



# Full wwPDB X-ray Structure Validation Report i

Nov 28, 2023 – 06:45 pm GMT

PDB ID : 1DYK  
Title : Laminin alpha 2 chain LG4-5 domain pair  
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Deposited on : 2000-02-01  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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

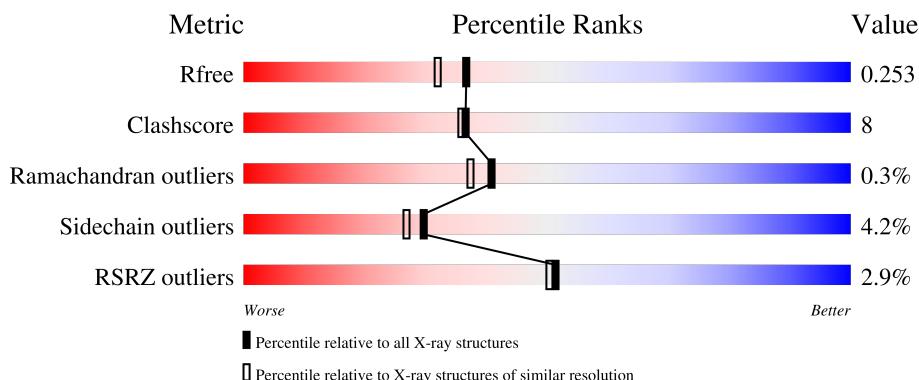
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	394	3%	76%	17%	• 5%

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3113 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 LAMININ ALPHA 2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C 2860	N 1806	O 496	S 544	14	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2773	ALA	VAL	conflict	UNP Q60675
A	2802	ALA	GLY	conflict	UNP Q60675
A	2810	ALA	GLY	conflict	UNP Q60675
A	2820	TYR	PHE	conflict	UNP Q60675
A	2829	ASP	SER	conflict	UNP Q60675
A	2831	SER	ARG	conflict	UNP Q60675
A	2878	VAL	GLY	conflict	UNP Q60675
A	2946	ALA	GLY	conflict	UNP Q60675
A	2953	LYS	ILE	conflict	UNP Q60675
A	2976	VAL	ILE	conflict	UNP Q60675
A	3022	HIS	TYR	conflict	UNP Q60675
A	3094	GLY	ALA	conflict	UNP Q60675

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0

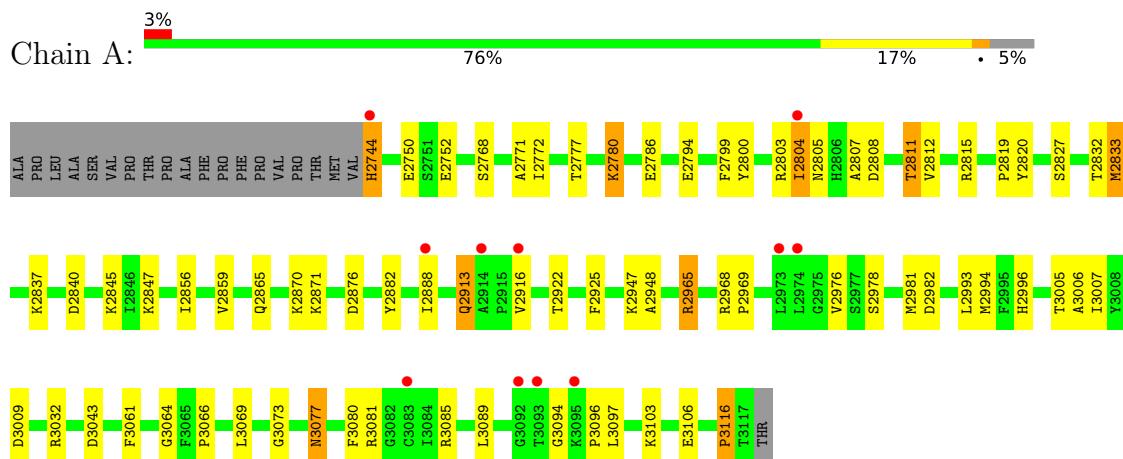
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	251	Total O 251 251	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: LAMININ ALPHA 2 CHAIN



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.60 Å    111.50 Å    124.80 Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-2.00) 94.3 (19.88-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	5.49 (at 2.01 Å)	Xtriage
Refinement program	X-PLOR	Depositor
$R$ , $R_{free}$	0.233 , 0.261 0.225 , 0.253	Depositor DCC
$R_{free}$ test set	2244 reflections (7.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 57.1	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.58	4/2918 (0.1%)	0.80	4/3950 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2833	MET	SD-CE	-6.73	1.40	1.77
1	A	2833	MET	CG-SD	5.44	1.95	1.81
1	A	3116	PRO	N-CD	5.32	1.55	1.47
1	A	3116	PRO	C-N	-5.23	1.22	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2833	MET	CG-SD-CE	15.82	125.52	100.20
1	A	3009	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	2840	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	2871	LYS	N-CA-C	5.56	126.02	111.00

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 MolProbit. 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	2860	0	2833	45	0
2	A	2	0	0	0	0
3	A	251	0	0	4	0
All	All	3113	0	2833	45	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 8.

