



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:40 PM UTC

PDB ID : 3IKL / pdb_00003ikl
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

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

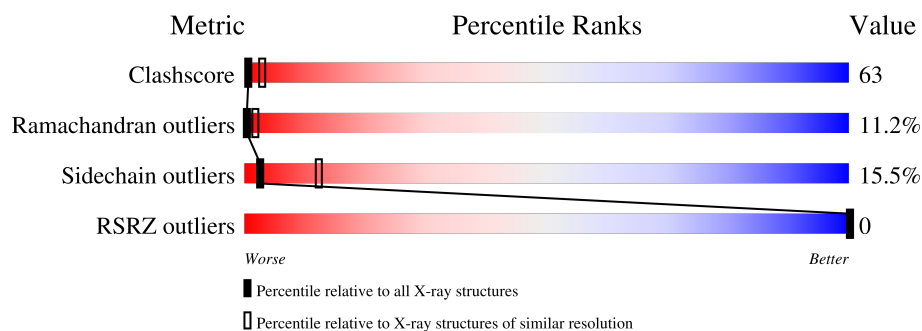
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

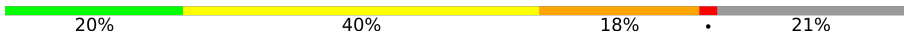
The reported resolution of this entry is 3.10 Å.

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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 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	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			

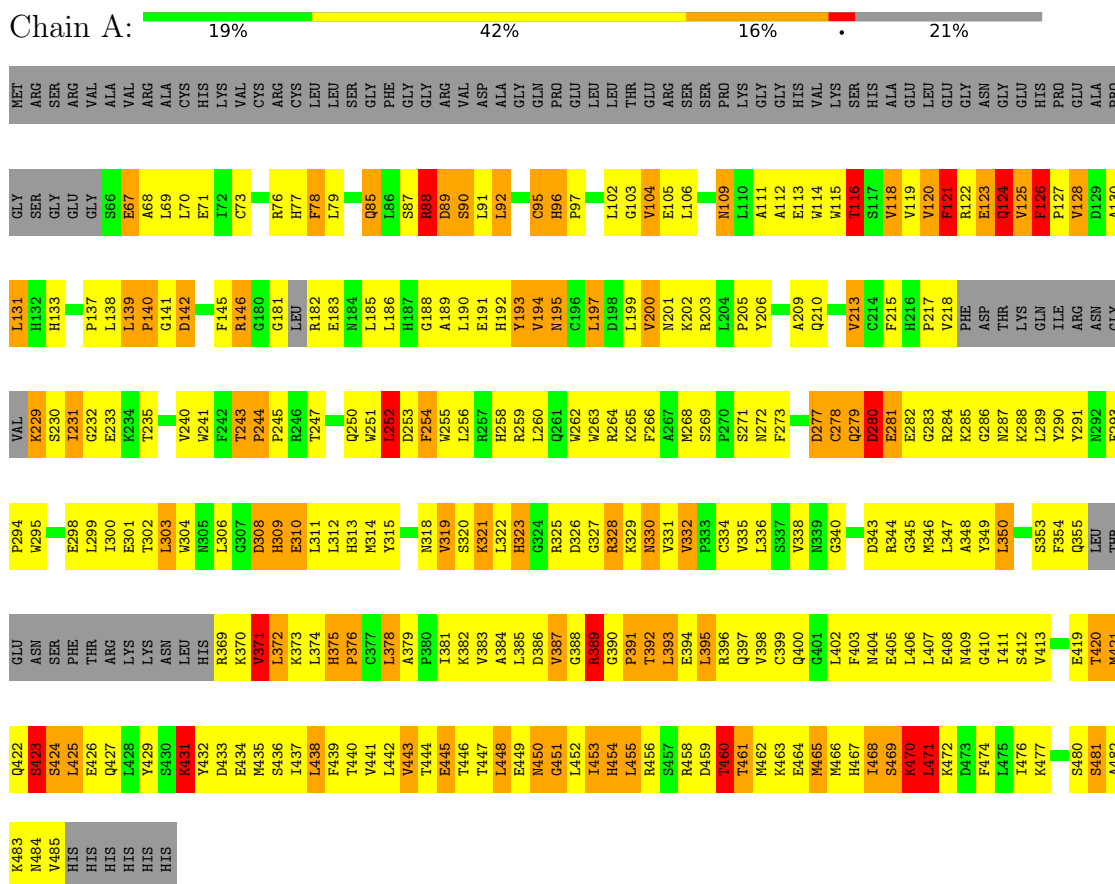
There are 16 discrepancies between the modelled and reference sequences:

