



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1GXV  
Title : SOLUTION STRUCTURE OF LYSOZYME AT LOW AND HIGH PRES-  
SURE  
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Deposited on : 2002-04-12

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

<http://wwpdb.org/validation/2016/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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

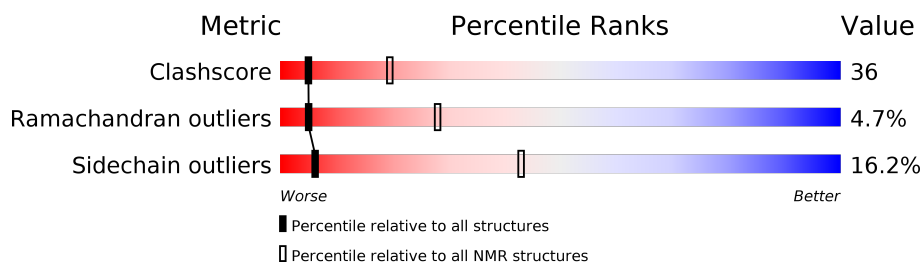
# 1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	2	129	 41% 47% 12% .

## 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 are 2 unique types of molecules in this entry. The entry contains 1975 atoms, of which 969 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LYSOZYME C.

Mol	Chain	Residues	Atoms						Trace
1	2	129	Total	C	H	N	O	S	0
			1960	613	959	193	185	10	

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		
2	2	5	Total	H	O
			15	10	5

i

- Molecule 1: LYSOZYME C

P79	C80	D87	I88	T88	V92	N93	C94	A95	K96	K97	I98	V99	S100	D101	G102	W111	R112	N113	R114	C115	K116	G117	T118	D119	W120	Q121	A122	W123	I124	R125	G126	G127	R128	L129																		
K1	R5	C6	E7	A11	M12	K13	R14	H15	G16	L17	D18	N19	Y20	R21	S24	W28	T40	Q41	M44	R45	M46	T47	D48	G49	T51	D52	Y53	G54	I55	L56	Q57	I58	N59	S60	R61	W62	C63	C64	N65	D66	G67	R68	T69	P70	G71	S72	R73	M74	L75	C76	W77	T78

## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *CHEMICAL SHIFT REFINEMENT*.

Of the 50 calculated structures, 1 were deposited, based on the following criterion: *ENERGY MINIMISED*.

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

Software name	Classification	Version
X-PLOR	refinement	
XPLOR	structure solution	

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.

There are no bond-length outliers.

There are no bond-angle outliers.

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	2	1001	959	959	71
2	2	5	10	0	1
All	All	1006	969	959	71

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:2:13:LYS:NZ	1:2:129:LEU:O	0.68	2.25
1:2:65:ASN:N	1:2:80:CYS:SG	0.67	2.67
1:2:5:ARG:NH1	1:2:122:ALA:O	0.66	2.26
1:2:20:TYR:CZ	1:2:21:ARG:NH1	0.63	2.67
1:2:76:CYS:O	1:2:97:LYS:NZ	0.62	2.29
1:2:21:ARG:NH2	1:2:100:SER:OG	0.62	2.25
1:2:15:HIS:O	1:2:96:LYS:NZ	0.61	2.28
1:2:17:LEU:HD22	1:2:28:TRP:CE2	0.61	2.30
1:2:13:LYS:NZ	1:2:129:LEU:OXT	0.61	2.32
1:2:65:ASN:C	1:2:80:CYS:SG	0.59	2.81
1:2:5:ARG:NH2	1:2:125:ARG:O	0.59	2.27
1:2:58:ILE:HG22	1:2:64:CYS:SG	0.58	2.38
1:2:1:LYS:NZ	1:2:7:GLU:OE2	0.58	2.32
1:2:115:CYS:O	1:2:117:GLY:N	0.58	2.37

