



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:27 PM UTC

PDB ID : 6EK5 / pdb_00006ek5
EMDB ID : EMD-3521
Title : Near-atomic resolution structure of a plant geminivirus determined by electron cryo-microscopy.
Authors : Grimm, C.; Bottcher, B.; Hipp, K.; Jeske, H.
Deposited on : 2017-09-25
Resolution : 4.20 Å(reported)

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

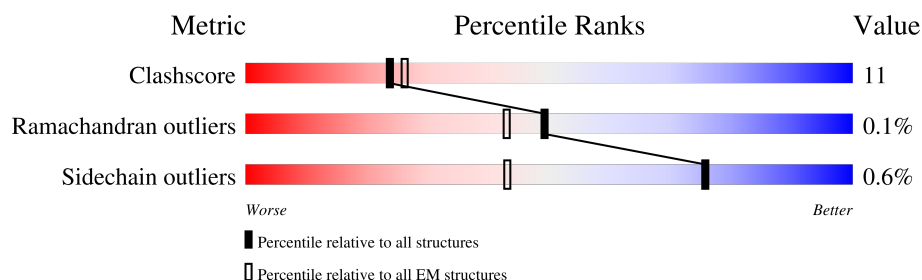
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	205	67% 21% • 11%
1	2	205	66% 22% 11%
1	3	205	65% 23% • 11%
1	A	205	62% 27% 11%
1	B	205	65% 23% 11%
1	B1	205	67% 21% 11%
1	B2	205	65% 23% • 11%
1	B3	205	65% 23% • 11%
1	BA	205	65% 23% 11%

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Mol	Chain	Length	Quality of chain
1	BB	205	
1	BC	205	
1	BD	205	
1	BE	205	
1	BF	205	
1	BG	205	
1	BH	205	
1	BI	205	
1	BJ	205	
1	BK	205	
1	BL	205	
1	BM	205	
1	BN	205	
1	BO	205	
1	BP	205	
1	BQ	205	
1	BR	205	
1	BS	205	
1	BT	205	
1	BU	205	
1	BV	205	
1	BW	205	
1	BX	205	
1	BY	205	
1	BZ	205	

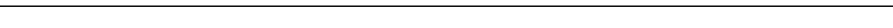
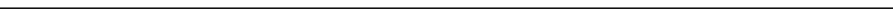
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Mol	Chain	Length	Quality of chain
1	Ba	205	 67% 22% 11%
1	Bb	205	 66% 23% 11%
1	Bc	205	 65% 24% 11%
1	Bd	205	 66% 23% 11%
1	Be	205	 65% 23% 11%
1	Bf	205	 66% 23% 11%
1	Bg	205	 66% 22% 11%
1	Bh	205	 66% 22% • 11%
1	Bi	205	 66% 23% 11%
1	Bj	205	 66% 23% 11%
1	Bk	205	 72% 23% • •
1	Bl	205	 65% 24% • 10%
1	Bm	205	 66% 23% 11%
1	Bn	205	 64% 24% 11%
1	Bo	205	 67% 22% 11%
1	Bp	205	 66% 23% 11%
1	Bq	205	 65% 23% • 11%
1	Br	205	 67% 22% 11%
1	Bs	205	 66% 22% 11%
1	Bt	205	 66% 23% 11%
1	Bu	205	 65% 24% 11%
1	Bv	205	 66% 24% 10%
1	Bw	205	 74% 21% • •
1	Bx	205	 66% 23% 11%
1	By	205	 66% 23% 11%

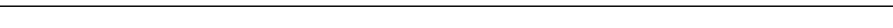
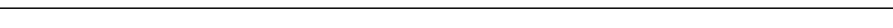
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Mol	Chain	Length	Quality of chain
1	Bz	205	
1	C	205	
1	D	205	
1	E	205	
1	F	205	
1	G	205	
1	H	205	
1	I	205	
1	J	205	
1	K	205	
1	L	205	
1	M	205	
1	N	205	
1	O	205	
1	P	205	
1	Q	205	
1	R	205	
1	S	205	
1	T	205	
1	U	205	
1	V	205	
1	W	205	
1	X	205	
1	Y	205	
1	Z	205	

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Mol	Chain	Length	Quality of chain
1	a	205	 66% 22% 11%
1	b	205	 66% 23% 11%
1	c	205	 66% 23% 11%
1	d	205	 67% 22% 11%
1	e	205	 66% 23% 11%
1	f	205	 66% 23% 11%
1	g	205	 67% 22% 11%
1	h	205	 66% 23% 11%
1	i	205	 66% 23% 11%
1	j	205	 65% 23% 11%
1	k	205	 72% 23% . .
1	l	205	 65% 24% . 10%
1	m	205	 67% 21% . 11%
1	n	205	 64% 25% 11%
1	o	205	 65% 23% 11%
1	p	205	 66% 23% 11%
1	q	205	 66% 22% 11%
1	r	205	 66% 23% 11%
1	s	205	 66% 23% 11%
1	t	205	 67% 21% . 11%
1	u	205	 66% 23% 11%
1	v	205	 65% 25% 10%
1	w	205	 73% 22% . .
1	x	205	 66% 23% 11%
1	y	205	 66% 22% 11%

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Mol	Chain	Length	Quality of chain
1	z	205	 66% 23% 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 165959 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 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	B	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	C	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	D	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	E	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	F	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	G	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	H	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		
1	I	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		
1	J	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	K	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	L	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	M	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	N	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	O	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	P	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Q	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		
1	S	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	T	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	U	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	V	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		
1	W	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		
1	X	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Y	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Z	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	BA	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	BB	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	BC	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	BD	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	a	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	b	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	c	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	d	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	e	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	f	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	g	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	h	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	j	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	m	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	n	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	o	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	p	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	q	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	r	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	s	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	t	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	u	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	x	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	y	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	z	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	3	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	1	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	2	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	k	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		
1	w	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		
1	l	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		
1	v	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BE	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BF	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BG	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BJ	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BP	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BS	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BT	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BU	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BX	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BY	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BZ	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	Ba	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	Bb	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	Bc	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	Bd	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BK	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BL	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BM	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BN	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	BO	183	Total 1495	C 956	N 270	O 260	S 9	0	0
1	Be	183	Total 1495	C 956	N 270	O 260	S 9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bf	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bg	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bh	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bi	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bj	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bm	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bn	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bo	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bp	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bq	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Br	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bs	183	Total	C	N	O	S	0	0
			1494	955	270	260	9		
1	Bt	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bu	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bx	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	By	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bz	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	B3	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	B1	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	B2	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	Bw	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BH	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		
1	BQ	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		
1	BV	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		
1	Bk	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		
1	Bv	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		
1	BI	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		
1	BR	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		
1	BW	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		
1	Bl	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		

