	0.17	31,35,37,39	0
3	GOL	A	4005	6/6	0.90	0.13	26,28,30,33	0
3	GOL	С	4008	6/6	0.93	0.14	35,39,40,42	0
3	GOL	С	4007	6/6	0.93	0.09	19,22,24,26	0
6	SO4	D	4011	5/5	0.93	0.14	70,71,71,71	0
2	NDG	В	4002	15/15	0.95	0.10	17,22,25,25	0
2	NDG	D	4004	15/15	0.97	0.15	18,22,23,25	0
2	NDG	A	4001	15/15	0.97	0.13	13,18,21,23	0
2	NDG	С	4003	15/15	0.97	0.14	18,19,22,25	0
5	MG	В	4013	1/1	0.99	0.03	30,30,30,30	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

