



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3IKL  
Title : Crystal structure of Pol gB delta-I4.  
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Deposited on : 2009-08-06  
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](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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

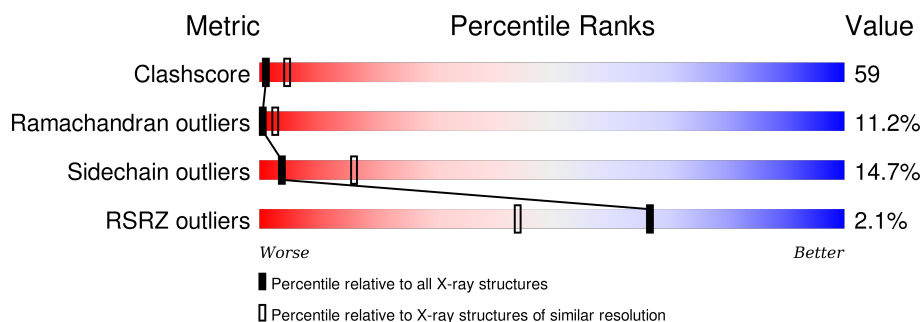
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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.

Mol	Chain	Length	Quality of chain
1	A	459	
1	B	459	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5866 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 DNA polymerase subunit gamma-2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2931	1877	515	523	16			
1	B	364	Total	C	N	O	S	0	0	0
			2935	1880	517	522	16			

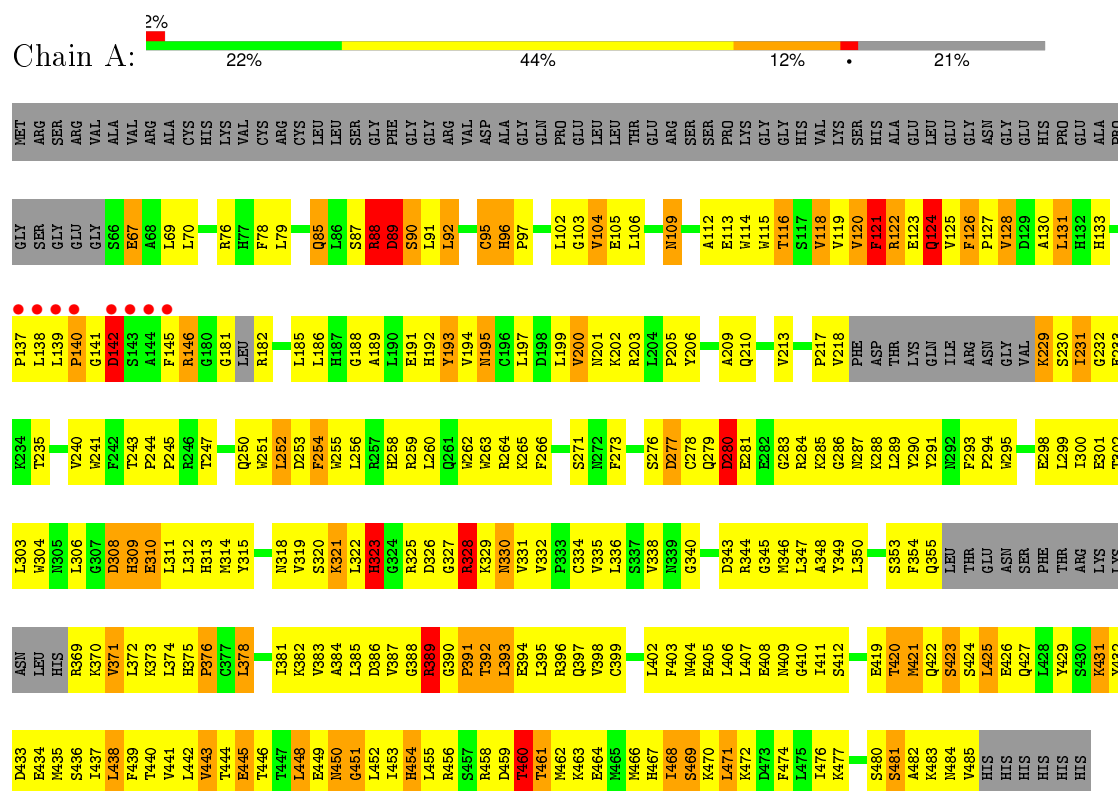
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLY	-	linker	UNP Q9UHN1
A	181	GLY	-	linker	UNP Q9UHN1
A	486	HIS	-	expression tag	UNP Q9UHN1
A	487	HIS	-	expression tag	UNP Q9UHN1
A	488	HIS	-	expression tag	UNP Q9UHN1
A	489	HIS	-	expression tag	UNP Q9UHN1
A	490	HIS	-	expression tag	UNP Q9UHN1
A	491	HIS	-	expression tag	UNP Q9UHN1
B	180	GLY	-	linker	UNP Q9UHN1
B	181	GLY	-	linker	UNP Q9UHN1
B	486	HIS	-	expression tag	UNP Q9UHN1
B	487	HIS	-	expression tag	UNP Q9UHN1
B	488	HIS	-	expression tag	UNP Q9UHN1
B	489	HIS	-	expression tag	UNP Q9UHN1
B	490	HIS	-	expression tag	UNP Q9UHN1
B	491	HIS	-	expression tag	UNP Q9UHN1

