



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:34 PM GMT

PDB ID : 1KSX
Title : Crystal Structures of Two Intermediates in the Assembly of the Papillomavirus Replication Initiation Complex
Authors : Enemark, E.J.; Stenlund, A.; Joshua-Tor, L.
Deposited on : 2002-01-14
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
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) : trunk26865

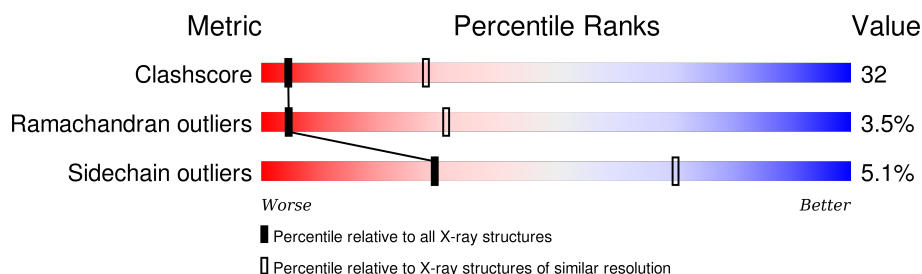
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)



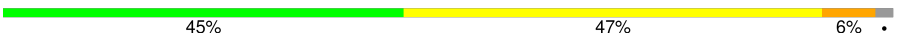


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	21	<div> <div>33%</div> <div>67%</div> </div>
1	G	21	<div> <div>33%</div> <div>67%</div> </div>
1	K	21	<div> <div>33%</div> <div>67%</div> </div>
1	O	21	<div> <div>33%</div> <div>67%</div> </div>
2	A	148	<div> <div>52%</div> <div>43%</div> <div>6%</div> </div>
2	B	148	<div> <div>43%</div> <div>49%</div> <div>6%</div> </div>
2	E	148	<div> <div>52%</div> <div>43%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	148	 44% 48% 6% •
2	I	148	 51% 45% • •
2	J	148	 45% 47% 6% •
2	M	148	 53% 43% • •
2	N	148	 43% 49% 6% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11044 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 DNA chain called E1 Recognition Sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	21	Total	C	N	O	P	0	0	0
			428	208	77	123	20			
1	G	21	Total	C	N	O	P	0	0	0
			428	208	77	123	20			
1	K	21	Total	C	N	O	P	0	0	0
			428	208	77	123	20			
1	O	21	Total	C	N	O	P	0	0	0
			428	208	77	123	20			

- Molecule 2 is a protein called REPLICATION PROTEIN E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	145	Total	C	N	O	S	7	0	0
			1164	754	200	201	9			
2	B	145	Total	C	N	O	S	7	0	0
			1164	754	200	201	9			
2	E	145	Total	C	N	O	S	7	0	0
			1164	754	200	201	9			
2	F	145	Total	C	N	O	S	7	0	0
			1164	754	200	201	9			
2	I	145	Total	C	N	O	S	7	0	0
			1164	754	200	201	9			
2	J	145	Total	C	N	O	S	7	0	0
			1164	754	200	201	9			
2	M	145	Total	C	N	O	S	7	0	0
			1164	754	200	201	9			
2	N	145	Total	C	N	O	S	7	0	0
			1164	754	200	201	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	CLONING ARTIFACT	UNP P03116

