wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 05:33 PM EDT

PDB ID	:	3IKL
Title	:	Crystal structure of Pol gB delta-I4.
Authors	:	Lee, Y.S.; Kennedy, W.D.; Yin, Y.W.
Deposited on	:	2009-08-06
Resolution	:	3.10 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

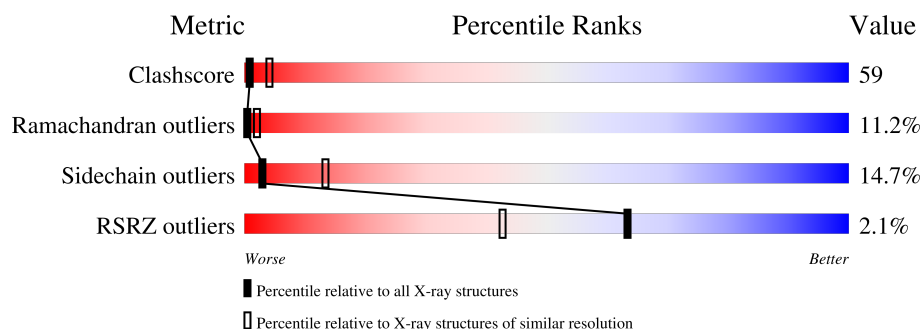|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	Percentile Ranks	Value
Clashscore		59
Ramachandran outliers		11.2%
Sidechain outliers		14.7%
RSRZ outliers		2.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 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 <=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	2% • 22% 44% 12% • 21%
1	B	459	2% • 23% 42% 13% • 21%

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			

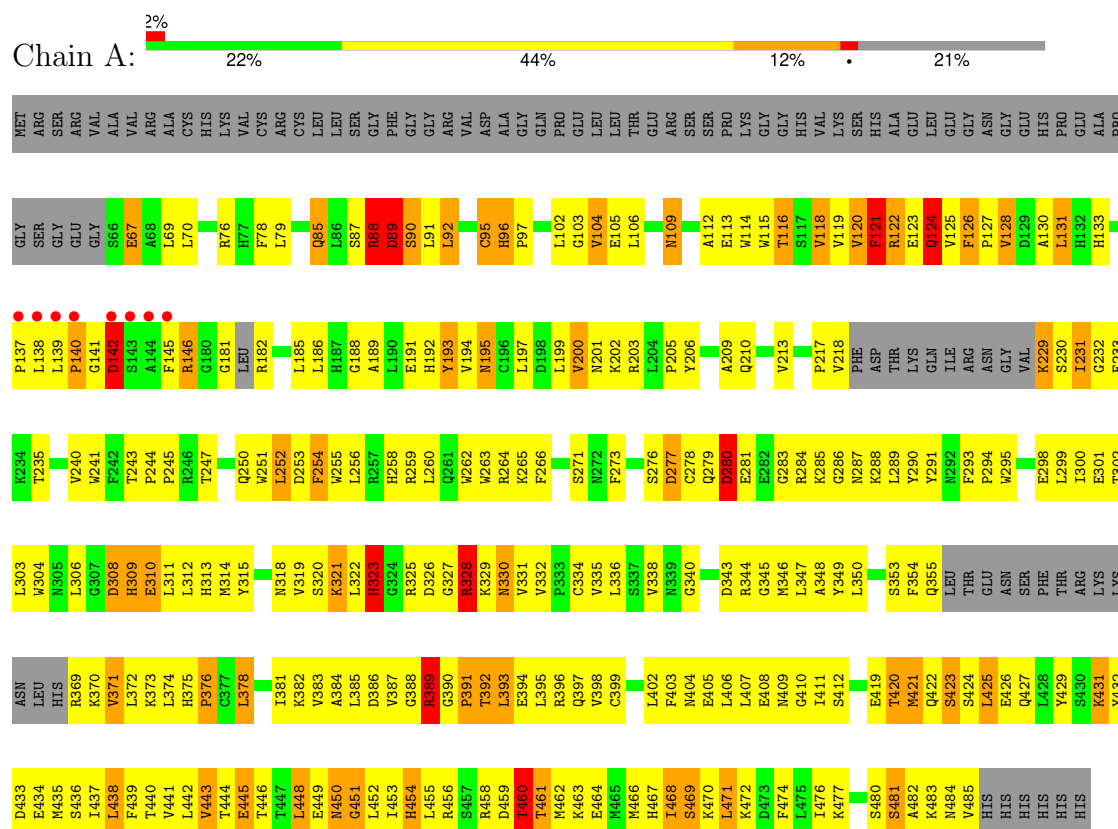There are 16 discrepancies between the modelled and reference sequences:

