Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 05:26 AM GMT

PDB ID	:	1I3V
Title	:	THREE-DIMENSIONAL STRUCTURE OF A LAMA VHH DOMAIN UN-LIGANDED
Authors	:	Spinelli, S.; Tegoni, M.; Frenken, L.; van Vliet, C.; Cambillau, C.
Deposited on	:	2001-02-16
Resolution	:	2.03 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.03 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
Rfree		0.253
Clashscore		15
Ramachandran outliers		1.6%
Sidechain outliers		7.7%
RSRZ outliers		3.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
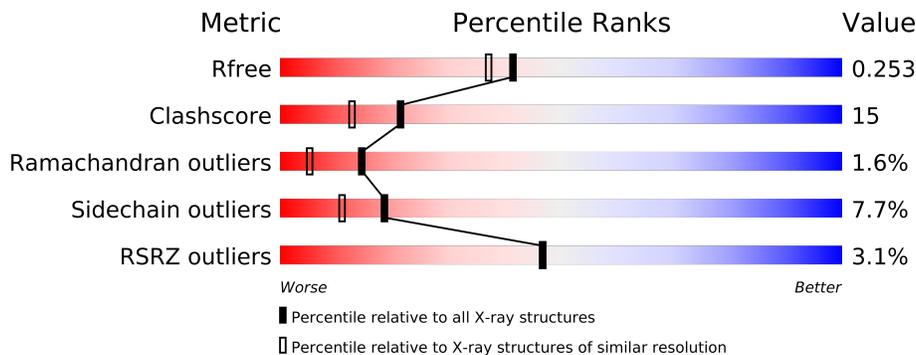
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	6003 (2.04-2.00)
Clashscore	79885	7467 (2.04-2.00)
Ramachandran outliers	78287	7370 (2.04-2.00)
Sidechain outliers	78261	7368 (2.04-2.00)
RSRZ outliers	66119	6006 (2.04-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	129	
1	B	129	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 2120 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ANTIBODY VHH LAMA DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			990	616	174	197	3			
1	B	129	Total	C	N	O	S	0	0	0
			984	613	171	197	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	68	Total	O	0	0
			68	68		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ANTIBODY VHH LAMA DOMAIN

Chain A:

• Molecule 1: ANTIBODY VHH LAMA DOMAIN

Chain B:
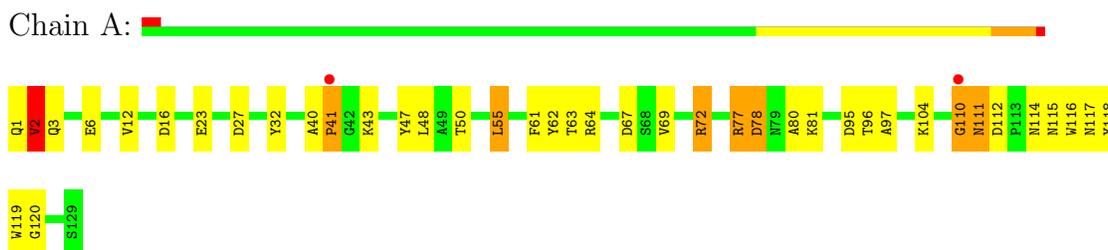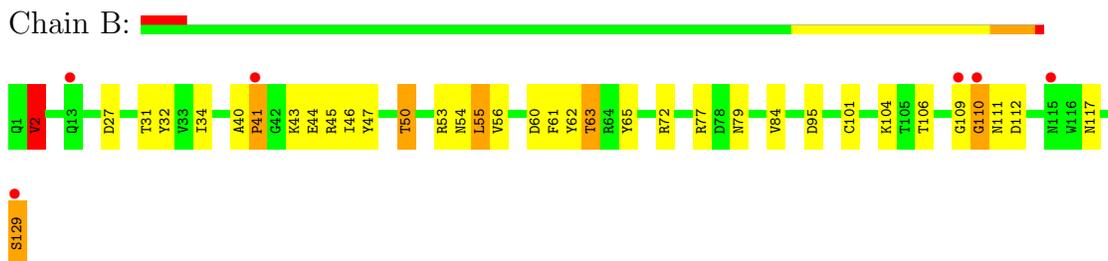
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	41.67Å 56.09Å 102.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.60 – 2.03 19.30 – 2.01	Depositor EDS
% Data completeness (in resolution range)	95.4 (14.60-2.03) 94.2 (19.30-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.250 0.214 , 0.253	Depositor DCC
R_{free} test set	1066 reflections (6.95%)	DCC
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	3 of 15610 reflections (0.019%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2120	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 86.88 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.1906e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

