



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:55 AM GMT

PDB ID : 1L13
Title : CONTRIBUTIONS OF HYDROGEN BONDS OF THR 157 TO THE THERMODYNAMIC STABILITY OF PHAGE T4 LYSOZYME
Authors : Dao-Pin, S.; Alber, T.; Matthews, B.W.
Deposited on : 1988-02-05
Resolution : 1.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

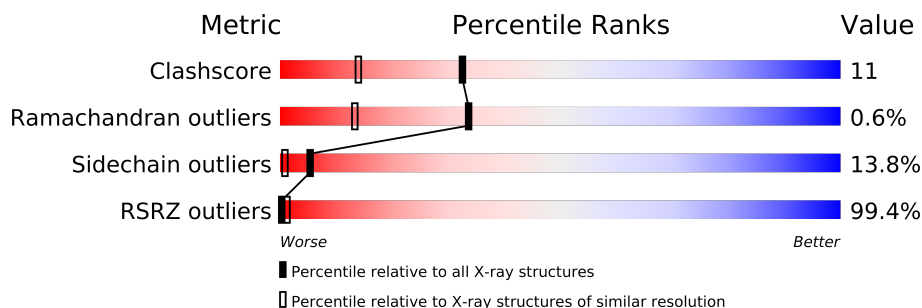
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.70 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	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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 ≥ 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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1431 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 T4 LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1313	825	241	240	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	ARG	THR	CONFLICT	UNP P00720

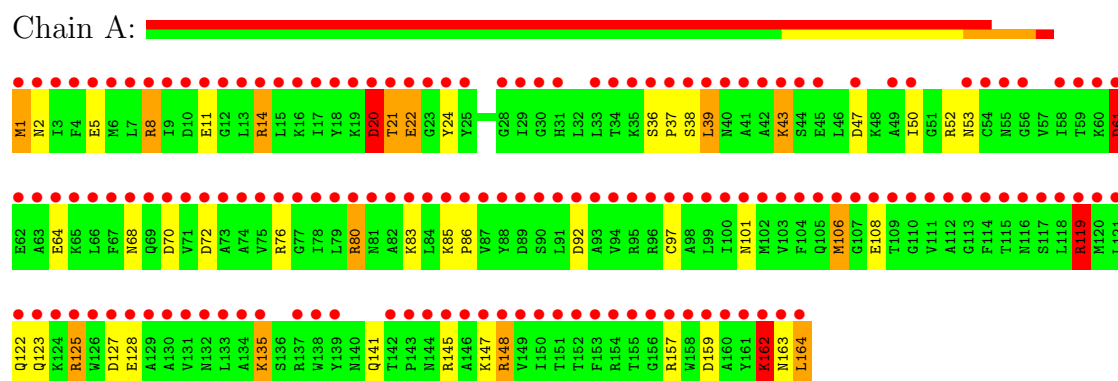
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	118	Total	O	0	0
			118	118		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: T4 LYSOZYME



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	61.10Å 61.10Å 97.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-1.70) 68.1 (20.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	126140.00 (at 1.70Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.174 , (Not available) 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.55 , 144.7	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 16037 reflections	Xtriage
F_o, F_c correlation	0.47	EDS
Total number of atoms	1431	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	1.12	4/1333 (0.3%)	1.61	27/1792 (1.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GLU	CD-OE2	6.97	1.33	1.25
1	A	128	GLU	CD-OE2	5.53	1.31	1.25
1	A	11	GLU	CD-OE1	-5.18	1.20	1.25
1	A	64	GLU	CD-OE2	5.01	1.31	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH1	12.97	126.79	120.30
1	A	8	ARG	NE-CZ-NH2	-12.45	114.07	120.30
1	A	80	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	A	14	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	20	ASP	CB-CG-OD2	-8.99	110.21	118.30
1	A	20	ASP	CB-CA-C	-8.24	93.93	110.40
1	A	61	ASP	N-CA-CB	-7.83	96.51	110.60
1	A	20	ASP	CB-CG-OD1	7.72	125.24	118.30
1	A	72	ASP	CB-CG-OD1	7.65	125.18	118.30
1	A	127	ASP	CB-CG-OD1	7.59	125.13	118.30
1	A	47	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	A	80	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	119	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	14	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	127	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	A	157	ARG	CD-NE-CZ	-6.50	114.50	123.60
1	A	22	GLU	CA-CB-CG	-6.44	99.22	113.40
1	A	125	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	92	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	162	LYS	CB-CA-C	-5.91	98.58	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	76	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	135	LYS	CB-CA-C	-5.62	99.17	110.40
1	A	70	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	145	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	148	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	A	21	THR	CA-CB-CG2	-5.02	105.38	112.40

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	1313	0	1340	30	0
2	A	118	0	0	4	0
All	All	1431	0	1340	30	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 11.

