



wwPDB EM Validation Summary Report ⓘ

Jan 26, 2025 – 12:06 AM JST

PDB ID : 8Y1L
EMDB ID : EMD-38839
Title : Cryo-EM structure of human N-terminally bound ATG9A-ATG2A-WIPI4 complex
Authors : Wang, Y.; Stjepanovic, G.
Deposited on : 2024-01-25
Resolution : 7.05 Å(reported)

This is a wwPDB EM Validation Summary 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) : 2.40

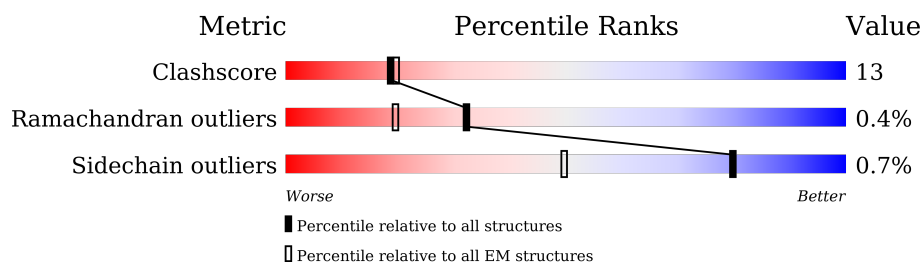
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.05 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	C	839	47% 9% 43%
1	D	839	48% 9% 43%
1	E	839	47% 9% 43%
2	A	360	99% .
3	B	1938	35% 8% 57%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15687 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 Autophagy-related protein 9A.

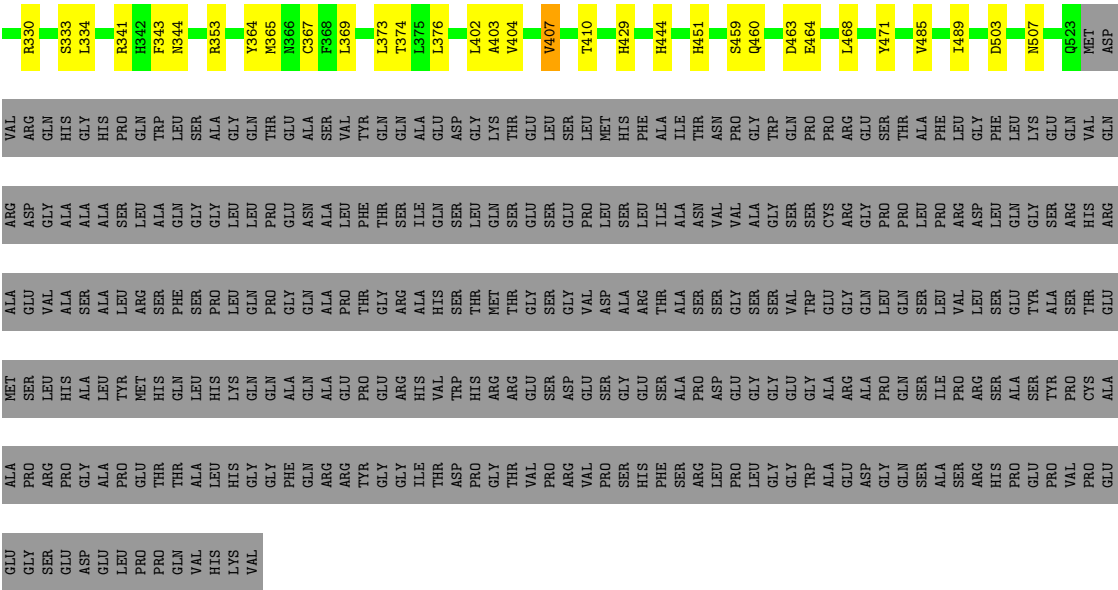
Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	475	Total	C	N	O	S	0	0
			2998	1891	559	543	5		
1	D	475	Total	C	N	O	S	0	0
			2926	1843	548	532	3		
1	E	475	Total	C	N	O	S	0	0
			2936	1858	538	535	5		

- Molecule 2 is a protein called WD repeat domain phosphoinositide-interacting protein 4.

