



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:40 PM BST

PDB ID : 2C9G
EMDB ID: : EMD-1178
Title : THE QUASI-ATOMIC MODEL OF THE ADENOVIRUS TYPE 3 PENTON
BASE DODECAHEDRON
Authors : Fuschiotti, P.; Schoehn, G.; Fender, P.; Fabry, C.M.S.; Hewat, E.A.;
Chroboczek, J.; Ruigrok, R.W.H.; Conway, J.F.
Deposited on : 2005-12-12
Resolution : 9.30 Å(reported)

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) : trunk27241

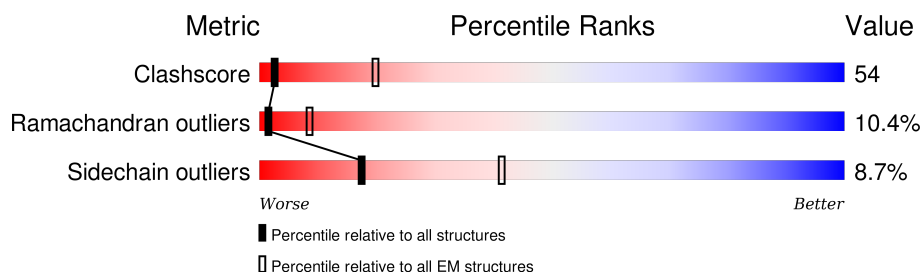
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.30 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	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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	523	 30% 44% 11% • 14%
1	B	523	 29% 45% 11% • 14%
1	C	523	 30% 45% 11% • 14%
1	D	523	 29% 45% 11% • 14%
1	E	523	 29% 46% 11% • 14%

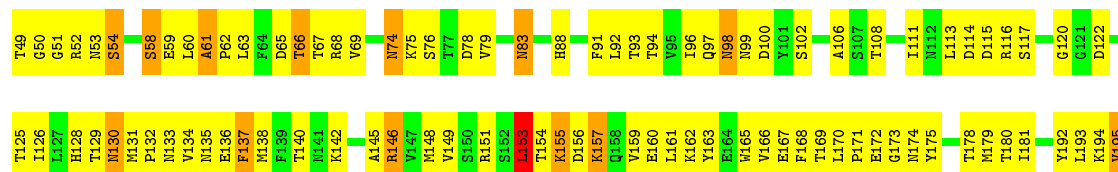
2 Entry composition

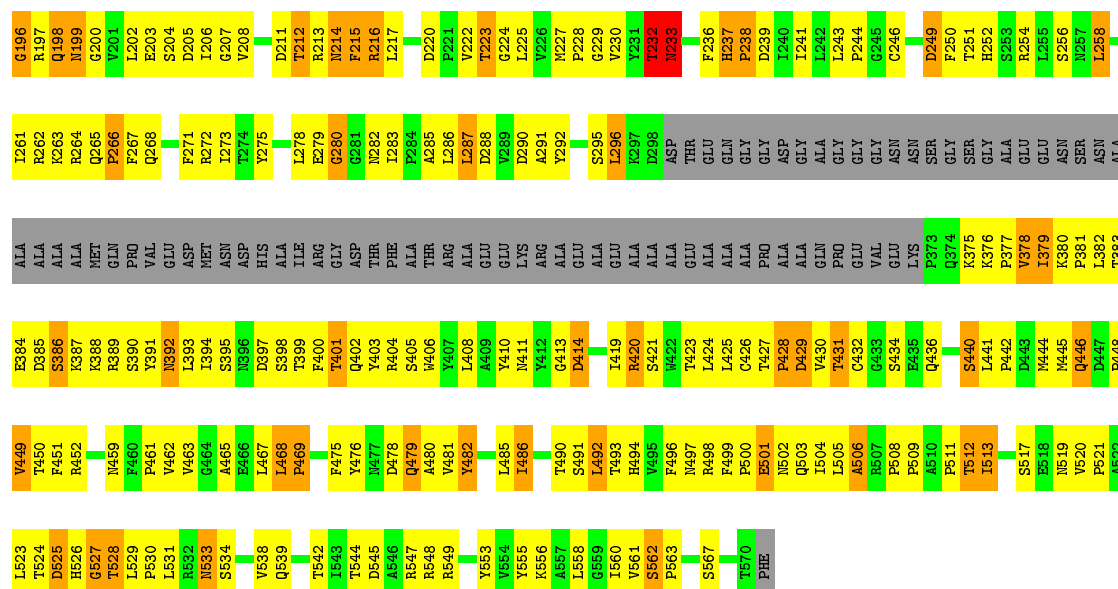
There is only 1 type of molecule in this entry. The entry contains 17840 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