There are 330 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ALA	ARG	conflict	UNP P03561
A	192	LEU	PRO	conflict	UNP P03561
A	194	CYS	GLY	conflict	UNP P03561
B	48	ALA	ARG	conflict	UNP P03561
B	192	LEU	PRO	conflict	UNP P03561
B	194	CYS	GLY	conflict	UNP P03561
C	48	ALA	ARG	conflict	UNP P03561
C	192	LEU	PRO	conflict	UNP P03561
C	194	CYS	GLY	conflict	UNP P03561
D	48	ALA	ARG	conflict	UNP P03561
D	192	LEU	PRO	conflict	UNP P03561
D	194	CYS	GLY	conflict	UNP P03561
E	48	ALA	ARG	conflict	UNP P03561
E	192	LEU	PRO	conflict	UNP P03561
E	194	CYS	GLY	conflict	UNP P03561
F	48	ALA	ARG	conflict	UNP P03561
F	192	LEU	PRO	conflict	UNP P03561
F	194	CYS	GLY	conflict	UNP P03561
G	48	ALA	ARG	conflict	UNP P03561
G	192	LEU	PRO	conflict	UNP P03561
G	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
H	48	ALA	ARG	conflict	UNP P03561
H	192	LEU	PRO	conflict	UNP P03561
H	194	CYS	GLY	conflict	UNP P03561
I	48	ALA	ARG	conflict	UNP P03561
I	192	LEU	PRO	conflict	UNP P03561
I	194	CYS	GLY	conflict	UNP P03561
J	48	ALA	ARG	conflict	UNP P03561
J	192	LEU	PRO	conflict	UNP P03561
J	194	CYS	GLY	conflict	UNP P03561
K	48	ALA	ARG	conflict	UNP P03561
K	192	LEU	PRO	conflict	UNP P03561
K	194	CYS	GLY	conflict	UNP P03561
L	48	ALA	ARG	conflict	UNP P03561
L	192	LEU	PRO	conflict	UNP P03561
L	194	CYS	GLY	conflict	UNP P03561
M	48	ALA	ARG	conflict	UNP P03561
M	192	LEU	PRO	conflict	UNP P03561
M	194	CYS	GLY	conflict	UNP P03561
N	48	ALA	ARG	conflict	UNP P03561
N	192	LEU	PRO	conflict	UNP P03561
N	194	CYS	GLY	conflict	UNP P03561
O	48	ALA	ARG	conflict	UNP P03561
O	192	LEU	PRO	conflict	UNP P03561
O	194	CYS	GLY	conflict	UNP P03561
P	48	ALA	ARG	conflict	UNP P03561
P	192	LEU	PRO	conflict	UNP P03561
P	194	CYS	GLY	conflict	UNP P03561
Q	48	ALA	ARG	conflict	UNP P03561
Q	192	LEU	PRO	conflict	UNP P03561
Q	194	CYS	GLY	conflict	UNP P03561
R	48	ALA	ARG	conflict	UNP P03561
R	192	LEU	PRO	conflict	UNP P03561
R	194	CYS	GLY	conflict	UNP P03561
S	48	ALA	ARG	conflict	UNP P03561
S	192	LEU	PRO	conflict	UNP P03561
S	194	CYS	GLY	conflict	UNP P03561
T	48	ALA	ARG	conflict	UNP P03561
T	192	LEU	PRO	conflict	UNP P03561
T	194	CYS	GLY	conflict	UNP P03561
U	48	ALA	ARG	conflict	UNP P03561
U	192	LEU	PRO	conflict	UNP P03561
U	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
V	48	ALA	ARG	conflict	UNP P03561
V	192	LEU	PRO	conflict	UNP P03561
V	194	CYS	GLY	conflict	UNP P03561
W	48	ALA	ARG	conflict	UNP P03561
W	192	LEU	PRO	conflict	UNP P03561
W	194	CYS	GLY	conflict	UNP P03561
X	48	ALA	ARG	conflict	UNP P03561
X	192	LEU	PRO	conflict	UNP P03561
X	194	CYS	GLY	conflict	UNP P03561
Y	48	ALA	ARG	conflict	UNP P03561
Y	192	LEU	PRO	conflict	UNP P03561
Y	194	CYS	GLY	conflict	UNP P03561
Z	48	ALA	ARG	conflict	UNP P03561
Z	192	LEU	PRO	conflict	UNP P03561
Z	194	CYS	GLY	conflict	UNP P03561
BA	48	ALA	ARG	conflict	UNP P03561
BA	192	LEU	PRO	conflict	UNP P03561
BA	194	CYS	GLY	conflict	UNP P03561
BB	48	ALA	ARG	conflict	UNP P03561
BB	192	LEU	PRO	conflict	UNP P03561
BB	194	CYS	GLY	conflict	UNP P03561
BC	48	ALA	ARG	conflict	UNP P03561
BC	192	LEU	PRO	conflict	UNP P03561
BC	194	CYS	GLY	conflict	UNP P03561
BD	48	ALA	ARG	conflict	UNP P03561
BD	192	LEU	PRO	conflict	UNP P03561
BD	194	CYS	GLY	conflict	UNP P03561
a	48	ALA	ARG	conflict	UNP P03561
a	192	LEU	PRO	conflict	UNP P03561
a	194	CYS	GLY	conflict	UNP P03561
b	48	ALA	ARG	conflict	UNP P03561
b	192	LEU	PRO	conflict	UNP P03561
b	194	CYS	GLY	conflict	UNP P03561
c	48	ALA	ARG	conflict	UNP P03561
c	192	LEU	PRO	conflict	UNP P03561
c	194	CYS	GLY	conflict	UNP P03561
d	48	ALA	ARG	conflict	UNP P03561
d	192	LEU	PRO	conflict	UNP P03561
d	194	CYS	GLY	conflict	UNP P03561
e	48	ALA	ARG	conflict	UNP P03561
e	192	LEU	PRO	conflict	UNP P03561
e	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
f	48	ALA	ARG	conflict	UNP P03561
f	192	LEU	PRO	conflict	UNP P03561
f	194	CYS	GLY	conflict	UNP P03561
g	48	ALA	ARG	conflict	UNP P03561
g	192	LEU	PRO	conflict	UNP P03561
g	194	CYS	GLY	conflict	UNP P03561
h	48	ALA	ARG	conflict	UNP P03561
h	192	LEU	PRO	conflict	UNP P03561
h	194	CYS	GLY	conflict	UNP P03561
i	48	ALA	ARG	conflict	UNP P03561
i	192	LEU	PRO	conflict	UNP P03561
i	194	CYS	GLY	conflict	UNP P03561
j	48	ALA	ARG	conflict	UNP P03561
j	192	LEU	PRO	conflict	UNP P03561
j	194	CYS	GLY	conflict	UNP P03561
m	48	ALA	ARG	conflict	UNP P03561
m	192	LEU	PRO	conflict	UNP P03561
m	194	CYS	GLY	conflict	UNP P03561
n	48	ALA	ARG	conflict	UNP P03561
n	192	LEU	PRO	conflict	UNP P03561
n	194	CYS	GLY	conflict	UNP P03561
o	48	ALA	ARG	conflict	UNP P03561
o	192	LEU	PRO	conflict	UNP P03561
o	194	CYS	GLY	conflict	UNP P03561
p	48	ALA	ARG	conflict	UNP P03561
p	192	LEU	PRO	conflict	UNP P03561
p	194	CYS	GLY	conflict	UNP P03561
q	48	ALA	ARG	conflict	UNP P03561
q	192	LEU	PRO	conflict	UNP P03561
q	194	CYS	GLY	conflict	UNP P03561
r	48	ALA	ARG	conflict	UNP P03561
r	192	LEU	PRO	conflict	UNP P03561
r	194	CYS	GLY	conflict	UNP P03561
s	48	ALA	ARG	conflict	UNP P03561
s	192	LEU	PRO	conflict	UNP P03561
s	194	CYS	GLY	conflict	UNP P03561
t	48	ALA	ARG	conflict	UNP P03561
t	192	LEU	PRO	conflict	UNP P03561
t	194	CYS	GLY	conflict	UNP P03561
u	48	ALA	ARG	conflict	UNP P03561
u	192	LEU	PRO	conflict	UNP P03561
u	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
x	48	ALA	ARG	conflict	UNP P03561
x	192	LEU	PRO	conflict	UNP P03561
x	194	CYS	GLY	conflict	UNP P03561
y	48	ALA	ARG	conflict	UNP P03561
y	192	LEU	PRO	conflict	UNP P03561
y	194	CYS	GLY	conflict	UNP P03561
z	48	ALA	ARG	conflict	UNP P03561
z	192	LEU	PRO	conflict	UNP P03561
z	194	CYS	GLY	conflict	UNP P03561
3	48	ALA	ARG	conflict	UNP P03561
3	192	LEU	PRO	conflict	UNP P03561
