Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 09:01 am GMT

PDB ID	:	9FWF
EMDB ID	:	EMD-50833
Title	:	N-VelcroVax HBcAg with SUMO-Affimer inserted at N-terminus (T=4 VLP)
Authors	:	Fatema, K.; Snowden, J.S.; Watson, A.; Sherry, L.; Ranson, N.A.; Stonehouse, N.J.; Rowlands, D.J.
Deposited on	:	2024-06-30
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

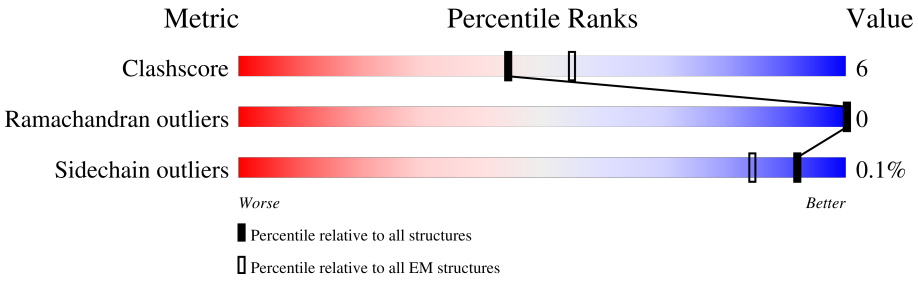
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	300	62% 12% 26%
1	B	300	61% 14% 25%
1	C	300	63% 11% 26%
1	D	300	59% 16% 25%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7222 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 N-VelcroVax HBcAg with SUMO-Affimer inserted at N-terminus.

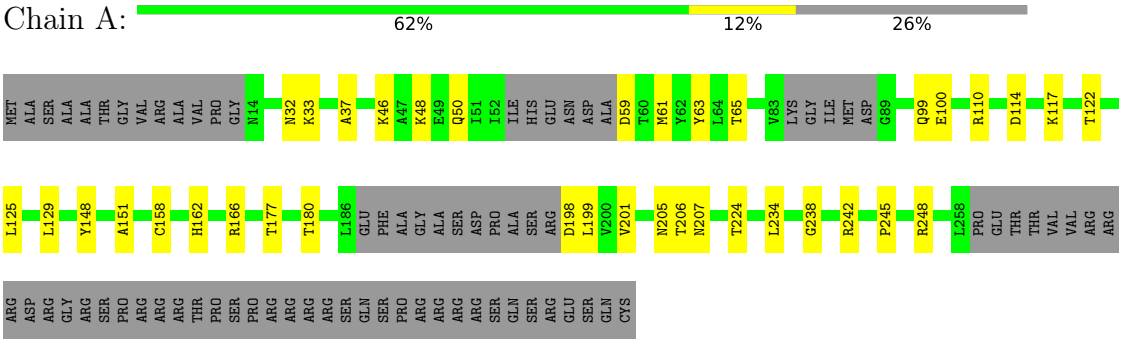
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1799	1165	298	330	6		
1	B	225	Total	C	N	O	S	0	0
			1812	1172	302	332	6		
1	C	222	Total	C	N	O	S	0	0
			1791	1159	297	329	6		
1	D	226	Total	C	N	O	S	0	0
			1820	1176	304	334	6		

3 Residue-property plots (i)

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. 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. 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.

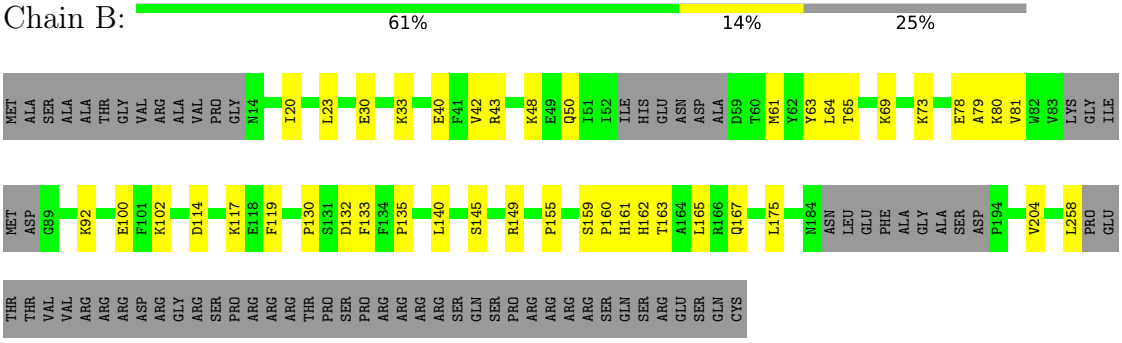
• Molecule 1: N-VelcroVax HBcAg with SUMO-Affimer inserted at N-terminus

