



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 09:17 am BST

PDB ID : 3PQ1
Title : Crystal structure of human mitochondrial poly(A) polymerase (PAPD1)
Authors : Bai, Y.; Srivastava, S.K.; Chang, J.H.; Tong, L.
Deposited on : 2010-11-25
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

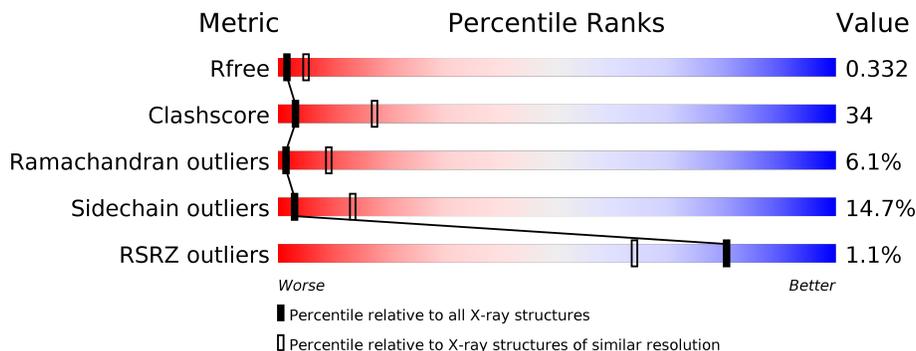
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 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	464	 % 36% 31% 8% • 23%
1	B	464	 % 29% 33% 7% • 31%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5351 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 Poly(A) RNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	355	2793	1782	474	520	11	6	0	0	0
1	B	321	2558	1629	438	475	10	6	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MSE	-	EXPRESSION TAG	UNP Q9NVV4
A	24	GLY	-	EXPRESSION TAG	UNP Q9NVV4
A	25	SER	-	EXPRESSION TAG	UNP Q9NVV4
A	26	SER	-	EXPRESSION TAG	UNP Q9NVV4
A	27	HIS	-	EXPRESSION TAG	UNP Q9NVV4
A	28	HIS	-	EXPRESSION TAG	UNP Q9NVV4
A	29	HIS	-	EXPRESSION TAG	UNP Q9NVV4
A	30	HIS	-	EXPRESSION TAG	UNP Q9NVV4
A	31	HIS	-	EXPRESSION TAG	UNP Q9NVV4
A	32	HIS	-	EXPRESSION TAG	UNP Q9NVV4
A	33	SER	-	EXPRESSION TAG	UNP Q9NVV4
A	34	SER	-	EXPRESSION TAG	UNP Q9NVV4
A	35	GLY	-	EXPRESSION TAG	UNP Q9NVV4
A	36	LEU	-	EXPRESSION TAG	UNP Q9NVV4
A	37	VAL	-	EXPRESSION TAG	UNP Q9NVV4
A	38	PRO	-	EXPRESSION TAG	UNP Q9NVV4
A	39	ARG	-	EXPRESSION TAG	UNP Q9NVV4
A	40	GLY	-	EXPRESSION TAG	UNP Q9NVV4
A	41	SER	-	EXPRESSION TAG	UNP Q9NVV4
A	42	HIS	-	EXPRESSION TAG	UNP Q9NVV4
A	43	MSE	-	EXPRESSION TAG	UNP Q9NVV4
A	151	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	152	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	153	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	154	UNK	-	SEE REMARK 999	UNP Q9NVV4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	155	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	156	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	157	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	325	ALA	ASP	ENGINEERED MUTATION	UNP Q9NVV4
A	464	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	465	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	466	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	467	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	468	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	469	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	470	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	471	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	472	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	473	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	474	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	475	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	476	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	477	UNK	-	SEE REMARK 999	UNP Q9NVV4
A	478	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	23	MSE	-	EXPRESSION TAG	UNP Q9NVV4
B	24	GLY	-	EXPRESSION TAG	UNP Q9NVV4
B	25	SER	-	EXPRESSION TAG	UNP Q9NVV4
B	26	SER	-	EXPRESSION TAG	UNP Q9NVV4
B	27	HIS	-	EXPRESSION TAG	UNP Q9NVV4
B	28	HIS	-	EXPRESSION TAG	UNP Q9NVV4
B	29	HIS	-	EXPRESSION TAG	UNP Q9NVV4
B	30	HIS	-	EXPRESSION TAG	UNP Q9NVV4
B	31	HIS	-	EXPRESSION TAG	UNP Q9NVV4
B	32	HIS	-	EXPRESSION TAG	UNP Q9NVV4
B	33	SER	-	EXPRESSION TAG	UNP Q9NVV4
B	34	SER	-	EXPRESSION TAG	UNP Q9NVV4
B	35	GLY	-	EXPRESSION TAG	UNP Q9NVV4
B	36	LEU	-	EXPRESSION TAG	UNP Q9NVV4
B	37	VAL	-	EXPRESSION TAG	UNP Q9NVV4
B	38	PRO	-	EXPRESSION TAG	UNP Q9NVV4
B	39	ARG	-	EXPRESSION TAG	UNP Q9NVV4
B	40	GLY	-	EXPRESSION TAG	UNP Q9NVV4
B	41	SER	-	EXPRESSION TAG	UNP Q9NVV4
B	42	HIS	-	EXPRESSION TAG	UNP Q9NVV4
B	43	MSE	-	EXPRESSION TAG	UNP Q9NVV4
B	151	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	152	UNK	-	SEE REMARK 999	UNP Q9NVV4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	153	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	154	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	155	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	156	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	157	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	325	ALA	ASP	ENGINEERED MUTATION	UNP Q9NVV4
B	464	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	465	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	466	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	467	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	468	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	469	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	470	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	471	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	472	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	473	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	474	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	475	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	476	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	477	UNK	-	SEE REMARK 999	UNP Q9NVV4
B	478	UNK	-	SEE REMARK 999	UNP Q9NVV4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.68Å 76.88Å 87.63Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	28.91 – 3.10 28.91 – 2.98	Depositor EDS
% Data completeness (in resolution range)	91.7 (28.91-3.10) 92.6 (28.91-2.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.00Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.247 , 0.328 0.255 , 0.332	Depositor DCC
R_{free} test set	1651 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtrriage
Anisotropy	0.261	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	5351	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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 [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	0.53	0/2750	0.69	3/3690 (0.1%)
1	B	0.50	0/2544	0.69	1/3413 (0.0%)
All	All	0.51	0/5294	0.69	4/7103 (0.1%)

