



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:18 PM GMT

PDB ID : 1T0K  
Title : Joint X-ray and NMR Refinement of Yeast L30e-mRNA complex  
Authors : Chao, J.A.; Williamson, J.R.  
Deposited on : 2004-04-09  
Resolution : 3.24 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

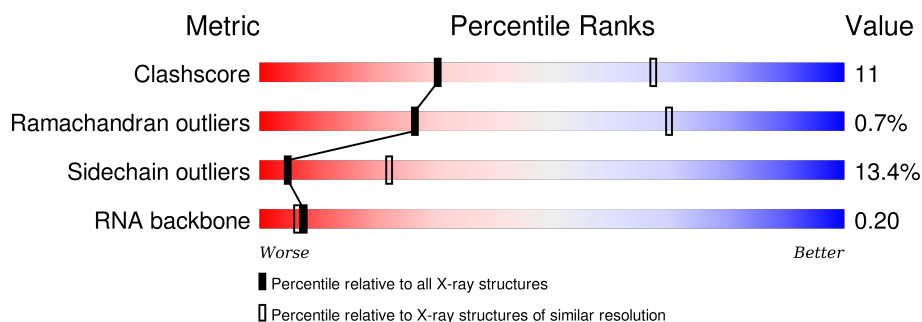
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.24 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	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RNA backbone	2183	1001 (3.74-2.74)

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. 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	13	
2	D	16	
3	A	381	
4	B	105	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4194 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 RNA chain called 5'-R(\*GP\*AP\*CP\*CP\*GP\*GP\*AP\*GP\*UP\*GP\*UP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			256	115	48	82	11			

- Molecule 2 is a RNA chain called 5'-R(\*G\*GP\*AP\*CP\*GP\*CP\*AP\*GP\*AP\*GP\*AP\*UP\*GP\*GP\*UP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	15	Total	C	N	O	P	0	0	0
			323	145	63	101	14			

- Molecule 3 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	365	Total	C	N	O	S	0	0	0
			2827	1819	460	542	6			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING MET	UNP P02928
A	367	ASN	-	CLONING ARTIFACT	UNP P02928
A	368	SER	-	CLONING ARTIFACT	UNP P02928
A	369	SER	-	CLONING ARTIFACT	UNP P02928
A	370	SER	-	CLONING ARTIFACT	UNP P02928
A	371	VAL	-	CLONING ARTIFACT	UNP P02928
A	372	PRO	-	CLONING ARTIFACT	UNP P02928
A	373	GLY	-	CLONING ARTIFACT	UNP P02928
A	374	ARG	-	CLONING ARTIFACT	UNP P02928
A	375	GLY	-	CLONING ARTIFACT	UNP P02928
A	376	SER	-	CLONING ARTIFACT	UNP P02928
A	377	ILE	-	CLONING ARTIFACT	UNP P02928

*Continued on next page...*

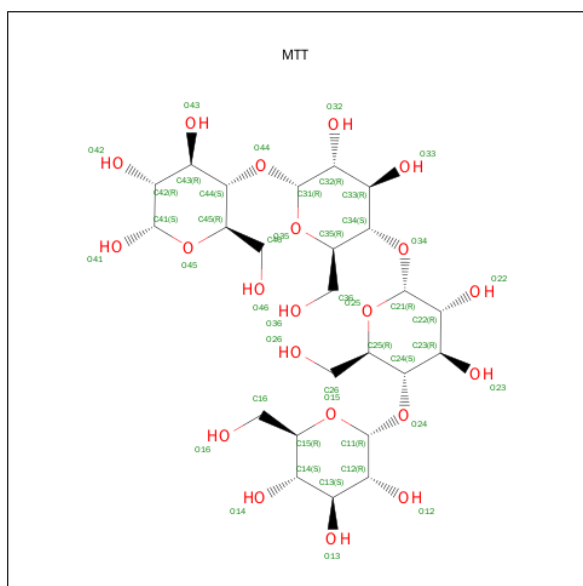
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	GLU	-	CLONING ARTIFACT	UNP P02928
A	379	GLY	-	CLONING ARTIFACT	UNP P02928
A	380	ARG	-	CLONING ARTIFACT	UNP P02928

- Molecule 4 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			

- Molecule 5 is MALTOTETRAOSE (three-letter code: MTT) (formula:  $C_{24}H_{42}O_{21}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			45	24	21		

### 3 Residue-property plots [i](#)

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.

Note EDS was not executed.

