



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 05:30 AM UTC

PDB ID : 6WUL / pdb_00006wul
EMDB ID : EMD-21915
Title : Mitochondrial SAM complex - dimer 1 in detergent
Authors : Ni, X.; Botos, I.; Diederichs, K.
Deposited on : 2020-05-04
Resolution : 3.20 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 : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

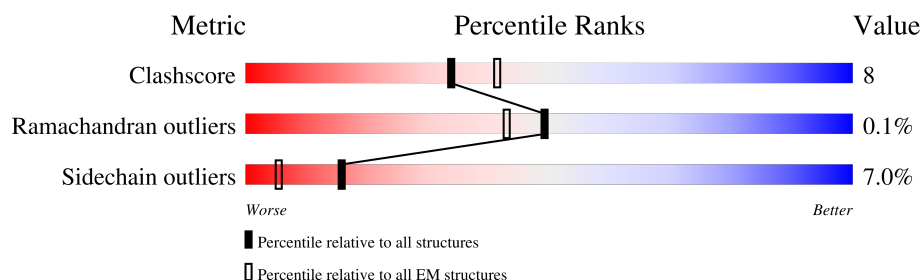
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	A	332	66% 21% • 11%
1	D	332	66% 20% • 11%
2	B	512	67% 18% • 13%
2	E	512	66% 19% • 13%
3	C	479	56% 16% • 28%
3	F	479	55% 16% • 28%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16386 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 Sam35.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	295	Total	C	N	O	S	0	0
			2284	1440	405	433	6		
1	D	295	Total	C	N	O	S	0	0
			2284	1440	405	433	6		

- Molecule 2 is a protein called Bac_surface_Ag domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	443	Total	C	N	O	S	0	0
			3295	2072	594	627	2		
2	E	443	Total	C	N	O	S	0	0
			3295	2072	594	627	2		

- Molecule 3 is a protein called Tom37 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	346	Total	C	N	O	S	0	0
			2614	1688	461	458	7		
3	F	346	Total	C	N	O	S	0	0
			2614	1688	461	458	7		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-34	MET	-	expression tag	UNP G2Q6R7
C	-33	SER	-	expression tag	UNP G2Q6R7
C	-32	SER	-	expression tag	UNP G2Q6R7
C	-31	ALA	-	expression tag	UNP G2Q6R7
C	-30	TRP	-	expression tag	UNP G2Q6R7
C	-29	SER	-	expression tag	UNP G2Q6R7
C	-28	HIS	-	expression tag	UNP G2Q6R7
C	-27	PRO	-	expression tag	UNP G2Q6R7
C	-26	GLN	-	expression tag	UNP G2Q6R7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-25	PHE	-	expression tag	UNP G2Q6R7
C	-24	GLU	-	expression tag	UNP G2Q6R7
C	-23	LYS	-	expression tag	UNP G2Q6R7
C	-21	GLY	-	expression tag	UNP G2Q6R7
C	-20	GLY	-	expression tag	UNP G2Q6R7
C	-19	GLY	-	expression tag	UNP G2Q6R7
C	-18	SER	-	expression tag	UNP G2Q6R7
C	-17	GLY	-	expression tag	UNP G2Q6R7
C	-16	GLY	-	expression tag	UNP G2Q6R7
C	-15	GLY	-	expression tag	UNP G2Q6R7
C	-14	SER	-	expression tag	UNP G2Q6R7
C	-13	GLY	-	expression tag	UNP G2Q6R7
C	-12	GLY	-	expression tag	UNP G2Q6R7
C	-11	SER	-	expression tag	UNP G2Q6R7
C	-10	ALA	-	expression tag	UNP G2Q6R7
C	-9	TRP	-	expression tag	UNP G2Q6R7
C	-8	SER	-	expression tag	UNP G2Q6R7
C	-7	HIS	-	expression tag	UNP G2Q6R7
C	-6	PRO	-	expression tag	UNP G2Q6R7
C	-5	GLN	-	expression tag	UNP G2Q6R7
C	-4	PHE	-	expression tag	UNP G2Q6R7
C	-3	GLU	-	expression tag	UNP G2Q6R7
C	-2	LYS	-	expression tag	UNP G2Q6R7
C	-1	GLY	-	expression tag	UNP G2Q6R7
C	0	GLY	-	expression tag	UNP G2Q6R7
F	-34	MET	-	expression tag	UNP G2Q6R7
F	-33	SER	-	expression tag	UNP G2Q6R7
F	-32	SER	-	expression tag	UNP G2Q6R7
F	-31	ALA	-	expression tag	UNP G2Q6R7
F	-30	TRP	-	expression tag	UNP G2Q6R7
F	-29	SER	-	expression tag	UNP G2Q6R7
F	-28	HIS	-	expression tag	UNP G2Q6R7
F	-27	PRO	-	expression tag	UNP G2Q6R7
F	-26	GLN	-	expression tag	UNP G2Q6R7
F	-25	PHE	-	expression tag	UNP G2Q6R7
F	-24	GLU	-	expression tag	UNP G2Q6R7
F	-23	LYS	-	expression tag	UNP G2Q6R7
F	-21	GLY	-	expression tag	UNP G2Q6R7
F	-20	GLY	-	expression tag	UNP G2Q6R7
F	-19	GLY	-	expression tag	UNP G2Q6R7
F	-18	SER	-	expression tag	UNP G2Q6R7
F	-17	GLY	-	expression tag	UNP G2Q6R7