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Chain	Residue	Modelled	Actual	Comment	Reference
A	157	SER	-	CLONING ARTIFACT	UNP P03116
A	158	ARG	-	CLONING ARTIFACT	UNP P03116
B	156	GLY	-	CLONING ARTIFACT	UNP P03116
B	157	SER	-	CLONING ARTIFACT	UNP P03116
B	158	ARG	-	CLONING ARTIFACT	UNP P03116
E	156	GLY	-	CLONING ARTIFACT	UNP P03116
E	157	SER	-	CLONING ARTIFACT	UNP P03116
E	158	ARG	-	CLONING ARTIFACT	UNP P03116
F	156	GLY	-	CLONING ARTIFACT	UNP P03116
F	157	SER	-	CLONING ARTIFACT	UNP P03116
F	158	ARG	-	CLONING ARTIFACT	UNP P03116
I	156	GLY	-	CLONING ARTIFACT	UNP P03116
I	157	SER	-	CLONING ARTIFACT	UNP P03116
I	158	ARG	-	CLONING ARTIFACT	UNP P03116
J	156	GLY	-	CLONING ARTIFACT	UNP P03116
J	157	SER	-	CLONING ARTIFACT	UNP P03116
J	158	ARG	-	CLONING ARTIFACT	UNP P03116
M	156	GLY	-	CLONING ARTIFACT	UNP P03116
M	157	SER	-	CLONING ARTIFACT	UNP P03116
M	158	ARG	-	CLONING ARTIFACT	UNP P03116
N	156	GLY	-	CLONING ARTIFACT	UNP P03116
N	157	SER	-	CLONING ARTIFACT	UNP P03116
N	158	ARG	-	CLONING ARTIFACT	UNP P03116

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	3	Total O 3 3	0	0
3	E	2	Total O 2 2	0	0
3	F	3	Total O 3 3	0	0
3	I	1	Total O 1 1	0	0
3	J	3	Total O 3 3	0	0
3	M	2	Total O 2 2	0	0
3	N	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	1	Total	O	0	0
			1	1		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

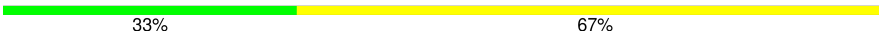
Note EDS was not executed.

• Molecule 1: E1 Recognition Sequence

Chain C: 



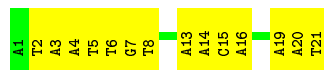
• Molecule 1: E1 Recognition Sequence

Chain G: 

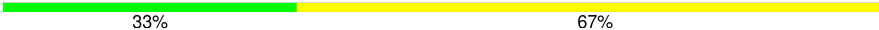


• Molecule 1: E1 Recognition Sequence

Chain K: 



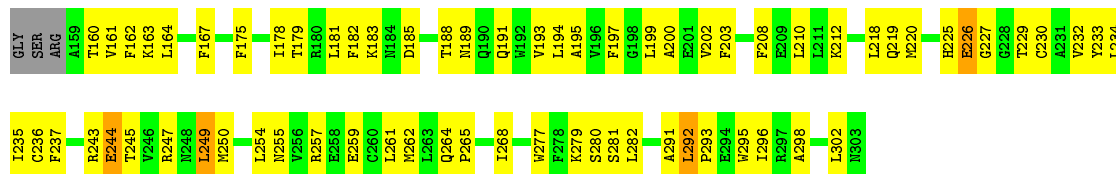
• Molecule 1: E1 Recognition Sequence

Chain O: 



• Molecule 2: REPLICATION PROTEIN E1

Chain A: 



- Molecule 2: REPLICATION PROTEIN E1

Chain M:

53%

43%



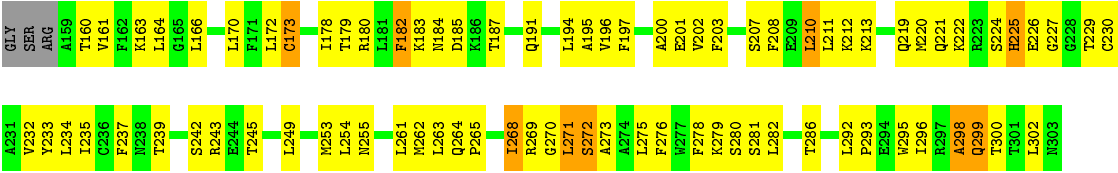
● Molecule 2: REPLICATION PROTEIN E1

Chain N:

43%

49%

6%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.25Å 103.65Å 125.00Å 90.00° 99.53° 90.00°	Depositor
Resolution (Å)	42.62 – 3.20	Depositor
% Data completeness (in resolution range)	90.5 (42.62-3.20)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.263 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11044	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