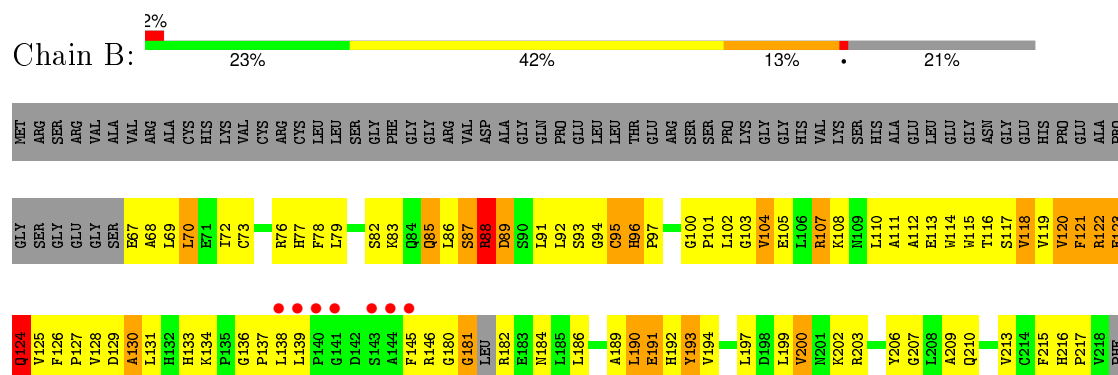
### 3 Residue-property plots

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.

- Molecule 1: DNA polymerase subunit gamma-2, mitochondrial



- Molecule 1: DNA polymerase subunit gamma-2, mitochondrial



V485	V413	A348	R284	ASP
HIS	W414		K285	THR
HIS	P415	Y351	G286	LYS
HIS	G416	D352	N287	GLN
HIS	Y417	S353	K288	ILE
HIS	L418	F354	L289	ARG
HIS	E419	Q355	Y290	ASN
	T420	LEU	Y291	GLY
	M421	THR		VAL
	Q422	GLU	P294	K229
	S423	ASN	W295	S230
	S424	SER	G296	I231
	L425	PHE	K297	G232
	E426	THR	E298	E233
	Q427	ARG		K234
	L428	LYS	I300	
		LYS	E301	V240
	K431	ASN	T302	W241
	Y432	LEU	I303	F242
	D433		W304	T243
			N305	P244
	I437		L306	P245
	L438			R246
	F439		H309	T247
	T440		E310	S248
	V441		L311	N249
	L442		L312	Q250
	T443		H313	W251
	T444		M314	L252
	E445		Y315	D253
	T446			F254
	T447			W255
	L448		N318	L256
	E449		V319	K257
			S320	H258
	I452		K321	R259
	I453		L322	L260
	H454		H323	Q261
	L455		G324	W262
	R456		R325	W263
	S457		D326	W264
	R458		G327	K265
	D459		R328	F266
	T460		K329	A267
	T461		N330	W268
	M462		V331	S269
			L395	P270
	M465		R396	P271
	M466		Q397	S271
			V398	W272
			C399	F273
	K472		L402	S274
	D473		F403	S275
			N404	S276
	K477		N405	D277
	Y478		G340	D278
	I479		L406	C279
	S480		E408	D280
	S481			E281
			I411	E282
				G283
			N484	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.43 Å 64.43 Å 260.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.82 – 3.10 45.82 – 3.10	Depositor EDS
% Data completeness (in resolution range)	74.6 (45.82-3.10) 74.7 (45.82-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 3.12 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.257 , 0.294 0.259 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 14.3	EDS
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 16475 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5866	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.46	0/3006	0.78	1/4067 (0.0%)
1	B	0.46	0/3011	0.76	1/4074 (0.0%)
All	All	0.46	0/6017	0.77	2/8141 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	GLN	N-CA-C	-6.04	94.69	111.00
1	B	455	LEU	CA-CB-CG	5.72	128.46	115.30

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	2931	0	2915	376	0
1	B	2935	0	2917	326	0
All	All	5866	0	5832	691	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 59.

The worst 5 of 691 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:231:ILE:H	1:A:231:ILE:HD12	1.16	1.10
1:B:392:THR:HG22	1:B:393:LEU:H	1.24	1.03
1:A:280:ASP:H	1:A:284:ARG:HA	1.23	1.03
1:A:448:LEU:HD23	1:A:448:LEU:H	1.23	1.02
1:A:450:ASN:HD21	1:A:452:LEU:HB2	1.24	1.01

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	358/459 (78%)	246 (69%)	75 (21%)	37 (10%)	1	4
1	B	358/459 (78%)	242 (68%)	73 (20%)	43 (12%)	0	2
All	All	716/918 (78%)	488 (68%)	148 (21%)	80 (11%)	0	3

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ARG
1	A	120	VAL
1	A	124	GLN
1	A	131	LEU
1	A	142	ASP

### 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	323/401 (80%)	271 (84%)	52 (16%)	3	13
1	B	323/401 (80%)	280 (87%)	43 (13%)	5	20
All	All	646/802 (80%)	551 (85%)	95 (15%)	4	16

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	LYS
1	B	70	LEU
1	B	455	LEU
1	A	445	GLU
1	A	460	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	B	124	GLN
1	B	375	HIS
1	A	454	HIS
1	B	192	HIS

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	364/459 (79%)	-0.07	8 (2%) 65 42	41, 74, 102, 136	0
1	B	364/459 (79%)	-0.06	7 (1%) 70 48	48, 73, 108, 127	0
All	All	728/918 (79%)	-0.07	15 (2%) 67 44	41, 73, 107, 136	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	LEU	9.9
1	A	139	LEU	9.4
1	B	140	PRO	8.0
1	A	140	PRO	6.9
1	B	139	LEU	4.6

### 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.