wwPDB EM Map/Model Validation Report (i)

Jul 3, 2016 – 05:07 AM EDT

PDB ID	:	5JM9
EMDB ID:	:	EMD-8167
Title	:	Structure of S. cerevesiae mApe1 dodecamer
Authors	:	Sachse, C.; Bertipaglia, C.
Deposited on	:	2016-04-28
Resolution	:	24.00 Å(reported)
Based on PDB ID	:	4R8F

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

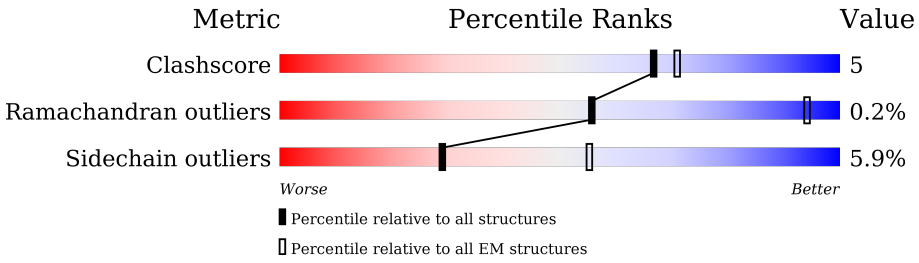
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 24.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	514	75% 10% • 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3418 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 Vacuolar aminopeptidase 1.

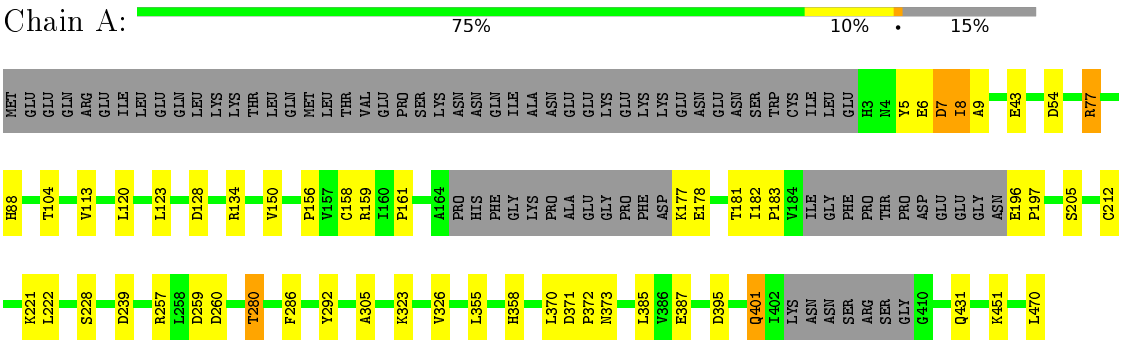
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	438	3418	2188	577	645	8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Vacuolar aminopeptidase 1

Chain A:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	5481	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI/PHILIPS CM12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	53000	Depositor
Image detector	Not provided	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	0.31	0/3493	0.59	0/4729

There are no bond length outliers.

There are no bond angle outliers.

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	3418	0	3387	33	0
All	All	3418	0	3387	33	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 5.

All (33) 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:7:ASP:HA	1:A:9:ALA:H	1.49	0.77
1:A:6:GLU:C	1:A:8:ILE:HG22	2.08	0.73
1:A:7:ASP:OD1	1:A:7:ASP:N	2.28	0.65
1:A:239:ASP:O	1:A:257:ARG:NH2	2.32	0.63
1:A:158:CYS:SG	1:A:182:ILE:HG21	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASP:HA	1:A:9:ALA:N	2.18	0.59
1:A:77:ARG:HH11	1:A:77:ARG:HG2	1.68	0.59
1:A:54:ASP:O	1:A:280:THR:HG23	2.06	0.54
1:A:181:THR:HA	1:A:182:ILE:HD12	1.91	0.53
1:A:6:GLU:C	1:A:7:ASP:OD1	2.49	0.51
1:A:161:PRO:HD3	1:A:183:PRO:HD2	1.93	0.51
1:A:181:THR:HG22	1:A:182:ILE:H	1.74	0.50
1:A:113:VAL:HG21	1:A:182:ILE:HD11	1.93	0.50
1:A:158:CYS:HB2	1:A:182:ILE:CG2	2.41	0.50
1:A:358:HIS:HB3	1:A:401:GLN:H	1.77	0.49
1:A:7:ASP:CA	1:A:9:ALA:H	2.24	0.49
1:A:196:GLU:HB3	1:A:197:PRO:HD3	1.96	0.48
1:A:395:ASP:OD1	1:A:451:LYS:HE3	2.14	0.47
1:A:259:ASP:HA	1:A:260:ASP:HA	1.72	0.47
1:A:358:HIS:ND1	1:A:401:GLN:HB2	2.30	0.47
1:A:355:LEU:CD2	1:A:358:HIS:CD2	3.00	0.45
1:A:370:LEU:O	1:A:401:GLN:HA	2.18	0.44
1:A:158:CYS:HB2	1:A:182:ILE:HG22	1.99	0.43
1:A:113:VAL:CG2	1:A:182:ILE:HD11	2.48	0.43
1:A:7:ASP:N	1:A:8:ILE:HG22	2.34	0.43
1:A:371:ASP:OD1	1:A:372:PRO:HD2	2.19	0.42
1:A:371:ASP:CG	1:A:373:ASN:O	2.58	0.41
1:A:128:ASP:HB3	1:A:156:PRO:HB3	2.02	0.41
1:A:150:VAL:HG22	1:A:222:LEU:HB2	2.03	0.41
1:A:77:ARG:NH1	1:A:77:ARG:HG2	2.35	0.41
1:A:292:TYR:CE1	1:A:305:ALA:HA	2.56	0.40
1:A:88:HIS:NE2	1:A:260:ASP:HB2	2.35	0.40
1:A:205:SER:HB2	1:A:228:SER:HA	2.04	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	430/514 (84%)	424 (99%)	5 (1%)	1 (0%)	52 86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ILE

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	370/439 (84%)	348 (94%)	22 (6%)	24 61

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	7	ASP
1	A	43	GLU
1	A	77	ARG
1	A	104	THR
1	A	120	LEU
1	A	123	LEU
1	A	134	ARG
1	A	159	ARG
1	A	177	LYS
1	A	178	GLU
1	A	212	CYS
1	A	221	LYS
1	A	280	THR
1	A	286	PHE
1	A	323	LYS
1	A	326	VAL
1	A	385	LEU
1	A	387	GLU
1	A	401	GLN

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Mol	Chain	Res	Type
1	A	431	GLN
1	A	470	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.