3	194	CYS	GLY	conflict	UNP P03561
1	48	ALA	ARG	conflict	UNP P03561
1	192	LEU	PRO	conflict	UNP P03561
1	194	CYS	GLY	conflict	UNP P03561
2	48	ALA	ARG	conflict	UNP P03561
2	192	LEU	PRO	conflict	UNP P03561
2	194	CYS	GLY	conflict	UNP P03561
k	48	ALA	ARG	conflict	UNP P03561
k	192	LEU	PRO	conflict	UNP P03561
k	194	CYS	GLY	conflict	UNP P03561
w	48	ALA	ARG	conflict	UNP P03561
w	192	LEU	PRO	conflict	UNP P03561
w	194	CYS	GLY	conflict	UNP P03561
l	48	ALA	ARG	conflict	UNP P03561
l	192	LEU	PRO	conflict	UNP P03561
l	194	CYS	GLY	conflict	UNP P03561
v	48	ALA	ARG	conflict	UNP P03561
v	192	LEU	PRO	conflict	UNP P03561
v	194	CYS	GLY	conflict	UNP P03561
BE	48	ALA	ARG	conflict	UNP P03561
BE	192	LEU	PRO	conflict	UNP P03561
BE	194	CYS	GLY	conflict	UNP P03561
BF	48	ALA	ARG	conflict	UNP P03561
BF	192	LEU	PRO	conflict	UNP P03561
BF	194	CYS	GLY	conflict	UNP P03561
BG	48	ALA	ARG	conflict	UNP P03561
BG	192	LEU	PRO	conflict	UNP P03561
BG	194	CYS	GLY	conflict	UNP P03561
BJ	48	ALA	ARG	conflict	UNP P03561
BJ	192	LEU	PRO	conflict	UNP P03561
BJ	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
BP	48	ALA	ARG	conflict	UNP P03561
BP	192	LEU	PRO	conflict	UNP P03561
BP	194	CYS	GLY	conflict	UNP P03561
BS	48	ALA	ARG	conflict	UNP P03561
BS	192	LEU	PRO	conflict	UNP P03561
BS	194	CYS	GLY	conflict	UNP P03561
BT	48	ALA	ARG	conflict	UNP P03561
BT	192	LEU	PRO	conflict	UNP P03561
BT	194	CYS	GLY	conflict	UNP P03561
BU	48	ALA	ARG	conflict	UNP P03561
BU	192	LEU	PRO	conflict	UNP P03561
BU	194	CYS	GLY	conflict	UNP P03561
BX	48	ALA	ARG	conflict	UNP P03561
BX	192	LEU	PRO	conflict	UNP P03561
BX	194	CYS	GLY	conflict	UNP P03561
BY	48	ALA	ARG	conflict	UNP P03561
BY	192	LEU	PRO	conflict	UNP P03561
BY	194	CYS	GLY	conflict	UNP P03561
BZ	48	ALA	ARG	conflict	UNP P03561
BZ	192	LEU	PRO	conflict	UNP P03561
BZ	194	CYS	GLY	conflict	UNP P03561
Ba	48	ALA	ARG	conflict	UNP P03561
Ba	192	LEU	PRO	conflict	UNP P03561
Ba	194	CYS	GLY	conflict	UNP P03561
Bb	48	ALA	ARG	conflict	UNP P03561
Bb	192	LEU	PRO	conflict	UNP P03561
Bb	194	CYS	GLY	conflict	UNP P03561
Bc	48	ALA	ARG	conflict	UNP P03561
Bc	192	LEU	PRO	conflict	UNP P03561
Bc	194	CYS	GLY	conflict	UNP P03561
Bd	48	ALA	ARG	conflict	UNP P03561
Bd	192	LEU	PRO	conflict	UNP P03561
Bd	194	CYS	GLY	conflict	UNP P03561
BK	48	ALA	ARG	conflict	UNP P03561
BK	192	LEU	PRO	conflict	UNP P03561
BK	194	CYS	GLY	conflict	UNP P03561
BL	48	ALA	ARG	conflict	UNP P03561
BL	192	LEU	PRO	conflict	UNP P03561
BL	194	CYS	GLY	conflict	UNP P03561
BM	48	ALA	ARG	conflict	UNP P03561
BM	192	LEU	PRO	conflict	UNP P03561
BM	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
BN	48	ALA	ARG	conflict	UNP P03561
BN	192	LEU	PRO	conflict	UNP P03561
BN	194	CYS	GLY	conflict	UNP P03561
BO	48	ALA	ARG	conflict	UNP P03561
BO	192	LEU	PRO	conflict	UNP P03561
BO	194	CYS	GLY	conflict	UNP P03561
Be	48	ALA	ARG	conflict	UNP P03561
Be	192	LEU	PRO	conflict	UNP P03561
Be	194	CYS	GLY	conflict	UNP P03561
Bf	48	ALA	ARG	conflict	UNP P03561
Bf	192	LEU	PRO	conflict	UNP P03561
Bf	194	CYS	GLY	conflict	UNP P03561
Bg	48	ALA	ARG	conflict	UNP P03561
Bg	192	LEU	PRO	conflict	UNP P03561
Bg	194	CYS	GLY	conflict	UNP P03561
Bh	48	ALA	ARG	conflict	UNP P03561
Bh	192	LEU	PRO	conflict	UNP P03561
Bh	194	CYS	GLY	conflict	UNP P03561
Bi	48	ALA	ARG	conflict	UNP P03561
Bi	192	LEU	PRO	conflict	UNP P03561
Bi	194	CYS	GLY	conflict	UNP P03561
Bj	48	ALA	ARG	conflict	UNP P03561
Bj	192	LEU	PRO	conflict	UNP P03561
Bj	194	CYS	GLY	conflict	UNP P03561
Bm	48	ALA	ARG	conflict	UNP P03561
Bm	192	LEU	PRO	conflict	UNP P03561
Bm	194	CYS	GLY	conflict	UNP P03561
Bn	48	ALA	ARG	conflict	UNP P03561
Bn	192	LEU	PRO	conflict	UNP P03561
Bn	194	CYS	GLY	conflict	UNP P03561
Bo	48	ALA	ARG	conflict	UNP P03561
Bo	192	LEU	PRO	conflict	UNP P03561
Bo	194	CYS	GLY	conflict	UNP P03561
Bp	48	ALA	ARG	conflict	UNP P03561
Bp	192	LEU	PRO	conflict	UNP P03561
Bp	194	CYS	GLY	conflict	UNP P03561
Bq	48	ALA	ARG	conflict	UNP P03561
Bq	192	LEU	PRO	conflict	UNP P03561
Bq	194	CYS	GLY	conflict	UNP P03561
Br	48	ALA	ARG	conflict	UNP P03561
Br	192	LEU	PRO	conflict	UNP P03561
Br	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
Bs	48	ALA	ARG	conflict	UNP P03561
Bs	192	LEU	PRO	conflict	UNP P03561
Bs	194	CYS	GLY	conflict	UNP P03561
Bt	48	ALA	ARG	conflict	UNP P03561
Bt	192	LEU	PRO	conflict	UNP P03561
Bt	194	CYS	GLY	conflict	UNP P03561
Bu	48	ALA	ARG	conflict	UNP P03561
Bu	192	LEU	PRO	conflict	UNP P03561
Bu	194	CYS	GLY	conflict	UNP P03561
Bx	48	ALA	ARG	conflict	UNP P03561
Bx	192	LEU	PRO	conflict	UNP P03561
Bx	194	CYS	GLY	conflict	UNP P03561
By	48	ALA	ARG	conflict	UNP P03561
By	192	LEU	PRO	conflict	UNP P03561
By	194	CYS	GLY	conflict	UNP P03561
Bz	48	ALA	ARG	conflict	UNP P03561
Bz	192	LEU	PRO	conflict	UNP P03561
Bz	194	CYS	GLY	conflict	UNP P03561
B3	48	ALA	ARG	conflict	UNP P03561
B3	192	LEU	PRO	conflict	UNP P03561
B3	194	CYS	GLY	conflict	UNP P03561
B1	48	ALA	ARG	conflict	UNP P03561
B1	192	LEU	PRO	conflict	UNP P03561
B1	194	CYS	GLY	conflict	UNP P03561
B2	48	ALA	ARG	conflict	UNP P03561
B2	192	LEU	PRO	conflict	UNP P03561
B2	194	CYS	GLY	conflict	UNP P03561
Bw	48	ALA	ARG	conflict	UNP P03561
Bw	192	LEU	PRO	conflict	UNP P03561
Bw	194	CYS	GLY	conflict	UNP P03561
BH	48	ALA	ARG	conflict	UNP P03561
BH	192	LEU	PRO	conflict	UNP P03561
BH	194	CYS	GLY	conflict	UNP P03561
BQ	48	ALA	ARG	conflict	UNP P03561
BQ	192	LEU	PRO	conflict	UNP P03561
BQ	194	CYS	GLY	conflict	UNP P03561
BV	48	ALA	ARG	conflict	UNP P03561
BV	192	LEU	PRO	conflict	UNP P03561
BV	194	CYS	GLY	conflict	UNP P03561
Bk	48	ALA	ARG	conflict	UNP P03561
Bk	192	LEU	PRO	conflict	UNP P03561
Bk	194	CYS	GLY	conflict	UNP P03561

