



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:06 AM GMT

PDB ID : 1OV7  
Title : T4 Lysozyme Cavity Mutant L99A/M102Q Bound with 2-Allyl-6-Methyl-Phenol  
Authors : Wei, B.Q.; Baase, W.A.; Weaver, L.H.; Matthews, B.W.; Shoichet, B.K.  
Deposited on : 2003-03-25  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

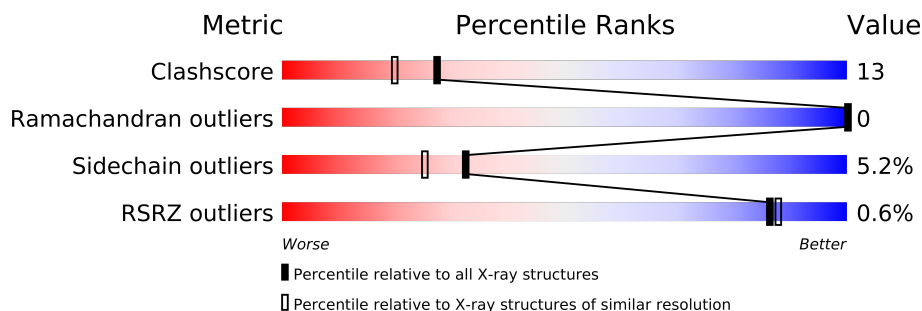
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	164	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CL	A	173	-	X
2	CL	A	178	-	X
3	LYL	A	407	-	X
4	BME	A	169	-	X
4	BME	A	170	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 1371 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1290	810	236	238	6			

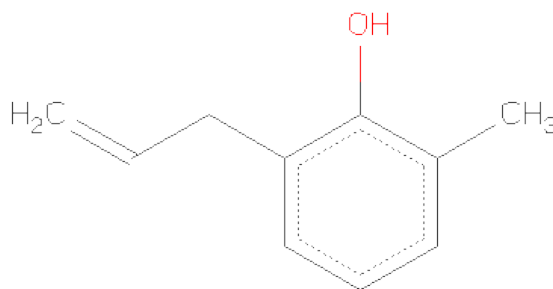
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	ALA	LEU	ENGINEERED	UNP P00720
A	102	GLN	MET	ENGINEERED	UNP P00720

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

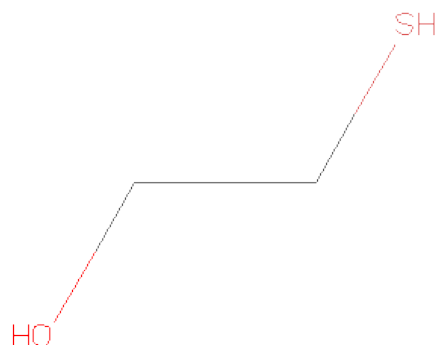
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		

- Molecule 3 is 2-ALLYL-6-METHYL-PHENOL (three-letter code: LYL) (formula: C<sub>10</sub>H<sub>12</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	10	1		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		

i

- Molecule 1: Lysozyme

N116	S117	L118	R119	M120	L121	Q122	Q123	K124	R125	W126	D127	R137	W138	Y139	P143	N144	R145	A146	K147	R148	R154	W158	D159	K162	ASN	LEU	M1	E5	D10	R14	L15	K16	I17	D20	T21	E22	M40	K43	S44	E45	L46	D47	G51	R52	D61	E62	D72	V75	R76	G77	I78	N81	A82	K83	L84	K85	P86	D89	D92	R96	V103	M106	G107	E108	V111	A112	G113	F114	T115
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.80Å 60.80Å 97.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	13.00 – 2.00 23.16 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.0 (13.00-2.00) 88.2 (23.16-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 1.90Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.189 , (Not available) 0.196 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 70.1	EDS
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 15011 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LYL, CL, BME

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	1.08	4/1310 (0.3%)	1.71	27/1764 (1.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	GLU	CD-OE2	6.30	1.32	1.25
1	A	108	GLU	CD-OE2	5.78	1.32	1.25
1	A	126	TRP	CD2-CE2	5.56	1.48	1.41
1	A	45	GLU	CD-OE2	5.13	1.31	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASP	CB-CG-OD1	10.30	127.57	118.30
1	A	127	ASP	CB-CG-OD1	10.12	127.41	118.30
1	A	127	ASP	CB-CG-OD2	-9.75	109.53	118.30
1	A	76	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A	89	ASP	CB-CG-OD2	-8.64	110.52	118.30
1	A	148	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	72	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	A	20	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	10	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	159	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	47	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	A	139	TYR	CB-CG-CD1	-6.65	117.01	121.00
1	A	159	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	119	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	154	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	103	VAL	CG1-CB-CG2	-5.92	101.44	110.90
1	A	96	ARG	NE-CZ-NH1	-5.84	117.38	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	148	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	14	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	61	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	20	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	92	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	40	ASN	CB-CA-C	5.30	121.01	110.40
1	A	137	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	145	ARG	CD-NE-CZ	-5.10	116.45	123.60
1	A	61	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1290	0	1310	34	0
2	A	2	0	0	0	0
3	A	11	0	12	11	0
4	A	8	0	12	2	0
5	A	60	0	0	0	0
All	All	1371	0	1334	34	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (34) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:LYS:HD2	1:A:17:ILE:N	1.83	0.92
1:A:78:ILE:HG12	3:A:407:LYL:H151	1.49	0.92
1:A:111:VAL:HG11	3:A:407:LYL:O6	1.73	0.86
1:A:123:GLN:NE2	1:A:125:ARG:HD2	1.91	0.84
1:A:1:MET:HA	1:A:5:GLU:OE1	1.77	0.84