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	0.76	1/1011 (0.1%)	1.59	12/1372 (0.9%)
1	B	0.77	1/1005 (0.1%)	0.98	6/1365 (0.4%)
All	All	0.77	2/2016 (0.1%)	1.32	18/2737 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	CYS	CB-SG	-6.04	1.72	1.82
1	A	77	ARG	CG-CD	5.43	1.65	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	ARG	NE-CZ-NH2	-31.48	104.56	120.30
1	A	77	ARG	NE-CZ-NH1	30.14	135.37	120.30
1	A	77	ARG	CD-NE-CZ	8.81	135.94	123.60
1	A	77	ARG	CG-CD-NE	-7.93	95.14	111.80
1	A	78	ASP	N-CA-CB	7.50	124.09	110.60
1	B	110	GLY	N-CA-C	7.49	131.81	113.10
1	A	78	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	2	VAL	CB-CA-C	-7.09	97.92	111.40
1	B	111	ASN	N-CA-C	6.89	129.59	111.00
1	B	129	SER	N-CA-C	-6.58	93.22	111.00
1	A	110	GLY	N-CA-C	6.24	128.71	113.10
1	A	72	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	78	ASP	CB-CA-C	-5.94	98.53	110.40
1	B	110	GLY	C-N-CA	5.55	135.58	121.70
1	B	110	GLY	O-C-N	5.45	131.41	122.70
1	A	55	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	78	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	B	2	VAL	CB-CA-C	-5.09	101.74	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	990	0	945	36	0
1	B	984	0	934	25	0
2	A	78	0	0	3	0
2	B	68	0	0	2	0
All	All	2120	0	1879	59	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (59) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:40:ALA:HB3	1:B:43:LYS:HE2	1.56	0.86
1:A:47:TYR:OH	1:A:50:THR:HG23	1.80	0.81
1:A:62:TYR:OH	1:A:64:ARG:HG3	1.85	0.77
1:A:112:ASP:HB3	1:A:114:ASN:HD22	1.49	0.77
1:A:78:ASP:OD1	1:A:80:ALA:HB3	1.84	0.76
1:B:56:VAL:HG12	1:B:60:ASP:O	1.92	0.69
1:B:47:TYR:OH	1:B:50:THR:HG22	1.92	0.69
1:B:40:ALA:CB	1:B:43:LYS:HE2	2.28	0.64
1:A:47:TYR:HE2	1:A:50:THR:HG22	1.63	0.62
1:B:40:ALA:HB3	1:B:43:LYS:CE	2.26	0.62
1:A:47:TYR:HE2	1:A:50:THR:CG2	2.14	0.60
1:B:2:VAL:CG2	1:B:32:TYR:CZ	2.85	0.59
1:B:54:ASN:HB2	2:B:132:HOH:O	2.02	0.58
1:A:3:GLN:OE1	1:B:109:GLY:N	2.35	0.57
1:A:61:PHE:CD2	1:A:77:ARG:HD3	2.39	0.57
1:A:47:TYR:CE2	1:A:50:THR:CG2	2.88	0.56
1:A:1:GLN:HB3	1:A:32:TYR:OH	2.06	0.56
1:A:104:LYS:HE2	1:A:116:TRP:CH2	2.41	0.56
1:A:104:LYS:HG2	1:A:116:TRP:CZ3	2.41	0.55
1:A:2:VAL:HG13	1:A:27:ASP:HB3	1.88	0.55
1:A:104:LYS:HA	1:A:117:ASN:HD22	1.72	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:78:ASP:CB	1:A:81:LYS:HZ3	2.21	0.54
1:B:77:ARG:HH21	1:B:79:ASN:HD21	1.54	0.53
1:A:12:VAL:HG22	1:A:16:ASP:HB2	1.90	0.53
1:A:78:ASP:CG	1:A:81:LYS:NZ	2.63	0.52
1:B:72:ARG:NH2	1:B:95:ASP:OD2	2.42	0.51
1:B:2:VAL:HG22	1:B:32:TYR:CZ	2.45	0.51
1:B:63:THR:HG21	2:B:153:HOH:O	2.12	0.50
1:A:78:ASP:CB	1:A:81:LYS:NZ	2.76	0.49
1:B:2:VAL:HG22	1:B:32:TYR:OH	2.13	0.48
1:A:78:ASP:CG	1:A:81:LYS:HZ3	2.16	0.48
1:A:47:TYR:CZ	1:A:50:THR:HG23	2.48	0.47
1:B:63:THR:HG23	1:B:65:TYR:CE2	2.48	0.47
1:A:111:ASN:N	1:A:111:ASN:OD1	2.46	0.47
1:A:12:VAL:CG2	1:A:16:ASP:HB2	2.44	0.47
1:B:34:ILE:HG13	1:B:84:VAL:HG21	1.97	0.47
1:B:55:LEU:HD13	1:B:61:PHE:CE2	2.50	0.47
1:A:40:ALA:HB1	1:A:41:PRO:HD2	1.97	0.46
1:B:2:VAL:HG13	1:B:27:ASP:HB3	1.98	0.45
1:A:47:TYR:CE2	1:A:50:THR:HG23	2.52	0.45
1:A:119:TRP:O	2:A:130:HOH:O	2.21	0.45
1:A:2:VAL:HG22	1:A:32:TYR:CZ	2.52	0.44
1:A:104:LYS:HG2	1:A:116:TRP:CE3	2.52	0.44
1:A:6:GLU:OE2	1:A:120:GLY:HA3	2.17	0.44
1:A:61:PHE:CE2	1:A:77:ARG:HD3	2.53	0.44
1:A:115:ASN:HB2	2:A:178:HOH:O	2.16	0.44
1:B:104:LYS:HA	1:B:117:ASN:HD22	1.83	0.44
1:B:77:ARG:HD3	1:B:79:ASN:HD21	1.83	0.43
1:A:72:ARG:NH2	1:A:95:ASP:OD2	2.47	0.43
1:B:47:TYR:OH	1:B:50:THR:CG2	2.62	0.42
1:A:23:GLU:OE2	1:B:62:TYR:OH	2.37	0.42
1:A:48:LEU:HD22	1:A:69:VAL:HG11	2.02	0.42
1:B:31:THR:O	1:B:53:ARG:NH1	2.49	0.42
1:B:47:TYR:CE2	1:B:50:THR:HG22	2.55	0.41
1:B:2:VAL:HG21	1:B:32:TYR:CZ	2.53	0.41
1:A:96:THR:O	1:A:97:ALA:HB2	2.21	0.41
1:A:50:THR:HG21	2:A:160:HOH:O	2.21	0.41
1:A:1:GLN:HB2	1:A:118:TYR:CZ	2.55	0.40
1:B:46:ILE:O	1:B:46:ILE:HG13	2.22	0.40