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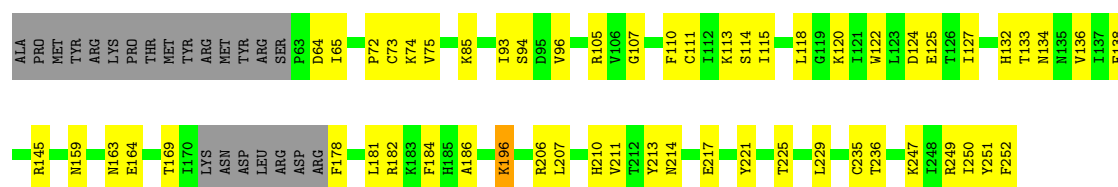
Chain	Residue	Modelled	Actual	Comment	Reference
Bv	48	ALA	ARG	conflict	UNP P03561
Bv	192	LEU	PRO	conflict	UNP P03561
Bv	194	CYS	GLY	conflict	UNP P03561
BI	48	ALA	ARG	conflict	UNP P03561
BI	192	LEU	PRO	conflict	UNP P03561
BI	194	CYS	GLY	conflict	UNP P03561
BR	48	ALA	ARG	conflict	UNP P03561
BR	192	LEU	PRO	conflict	UNP P03561
BR	194	CYS	GLY	conflict	UNP P03561
BW	48	ALA	ARG	conflict	UNP P03561
BW	192	LEU	PRO	conflict	UNP P03561
BW	194	CYS	GLY	conflict	UNP P03561
Bl	48	ALA	ARG	conflict	UNP P03561
Bl	192	LEU	PRO	conflict	UNP P03561
Bl	194	CYS	GLY	conflict	UNP P03561