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

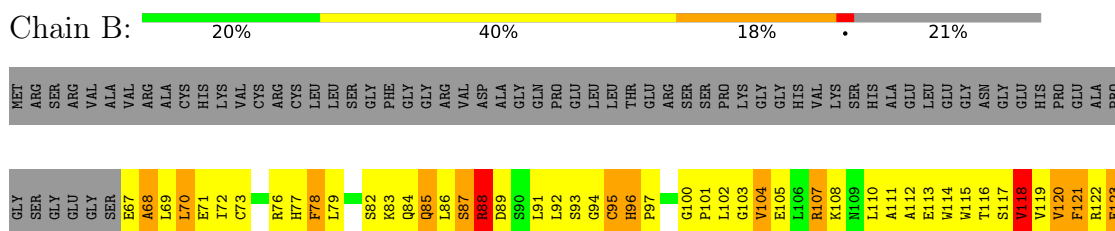
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



HIS	G416	G417	L418	E419	M421	Q422	S423	S424	L425	E426	Q427	L428	K431	D433	L437	L438	F439	T440	V441	L442	V443	T444	E445	T446	T447	L448	E449	L452	I453	H454	L455	R456	S457	R458	D459	T460	T461	M462	M465	M466	K472	D473	K477	Y478	I479	S480	S481	M484	V485	HIS	HIS								
HIS	S353	F354	Q355	LEU	THR	GLU	ASN	SER	PHE	THR	ARG	LYS	LYS	ASN	LEU	H368	R369	K370	V371	L372	K373	L374	H375	F376	G377	L378	K382	V383	A384	L385	D386	V387	G388	R389	G390	P391	T392	L393	E394	L395	R396	Q397	V398	C399	Q400	G401	L402	F403	M404	E405	L406	L407	E408	I411	S412	V413	W414	P415	
HIS	L289	Y290	Y291	P294	W295	G296	K297	E298	L299	I300	E301	T302	L303	W304	N305	L306	G307	T308	H309	E310	L311	L312	H313	M314	Y315	N318	V319	S320	K321	L322	H323	G324	R325	D326	G327	R328	K329	M330	V331	V332	P333	C334	V335	L336	S337	V338	N339	G340	D341	R344	G345	M346	L347	A348	Y351	D352			
ARG	ASN	GLY	VAL	K229	S230	I231	G232	E233	K234	V240	W241	F242	T243	P244	P245	R246	T247	S248	N249	Q250	W251	L252	D253	F254	W255	L256	R257	H258	R259	L260	Q261	W262	W263	R264	K265	F266	A267	M268	S269	P270	S271	M272	F273	S274	S275	S276	D277	C278	Q279	D280	E281	E282	G283	R284	K285	G286	LYS	N287	K288
Q124	V125	F126	P127	V128	D129	A130	L131	H132	H133	K134	P135	G136	P137	L138	L139	F145	R146	G180	G181	LEU	R182	E183	L186	A189	L190	E191	H192	Y193	V194	L197	D198	L199	V200	M201	K202	R203	Y206	G207	L208	A209	Q210	V213	C214	F215	H216	P217	V218	PHE	ASP	THR	LYS	GLN	ILE						

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	64.43Å 64.43Å 260.70Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.294 0.258 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.450 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5866	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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	0.56	0/3006	1.18	40/4067 (1.0%)
1	B	0.54	0/3011	1.17	37/4074 (0.9%)
All	All	0.55	0/6017	1.17	77/8141 (0.9%)

There are no bond length outliers.

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	PHE	N-CA-C	-10.24	101.28	113.88
1	B	197	LEU	N-CA-C	-9.77	101.87	113.88
1	B	332	VAL	CA-C-N	9.16	129.72	119.92
1	B	332	VAL	C-N-CA	9.16	129.72	119.92
1	B	78	PHE	N-CA-C	-9.02	102.78	113.88

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	399	0
1	B	2935	0	2917	344	0
All	All	5866	0	5832	732	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 63.

The worst 5 of 732 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:A:280:ASP:H	1:A:284:ARG:HA	1.23	1.03
1:B:392:THR:HG22	1:B:393:LEU:H	1.24	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%)	0	2
1	B	358/459 (78%)	242 (68%)	73 (20%)	43 (12%)	0	1
All	All	716/918 (78%)	488 (68%)	148 (21%)	80 (11%)	0	2

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%)	2	11
1	B	323/401 (80%)	275 (85%)	48 (15%)	3	13
All	All	646/802 (80%)	546 (84%)	100 (16%)	2	12

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	118	VAL
1	B	284	ARG
1	B	484	ASN
1	B	139	LEU
1	B	248	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	313	HIS
1	B	318	ASN
1	B	400	GLN
1	A	305	ASN
1	A	287	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 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	364/459 (79%)	-1.41	0 100 100	41, 74, 102, 136	0
1	B	364/459 (79%)	-1.39	0 100 100	48, 73, 108, 127	0
All	All	728/918 (79%)	-1.40	0 100 100	41, 73, 107, 136	0

There are no RSRZ outliers to report.

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.