



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 02:33 pm GMT

PDB ID : 3A3Y  
Title : Crystal structure of the sodium-potassium pump with bound potassium and ouabain  
Authors : Ogawa, H.; Shinoda, T.; Cornelius, F.; Toyoshima, C.  
Deposited on : 2009-06-23  
Resolution : 2.80 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](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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

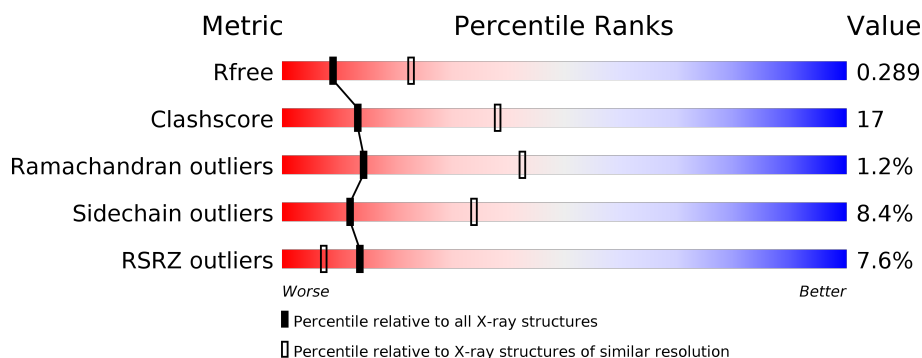
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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. 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	1028	<div> <div>7%</div> <div>61%</div> <div>32%</div> <div>• •</div> </div>
2	B	305	<div> <div>10%</div> <div>50%</div> <div>32%</div> <div>5%</div> <div>13%</div> </div>
3	G	74	<div> <div>32%</div> <div>19%</div> <div>49%</div> </div>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10308 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 Na, K-ATPase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	992	Total	C	N	O	S	0	0	0
			7675	4886	1290	1453	46			

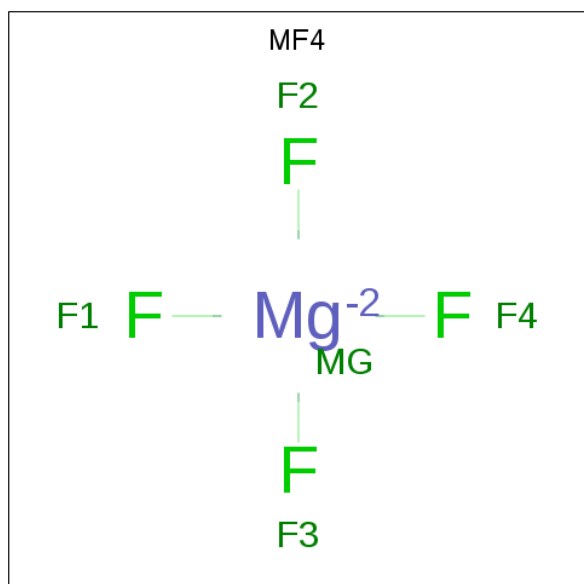
- Molecule 2 is a protein called NA<sup>+</sup>,K<sup>+</sup>-ATPASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	265	Total	C	N	O	S	0	0	0
			2151	1392	356	392	11			

- Molecule 3 is a protein called Phospholemman-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	38	Total	C	N	O	S	0	0	0
			296	195	49	51	1			

- Molecule 4 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F<sub>4</sub>Mg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	F	Mg	0	0
			5	4	1		

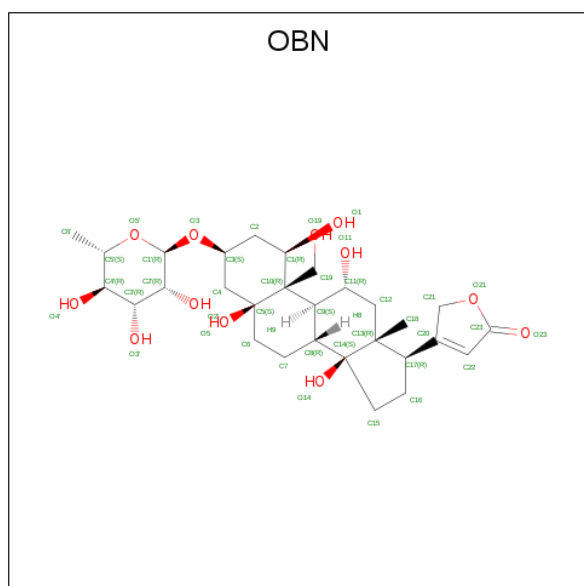
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