All (30) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:ASP:HB3	1:A:22:GLU:H	1.29	0.97
1:A:20:ASP:HB2	1:A:24:TYR:H	1.27	0.94
1:A:97:CYS:SG	2:A:213:HOH:O	2.31	0.89
1:A:148:ARG:HD3	1:A:164:LEU:CD2	2.04	0.88
1:A:20:ASP:HB3	1:A:22:GLU:N	2.00	0.75
1:A:148:ARG:HD3	1:A:164:LEU:HD23	1.71	0.71
1:A:148:ARG:HD3	1:A:164:LEU:HD21	1.74	0.69
1:A:20:ASP:HB2	1:A:24:TYR:N	2.06	0.68
1:A:80:ARG:NH2	2:A:277:HOH:O	2.31	0.62
1:A:1:MET:HA	1:A:5:GLU:OE1	2.01	0.61
1:A:164:LEU:N	1:A:164:LEU:HD13	2.17	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:LEU:HD13	1:A:43:LYS:HE2	1.88	0.54
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.74	0.53
1:A:164:LEU:N	1:A:164:LEU:CD1	2.73	0.52
1:A:119:ARG:HH11	1:A:119:ARG:HB3	1.74	0.52
1:A:148:ARG:CD	1:A:164:LEU:HD23	2.41	0.49
1:A:85:LYS:N	1:A:86:PRO:HD2	2.27	0.48
1:A:21:THR:HG22	1:A:21:THR:O	2.15	0.46
1:A:52:ARG:HG3	1:A:52:ARG:NH1	2.30	0.46
1:A:106:MET:HB2	1:A:106:MET:HE2	1.76	0.45
1:A:61:ASP:HB2	2:A:182:HOH:O	2.17	0.44
1:A:159:ASP:O	1:A:162:LYS:HB2	2.17	0.44
1:A:85:LYS:N	1:A:86:PRO:CD	2.80	0.43
1:A:123:GLN:HE21	1:A:125:ARG:HD2	1.82	0.43
1:A:85:LYS:HB3	1:A:86:PRO:HD3	2.00	0.42
1:A:163:ASN:O	1:A:164:LEU:OXT	2.37	0.42
1:A:1:MET:HG3	1:A:2:ASN:N	2.35	0.42
1:A:36:SER:HA	1:A:37:PRO:HD3	1.79	0.41
1:A:50:ILE:HG22	1:A:52:ARG:HG2	2.01	0.41
1:A:68:ASN:ND2	2:A:185:HOH:O	2.53	0.41

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	162/164 (99%)	158 (98%)	3 (2%)	1 (1%)	33	13

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ASP

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	138/138 (100%)	119 (86%)	19 (14%)	5 1

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	ARG
1	A	14	ARG
1	A	20	ASP
1	A	38	SER
1	A	39	LEU
1	A	43	LYS
1	A	53	ASN
1	A	61	ASP
1	A	83	LYS
1	A	101	ASN
1	A	106	MET
1	A	119	ARG
1	A	122	GLN
1	A	135	LYS
1	A	141	GLN
1	A	147	LYS
1	A	162	LYS
1	A	164	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	101	ASN
1	A	123	GLN
1	A	144	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 ⓘ

There are no ligands in this entry.

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, 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	154/164 (93%)	12.83	153 (99%) 0 1	10, 21, 39, 74	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	PHE	40.0
1	A	111	VAL	37.9
1	A	97	CYS	33.0
1	A	86	PRO	29.8
1	A	78	ILE	27.7
1	A	84	LEU	24.7
1	A	103	VAL	24.3
1	A	25	TYR	23.7
1	A	71	VAL	23.7
1	A	33	LEU	23.7
1	A	131	VAL	22.9
1	A	39	LEU	22.7
1	A	17	ILE	22.4
1	A	118	LEU	22.2
1	A	102	MET	21.8
1	A	75	VAL	21.5
1	A	98	ALA	21.3
1	A	53	ASN	20.9
1	A	112	ALA	20.5
1	A	24	TYR	20.1
1	A	115	THR	20.0
1	A	126	TRP	19.6
1	A	121	LEU	18.8
1	A	36	SER	18.6
1	A	58	ILE	18.2
1	A	59	THR	18.1
1	A	82	ALA	18.1

