wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 01:35 PM EST

PDB ID	:	150L
Title	:	CONSERVATION OF SOLVENT-BINDING SITES IN 10 CRYSTAL FORMS OF T4 LYSOZYME
Authors	:	Faber, H.R.; Matthews, B.W.
Deposited on	:	1994-01-25
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

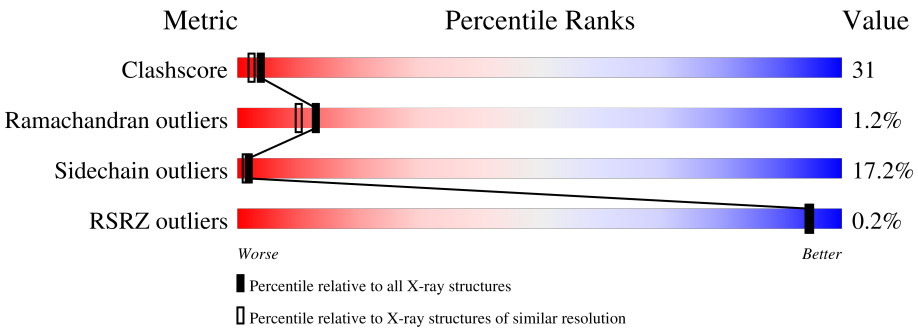
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	164	% 47% 39% 13% •
1	B	164	41% 35% 21% ••
1	C	164	61% 28% 9% ••
1	D	164	41% 40% 16% ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5327 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	164	1303	821	235	241	6	0	0	0
1	B	162	1284	809	233	236	6	0	0	0
1	C	162	1288	811	234	237	6	0	0	0
1	D	162	1288	811	234	237	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ILE	MET	conflict	UNP P00720
B	6	ILE	MET	conflict	UNP P00720
C	6	ILE	MET	conflict	UNP P00720
D	6	ILE	MET	conflict	UNP P00720

- Molecule 2 is water.

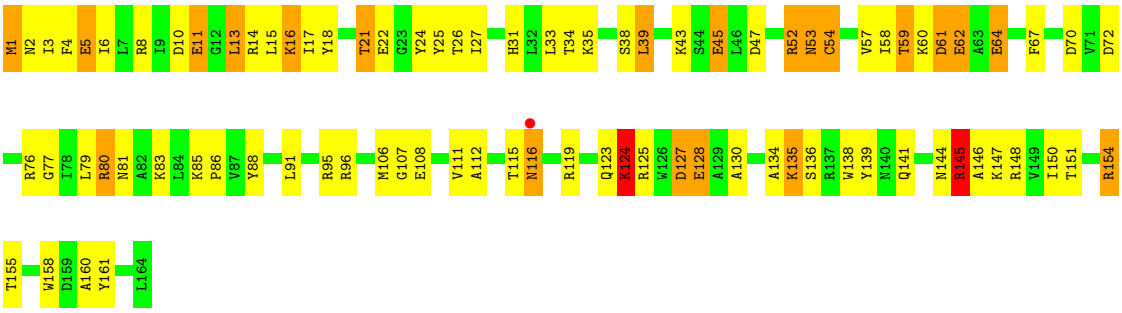
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	58	58	58	0	0
2	B	21	21	21	0	0
2	C	49	49	49	0	0
2	D	36	36	36	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