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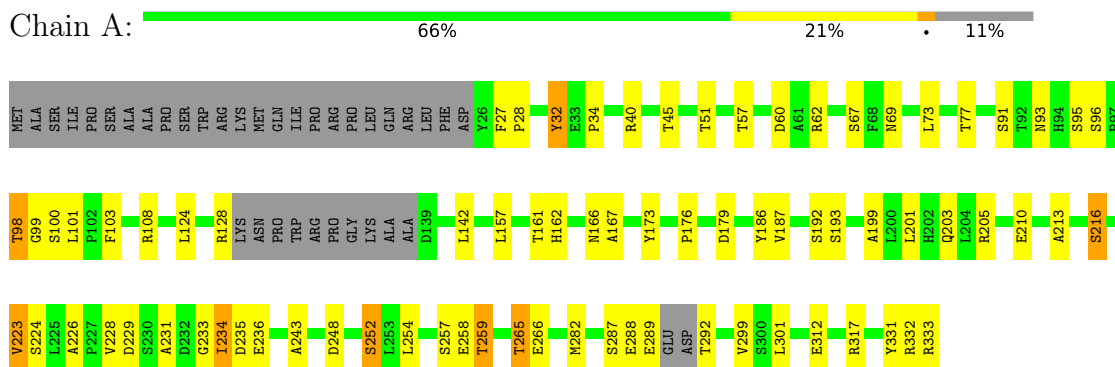
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-16	GLY	-	expression tag	UNP G2Q6R7
F	-15	GLY	-	expression tag	UNP G2Q6R7
F	-14	SER	-	expression tag	UNP G2Q6R7
F	-13	GLY	-	expression tag	UNP G2Q6R7
F	-12	GLY	-	expression tag	UNP G2Q6R7
F	-11	SER	-	expression tag	UNP G2Q6R7
F	-10	ALA	-	expression tag	UNP G2Q6R7
F	-9	TRP	-	expression tag	UNP G2Q6R7
F	-8	SER	-	expression tag	UNP G2Q6R7
F	-7	HIS	-	expression tag	UNP G2Q6R7
F	-6	PRO	-	expression tag	UNP G2Q6R7
F	-5	GLN	-	expression tag	UNP G2Q6R7
F	-4	PHE	-	expression tag	UNP G2Q6R7
F	-3	GLU	-	expression tag	UNP G2Q6R7
F	-2	LYS	-	expression tag	UNP G2Q6R7
F	-1	GLY	-	expression tag	UNP G2Q6R7
F	0	GLY	-	expression tag	UNP G2Q6R7

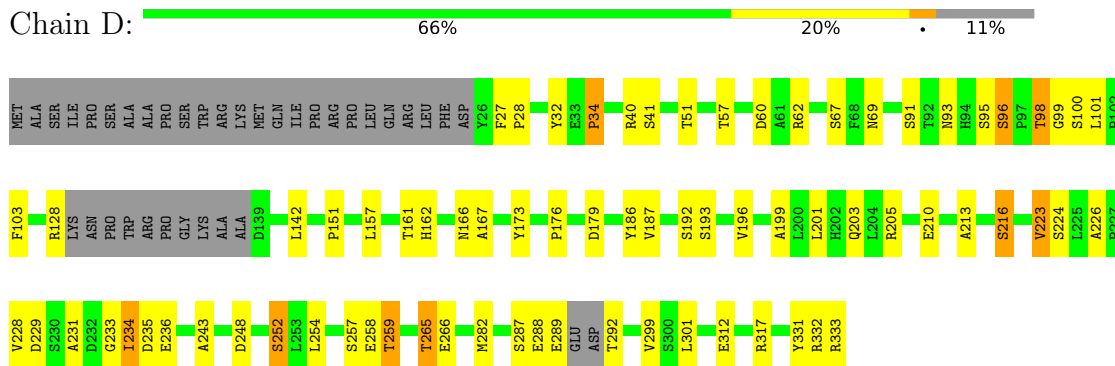
3 Residue-property plots

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.