3 Residue-property plots

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.

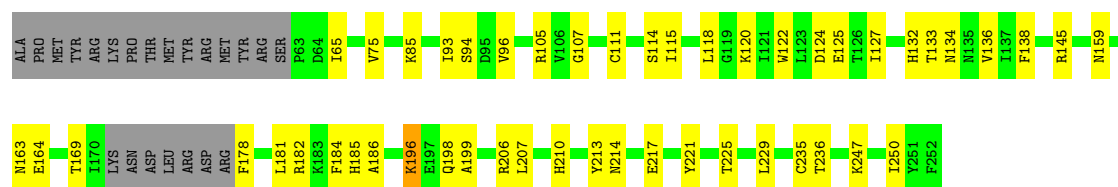
- Molecule 1: Capsid protein

Chain A: 



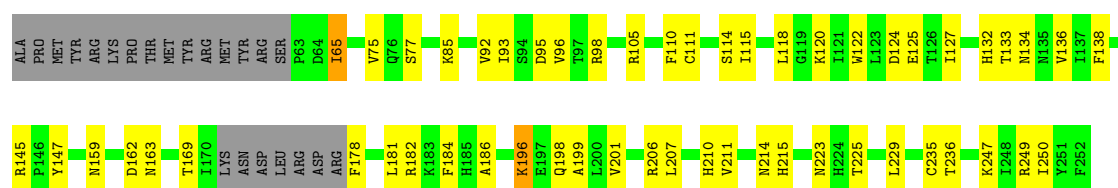
- Molecule 1: Capsid protein

Chain B: 



- Molecule 1: Capsid protein

Chain C: 



- Molecule 1: Capsid protein

Chain D: 





- Molecule 1: Capsid protein

Chain E: 66% 23% 11%



- Molecule 1: Capsid protein

Chain F: 65% 23% 11%



- Molecule 1: Capsid protein

Chain G: 64% 24% 11%



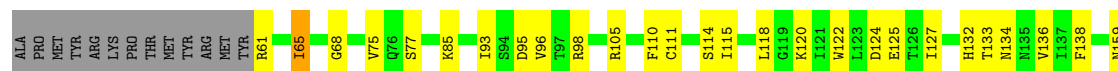
- Molecule 1: Capsid protein

Chain H: 72% 24% ..



- Molecule 1: Capsid protein

Chain I: 65% 24% • 10%





- Molecule 1: Capsid protein

Chain J: 66% 22% 11%



- Molecule 1: Capsid protein

Chain K: 66% 23% 11%



- Molecule 1: Capsid protein

Chain L: 66% 23% 11%



- Molecule 1: Capsid protein

Chain M: 67% 22% 11%



- Molecule 1: Capsid protein

Chain N: 66% 23% 11%





- Molecule 1: Capsid protein

Chain O: 66% 22% 11%



- Molecule 1: Capsid protein

Chain P: 63% 26% 11%



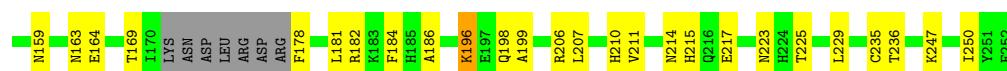
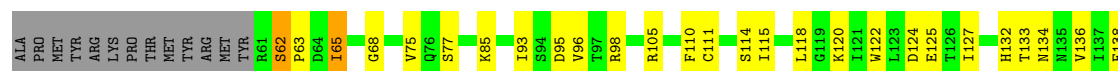
- Molecule 1: Capsid protein

