

Full wwPDB NMR Structure Validation Report (i)

Feb 24, 2022 – 06:56 AM EST

PDB ID	:	1Z7P
Title	:	Solution structure of reduced glutaredoxin C1 from Populus tremula x tremu-
		loides
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Deposited on	:	2005-03-26

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

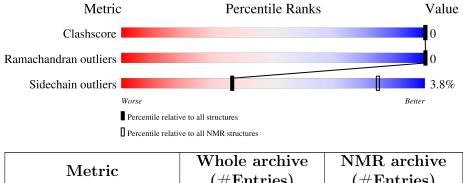
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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	(# Entries)	(#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 >=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 <=5%

Mol	Chain	Length	Quality of chain		
1	А	117	90%	•	9%



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues							
Well-defined core Residue range (total) Backbone RMSD (Å) Medoid mod							
1	A:4-A:110 (107)	0.26	16				

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 6, 7, 8, 9, 10, 12, 13, 14, 16, 17, 18, 19
2	3, 4, 5
3	11, 20
4	1, 15



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1775 atoms, of which 897 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called glutaredoxin.

Mol	Chain	Residues		Atoms					Trace
1	٨	117	Total	С	Н	Ν	0	S	0
1 A	117	1775	550	897	154	170	4	0	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	cloning artifact	UNP Q5PSJ1
A	2	ALA	-	cloning artifact	UNP Q5PSJ1
А	113	ASN	-	SEE REMARK 999	UNP Q5PSJ1
А	114	PRO	-	SEE REMARK 999	UNP Q5PSJ1
A	115	ALA	-	SEE REMARK 999	UNP Q5PSJ1
А	116	GLN	-	SEE REMARK 999	UNP Q5PSJ1
А	117	LEU	-	SEE REMARK 999	UNP Q5PSJ1

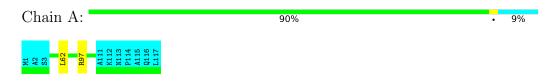


4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: glutaredoxin

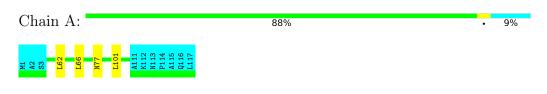


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

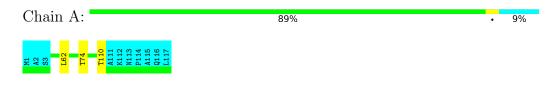
4.2.1 Score per residue for model 1

• Molecule 1: glutaredoxin



4.2.2 Score per residue for model 2

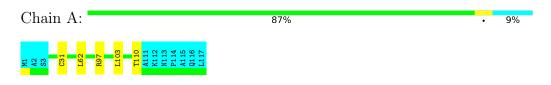
• Molecule 1: glutaredoxin





4.2.3 Score per residue for model 3

• Molecule 1: glutaredoxin



4.2.4 Score per residue for model 4

• Molecule 1: glutaredoxin

Chain A	:				85%	6%	9%
M1 A2 N35 N35	L62 L66	R97 N98	L101	T110 A111 K112 N113 P114			

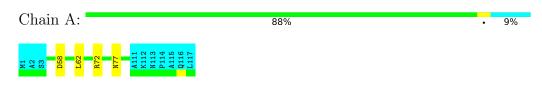
4.2.5 Score per residue for model 5

• Molecule 1: glutaredoxin

Chain A:	89%	•	9%
MI A2 A2 A2 A1 0 0 114 0 114 0 114 0 114 0 115 0 115 0 117 0 117 0 117			

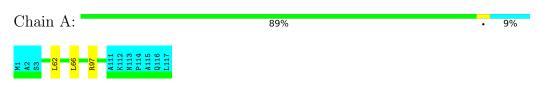
4.2.6 Score per residue for model 6

• Molecule 1: glutaredoxin



4.2.7 Score per residue for model 7

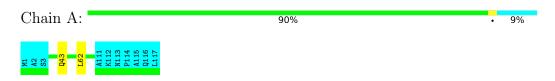
 \bullet Molecule 1: glutared oxin





4.2.8 Score per residue for model 8

• Molecule 1: glutaredoxin



4.2.9 Score per residue for model 9

• Molecule 1: glutaredoxin

Chain A:	90%	·	9%
M1 83 83 83 81 162 81114 81117 81117 81117 81117 81117 81117 81117 81117 81117 81117 81117 81117 81117 81118 8118 811181			

4.2.10 Score per residue for model 10

• Molecule 1: glutaredoxin

Chain A:	87%	•	9%
M1 83 83 83 83 83 83 83 83 83 83 83 8111 81112 81113 81115 81115 81115 81115 81115 81115			

