



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1XB2 / pdb_00001xb2
Title : Crystal Structure of Bos taurus mitochondrial Elongation Factor Tu/Ts Complex
Authors : Jeppesen, M.G.; Navratil, T.; Spremulli, L.L.; Nyborg, J.
Deposited on : 2004-08-27
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

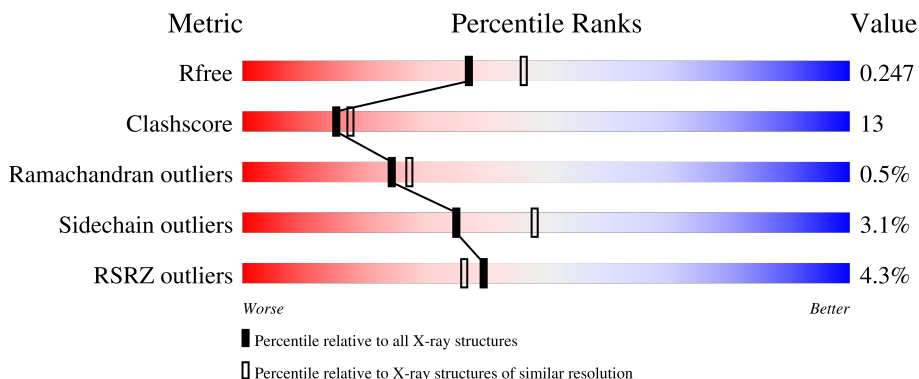
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	409	5% 61% 25% • 10%
2	B	291	2% 74% 19% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5294 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 Elongation factor Tu, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	Se	0	1	0
			2864	1810	500	537	5	12			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	MSE	MET	modified residue	UNP P49410
A	158	MSE	MET	modified residue	UNP P49410
A	191	MSE	MET	modified residue	UNP P49410
A	308	MSE	MET	modified residue	UNP P49410
A	340	MSE	MET	modified residue	UNP P49410
A	375	MSE	MET	modified residue	UNP P49410
A	378	MSE	MET	modified residue	UNP P49410
A	385	MSE	MET	modified residue	UNP P49410
A	399	MSE	MET	modified residue	UNP P49410
A	414	MSE	MET	modified residue	UNP P49410
A	442	MSE	MET	modified residue	UNP P49410

- Molecule 2 is a protein called Elongation factor Ts, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	276	Total	C	N	O	S	0	0	0
			2108	1329	369	399	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	LEU	-	expression tag	UNP P43896
B	340	GLU	-	expression tag	UNP P43896
B	341	HIS	-	expression tag	UNP P43896
B	342	HIS	-	expression tag	UNP P43896
B	343	HIS	-	expression tag	UNP P43896

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Chain	Residue	Modelled	Actual	Comment	Reference
B	344	HIS	-	expression tag	UNP P43896
B	345	HIS	-	expression tag	UNP P43896
B	346	HIS	-	expression tag	UNP P43896

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total 152	O 152	0	0
3	B	170	Total 170	O 170	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.00Å 149.30Å 70.00Å 90.00° 125.20° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.20) 98.3 (30.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.247 0.229 , 0.247	Depositor DCC
R_{free} test set	3186 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5294	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.69	12/2906 (0.4%)	0.93	9/3917 (0.2%)
2	B	0.42	0/2144	0.89	8/2889 (0.3%)
All	All	0.59	12/5050 (0.2%)	0.91	17/6806 (0.2%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	414	MSE	SE-CE	-10.58	1.63	1.95
1	A	399	MSE	SE-CE	-10.14	1.65	1.95
1	A	191	MSE	SE-CE	-7.52	1.72	1.95
1	A	308	MSE	SE-CE	-6.94	1.74	1.95
1	A	158	MSE	SE-CE	-6.57	1.75	1.95

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	A	119	ALA	N-CA-C	7.79	119.55	111.14
1	A	187	GLN	CG-CD-NE2	6.66	126.39	116.40
2	B	236	SER	CA-C-N	6.50	126.64	119.87
2	B	236	SER	C-N-CA	6.50	126.64	119.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2864	0	2917	100	0
2	B	2108	0	2135	40	0
3	A	152	0	0	16	0
3	B	170	0	0	5	0
All	All	5294	0	5052	135	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 13.

The worst 5 of 135 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:308:MSE:HE3	1:A:313:LEU:HD22	1.58	0.84
1:A:361:LYS:HE3	1:A:367:HIS:NE2	1.94	0.83
2:B:162:CYS:HG	2:B:217:TRP:CG	1.97	0.83
1:A:183:ALA:HB3	1:A:187:GLN:OE1	1.82	0.79
1:A:361:LYS:HG3	1:A:367:HIS:CD2	2.18	0.78

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	
1	A	366/409 (90%)	345 (94%)	18 (5%)	3 (1%)	16	16
2	B	274/291 (94%)	263 (96%)	11 (4%)	0	100	100
All	All	640/700 (91%)	608 (95%)	29 (4%)	3 (0%)	24	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	ASP

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Mol	Chain	Res	Type
1	A	187	GLN
1	A	183	ALA

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	314/331 (95%)	303 (96%)	11 (4%)	32	43
2	B	228/240 (95%)	221 (97%)	7 (3%)	35	48
All	All	542/571 (95%)	524 (97%)	18 (3%)	35	45

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	234	MET
2	B	319	SER
2	B	294	THR
1	A	375[A]	MSE
2	B	220	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	448	ASN
2	B	153	GLN
2	B	163	GLN
2	B	314	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	358/409 (87%)	0.56	22 (6%) 27 24	27, 53, 86, 97	0
2	B	276/291 (94%)	0.17	5 (1%) 67 64	26, 42, 74, 94	0
All	All	634/700 (90%)	0.39	27 (4%) 40 36	26, 48, 83, 97	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	VAL	4.2
1	A	452	SER	3.5
1	A	185	ALA	3.2
2	B	288	PRO	3.1
1	A	115	TYR	3.0

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 oligosaccharides 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.