



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:56 am BST

PDB ID : 6DBG  
Title : Crystal Structure of VHH R303 in complex with InlB-LRR-IR  
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Deposited on : 2018-05-03  
Resolution : 1.51 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 ⓘ 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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

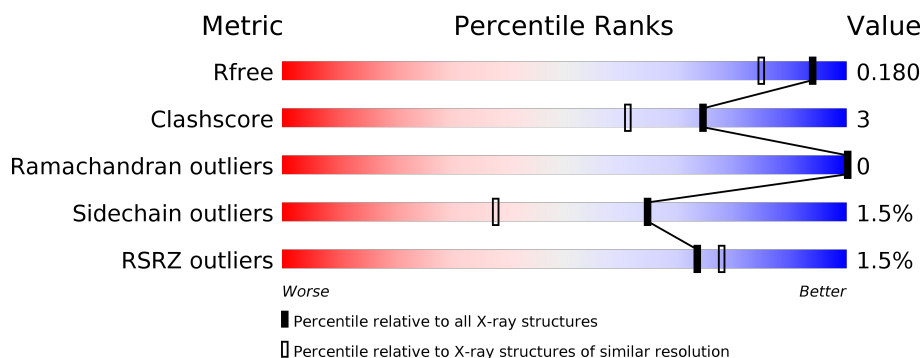
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.51 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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 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	301	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>89%</span> <span>5% • 5%</span> </div> </div>
1	B	301	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>89%</span> <span>5% • 5%</span> </div> </div>
2	C	142	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 73%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>73%</span> <span>11% 17%</span> </div> </div>
2	D	142	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 85%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>3%</span> <span>85%</span> <span>• 14%</span> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13440 atoms, of which 6098 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 Internalin B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	H	N	O	S	0	3	0
			4466	1423	2237	367	438	1			
1	B	286	Total	C	H	N	O	S	0	6	0
			4555	1443	2291	377	443	1			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	expression tag	UNP C6ZUN6
A	34	ALA	-	expression tag	UNP C6ZUN6
A	35	MET	-	expression tag	UNP C6ZUN6
A	322	ASN	-	expression tag	UNP C6ZUN6
A	323	LEU	-	expression tag	UNP C6ZUN6
A	324	TYR	-	expression tag	UNP C6ZUN6
A	325	PHE	-	expression tag	UNP C6ZUN6
A	326	GLN	-	expression tag	UNP C6ZUN6
A	327	GLY	-	expression tag	UNP C6ZUN6
A	328	HIS	-	expression tag	UNP C6ZUN6
A	329	HIS	-	expression tag	UNP C6ZUN6
A	330	HIS	-	expression tag	UNP C6ZUN6
A	331	HIS	-	expression tag	UNP C6ZUN6
A	332	HIS	-	expression tag	UNP C6ZUN6
A	333	HIS	-	expression tag	UNP C6ZUN6
B	33	GLY	-	expression tag	UNP C6ZUN6
B	34	ALA	-	expression tag	UNP C6ZUN6
B	35	MET	-	expression tag	UNP C6ZUN6
B	322	ASN	-	expression tag	UNP C6ZUN6
B	323	LEU	-	expression tag	UNP C6ZUN6
B	324	TYR	-	expression tag	UNP C6ZUN6
B	325	PHE	-	expression tag	UNP C6ZUN6
B	326	GLN	-	expression tag	UNP C6ZUN6
B	327	GLY	-	expression tag	UNP C6ZUN6
B	328	HIS	-	expression tag	UNP C6ZUN6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	329	HIS	-	expression tag	UNP C6ZUN6
B	330	HIS	-	expression tag	UNP C6ZUN6
B	331	HIS	-	expression tag	UNP C6ZUN6
B	332	HIS	-	expression tag	UNP C6ZUN6
B	333	HIS	-	expression tag	UNP C6ZUN6

- Molecule 2 is a protein called VHH R303.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	118	Total	C	H	N	O	S	0	2	0
			1647	540	775	150	176	6			
2	D	122	Total	C	H	N	O	S	0	2	0
			1687	553	795	154	179	6			

- Molecule 3 is water.