Chain Q: 73% 23% 4%



- Molecule 1: Capsid protein

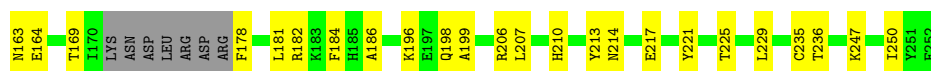
Chain R: 64% 24% 12%



- Molecule 1: Capsid protein

Chain S: 66% 23% 11%





- Molecule 1: Capsid protein

Chain T: 66% 23% 11%



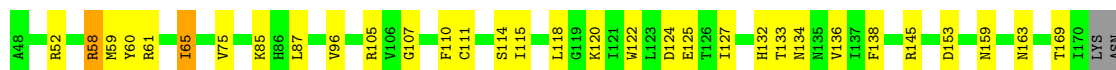
- Molecule 1: Capsid protein

Chain U: 65% 23% 11%



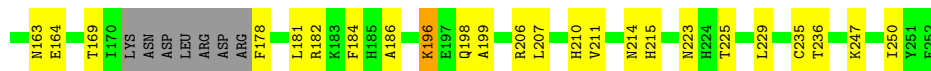
- Molecule 1: Capsid protein

Chain V: 73% 22% 5%



- Molecule 1: Capsid protein

Chain W: 65% 24% 10%



- Molecule 1: Capsid protein

Chain X: 66% 22% 11%





- Molecule 1: Capsid protein

Chain Y: 64% 24% 11%



- Molecule 1: Capsid protein

Chain Z: 67% 22% 11%



- Molecule 1: Capsid protein

Chain BA: 65% 23% 11%



- Molecule 1: Capsid protein

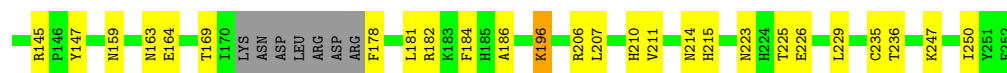
Chain BB: 67% 21% 11%



- Molecule 1: Capsid protein

Chain BC: 64% 24% 11%





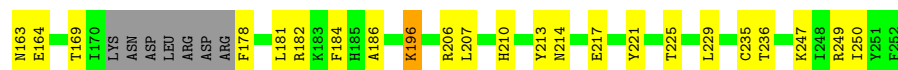
- Molecule 1: Capsid protein

Chain BD: 66% 22% 11%



- Molecule 1: Capsid protein

Chain a: 66% 22% 11%



- Molecule 1: Capsid protein

Chain b: 66% 23% 11%



- Molecule 1: Capsid protein

Chain c: 66% 23% 11%



- Molecule 1: Capsid protein

Chain d: 67% 22% 11%

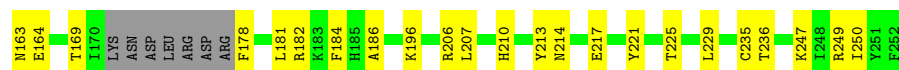




- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein





- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

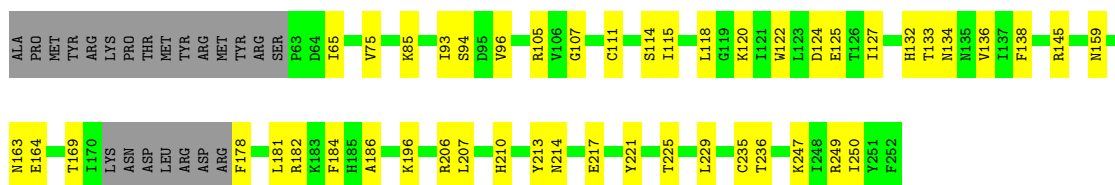


- Molecule 1: Capsid protein



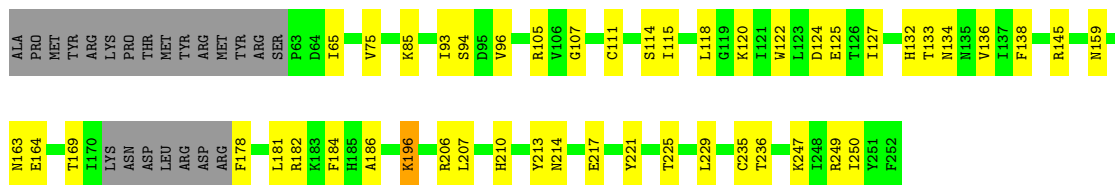
- Molecule 1: Capsid protein





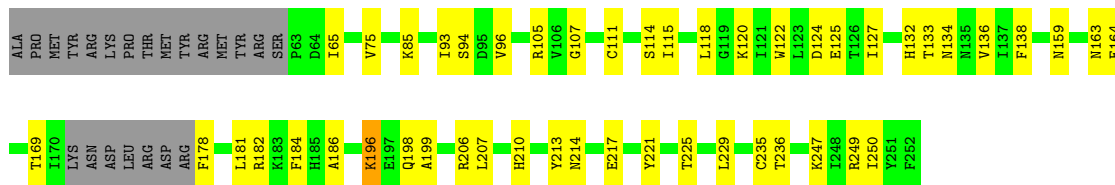
