wwPDB EM Validation Summary Report

Jan 2, 2025 – 10:08 AM EST

PDB ID	:	9EK2
EMDB ID	:	EMD-52059
Title	:	HIV-1 immature L20K/E73K/A82T matrix protein p17 lattice
Authors	:	Rey, J.S.; Perilla, J.R.; Chen, L.; Zhang, P.
Deposited on	:	2024-11-30
Resolution	:	8.30 Å(reported)
Based on initial models	:	7TBP, 2LYB

This is a wwPDB EM 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

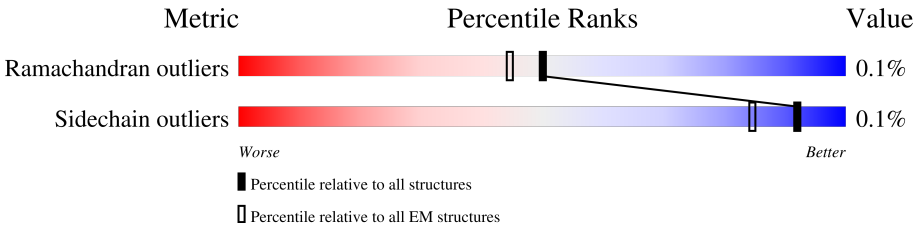
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.30 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	115	97%
1	B	115	99%
1	C	115	97%
1	D	115	99%
1	E	115	98%
1	F	115	99%
1	G	115	100%
1	H	115	98%
1	I	115	99%
1	J	115	100%

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Mol	Chain	Length	Quality of chain
1	K	115	98%
1	L	115	99%
1	M	115	98%
1	N	115	100%
1	O	115	99%
1	P	115	98%
1	Q	115	98%
1	R	115	100%
1	S	115	97%
1	T	115	100%
1	U	115	99%
1	V	115	99%
1	W	115	100%
1	X	115	100%
1	Y	115	98%
1	Z	115	99%
1	a	115	97%
1	b	115	97%
1	c	115	98%
1	d	115	98%
1	e	115	97%
1	f	115	100%
1	g	115	98%
1	h	115	97%
1	i	115	98%

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Mol	Chain	Length	Quality of chain
1	j	115	100%
1	k	115	98%
1	l	115	99%
1	m	115	97%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 36504 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 Matrix protein p17.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	D	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	e	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	h	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	k	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	G	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	J	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	M	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	P	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	S	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	V	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	Y	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	b	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	B	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	E	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	f	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	i	115	Total	C	N	O	S	0	0
			921	576	171	172	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	l	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	H	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	K	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	N	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	Q	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	T	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	W	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	Z	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	c	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	C	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	F	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	g	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	j	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	m	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	I	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	L	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	O	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	R	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	U	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	X	115	Total	C	N	O	S	0	0
			921	576	171	172	2		
1	a	115	Total	C	N	O	S	0	0
			921	576	171	172	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	d	115	Total	C	N	O	S	0	0
			921	576	171	172	2		

