



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:29 pm GMT

PDB ID : 5G4F
EMDB ID: : EMD-3436
Title : Structure of the ADP-bound VAT complex
Authors : Huang, R.; Ripstein, Z.A.; Augustyniak, R.; Lazniewski, M.; Ginalski, K.;
Kay, L.E.; Rubinstein, J.L.
Deposited on : 2016-05-12
Resolution : 7.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

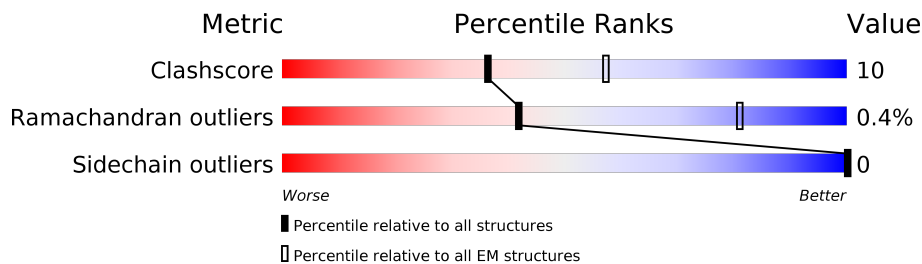
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.00 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	726	76% 23%
1	B	726	79% 20% .
1	C	726	77% 23% .
1	D	726	76% 24%
1	E	726	78% 21%
1	P	726	77% 22% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 69210 atoms, of which 35130 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.

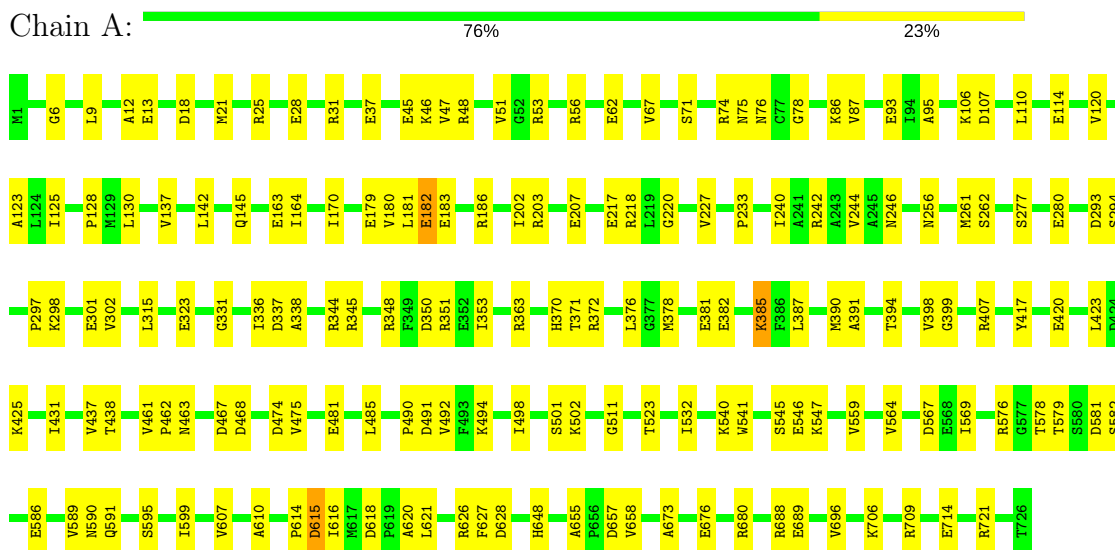
- Molecule 1 is a protein called VCP-LIKE ATPASE.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	726	Total 11535	C 3573	H 5855	N 997	O 1089	S 21	0	0
1	B	726	Total 11535	C 3573	H 5855	N 997	O 1089	S 21	0	0
1	C	726	Total 11535	C 3573	H 5855	N 997	O 1089	S 21	0	0
1	D	726	Total 11535	C 3573	H 5855	N 997	O 1089	S 21	0	0
1	E	726	Total 11535	C 3573	H 5855	N 997	O 1089	S 21	0	0
1	P	726	Total 11535	C 3573	H 5855	N 997	O 1089	S 21	0	0