Chain A:



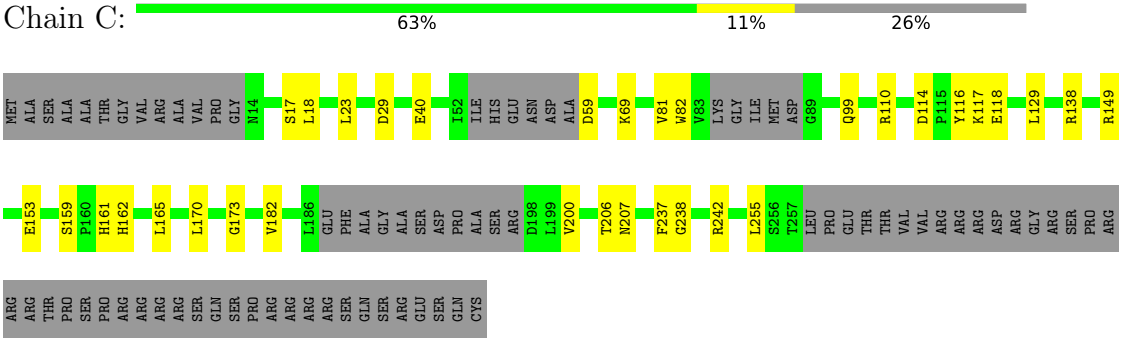
• Molecule 1: N-VelcroVax HBcAg with SUMO-Affimer inserted at N-terminus

Chain B:



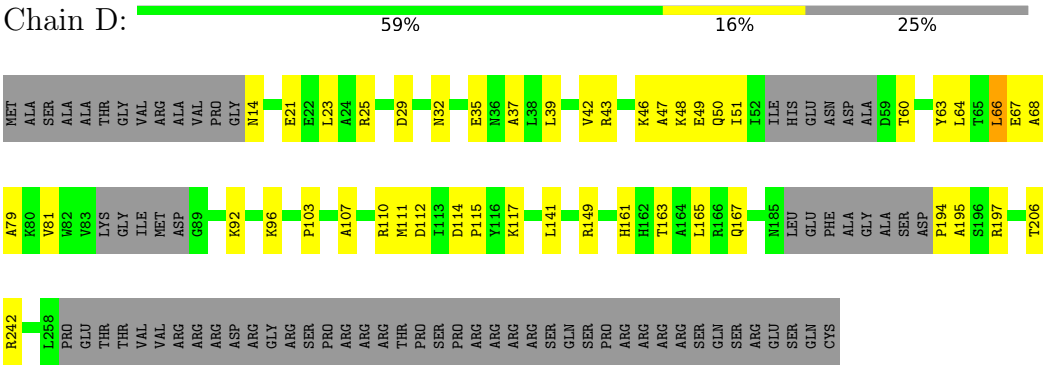
• Molecule 1: N-VelcroVax HBcAg with SUMO-Affimer inserted at N-terminus

Chain C:



• Molecule 1: N-VelcroVax HBcAg with SUMO-Affimer inserted at N-terminus

Chain D:


59%
16%
25%
MET ALA SER ALA ALA THR GLY VAL ARG ALA VAL PRO GLY N14 E21 E22 L23 A24 R25 D29 N32 E35 N36 A37 L38 L39 V42 R43 K46 A47 K48 E49 Q50 I51 I52 ILE HIS GLU ASN ASP ALA D59 T60 Y63 L64 T65 L66 E67 A68 K74 E78
A79 K80 V81 W82 V83 LYS GLY ILE MET ASP G89 K92 K96 P103 A107 R110 M111 D112 I113 D114 P115 Y116 K117 L141 R149 H161 H162 T163 A164 L165 R166 Q167 N185 LEU GLU PHE ALA GLY ALA SER ASP P194 A195 S196 R197 T206 N207 G238
R242 L258 PRO GLU THR THR VAL VAL ARG ARG ARG ASP ARG GLY ARG SER PRO ARG ARG ARG THR PRO SER PRO ARG ARG ARG ARG SER GLN SER PRO ARG ARG ARG ARG SER GLN SER ARG GLU SER GLN CYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	56416	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

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	0.49	0/1841	0.59	0/2496
1	B	0.47	0/1855	0.60	1/2514 (0.0%)
1	C	0.46	0/1833	0.58	2/2485 (0.1%)
1	D	0.46	0/1863	0.58	2/2525 (0.1%)
All	All	0.47	0/7392	0.59	5/10020 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	255	LEU	CA-CB-CG	5.93	128.95	115.30
1	C	29	ASP	CB-CG-OD1	5.75	123.47	118.30
1	D	66	LEU	CA-CB-CG	5.26	127.40	115.30
1	B	258	LEU	CA-CB-CG	5.23	127.33	115.30
1	D	23	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1799	0	1788	21	0
1	B	1812	0	1802	25	0
1	C	1791	0	1777	21	0
1	D	1820	0	1808	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7222	0	7175	89	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 6.