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	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	507	TRP	CA-CB-CG	10.60	133.84	113.70
1	A	507	TRP	CA-CB-CG	9.49	131.73	113.70
1	A	392	SER	N-CA-C	-5.20	96.96	111.00
1	A	507	TRP	N-CA-CB	-5.10	101.41	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	391	ARG	Peptide

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	2793	0	2688	202	0
1	B	2558	0	2478	195	0
All	All	5351	0	5166	355	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 34.

The worst 5 of 355 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:B:507:TRP:HZ3	1:B:511:GLN:OE1	1.32	1.10
1:A:131:THR:HA	1:B:267:MSE:O	1.55	1.03
1:A:84:GLU:O	1:A:85:LYS:HD3	1.64	0.97
1:A:507:TRP:CZ3	1:A:511:GLN:OE1	2.18	0.96
1:B:507:TRP:CZ3	1:B:511:GLN:OE1	2.18	0.96

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	316/464 (68%)	241 (76%)	53 (17%)	22 (7%)	1 7
1	B	291/464 (63%)	232 (80%)	44 (15%)	15 (5%)	2 12
All	All	607/928 (65%)	473 (78%)	97 (16%)	37 (6%)	1 9

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	TYR

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Mol	Chain	Res	Type
1	A	100	PRO
1	A	101	ILE
1	A	102	ASN
1	A	201	GLU

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	300/388 (77%)	257 (86%)	43 (14%)	3	14
1	B	278/388 (72%)	236 (85%)	42 (15%)	3	12
All	All	578/776 (74%)	493 (85%)	85 (15%)	3	13

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	B	102	ASN
1	B	432	GLN
1	A	451	PHE
1	B	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	433	ASN
1	B	67	GLN
1	B	389	GLN
1	A	511	GLN
1	B	128	GLN

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 carbohydrates 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	332/464 (71%)	-0.31	3 (0%) 84 69	17, 43, 83, 108	0
1	B	305/464 (65%)	-0.23	4 (1%) 77 59	17, 45, 85, 119	0
All	All	637/928 (68%)	-0.27	7 (1%) 80 64	17, 44, 85, 119	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	PHE	3.0
1	B	493	SER	2.8
1	B	374	TRP	2.4
1	A	263	GLY	2.4
1	B	491	SER	2.4

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 carbohydrates 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.