



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Sep 7, 2019 – 02:13 PM EDT

PDB ID : 6PPB
EMDB ID: : EMD-20432
Title : Kaposi's sarcoma-associated herpesvirus (KSHV), C5 portal vertex structure
Authors : Gong, D.; Dai, X.; Jih, J.; Liu, Y.T.; Bi, G.Q.; Sun, R.; Zhou, Z.H.
Deposited on : 2019-07-06
Resolution : 4.30 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

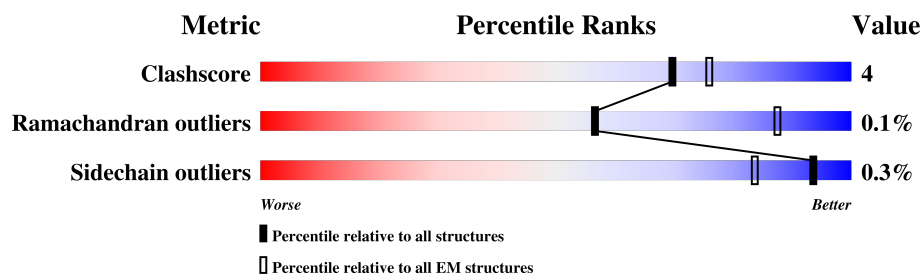
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	k	454	76% 24%
2	l	549	15% 85%
2	m	549	15% 85%
3	n	2635	98%
3	o	2635	98%
4	S	1376	82% 11% 7%
4	T	1376	87% 12% .
4	W	1376	85% 14% .
4	X	1376	82% 11% 6%

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Mol	Chain	Length	Quality of chain
5	5	331	<div><div></div><div>70%11%19%</div></div>
5	b	331	<div><div></div><div>96%. .</div></div>
6	6	305	<div><div></div><div>88%9%. .</div></div>
6	7	305	<div><div></div><div>88%8%. .</div></div>
6	c	305	<div><div></div><div>96%.</div></div>
6	d	305	<div><div></div><div>98%.</div></div>
7	0	170	<div><div></div><div>43%.54%</div></div>
7	1	170	<div><div></div><div>45%.54%</div></div>
7	2	170	<div><div></div><div>44%.54%</div></div>
7	3	170	<div><div></div><div>45%.54%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 62671 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 Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	k	344	Total	C	N	O	S	0	0
			2680	1722	467	477	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	165	PRO	LEU	conflict	UNP Q76RH8
k	281	SER	GLY	conflict	UNP Q76RH8

- Molecule 2 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	l	83	Total	C	N	O	S	0	0
			686	429	135	119	3		
2	m	80	Total	C	N	O	S	0	0
			645	406	121	115	3		

- Molecule 3 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	n	40	Total	C	N	O	0	0
			323	209	56	58		
3	o	40	Total	C	N	O	0	0
			323	209	56	58		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	2220	THR	PRO	conflict	UNP Q2HR64
o	2220	THR	PRO	conflict	UNP Q2HR64

- Molecule 4 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	1281	Total	C	N	O	S	0	0
			10061	6401	1739	1852	69		
4	T	1360	Total	C	N	O	S	0	0
			10667	6776	1851	1967	73		
4	W	1354	Total	C	N	O	S	0	0
			10622	6748	1842	1960	72		
4	X	1288	Total	C	N	O	S	0	0
			10108	6421	1755	1861	71		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1146	PRO	SER	conflict	UNP Q2HRA7
S	1157	ALA	THR	conflict	UNP Q2HRA7
T	1146	PRO	SER	conflict	UNP Q2HRA7
T	1157	ALA	THR	conflict	UNP Q2HRA7
W	1146	PRO	SER	conflict	UNP Q2HRA7
W	1157	ALA	THR	conflict	UNP Q2HRA7
X	1146	PRO	SER	conflict	UNP Q2HRA7
X	1157	ALA	THR	conflict	UNP Q2HRA7

- Molecule 5 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	321	Total	C	N	O	S	0	0
			2478	1586	424	453	15		
5	5	268	Total	C	N	O	S	0	0
			2074	1336	344	381	13		