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	LYS	LEU	engineered mutation	UNP P12497
A	73	LYS	GLU	engineered mutation	UNP P12497
A	82	THR	ALA	engineered mutation	UNP P12497
D	20	LYS	LEU	engineered mutation	UNP P12497
D	73	LYS	GLU	engineered mutation	UNP P12497
D	82	THR	ALA	engineered mutation	UNP P12497
e	20	LYS	LEU	engineered mutation	UNP P12497
e	73	LYS	GLU	engineered mutation	UNP P12497
e	82	THR	ALA	engineered mutation	UNP P12497
h	20	LYS	LEU	engineered mutation	UNP P12497
h	73	LYS	GLU	engineered mutation	UNP P12497
h	82	THR	ALA	engineered mutation	UNP P12497
k	20	LYS	LEU	engineered mutation	UNP P12497
k	73	LYS	GLU	engineered mutation	UNP P12497
k	82	THR	ALA	engineered mutation	UNP P12497
G	20	LYS	LEU	engineered mutation	UNP P12497
G	73	LYS	GLU	engineered mutation	UNP P12497
G	82	THR	ALA	engineered mutation	UNP P12497
J	20	LYS	LEU	engineered mutation	UNP P12497
J	73	LYS	GLU	engineered mutation	UNP P12497
J	82	THR	ALA	engineered mutation	UNP P12497
M	20	LYS	LEU	engineered mutation	UNP P12497
M	73	LYS	GLU	engineered mutation	UNP P12497
M	82	THR	ALA	engineered mutation	UNP P12497
P	20	LYS	LEU	engineered mutation	UNP P12497
P	73	LYS	GLU	engineered mutation	UNP P12497
P	82	THR	ALA	engineered mutation	UNP P12497
S	20	LYS	LEU	engineered mutation	UNP P12497
S	73	LYS	GLU	engineered mutation	UNP P12497
S	82	THR	ALA	engineered mutation	UNP P12497
V	20	LYS	LEU	engineered mutation	UNP P12497
V	73	LYS	GLU	engineered mutation	UNP P12497
V	82	THR	ALA	engineered mutation	UNP P12497
Y	20	LYS	LEU	engineered mutation	UNP P12497
Y	73	LYS	GLU	engineered mutation	UNP P12497
Y	82	THR	ALA	engineered mutation	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
b	20	LYS	LEU	engineered mutation	UNP P12497
b	73	LYS	GLU	engineered mutation	UNP P12497
b	82	THR	ALA	engineered mutation	UNP P12497
B	20	LYS	LEU	engineered mutation	UNP P12497
B	73	LYS	GLU	engineered mutation	UNP P12497
B	82	THR	ALA	engineered mutation	UNP P12497
E	20	LYS	LEU	engineered mutation	UNP P12497
E	73	LYS	GLU	engineered mutation	UNP P12497
E	82	THR	ALA	engineered mutation	UNP P12497
f	20	LYS	LEU	engineered mutation	UNP P12497
f	73	LYS	GLU	engineered mutation	UNP P12497
f	82	THR	ALA	engineered mutation	UNP P12497
i	20	LYS	LEU	engineered mutation	UNP P12497
i	73	LYS	GLU	engineered mutation	UNP P12497
i	82	THR	ALA	engineered mutation	UNP P12497
l	20	LYS	LEU	engineered mutation	UNP P12497
l	73	LYS	GLU	engineered mutation	UNP P12497
l	82	THR	ALA	engineered mutation	UNP P12497
H	20	LYS	LEU	engineered mutation	UNP P12497
H	73	LYS	GLU	engineered mutation	UNP P12497
H	82	THR	ALA	engineered mutation	UNP P12497
K	20	LYS	LEU	engineered mutation	UNP P12497
K	73	LYS	GLU	engineered mutation	UNP P12497
K	82	THR	ALA	engineered mutation	UNP P12497
N	20	LYS	LEU	engineered mutation	UNP P12497
N	73	LYS	GLU	engineered mutation	UNP P12497
N	82	THR	ALA	engineered mutation	UNP P12497
Q	20	LYS	LEU	engineered mutation	UNP P12497
Q	73	LYS	GLU	engineered mutation	UNP P12497
Q	82	THR	ALA	engineered mutation	UNP P12497
T	20	LYS	LEU	engineered mutation	UNP P12497
T	73	LYS	GLU	engineered mutation	UNP P12497
T	82	THR	ALA	engineered mutation	UNP P12497
W	20	LYS	LEU	engineered mutation	UNP P12497
W	73	LYS	GLU	engineered mutation	UNP P12497
W	82	THR	ALA	engineered mutation	UNP P12497
Z	20	LYS	LEU	engineered mutation	UNP P12497
Z	73	LYS	GLU	engineered mutation	UNP P12497
Z	82	THR	ALA	engineered mutation	UNP P12497
c	20	LYS	LEU	engineered mutation	UNP P12497
c	73	LYS	GLU	engineered mutation	UNP P12497
c	82	THR	ALA	engineered mutation	UNP P12497