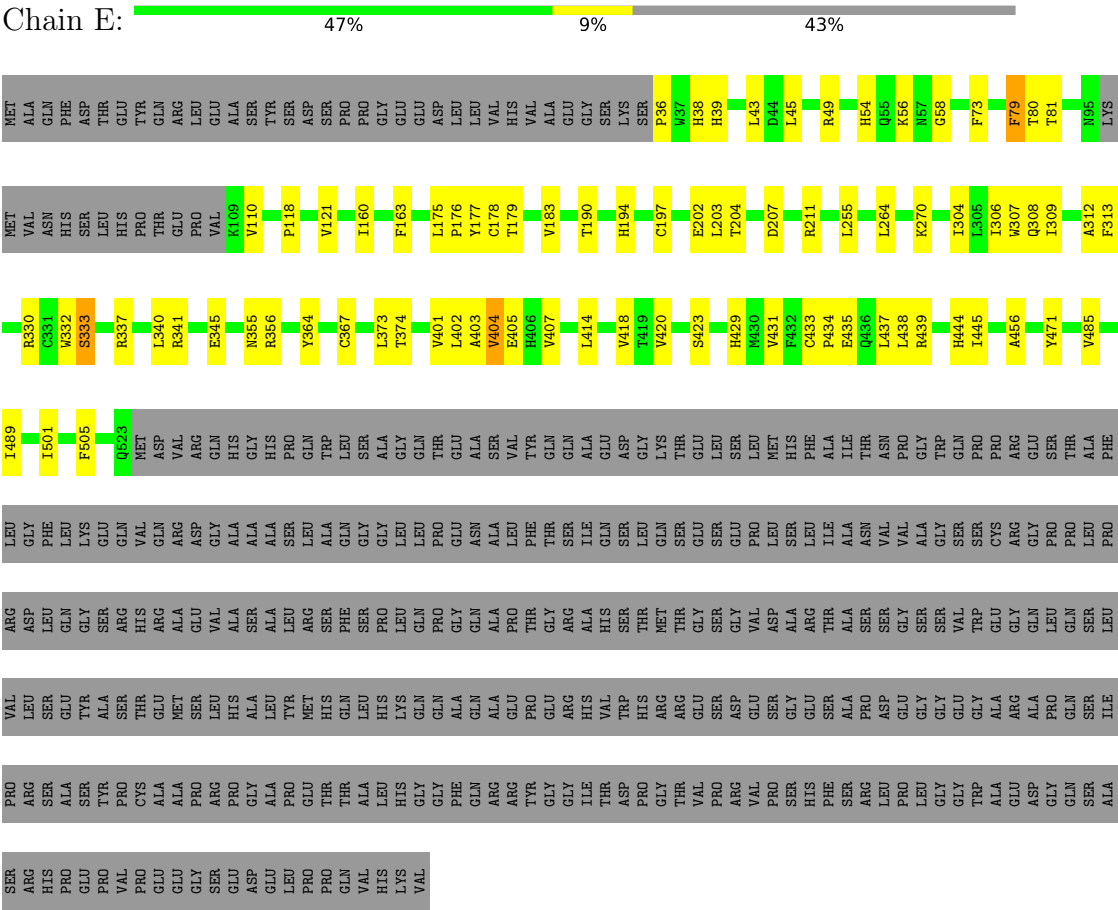
Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	360	Total	C	N	O	0	0
			1777	1057	360	360		

- Molecule 3 is a protein called Autophagy-related protein 2 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	830	Total	C	N	O	S	0	0
			5050	3121	934	980	15		



• Molecule 1: Autophagy-related protein 9A



• Molecule 2: WD repeat domain phosphoinositide-interacting protein 4







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232894	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 ($e^-/\text{\AA}^2$)	51.46	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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	C	0.50	0/3061	0.63	3/4225 (0.1%)
1	D	0.48	0/2983	0.63	2/4119 (0.0%)
1	E	0.50	0/3005	0.65	3/4157 (0.1%)
2	A	0.35	0/1776	0.73	0/2471
3	B	0.26	0/5077	0.56	1/6963 (0.0%)
All	All	0.42	0/15902	0.62	9/21935 (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	D	0	1
2	A	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	LEU	N-CA-C	7.26	130.61	111.00
1	D	367	CYS	N-CA-C	7.05	130.04	111.00
1	C	404	VAL	N-CA-C	-7.03	92.02	111.00
1	C	465	PHE	N-CA-C	-5.63	95.80	111.00
1	E	404	VAL	N-CA-C	-5.56	96.00	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	359	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	D	308	GLN	Mainchain

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	C	2998	0	2145	91	0
1	D	2926	0	2016	56	0
1	E	2936	0	1987	86	0
2	A	1777	0	789	2	0
3	B	5050	0	3675	110	0
All	All	15687	0	10612	335	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 13.

The worst 5 of 335 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:E:340:LEU:HD22	1:E:445:ILE:CG2	1.67	1.23
1:E:364:TYR:CE1	1:E:438:LEU:HD21	1.83	1.13
1:C:368:PHE:CZ	1:C:433:CYS:HB3	1.92	1.05
1:E:45:LEU:HD23	1:E:45:LEU:O	1.63	0.97
1:C:438:LEU:HD12	1:C:456:ALA:CB	1.95	0.97

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	C	471/839 (56%)	437 (93%)	33 (7%)	1 (0%)	44	78
1	D	471/839 (56%)	431 (92%)	38 (8%)	2 (0%)	30	68
1	E	471/839 (56%)	432 (92%)	37 (8%)	2 (0%)	30	68
2	A	358/360 (99%)	345 (96%)	11 (3%)	2 (1%)	22	60
3	B	776/1938 (40%)	677 (87%)	96 (12%)	3 (0%)	30	68
All	All	2547/4815 (53%)	2322 (91%)	215 (8%)	10 (0%)	32	68

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	282	LYS
3	B	673	LEU
1	D	407	VAL
1	D	179	THR
3	B	602	ARG

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	C	165/717 (23%)	164 (99%)	1 (1%)	84	88
1	D	142/717 (20%)	140 (99%)	2 (1%)	62	75
1	E	147/717 (20%)	146 (99%)	1 (1%)	81	87
3	B	304/1662 (18%)	303 (100%)	1 (0%)	91	92
All	All	758/3813 (20%)	753 (99%)	5 (1%)	80	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	469	PHE
1	D	313	PHE
1	D	341	ARG

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Mol	Chain	Res	Type
1	E	79	PHE
3	B	1103	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	217	ASN
1	D	366	ASN
3	B	802	GLN
1	E	342	HIS
1	E	406	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.