



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:59 AM UTC

PDB ID : 3TAL / pdb_00003tal
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

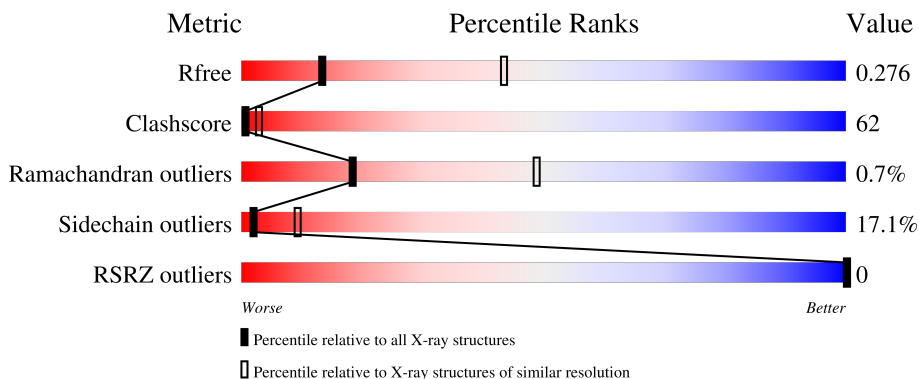
1 Overall quality at a glance

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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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 ≥ 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	

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
			Total	C	N	O	Se			
1	A	424	3420	2188	587	638	7	0	0	0
1	B	421	3411	2186	584	634	7	0	0	0

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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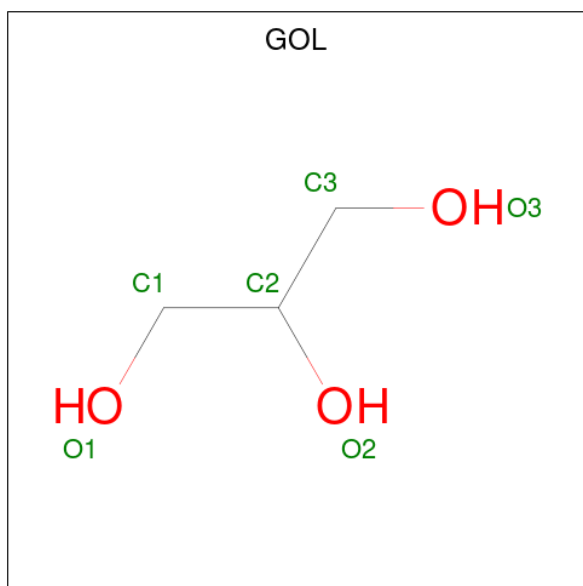
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q8U1N8
B	-13	HIS	-	expression tag	UNP Q8U1N8
B	-12	HIS	-	expression tag	UNP Q8U1N8
B	-11	HIS	-	expression tag	UNP Q8U1N8
B	-10	HIS	-	expression tag	UNP Q8U1N8
B	-9	SER	-	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 (CCD ID: 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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

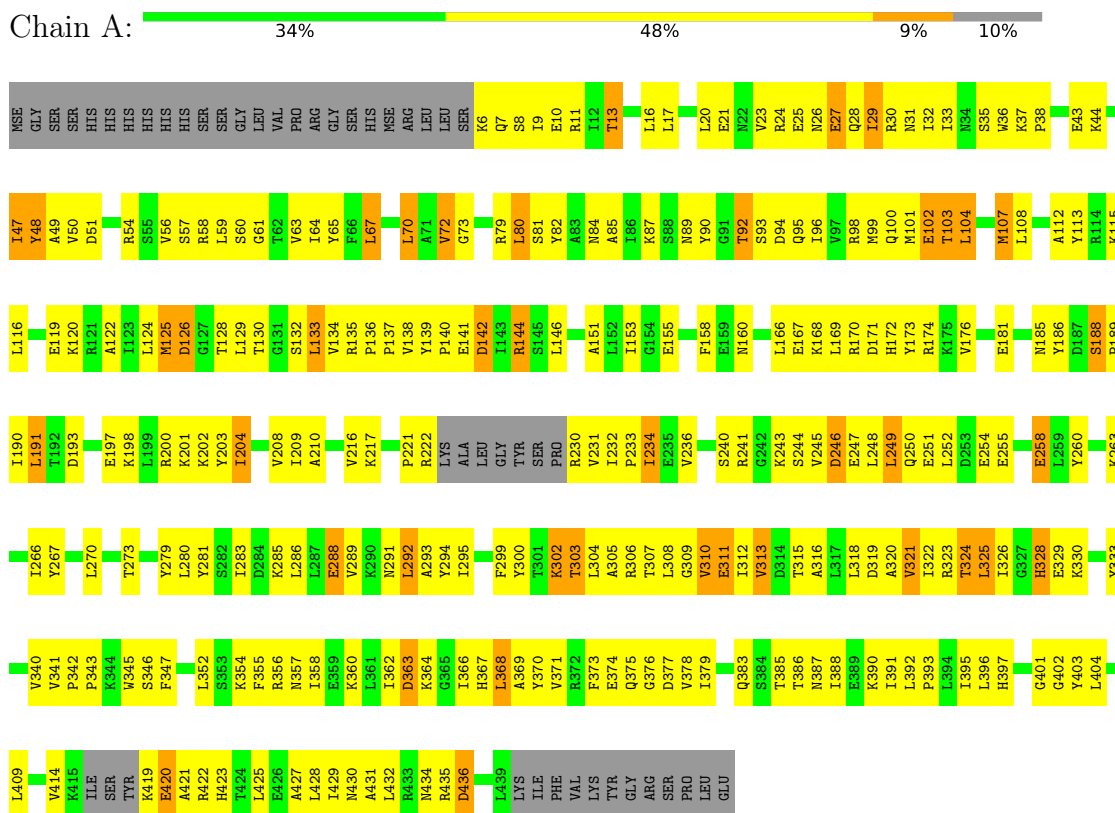
- Molecule 4 is water.