- Molecule 1: Capsid protein

Chain q: 66% 22% 11%



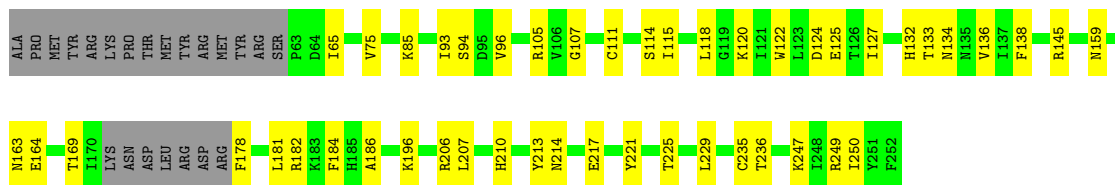
- Molecule 1: Capsid protein

Chain r: 66% 23% 11%



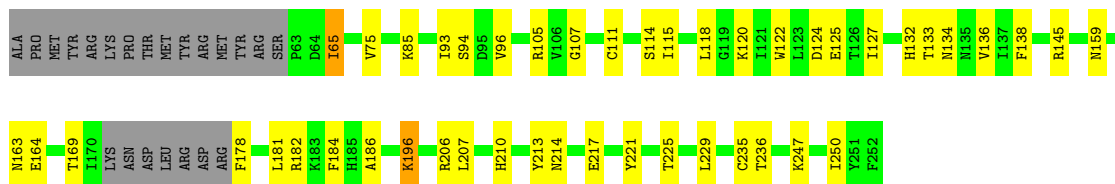
- Molecule 1: Capsid protein

Chain s: 66% 23% 11%



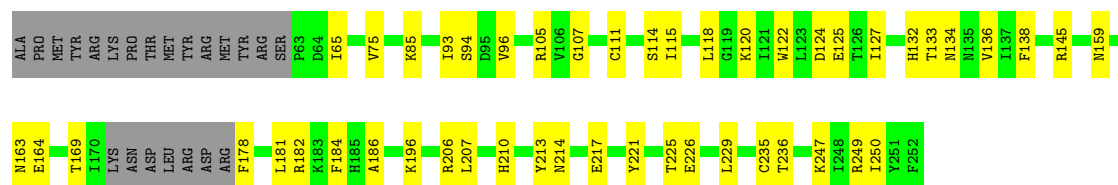
- Molecule 1: Capsid protein

Chain t: 67% 21% 11%



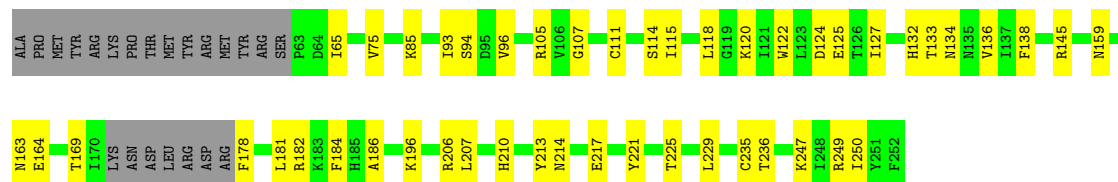
- Molecule 1: Capsid protein

Chain u: 66% 23% 11%



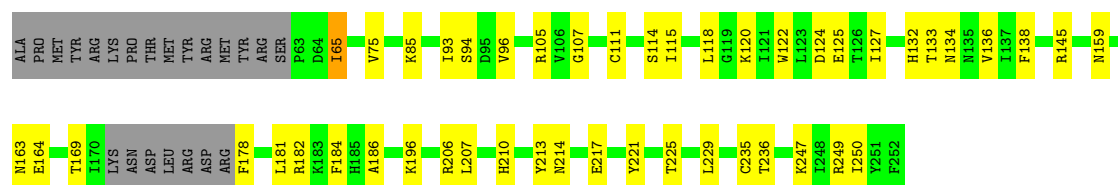
- Molecule 1: Capsid protein

Chain x: 66% 23% 11%



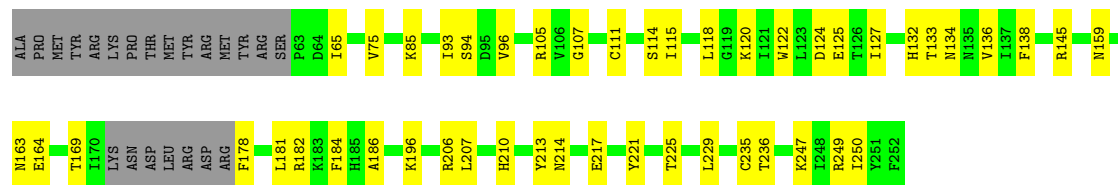
- Molecule 1: Capsid protein

Chain y: 66% 22% 11%



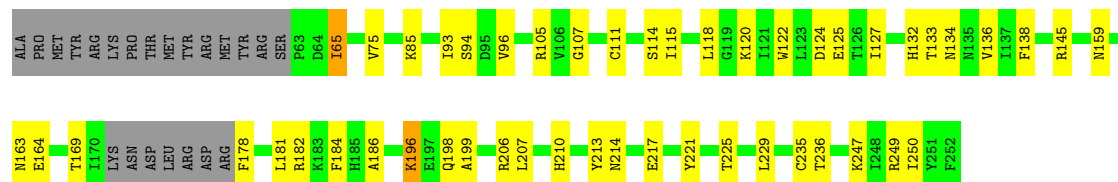
- Molecule 1: Capsid protein

Chain z: 66% 23% 11%



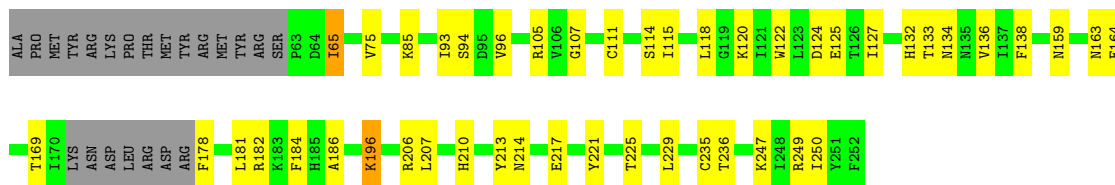
- Molecule 1: Capsid protein

Chain 3: 65% 23% 11%

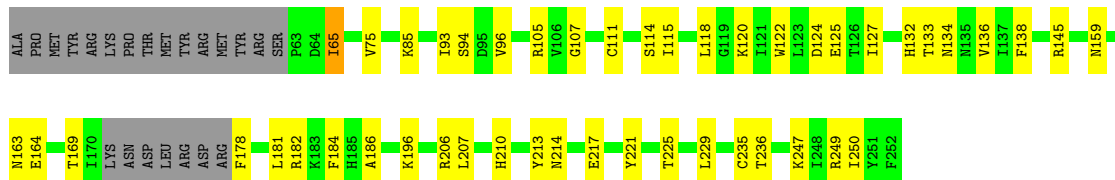


- Molecule 1: Capsid protein

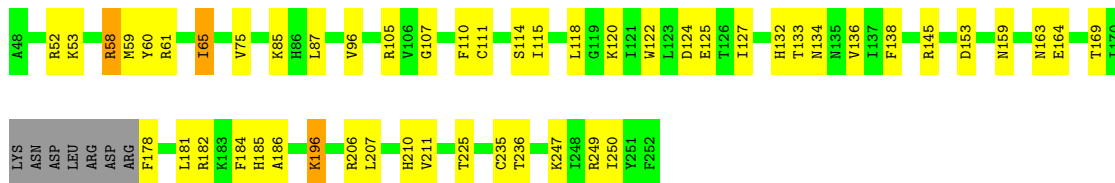
Chain 1: 67% 21% 11%



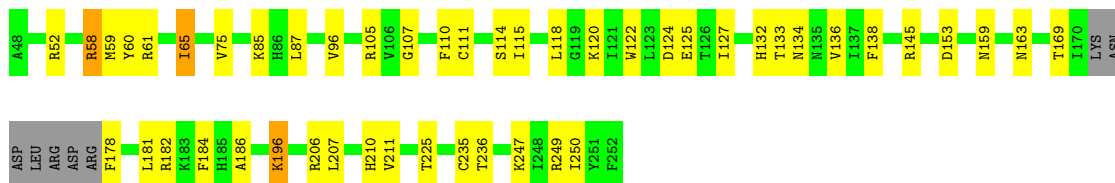
- Molecule 1: Capsid protein



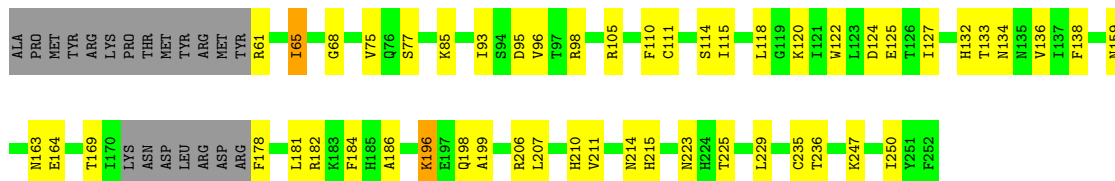
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

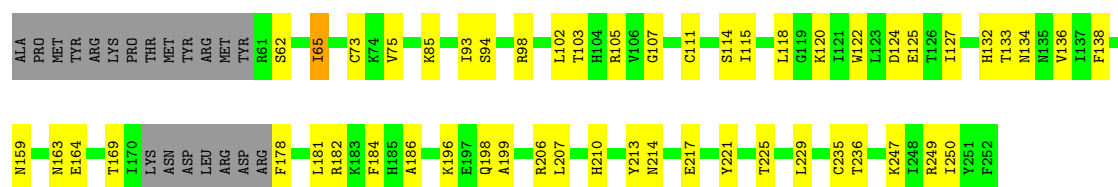


- Molecule 1: Capsid protein

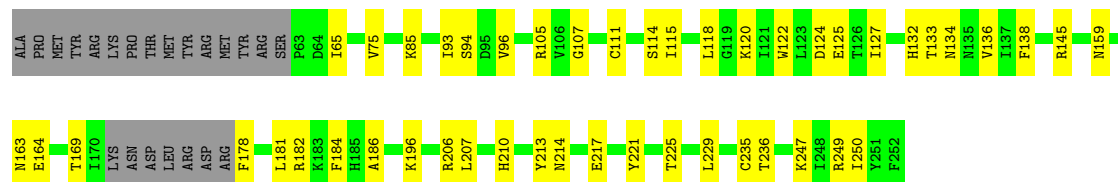


- Molecule 1: Capsid protein

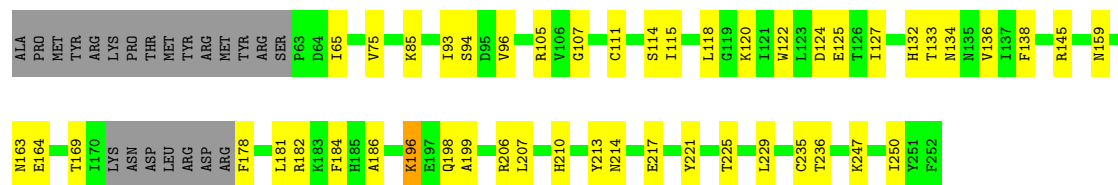




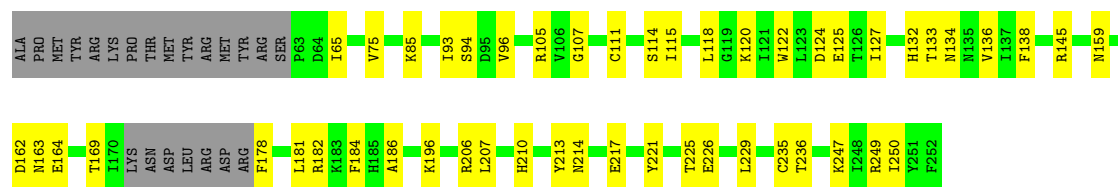
- Molecule 1: Capsid protein



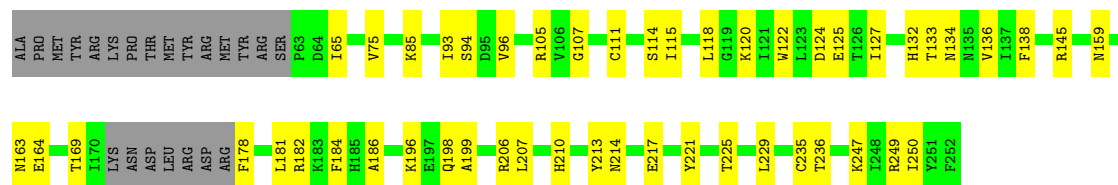
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