All (89) 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:238:GLY:O	1:A:242:ARG:HB2	1.93	0.67
1:D:114:ASP:HB3	1:D:117:LYS:HB2	1.79	0.65
1:D:67:GLU:HB2	1:D:74:LYS:HD2	1.82	0.62
1:D:163:THR:O	1:D:167:GLN:NE2	2.33	0.62
1:A:110:ARG:O	1:B:149:ARG:NH1	2.35	0.60
1:D:48:LYS:HB2	1:D:63:TYR:HB2	1.84	0.59
1:B:114:ASP:HB3	1:B:117:LYS:HB2	1.85	0.59
1:C:110:ARG:O	1:D:149:ARG:NH2	2.36	0.57
1:B:50:GLN:HB2	1:B:61:MET:HB3	1.86	0.57
1:C:149:ARG:NH2	1:D:110:ARG:O	2.38	0.56
1:B:40:GLU:HG2	1:B:69:LYS:HD2	1.88	0.56
1:B:163:THR:O	1:B:167:GLN:NE2	2.40	0.55
1:D:46:LYS:NZ	1:D:78:GLU:OE2	2.41	0.54
1:B:65:THR:HG22	1:B:78:GLU:HG2	1.90	0.53
1:B:145:SER:O	1:B:149:ARG:HB2	2.09	0.53
1:D:66:LEU:HD22	1:D:79:ALA:HB2	1.91	0.53
1:C:149:ARG:HG3	1:D:111:MET:HG2	1.89	0.53
1:A:48:LYS:HB3	1:A:63:TYR:HB2	1.91	0.52
1:D:161:HIS:O	1:D:165:LEU:HB2	2.10	0.52
1:A:201:VAL:O	1:A:205:ASN:ND2	2.43	0.51
1:B:130:PRO:HD2	1:B:133:PHE:HB2	1.92	0.51
1:C:23:LEU:HD22	1:C:81:VAL:HG21	1.92	0.51
1:A:117:LYS:HZ2	1:B:155:PRO:HB3	1.76	0.51
1:D:50:GLN:NE2	1:D:51:ILE:O	2.44	0.51
1:A:99:GLN:HG3	1:A:100:GLU:HG3	1.94	0.50
1:D:42:VAL:HG23	1:D:43:ARG:HG2	1.94	0.50
1:C:82:TRP:HB3	1:C:99:GLN:HE22	1.75	0.50
1:A:32:ASN:ND2	1:A:37:ALA:O	2.44	0.50
1:A:148:TYR:HH	1:A:224:THR:HG1	1.58	0.50
1:B:80:LYS:HB3	1:B:100:GLU:HB3	1.93	0.49
1:C:114:ASP:HB2	1:C:117:LYS:HB2	1.94	0.49
1:B:64:LEU:HB2	1:B:79:ALA:HB3	1.93	0.49
1:C:59:ASP:OD2	1:C:59:ASP:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LYS:HB2	1:B:63:TYR:HB2	1.95	0.49
1:D:14:ASN:N	1:D:49:GLU:OE2	2.45	0.48
1:D:81:VAL:HG11	1:D:96:LYS:HE2	1.95	0.47
1:D:194:PRO:O	1:D:197:ARG:NE	2.45	0.47
1:C:17:SER:OG	1:C:18:LEU:N	2.47	0.47
1:A:177:THR:HA	1:A:180:THR:HG22	1.97	0.47
1:B:119:PHE:HE1	1:B:160:PRO:HB2	1.79	0.46
1:D:92:LYS:HD3	1:D:92:LYS:HA	1.78	0.46
1:C:138:ARG:NH1	1:D:103:PRO:O	2.48	0.46
1:D:21:GLU:O	1:D:25:ARG:HB2	2.15	0.46
1:A:245:PRO:HA	1:A:248:ARG:HG2	1.99	0.45
1:C:170:LEU:HD13	1:D:115:PRO:HG3	1.98	0.45
1:C:173:GLY:HA2	1:D:107:ALA:HB1	1.99	0.45
1:D:46:LYS:HE2	1:D:48:LYS:HG3	1.99	0.45
1:C:161:HIS:O	1:C:165:LEU:HB2	2.17	0.45
1:A:50:GLN:O	1:A:61:MET:N	2.48	0.45
1:D:194:PRO:HB2	1:D:195:ALA:H	1.60	0.45
1:D:238:GLY:O	1:D:242:ARG:HG2	2.17	0.45
1:C:238:GLY:O	1:C:242:ARG:HG2	2.17	0.44
1:B:42:VAL:HG12	1:B:43:ARG:HB2	1.98	0.44
1:A:129:LEU:HD13	1:A:234:LEU:HD23	1.98	0.44
1:B:23:LEU:HD22	1:B:81:VAL:HG21	1.98	0.44
1:B:20:ILE:HA	1:B:23:LEU:HD12	1.98	0.44
