



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:38 AM UTC

PDB ID : 6BFI / pdb_00006bfi
Title : Vinculin homolog in a sponge (phylum Porifera) reveals vertebrate-like cell adhesions involved in early multicellular evolution
Authors : Weis, W.I.; Chodaparambil, J.V.
Deposited on : 2017-10-26
Resolution : 2.30 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

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

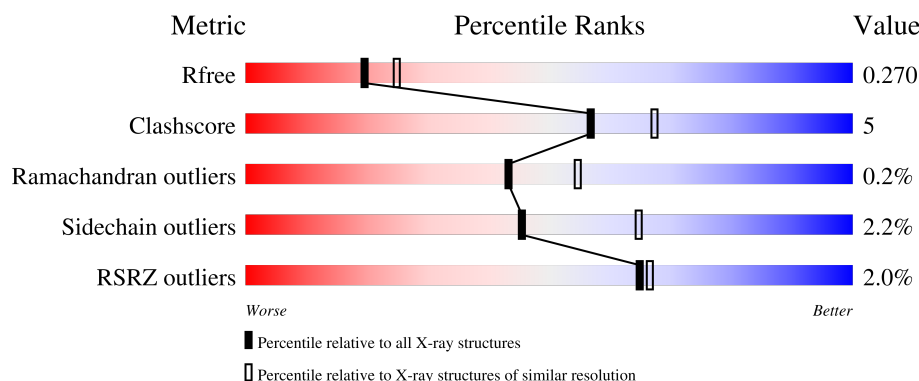
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	846	 2% 83% 12% 5%
1	B	846	 2% 82% 13% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12363 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 VIN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	805	Total	C	N	O	S	0	2	0
			6124	3804	1098	1186	36			
1	B	806	Total	C	N	O	S	0	0	0
			6106	3794	1091	1185	36			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	62	Total	O	0	0
			62	62		
2	B	71	Total	O	0	0
			71	71		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.34Å 93.68Å 101.63Å 114.81° 93.29° 90.23°	Depositor
Resolution (Å)	36.50 – 2.30 36.50 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.6 (36.50-2.30) 92.6 (36.50-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.218 , 0.266 0.223 , 0.270	Depositor DCC
R_{free} test set	7546 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12363	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 6.31% 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](#)

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	0.13	0/6190	0.29	0/8348
1	B	0.13	0/6169	0.28	0/8322
All	All	0.13	0/12359	0.29	0/16670

There are no bond length outliers.

There are no bond angle outliers.

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	6124	0	6295	55	0
1	B	6106	0	6272	59	0
2	A	62	0	0	2	0
2	B	71	0	0	0	0
All	All	12363	0	12567	113	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 5.