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	127/129 (98%)	122 (96%)	3 (2%)	2 (2%)	14	5
1	B	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	14	5
All	All	254/258 (98%)	243 (96%)	7 (3%)	4 (2%)	14	5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	GLY
1	B	110	GLY
1	B	41	PRO
1	A	41	PRO

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	104/104 (100%)	98 (94%)	6 (6%)	28	20
1	B	103/104 (99%)	93 (90%)	10 (10%)	12	6
All	All	207/208 (100%)	191 (92%)	16 (8%)	18	11

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	43	LYS
1	A	55	LEU
1	A	63	THR
1	A	67	ASP

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Mol	Chain	Res	Type
1	A	111	ASN
1	B	2	VAL
1	B	41	PRO
1	B	44	GLU
1	B	45	ARG
1	B	50	THR
1	B	55	LEU
1	B	63	THR
1	B	106	THR
1	B	112	ASP
1	B	129	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	54	ASN
1	A	79	ASN
1	A	114	ASN
1	A	117	ASN
1	B	1	GLN
1	B	3	GLN
1	B	79	ASN
1	B	114	ASN
1	B	117	ASN
1	B	124	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 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

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, 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	129/129 (100%)	0.12	2 (1%)	68　69	12, 23, 39, 49	0
1	B	129/129 (100%)	0.18	6 (4%)	30　29	13, 23, 41, 51	0
All	All	258/258 (100%)	0.15	8 (3%)	47　47	12, 23, 41, 51	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	GLY	4.6
1	B	41	PRO	3.2
1	A	110	GLY	3.1
1	B	129	SER	3.0
1	B	110	GLY	2.5
1	B	115	ASN	2.4
1	A	41	PRO	2.3
1	B	13	GLN	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.