1:C:182:VAL:HG11	1:C:200:VAL:HG11	2.00	0.44
1:D:47:ALA:HA	1:D:64:LEU:HA	1.99	0.44
1:C:59:ASP:HB2	1:C:82:TRP:HE1	1.83	0.43
1:B:92:LYS:HD3	1:B:92:LYS:HA	1.87	0.43
1:C:159:SER:OG	1:C:162:HIS:ND1	2.50	0.43
1:C:206:THR:OG1	1:C:207:ASN:ND2	2.51	0.43
1:B:159:SER:OG	1:B:162:HIS:ND1	2.46	0.43
1:C:40:GLU:O	1:C:69:LYS:N	2.51	0.43
1:A:206:THR:OG1	1:A:207:ASN:N	2.52	0.43
1:A:46:LYS:H	1:A:65:THR:HB	1.84	0.43
1:D:51:ILE:HG13	1:D:60:THR:HG22	2.00	0.43
1:D:35:GLU:HG3	1:D:37:ALA:HB2	2.01	0.43
1:C:129:LEU:HD22	1:C:237:PHE:HD2	1.83	0.42
1:A:198:ASP:HB3	1:A:199:LEU:H	1.62	0.42
1:B:102:LYS:HA	1:B:102:LYS:HD3	1.88	0.42
1:A:114:ASP:HB3	1:A:117:LYS:HB2	2.00	0.42
1:A:122:THR:HG23	1:A:125:LEU:H	1.84	0.42
1:B:30:GLU:HA	1:B:33:LYS:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:HIS:O	1:B:165:LEU:HB2	2.19	0.42
1:B:175:LEU:HD21	1:B:204:VAL:HB	2.02	0.42
1:B:73:LYS:HA	1:B:73:LYS:HD2	1.87	0.42
1:D:206:THR:OG1	1:D:207:ASN:ND2	2.52	0.41
1:A:59:ASP:OD2	1:A:59:ASP:N	2.53	0.41
1:A:158:CYS:HB2	1:A:162:HIS:CD2	2.55	0.41
1:D:29:ASP:HA	1:D:32:ASN:HD22	1.85	0.41
1:A:33:LYS:HA	1:A:33:LYS:HD3	1.94	0.41
1:D:141:LEU:HD23	1:D:141:LEU:HA	1.85	0.41
1:C:153:GLU:OE2	1:D:112:ASP:N	2.53	0.41
1:B:135:PRO:HG2	1:B:140:LEU:HG	2.02	0.40
1:C:118:GLU:H	1:C:118:GLU:HG2	1.59	0.40
1:B:132:ASP:OD1	1:B:132:ASP:N	2.52	0.40
1:D:39:LEU:HB3	1:D:68:ALA:HB1	2.03	0.40
1:A:151:ALA:O	1:A:166:ARG:NH1	2.48	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 PDB entries followed by that with respect to all EM entries.

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	215/300 (72%)	207 (96%)	8 (4%)	0	100	100
1	B	217/300 (72%)	203 (94%)	14 (6%)	0	100	100
1	C	214/300 (71%)	206 (96%)	8 (4%)	0	100	100
1	D	218/300 (73%)	209 (96%)	9 (4%)	0	100	100
All	All	864/1200 (72%)	825 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	194/258 (75%)	194 (100%)	0	100 100
1	B	195/258 (76%)	195 (100%)	0	100 100
1	C	193/258 (75%)	192 (100%)	1 (0%)	86 91
1	D	196/258 (76%)	196 (100%)	0	100 100
All	All	778/1032 (75%)	777 (100%)	1 (0%)	92 96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	116	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	50	GLN
1	A	205	ASN
1	B	31	HIS
1	B	167	GLN
1	B	184	ASN
1	C	99	GLN
1	C	161	HIS
1	C	202	ASN
1	C	207	ASN
1	D	167	GLN
1	D	207	ASN
1	D	219	HIS

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 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.