All (45) 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:2981:MET:SD	3:A:2161:HOH:O	2.45	0.73
1:A:2845:LYS:NZ	3:A:2073:HOH:O	2.21	0.72
1:A:2856:ILE:HG12	1:A:2865:GLN:HG3	1.73	0.71
1:A:2803:ARG:HD3	1:A:2807:ALA:HB3	1.78	0.65
1:A:2800:TYR:HD1	1:A:2811:THR:HG23	1.62	0.64
1:A:2827:SER:HB3	1:A:2870:LYS:HB2	1.80	0.64
1:A:2803:ARG:HB3	1:A:2876:ASP:O	1.98	0.63
1:A:3103:LYS:O	1:A:3103:LYS:HG2	1.99	0.62
1:A:2750:GLU:OE1	1:A:2968:ARG:NH2	2.31	0.61
1:A:3080:PHE:HA	3:A:2230:HOH:O	1.98	0.61
1:A:3077:ASN:HD22	1:A:3077:ASN:H	1.50	0.60
1:A:2968:ARG:HG3	1:A:3081:ARG:HB3	1.84	0.58
1:A:2819:PRO:HG3	1:A:2859:VAL:HG21	1.86	0.56
1:A:2777:THR:O	1:A:2780:LYS:HG2	2.05	0.55
1:A:2772:ILE:HD13	1:A:2916:VAL:HG13	1.87	0.54
1:A:2994:MET:HG2	1:A:3007:ILE:HG12	1.90	0.53
1:A:2965:ARG:NH2	1:A:3116:PRO:O	2.39	0.53
1:A:2981:MET:O	1:A:2982:ASP:HB2	2.10	0.51
1:A:2804:ILE:CG2	1:A:2805:ASN:N	2.73	0.50
1:A:2786:GLU:HB3	1:A:2847:LYS:HG3	1.92	0.50
1:A:3032:ARG:HH12	1:A:3043:ASP:HB3	1.79	0.48
1:A:2777:THR:O	1:A:2780:LYS:CG	2.61	0.48
1:A:2976:VAL:O	1:A:2976:VAL:HG13	2.14	0.47
1:A:2947:LYS:HB3	1:A:3106:GLU:HB3	1.97	0.47
1:A:2978:SER:HB3	1:A:2981:MET:O	2.14	0.47
1:A:2996:HIS:HB2	1:A:3073:GLY:O	2.14	0.47
1:A:2815:ARG:HB2	1:A:2820:TYR:CE2	2.50	0.46
1:A:2913:GLN:H	1:A:2913:GLN:CD	2.18	0.45
1:A:3032:ARG:HH11	1:A:3032:ARG:HG3	1.81	0.45
1:A:2804:ILE:HG23	1:A:2805:ASN:N	2.31	0.45
1:A:2803:ARG:HG2	1:A:2808:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2744:HIS:HA	1:A:2969:PRO:HD3	1.98	0.44
1:A:2794:GLU:OE2	1:A:2837:LYS:NZ	2.49	0.44
1:A:3061:PHE:HB3	1:A:3064:GLY:O	2.17	0.44
1:A:2888:ILE:HG12	3:A:2093:HOH:O	2.16	0.43
1:A:3094:GLY:O	1:A:3096:PRO:HD3	2.19	0.43
1:A:2752:GLU:HA	1:A:2752:GLU:OE1	2.19	0.43
1:A:3005:THR:HG22	1:A:3006:ALA:N	2.34	0.42
1:A:2812:VAL:HA	1:A:2820:TYR:O	2.19	0.42
1:A:3066:PRO:HD2	1:A:3069:LEU:HD12	2.01	0.42
1:A:2744:HIS:ND1	1:A:2744:HIS:N	2.69	0.41
1:A:3077:ASN:HD22	1:A:3077:ASN:N	2.14	0.41
1:A:2799:PHE:HA	1:A:2882:TYR:O	2.20	0.41
1:A:2768:SER:HA	1:A:2925:PHE:O	2.20	0.40
1:A:2771:ALA:O	1:A:2922:THR:HG22	2.22	0.40

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	372/394 (94%)	348 (94%)	23 (6%)	1 (0%)	41 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2948	ALA

#### 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	311/328 (95%)	298 (96%)	13 (4%)	30   27

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2744	HIS
1	A	2780	LYS
1	A	2804	ILE
1	A	2811	THR
1	A	2832	THR
1	A	2833	MET
1	A	2913	GLN
1	A	2965	ARG
1	A	2993	LEU
1	A	3077	ASN
1	A	3085	ARG
1	A	3089	LEU
1	A	3097	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2761	GLN
1	A	2933	ASN
1	A	3077	ASN
1	A	3100	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

Of 2 ligands modelled in this entry, 2 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, 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	374/394 (94%)	0.13	11 (2%) 51 50	10, 20, 39, 52	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3093	THR	5.8
1	A	3092	GLY	4.5
1	A	2744	HIS	4.3
1	A	2804	ILE	4.1
1	A	2888	ILE	3.0
1	A	3083	CYS	2.4
1	A	2973	LEU	2.3
1	A	2914	ALA	2.3
1	A	3095	LYS	2.1
1	A	2974	LEU	2.0
1	A	2916	VAL	2.0

### 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CA	A	4001	1/1	0.93	0.07	35,35,35,35	0
2	CA	A	4002	1/1	0.99	0.07	15,15,15,15	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.