



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 19, 2024 – 07:35 PM EDT

PDB ID : 3TAL  
Title : Crystal structure of NurA with manganese  
Authors : Chae, J.; Kim, Y.C.; Cho, Y.  
Deposited on : 2011-08-04  
Resolution : 3.15 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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

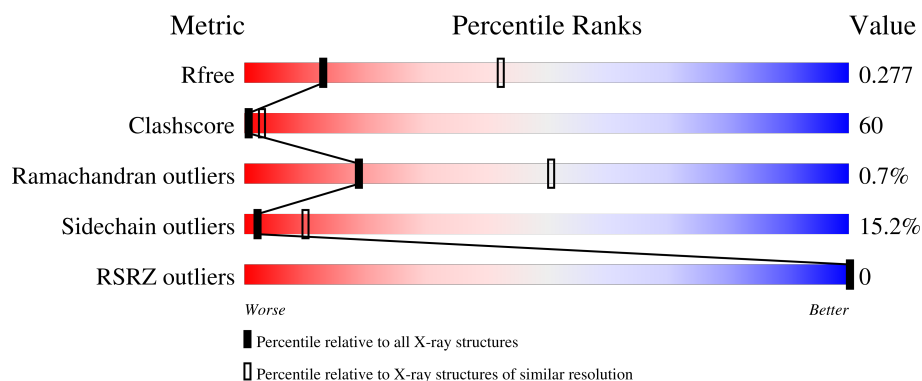
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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))
$R_{free}$	164625	2168 (3.20-3.12)
Clashscore	180529	2333 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)

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	<div> <div></div> <div>34%</div> <div>48%</div> <div>8%</div> <div>10%</div> </div>
1	B	471	<div> <div></div> <div>25%</div> <div>53%</div> <div>11%</div> <div>11%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6861 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	424	Total	C	N	O	Se	0	0	0
			3420	2188	587	638	7			
1	B	421	Total	C	N	O	Se	0	0	0
			3411	2186	584	634	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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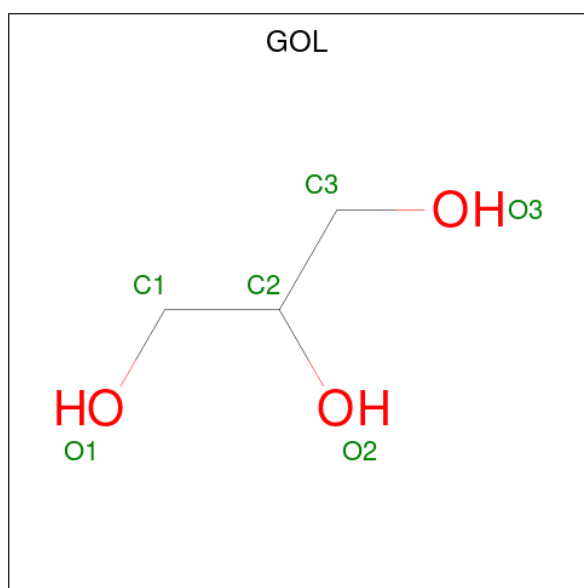
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q8U1N8
B	-13	HIS	-	expression tag	UNP Q8U1N8
B	-12	HIS	-	expression tag	UNP Q8U1N8
B	-11	HIS	-	expression tag	UNP Q8U1N8
B	-10	HIS	-	expression tag	UNP Q8U1N8
B	-9	SER	-	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 MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

