



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:38 PM BST

PDB ID : 1N03
EMDB ID: : unknown
Title : Model for Active RecA Filament
Authors : VanLoock, M.S.; Yu, X.; Yang, S.; Lai, A.L.; Low, C.; Campbell, M.J.; Egelman, E.H.
Deposited on : 2002-10-10
Resolution : 20.00 Å(reported)
Based on PDB ID : 1REA

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 : 1.7.1 (RC1), CSD as537be (2016)
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

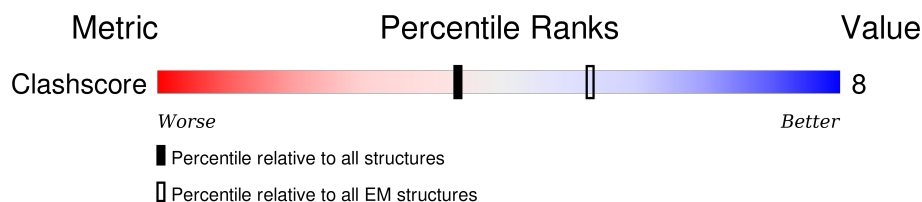
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY







The reported resolution of this entry is 20.00 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

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	352	 81% 5% 14%
1	B	352	 85% • 14%
1	C	352	 85% • 14%
1	D	352	 85% • 14%
1	E	352	 85% • 14%
1	F	352	 85% • 14%
1	G	352	 82% 5% 14%

2 Entry composition [i](#)

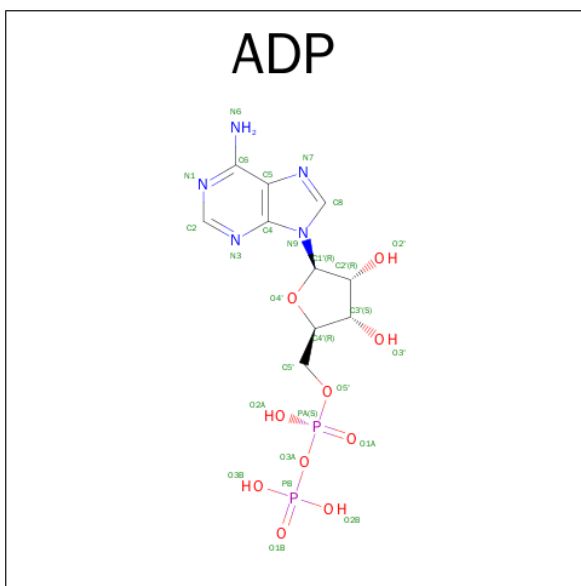
There are 2 unique types of molecules in this entry. The entry contains 2310 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RecA protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	303	Total C 303 303	0	303
1	B	303	Total C 303 303	0	303
1	C	303	Total C 303 303	0	303
1	D	303	Total C 303 303	0	303
1	E	303	Total C 303 303	0	303
1	F	303	Total C 303 303	0	303
1	G	303	Total C 303 303	0	303

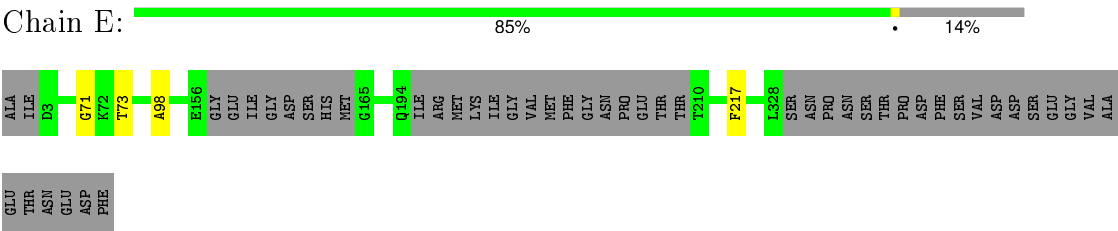
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



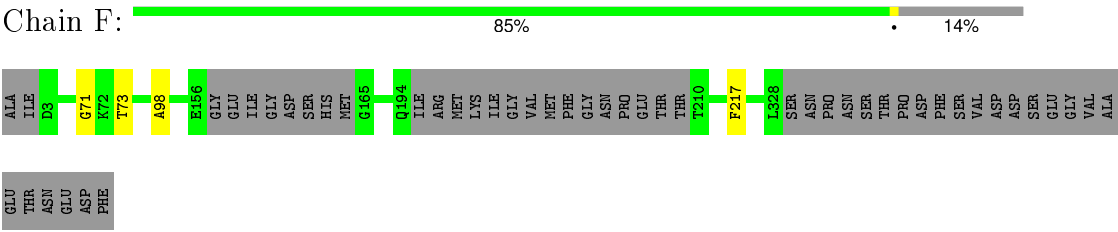
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0
2	G	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 1: RecA protein