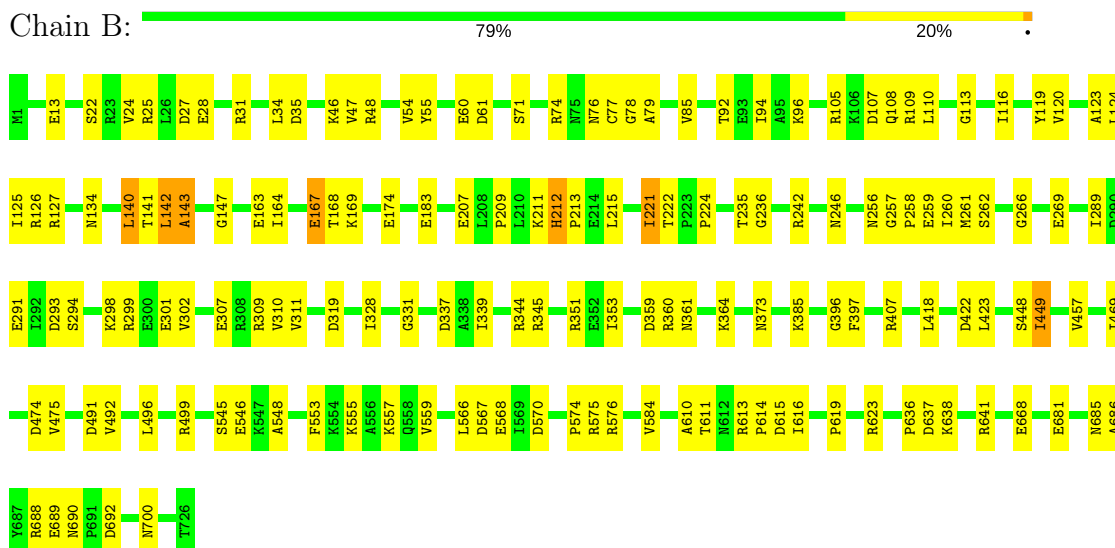
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: VCP-LIKE ATPASE