All (113) 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:695:VAL:HG11	1:A:811:ILE:HD11	1.63	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:VAL:HG11	1:B:811:ILE:HD11	1.67	0.75
1:B:10:LEU:HD11	1:B:124:MET:HE3	1.70	0.73
1:A:362:GLN:OE1	1:A:365:ARG:NH2	2.27	0.68
1:B:176:GLU:OE2	1:B:199:ARG:NH2	2.31	0.64
1:A:168:MET:HE3	1:A:202:ILE:HD11	1.82	0.61
1:A:362:GLN:NE2	1:A:498:GLU:OE2	2.31	0.61
1:A:58:ALA:HA	1:A:61:MET:HE2	1.84	0.60
1:B:304:ARG:NH2	1:B:427:SER:OG	2.34	0.60
1:B:372:VAL:HG21	1:B:494:ILE:HG13	1.83	0.60
1:A:517:ILE:HD13	1:A:526:LYS:HB3	1.84	0.59
1:B:303:ARG:NH2	1:B:326:ASP:OD2	2.35	0.59
1:B:152:ASP:N	1:B:152:ASP:OD1	2.36	0.59
1:B:683:GLN:HB2	1:B:834:LYS:HE2	1.84	0.59
1:B:574:PRO:HA	1:B:577:ILE:HG12	1.85	0.58
1:B:21:VAL:HG13	1:B:112:ALA:HB1	1.85	0.58
1:A:203:PRO:HA	1:A:206:ILE:HG12	1.85	0.57
1:A:751:ARG:NH2	2:A:902:HOH:O	2.36	0.57
1:B:750:LYS:HA	1:B:753:LYS:HG2	1.86	0.57
1:B:214:LEU:HB3	1:B:465:ASN:HD21	1.69	0.57
1:B:44:VAL:HG11	1:B:89:SER:HA	1.88	0.56
1:A:142:GLN:HE22	1:A:243:GLU:HG2	1.70	0.56
1:B:744:ALA:HB2	1:B:756:LEU:HD23	1.87	0.56
1:A:744:ALA:HB2	1:A:756:LEU:HD23	1.88	0.56
1:B:324:GLU:OE2	1:B:356:LYS:NZ	2.39	0.55
1:B:580:LYS:HA	1:B:583:VAL:HG13	1.89	0.55
1:B:276:HIS:CG	1:B:621:ARG:HD3	2.42	0.55
1:A:29:GLU:OE2	1:A:717:ARG:N	2.39	0.54
1:B:513:GLU:OE2	1:B:516:ARG:NH1	2.41	0.54
1:A:68:GLU:HG3	1:B:570:LYS:HA	1.90	0.53
1:A:698:MET:HE2	1:A:732:ASN:HB3	1.91	0.53
1:A:372:VAL:HG21	1:A:494:ILE:HG13	1.90	0.53
1:B:44:VAL:HG21	1:B:92:ALA:HB2	1.91	0.53
1:B:705:MET:HE3	1:B:729:ILE:HD12	1.90	0.52
1:B:124:MET:HA	1:B:124:MET:HE2	1.90	0.52
1:A:521:GLU:OE2	1:A:592:GLN:NE2	2.41	0.51
1:B:824:ASP:OD1	1:B:825:SER:N	2.43	0.51
1:A:184:ASN:ND2	1:A:255:PHE:H	2.09	0.51
1:B:279:GLN:HG3	1:B:357:LEU:HD23	1.92	0.51
1:A:818:CYS:SG	1:A:832:TRP:NE1	2.84	0.51
1:A:610:ARG:O	1:A:614:GLU:HB2	2.11	0.50
1:B:62:VAL:O	1:B:71:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD13	1:B:209:ILE:HG21	1.94	0.50
1:A:113:ARG:HD3	1:A:780:SER:HB3	1.94	0.49
1:A:142:GLN:NE2	1:A:243:GLU:HG2	2.28	0.49
1:A:342:ASP:O	1:A:347:ARG:NH1	2.47	0.48
1:B:179:HIS:CG	1:B:180:PRO:HD3	2.49	0.48
1:A:27:PHE:CE1	1:A:38:GLU:HG3	2.49	0.48
1:A:218:LYS:HD3	1:A:218:LYS:HA	1.74	0.48
1:B:61:MET:HB3	1:B:61:MET:HE2	1.83	0.48
1:A:303:ARG:HE	1:A:322:ALA:HB1	1.79	0.48
1:A:157:LEU:O	1:A:161:LEU:HB2	2.13	0.47
1:B:75:PRO:HA	1:B:78:MET:HE2	1.96	0.47
1:B:513:GLU:HG2	1:B:530:LYS:HE2	1.95	0.47
1:A:744:ALA:O	1:A:753:LYS:NZ	2.44	0.47
1:B:674:ALA:HA	1:B:804:MET:HE2	1.97	0.47
1:A:7:THR:HG22	1:A:10:LEU:H	1.79	0.46
1:B:697:GLN:HG3	1:B:701:LYS:HE2	1.96	0.46
1:B:153:VAL:HG23	1:B:155:ALA:H	1.80	0.46
1:A:184:ASN:HD21	1:A:255:PHE:H	1.62	0.46
1:A:130:GLU:O	1:A:134:MET:HG3	2.15	0.46
1:B:126:ALA:O	1:B:130:GLU:HG2	2.16	0.46
1:B:553:GLU:HG2	1:B:750:LYS:HE3	1.99	0.45
1:A:375:ASP:OD2	1:A:420:THR:OG1	2.34	0.45
1:B:202:ILE:HB	1:B:203:PRO:HD3	1.97	0.45
1:B:27:PHE:CE1	1:B:38:GLU:HG3	2.52	0.45
1:A:303:ARG:NH2	1:A:326:ASP:OD2	2.50	0.45
1:B:680:GLU:HG2	1:B:808:LYS:HG3	1.99	0.44
1:A:256:GLU:OE1	1:A:256:GLU:N	2.50	0.44
1:A:574:PRO:HA	1:A:577:ILE:HG12	1.99	0.44
1:A:172:MET:O	1:A:176:GLU:HB2	2.17	0.43
1:A:719:LYS:NZ	1:A:781:MET:O	2.51	0.43
1:A:61:MET:HE3	1:A:70:PHE:HZ	1.83	0.43
1:A:74:LEU:HB3	1:A:75:PRO:HD3	2.01	0.43
1:B:121:ASP:HA	1:B:124:MET:HB2	2.00	0.43
1:B:142:GLN:HB2	1:B:242:ILE:HG21	2.00	0.43
1:B:54:LEU:HD23	1:B:122:LEU:HD23	1.99	0.43
1:B:696:LYS:O	1:B:700:ARG:HG3	2.19	0.43
1:A:108:LEU:O	1:A:112:ALA:HB2	2.19	0.43
1:A:580:LYS:O	1:A:583:VAL:HG22	2.19	0.43
1:B:580:LYS:O	1:B:583:VAL:HG22	2.19	0.43
1:B:207:SER:O	1:B:211:VAL:HG13	2.19	0.43
1:B:530:LYS:HD3	1:B:530:LYS:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:HIS:CG	1:A:180:PRO:HD3	2.54	0.42
1:B:148:ALA:HA	1:B:151:ILE:HD13	2.00	0.42
1:B:551:ASN:OD1	1:B:751:ARG:HG3	2.18	0.42
1:A:199[A]:ARG:NH1	2:A:908:HOH:O	2.52	0.42
1:A:190:MET:O	1:A:194:GLU:HG2	2.20	0.42
1:A:705:MET:HE3	1:A:729:ILE:HD12	2.01	0.42
1:A:619:PRO:HA	1:A:620:PRO:HD3	1.95	0.42
1:A:674:ALA:HA	1:A:804:MET:HE3	2.01	0.42
1:B:67:ASP:HB3	1:B:70:PHE:HB3	2.02	0.42
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.84	0.42
1:B:208:SER:O	1:B:211:VAL:HG22	2.19	0.42
1:A:705:MET:O	1:A:709:THR:HG23	2.20	0.42
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.89	0.42
1:B:500:MET:SD	1:B:541:VAL:HG13	2.60	0.41
1:A:763:ILE:N	1:A:764:PRO:HD2	2.35	0.41
1:B:708:TYR:CE2	1:B:721:ASP:HB3	2.55	0.41
1:B:83:GLN:O	1:B:86:VAL:HG12	2.20	0.41
1:B:403:PHE:CG	1:B:460:LEU:HD22	2.55	0.41
1:A:682:ASP:HA	1:A:696:LYS:HE3	2.02	0.41
1:A:157:LEU:HD13	1:A:209:ILE:HG21	2.01	0.41
1:B:430:CYS:HB3	1:B:493:VAL:HG13	2.03	0.41
1:A:226:ASP:OD2	1:A:457:ARG:HD2	2.21	0.41
1:A:494:ILE:HD13	1:A:494:ILE:HA	1.87	0.41
1:A:549:ALA:HB2	1:A:561:LEU:HD23	2.03	0.41
1:A:668:ASN:HB3	1:A:671:HIS:HB3	2.03	0.41
1:B:763:ILE:N	1:B:764:PRO:HD2	2.35	0.41
1:A:186:ALA:O	1:A:190:MET:HG3	2.21	0.40
1:B:382:PRO:HG2	1:B:413:HIS:CG	2.56	0.40
1:B:511:VAL:HG13	1:B:599:ALA:HB1	2.02	0.40
1:B:103:GLU:O	1:B:107:LYS:HB2	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	797/846 (94%)	780 (98%)	15 (2%)	2 (0%)	36	46
1	B	796/846 (94%)	775 (97%)	20 (2%)	1 (0%)	48	60
All	All	1593/1692 (94%)	1555 (98%)	35 (2%)	3 (0%)	43	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	SER
1	A	620	PRO
1	B	102	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	654/686 (95%)	639 (98%)	15 (2%)	44	63
1	B	652/686 (95%)	638 (98%)	14 (2%)	47	66
All	All	1306/1372 (95%)	1277 (98%)	29 (2%)	45	65