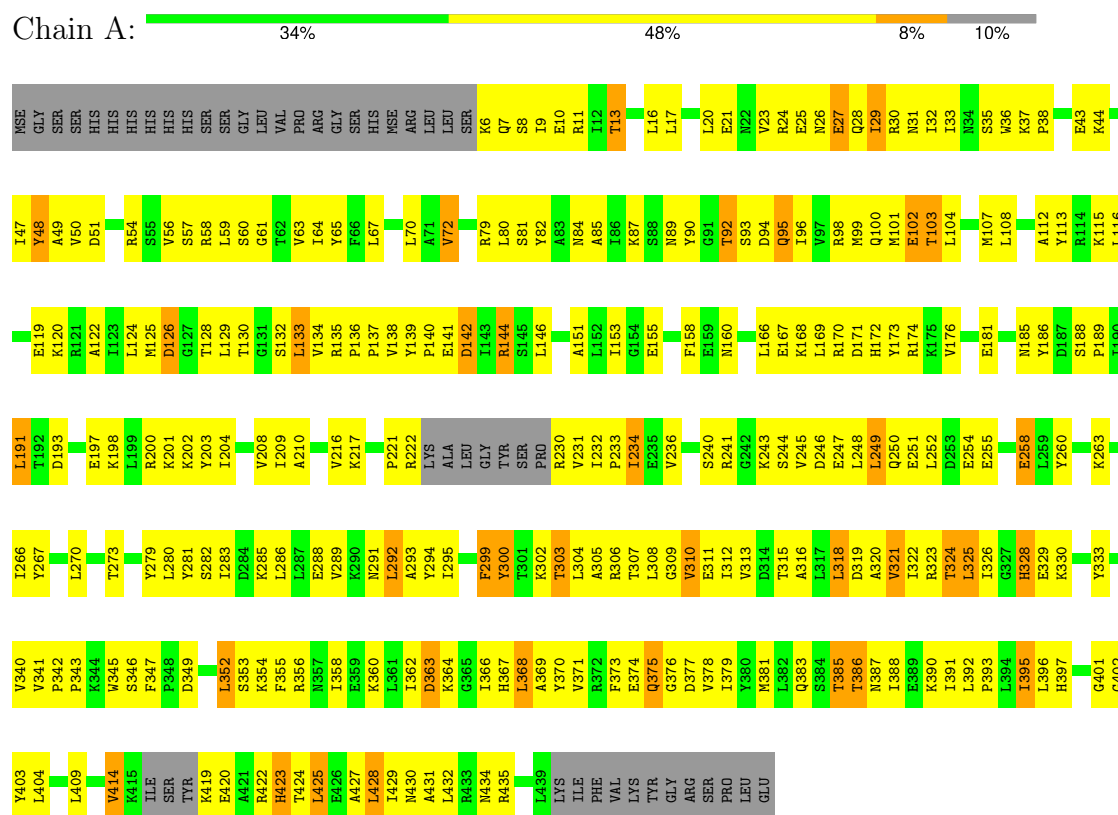
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	7	Total	O	0	0
			7	7		

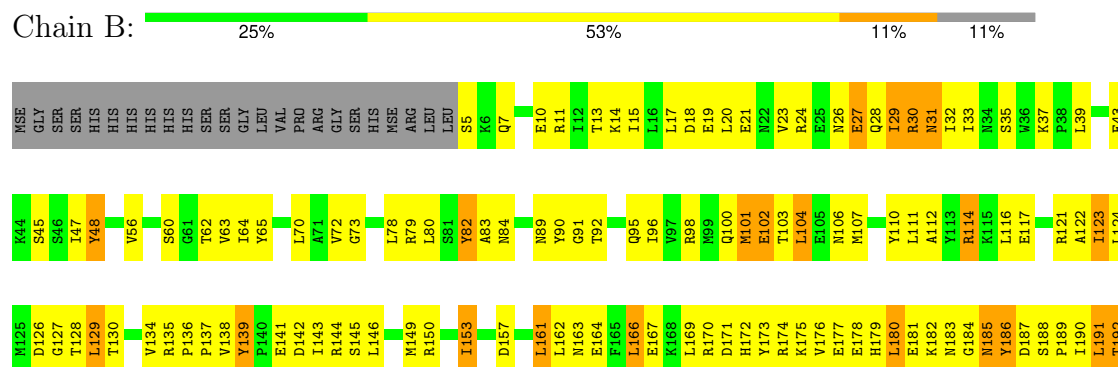
### 3 Residue-property plots

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: DNA double-strand break repair protein nurA