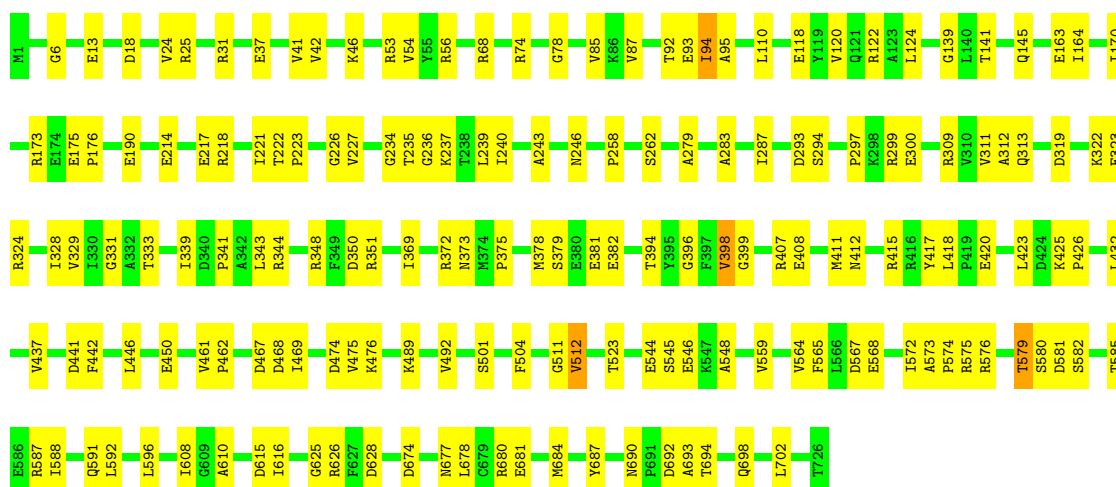


• Molecule 1: VCP-LIKE ATPASE



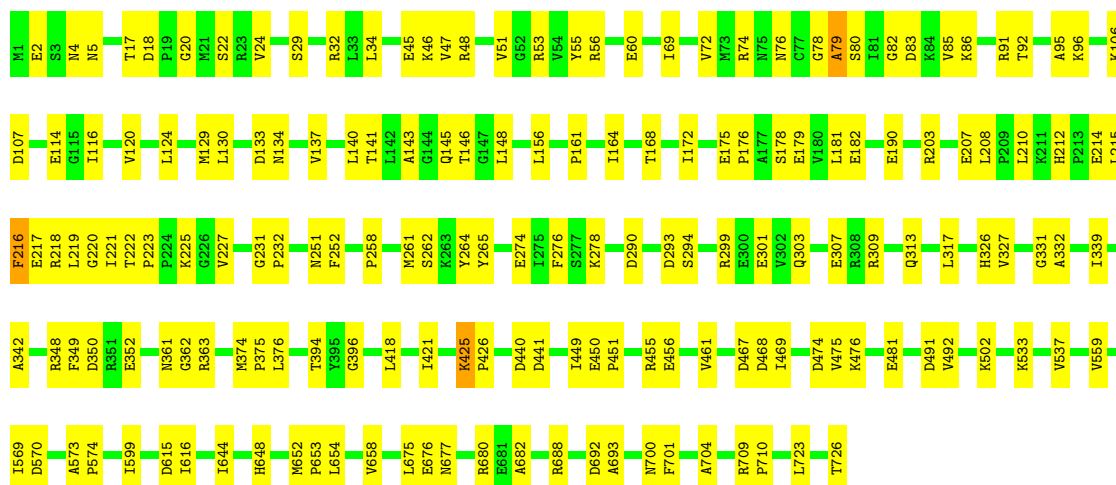
• Molecule 1: VCP-LIKE ATPASE





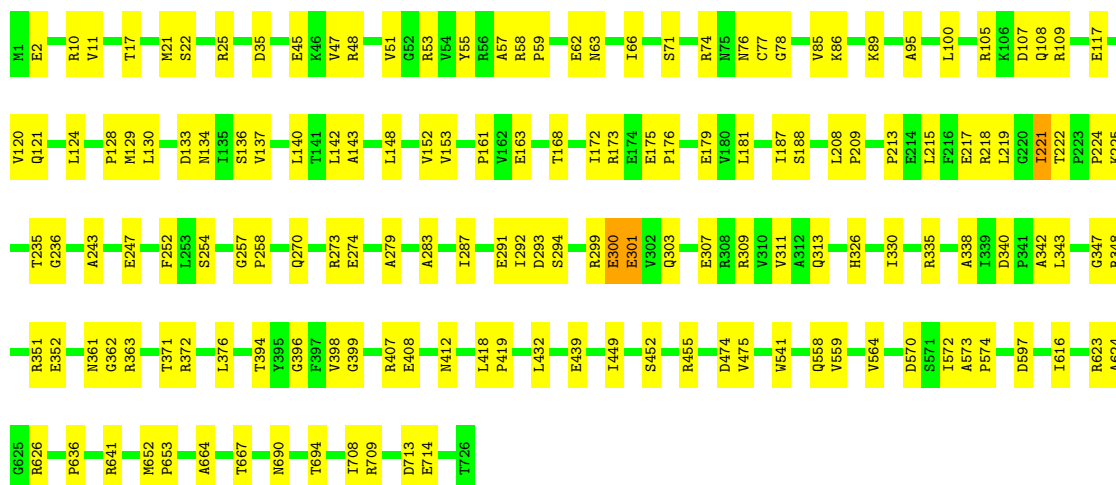
• Molecule 1: VCP-LIKE ATPASE

Chain D: 76% 24%

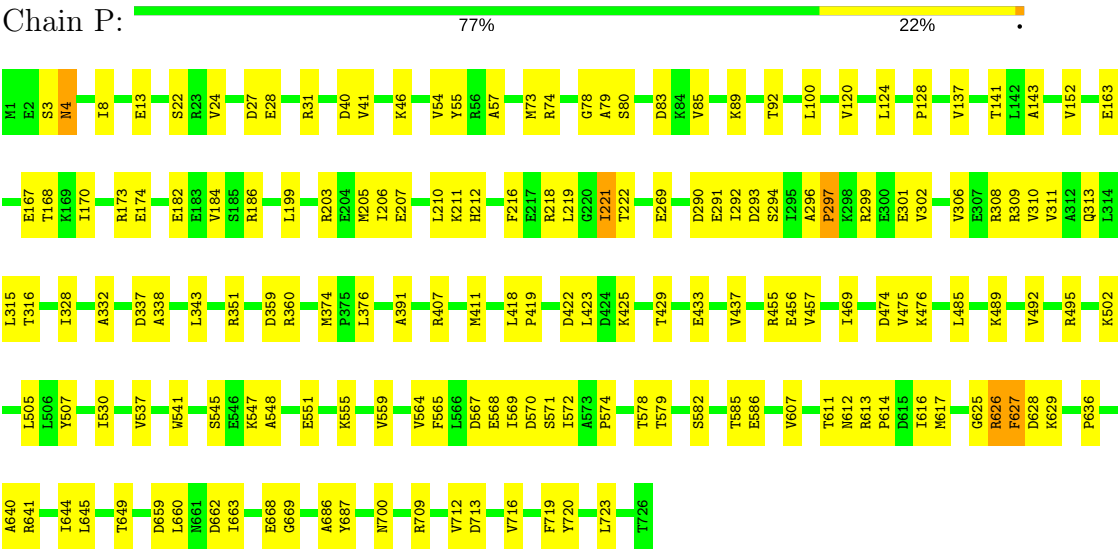


• Molecule 1: VCP-LIKE ATPASE

Chain E: 78% 21%



● Molecule 1: VCP-LIKE ATPASE



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH MICROGRAPH	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	34483	Depositor
Image detector	GATAN K2 SUMMIT (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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.25	0/5763	0.44	0/7778
1	B	0.28	1/5763 (0.0%)	0.45	1/7778 (0.0%)
1	C	0.24	0/5763	0.43	0/7778
1	D	0.24	0/5763	0.45	0/7778
1	E	0.24	0/5763	0.44	0/7778
1	P	0.25	0/5763	0.43	0/7778
All	All	0.25	1/34578 (0.0%)	0.44	1/46668 (0.0%)

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	4
1	B	0	3
1	C	0	4
1	D	0	2
1	E	0	2
1	P	0	4
All	All	0	19

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	613	ARG	C-N	10.34	1.53	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	LEU	CA-CB-CG	5.96	129.00	115.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	GLU	Peptide
1	A	298	LYS	Peptide
1	A	385	LYS	Peptide
1	A	463	ASN	Peptide
1	B	142	LEU	Peptide

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	5680	5855	5855	111	0
1	B	5680	5855	5855	116	0
1	C	5680	5855	5855	113	0
1	D	5680	5855	5855	131	0
1	E	5680	5855	5855	108	0
1	P	5680	5855	5855	123	0