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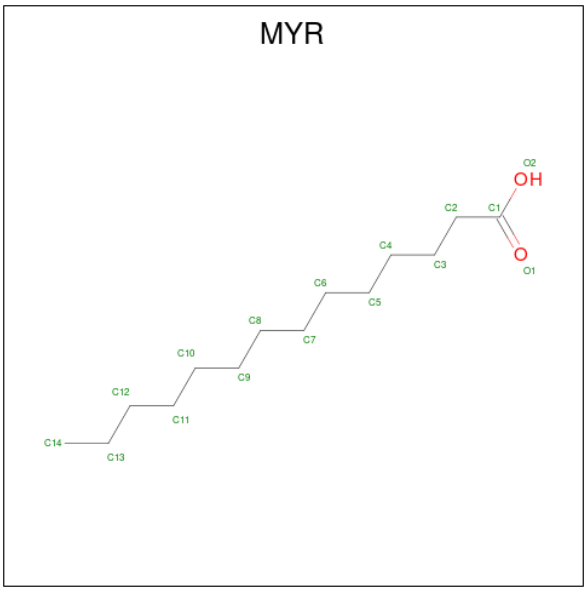
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	LYS	LEU	engineered mutation	UNP P12497
C	73	LYS	GLU	engineered mutation	UNP P12497
C	82	THR	ALA	engineered mutation	UNP P12497
F	20	LYS	LEU	engineered mutation	UNP P12497
F	73	LYS	GLU	engineered mutation	UNP P12497
F	82	THR	ALA	engineered mutation	UNP P12497
g	20	LYS	LEU	engineered mutation	UNP P12497
g	73	LYS	GLU	engineered mutation	UNP P12497
g	82	THR	ALA	engineered mutation	UNP P12497
j	20	LYS	LEU	engineered mutation	UNP P12497
j	73	LYS	GLU	engineered mutation	UNP P12497
j	82	THR	ALA	engineered mutation	UNP P12497
m	20	LYS	LEU	engineered mutation	UNP P12497
m	73	LYS	GLU	engineered mutation	UNP P12497
m	82	THR	ALA	engineered mutation	UNP P12497
I	20	LYS	LEU	engineered mutation	UNP P12497
I	73	LYS	GLU	engineered mutation	UNP P12497
I	82	THR	ALA	engineered mutation	UNP P12497
L	20	LYS	LEU	engineered mutation	UNP P12497
L	73	LYS	GLU	engineered mutation	UNP P12497
L	82	THR	ALA	engineered mutation	UNP P12497
O	20	LYS	LEU	engineered mutation	UNP P12497
O	73	LYS	GLU	engineered mutation	UNP P12497
O	82	THR	ALA	engineered mutation	UNP P12497
R	20	LYS	LEU	engineered mutation	UNP P12497
R	73	LYS	GLU	engineered mutation	UNP P12497
R	82	THR	ALA	engineered mutation	UNP P12497
U	20	LYS	LEU	engineered mutation	UNP P12497
U	73	LYS	GLU	engineered mutation	UNP P12497
U	82	THR	ALA	engineered mutation	UNP P12497
X	20	LYS	LEU	engineered mutation	UNP P12497
X	73	LYS	GLU	engineered mutation	UNP P12497
X	82	THR	ALA	engineered mutation	UNP P12497
a	20	LYS	LEU	engineered mutation	UNP P12497
a	73	LYS	GLU	engineered mutation	UNP P12497
a	82	THR	ALA	engineered mutation	UNP P12497
d	20	LYS	LEU	engineered mutation	UNP P12497
d	73	LYS	GLU	engineered mutation	UNP P12497
d	82	THR	ALA	engineered mutation	UNP P12497

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C O 15 14 1	0
2	D	1	Total C O 15 14 1	0
2	e	1	Total C O 15 14 1	0
2	h	1	Total C O 15 14 1	0
2	k	1	Total C O 15 14 1	0
2	G	1	Total C O 15 14 1	0
2	J	1	Total C O 15 14 1	0
2	M	1	Total C O 15 14 1	0
2	P	1	Total C O 15 14 1	0
2	S	1	Total C O 15 14 1	0
2	V	1	Total C O 15 14 1	0
2	Y	1	Total C O 15 14 1	0
2	b	1	Total C O 15 14 1	0
2	B	1	Total C O 15 14 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	E	1	Total C O 15 14 1	0
2	f	1	Total C O 15 14 1	0
2	i	1	Total C O 15 14 1	0
2	l	1	Total C O 15 14 1	0
2	H	1	Total C O 15 14 1	0
2	K	1	Total C O 15 14 1	0
2	N	1	Total C O 15 14 1	0
2	Q	1	Total C O 15 14 1	0
2	T	1	Total C O 15 14 1	0
2	W	1	Total C O 15 14 1	0
2	Z	1	Total C O 15 14 1	0
2	c	1	Total C O 15 14 1	0
2	C	1	Total C O 15 14 1	0
2	F	1	Total C O 15 14 1	0
2	g	1	Total C O 15 14 1	0
2	j	1	Total C O 15 14 1	0
2	m	1	Total C O 15 14 1	0
2	I	1	Total C O 15 14 1	0
2	L	1	Total C O 15 14 1	0
2	O	1	Total C O 15 14 1	0
2	R	1	Total C O 15 14 1	0

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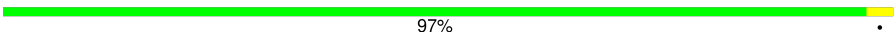
Mol	Chain	Residues	Atoms			AltConf
2	U	1	Total	C	O	0
			15	14	1	
2	X	1	Total	C	O	0
			15	14	1	
2	a	1	Total	C	O	0
			15	14	1	
2	d	1	Total	C	O	0
			15	14	1	

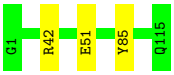
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Matrix protein p17

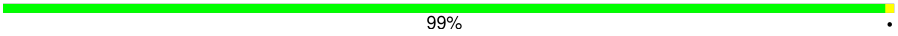
Chain A:





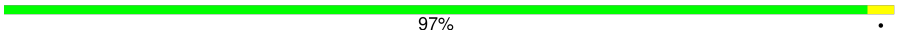
- Molecule 1: Matrix protein p17

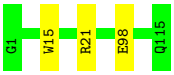
Chain D:



- Molecule 1: Matrix protein p17

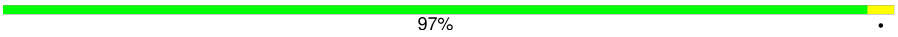
Chain e:

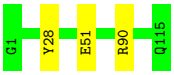




- Molecule 1: Matrix protein p17

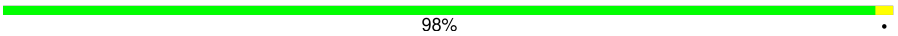
Chain h:





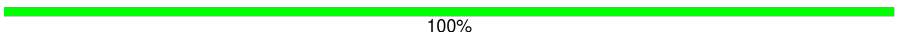
- Molecule 1: Matrix protein p17

Chain k:



- Molecule 1: Matrix protein p17

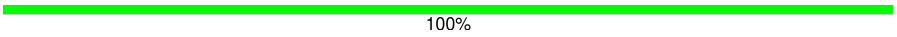
Chain G:



There are no outlier residues recorded for this chain.

• Molecule 1: Matrix protein p17

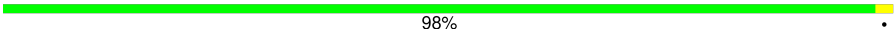
Chain J:



There are no outlier residues recorded for this chain.

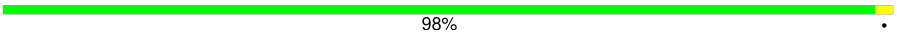
• Molecule 1: Matrix protein p17

Chain M:



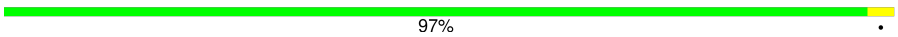
• Molecule 1: Matrix protein p17

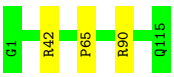
Chain P:



• Molecule 1: Matrix protein p17

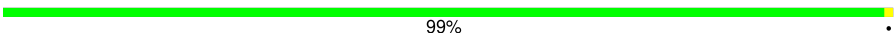
Chain S:





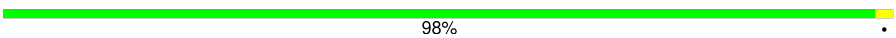
• Molecule 1: Matrix protein p17

Chain V:



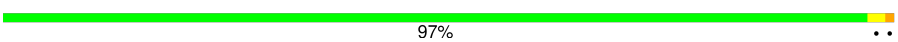
• Molecule 1: Matrix protein p17

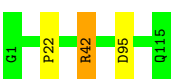
Chain Y:



• Molecule 1: Matrix protein p17

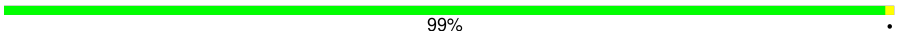
Chain b:





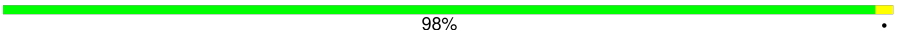
• Molecule 1: Matrix protein p17

Chain B:



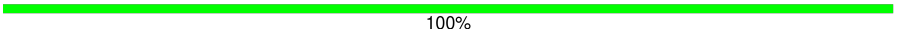
- Molecule 1: Matrix protein p17

Chain E:



- Molecule 1: Matrix protein p17

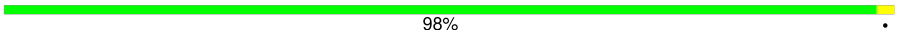
Chain f:



There are no outlier residues recorded for this chain.

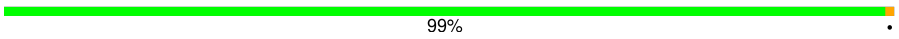
- Molecule 1: Matrix protein p17

Chain i:



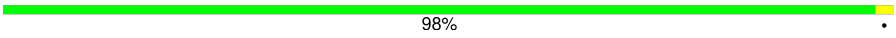
- Molecule 1: Matrix protein p17

Chain l:



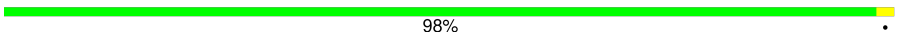
- Molecule 1: Matrix protein p17

Chain H:



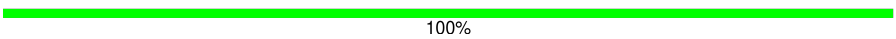
- Molecule 1: Matrix protein p17

Chain K:



- Molecule 1: Matrix protein p17

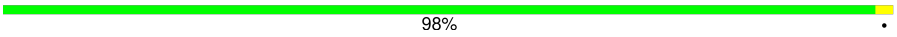
Chain N:



There are no outlier residues recorded for this chain.