- Molecule 6 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	c	294	Total	C	N	O	S	0	0
			2330	1485	397	434	14		
6	d	300	Total	C	N	O	S	0	0
			2365	1505	401	444	15		
6	6	294	Total	C	N	O	S	0	0
			2330	1485	397	434	14		
6	7	294	Total	C	N	O	S	0	0
			2315	1478	391	431	15		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	11	LEU	PHE	conflict	UNP Q98832
c	117	LEU	PHE	conflict	UNP Q98832
c	134	ILE	PRO	conflict	UNP Q98832
c	167	GLY	ASP	conflict	UNP Q98832
d	11	LEU	PHE	conflict	UNP Q98832
d	117	LEU	PHE	conflict	UNP Q98832
d	134	ILE	PRO	conflict	UNP Q98832
d	167	GLY	ASP	conflict	UNP Q98832
6	11	LEU	PHE	conflict	UNP Q98832
6	117	LEU	PHE	conflict	UNP Q98832
6	134	ILE	PRO	conflict	UNP Q98832
6	167	GLY	ASP	conflict	UNP Q98832
7	11	LEU	PHE	conflict	UNP Q98832
7	117	LEU	PHE	conflict	UNP Q98832
7	134	ILE	PRO	conflict	UNP Q98832
7	167	GLY	ASP	conflict	UNP Q98832

- Molecule 7 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	0	78	Total 666	C 418	N 130	O 115	S 3	0	0
7	1	78	Total 666	C 418	N 130	O 115	S 3	0	0
7	2	78	Total 666	C 418	N 130	O 115	S 3	0	0
7	3	78	Total 666	C 418	N 130	O 115	S 3	0	0

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- Molecule 1: Capsid vertex component 1

[illegible]

- Molecule 2: Capsid vertex component 2

[illegible]

- Molecule 2: Capsid vertex component 2

Chain m:  15% 85%

[illegible]

- Molecule 3: Large tegument protein deneddylase

Chain n: 98%

ILE	ALA	TYR	THR	VAL	SER	GLY	MET
ASN	GLY	GLY	GLU	LEU	LEU	ARG	ALA
GLY	GLU	ASN	THR	LEU	SER	ARG	ALA
THR	THR	LYS	SER	TYR	VAL	ASP	PRO
SER	SER	GLY	PRO	ILE	LEU	LEU	LEU
VAL	VAL	ARG	SER	ALA	SER	LEU	TYR
ASP	THR	GLY	VAL	THR	ASN	ARG	MET
ASP	GLU	GLY	SER	HIS	ASN	GLY	GLY
VAL	THR	ASN	PRO	ASP	TYR	LYS	MET
SER	PRO	LYS	ALA	THR	ALA	SER	ALA
GLY	GLY	GLY	PRO	GLU	GLY	GLY	ALA
PRO	PRO	ARG	THR	TYR	THR	MET	SER
GLU	GLU	GLY	GLU	THR	VAL	LEU	THR
ASN	ASN	LYS	PRO	CYS	TYR	PHE	GLN
PRO	PRO	THR	LEU	PHE	LEU	ARG	ALA
THR	THR	GLY	ARG	LEU	ILE	GLN	ASN
ALA	ALA	GLY	ASP	TYR	ILE	TYR	CYS
ARG	ARG	GLY	SER	PHE	ILE	ALA	ILE
PRO	PRO	GLY	THR	ILE	CYS	GLN	PHE
ASP	ASP	ASN	THR	PRO	GLN	LEU	GLY
THR	THR	GLY	GLN	HIS	SER	HIS	GLY
GLU	GLU	GLY	SER	ASP	LYS	HIS	HIS
ASP	GLU	GLY	GLN	THR	ALA	ILE	ALA
PRO	PRO	ARG	ASP	ILE	GLY	PRO	GLY
THR	THR	GLY	GLU	SER	ALA	GLY	SER
PRO	PRO	GLY	THR	PRO	ILE	PHE	GLN
GLY	GLY	HIS	ARG	GLU	VAL	LEU	CYS
ALA	ALA	GLN	VAL	HIS	TYR	ALA	VAL
THR	THR	PRO	VAL	THR	TYR	THR	MET
ALA	ALA	PRO	ILE	ARG	MET	LYS	LEU
LEU	LEU	HIS	PRO	THR	PHE	ILE	ALA
ASP	ASP	ILE	PRO	ILE	ASP	PHE	SER
THR	SER	THR	TYR	VAL	PRO	GLN	TYR
PRO	ASP	ALA	ASP	PHE	HIS	SER	SER
LEU	LEU	GLU	PRO	GLU	CYS	PRO	TYR
THR	THR	HIS	THR	GLU	ILE	GLU	ASN
ILE	ALA	MET	ASP	LEU	PRO	PHE	ASN
THR	THR	ASP	ARG	HIS	ASN	TYR	GLU
ALA	ARG	GLN	PRO	GLY	ILE	GLY	THR
ASP	GLY	SER	ARG	PRO	PRO	LEU	PRO
GLN	LYS	ASP	PRO	ARG	ASN	ILE	LEU
LYS	GLY	GLY	PRO	VAL	SER	GLY	VAL
THR	THR	GLN	HIS	ILE	PRO	GLN	ASP
ASN	PHE	ALA	ASP	SER	HIS	ALA	ALA
THR	SER	GLY	ARG	ARG	VAL	ALA	SER
ASN	SER	ASP	PRO	GLY	ILE	ILE	LEU
HIS	LEU	ASP	PRO	VAL	LYS	ARG	ASP
PRO	LYS	MET	GLU	GLU	THR	GLY	ASP
GLY	GLU	ASP	GLN	SER	ASN	PRO	LEU
LYS	SER	SER	ALA	CYS	ASP	PHE	GLY
ALA	TYR	THR	ALA	SER	VAL	ILE	GLY








