



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:54 pm GMT

PDB ID : 1XWJ
Title : Vinculin head (1-258) in complex with the talin vinculin binding site 3 (1945-1969)
Authors : Gingras, A.R.; Papagrigoriou, E.; Barsukov, I.L.; Critchley, D.R.; Emsley, J.
Deposited on : 2004-11-01
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

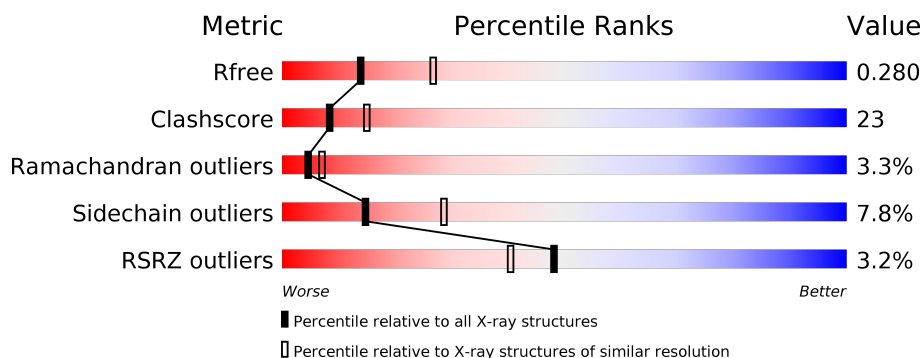
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	280	<div> <div>3%</div> <div> <div></div> <div>49%</div> <div>38%</div> <div>•</div> <div>10%</div> </div> </div>
2	B	26	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2144 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 Vinculin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	253	1925	1212	328	371	14	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP P12003
A	-20	GLY	-	EXPRESSION TAG	UNP P12003
A	-19	SER	-	EXPRESSION TAG	UNP P12003
A	-18	SER	-	EXPRESSION TAG	UNP P12003
A	-17	HIS	-	EXPRESSION TAG	UNP P12003
A	-16	HIS	-	EXPRESSION TAG	UNP P12003
A	-15	HIS	-	EXPRESSION TAG	UNP P12003
A	-14	HIS	-	EXPRESSION TAG	UNP P12003
A	-13	HIS	-	EXPRESSION TAG	UNP P12003
A	-12	HIS	-	EXPRESSION TAG	UNP P12003
A	-11	SER	-	EXPRESSION TAG	UNP P12003
A	-10	SER	-	EXPRESSION TAG	UNP P12003
A	-9	GLY	-	EXPRESSION TAG	UNP P12003
A	-8	LEU	-	EXPRESSION TAG	UNP P12003
A	-7	VAL	-	EXPRESSION TAG	UNP P12003
A	-6	PRO	-	EXPRESSION TAG	UNP P12003
A	-5	ARG	-	EXPRESSION TAG	UNP P12003
A	-4	GLY	-	EXPRESSION TAG	UNP P12003
A	-3	SER	-	EXPRESSION TAG	UNP P12003
A	-2	HIS	-	EXPRESSION TAG	UNP P12003
A	-1	MET	-	EXPRESSION TAG	UNP P12003
A	0	MET	-	EXPRESSION TAG	UNP P12003

- Molecule 2 is a protein called Talin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	24	Total	C	N	O	0	0	0
			173	109	33	31			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	4	Total	O	0	0
			4	4		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	52.17Å 72.43Å 96.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.95 – 2.60 28.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.9 (28.95-2.60) 90.0 (28.95-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.281 0.242 , 0.280	Depositor DCC
R_{free} test set	552 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	1.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2144	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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	0.37	0/1948	0.58	0/2644
2	B	0.36	0/173	0.54	0/230
All	All	0.37	0/2121	0.58	0/2874

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	TYR	Sidechain

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	1925	0	1961	96	0
2	B	173	0	184	8	0
3	A	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	1	0
All	All	2144	0	2145	98	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 23.

