



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 05:44 PM EDT

PDB ID : 3TAI  
Title : Crystal structure of NurA  
Authors : Chae, J.; Kim, Y.C.; Cho, Y.  
Deposited on : 2011-08-04  
Resolution : 2.82 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)

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

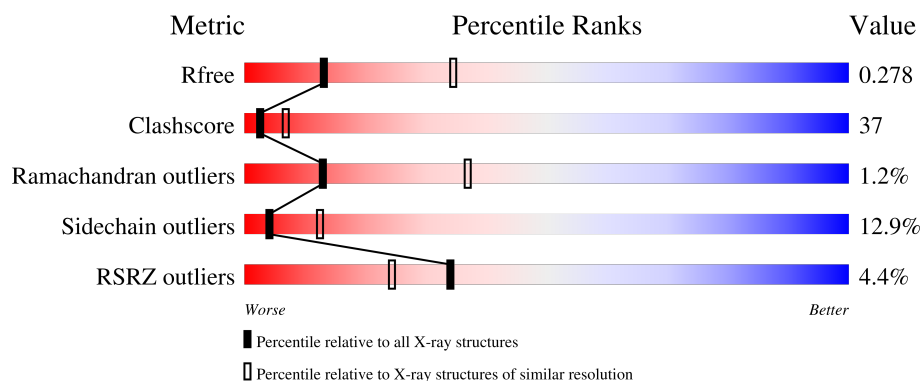
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 of 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	471	
1	B	471	

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	GOL	A	455	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7002 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 DNA double-strand break repair protein nurA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	Se	0	0	0
			3471	2223	595	646	7			
1	B	430	Total	C	N	O	Se	0	0	0
			3470	2223	594	646	7			

There are 40 discrepancies between the modelled and reference sequences:

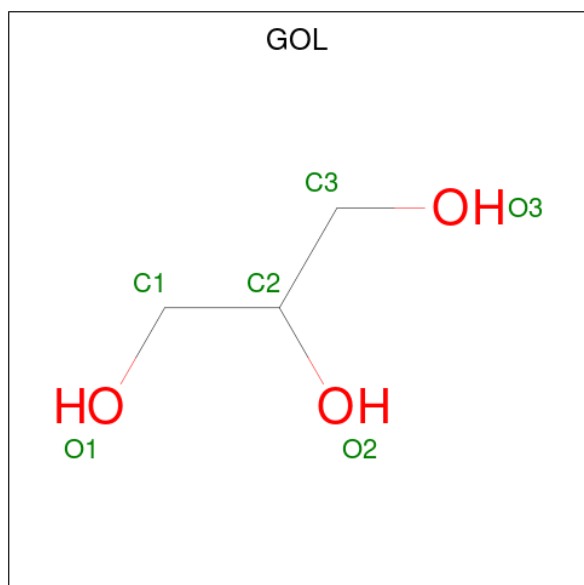
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP Q8U1N8
A	-18	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-17	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-16	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-15	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-14	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-13	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-12	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-11	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-10	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-9	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-8	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-7	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-6	LEU	-	EXPRESSION TAG	UNP Q8U1N8
A	-5	VAL	-	EXPRESSION TAG	UNP Q8U1N8
A	-4	PRO	-	EXPRESSION TAG	UNP Q8U1N8
A	-3	ARG	-	EXPRESSION TAG	UNP Q8U1N8
A	-2	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-1	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	0	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-19	MSE	-	EXPRESSION TAG	UNP Q8U1N8
B	-18	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-17	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-16	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-15	HIS	-	EXPRESSION TAG	UNP Q8U1N8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-13	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-12	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-11	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-10	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-9	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-8	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-7	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-6	LEU	-	EXPRESSION TAG	UNP Q8U1N8
B	-5	VAL	-	EXPRESSION TAG	UNP Q8U1N8
B	-4	PRO	-	EXPRESSION TAG	UNP Q8U1N8
B	-3	ARG	-	EXPRESSION TAG	UNP Q8U1N8
B	-2	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-1	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	0	HIS	-	EXPRESSION TAG	UNP Q8U1N8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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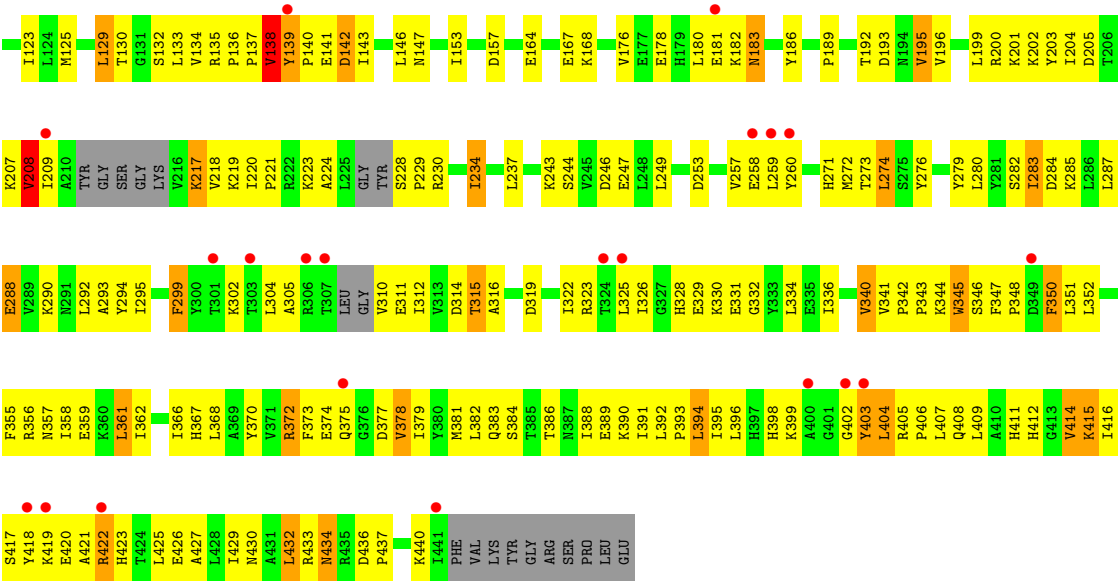
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	4	Total	O	0	0
			4	4		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.00Å 114.21Å 122.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.82 31.73 – 2.49	Depositor EDS
% Data completeness (in resolution range)	95.7 (29.55-2.82) 89.0 (31.73-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.202 , 0.276 0.197 , 0.278	Depositor DCC
$R_{free}$ test set	1141 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.0	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 71.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: GOL