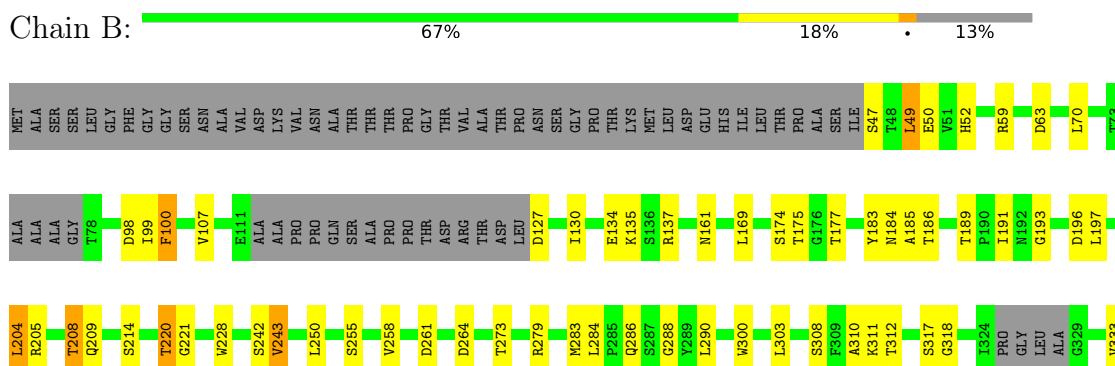
- Molecule 1: Sam35



- Molecule 1: Sam35



- Molecule 2: Bac_surface_Ag domain-containing protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	117339	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	69	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k 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	A	0.23	0/2339	0.46	1/3185 (0.0%)
1	D	0.23	0/2339	0.46	1/3185 (0.0%)
2	B	0.25	0/3355	0.53	2/4546 (0.0%)
2	E	0.25	0/3355	0.53	2/4546 (0.0%)
3	C	0.23	0/2688	0.47	0/3673
3	F	0.23	0/2688	0.47	0/3673
All	All	0.24	0/16764	0.49	6/22808 (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	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	193	GLY	CA-C-N	6.07	130.04	121.61
2	B	193	GLY	C-N-CA	6.07	130.04	121.61
2	E	193	GLY	CA-C-N	6.04	130.01	121.61
2	E	193	GLY	C-N-CA	6.04	130.01	121.61
1	D	32	TYR	N-CA-C	5.35	116.86	110.44

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	PRO	Peptide
1	D	34	PRO	Peptide

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	2284	0	2241	46	0
1	D	2284	0	2241	44	0
2	B	3295	0	3311	55	0
2	E	3295	0	3311	58	0
3	C	2614	0	2621	44	0
3	F	2614	0	2621	46	0
All	All	16386	0	16346	269	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 8.

The worst 5 of 269 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)
3:C:11:ALA:HB1	3:C:145:ALA:HB1	1.66	0.77
3:F:11:ALA:HB1	3:F:145:ALA:HB1	1.66	0.76
1:A:162:HIS:O	1:A:166:ASN:ND2	2.21	0.74
1:D:162:HIS:O	1:D:166:ASN:ND2	2.21	0.73
1:A:259:THR:O	1:A:259:THR:OG1	2.10	0.69

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	289/332 (87%)	251 (87%)	38 (13%)	0	100	100
1	D	289/332 (87%)	251 (87%)	38 (13%)	0	100	100
2	B	435/512 (85%)	376 (86%)	59 (14%)	0	100	100
2	E	435/512 (85%)	376 (86%)	59 (14%)	0	100	100
3	C	338/479 (71%)	299 (88%)	38 (11%)	1 (0%)	36	68
3	F	338/479 (71%)	299 (88%)	38 (11%)	1 (0%)	36	68
All	All	2124/2646 (80%)	1852 (87%)	270 (13%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	19	ALA
3	F	19	ALA

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	241/272 (89%)	225 (93%)	16 (7%)	15	47
1	D	241/272 (89%)	225 (93%)	16 (7%)	15	47
2	B	344/394 (87%)	314 (91%)	30 (9%)	9	36
2	E	344/394 (87%)	314 (91%)	30 (9%)	9	36
3	C	258/337 (77%)	245 (95%)	13 (5%)	22	55
3	F	258/337 (77%)	245 (95%)	13 (5%)	22	55
All	All	1686/2006 (84%)	1568 (93%)	118 (7%)	16	45

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	390	LEU

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Mol	Chain	Res	Type
3	F	109	THR
1	D	265	THR
3	F	52	LEU
2	E	446	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	310	ASN
2	E	385	HIS
3	F	137	ASN
2	E	423	ASN
2	E	286	GLN

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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21915. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.