- Molecule 1: DNA double-strand break repair protein nurA



LEU	E389	K390	I326	GLY	E391	HIS	L261
GLU	L392	P393	L394	K330	E331	GLU	I266
	L395	I396	Y333	G332	D268	E269	Y267
	L397	H398	L334	E335	L270	H271	L270
	L399	A400		I336	H272	T273	K202
	GLY	V340	V341		L274	K275	Y203
	GLY	P342	P343		Y276	S275	I204
	L404	K344	K345		I277	E278	D205
	R405	L346	S346		Y279	L280	T206
	P406	L407	F347		L281	Y281	K207
	Q408	L409	P348		S282	I283	V208
	L410	F349	S349		D284	K285	ILE
	H411	F350	L351		L286	K287	ALA
	H412	L352	L353		L287	E288	TYR
	G413	S353	K354		N291	L292	GLY
	V414	F355	F356		A293	Y294	SER
	K415	N357	I358		L295	A296	GLY
	I416	E359	K360		K297	S298	
	S417	L361	I362		T301	K302	V216
	Y418	D363	K364		L303	L304	K217
	K419	G365	I366		A305	R306	V218
	L420	E426	L427		THR	LEU	K219
	E427	R433	K434		GLY	S240	I220
	L428	R435	L436		V310	E311	K223
	I429	P437	A438		I312	K243	A224
		L439	D377		V313	S244	L225
		K440	V378		D314	V245	G226
			I379		L317	E247	Y227
	L432	PHE	Y380		L318	L248	S228
	R433	VAL	K381		D319	L249	P229
	M434	LVS	L382		A320	Q250	R230
	R435	TYR	Q383		V321	K256	V231
	D436	GLY	S384		I322	V257	I232
	P437	ARG	T385		R323	E258	P233
	A438	SER	I388		T324	L259	I234
	L439	PRO					E235
	L440						V236

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.80Å 114.65Å 121.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 3.15 29.48 – 3.15	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.48-3.15) 95.5 (29.48-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.218 , 0.285 0.216 , 0.277	Depositor DCC
$R_{free}$ test set	1623 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.2	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 102.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6861	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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 lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.34	0/3470	0.60	0/4670
1	B	0.32	0/3459	0.62	1/4652 (0.0%)
All	All	0.33	0/6929	0.61	1/9322 (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	B	0	2

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	B	274	LEU	CA-CB-CG	5.97	129.03	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	228	SER	Peptide
1	B	417	SER	Peptide

### 5.2 Too-close contacts

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	3420	0	3526	400	0
1	B	3411	0	3532	474	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	8	3	0
4	A	13	0	0	3	0
4	B	7	0	0	1	0
All	All	6861	0	7066	829	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 60.

The worst 5 of 829 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:B:172:HIS:ND1	1:B:191:LEU:HD11	1.57	1.20
1:A:54:ARG:HB3	1:A:101:MSE:HE3	1.29	1.14
1:B:98:ARG:HH22	1:B:137:PRO:HB3	0.99	1.10
1:A:244:SER:HA	1:B:244:SER:HA	1.24	1.09
1:A:240:SER:HB3	1:A:243:LYS:HD2	1.31	1.08

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	418/471 (89%)	370 (88%)	46 (11%)	2 (0%)	25	57
1	B	411/471 (87%)	345 (84%)	62 (15%)	4 (1%)	13	43
All	All	829/942 (88%)	715 (86%)	108 (13%)	6 (1%)	19	51

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ILE
1	A	310	VAL
1	B	27	GLU
1	B	312	ILE
1	B	230	ARG

### 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	378/410 (92%)	325 (86%)	53 (14%)	3	12
1	B	380/410 (93%)	318 (84%)	62 (16%)	2	8
All	All	758/820 (92%)	643 (85%)	115 (15%)	2	10

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	82	TYR
1	B	422	ARG
1	B	166	LEU
1	B	418	TYR
1	B	350	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	185	ASN
1	B	398	HIS
1	B	411	HIS
1	B	408	GLN
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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z  > 2$
3	GOL	A	454	-	5,5,5	0.36	0	5,5,5	0.38	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	GOL	A	454	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	454	GOL	O1-C1-C2-O2
3	A	454	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	454	GOL	3	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	417/471 (88%)	-0.76	0 100 100	52, 103, 201, 270	0
1	B	414/471 (87%)	-0.68	0 100 100	72, 130, 200, 374	0
All	All	831/942 (88%)	-0.72	0 100 100	52, 118, 201, 374	0

There are no RSRZ outliers to report.

### 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(Å <sup>2</sup> )	Q<0.9
2	MN	B	453	1/1	0.76	0.12	235,235,235,235	0
3	GOL	A	454	6/6	0.91	0.16	95,114,126,129	0
2	MN	A	453	1/1	0.97	0.05	131,131,131,131	0
2	MN	A	452	1/1	0.99	0.05	93,93,93,93	0
2	MN	B	452	1/1	0.99	0.05	103,103,103,103	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.