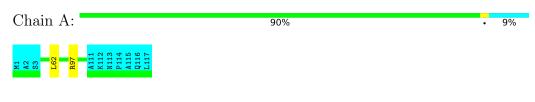
4.2.11 Score per residue for model 11

• Molecule 1: glutaredoxin

Chain A: • 9%

4.2.12 Score per residue for model 12

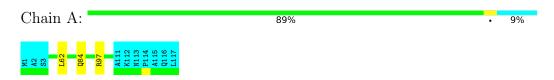
• Molecule 1: glutaredoxin





4.2.13 Score per residue for model 13

• Molecule 1: glutaredoxin



4.2.14 Score per residue for model 14

• Molecule 1: glutaredoxin

Chain A:				86%	5%	% 9%
M1 A2 S3 K4 Q5 N35	L62 R97 N98	L101	A111 K112 N113 P114 A115 Q116 L117			

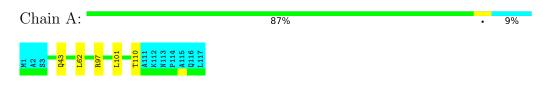
4.2.15 Score per residue for model 15

• Molecule 1: glutaredoxin

Chain A:	86%	5% 9%
M1 83 83 84 84 84 84 84 84 101 100 1103 1103 1114 81114 81114 81114 81114 81114	0116 1117	

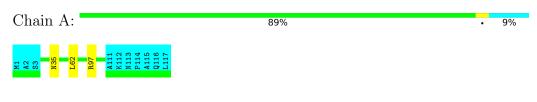
4.2.16 Score per residue for model 16 (medoid)

• Molecule 1: glutaredoxin



4.2.17 Score per residue for model 17

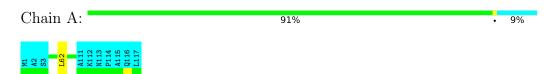
 \bullet Molecule 1: glutared oxin





4.2.18 Score per residue for model 18

• Molecule 1: glutaredoxin



4.2.19 Score per residue for model 19

• Molecule 1: glutaredoxin

Chain A:			86%	5% 9%
M1 A2 S3 L62 T74	T90 L101 L103 L103	T110 A111 K112 N113 P114 A115 Q116 L117		

4.2.20 Score per residue for model 20

• Molecule 1: glutaredoxin

Chain A:	87%	•	9%
M1 A2 B3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3			



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics simulated annealing.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	1.0.6
Amber	refinement	7

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	B	ond lengths	Bond angles		
	Unam	RMSZ	$\#Z{>}5$	RMSZ	#Z > 5	
1	А	$0.57 {\pm} 0.00$	$0{\pm}0/819$ ($0.0{\pm}$ 0.0%)	$0.84{\pm}0.01$	$1{\pm}0/1109$ ($0.1{\pm}$ 0.0%)	
All	All	0.57	0/16380 ($0.0%$)	0.84	13/22180~(~0.1%)	

There are no bond-length outliers.

All unique angle outliers are listed below.

Mo	ol (Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$\mathrm{Ideal}(^{o})$	Moo Worst	lels Total
1		A	97	ARG	NE-CZ-NH2	-6.15	117.23	120.30	10	13

There are no chirality outliers.

There are no planarity outliers.

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.

Mo	Chain	Non-H	H(model)	H(added)	Clashes
All	All	16140	16420	16440	-

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is -.

There are no clashes.



6.3 Torsion angles (i)

6.3.1 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 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	Perce	ntiles
1	А	107/117~(91%)	103 ± 2 (96 $\pm2\%$)	$4\pm2~(4\pm2\%)$	0±0 (0±0%)	100	100
All	All	2140/2340~(91%)	2061 (96%)	79~(4%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	87/94~(93%)	84 ± 2 (96 $\pm2\%$)	$3\pm2~(4\pm2\%)$	36	84
All	All	1740/1880~(93%)	1674 (96%)	66 (4%)	36	84

All 18 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	62	LEU	20
1	А	101	LEU	7
1	А	110	THR	7
1	А	66	LEU	6
1	А	77	ASN	3
1	А	103	LEU	3
1	А	35	ASN	3
1	А	5	GLN	3
1	А	74	THR	2
1	А	31	CYS	2
1	А	98	ASN	2
1	А	43	GLN	2
1	А	58	ASP	1

Continued on next page...



Mol	Chain	Res	Type	Models (Total)
1	А	72	ARG	1
1	А	28	LYS	1
1	А	93	GLU	1
1	А	84	GLN	1
1	А	90	THR	1

Continued from previous page...

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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