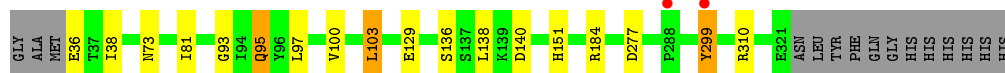
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	416	Total	O	0	0
			416	416		
3	B	433	Total	O	0	0
			433	433		
3	C	117	Total	O	0	0
			117	117		
3	D	119	Total	O	0	0
			119	119		

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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: Internalin B

Chain A: 




- Molecule 1: Internalin B

Chain B: 




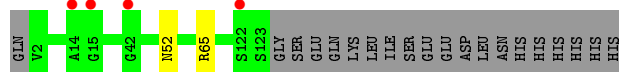
- Molecule 2: VHH R303

Chain C: 



- Molecule 2: VHH R303

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.89 Å   66.95 Å   73.83 Å 116.67°   97.73°   95.08°	Depositor
Resolution (Å)	43.20 – 1.51 43.20 – 1.51	Depositor EDS
% Data completeness (in resolution range)	93.5 (43.20-1.51) 93.5 (43.20-1.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 1.51 Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.160   ,   0.180 0.161   ,   0.180	Depositor DCC
$R_{free}$ test set	6121 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% 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, 0.333 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	0.59	1/2273 (0.0%)	0.71	1/3093 (0.0%)
1	B	0.56	0/2319	0.71	2/3154 (0.1%)
2	C	0.50	0/894	0.65	0/1213
2	D	0.48	0/915	0.65	0/1245
All	All	0.55	1/6401 (0.0%)	0.69	3/8705 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	TYR	CB-CG	-5.52	1.43	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	222	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	B	222	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	184	ARG	NE-CZ-NH2	-5.30	117.65	120.30

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	2229	2237	2240	14	0
1	B	2264	2291	2302	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	872	775	778	10	0
2	D	892	795	799	5	0
3	A	416	0	0	4	4
3	B	433	0	0	8	3
3	C	117	0	0	5	0
3	D	119	0	0	5	1
All	All	7342	6098	6119	40	4

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 3.