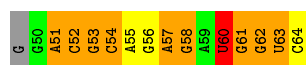
- Molecule 1: 5'-R(\*GP\*AP\*CP\*CP\*GP\*GP\*AP\*GP\*UP\*GP\*UP\*CP\*C)-3'

Chain C: 



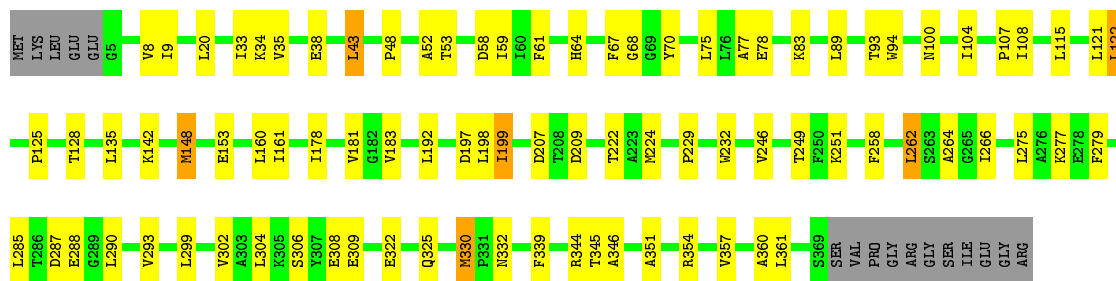
- Molecule 2: 5'-R(\*G\*GP\*AP\*CP\*GP\*CP\*AP\*GP\*AP\*GP\*AP\*UP\*GP\*GP\*UP\*C)-3'

Chain D: 



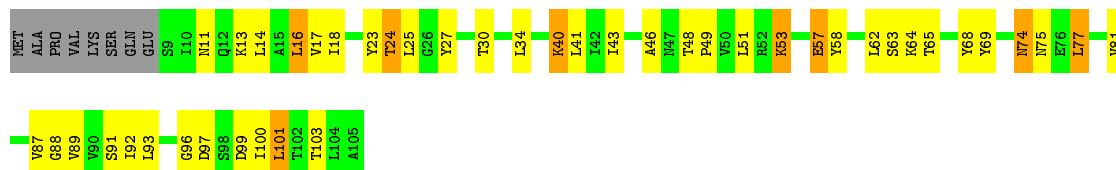
- Molecule 3: Maltose-binding periplasmic protein

Chain A: 



- Molecule 4: 60S ribosomal protein L30

Chain B: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.01Å 136.01Å 123.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.00 – 3.24	Depositor
% Data completeness (in resolution range)	(Not available) (26.00-3.24)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.261 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MTT

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	C	0.72	0/286	0.74	0/445
2	D	0.86	0/362	0.96	0/564
3	A	0.70	0/2896	0.61	0/3933
4	B	0.81	0/751	0.88	0/1008
All	All	0.74	0/4295	0.71	0/5950

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	D	0	1
3	A	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	344	ARG	Sidechain
1	C	9	C	Sidechain
2	D	60	U	Sidechain

## 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	C	256	0	132	5	0
2	D	323	0	165	19	0
3	A	2827	0	2792	37	0
4	B	743	0	797	33	0
5	A	45	0	41	1	0
All	All	4194	0	3927	89	0

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 11.

The worst 5 of 89 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)
3:A:199:ILE:HD13	3:A:351:ALA:HB1	1.63	0.80
4:B:24:THR:HG22	4:B:93:LEU:HD11	1.76	0.67
3:A:293:VAL:HG12	3:A:299:LEU:HD21	1.79	0.65
3:A:122:LEU:HD11	3:A:135:LEU:HD21	1.77	0.65
4:B:53:LYS:O	4:B:57:GLU:HB2	2.00	0.60

There are no symmetry-related clashes.

## 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
3	A	363/381 (95%)	331 (91%)	31 (8%)	1 (0%)	46 83

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	95/105 (90%)	80 (84%)	13 (14%)	2 (2%)	9	44
All	All	458/486 (94%)	411 (90%)	44 (10%)	3 (1%)	26	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	262	LEU
4	B	46	ALA
4	B	96	GLY

### 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	
3	A	292/305 (96%)	256 (88%)	36 (12%)	6	27
4	B	81/88 (92%)	67 (83%)	14 (17%)	2	12
All	All	373/393 (95%)	323 (87%)	50 (13%)	5	22

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	262	LEU
3	A	306	SER
4	B	74	ASN
3	A	277	LYS
3	A	288	GLU

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

Mol	Chain	Res	Type
3	A	272	ASN
3	A	335	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	11/13 (84%)	5 (45%)	0
2	D	14/16 (87%)	10 (71%)	3 (21%)
All	All	25/29 (86%)	15 (60%)	3 (12%)

5 of 15 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	11	G
1	C	12	A
1	C	13	G
1	C	15	G
1	C	16	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	51	A
2	D	58	G
2	D	62	G

## 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 ⓘ

1 ligand is modelled in this entry.

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
5	MTT	A	381	-	48,48,48	1.07	4 (8%)	71,71,71	1.69	11 (15%)

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
5	MTT	A	381	-	-	0/20/100/100	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	381	MTT	O34-C34	-2.40	1.37	1.43
5	A	381	MTT	O44-C44	-2.31	1.38	1.43
5	A	381	MTT	O45-C45	-2.14	1.39	1.44
5	A	381	MTT	O45-C41	-2.08	1.39	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	381	MTT	O43-C43-C42	-2.98	103.62	110.34
5	A	381	MTT	O34-C21-O25	-2.36	104.72	110.68
5	A	381	MTT	O42-C42-C43	-2.12	105.58	110.34
5	A	381	MTT	C43-C44-C45	2.07	115.52	110.84
5	A	381	MTT	C31-O44-C44	2.14	123.59	118.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	381	MTT	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.