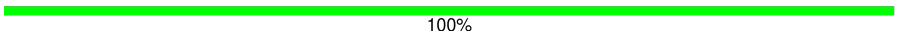
• Molecule 1: Matrix protein p17

Chain Q:



• Molecule 1: Matrix protein p17

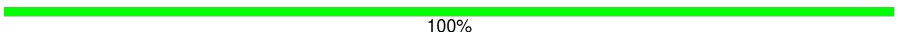
Chain T:



There are no outlier residues recorded for this chain.

• Molecule 1: Matrix protein p17

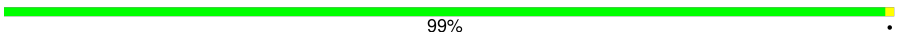
Chain W:



There are no outlier residues recorded for this chain.

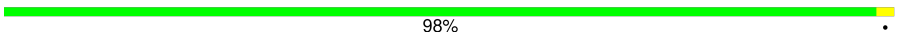
• Molecule 1: Matrix protein p17

Chain Z:



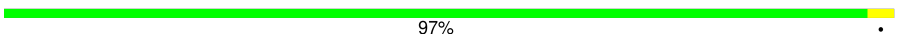
• Molecule 1: Matrix protein p17

Chain c:



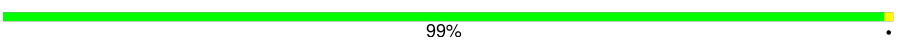
• Molecule 1: Matrix protein p17

Chain C:



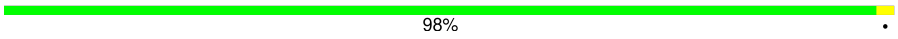
• Molecule 1: Matrix protein p17

Chain F:



• Molecule 1: Matrix protein p17

Chain g:



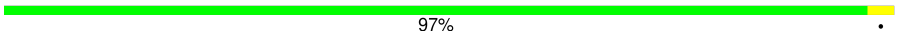
• Molecule 1: Matrix protein p17

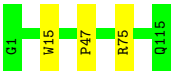
Chain j:

There are no outlier residues recorded for this chain.

• Molecule 1: Matrix protein p17

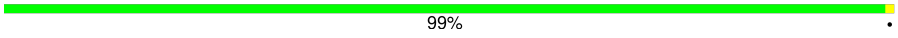
Chain m:





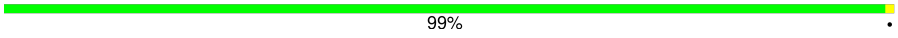
• Molecule 1: Matrix protein p17

Chain I:



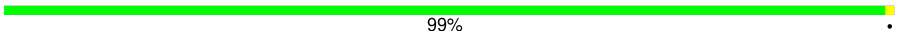
• Molecule 1: Matrix protein p17

Chain L:



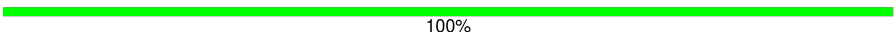
• Molecule 1: Matrix protein p17

Chain O:



• Molecule 1: Matrix protein p17

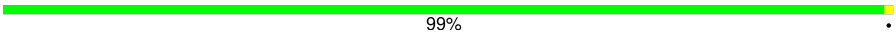
Chain R:



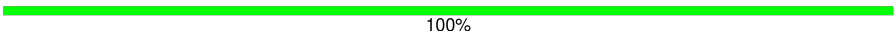
There are no outlier residues recorded for this chain.

• Molecule 1: Matrix protein p17

Chain U:

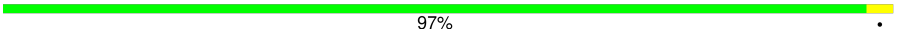


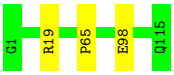
• Molecule 1: Matrix protein p17

Chain X: 

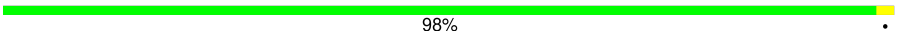
There are no outlier residues recorded for this chain.

• Molecule 1: Matrix protein p17

Chain a: 



• Molecule 1: Matrix protein p17

Chain d: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	8600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	123	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	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: MYR

