



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:40 PM BST

PDB ID : 1LD4
Title : Placement of the Structural Proteins in Sindbis Virus
Authors : Zhang, W.; Mukhopadhyay, S.; Pletnev, S.V.; Baker, T.S.; Kuhn, R.J.; Rossmann, M.G.
Deposited on : 2002-04-08
Resolution : 11.40 Å (reported)
Based on PDB ID : 1SVB, 1YSA, 1I9W

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

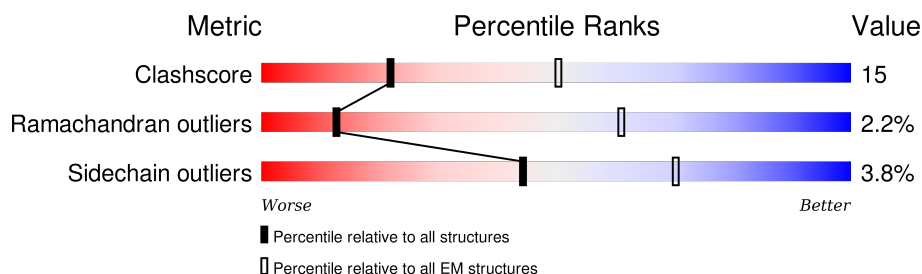
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.40 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	264	47% 9% . 43%
1	B	264	48% 8% . 43%
1	C	264	48% 8% . 43%
1	D	264	48% 8% . 43%
2	E	57	49% 51%
2	F	57	49% 51%
2	G	57	49% 51%
2	H	57	49% 51%
2	I	57	49% 51%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	57	<div><div></div><div>49%</div><div>51%</div></div>
2	K	57	<div><div></div><div>49%</div><div>51%</div></div>
2	L	57	<div><div></div><div>49%</div><div>51%</div></div>
3	M	439	<div><div></div><div>54%</div><div>28%</div><div>•</div><div>16%</div></div>
3	N	439	<div><div></div><div>55%</div><div>28%</div><div>•</div><div>16%</div></div>
3	O	439	<div><div></div><div>55%</div><div>28%</div><div>•</div><div>16%</div></div>
3	P	439	<div><div></div><div>55%</div><div>27%</div><div>•</div><div>16%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15680 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 Coat protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		
1	B	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		
1	C	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		
1	D	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		

- Molecule 2 is a protein called GENERAL CONTROL PROTEIN GCN4.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	E	28	Total	C	0	28
			28	28		
2	F	28	Total	C	0	28
			28	28		
2	G	28	Total	C	0	28
			28	28		
2	H	28	Total	C	0	28
			28	28		
2	I	28	Total	C	0	28
			28	28		
2	J	28	Total	C	0	28
			28	28		
2	K	28	Total	C	0	28
			28	28		
2	L	28	Total	C	0	28
			28	28		

- Molecule 3 is a protein called Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		
3	O	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		
3	P	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		

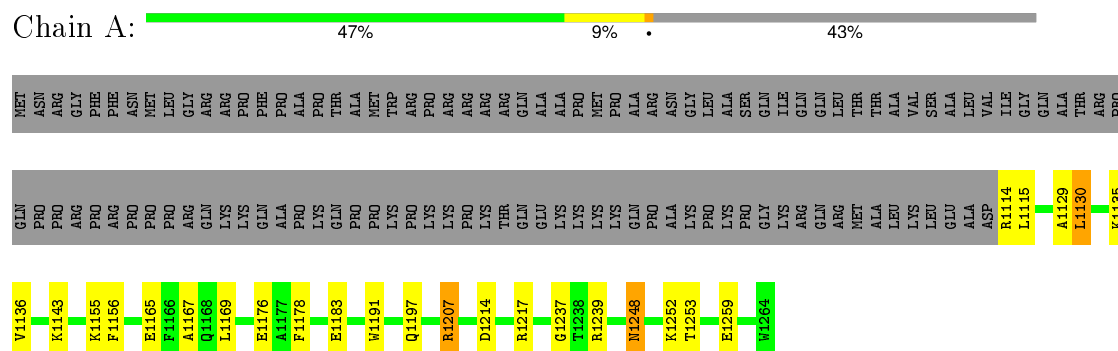
- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
4	P	6	Total	X	0
			6	6	
4	J	1	Total	X	0
			1	1	
4	H	1	Total	X	0
			1	1	
4	N	6	Total	X	0
			6	6	
4	O	8	Total	X	0
			8	8	
4	L	1	Total	X	0
			1	1	
4	F	2	Total	X	0
			2	2	
4	M	7	Total	X	0
			7	7	