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	C	0.62	0/480	0.84	0/739
1	G	0.63	0/480	0.84	0/739
1	K	0.62	0/480	0.84	0/739
1	O	0.63	0/480	0.85	0/739
2	A	0.42	0/1190	0.64	0/1602
2	B	0.39	0/1190	0.67	0/1602
2	E	0.42	0/1190	0.64	0/1602
2	F	0.39	0/1190	0.67	0/1602
2	I	0.42	0/1190	0.63	0/1602
2	J	0.39	0/1190	0.67	0/1602
2	M	0.42	0/1190	0.64	0/1602
2	N	0.39	0/1190	0.67	0/1602
All	All	0.45	0/11440	0.69	0/15772

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	C	428	0	241	37	0
1	G	428	0	241	59	0
1	K	428	0	241	39	0
1	O	428	0	241	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1164	0	1189	63	0
2	B	1164	0	1189	79	0
2	E	1164	0	1189	63	0
2	F	1164	0	1189	76	0
2	I	1164	0	1189	86	0
2	J	1164	0	1189	76	0
2	M	1164	0	1189	63	0
2	N	1164	0	1189	80	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	E	2	0	0	0	0
3	F	3	0	0	0	0
3	I	1	0	0	0	0
3	J	3	0	0	0	0
3	M	2	0	0	0	0
3	N	3	0	0	0	0
3	O	1	0	0	0	0
All	All	11044	0	10476	690	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 32.

The worst 5 of 690 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:G:21:DT:H71	2:I:162:PHE:CE2	1.40	1.56
1:G:21:DT:C7	2:I:162:PHE:CZ	2.07	1.38
1:G:21:DT:H73	2:I:162:PHE:CZ	1.64	1.30
1:G:21:DT:C7	2:I:162:PHE:CE2	2.16	1.26
1:O:3:DA:H2"	1:O:4:DA:C8	1.95	1.02

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
2	A	143/148 (97%)	119 (83%)	21 (15%)	3 (2%)	9	46
2	B	143/148 (97%)	121 (85%)	15 (10%)	7 (5%)	3	22
2	E	143/148 (97%)	119 (83%)	21 (15%)	3 (2%)	9	46
2	F	143/148 (97%)	121 (85%)	15 (10%)	7 (5%)	3	22
2	I	143/148 (97%)	119 (83%)	21 (15%)	3 (2%)	9	46
2	J	143/148 (97%)	121 (85%)	15 (10%)	7 (5%)	3	22
2	M	143/148 (97%)	119 (83%)	21 (15%)	3 (2%)	9	46
2	N	143/148 (97%)	121 (85%)	15 (10%)	7 (5%)	3	22
All	All	1144/1184 (97%)	960 (84%)	144 (13%)	40 (4%)	4	31

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	271	LEU
2	B	299	GLN
2	F	271	LEU
2	F	299	GLN
2	J	271	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 X-ray entries followed by that with respect to entries of similar resolution.

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	
2	A	127/129 (98%)	120 (94%)	7 (6%)	27	68
2	B	127/129 (98%)	121 (95%)	6 (5%)	32	73
2	E	127/129 (98%)	120 (94%)	7 (6%)	27	68
2	F	127/129 (98%)	121 (95%)	6 (5%)	32	73
2	I	127/129 (98%)	120 (94%)	7 (6%)	27	68
2	J	127/129 (98%)	121 (95%)	6 (5%)	32	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	127/129 (98%)	120 (94%)	7 (6%)	27	68
2	N	127/129 (98%)	121 (95%)	6 (5%)	32	73
All	All	1016/1032 (98%)	964 (95%)	52 (5%)	29	70

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	225	HIS
2	I	226	GLU
2	N	221	GLN
2	F	239	THR
2	I	188	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	238	ASN
2	I	225	HIS
2	N	238	ASN
2	F	264	GLN
2	J	191	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 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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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