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	7	THR
1	A	146	ASP
1	A	150	VAL
1	A	174	VAL
1	A	211	VAL
1	A	217	VAL
1	A	290	SER
1	A	363	GLU
1	A	494	ILE

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Mol	Chain	Res	Type
1	A	524	SER
1	A	548	GLU
1	A	583	VAL
1	A	621	ARG
1	A	665	LYS
1	B	5	PHE
1	B	35	LEU
1	B	43	LEU
1	B	83	GLN
1	B	150	VAL
1	B	152	ASP
1	B	174	VAL
1	B	206	ILE
1	B	211	VAL
1	B	236	GLN
1	B	528	ILE
1	B	556	GLU
1	B	583	VAL
1	B	731	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	236	GLN
1	A	537	GLN
1	A	668	ASN
1	B	82	GLN
1	B	184	ASN
1	B	539	ASN
1	B	671	HIS

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 [i](#)

There are no oligosaccharides 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, 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	805/846 (95%)	0.35	16 (1%) 65 66	33, 71, 118, 177	2 (0%)
1	B	806/846 (95%)	0.34	16 (1%) 65 66	44, 72, 123, 165	0
All	All	1611/1692 (95%)	0.35	32 (1%) 65 66	33, 71, 119, 177	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	GLY	4.3
1	B	217	VAL	3.9
1	B	717	ARG	3.8
1	A	627	LEU	3.7
1	B	389	ALA	3.6
1	A	713	SER	2.9
1	A	285	GLY	2.8
1	A	62	VAL	2.8
1	A	591	ILE	2.6
1	B	646	LEU	2.4
1	A	206	ILE	2.4
1	B	150	VAL	2.4
1	A	1	MET	2.4
1	A	664	PRO	2.3
1	B	380	GLY	2.3
1	B	783	GLY	2.3
1	B	836	GLY	2.3
1	B	224	MET	2.2
1	B	285	GLY	2.2
1	A	763	ILE	2.2
1	A	626	GLU	2.2
1	A	219	ASP	2.2
1	B	664	PRO	2.2
1	A	685	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	222	SER	2.1
1	A	737	LEU	2.1
1	A	717	ARG	2.1
1	B	1	MET	2.1
1	A	739	LEU	2.1
1	B	572	ILE	2.1
1	B	713	SER	2.0
1	B	36	LEU	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 oligosaccharides 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.