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

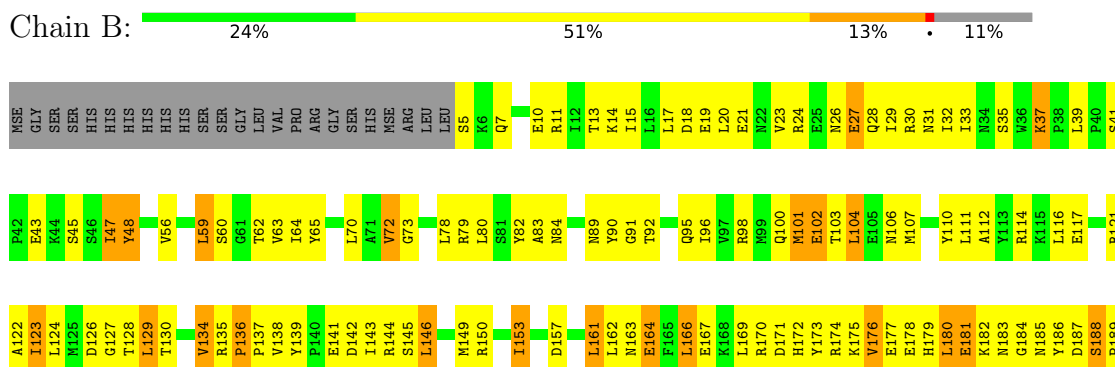
3 Residue-property plots

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



GLY	T385	R323	V257	I190
ARG	I388	I324	E288	L191
SER	E389	I326	L259	T192
PRO	K390	GLY	Y260	D193
LEU	I391	HIS	L261	N194
GLU	L392	GLU	I266	V195
	P393	K390	Y267	V196
	L394	E331	D268	E197
	I395	G332	A269	K198
	L396	Y333	L270	L199
	H397	L394	H271	R200
	H398	E335	M272	K201
	K399	I336	I273	K202
	A400	V340	L274	Y203
	GLY	V341	S275	I204
	TYR	P342	Y276	D205
	L404	P343	I277	T206
	R405	K344	E278	K207
	P406	W345	Y279	V208
	L407	S346	L280	ILE
	Q408	F347	Y281	ALA
	L409	P348	S282	TYR
	A410	I349	I283	GLY
	H411	F350	D284	SER
	H412	L351	K285	GLY
	V414	L352	E288	K215
	K415	S353	N291	V216
	I416	K354	L292	K217
	S417	F355	A293	V218
	Y418	R356	L294	K219
	K419	N357	Y294	I220
	E420	I358	I295	K223
	A421	K360	A296	A224
	R422	L361	K297	G226
	H423	I362	S298	Y227
	T424	D363	T301	S228
	L425	K364	K302	P229
	E426	G365	I303	R230
	A427	I366	L304	V231
	L428	H367	A305	I232
	I429	L368	R306	P233
	M430	A369	THR	I234
	A431	Y370	LEU	E235
	R433	V371	GLY	V236
	N434	F373	V310	S240
	R435	E374	E311	R241
	D436	Q375	I312	G242
	P437	G376	V313	K243
	A438	D377	D314	S244
	L439	V378	D314	V245
	K440	I379	L317	D246
	I44	Y380	L318	E247
	PHE	M381	L318	L248
	VAL	L382	D319	L249
	LYS	Q383	A320	Q250
	TYR	S384	V321	K256
			I322	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.218 , 0.285 0.219 , 0.276	Depositor DCC
R_{free} test set	1694 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	97.2	Xtrriage
Anisotropy	0.133	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 102.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6861	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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	0.44	0/3470	0.93	8/4670 (0.2%)
1	B	0.43	0/3459	0.98	19/4652 (0.4%)
All	All	0.43	0/6929	0.96	27/9322 (0.3%)

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.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	SER	CA-C-N	7.81	127.44	119.56
1	B	188	SER	C-N-CA	7.81	127.44	119.56
1	B	257	VAL	CB-CA-C	-7.38	104.80	111.74
1	B	228	SER	CA-C-N	-7.13	110.93	119.84
1	B	228	SER	C-N-CA	-7.13	110.93	119.84

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 [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	3420	0	3526	411	0
1	B	3411	0	3532	490	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	856	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 62.

The worst 5 of 856 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	360/471 (76%)	315 (88%)	44 (12%)	1 (0%)	36	64
1	B	244/471 (52%)	198 (81%)	43 (18%)	3 (1%)	10	37
All	All	604/942 (64%)	513 (85%)	87 (14%)	4 (1%)	18	49

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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	311/410 (76%)	264 (85%)	47 (15%)	3	13
1	B	351/410 (86%)	285 (81%)	66 (19%)	1	8
All	All	662/820 (81%)	549 (83%)	113 (17%)	2	9

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	129	LEU
1	B	424	THR
1	B	199	LEU
1	B	422	ARG
1	B	385	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	408	GLN
1	B	411	HIS

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Mol	Chain	Res	Type
1	A	367	HIS
1	B	172	HIS
1	B	185	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 95th 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 ²)	Q<0.9
1	A	417/471 (88%)	-0.62	0 100 100	52, 103, 201, 270	0
1	B	414/471 (87%)	-0.53	0 100 100	72, 130, 200, 374	0
All	All	831/942 (88%)	-0.57	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 oligosaccharides 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, 95th 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
2	MN	B	453	1/1	0.77	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	0.96	0.04	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.