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	A	1.00	2/933 (0.2%)	0.81	2/1247 (0.2%)
1	B	0.87	0/933	0.81	1/1247 (0.1%)
1	C	0.91	3/933 (0.3%)	0.81	0/1247
1	D	0.89	0/933	0.88	1/1247 (0.1%)
1	E	0.90	1/933 (0.1%)	0.78	1/1247 (0.1%)
1	F	0.90	0/933	0.81	1/1247 (0.1%)
1	G	0.86	0/933	0.75	0/1247
1	H	0.87	0/933	0.85	2/1247 (0.2%)
1	I	0.90	1/933 (0.1%)	0.74	0/1247
1	J	0.88	0/933	0.77	0/1247
1	K	0.94	0/933	0.90	2/1247 (0.2%)
1	L	0.91	1/933 (0.1%)	0.80	0/1247
1	M	0.88	1/933 (0.1%)	0.80	1/1247 (0.1%)
1	N	0.86	0/933	0.79	0/1247
1	O	0.88	0/933	0.80	1/1247 (0.1%)
1	P	0.85	0/933	0.83	1/1247 (0.1%)
1	Q	0.95	2/933 (0.2%)	0.80	0/1247
1	R	0.85	0/933	0.71	0/1247
1	S	0.90	1/933 (0.1%)	0.84	2/1247 (0.2%)
1	T	0.89	0/933	0.81	0/1247
1	U	0.90	0/933	0.75	0/1247
1	V	0.88	1/933 (0.1%)	0.76	0/1247
1	W	0.92	0/933	0.79	0/1247
1	X	0.88	0/933	0.80	0/1247
1	Y	0.88	1/933 (0.1%)	0.79	1/1247 (0.1%)
1	Z	0.83	0/933	0.76	0/1247
1	a	0.92	2/933 (0.2%)	0.76	1/1247 (0.1%)
1	b	0.89	1/933 (0.1%)	0.78	1/1247 (0.1%)
1	c	0.91	1/933 (0.1%)	0.78	1/1247 (0.1%)
1	d	0.86	1/933 (0.1%)	0.77	1/1247 (0.1%)
1	e	0.93	2/933 (0.2%)	0.79	0/1247
1	f	0.88	0/933	0.82	0/1247

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	g	0.91	1/933 (0.1%)	0.78	1/1247 (0.1%)
1	h	0.87	1/933 (0.1%)	0.81	2/1247 (0.2%)
1	i	0.89	0/933	0.82	2/1247 (0.2%)
1	j	0.90	0/933	0.78	0/1247
1	k	0.89	1/933 (0.1%)	0.78	0/1247
1	l	0.87	1/933 (0.1%)	0.81	0/1247
1	m	0.95	2/933 (0.2%)	0.82	1/1247 (0.1%)
All	All	0.89	27/36387 (0.1%)	0.80	26/48633 (0.1%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	TYR	CB-CG	-7.16	1.41	1.51
1	E	22	PRO	N-CD	-6.82	1.38	1.47
1	e	15	TRP	CZ3-CH2	-6.65	1.29	1.40
1	S	65	PRO	N-CD	-6.31	1.39	1.47
1	g	22	PRO	N-CD	-6.03	1.39	1.47

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	90	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	K	75	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	H	19	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	S	90	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	b	42	ARG	NE-CZ-NH2	-7.50	116.55	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	113/115 (98%)	113 (100%)	0	0	100	100
1	B	113/115 (98%)	113 (100%)	0	0	100	100
1	C	113/115 (98%)	113 (100%)	0	0	100	100
1	D	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	E	113/115 (98%)	113 (100%)	0	0	100	100
1	F	113/115 (98%)	113 (100%)	0	0	100	100
1	G	113/115 (98%)	113 (100%)	0	0	100	100
1	H	113/115 (98%)	113 (100%)	0	0	100	100
1	I	113/115 (98%)	113 (100%)	0	0	100	100
1	J	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	K	113/115 (98%)	113 (100%)	0	0	100	100
1	L	113/115 (98%)	113 (100%)	0	0	100	100
1	M	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	N	113/115 (98%)	113 (100%)	0	0	100	100
1	O	113/115 (98%)	113 (100%)	0	0	100	100
1	P	113/115 (98%)	113 (100%)	0	0	100	100
1	Q	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	R	113/115 (98%)	113 (100%)	0	0	100	100
1	S	113/115 (98%)	113 (100%)	0	0	100	100
1	T	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
1	U	113/115 (98%)	112 (99%)	0	1 (1%)	14	52
1	V	113/115 (98%)	113 (100%)	0	0	100	100
1	W	113/115 (98%)	113 (100%)	0	0	100	100
1	X	113/115 (98%)	113 (100%)	0	0	100	100
1	Y	113/115 (98%)	113 (100%)	0	0	100	100
1	Z	113/115 (98%)	113 (100%)	0	0	100	100
1	a	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
1	b	113/115 (98%)	113 (100%)	0	0	100	100
1	c	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
1	d	113/115 (98%)	113 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	e	113/115 (98%)	112 (99%)	0	1 (1%)	14 52
1	f	113/115 (98%)	113 (100%)	0	0	100 100
1	g	113/115 (98%)	113 (100%)	0	0	100 100
1	h	113/115 (98%)	112 (99%)	1 (1%)	0	100 100
1	i	113/115 (98%)	113 (100%)	0	0	100 100
1	j	113/115 (98%)	113 (100%)	0	0	100 100
1	k	113/115 (98%)	113 (100%)	0	0	100 100
1	l	113/115 (98%)	111 (98%)	1 (1%)	1 (1%)	14 52
1	m	113/115 (98%)	112 (99%)	1 (1%)	0	100 100
All	All	4407/4485 (98%)	4392 (100%)	12 (0%)	3 (0%)	50 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	e	21	ARG
1	l	11	GLU
1	U	21	ARG