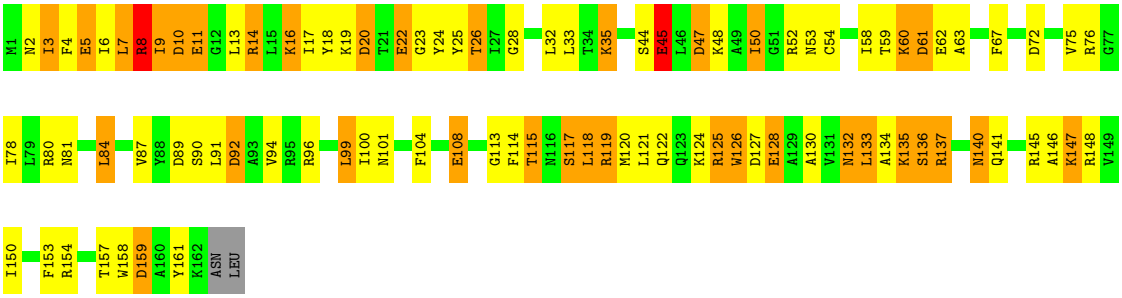
• Molecule 1: T4 LYSOZYME

Chain A:



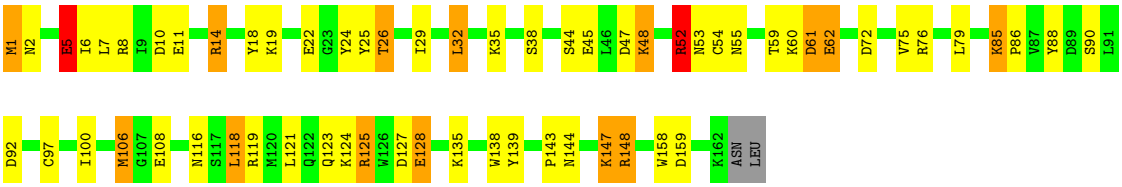
• Molecule 1: T4 LYSOZYME

Chain B:



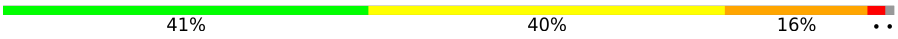
• Molecule 1: T4 LYSOZYME

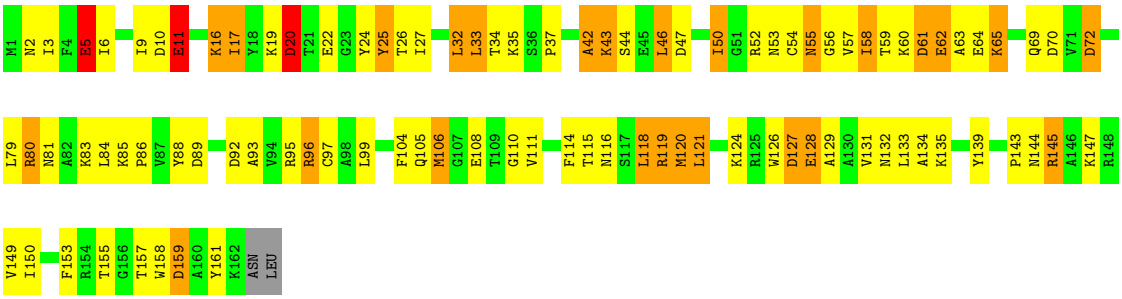
Chain C:



• Molecule 1: T4 LYSOZYME

Chain D:


41%
40%
16%


M1 N2 I3 F4 E5 I6 I9 D10 E11 K16 I17 Y18 K19 D20 T21 E22 G23 Y24 Y25 T26 I27 L32 L33 T34 K35 S36 P37 A42 K43 S44 E45 L46 D47 I50 G51 R52 N53 C54 N55 G56 V57 I58 T59 K60 D61 E62 A63 E64 K65 Q69 D70 V71 D72
L79 R80 N81 A82 K83 L84 K85 P86 V87 Y88 D89 D92 A93 Y94 R95 R96 C97 A98 L99 F104 Q105 M106 G107 E108 T109 G110 V111 F114 T115 N116 S117 L118 R119 M120 L121 K124 R125 W126 D127 E128 A129 A130 V131 N132 L133 A134 K135 Y139 P143 N144 R145 A146 K147 R148
V149 I150 F153 R154 T155 G156 T157 W158 D159 A160 Y161 K162 ASN LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.20Å 73.80Å 150.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20 7.88 – 2.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.20) 84.4 (7.88-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.22Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.210 , (Not available) 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 102.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5327	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 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 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	1.11	5/1323 (0.4%)	1.51	18/1782 (1.0%)
1	B	1.08	8/1304 (0.6%)	1.52	25/1758 (1.4%)
1	C	1.17	7/1308 (0.5%)	1.50	17/1763 (1.0%)
1	D	1.10	7/1308 (0.5%)	1.59	29/1763 (1.6%)
All	All	1.12	27/5243 (0.5%)	1.53	89/7066 (1.3%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	GLU	CD-OE2	8.55	1.35	1.25
1	B	5	GLU	CD-OE2	7.68	1.34	1.25
1	C	108	GLU	CD-OE2	7.17	1.33	1.25
1	D	5	GLU	CD-OE1	7.08	1.33	1.25
1	A	64	GLU	CD-OE1	6.87	1.33	1.25