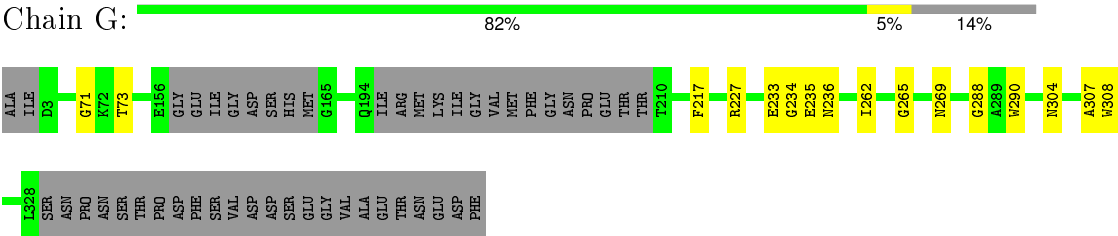




• Molecule 1: RecA protein



• Molecule 1: RecA protein



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 [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	303	0	0	3	17
1	B	303	0	0	4	0
1	C	303	0	0	4	0
1	D	303	0	0	4	0
1	E	303	0	0	4	0
1	F	303	0	0	4	0
1	G	303	0	0	3	14
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	2	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
2	F	27	0	12	2	0
2	G	27	0	12	2	3
All	All	2310	0	84	20	17

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 20 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:F:73:THR:CA	2:F:506:ADP:O1A	2.50	0.60
1:G:73:THR:CA	2:G:507:ADP:O1A	2.50	0.60
1:B:73:THR:CA	2:B:502:ADP:O1A	2.50	0.60
1:C:73:THR:CA	2:C:503:ADP:O1A	2.50	0.60
1:E:73:THR:CA	2:E:505:ADP:O1A	2.50	0.60

The worst 5 of 17 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLU:CA	2:G:507:ADP:C2[1_556]	0.87	1.33
1:A:58:MET:CA	1:G:307:ALA:CA[1_556]	1.03	1.17
1:A:127:GLU:CA	2:G:507:ADP:N3[1_556]	1.11	1.09
1:A:52:GLY:CA	1:G:290:TRP:CA[1_556]	1.27	0.93
1:A:38:GLU:CA	1:G:308:TRP:CA[1_556]	1.27	0.93

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADP	A	501	-	24,29,29	1.07	2 (8%)	23,45,45	1.49	4 (17%)
2	ADP	B	502	-	24,29,29	1.06	2 (8%)	23,45,45	1.49	4 (17%)
2	ADP	C	503	-	24,29,29	1.06	2 (8%)	23,45,45	1.49	4 (17%)
2	ADP	D	504	-	24,29,29	1.06	2 (8%)	23,45,45	1.49	4 (17%)
2	ADP	E	505	-	24,29,29	1.06	2 (8%)	23,45,45	1.49	4 (17%)
2	ADP	F	506	-	24,29,29	1.06	2 (8%)	23,45,45	1.49	4 (17%)
2	ADP	G	507	-	24,29,29	1.06	2 (8%)	23,45,45	1.49	4 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	501	-	-	0/12/32/32	0/3/3/3
2	ADP	B	502	-	-	0/12/32/32	0/3/3/3
2	ADP	C	503	-	-	0/12/32/32	0/3/3/3
2	ADP	D	504	-	-	0/12/32/32	0/3/3/3
2	ADP	E	505	-	-	0/12/32/32	0/3/3/3
2	ADP	F	506	-	-	0/12/32/32	0/3/3/3
2	ADP	G	507	-	-	0/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	ADP	PB-O2B	-2.29	1.46	1.54
2	A	501	ADP	PB-O2B	-2.28	1.46	1.54
2	G	507	ADP	PB-O2B	-2.28	1.46	1.54
2	F	506	ADP	PB-O2B	-2.27	1.46	1.54
2	E	505	ADP	PB-O2B	-2.27	1.46	1.54

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	507	ADP	O2'-C2'-C1'	-2.24	104.60	111.61
2	E	505	ADP	O2'-C2'-C1'	-2.24	104.61	111.61
2	B	502	ADP	O2'-C2'-C1'	-2.23	104.62	111.61
2	C	503	ADP	O2'-C2'-C1'	-2.23	104.63	111.61
2	F	506	ADP	O2'-C2'-C1'	-2.23	104.64	111.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ADP	2	0
2	B	502	ADP	2	0
2	C	503	ADP	2	0
2	D	504	ADP	2	0
2	E	505	ADP	2	0
2	F	506	ADP	2	0
2	G	507	ADP	2	3

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.