All (98) 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:142:GLU:O	1:A:145:THR:HG22	1.69	0.92
1:A:178:GLN:HE21	1:A:187:ARG:HD2	1.40	0.87
1:A:34:LYS:HE3	1:A:34:LYS:HA	1.63	0.80
1:A:215:LYS:HD3	1:A:215:LYS:O	1.81	0.79
1:A:24:ILE:O	1:A:29:GLY:HA3	1.83	0.78
1:A:3:PHE:O	1:A:182:THR:HG21	1.84	0.76
1:A:64:THR:HG21	1:A:69:LEU:HD23	1.68	0.74
1:A:152:THR:HG22	1:A:154:GLU:H	1.51	0.74
1:A:149:VAL:HG23	1:A:150:VAL:N	2.02	0.73
1:A:229:ARG:HH11	1:A:230:ASN:HD21	1.41	0.67
1:A:90:ALA:HB1	1:A:107:LEU:HD22	1.77	0.67
1:A:101:VAL:N	1:A:102:PRO:HD2	2.10	0.66
1:A:184:GLN:HE22	1:A:187:ARG:NH1	1.93	0.65
1:A:69:LEU:HD12	1:A:124:THR:HG22	1.79	0.65
1:A:149:VAL:HG23	1:A:150:VAL:H	1.63	0.63
1:A:34:LYS:CA	1:A:34:LYS:HE3	2.31	0.60
1:A:19:ILE:O	1:A:23:VAL:HG23	2.01	0.60
1:A:189:MET:HE1	1:A:245:ARG:NH2	2.17	0.59
1:A:41:ALA:HB3	1:A:42:PRO:CD	2.32	0.59
1:A:34:LYS:O	1:A:35:ALA:HB3	2.04	0.57
1:A:68:ILE:H	1:A:68:ILE:HD12	1.70	0.55
1:A:163:LEU:HD11	1:A:167:MET:HE2	1.87	0.55
1:A:184:GLN:HA	1:A:184:GLN:HE21	1.72	0.54
1:A:181:LEU:HB2	1:A:187:ARG:HG2	1.89	0.54
1:A:217:THR:HG22	1:A:219:SER:H	1.73	0.54
1:A:174:ILE:HD13	1:A:243:ILE:HD13	1.88	0.54
1:A:152:THR:HB	1:A:155:ASP:OD2	2.08	0.54
1:A:90:ALA:HB2	1:A:106:TYR:HB3	1.89	0.54
1:A:15:VAL:HG12	1:A:115:LEU:HD11	1.91	0.53
1:A:94:LEU:HD13	1:A:103:ALA:HB1	1.91	0.53
1:A:101:VAL:N	1:A:102:PRO:CD	2.72	0.52
1:A:206:SER:O	1:A:210:ILE:HG13	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD12	1:A:94:LEU:HD23	1.92	0.52
1:A:184:GLN:NE2	1:A:187:ARG:NH1	2.57	0.52
1:A:0:MET:N	1:A:1:PRO:HD2	2.25	0.52
1:A:22:LEU:HD22	2:B:1965:LEU:HD22	1.92	0.52
1:A:18:GLN:HE22	2:B:1962:SER:CB	2.22	0.52
1:A:94:LEU:HD13	1:A:103:ALA:CB	2.40	0.51
1:A:19:ILE:HD12	1:A:115:LEU:HD12	1.92	0.51
1:A:42:PRO:HB2	2:B:1964:VAL:HG22	1.91	0.51
1:A:15:VAL:HG21	2:B:1958:SER:OG	2.10	0.51
1:A:240:ILE:O	1:A:244:ILE:HG13	2.11	0.51
1:A:224:GLU:OE1	1:A:224:GLU:HA	2.12	0.50
1:A:27:GLU:HG3	1:A:105:ASP:OD2	2.10	0.50
1:A:174:ILE:CD1	1:A:243:ILE:HG21	2.42	0.49
1:A:123:LEU:O	1:A:127:GLU:HG3	2.13	0.49
1:A:6:ARG:HD3	1:A:180:GLU:HA	1.95	0.49
1:A:153:MET:O	1:A:157:VAL:HG23	2.13	0.49
1:A:52:ASN:HD22	1:A:55:ARG:HH21	1.60	0.49
1:A:15:VAL:CG1	1:A:115:LEU:HD11	2.44	0.48
1:A:13:GLU:N	1:A:14:PRO:HD2	2.28	0.48
1:A:34:LYS:O	1:A:34:LYS:HG3	2.13	0.48
1:A:146:VAL:O	1:A:149:VAL:HG22	2.14	0.47
1:A:242:GLU:HA	1:A:242:GLU:OE1	2.14	0.47
1:A:36:ILE:HD11	1:A:104:ARG:CZ	2.45	0.47
1:A:136:VAL:HG21	1:A:173:MET:SD	2.55	0.47
1:A:149:VAL:O	1:A:150:VAL:HB	2.15	0.47
1:A:89:ARG:HA	1:A:89:ARG:HD2	1.69	0.46
1:A:52:ASN:ND2	1:A:55:ARG:HH21	2.14	0.46
1:A:57:GLY:O	1:A:60:THR:HB	2.16	0.46
1:A:48:ALA:O	1:A:51:SER:HB3	2.17	0.45
1:A:27:GLU:OE1	1:A:27:GLU:N	2.50	0.45
1:A:19:ILE:CD1	1:A:115:LEU:HD12	2.47	0.45
1:A:69:LEU:HD12	1:A:124:THR:CG2	2.45	0.45
1:A:99:TYR:HA	1:A:104:ARG:HH12	1.81	0.45
1:A:184:GLN:HA	1:A:184:GLN:NE2	2.32	0.45
1:A:121:LEU:CD2	2:B:1950:LEU:HD11	2.47	0.45
1:A:11:ILE:HG22	1:A:12:LEU:HD13	1.98	0.45
1:A:50:VAL:HG13	1:A:80:VAL:CG1	2.46	0.44
1:A:174:ILE:HD11	1:A:243:ILE:HG21	2.00	0.44
1:A:175:ASP:O	1:A:179:GLN:HG3	2.17	0.44
1:A:34:LYS:O	1:A:35:ALA:CB	2.66	0.44
1:A:143:TYR:OH	1:A:159:TYR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:MET:CE	1:A:245:ARG:NH2	2.80	0.44
1:A:152:THR:HG22	1:A:154:GLU:N	2.27	0.44
1:A:201:LEU:HB3	1:A:202:PRO:HD3	1.99	0.44
1:A:214:THR:OG1	1:A:222:ILE:HD13	2.18	0.44
1:A:211:PHE:O	1:A:215:LYS:HB2	2.18	0.43
1:A:73:MET:HB3	1:A:74:PRO:HD3	2.01	0.43
1:A:71:ARG:CG	1:A:72:ASP:N	2.82	0.43
1:A:178:GLN:HG3	1:A:191:VAL:HG23	2.01	0.43
1:A:23:VAL:O	1:A:27:GLU:O	2.36	0.43
2:B:1960:LYS:NZ	3:B:5:HOH:O	2.52	0.43
1:A:143:TYR:OH	1:A:162:ASN:HB2	2.18	0.43
1:A:41:ALA:HB3	1:A:42:PRO:HD3	2.00	0.43
1:A:189:MET:CE	1:A:245:ARG:HH21	2.32	0.42
2:B:1968:LEU:C	2:B:1969:GLN:NE2	2.72	0.42
1:A:87:LEU:HA	1:A:87:LEU:HD12	1.92	0.42
1:A:201:LEU:HA	1:A:201:LEU:HD23	1.89	0.42
1:A:89:ARG:HD2	1:A:92:GLN:NE2	2.35	0.41
1:A:121:LEU:HD22	2:B:1950:LEU:HD11	2.01	0.41
1:A:189:MET:HE1	1:A:245:ARG:HH21	1.84	0.41
1:A:68:ILE:HD12	1:A:68:ILE:N	2.36	0.41
1:A:104:ARG:HH21	1:A:104:ARG:HG3	1.85	0.41
1:A:149:VAL:CG2	1:A:150:VAL:N	2.73	0.41
1:A:2:VAL:HG12	1:A:182:THR:HG21	2.04	0.40
1:A:184:GLN:HE21	1:A:184:GLN:CA	2.30	0.40
1:A:178:GLN:O	1:A:187:ARG:HD2	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	251/280 (90%)	230 (92%)	12 (5%)	9 (4%)	4 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	22/26 (85%)	22 (100%)	0	0	100	100
All	All	273/306 (89%)	252 (92%)	12 (4%)	9 (3%)	4	7