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:LYS:HD2	1:A:17:ILE:H	1.54	0.71
1:A:72:ASP:OD2	1:A:76:ARG:NH2	2.28	0.65
1:A:103:VAL:HG21	3:A:407:LYL:C15	2.28	0.64
1:A:1:MET:HG2	1:A:158:TRP:CE3	2.39	0.58
1:A:116:ASN:OD1	1:A:119:ARG:NH2	2.36	0.57
1:A:123:GLN:HE21	1:A:125:ARG:HD2	1.66	0.57
1:A:78:ILE:HG12	3:A:407:LYL:C15	2.32	0.55
1:A:85:LYS:N	1:A:86:PRO:CD	2.70	0.54
1:A:1:MET:HG2	1:A:158:TRP:CD2	2.44	0.53
1:A:81:ASN:HB3	1:A:84:LEU:HB2	1.90	0.52
1:A:103:VAL:CG2	3:A:407:LYL:C15	2.88	0.51
1:A:103:VAL:CG2	3:A:407:LYL:H153	2.43	0.49
1:A:143:PRO:O	1:A:147:LYS:HG3	2.13	0.48
1:A:111:VAL:CG1	3:A:407:LYL:H13	2.45	0.47
1:A:103:VAL:HG21	3:A:407:LYL:H153	1.96	0.46
1:A:106:MET:HE2	1:A:111:VAL:HG22	1.97	0.46
1:A:84:LEU:HD13	3:A:407:LYL:H152	1.97	0.46
1:A:103:VAL:HG21	3:A:407:LYL:H152	1.99	0.44
1:A:106:MET:HE1	1:A:114:PHE:CZ	2.52	0.44
1:A:51:GLY:O	1:A:52:ARG:HB3	2.16	0.44
1:A:72:ASP:OD1	4:A:169:BME:O1	2.29	0.43
1:A:75:VAL:CG1	4:A:169:BME:S2	3.07	0.42
1:A:103:VAL:CG2	3:A:407:LYL:H152	2.50	0.42
1:A:106:MET:CE	1:A:111:VAL:HG22	2.50	0.42
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.83	0.41
1:A:111:VAL:HG12	1:A:111:VAL:O	2.20	0.41
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.85	0.41
1:A:114:PHE:O	1:A:118:LEU:HG	2.22	0.40
1:A:84:LEU:C	1:A:86:PRO:HD2	2.41	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 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 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	160/164 (98%)	153 (96%)	7 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	135/137 (98%)	128 (95%)	7 (5%)	32	25

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	22	GLU
1	A	43	LYS
1	A	44	SER
1	A	83	LYS
1	A	108	GLU
1	A	162	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	140	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z  > 2$
4	BME	A	169	-	3,3,3	0.37	0	2,2,2	0.81	0
4	BME	A	170	-	3,3,3	0.33	0	2,2,2	1.26	0
3	LYL	A	407	-	11,11,11	0.47	0	14,14,14	1.63	4 (28%)

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
4	BME	A	169	-	-	0/1/1/1	0/0/0/0
4	BME	A	170	-	-	0/1/1/1	0/0/0/0
3	LYL	A	407	-	-	0/3/3/3	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	407	LYL	C15-C5-C2	2.72	124.71	120.53
3	A	407	LYL	C15-C5-C8	-2.41	115.23	120.33
3	A	407	LYL	C3-C1-C2	2.37	120.83	117.95
3	A	407	LYL	O6-C2-C5	2.10	125.07	119.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	162/164 (98%)	-0.63	1 (0%) 86 88	6, 17, 52, 76	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	ALA	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	LYL	A	407	11/11	0.45	10.72	0,33,47,59	0
4	BME	A	169	4/4	0.24	6.07	51,64,80,82	0
4	BME	A	170	4/4	0.23	5.92	25,37,64,66	0
2	CL	A	173	1/1	0.13	5.13	53,53,53,53	0
2	CL	A	178	1/1	0.12	3.90	42,42,42,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.