[illegible]

[illegible]

HIS	PRO	THR	GLN	THR	PRO	VAL	PRO
	PRO	THR	GLN	THR	PRO	ILE	SER
ILE	ILE	SER	GLY	GLY	PRO	ASP	PRO
	ILE	SER	GLY	GLY	PRO	ARG	THR
MET	TRP	GLN	SER	SER	THR	PRO	PRO
	SER	PRO	THR	THR	PRO	LYS	PRO
PRO	PRO	ILE	ARG	ARG	PRO	PRO	LYS
	ILE	ARG	ASN	ASN	HIS	VAL	PRO
VAL	VAL	VAL	GLU	GLU	ALA	ALA	ARG
	VAL	VAL	GLU	GLU	ALA	SER	ARG
PRO	PRO	ASP	ALA	ALA	ILE	ALA	GLU
	PRO	ASP	ALA	ALA	ILE	ALA	GLU
ILE	ILE	ASP	PRO	PRO	ILE	THR	THR
	ILE	ASP	PRO	PRO	ILE	THR	THR
SER	SER	LYS	PRO	ILE	ARG	ALA	GLN
	SER	LYS	PRO	ILE	ARG	PHE	GLU
LEU	LEU	SER	LEU	SER	VAL	ARG	PRO
	LEU	SER	LEU	SER	VAL	ARG	PRO
GLN	GLN	PRO	GLU	GLU	MET	LEU	LYS
	GLN	PRO	GLU	GLU	MET	LEU	LYS
T2596	ASN	PRO	SER	GLN	THR	PRO	THR
	ASN	PRO	SER	GLN	THR	PRO	THR
L2635	THR	THR	ASN	THR	GLN	THR	ALA
	THR	THR	ASN	THR	GLN	THR	ALA
LEU	LEU	VAL	ALA	PRO	PRO	ALA	LEU
	LEU	VAL	ALA	PRO	PRO	ALA	LEU
GLU	GLU	GLU	VAL	MET	MET	LEU	VAL
	GLU	GLU	VAL	MET	MET	LEU	VAL
ARG	ARG	TYR	ALA	THR	ASP	GLU	ARG
	ARG	TYR	ALA	THR	ASP	GLU	ARG
PRO	PRO	ARG	ALA	THR	THR	THR	PRO
	PRO	ARG	ALA	THR	THR	THR	PRO
ILE	ILE	GLY	PRO	HIS	THR	THR	THR
	ILE	GLY	PRO	HIS	THR	THR	THR
THR	THR	ALA	ARG	ALA	GLU	ALA	VAL
	THR	ALA	ARG	ALA	GLU	ALA	VAL
SER	SER	THR	THR	ASP	THR	THR	THR
	SER	THR	THR	ASP	THR	THR	THR
PRO	PRO	GLY	VAL	VAL	GLY	GLY	ARG
	PRO	GLY	VAL	VAL	GLY	GLY	ARG
GLY	GLY	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
ALA	ALA	THR	THR	THR	THR	THR	THR
	ALA	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
LEU	LEU	THR	THR	THR	THR	THR	THR
	LEU	THR	THR	THR	THR	THR	THR
VAL	VAL	THR	THR	THR	THR	THR	THR
	VAL	THR	THR	THR	THR	THR	THR
GLU	GLU	THR	THR	THR	THR	THR	THR
	GLU	THR	THR	THR	THR	THR	THR
ARG	ARG	THR	THR	THR	THR	THR	THR
	ARG	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
ILE	ILE	THR	THR	THR	THR	THR	THR
	ILE	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
SER	SER	THR	THR	THR	THR	THR	THR
	SER	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
GLY	GLY	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
ALA	ALA	THR	THR	THR	THR	THR	THR
	ALA	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
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LEU	LEU	THR	THR	THR	THR	THR	THR
	LEU	THR	THR	THR	THR	THR	THR
VAL	VAL	THR	THR	THR	THR	THR	THR
	VAL	THR	THR	THR	THR	THR	THR
GLU	GLU	THR	THR	THR	THR	THR	THR
	GLU	THR	THR	THR	THR	THR	THR
ARG	ARG	THR	THR	THR	THR	THR	THR
	ARG	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
ILE	ILE	THR	THR	THR	THR	THR	THR
	ILE	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
SER	SER	THR	THR	THR	THR	THR	THR
	SER	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
GLY	GLY	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
ALA	ALA	THR	THR	THR	THR	THR	THR
	ALA	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
LEU	LEU	THR	THR	THR	THR	THR	THR
	LEU	THR	THR	THR	THR	THR	THR
VAL	VAL	THR	THR	THR	THR	THR	THR
	VAL	THR	THR	THR	THR	THR	THR
GLU	GLU	THR	THR	THR	THR	THR	THR
	GLU	THR	THR	THR	THR	THR	THR
ARG	ARG	THR	THR	THR	THR	THR	THR
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	PRO	THR	THR	THR	THR	THR	THR
ILE	ILE	THR	THR	THR	THR	THR	THR
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SER	SER	THR	THR	THR	THR	THR	THR
	SER	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
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GLY	GLY	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
ALA	ALA	THR	THR	THR	THR	THR	THR