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	32	ASP
1	A	149	VAL
1	A	25	MET
1	A	26	HIS
1	A	150	VAL
1	A	35	ALA
1	A	37	PRO
1	A	220	GLN

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	213/247 (86%)	195 (92%)	18 (8%)	12	24
2	B	17/22 (77%)	17 (100%)	0	100	100
All	All	230/269 (86%)	212 (92%)	18 (8%)	15	29

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	27	GLU
1	A	34	LYS
1	A	62	GLN
1	A	67	GLN
1	A	87	LEU
1	A	94	LEU

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Mol	Chain	Res	Type
1	A	106	TYR
1	A	109	ASP
1	A	141	LEU
1	A	169	LYS
1	A	201	LEU
1	A	204	LEU
1	A	215	LYS
1	A	224	GLU
1	A	226	LEU
1	A	228	ASN
1	A	249	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	17	GLN
1	A	18	GLN
1	A	26	HIS
1	A	47	GLN
1	A	52	ASN
1	A	62	GLN
1	A	67	GLN
1	A	92	GLN
1	A	95	GLN
1	A	178	GLN
1	A	179	GLN
1	A	184	GLN
1	A	192	ASN
1	A	195	ASN
1	A	216	ASN
1	A	228	ASN
1	A	230	ASN
2	B	1969	GLN

5.3.3 RNA ⓘ

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 [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	253/280 (90%)	0.05	8 (3%)	48	40	38, 55, 86, 106	0
2	B	24/26 (92%)	0.23	1 (4%)	37	29	46, 58, 79, 83	0
All	All	277/306 (90%)	0.06	9 (3%)	48	40	38, 55, 86, 106	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	VAL	4.1
1	A	251	SER	3.2
1	A	32	ASP	3.2
1	A	27	GLU	3.0
1	A	36	ILE	2.8
1	A	26	HIS	2.7
2	B	1969	GLN	2.5
1	A	33	GLY	2.2
1	A	28	GLU	2.2

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 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.