All	All	34080	35130	35130	664	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 10.

The worst 5 of 664 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:D:107:ASP:OD1	1:E:218:ARG:NH2	2.02	0.93
1:E:55:TYR:OH	1:E:163:GLU:OE2	1.88	0.89
1:E:221:ILE:HG22	1:E:222:THR:H	1.37	0.88
1:E:120:VAL:O	1:E:124:LEU:N	2.06	0.88
1:P:570:ASP:OD2	1:P:611:THR:OG1	1.89	0.88

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 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	724/726 (100%)	662 (91%)	58 (8%)	4 (1%)	28	71
1	B	724/726 (100%)	662 (91%)	58 (8%)	4 (1%)	28	71
1	C	724/726 (100%)	662 (91%)	58 (8%)	4 (1%)	28	71
1	D	724/726 (100%)	661 (91%)	60 (8%)	3 (0%)	38	77
1	E	724/726 (100%)	677 (94%)	45 (6%)	2 (0%)	44	81
1	P	724/726 (100%)	663 (92%)	59 (8%)	2 (0%)	44	81
All	All	4344/4356 (100%)	3987 (92%)	338 (8%)	19 (0%)	42	77

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	221	ILE
1	E	301	GLU
1	B	221	ILE
1	C	221	ILE
1	C	512	VAL

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 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	626/626 (100%)	626 (100%)	0	100	100
1	B	626/626 (100%)	626 (100%)	0	100	100
1	C	626/626 (100%)	626 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	626/626 (100%)	626 (100%)	0	100	100
1	E	626/626 (100%)	626 (100%)	0	100	100
1	P	626/626 (100%)	626 (100%)	0	100	100
All	All	3756/3756 (100%)	3756 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	212	HIS
1	E	303	GLN
1	P	412	ASN
1	E	145	GLN
1	P	590	ASN

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 ⓘ

There are no chain breaks in this entry.