	ALA	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
LEU	LEU	THR	THR	THR	THR	THR	THR
	LEU	THR	THR	THR	THR	THR	THR
VAL	VAL	THR	THR	THR	THR	THR	THR
	VAL	THR	THR	THR	THR	THR	THR
GLU	GLU	THR	THR	THR	THR	THR	THR
	GLU	THR	THR	THR	THR	THR	THR
ARG	ARG	THR	THR	THR	THR	THR	THR
	ARG	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
ILE	ILE	THR	THR	THR	THR	THR	THR
	ILE	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
SER	SER	THR	THR	THR	THR	THR	THR
	SER	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
GLY	GLY	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
ALA	ALA	THR	THR	THR	THR	THR	THR
	ALA	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
LEU	LEU	THR	THR	THR	THR	THR	THR
	LEU	THR	THR	THR	THR	THR	THR
VAL	VAL	THR	THR	THR	THR	THR	THR
	VAL	THR	THR	THR	THR	THR	THR
GLU	GLU	THR	THR	THR	THR	THR	THR
	GLU	THR	THR	THR	THR	THR	THR
ARG	ARG	THR	THR	THR	THR	THR	THR
	ARG	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
ILE	ILE	THR	THR	THR	THR	THR	THR
	ILE	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
SER	SER	THR	THR	THR	THR	THR	THR
	SER	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
GLY	GLY	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
ALA	ALA	THR	THR	THR	THR	THR	THR
	ALA	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
LEU	LEU	THR	THR	THR	THR	THR	THR
	LEU	THR	THR	THR	THR	THR	THR
VAL	VAL	THR	THR	THR	THR	THR	THR
	VAL	THR	THR	THR	THR	THR	THR
GLU	GLU	THR	THR	THR	THR	THR	THR
	GLU	THR	THR	THR	THR	THR	THR
ARG	ARG	THR	THR	THR	THR	THR	THR
	ARG	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
ILE	ILE	THR	THR	THR	THR	THR	THR
	ILE	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
SER	SER	THR	THR	THR	THR	THR	THR
	SER	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
GLY	GLY	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
ALA	ALA	THR	THR	THR	THR	THR	THR
	ALA	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
LEU	LEU	THR	THR	THR	THR	THR	THR
	LEU	THR	THR	THR	THR	THR	THR
VAL	VAL	THR	THR	THR	THR	THR	THR
	VAL	THR	THR	THR	THR	THR	THR
GLU	GLU	THR	THR	THR	THR	THR	THR
	GLU	THR	THR	THR	THR	THR	THR
ARG	ARG	THR	THR	THR	THR	THR	THR
	ARG	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
ILE	ILE	THR	THR	THR	THR	THR	THR
	ILE	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
SER	SER	THR	THR	THR	THR	THR	THR
	SER	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
GLY	GLY	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
ALA	ALA	THR	THR	THR	THR	THR	THR
	ALA	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
LEU	LEU	THR	THR	THR	THR	THR	THR
	LEU	THR	THR	THR	THR	THR	THR
VAL	VAL	THR	THR	THR	THR	THR	THR
	VAL	THR	THR	THR	THR	THR	THR
GLU	GLU	THR	THR	THR	THR	THR	THR
	GLU	THR	THR	THR	THR	THR	THR
ARG	ARG	THR	THR	THR	THR	THR	THR
	ARG	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
ILE	ILE	THR	THR	THR	THR	THR	THR
	ILE	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
SER	SER	THR	THR	THR	THR	THR	THR
	SER	THR	THR	THR	THR	THR	THR
PRO	PRO	THR	THR	THR	THR	THR	THR
	PRO	THR	THR	THR	THR	THR	THR
GLY	GLY	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
ALA	ALA	THR	THR	THR	THR	THR	THR
	ALA	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR
LEU	LEU	THR	THR	THR	THR	THR	THR
	LEU	THR	THR	THR	THR	THR	THR
VAL	VAL	THR	THR	THR	THR	THR	THR
	VAL	THR	THR	THR	THR	THR	THR
GL							