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Mol	Chain	Res	Type	RSRZ
1	A	150	ILE	18.0
1	A	18	TYR	17.3
1	A	109	THR	17.3
1	A	110	GLY	17.2
1	A	129	ALA	17.1
1	A	37	PRO	17.1
1	A	79	LEU	17.0
1	A	41	ALA	17.0
1	A	114	PHE	16.9
1	A	43	LYS	16.9
1	A	38	SER	16.7
1	A	164	LEU	16.6
1	A	95	ARG	16.4
1	A	113	GLY	16.3
1	A	122	GLN	16.1
1	A	117	SER	16.1
1	A	163	ASN	16.0
1	A	120	MET	15.4
1	A	12	GLY	15.2
1	A	44	SER	15.2
1	A	116	ASN	14.5
1	A	135	LYS	14.4
1	A	99	LEU	14.1
1	A	16	LYS	14.0
1	A	143	PRO	14.0
1	A	91	LEU	13.9
1	A	100	ILE	13.9
1	A	13	LEU	13.8
1	A	40	ASN	13.8
1	A	85	LYS	13.8
1	A	15	LEU	13.7
1	A	127	ASP	13.6
1	A	119	ARG	13.5
1	A	130	ALA	13.4
1	A	83	LYS	13.3
1	A	19	LYS	13.3
1	A	88	TYR	13.2
1	A	158	TRP	13.1
1	A	104	PHE	13.0
1	A	94	VAL	13.0
1	A	87	VAL	12.8
1	A	77	GLY	12.8

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Mol	Chain	Res	Type	RSRZ
1	A	80	ARG	12.7
1	A	72	ASP	12.6
1	A	55	ASN	12.4
1	A	81	ASN	12.3
1	A	108	GLU	12.0
1	A	132	ASN	11.9
1	A	42	ALA	11.9
1	A	149	VAL	11.8
1	A	60	LYS	11.5
1	A	54	CYS	11.5
1	A	123	GLN	11.3
1	A	45	GLU	11.2
1	A	128	GLU	10.9
1	A	56	GLY	10.9
1	A	156	GLY	10.9
1	A	148	ARG	10.8
1	A	9	ILE	10.8
1	A	145	ARG	10.7
1	A	28	GLY	10.6
1	A	14	ARG	10.6
1	A	34	THR	10.5
1	A	139	TYR	10.4
1	A	4	PHE	10.3
1	A	144	ASN	10.2
1	A	90	SER	10.2
1	A	125	ARG	10.1
1	A	35	LYS	9.9
1	A	2	ASN	9.9
1	A	74	ALA	9.6
1	A	29	ILE	9.3
1	A	162	LYS	9.3
1	A	73	ALA	9.3
1	A	47	ASP	9.1
1	A	89	ASP	9.1
1	A	92	ASP	9.1
1	A	101	ASN	9.0
1	A	134	ALA	9.0
1	A	66	LEU	8.9
1	A	107	GLY	8.9
1	A	7	LEU	8.8
1	A	161	TYR	8.8
1	A	151	THR	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	138	TRP	8.6
1	A	61	ASP	8.6
1	A	6	MET	8.6
1	A	67	PHE	8.4
1	A	155	THR	8.3
1	A	93	ALA	8.3
1	A	154	ARG	8.2
1	A	63	ALA	8.2
1	A	159	ASP	8.1
1	A	3	ILE	8.1
1	A	133	LEU	8.0
1	A	152	THR	8.0
1	A	146	ALA	8.0
1	A	23	GLY	7.7
1	A	76	ARG	7.6
1	A	64	GLU	7.3
1	A	49	ALA	7.0
1	A	160	ALA	7.0
1	A	1	MET	6.8
1	A	105	GLN	6.8
1	A	69	GLN	6.6
1	A	50	ILE	6.6
1	A	124	LYS	6.5
1	A	8	ARG	6.4
1	A	96	ARG	6.4
1	A	106	MET	6.4
1	A	31	HIS	6.3
1	A	11	GLU	6.2
1	A	137	ARG	5.9
1	A	20	ASP	5.9
1	A	70	ASP	5.4
1	A	68	ASN	5.1
1	A	22	GLU	4.7
1	A	142	THR	4.4
1	A	5	GLU	4.4
1	A	157	ARG	4.1
1	A	147	LYS	3.9
1	A	65	LYS	3.8
1	A	30	GLY	3.7
1	A	10	ASP	3.2
1	A	62	GLU	3.2
1	A	21	THR	3.0

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.