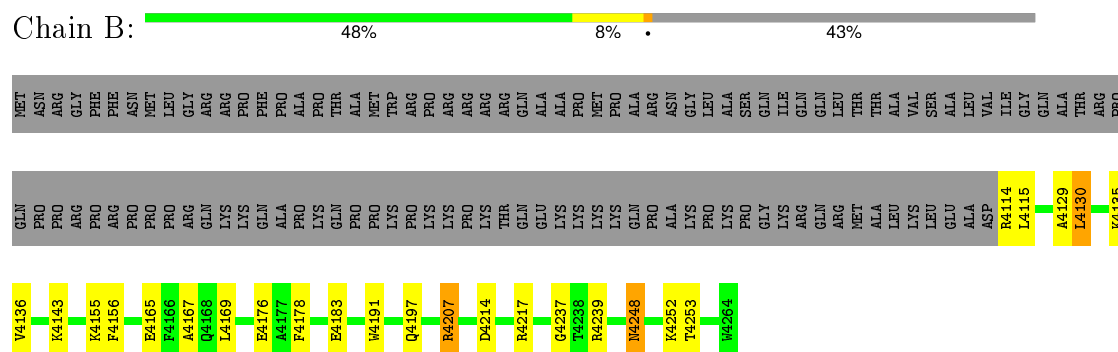
3 Residue-property plots [i](#)

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. 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. 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.