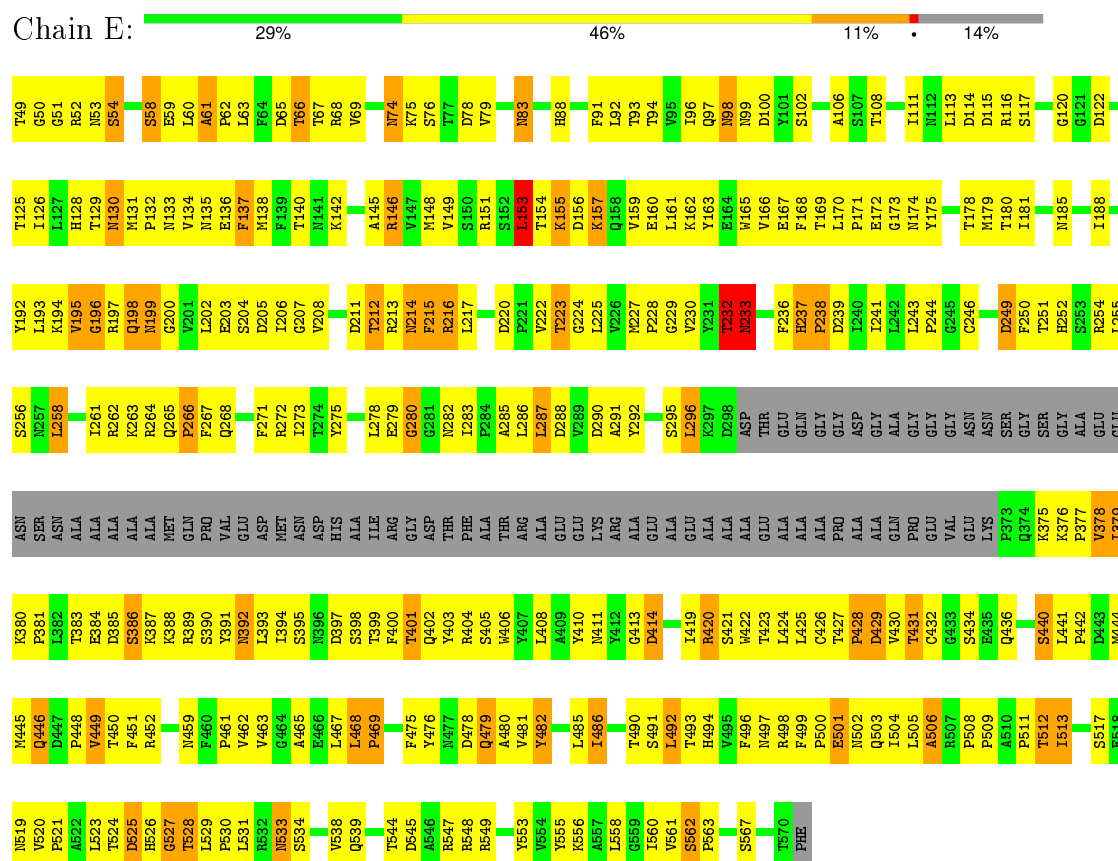
- Molecule 1 is a protein called PENTON PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	B	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	C	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	D	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	E	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		





● Molecule 1: PENTON PROTEIN



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	AMPLITUDE, PHASE	Depositor
Microscope	JEOL 2010F	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.57	0/3652	0.81	2/4971 (0.0%)
1	B	0.57	0/3652	0.81	2/4971 (0.0%)
1	C	0.57	0/3652	0.81	2/4971 (0.0%)
1	D	0.57	0/3652	0.81	2/4971 (0.0%)
1	E	0.57	0/3652	0.81	2/4971 (0.0%)
All	All	0.57	0/18260	0.81	10/24855 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	207	GLY	N-CA-C	5.62	127.14	113.10
1	D	207	GLY	N-CA-C	5.60	127.10	113.10
1	A	207	GLY	N-CA-C	5.58	127.06	113.10
1	C	207	GLY	N-CA-C	5.58	127.06	113.10
1	B	207	GLY	N-CA-C	5.58	127.06	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3568	0	3498	414	0
1	B	3568	0	3498	421	0
1	C	3568	0	3498	421	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3568	0	3498	424	0
1	E	3568	0	3498	422	0
All	All	17840	0	17490	1895	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 54.

The worst 5 of 1895 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:B:452:ARG:HH21	1:C:99:ASN:HB3	1.14	1.13
1:C:452:ARG:HH21	1:D:99:ASN:HB3	1.14	1.11
1:D:452:ARG:HH21	1:E:99:ASN:HB3	1.14	1.10
1:A:99:ASN:HB3	1:E:452:ARG:HH21	1.14	1.07
1:A:452:ARG:HH21	1:B:99:ASN:HB3	1.14	1.06

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	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	1	12
1	B	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	1	12
1	C	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	1	12
1	D	444/523 (85%)	323 (73%)	75 (17%)	46 (10%)	1	12
1	E	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	1	12
All	All	2220/2615 (85%)	1619 (73%)	371 (17%)	230 (10%)	1	12

5 of 230 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	59	GLU
1	A	130	ASN
1	A	137	PHE
1	A	296	LEU

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	404/451 (90%)	369 (91%)	35 (9%)	13	45
1	B	404/451 (90%)	369 (91%)	35 (9%)	13	45
1	C	404/451 (90%)	369 (91%)	35 (9%)	13	45
1	D	404/451 (90%)	369 (91%)	35 (9%)	13	45
1	E	404/451 (90%)	369 (91%)	35 (9%)	13	45
All	All	2020/2255 (90%)	1845 (91%)	175 (9%)	17	45

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	214	ASN
1	C	501	GLU
1	E	429	ASP
1	C	232	THR
1	C	287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	99	ASN
1	C	459	ASN
1	E	265	GLN
1	C	128	HIS
1	C	214	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 [i](#)

There are no chain breaks in this entry.