5.3.2 Protein sidechains (i)

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	100/100 (100%)	100 (100%)	0	100 100
1	B	100/100 (100%)	100 (100%)	0	100 100
1	C	100/100 (100%)	100 (100%)	0	100 100
1	D	100/100 (100%)	100 (100%)	0	100 100
1	E	100/100 (100%)	100 (100%)	0	100 100
1	F	100/100 (100%)	100 (100%)	0	100 100
1	G	100/100 (100%)	100 (100%)	0	100 100
1	H	100/100 (100%)	100 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	100/100 (100%)	100 (100%)	0	100	100
1	J	100/100 (100%)	100 (100%)	0	100	100
1	K	100/100 (100%)	100 (100%)	0	100	100
1	L	100/100 (100%)	100 (100%)	0	100	100
1	M	100/100 (100%)	100 (100%)	0	100	100
1	N	100/100 (100%)	100 (100%)	0	100	100
1	O	100/100 (100%)	100 (100%)	0	100	100
1	P	100/100 (100%)	99 (99%)	1 (1%)	73	82
1	Q	100/100 (100%)	100 (100%)	0	100	100
1	R	100/100 (100%)	100 (100%)	0	100	100
1	S	100/100 (100%)	100 (100%)	0	100	100
1	T	100/100 (100%)	100 (100%)	0	100	100
1	U	100/100 (100%)	100 (100%)	0	100	100
1	V	100/100 (100%)	100 (100%)	0	100	100
1	W	100/100 (100%)	100 (100%)	0	100	100
1	X	100/100 (100%)	100 (100%)	0	100	100
1	Y	100/100 (100%)	100 (100%)	0	100	100
1	Z	100/100 (100%)	99 (99%)	1 (1%)	73	82
1	a	100/100 (100%)	100 (100%)	0	100	100
1	b	100/100 (100%)	98 (98%)	2 (2%)	50	68
1	c	100/100 (100%)	100 (100%)	0	100	100
1	d	100/100 (100%)	100 (100%)	0	100	100
1	e	100/100 (100%)	100 (100%)	0	100	100
1	f	100/100 (100%)	100 (100%)	0	100	100
1	g	100/100 (100%)	100 (100%)	0	100	100
1	h	100/100 (100%)	100 (100%)	0	100	100
1	i	100/100 (100%)	100 (100%)	0	100	100
1	j	100/100 (100%)	100 (100%)	0	100	100
1	k	100/100 (100%)	99 (99%)	1 (1%)	73	82
1	l	100/100 (100%)	100 (100%)	0	100	100
1	m	100/100 (100%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3900/3900 (100%)	3895 (100%)	5 (0%)	92 95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	k	52	THR
1	P	52	THR
1	b	42	ARG
1	b	95	ASP
1	Z	42	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	b	88	HIS
1	O	62	GLN
1	a	89	GLN
1	S	88	HIS
1	P	64	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