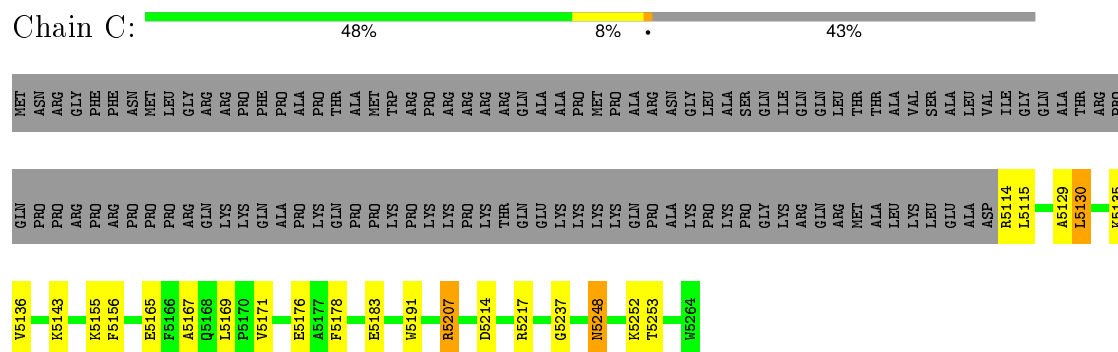
- Molecule 1: Coat protein C



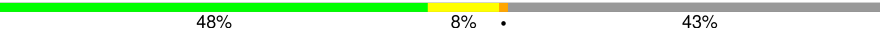
- Molecule 1: Coat protein C

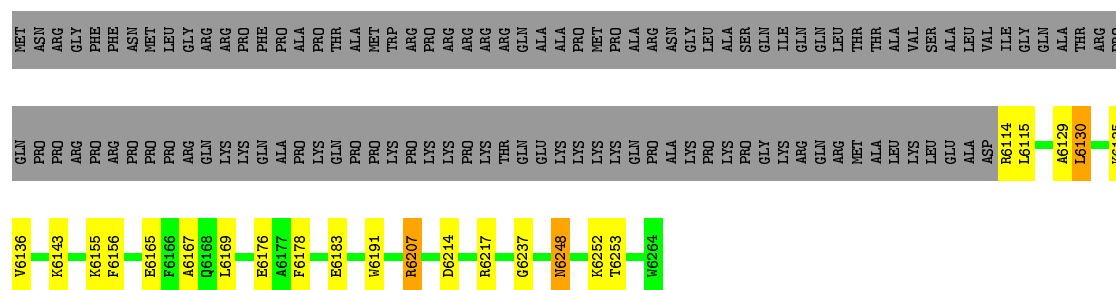


- Molecule 1: Coat protein C



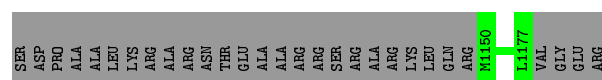
- Molecule 1: Coat protein C

Chain D:  48% 8% 43%



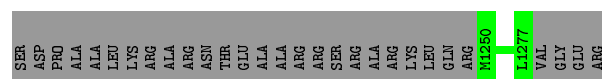
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain E:  49% 51%



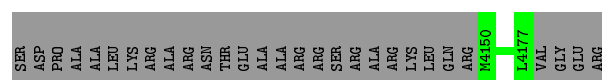
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain F:  49% 51%



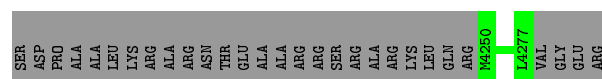
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain G:  49% 51%



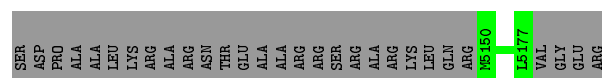
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain H:  49% 51%



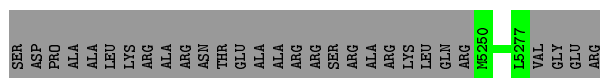
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain I:  49% 51%



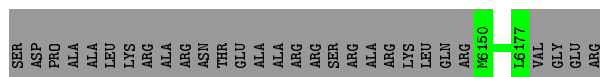
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain J:  49% 51%



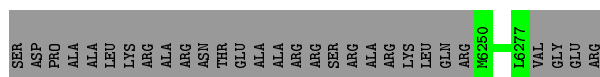
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain K: 49% 51%



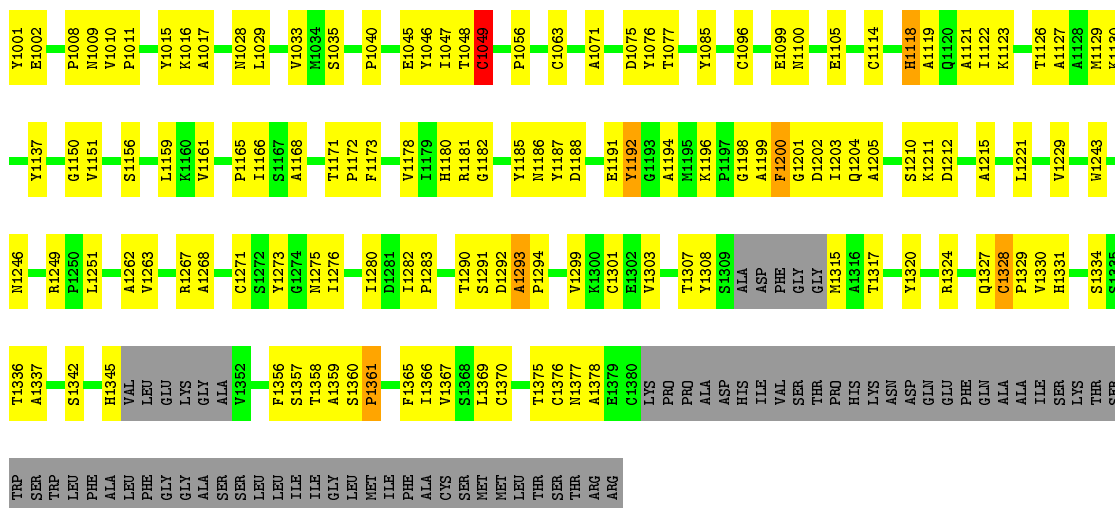
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain L: 49% 51%