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	0.52	0/3523	0.72	1/4741 (0.0%)
1	B	0.46	0/3520	0.66	0/4738
All	All	0.49	0/7043	0.69	1/9479 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	62	THR	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ARG	Sidechain

### 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	3471	0	3587	271	0
1	B	3470	0	3586	295	0
2	A	36	0	48	9	0
2	B	6	0	8	2	0
3	A	15	0	0	3	0
3	B	4	0	0	0	0
All	All	7002	0	7229	522	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 37.

The worst 5 of 522 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:54:ARG:HB3	1:A:101:MSE:HE3	1.26	1.11
1:A:138:VAL:HG13	1:A:142:ASP:OD1	1.54	1.07
1:B:347:PHE:HB3	1:B:352:LEU:HD11	1.37	1.05
1:A:135:ARG:NH2	1:B:90:TYR:HB2	1.73	1.04
1:B:67:LEU:HD22	1:B:101:MSE:HE2	1.39	1.03

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	424/471 (90%)	390 (92%)	31 (7%)	3 (1%)	22	51
1	B	422/471 (90%)	382 (90%)	33 (8%)	7 (2%)	9	27
All	All	846/942 (90%)	772 (91%)	64 (8%)	10 (1%)	13	37

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ILE
1	B	43	GLU
1	B	139	TYR
1	A	420	GLU
1	B	42	PRO

### 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	385/410 (94%)	337 (88%)	48 (12%)	4	14
1	B	385/410 (94%)	334 (87%)	51 (13%)	4	11
All	All	770/820 (94%)	671 (87%)	99 (13%)	4	12

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	90	TYR
1	B	274	LEU
1	B	129	LEU
1	B	199	LEU
1	B	299	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	271	HIS
1	B	408	GLN
1	B	423	HIS
1	B	412	HIS
1	A	397	HIS

### 5.3.3 RNA ⓘ

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](#)

7 ligands 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	GOL	B	452	-	5,5,5	0.39	0	5,5,5	0.43	0
2	GOL	A	455	-	5,5,5	0.29	0	5,5,5	0.91	0
2	GOL	A	454	-	5,5,5	0.47	0	5,5,5	0.43	0
2	GOL	A	456	-	5,5,5	0.45	0	5,5,5	0.31	0
2	GOL	A	457	-	5,5,5	0.38	0	5,5,5	0.32	0
2	GOL	A	452	-	5,5,5	0.37	0	5,5,5	0.30	0
2	GOL	A	453	-	5,5,5	0.38	0	5,5,5	0.31	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
2	GOL	B	452	-	-	2/4/4/4	-
2	GOL	A	455	-	-	4/4/4/4	-
2	GOL	A	454	-	-	4/4/4/4	-
2	GOL	A	456	-	-	2/4/4/4	-
2	GOL	A	457	-	-	4/4/4/4	-
2	GOL	A	452	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	453	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	452	GOL	O1-C1-C2-C3
2	A	452	GOL	C1-C2-C3-O3
2	A	453	GOL	O1-C1-C2-C3
2	A	453	GOL	C1-C2-C3-O3
2	A	454	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	452	GOL	2	0
2	A	455	GOL	6	0
2	A	456	GOL	1	0
2	A	452	GOL	2	0
2	A	453	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<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	423/471 (89%)	-0.30	11 (2%) 56 46	41, 79, 150, 209	0
1	B	423/471 (89%)	0.02	26 (6%) 21 13	51, 104, 174, 265	0
All	All	846/942 (89%)	-0.14	37 (4%) 34 24	41, 91, 162, 265	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	LEU	6.9
1	B	403	TYR	6.8
1	A	139	TYR	4.0
1	B	31	ASN	3.8
1	B	258	GLU	3.6

### 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<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
2	GOL	A	452	6/6	0.60	0.31	83,118,124,130	0
2	GOL	A	457	6/6	0.84	0.25	93,115,118,121	0
2	GOL	A	453	6/6	0.85	0.14	96,115,118,118	0
2	GOL	A	454	6/6	0.86	0.27	77,104,111,117	0
2	GOL	A	455	6/6	0.87	0.29	68,78,79,91	0
2	GOL	A	456	6/6	0.88	0.46	83,96,100,103	0
2	GOL	B	452	6/6	0.92	0.69	110,131,142,147	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.