- Molecule 4: Major capsid protein

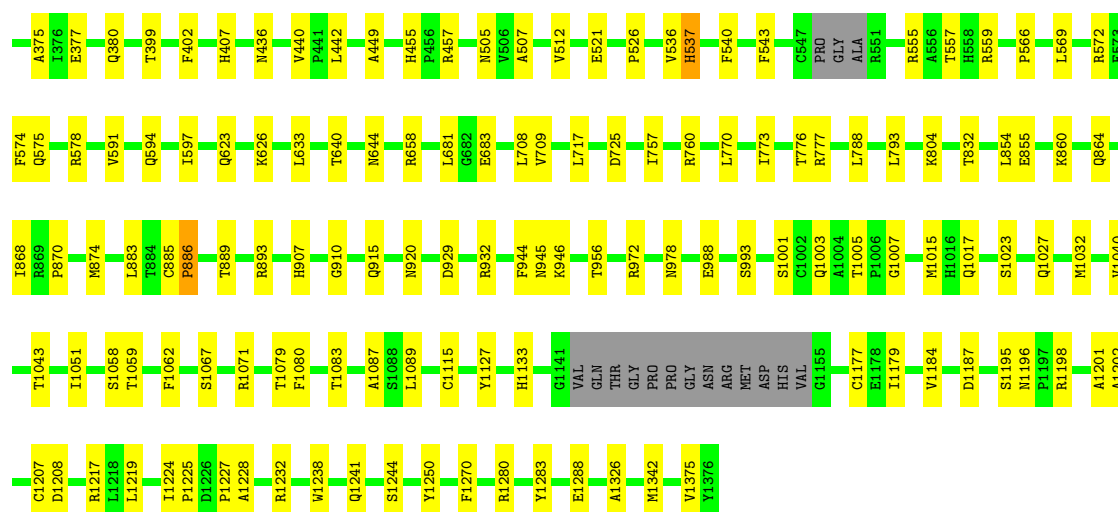
Chain S:  82% 11% 7%

[illegible]

