



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:41 PM GMT

PDB ID : 4CWU
Title : CRYSTAL STRUCTURE DERIVED MODELS OF ADENOVIRUS CE-
MENT PROTEINS AT 3.8Å
Authors : Reddy, V.S.; Nemerow, G.R.
Deposited on : 2014-04-03
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **NOT EXECUTED**
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **FAILED**
EDS : **NOT EXECUTED**
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-20026919

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

There are no percentiles available for this entry.

MolProbity and EDS were not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 98419 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 HEXON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	B	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	C	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	D	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	E	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	F	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	G	918	Total	C	N	O	S	0	0	0
			7352	4673	1244	1399	36			
1	H	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	I	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	J	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	K	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			
1	L	913	Total	C	N	O	S	0	0	0
			7320	4656	1238	1390	36			

- Molecule 2 is a protein called PENTON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	440	Total	C	N	O	S	0	0	0
			3524	2230	611	671	12			

- Molecule 3 is a protein called PRE-CAPSID VERTEX PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	283	Total	C	N	O	S	0	0	0
			2198	1353	406	433	6			

- Molecule 4 is a protein called HEXON-INTERLACING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	57	Total	C	N	O	S	0	0	0
			394	242	70	80	2			
4	Q	81	Total	C	N	O	S	0	0	0
			573	355	100	116	2			
4	R	49	Total	C	N	O	S	0	0	0
			328	200	56	71	1			
4	S	58	Total	C	N	O	S	0	0	0
			401	245	71	84	1			

- Molecule 5 is a protein called CORE-CAPSID BRIDGING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	T	72	Total	C	N	O	S	0	0	0
			518	319	95	103	1			

- Molecule 6 is a protein called PRE-PROTEIN VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	U	143	Total	C	N	O	S	0	0	0
			1118	696	201	218	3			
6	V	23	Total	C	N	O		0	0	0
			188	116	29	43				

- Molecule 7 is a protein called PRE-HEXON-LINKING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	X	111	Total	C	N	O	S	0	0	0
			865	549	155	159	2			
7	Y	56	Total	C	N	O	S	0	0	0
			440	274	87	77	2			

MolProbity and EDS were not executed - this section will therefore be empty.

3 Data and refinement statistics

Xtriage (Phenix) failed to run properly; EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	853.79Å 854.45Å 865.39Å 60.40° 60.42° 61.98°	Depositor
Resolution (Å)	15.00 – 3.80	Depositor
% Data completeness (in resolution range)	17.0 (15.00-3.80)	Depositor
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.368 , 0.382	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	98419	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity was not executed - this section will therefore be empty.

4.2 Too-close contacts [i](#)

MolProbity was not executed - this section will therefore be empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity was not executed - this section will therefore be empty.

4.3.2 Protein sidechains [i](#)

MolProbity was not executed - this section will therefore be empty.

4.3.3 RNA [i](#)

MolProbity was not executed - this section will therefore be empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

validation-pack was not executed - this section will therefore be empty.

4.5 Carbohydrates [i](#)

validation-pack was not executed - this section will therefore be empty.

4.6 Ligand geometry [i](#)

validation-pack was not executed - this section will therefore be empty.

4.7 Other polymers [i](#)

validation-pack was not executed - this section will therefore be empty.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

5.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

5.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

5.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.