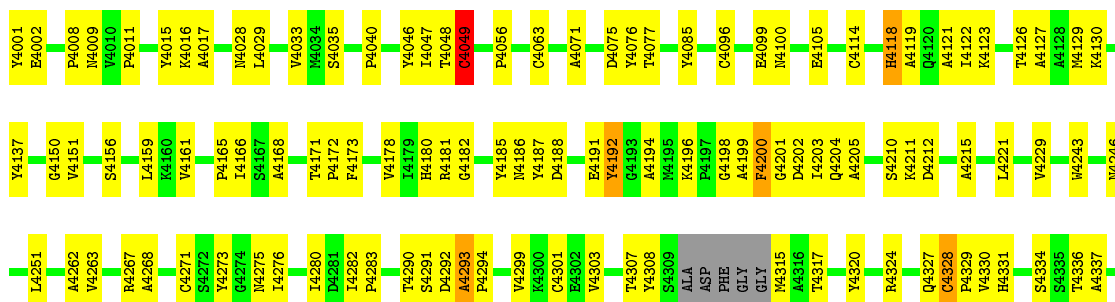
- Molecule 3: Spike glycoprotein E1

Chain M: 54% 28% 16%



- Molecule 3: Spike glycoprotein E1

Chain N: 55% 28% 16%



S4342	LEU
H4345	PHE
VAL	ALA
LEU	LEU
GLU	PHE
LYS	GLY
GLY	ALA
V4352	SER
F4356	LEU
S4357	LEU
T4358	ILE
A4359	ILE
S4360	GLY
P4361	LEU
F4365	MET
I4366	ILE
V4367	PHE
S4368	ALA
L4369	CYS
C4370	SER
T4375	SER
C4376	THR
M4377	THR
A4378	ARG
E4379	ARG
C4380	LYS
LYS	PRO
PRO	PRO
ALA	ALA
ASP	ASP
HIS	HIS
ILE	ILE
VAL	VAL
SER	SER
THR	THR
PRO	PRO
HIS	HIS
LYS	LYS
ASN	ASN
ASP	ASP
GLN	GLN
GLU	GLU
PHE	PHE
GLN	GLN
ALA	ALA
ALA	ALA
ILE	ILE
SER	SER
LYS	LYS
THR	THR
SER	SER
TRP	TRP
SER	TRP

• Molecule 3: Spike glycoprotein E1

Chain O:  55% 28% 16%

LEU	PHE	ALA	LEU	PHE	GLY	GLY	ALA	SER	SER	LEU	LEU	LEU	LEU	ILE	PHE	ALA	CYS	SER	SER	LEU	THR	SER	THR	ARG	ARG	LYS	PRO	PRO	ALA	ASP	HIS	ILE	VAL	SER	GLY	THR	PRO	HIS	LYS	ASN	ASP	GLN	GLU	PHE	GLN	ALA	ALA	ILE	SER	LYS	THR	SER	TRP	SER	TRP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
S5342			H5345	VAL	LEU	GLU	GLY	ALA	V5352	F5356	S5357	T5358	A5359	S5360	P5361	F5365	L5366	S5367	L5368	C5370	T5375	C5376	N5377	E5379	C5380	LYS	PRO	PRO	ALA	ASP	HIS	ILE	VAL	SER	GLY	THR	PRO	HIS	LYS	ASN	ASP	GLN	GLU	PHE	GLN	ALA	ALA	ILE	SER	LYS	THR	SER	TRP	SER	TRP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
P5250	L5251	A5262	V5263	R5267	A5268	C5271	S5272	Y5273	G5274	N5275	L5276	I5280	D5281	P5282	P5283	T5290	S5291	D5292	A5293	P5294	V5299	K5300	C5301	F5302	V5303	T5307	Y5308	S5309	ALA	ASP	PHE	GLY	M5315	A5316	T5317	Y5320	R5324	Q5327	C5328	P5329	V5330	H5331	S5334	S5335	T5336	A5337																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
K5130	Y5137	G5150	S5156	L5159	V5161	P5165	L5166	S5167	A5168	T5171	P5172	F5173	V5178	I5179	H5180	A5181	G5182	Y5185	N5186	Y5187	D5188	Y5192	K5196	P5197	G5198	A5199	F5200	G5201	D5202	T5203	Q5204	A5205	S5210	K5211	D5212	A5215	L5221	V5229	W5243	N5246	P5249																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								