- Molecule 4: Major capsid protein

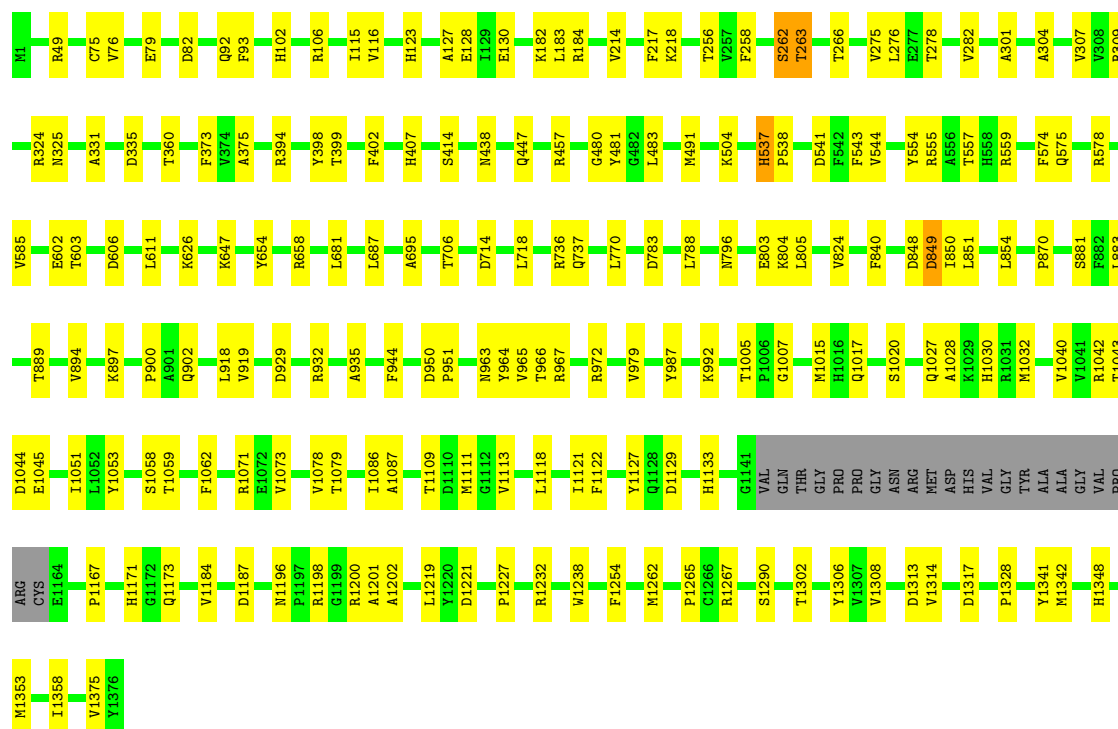
Chain T: 87% 12%

Y1	F10	P11	N18	K41	R44	L71	G75	E79	D82	I87	I91	Q92	F93	K94	I96	A101	Y114	J115	V116	I129	E130	P146	F149	K182	L195	S211	V275	T278	T279	V293	A304	R332	D346	V368
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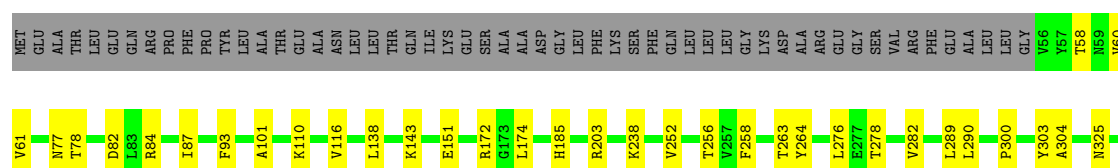
• Molecule 4: Major capsid protein

