



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 21, 2018 – 02:23 am GMT

PDB ID : 1UXC  
Title : FRUCTOSE REPRESSOR DNA-BINDING DOMAIN, NMR, MINIMIZED STRUCTURE  
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Deposited on : 1996-12-26

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp>

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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk30686  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

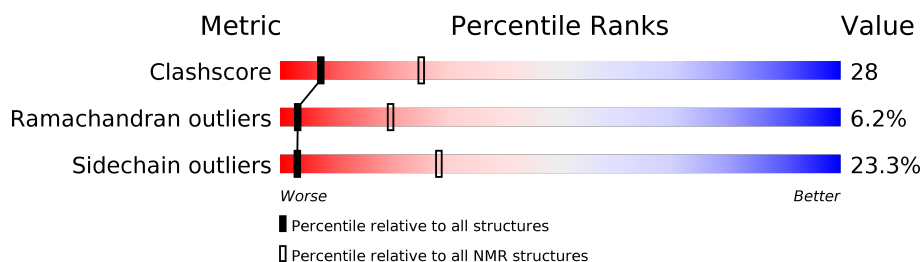
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	65	<div> <div></div> <div>34%</div> <div>32%</div> <div>11%</div> <div>23%</div> </div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition [i](#)

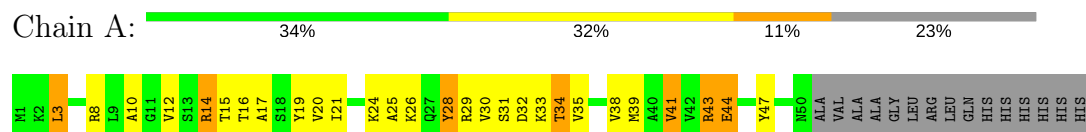
There is only 1 type of molecule in this entry. The entry contains 808 atoms, of which 411 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FRUCTOSE REPRESSOR.

Mol	Chain	Residues	Atoms						Trace
1	A	50	Total	C	H	N	O	S	0
			808	247	411	75	73	2	



- Molecule 1: FRUCTOSE REPRESSOR



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

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	Planarity
1	A	0	4
All	All	0	4

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	29	ARG	Sidechain
1	A	14	ARG	Sidechain
1	A	43	ARG	Sidechain
1	A	8	ARG	Sidechain

### 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	397	411	411	23
All	All	397	411	411	23

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 28.





All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:25:ALA:HB1	1:A:30:VAL:HG23	0.76	1.57
1:A:20:VAL:HG21	1:A:38:VAL:HB	0.76	1.56
1:A:25:ALA:HB1	1:A:30:VAL:CG2	0.59	2.28
1:A:20:VAL:HG22	1:A:39:MET:HE2	0.57	1.77
1:A:20:VAL:HG13	1:A:39:MET:SD	0.55	2.42
1:A:24:LYS:HB3	1:A:28:TYR:CE2	0.54	2.37
1:A:25:ALA:CB	1:A:30:VAL:HG23	0.53	2.32
1:A:10:ALA:HB1	1:A:38:VAL:HA	0.52	1.81
1:A:17:ALA:HA	1:A:38:VAL:HG11	0.52	1.82
1:A:25:ALA:CB	1:A:30:VAL:CG2	0.51	2.88
1:A:21:ILE:HD13	1:A:47:TYR:CD2	0.49	2.43
1:A:3:LEU:HD22	1:A:14:ARG:O	0.48	2.09
1:A:20:VAL:HG11	1:A:39:MET:N	0.46	2.25
1:A:20:VAL:HG11	1:A:38:VAL:C	0.45	2.31
1:A:20:VAL:HB	1:A:38:VAL:CG1	0.45	2.41
1:A:19:TYR:CD1	1:A:28:TYR:CD2	0.43	3.06
1:A:25:ALA:HA	1:A:30:VAL:HG22	0.43	1.90
1:A:41:VAL:HA	1:A:44:GLU:HG2	0.43	1.90
1:A:30:VAL:HB	1:A:34:THR:HB	0.42	1.90
1:A:30:VAL:HG23	1:A:30:VAL:O	0.42	2.13
1:A:35:VAL:O	1:A:39:MET:CG	0.42	2.67
1:A:20:VAL:CG1	1:A:38:VAL:HG12	0.42	2.45
1:A:20:VAL:HG13	1:A:39:MET:CG	0.41	2.45

## 6.3 Torsion angles

### 6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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	48/65 (74%)	40 (83%)	5 (10%)	3 (6%)		
All	All	48/65 (74%)	40 (83%)	5 (10%)	3 (6%)		

All 3 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	12	VAL

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Mol	Chain	Res	Type
1	A	31	SER
1	A	28	TYR

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	43/54 (80%)	33 (77%)	10 (23%)	3	28
All	All	43/54 (80%)	33 (77%)	10 (23%)	3	28

All 10 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	33	LYS
1	A	43	ARG
1	A	16	THR
1	A	3	LEU
1	A	41	VAL
1	A	34	THR
1	A	15	THR
1	A	44	GLU
1	A	26	LYS
1	A	32	ASP

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided