



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:49 AM UTC

PDB ID : 4XQK / pdb_00004xqk
Title : ATP-dependent Type ISP restriction-modification enzyme LlaBIII bound to DNA
Authors : Chand, M.K.; Saikrishnan, K.
Deposited on : 2015-01-19
Resolution : 2.70 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

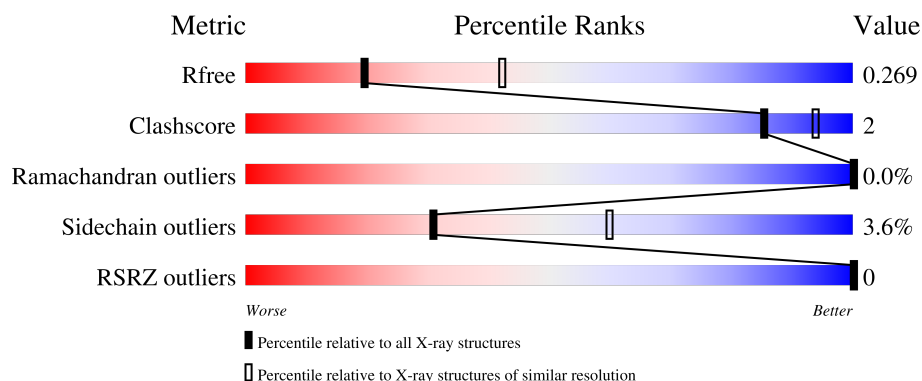
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	1578	 89% 7% • •
1	B	1578	 85% 9% • 6%
2	C	28	 100%
2	E	28	 100%
3	D	28	 93% 7%

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Mol	Chain	Length	Quality of chain
3	F	28	 93% 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 49902 atoms, of which 24156 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 LlaBIII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1517	Total	C	H	N	O	S	0	0	0
			23551	7549	11680	1983	2302	37			
1	B	1484	Total	C	H	N	O	S	0	0	0
			22688	7279	11247	1920	2205	37			

- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	28	Total	C	H	N	O	P	0	0	0
			871	271	305	101	167	27			
2	E	28	Total	C	H	N	O	P	0	0	0
			871	271	305	101	167	27			

- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	28	Total	C	H	N	O	P	0	0	0
			890	274	315	110	164	27			
3	F	28	Total	C	H	N	O	P	0	0	0
			880	274	304	110	165	27			

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total K 2 2	0	0
4	B	1	Total K 1 1	0	0

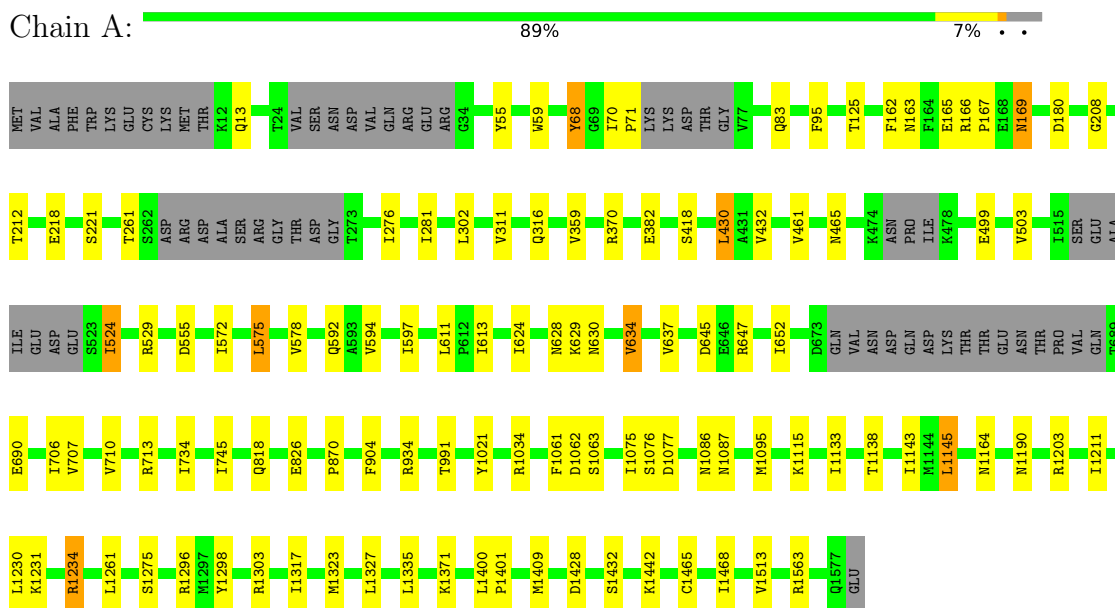
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	73	Total 73	O 73	0	0
5	B	44	Total 44	O 44	0	0
5	C	6	Total 6	O 6	0	0
5	D	11	Total 11	O 11	0	0
5	E	10	Total 10	O 10	0	0
5	F	4	Total 4	O 4	0	0

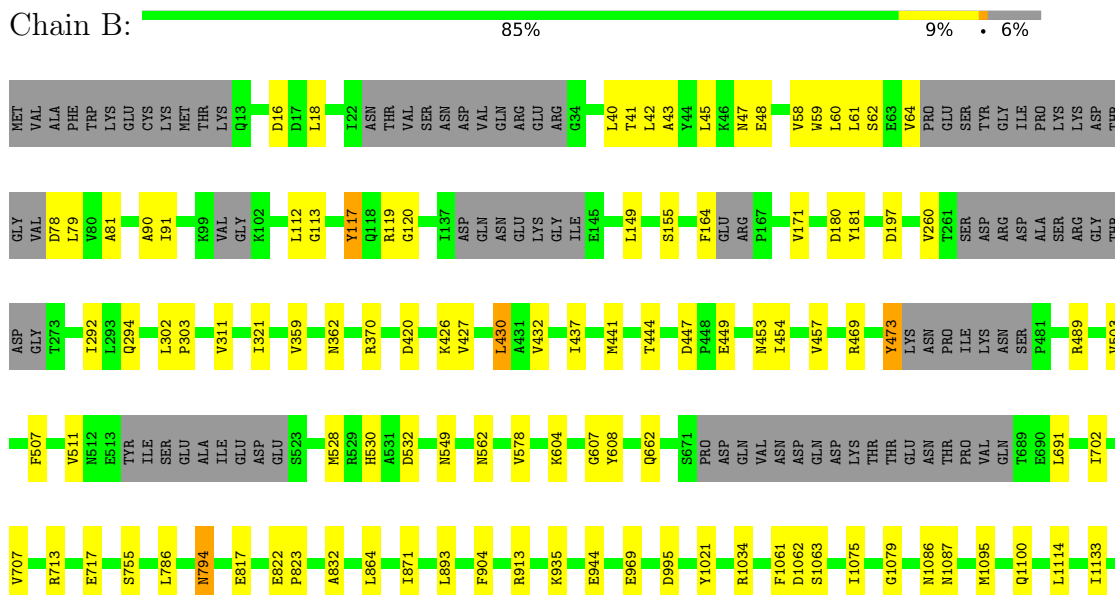
3 Residue-property plots

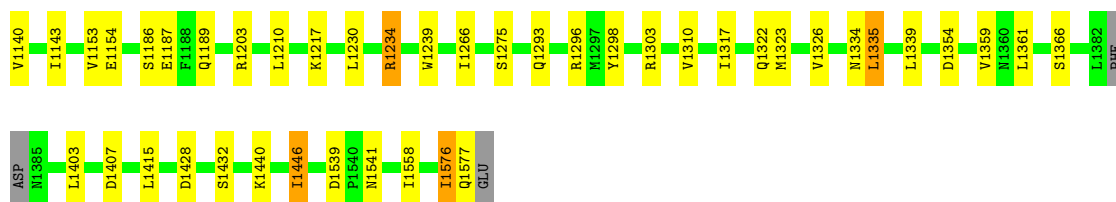
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: LlaBIH



• Molecule 1: LlaBIH





- Molecule 2: DNA (28-MER)

Chain C: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (28-MER)

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: DNA (28-MER)

Chain D: 93% 7%



- Molecule 3: DNA (28-MER)

Chain F: 93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.88Å 112.66Å 146.21Å 103.30° 90.88° 105.79°	Depositor
Resolution (Å)	48.22 – 2.70 48.22 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.22-2.70) 92.1 (48.22-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.218 , 0.260 0.228 , 0.269	Depositor DCC
R_{free} test set	4970 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.147 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	49902	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
K

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	0.28	0/12101	0.64	3/16403 (0.0%)
1	B	0.28	0/11656	0.66	0/15815
2	C	0.23	0/633	0.44	0/974
2	E	0.24	0/633	0.46	0/974
3	D	0.25	0/646	0.47	0/997
3	F	0.24	0/647	0.42	0/998
All	All	0.28	0/26316	0.63	3/36161 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	ILE	N-CA-C	5.30	116.03	110.62
1	A	165	GLU	N-CA-C	-5.11	106.14	112.38
1	A	991	THR	N-CA-C	5.00	117.71	109.76

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	11871	11680	11483	51	0
1	B	11441	11247	10965	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	566	305	317	0	0
2	E	566	305	317	0	0
3	D	575	315	313	2	0
3	F	576	304	316	2	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	73	0	0	1	0
5	B	44	0	0	0	0
5	C	6	0	0	0	0
5	D	11	0	0	0	0
5	E	10	0	0	0	0
5	F	4	0	0	1	0
All	All	25746	24156	23711	109	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 2.

The worst 5 of 109 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:893:LEU:O	1:B:935:LYS:NZ	2.16	0.79
1:A:1034:ARG:NH2	1:A:1061:PHE:O	2.20	0.75
1:A:690:GLU:N	1:A:690:GLU:OE1	2.21	0.73
1:A:359:VAL:O	1:A:370:ARG:NH1	2.25	0.69
1:B:707:VAL:O	1:B:713:ARG:NH2	2.30	0.65

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	1503/1578 (95%)	1454 (97%)	49 (3%)	0	100	100
1	B	1462/1578 (93%)	1391 (95%)	70 (5%)	1 (0%)	48	73
All	All	2965/3156 (94%)	2845 (96%)	119 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1440	LYS

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	1266/1407 (90%)	1235 (98%)	31 (2%)	43	72
1	B	1194/1407 (85%)	1136 (95%)	58 (5%)	22	49
All	All	2460/2814 (87%)	2371 (96%)	89 (4%)	31	60

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	702	ILE
1	B	1187	GLU
1	B	794	ASN
1	B	1021	TYR
1	B	1217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1018	ASN
1	B	1476	ASN
1	A	1367	GLN
1	B	92	GLN
1	B	200	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1517/1578 (96%)	-1.21	0 100 100	32, 70, 103, 128	0
1	B	1484/1578 (94%)	-1.16	0 100 100	36, 77, 123, 150	0
2	C	28/28 (100%)	-1.77	0 100 100	40, 68, 112, 121	0
2	E	28/28 (100%)	-1.76	0 100 100	43, 69, 106, 107	0
3	D	28/28 (100%)	-1.78	0 100 100	40, 75, 129, 150	0
3	F	28/28 (100%)	-1.76	0 100 100	42, 80, 114, 117	0
All	All	3113/3268 (95%)	-1.20	0 100 100	32, 73, 113, 150	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	A	1601	1/1	0.99	0.06	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	A	1602	1/1	1.00	0.03	83,83,83,83	0
4	K	B	1601	1/1	1.00	0.05	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.