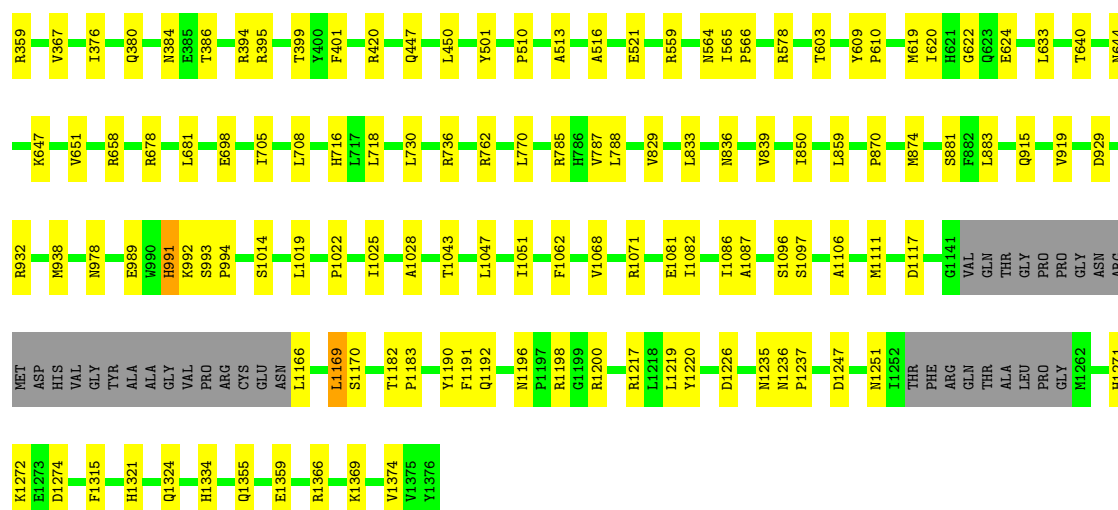
Chain W: 85% 14%



• Molecule 4: Major capsid protein

Chain X: 82% 11% 6%





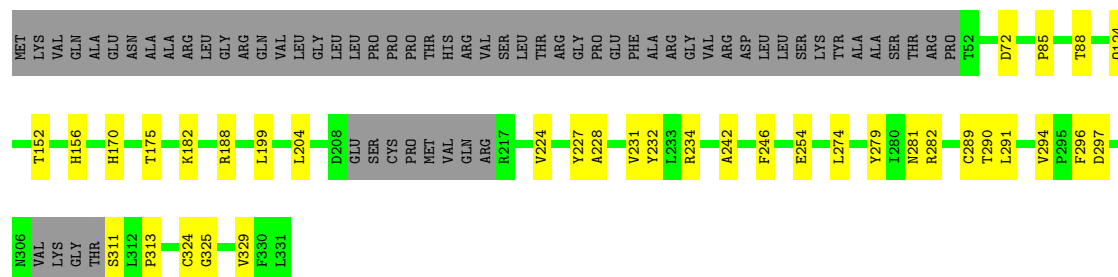
- Molecule 5: Triplex capsid protein 1

Chain b: 96%



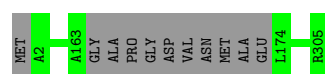
- Molecule 5: Triplex capsid protein 1

Chain 5: 70%



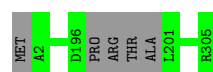
- Molecule 6: Triplex capsid protein 2

Chain c: 96%

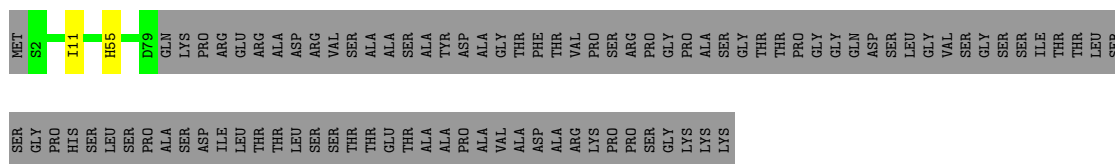


- Molecule 6: Triplex capsid protein 2

Chain d: 98%



- Molecule 6: Triplex capsid protein 2



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	39773	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	k	0.31	0/2753	0.52	1/3755 (0.0%)
2	l	0.27	0/698	0.48	0/942
2	m	0.25	0/656	0.45	0/887
3	n	0.32	0/326	0.45	0/437
3	o	0.32	0/326	0.45	0/437
4	S	0.32	0/10300	0.56	3/13998 (0.0%)
4	T	0.34	0/10919	0.58	1/14839 (0.0%)
4	W	0.32	0/10874	0.57	1/14780 (0.0%)
4	X	0.33	0/10350	0.56	1/14071 (0.0%)
5	5	0.30	0/2127	0.58	2/2891 (0.1%)
5	b	0.32	0/2540	0.60	2/3452 (0.1%)
6	6	0.30	0/2376	0.59	0/3234
6	7	0.29	0/2360	0.58	1/3210 (0.0%)
6	c	0.30	0/2376	0.56	0/3234
6	d	0.30	0/2411	0.55	0/3281
7	0	0.27	0/682	0.47	0/919
7	1	0.27	0/682	0.47	0/919
7	2	0.27	0/682	0.47	0/919
7	3	0.27	0/682	0.47	0/919
All	All	0.32	0/64120	0.56	12/87124 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	S	0	2
4	T	0	5
4	W	0	5
4	X	0	1
All	All	0	13

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	297	ASP	CB-CG-OD1	8.70	126.13	118.30
5	b	297	ASP	CB-CG-OD1	8.55	126.00	118.30
5	b	274	LEU	CA-CB-CG	5.95	128.99	115.30
4	T	708	LEU	CA-CB-CG	5.68	128.37	115.30
5	5	296	PHE	C-N-CA	5.67	135.87	121.70

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	S	991	HIS	Peptide
4	S	992	LYS	Peptide
4	T	10	PHE	Peptide
4	T	505	ASN	Peptide
4	T	537	HIS	Peptide