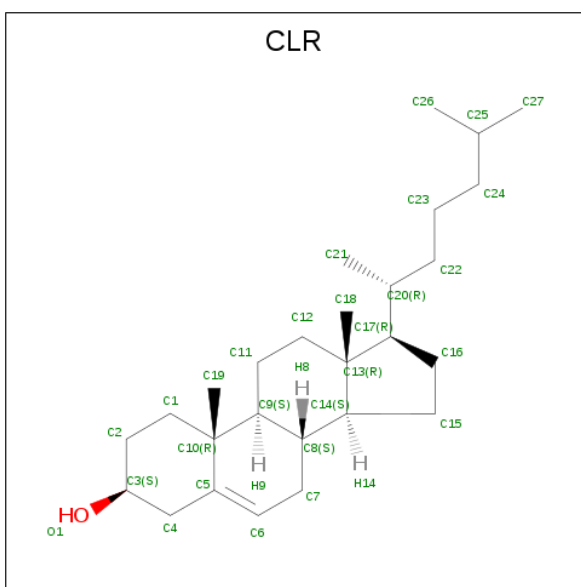
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total K 3 3	0	0

- Molecule 7 is OUABAIN (three-letter code: OBN) (formula:  $\text{C}_{29}\text{H}_{44}\text{O}_{12}$ ).



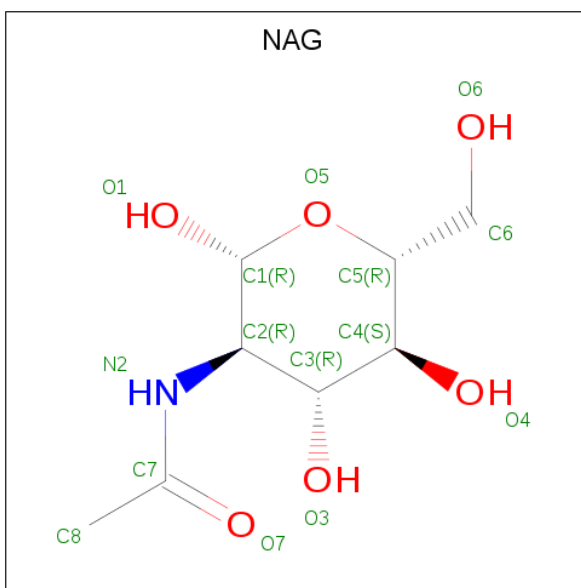
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			41	29	12		

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			28	27	1		

- Molecule 9 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

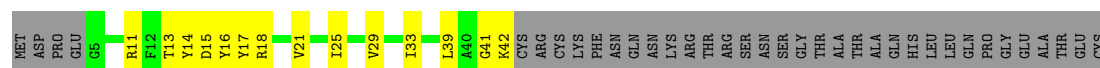


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	65	Total 65	O 65	0	0
10	G	1	Total 1	O 1	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.88Å 50.72Å 163.34Å 90.00° 104.63° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 43.58 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.80) 99.9 (43.58-2.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.41 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.247 , 0.293 0.245 , 0.289	Depositor DCC
$R_{free}$ test set	1342 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 72.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: OBN, MG, NAG, K, MF4, CLR

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	0.37	0/7825	0.55	0/10616
2	B	0.35	0/2205	0.54	0/2970
3	G	0.39	0/300	0.53	0/407
All	All	0.37	0/10330	0.55	0/13993

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1015	GLY	Peptide

### 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	7675	0	7700	270	0
2	B	2151	0	2127	81	0
3	G	296	0	312	11	0
4	A	5	0	0	1	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0
7	A	41	0	44	7	0
8	B	28	0	46	2	0
9	B	42	0	39	3	0
10	A	65	0	0	3	0
10	G	1	0	0	0	0
All	All	10308	0	10268	355	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 17.

