



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6ERP / pdb_00006erp
Title : Structure of the human mitochondrial transcription initiation complex at the LSP promoter
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Deposited on : 2017-10-18
Resolution : 4.50 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
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

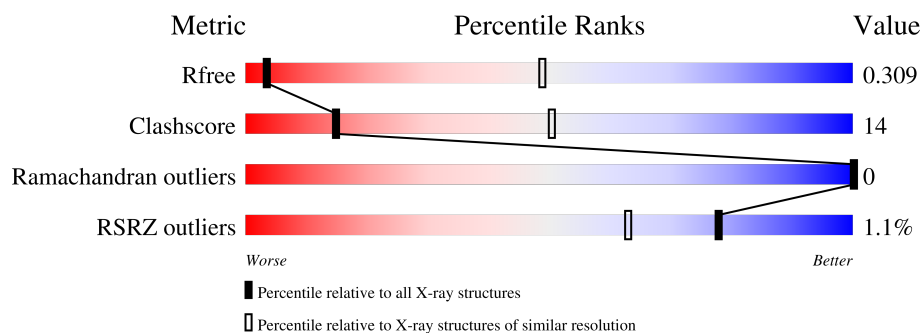
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27644 atoms, of which 42 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 Transcription factor A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	192	Total	C	N	O	S	0	0	0
			1615	1019	291	300	5			
1	G	192	Total	C	N	O	S	0	0	0
			1615	1019	291	300	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	41	ASN	-	expression tag	UNP Q00059
C	42	ALA	-	expression tag	UNP Q00059
C	49	SER	CYS	conflict	UNP Q00059
G	41	ASN	-	expression tag	UNP Q00059
G	42	ALA	-	expression tag	UNP Q00059
G	49	SER	CYS	conflict	UNP Q00059

- Molecule 2 is a DNA chain called Non-Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	46	Total	C	N	O	P	0	0	0
			952	454	176	277	45			
2	H	46	Total	C	N	O	P	0	0	0
			952	454	176	277	45			

- Molecule 3 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	45	Total	C	N	O	P	0	0	0
			907	434	163	266	44			
3	I	45	Total	C	N	O	P	0	0	0
			907	434	163	266	44			

- Molecule 4 is a protein called DNA-directed RNA polymerase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1011	Total	C	N	O	S	0	0	0
			8028	5107	1452	1418	51			
4	B	1003	Total	C	N	O	S	0	0	0
			7974	5073	1444	1406	51			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	-	expression tag	UNP O00411
A	104	ALA	-	expression tag	UNP O00411
A	555	ALA	GLU	engineered mutation	UNP O00411
B	103	ASN	-	expression tag	UNP O00411
B	104	ALA	-	expression tag	UNP O00411
B	555	ALA	GLU	engineered mutation	UNP O00411

- Molecule 5 is a protein called Dimethyladenosine transferase 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	288	Total	C	H	N	O	S	0	0
			2347	1506	21	397	408	15		
5	J	288	Total	C	H	N	O	S	0	0
			2347	1506	21	397	408	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	20	ASN	-	expression tag	UNP Q9H5Q4
F	21	ALA	GLY	conflict	UNP Q9H5Q4
J	20	ASN	-	expression tag	UNP Q9H5Q4
J	21	ALA	GLY	conflict	UNP Q9H5Q4

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.91Å 197.03Å 137.21Å 90.00° 99.87° 90.00°	Depositor
Resolution (Å)	49.58 – 4.50 49.58 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.58-4.50) 98.7 (49.58-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 4.45Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.270 , 0.310 0.273 , 0.309	Depositor DCC
R_{free} test set	1595 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	276.0	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 308.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27644	wwPDB-VP
Average B, all atoms (Å ²)	379.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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.

4 Model quality [i](#)

4.1 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	C	0.09	0/1646	0.26	0/2202
1	G	0.08	0/1646	0.26	0/2202
2	D	0.19	0/1068	0.39	0/1648
2	H	0.20	0/1068	0.39	0/1648
3	E	0.22	0/1014	0.54	3/1557 (0.2%)
3	I	0.22	0/1014	0.54	3/1557 (0.2%)
4	A	0.09	0/8213	0.28	0/11132
4	B	0.09	0/8157	0.28	0/11053
5	F	0.08	0/2380	0.25	0/3213
5	J	0.07	0/2380	0.25	0/3213
All	All	0.11	0/28586	0.31	6/39425 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	19	DA	OP2-P-O3'	-8.98	81.06	108.00
3	I	19	DA	OP2-P-O3'	-8.82	81.54	108.00
3	E	19	DA	OP1-P-O3'	-7.56	85.32	108.00
3	I	19	DA	OP1-P-O3'	-7.43	85.70	108.00
3	E	20	DT	OP1-P-OP2	5.69	137.06	120.00

There are no chirality outliers.

There are no planarity outliers.

4.2 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	1615	0	1655	56	0
1	G	1615	0	1655	50	0
2	D	952	0	523	36	0
2	H	952	0	523	20	0
3	E	907	0	508	58	0
3	I	907	0	508	52	0
4	A	8028	0	8092	213	0
4	B	7974	0	8039	208	0
5	F	2326	21	2375	64	0
5	J	2326	21	2375	51	0
All	All	27602	42	26253	741	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 14.

The worst 5 of 741 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)
4:B:363:GLN:HB3	4:B:364:LEU:HG	1.28	1.13
4:A:363:GLN:HB3	4:A:364:LEU:HG	1.34	1.07
1:G:152:LEU:HD21	1:G:230:LEU:HD13	1.41	1.02
5:F:89:LEU:HD11	5:F:116:ALA:HB1	1.42	1.00
5:J:114:LEU:HB3	5:J:140:LEU:HD11	1.43	0.99

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	C	190/205 (93%)	184 (97%)	6 (3%)	0	100	100
1	G	190/205 (93%)	187 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1001/1128 (89%)	962 (96%)	39 (4%)	0	100	100
4	B	991/1128 (88%)	958 (97%)	33 (3%)	0	100	100
5	F	282/377 (75%)	271 (96%)	11 (4%)	0	100	100
5	J	282/377 (75%)	272 (96%)	10 (4%)	0	100	100
All	All	2936/3420 (86%)	2834 (96%)	102 (4%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	C	192/205 (93%)	-0.38	1 (0%) 87 75	312, 394, 446, 483	0
1	G	192/205 (93%)	-0.48	0 100 100	405, 477, 524, 533	0
2	D	46/50 (92%)	0.01	0 100 100	337, 410, 526, 562	0
2	H	46/50 (92%)	0.05	0 100 100	415, 474, 534, 545	0
3	E	45/50 (90%)	-0.10	0 100 100	359, 433, 502, 518	0
3	I	45/50 (90%)	-0.02	0 100 100	413, 483, 558, 625	0
4	A	1011/1128 (89%)	-0.09	17 (1%) 69 55	246, 329, 411, 462	0
4	B	1003/1128 (88%)	-0.20	10 (0%) 79 64	269, 356, 432, 478	0
5	F	288/377 (76%)	-0.28	1 (0%) 90 80	287, 345, 461, 501	0
5	J	288/377 (76%)	-0.30	5 (1%) 69 55	325, 410, 579, 648	0
All	All	3156/3620 (87%)	-0.20	34 (1%) 78 63	246, 362, 500, 648	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1032	LEU	5.7
4	A	815	HIS	5.3
5	J	254	TRP	4.8
4	B	1032	LEU	4.0
4	A	297	LEU	3.4

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.