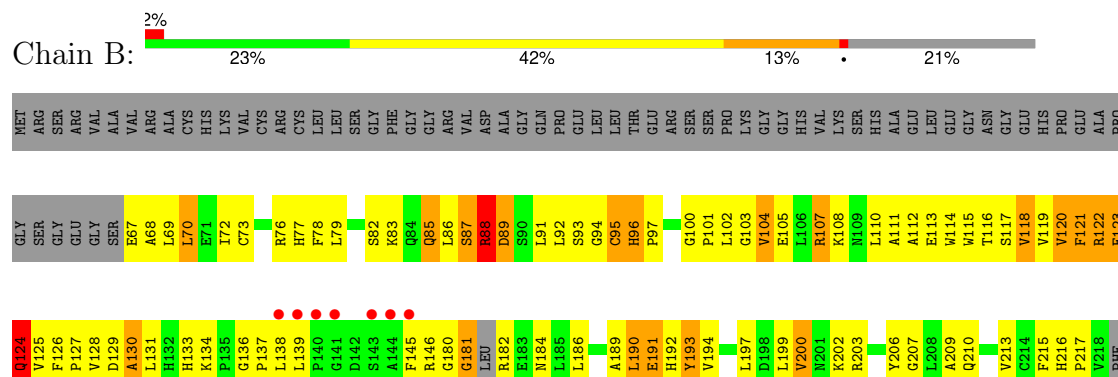| Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLY	-	linker	UNP Q9UHN1
A	181	GLY	-	linker	UNP Q9UHN1
A	486	HIS	-	expression tag	UNP Q9UHN1
A	487	HIS	-	expression tag	UNP Q9UHN1
A	488	HIS	-	expression tag	UNP Q9UHN1
A	489	HIS	-	expression tag	UNP Q9UHN1
A	490	HIS	-	expression tag	UNP Q9UHN1
A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

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ASP THR LYS GLN ILE 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 N272 F273 S274 S275 S276 D277 C278 Q279 D280 E281 E282 G283

R284 K285 G286 N287 K288 L289 Y290 Y291 P294 W295 G296 K297 E298 L299 I300 E301 T302 L303 W304 N305 L306 H309 E310 L311 L312 H313 M314 Y315 N318 V319 S320 K321 L322 H323 G324 R325 D326 G327 R328 K329 N330 V331 V332 P333 C334 V335 L336 S337 V338 N339 G340 D341 R344 G345 M346 L347

A348 Y351 D352 S353 F354 Q355 LEU THR GLU ASN SER PHE THR ARG LYS LYS ASN LEU H368 R369 K370 V371 L372 K373 L374 H375 P376 C377 L378 K382 V383 A384 L385 D386 V387 G388 R389 G390 P391 T392 L393 E394 L395 R396 Q397 V398 C399 L402 F403 N404 E405 L406 L407 E408 I411 S412

V413 W414 P415 G416 Y417 L418 E419 T420 M421 Q422 S423 S424 L425 E426 Q427 L428 K431 Y432 D433 I437 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 N484

V485 HIS HIS HIS HIS HIS

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
$< I/\sigma(I) >$ [1]	2.15 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.294 0.259 , (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)	0.29 , 14.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.450 for h,-k,-l	Xtriage
F_o,F_c correlation	0.88	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.46	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(^{o})	Ideal(^{o})
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 ⓘ

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: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 ⓘ

5.3.1   Protein backbone ⓘ

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	3
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 ⓘ

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	10
1	B	323/401 (80%)	280 (87%)	43 (13%)	4	16
All	All	646/802 (80%)	551 (85%)	95 (15%)	3	13

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

Mol	Chain	Res	Type
1	B	95	CYS
1	B	271	SER
1	B	122	ARG
1	B	216	HIS
1	B	312	LEU

Sometimes 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	454	HIS
1	B	400	GLN
1	B	192	HIS
1	B	318	ASN
1	B	124	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.09	8 (2%)	62	41	41, 74, 102, 136	0
1	B	364/459 (79%)	-0.09	7 (1%)	66	46	48, 73, 108, 127	0
All	All	728/918 (79%)	-0.09	15 (2%)	63	43	41, 73, 107, 136	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	LEU	9.6
1	A	139	LEU	9.1
1	B	140	PRO	7.7
1	A	140	PRO	6.7
1	B	139	LEU	4.4

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 monosaccharides 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.