• Molecule 3: Spike glycoprotein E1

Chain P:  55% 27% 16%

LEU	PHE	GLY	GLY	ALA	GLY	SER	SER	LEU	ILE	ILE	PHE	ALA	CYS	MET	MET	LEU	THR	SER	THR	ARG	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--

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	each viral image was CTF corrected before reconstruction, based on the following equation: $F(\text{corr})=F(\text{obs})/[CTF +wiener]$	Depositor
Microscope	PHILLIPS CM200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1840	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2580	Depositor
Magnification	38000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.52	0/1190	0.81	1/1607 (0.1%)
1	B	0.52	0/1190	0.81	1/1607 (0.1%)
1	C	0.52	0/1190	0.81	1/1607 (0.1%)
1	D	0.52	0/1190	0.81	1/1607 (0.1%)
3	M	0.34	0/2743	0.54	0/3740
3	N	0.34	0/2743	0.54	0/3740
3	O	0.34	0/2743	0.54	0/3740
3	P	0.34	0/2743	0.54	0/3740
All	All	0.41	0/15732	0.63	4/21388 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	6130	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	1130	LEU	CA-CB-CG	5.10	127.04	115.30
1	B	4130	LEU	CA-CB-CG	5.09	127.02	115.30
1	C	5130	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1162	0	1131	16	0
1	B	1162	0	1131	11	0
1	C	1162	0	1131	14	0
1	D	1162	0	1131	9	0
2	E	28	0	0	0	0
2	F	28	0	0	0	0
2	G	28	0	0	0	0
2	H	28	0	0	0	0
2	I	28	0	0	0	0
2	J	28	0	0	0	0
2	K	28	0	0	0	0
2	L	28	0	0	0	0
3	M	2694	0	2605	139	0
3	N	2694	0	2605	135	0
3	O	2694	0	2605	91	0
3	P	2694	0	2605	95	0
4	F	2	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
4	M	7	0	0	0	0
4	N	6	0	0	0	0
4	O	8	0	0	0	0
4	P	6	0	0	0	0
All	All	15680	0	14944	464	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 15.

The worst 5 of 464 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)
3:M:1194:ALA:CB	3:N:4151:VAL:HG12	1.36	1.54
3:M:1151:VAL:HG12	3:N:4194:ALA:CB	1.36	1.48
3:M:1151:VAL:CG1	3:N:4194:ALA:CB	2.05	1.34
3:M:1194:ALA:CB	3:N:4151:VAL:CG1	2.05	1.31
3:O:5330:VAL:HG22	3:O:5369:LEU:CA	1.62	1.29

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	A	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
1	B	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
1	C	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
1	D	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
3	M	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	41
3	N	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	41
3	O	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	41
3	P	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	41
All	All	1988/2812 (71%)	1656 (83%)	288 (14%)	44 (2%)	13	49

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	1126	THR
3	M	1361	PRO
3	N	4126	THR
3	N	4361	PRO
3	O	5126	THR

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	122/218 (56%)	115 (94%)	7 (6%)	25	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	122/218 (56%)	115 (94%)	7 (6%)	25	62
1	C	122/218 (56%)	115 (94%)	7 (6%)	25	62
1	D	122/218 (56%)	115 (94%)	7 (6%)	25	62
3	M	299/370 (81%)	290 (97%)	9 (3%)	48	77
3	N	299/370 (81%)	290 (97%)	9 (3%)	48	77
3	O	299/370 (81%)	290 (97%)	9 (3%)	48	77
3	P	299/370 (81%)	290 (97%)	9 (3%)	48	77
All	All	1684/2352 (72%)	1620 (96%)	64 (4%)	44	73

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	1035	SER
3	M	1292	ASP
3	P	6192	TYR
3	M	1049	CYS
3	M	1192	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	1073	HIS
3	M	1355	HIS
3	P	6331	HIS
3	M	1100	ASN
3	M	1331	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

Of 32 ligands modelled in this entry, 32 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.