All (40) 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)
2:D:52:ASN:ND2	3:D:201:HOH:O	1.89	0.92
1:B:260:LYS:NZ	3:B:401:HOH:O	1.95	0.85
2:D:52:ASN:OD1	3:D:202:HOH:O	1.95	0.85
1:B:270:GLU:HG2	3:B:402:HOH:O	1.76	0.83
2:C:5:GLU:OE1	3:C:201:HOH:O	2.02	0.77
1:A:140:ASP:OD2	3:A:401:HOH:O	2.01	0.76
1:B:270:GLU:OE2	3:B:402:HOH:O	2.06	0.72
2:D:65:ARG:O	3:D:203:HOH:O	2.06	0.72
2:C:123:SER:O	3:C:203:HOH:O	2.11	0.68
2:C:74:ASN:OD1	3:C:202:HOH:O	2.09	0.68
1:B:252:ASN:ND2	3:B:403:HOH:O	2.07	0.68
2:C:65:ARG:O	3:C:204:HOH:O	2.12	0.66
1:A:36:GLU:N	3:A:404:HOH:O	2.29	0.65
1:A:299:TYR:OH	1:A:310:ARG:HD3	2.03	0.58
1:A:73:ASN:ND2	3:A:407:HOH:O	2.35	0.58
1:B:95:GLN:HG2	3:B:471:HOH:O	2.06	0.55
1:A:93:GLY:N	1:A:95:GLN:OE1	2.38	0.54
1:B:73:ASN:OD1	3:B:405:HOH:O	2.19	0.54
1:B:270:GLU:CG	3:B:402:HOH:O	2.47	0.53
2:C:89:GLU:HG3	3:C:215:HOH:O	2.10	0.52
1:B:81:ILE:HB	1:B:103:LEU:HD23	1.94	0.49
2:D:52:ASN:CB	3:D:202:HOH:O	2.60	0.49
1:A:299:TYR:OH	1:A:310:ARG:CD	2.60	0.49
2:D:52:ASN:CG	3:D:202:HOH:O	2.46	0.47
1:B:245:LYS:NZ	3:B:404:HOH:O	2.16	0.47
2:C:6:GLU:OE1	2:C:117:THR:HG23	2.15	0.47
1:B:173[B]:ASN:ND2	1:B:195:ASP:OD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:14:ALA:N	2:C:122:SER:O	2.44	0.46
1:A:38:ILE:O	1:A:38:ILE:HG13	2.15	0.46
1:A:97:LEU:HB3	1:A:100[B]:VAL:HG23	1.97	0.46
1:A:136[A]:SER:OG	3:A:402:HOH:O	2.21	0.46
1:B:124:TRP:CE3	2:C:107:LEU:HD11	2.50	0.45
1:A:81:ILE:HB	1:A:103:LEU:HD23	1.99	0.43
1:A:129:GLU:OE2	1:A:151:HIS:ND1	2.45	0.43
2:C:68:PHE:CZ	2:C:83:MET:HE2	2.54	0.42
1:A:299:TYR:CE1	1:A:310:ARG:HD3	2.54	0.41
1:A:299:TYR:CZ	1:A:310:ARG:CG	3.03	0.41
1:A:299:TYR:CZ	1:A:310:ARG:HD3	2.56	0.41
2:C:36:TRP:CZ3	2:C:81:LEU:HB2	2.56	0.41
1:B:114:LYS:N	1:B:115:PRO:CD	2.85	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:407:HOH:O	3:B:495:HOH:O[1_544]	1.79	0.41
3:A:711:HOH:O	3:B:788:HOH:O[1_655]	1.81	0.39
3:A:736:HOH:O	3:B:760:HOH:O[1_655]	1.96	0.24
3:A:716:HOH:O	3:D:307:HOH:O[1_655]	2.02	0.18

## 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	287/301 (95%)	279 (97%)	8 (3%)	0	100	100
1	B	290/301 (96%)	283 (98%)	7 (2%)	0	100	100
2	C	116/142 (82%)	114 (98%)	2 (2%)	0	100	100
2	D	122/142 (86%)	119 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	815/886 (92%)	795 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	253/276 (92%)	249 (98%)	4 (2%)	62	35
1	B	263/276 (95%)	257 (98%)	6 (2%)	50	20
2	C	88/120 (73%)	87 (99%)	1 (1%)	73	52
2	D	89/120 (74%)	89 (100%)	0	100	100
All	All	693/792 (88%)	682 (98%)	11 (2%)	65	35

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	103	LEU
1	A	138	LEU
1	A	277	ASP
1	B	65	SER
1	B	95	GLN
1	B	138	LEU
1	B	173[A]	ASN
1	B	173[B]	ASN
1	B	277	ASP
2	C	52	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	286/301 (95%)	-0.18	2 (0%) 87 90	11, 18, 37, 48	0
1	B	286/301 (95%)	-0.24	4 (1%) 75 79	11, 18, 36, 54	0
2	C	118/142 (83%)	-0.02	2 (1%) 70 74	13, 28, 48, 63	0
2	D	122/142 (85%)	0.13	4 (3%) 46 51	14, 29, 50, 74	0
All	All	812/886 (91%)	-0.13	12 (1%) 73 78	11, 20, 44, 74	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	PRO	3.7
1	A	299	TYR	3.4
2	D	14	ALA	3.1
2	D	42	GLY	2.9
1	B	288	PRO	2.6
2	D	122[A]	SER	2.3
1	B	39	THR	2.2
1	B	290	PHE	2.1
2	C	27	HIS	2.1
2	D	15	GLY	2.1
1	B	134	ASP	2.1
2	C	66	ASP	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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.