39 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	MYR	m	201	1	13,14,15	0.50	0	12,13,15	0.39	0
2	MYR	Y	201	1	13,14,15	0.50	0	12,13,15	0.32	0
2	MYR	a	201	1	13,14,15	0.52	0	12,13,15	0.38	0
2	MYR	M	201	1	13,14,15	0.54	0	12,13,15	0.27	0
2	MYR	h	201	1	13,14,15	0.49	0	12,13,15	0.35	0
2	MYR	Z	201	1	13,14,15	0.53	0	12,13,15	0.33	0
2	MYR	B	201	1	13,14,15	0.53	0	12,13,15	0.33	0
2	MYR	l	201	1	13,14,15	0.52	0	12,13,15	0.37	0
2	MYR	G	201	1	13,14,15	0.53	0	12,13,15	0.34	0
2	MYR	b	201	1	13,14,15	0.51	0	12,13,15	0.33	0
2	MYR	V	201	1	13,14,15	0.51	0	12,13,15	0.26	0
2	MYR	f	201	1	13,14,15	0.51	0	12,13,15	0.30	0
2	MYR	H	201	1	13,14,15	0.52	0	12,13,15	0.40	0
2	MYR	c	201	1	13,14,15	0.91	1 (7%)	12,13,15	1.35	1 (8%)
2	MYR	A	201	1	13,14,15	0.49	0	12,13,15	0.33	0
2	MYR	W	201	1	13,14,15	0.50	0	12,13,15	0.33	0
2	MYR	i	201	1	13,14,15	0.54	0	12,13,15	0.30	0
2	MYR	Q	201	1	13,14,15	0.54	0	12,13,15	0.38	0
2	MYR	F	201	1	13,14,15	0.50	0	12,13,15	0.38	0
2	MYR	E	201	1	13,14,15	0.51	0	12,13,15	0.33	0
2	MYR	C	201	1	13,14,15	0.47	0	12,13,15	0.42	0
2	MYR	N	201	1	13,14,15	0.51	0	12,13,15	0.33	0
2	MYR	U	201	1	13,14,15	0.52	0	12,13,15	0.31	0
2	MYR	R	201	1	13,14,15	0.55	0	12,13,15	1.13	1 (8%)
2	MYR	O	201	1	13,14,15	0.51	0	12,13,15	0.33	0
2	MYR	L	201	1	13,14,15	0.49	0	12,13,15	0.23	0
2	MYR	I	201	1	13,14,15	0.51	0	12,13,15	0.30	0
2	MYR	k	201	1	13,14,15	0.49	0	12,13,15	0.34	0
2	MYR	P	201	1	13,14,15	0.53	0	12,13,15	0.31	0
2	MYR	g	201	1	13,14,15	0.50	0	12,13,15	0.33	0
2	MYR	e	201	1	13,14,15	0.51	0	12,13,15	0.43	0
2	MYR	j	201	1	13,14,15	0.52	0	12,13,15	0.25	0
2	MYR	D	201	1	13,14,15	0.57	0	12,13,15	0.43	0
2	MYR	S	201	1	13,14,15	0.77	0	12,13,15	0.73	0
2	MYR	J	201	1	13,14,15	0.51	0	12,13,15	0.33	0
2	MYR	K	201	1	13,14,15	0.50	0	12,13,15	0.32	0
2	MYR	T	201	1	13,14,15	0.52	0	12,13,15	0.35	0
2	MYR	d	201	1	13,14,15	0.47	0	12,13,15	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MYR	X	201	1	13,14,15	0.57	0	12,13,15	0.54	0

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	MYR	m	201	1	-	0/12/12/13	-
2	MYR	Y	201	1	-	1/12/12/13	-
2	MYR	a	201	1	-	0/12/12/13	-
2	MYR	M	201	1	-	2/12/12/13	-
2	MYR	h	201	1	-	1/12/12/13	-
2	MYR	Z	201	1	-	0/12/12/13	-
2	MYR	B	201	1	-	2/12/12/13	-
2	MYR	l	201	1	-	1/12/12/13	-
2	MYR	G	201	1	-	1/12/12/13	-
2	MYR	b	201	1	-	0/12/12/13	-
2	MYR	V	201	1	-	2/12/12/13	-
2	MYR	f	201	1	-	0/12/12/13	-
2	MYR	H	201	1	-	2/12/12/13	-
2	MYR	c	201	1	-	2/12/12/13	-
2	MYR	A	201	1	-	0/12/12/13	-
2	MYR	W	201	1	-	0/12/12/13	-
2	MYR	i	201	1	-	4/12/12/13	-
2	MYR	Q	201	1	-	2/12/12/13	-
2	MYR	F	201	1	-	0/12/12/13	-
2	MYR	E	201	1	-	0/12/12/13	-
2	MYR	C	201	1	-	4/12/12/13	-
2	MYR	N	201	1	-	3/12/12/13	-
2	MYR	U	201	1	-	0/12/12/13	-
2	MYR	R	201	1	-	5/12/12/13	-
2	MYR	O	201	1	-	0/12/12/13	-
2	MYR	L	201	1	-	3/12/12/13	-
2	MYR	I	201	1	-	1/12/12/13	-
2	MYR	k	201	1	-	1/12/12/13	-
2	MYR	P	201	1	-	0/12/12/13	-
2	MYR	g	201	1	-	1/12/12/13	-
2	MYR	e	201	1	-	2/12/12/13	-
2	MYR	j	201	1	-	1/12/12/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	D	201	1	-	1/12/12/13	-
2	MYR	S	201	1	-	5/12/12/13	-
2	MYR	J	201	1	-	2/12/12/13	-
2	MYR	K	201	1	-	1/12/12/13	-
2	MYR	T	201	1	-	0/12/12/13	-
2	MYR	d	201	1	-	2/12/12/13	-
2	MYR	X	201	1	-	1/12/12/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	c	201	MYR	C3-C2	2.12	1.61	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	c	201	MYR	C5-C4-C3	4.53	137.26	114.37
2	R	201	MYR	C5-C4-C3	2.50	126.99	114.37

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	h	201	MYR	O1-C1-C2-C3
2	k	201	MYR	O1-C1-C2-C3
2	J	201	MYR	O1-C1-C2-C3
2	V	201	MYR	O1-C1-C2-C3
2	i	201	MYR	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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.