The worst 5 of 355 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:905:GLN:HE21	2:B:183:ARG:H	1.13	0.96
1:A:328:ILE:HG13	1:A:329:VAL:H	1.30	0.94
1:A:102:ILE:HA	1:A:105:TRP:HD1	1.32	0.94
1:A:44:HIS:H	1:A:44:HIS:CD2	1.83	0.93
1:A:894:TRP:HB2	2:B:83:TYR:HE1	1.38	0.88

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	990/1028 (96%)	902 (91%)	78 (8%)	10 (1%)	<b>17</b> 48
2	B	259/305 (85%)	216 (83%)	37 (14%)	6 (2%)	<b>7</b> <b>23</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	36/74 (49%)	32 (89%)	4 (11%)	0	100	100
All	All	1285/1407 (91%)	1150 (90%)	119 (9%)	16 (1%)	14	42

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ASP
1	A	329	VAL
1	A	566	ASN
1	A	576	PRO
2	B	85	ILE

### 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	840/869 (97%)	770 (92%)	70 (8%)	12	34
2	B	232/266 (87%)	210 (90%)	22 (10%)	9	27
3	G	31/62 (50%)	30 (97%)	1 (3%)	42	76
All	All	1103/1197 (92%)	1010 (92%)	93 (8%)	12	34

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	538	PHE
1	A	719	VAL
2	B	226	ILE
1	A	548	LEU
1	A	656	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	838	ASN
1	A	905	GLN
2	B	243	GLN
1	A	846	ASN
1	A	904	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
4	MF4	A	2001	-	0,4,4	0.00	-	0,6,6	0.00	-
7	OBN	A	6000	-	44,46,46	0.74	1 (2%)	69,76,76	1.60	11 (15%)
8	CLR	B	3001	-	31,31,31	0.48	0	48,48,48	1.29	6 (12%)
9	NAG	B	4001	-	14,14,15	0.54	0	17,19,21	0.97	1 (5%)
9	NAG	B	4002	-	14,14,15	0.57	0	17,19,21	1.08	1 (5%)
9	NAG	B	4021	-	14,14,15	0.48	0	17,19,21	0.94	1 (5%)

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
4	MF4	A	2001	-	-	0/0/0/0	0/0/0/0
7	OBN	A	6000	-	-	0/11/116/116	0/6/6/6
8	CLR	B	3001	-	-	0/10/68/68	0/4/4/4
9	NAG	B	4001	-	-	0/6/23/26	0/1/1/1
9	NAG	B	4002	-	-	0/6/23/26	0/1/1/1
9	NAG	B	4021	-	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	6000	OBN	O21-C23	3.44	1.45	1.36

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	6000	OBN	C15-C14-C8	-3.60	110.98	116.07
7	A	6000	OBN	C12-C11-C9	-3.59	107.69	112.62
7	A	6000	OBN	C18-C13-C12	-3.29	106.52	111.10
7	A	6000	OBN	C17-C20-C22	-3.19	120.30	128.85
8	B	3001	CLR	C3-C4-C5	-2.94	106.90	112.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	MF4	1	0
7	A	6000	OBN	7	0
8	B	3001	CLR	2	0
9	B	4001	NAG	2	0
9	B	4002	NAG	2	0
9	B	4021	NAG	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	992/1028 (96%)	0.27	69 (6%) 16 9	23, 48, 111, 161	0
2	B	265/305 (86%)	0.66	30 (11%) 5 2	45, 86, 120, 127	0
3	G	38/74 (51%)	-0.22	0 100 100	37, 46, 85, 89	0
All	All	1295/1407 (92%)	0.33	99 (7%) 14 7	23, 54, 116, 161	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	GLY	6.9
1	A	131	TYR	6.3
1	A	317	TRP	6.3
1	A	90	ILE	6.3
1	A	313	LEU	6.2

### 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](#)

There are no carbohydrates 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<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
9	NAG	B	4021	14/15	0.48	0.39	116,117,117,117	0
9	NAG	B	4002	14/15	0.63	0.32	109,110,111,111	0
8	CLR	B	3001	28/28	0.81	0.34	86,88,89,89	0
7	OBN	A	6000	41/41	0.84	0.19	93,95,98,98	0
9	NAG	B	4001	14/15	0.87	0.22	101,102,102,102	0
4	MF4	A	2001	5/5	0.94	0.24	23,23,24,27	0
6	K	A	2005	1/1	0.94	0.10	76,76,76,76	0
6	K	A	2004	1/1	0.95	0.10	72,72,72,72	0
5	MG	A	2002	1/1	0.97	0.19	25,25,25,25	0
6	K	A	2003	1/1	0.97	0.14	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.