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:2:14:ARG:NH1	1:2:15:HIS:CE1	0.58	2.72
1:2:13:LYS:NZ	1:2:129:LEU:C	0.57	2.58
1:2:16:GLY:O	1:2:96:LYS:NZ	0.56	2.32
1:2:14:ARG:NH1	1:2:15:HIS:NE2	0.56	2.54
1:2:119:ASP:O	1:2:123:TRP:NE1	0.56	2.29
1:2:126:GLY:O	1:2:128:ARG:N	0.55	2.36
1:2:15:HIS:HB3	1:2:92:VAL:HG11	0.55	1.77
1:2:99:VAL:O	1:2:99:VAL:HG13	0.55	2.01
1:2:74:ASN:N	2:2:133:HOH:O	0.53	2.41
1:2:124:ILE:O	1:2:125:ARG:C	0.52	2.46
1:2:98:ILE:O	1:2:100:SER:N	0.52	2.40
1:2:1:LYS:N	1:2:41:GLN:OE1	0.52	2.33
1:2:14:ARG:NH1	1:2:89:THR:OG1	0.51	2.34
1:2:11:ALA:O	1:2:15:HIS:ND1	0.51	2.24
1:2:65:ASN:O	1:2:80:CYS:SG	0.50	2.69
1:2:53:TYR:N	1:2:53:TYR:CD1	0.50	2.79
1:2:63:TRP:CZ3	1:2:98:ILE:HG23	0.49	2.42
1:2:101:ASP:CG	1:2:102:GLY:N	0.49	2.66
1:2:112:ARG:CZ	1:2:112:ARG:CB	0.48	2.90
1:2:77:ASN:ND2	1:2:77:ASN:O	0.48	2.44
1:2:94:CYS:SG	1:2:98:ILE:CD1	0.48	3.01
1:2:127:CYS:O	1:2:129:LEU:N	0.48	2.43
1:2:44:ASN:O	1:2:51:THR:HG23	0.48	2.08
1:2:1:LYS:HZ1	1:2:7:GLU:CD	0.47	2.10
1:2:55:ILE:HG23	1:2:56:LEU:N	0.47	2.23
1:2:15:HIS:NE2	1:2:89:THR:OG1	0.47	2.47
1:2:111:TRP:HA	1:2:115:CYS:SG	0.47	2.50
1:2:87:ASP:OD1	1:2:89:THR:OG1	0.46	2.32
1:2:75:LEU:N	1:2:75:LEU:CD1	0.46	2.78
1:2:59:ASN:OD1	1:2:61:ARG:HB3	0.46	2.11
1:2:21:ARG:NH1	1:2:21:ARG:CG	0.46	2.77
1:2:65:ASN:CB	1:2:74:ASN:HD22	0.45	2.23
1:2:128:ARG:NH1	1:2:128:ARG:CG	0.45	2.78
1:2:1:LYS:N	1:2:40:THR:OG1	0.45	2.31
1:2:53:TYR:OH	1:2:68:ARG:NE	0.45	2.50
1:2:19:ASN:H	1:2:24:SER:HA	0.45	1.71
1:2:61:ARG:CD	1:2:71:GLY:O	0.45	2.64
1:2:65:ASN:ND2	1:2:72:SER:HB3	0.44	2.27
1:2:65:ASN:OD1	1:2:66:ASP:N	0.44	2.51
1:2:14:ARG:NH2	1:2:87:ASP:OD2	0.44	2.35
1:2:58:ILE:HG23	1:2:63:TRP:CB	0.43	2.42
1:2:65:ASN:HB2	1:2:74:ASN:HD22	0.43	1.73

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:2:15:HIS:CD2	1:2:89:THR:HA	0.43	2.49
1:2:21:ARG:HH11	1:2:21:ARG:CG	0.42	2.27
1:2:60:SER:HA	1:2:64:CYS:O	0.42	2.14
1:2:73:ARG:O	1:2:74:ASN:CB	0.42	2.67
1:2:47:THR:O	1:2:48:ASP:C	0.42	2.56
1:2:15:HIS:NE2	1:2:89:THR:HA	0.41	2.31
1:2:47:THR:O	1:2:49:GLY:N	0.41	2.53
1:2:94:CYS:SG	1:2:98:ILE:HD11	0.41	2.56
1:2:69:THR:O	1:2:71:GLY:N	0.41	2.54
1:2:119:ASP:CG	1:2:121:GLN:H	0.41	2.19
1:2:53:TYR:OH	1:2:68:ARG:NH2	0.41	2.53
1:2:101:ASP:CG	1:2:102:GLY:H	0.40	2.20
1:2:111:TRP:CD1	1:2:115:CYS:HB2	0.40	2.52
1:2:12:MET:SD	1:2:17:LEU:HD13	0.40	2.57
1:2:45:ARG:HG3	1:2:46:ASN:N	0.40	2.31

## 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	2	127/129 (98%)	99 (78%)	22 (17%)	6 (5%)	5	28
All	All	127/129 (98%)	99 (78%)	22 (17%)	6 (5%)	5	28

All 6 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	2	57	GLN
1	2	70	PRO
1	2	116	LYS
1	2	128	ARG
1	2	99	VAL
1	2	127	CYS

### 6.3.2 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 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	2	105/105 (100%)	88 (84%)	17 (16%)	6	43
All	All	105/105 (100%)	88 (84%)	17 (16%)	6	43

All 17 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	2	113	ASN
1	2	52	ASP
1	2	58	ILE
1	2	44	ASN
1	2	56	LEU
1	2	128	ARG
1	2	77	ASN
1	2	119	ASP
1	2	73	ARG
1	2	46	ASN
1	2	123	TRP
1	2	112	ARG
1	2	21	ARG
1	2	5	ARG
1	2	12	MET
1	2	78	ILE
1	2	129	LEU

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 [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

No chemical shift data were provided