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	k	2680	0	2675	0	0
2	l	686	0	704	0	0
2	m	645	0	653	0	0
3	n	323	0	353	0	0
3	o	323	0	353	0	0
4	S	10061	0	9954	92	0
4	T	10667	0	10542	96	0
4	W	10622	0	10500	107	0
4	X	10108	0	9980	92	0
5	5	2074	0	2050	19	0
5	b	2478	0	2466	0	0
6	6	2330	0	2354	18	0
6	7	2315	0	2335	14	0
6	c	2330	0	2354	0	0
6	d	2365	0	2379	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	0	666	0	647	4	0
7	1	666	0	647	2	0
7	2	666	0	647	4	0
7	3	666	0	647	2	0
All	All	62671	0	62240	404	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 4.

The worst 5 of 404 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)
4:S:777:ARG:NH2	4:S:885:CYS:O	2.27	0.67
4:T:536:VAL:HG13	4:T:1244:SER:HA	1.77	0.66
4:S:770:LEU:HD21	4:S:883:LEU:HD22	1.76	0.66
4:W:770:LEU:HD21	4:W:883:LEU:HD22	1.76	0.66
4:W:929:ASP:OD1	4:W:932:ARG:NH2	2.29	0.66

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 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	k	334/454 (74%)	322 (96%)	12 (4%)	0	100	100
2	l	81/549 (15%)	81 (100%)	0	0	100	100
2	m	76/549 (14%)	75 (99%)	1 (1%)	0	100	100
3	n	38/2635 (1%)	38 (100%)	0	0	100	100
3	o	38/2635 (1%)	38 (100%)	0	0	100	100
4	S	1273/1376 (92%)	1179 (93%)	92 (7%)	2 (0%)	49	84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	T	1354/1376 (98%)	1273 (94%)	78 (6%)	3 (0%)	49	84
4	W	1350/1376 (98%)	1287 (95%)	61 (4%)	2 (0%)	53	88
4	X	1282/1376 (93%)	1201 (94%)	79 (6%)	2 (0%)	49	84
5	5	262/331 (79%)	250 (95%)	12 (5%)	0	100	100
5	b	315/331 (95%)	307 (98%)	8 (2%)	0	100	100
6	6	290/305 (95%)	275 (95%)	15 (5%)	0	100	100
6	7	288/305 (94%)	275 (96%)	13 (4%)	0	100	100
6	c	290/305 (95%)	282 (97%)	8 (3%)	0	100	100
6	d	296/305 (97%)	292 (99%)	4 (1%)	0	100	100
7	0	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	1	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	2	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	3	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
All	All	7871/14888 (53%)	7475 (95%)	387 (5%)	9 (0%)	56	88

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	W	263	THR
4	T	10	PHE
4	X	992	LYS
4	S	992	LYS
4	S	993	SER

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	k	293/377 (78%)	293 (100%)	0	100	100
2	l	76/473 (16%)	76 (100%)	0	100	100
2	m	71/473 (15%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	n	35/2239 (2%)	35 (100%)	0	100	100
3	o	35/2239 (2%)	35 (100%)	0	100	100
4	S	1094/1166 (94%)	1086 (99%)	8 (1%)	85	92
4	T	1154/1166 (99%)	1154 (100%)	0	100	100
4	W	1150/1166 (99%)	1149 (100%)	1 (0%)	94	97
4	X	1097/1166 (94%)	1092 (100%)	5 (0%)	90	94
5	5	229/281 (82%)	229 (100%)	0	100	100
5	b	272/281 (97%)	272 (100%)	0	100	100
6	6	267/274 (97%)	266 (100%)	1 (0%)	92	95
6	7	264/274 (96%)	259 (98%)	5 (2%)	60	80
6	c	267/274 (97%)	267 (100%)	0	100	100
6	d	270/274 (98%)	270 (100%)	0	100	100
7	0	70/141 (50%)	70 (100%)	0	100	100
7	1	70/141 (50%)	70 (100%)	0	100	100
7	2	70/141 (50%)	70 (100%)	0	100	100
7	3	70/141 (50%)	70 (100%)	0	100	100
All	All	6854/12687 (54%)	6834 (100%)	20 (0%)	93	96

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	X	143	LYS
4	X	325	ASN
6	7	78	ARG
4	S	1235	ASN
4	W	1113	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
4	W	816	ASN
4	X	428	GLN
7	0	55	HIS
4	W	978	ASN
4	X	102	HIS

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.