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	ARG	NE-CZ-NH1	13.26	126.93	120.30
1	A	145	ARG	NE-CZ-NH2	-10.65	114.98	120.30
1	D	89	ASP	CB-CG-OD2	-9.77	109.51	118.30
1	B	72	ASP	CB-CG-OD2	9.43	126.78	118.30
1	A	61	ASP	CB-CG-OD1	-9.01	110.19	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1303	0	1325	86	0
1	B	1284	0	1302	105	0
1	C	1288	0	1308	45	1
1	D	1288	0	1308	89	1
2	A	58	0	0	6	0
2	B	21	0	0	2	0
2	C	49	0	0	0	0
2	D	36	0	0	2	0
All	All	5327	0	5243	319	1

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 31.

The worst 5 of 319 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG2	1:A:6:ILE:HD11	1.37	1.05
1:A:116:ASN:H	1:A:116:ASN:ND2	1.51	1.04
1:C:75:VAL:HG22	1:C:100:ILE:HD11	1.40	1.03
1:A:125:ARG:HB3	1:A:128:GLU:HG3	1.38	1.01
1:D:155:THR:HG22	1:D:157:THR:HG23	1.43	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LYS:NZ	1:D:72:ASP:OD1[3_645]	2.06	0.14

5.3 Torsion angles (i)

5.3.1 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 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%)	152 (94%)	8 (5%)	2 (1%)	13	10
1	B	160/164 (98%)	140 (88%)	16 (10%)	4 (2%)	5	3
1	C	160/164 (98%)	148 (92%)	11 (7%)	1 (1%)	25	26
1	D	160/164 (98%)	146 (91%)	13 (8%)	1 (1%)	25	26
All	All	642/656 (98%)	586 (91%)	48 (8%)	8 (1%)	13	10

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	LYS
1	B	53	ASN
1	A	135	LYS
1	C	124	LYS
1	B	132	ASN

5.3.2 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 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	137/138 (99%)	116 (85%)	21 (15%)	2	2
1	B	134/138 (97%)	102 (76%)	32 (24%)	0	0
1	C	135/138 (98%)	117 (87%)	18 (13%)	4	3
1	D	135/138 (98%)	113 (84%)	22 (16%)	2	2
All	All	541/552 (98%)	448 (83%)	93 (17%)	2	1

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	26	THR
1	D	5	GLU
1	C	38	SER
1	C	90	SER
1	D	17	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	132	ASN
1	D	144	ASN
1	B	2	ASN
1	B	68	ASN
1	B	144	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	164/164 (100%)	-0.30	1 (0%) 89 88	12, 29, 52, 59	0
1	B	162/164 (98%)	-0.36	0 100 100	18, 37, 58, 71	0
1	C	162/164 (98%)	-0.54	0 100 100	15, 27, 49, 63	0
1	D	162/164 (98%)	-0.47	0 100 100	13, 35, 55, 65	0
All	All	650/656 (99%)	-0.42	1 (0%) 95 94	12, 33, 55, 71	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	ASN	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.