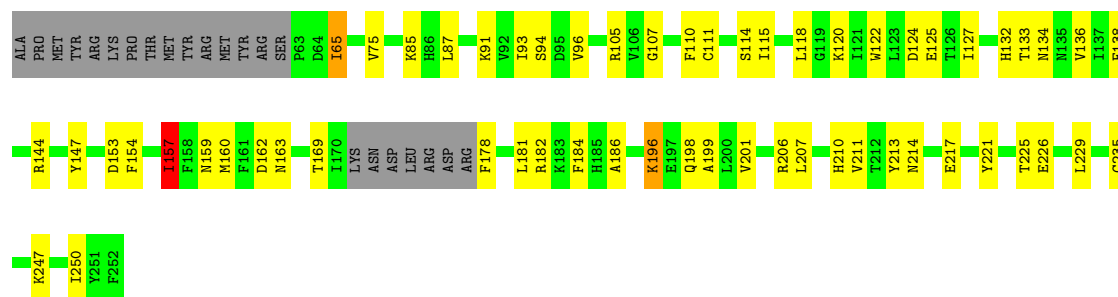


- Molecule 1: Capsid protein



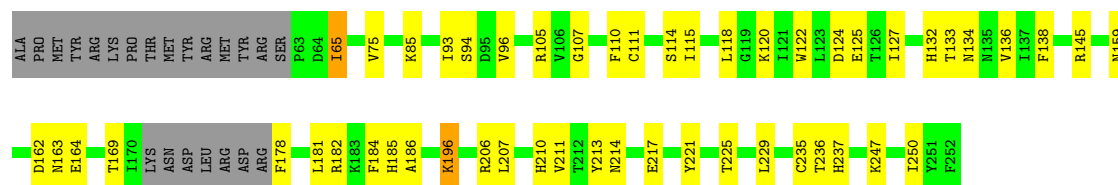
- Molecule 1: Capsid protein





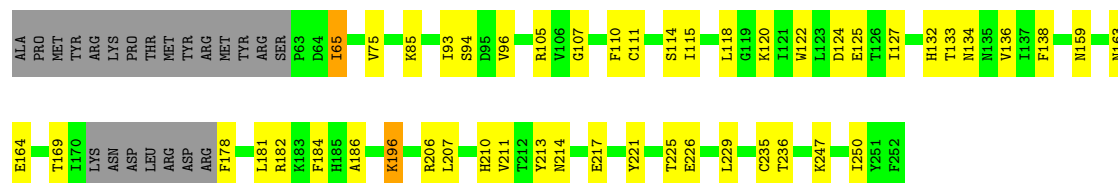
• Molecule 1: Capsid protein

Chain BS: 64% 24% 11%



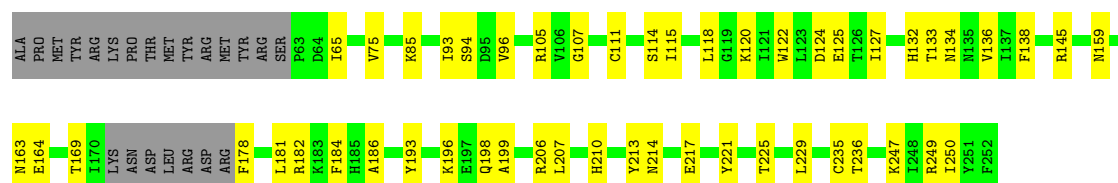
• Molecule 1: Capsid protein

Chain BT: 66% 22% 11%



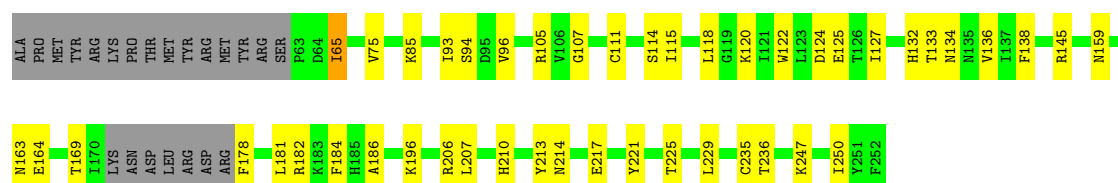
• Molecule 1: Capsid protein

Chain BU: 65% 24% 11%



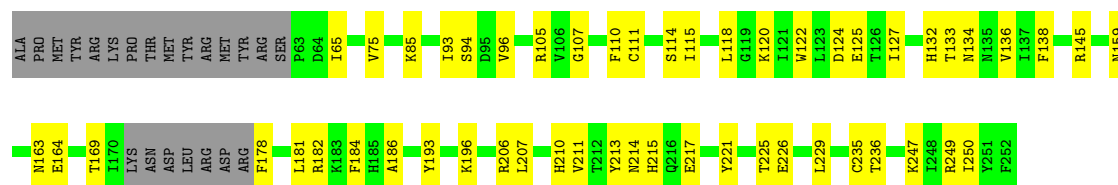
• Molecule 1: Capsid protein

Chain BX: 67% 22% 11%



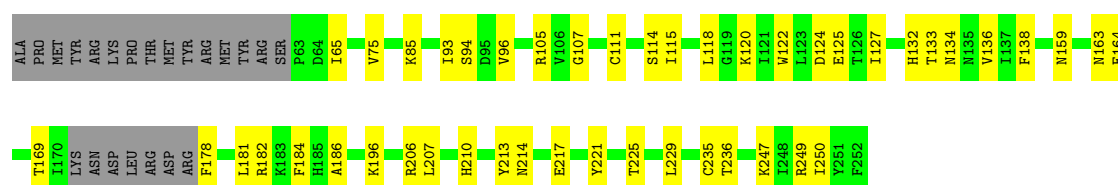
- Molecule 1: Capsid protein

Chain BY:  64% 25% 11%



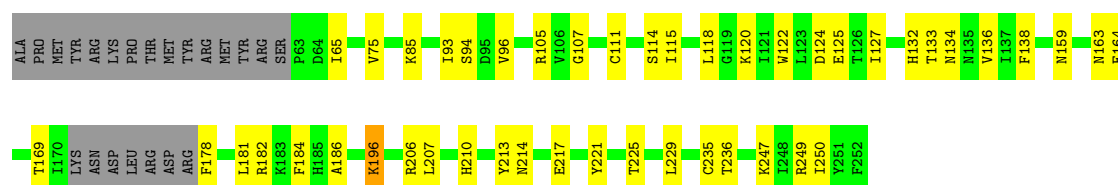
- Molecule 1: Capsid protein

Chain BZ:  67% 22% 11%



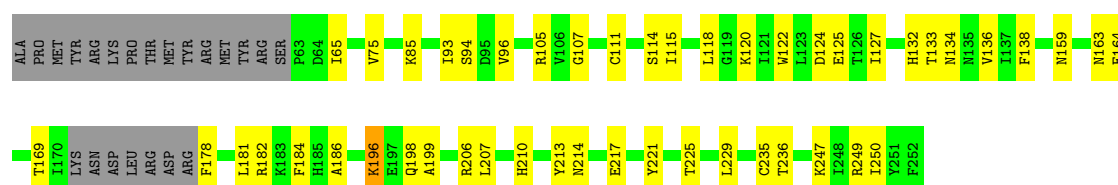
- Molecule 1: Capsid protein

Chain Ba:  67% 22% 11%



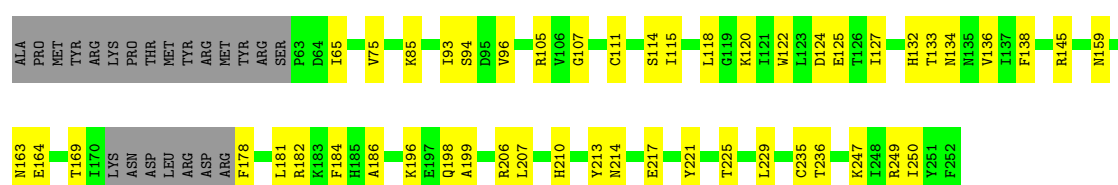
- Molecule 1: Capsid protein

Chain Bb:  66% 23% 11%



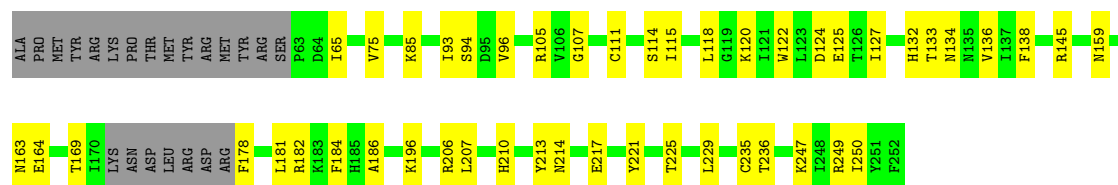
- Molecule 1: Capsid protein

Chain Bc:  65% 24% 11%



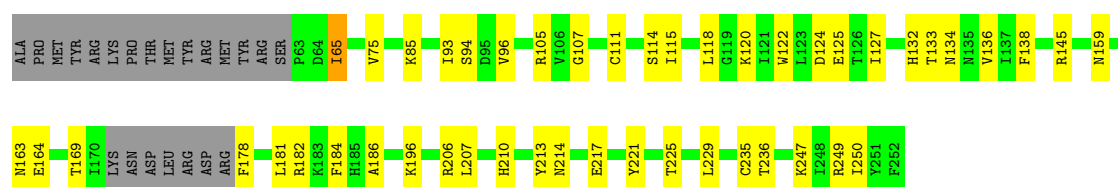
- Molecule 1: Capsid protein

Chain Bd:  66% 23% 11%



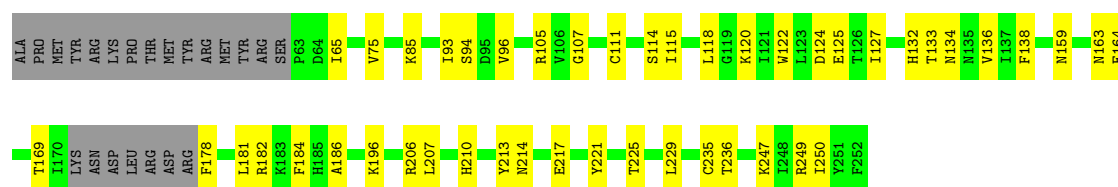
- Molecule 1: Capsid protein

Chain BK:  66% 22% 11%



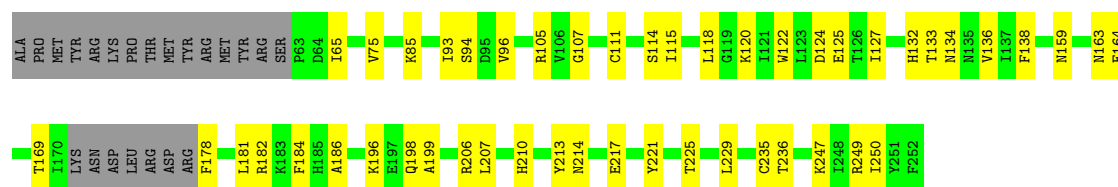
- Molecule 1: Capsid protein

Chain BL:  67% 22% 11%



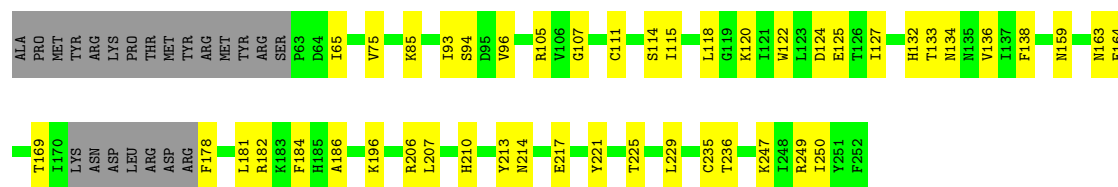
- Molecule 1: Capsid protein

Chain BM:  66% 23% 11%



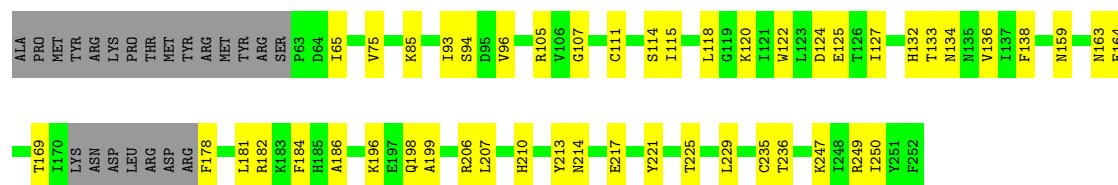
- Molecule 1: Capsid protein

Chain BN:  67% 22% 11%



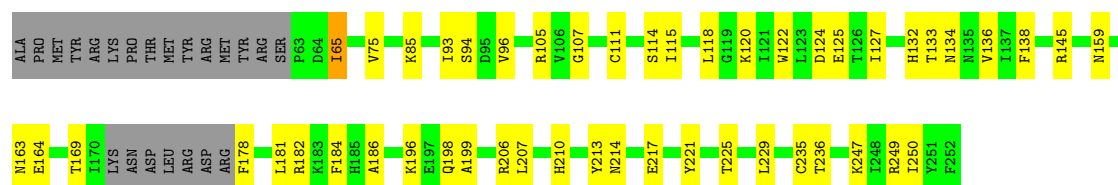
- Molecule 1: Capsid protein

Chain BO:  66% 23% 11%



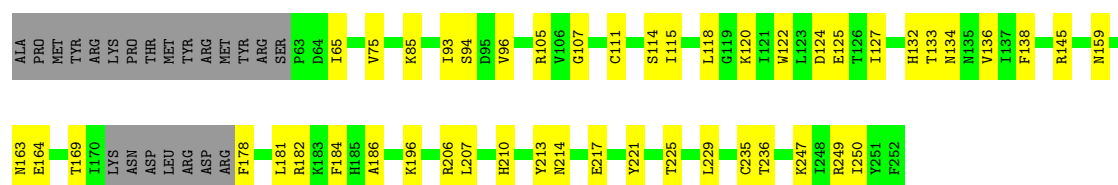
- Molecule 1: Capsid protein

Chain Be:  65% 23% 11%



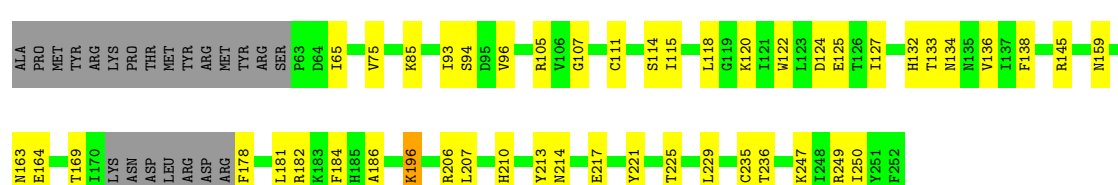
- Molecule 1: Capsid protein

Chain Bf:  66% 23% 11%



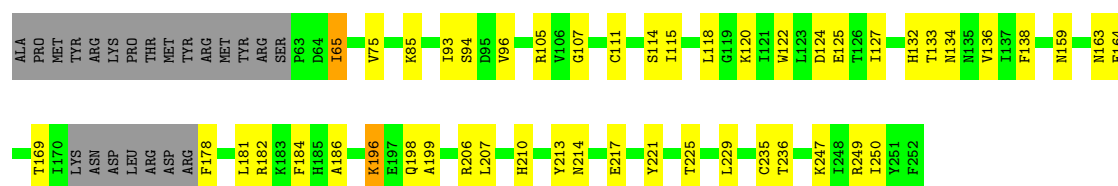
- Molecule 1: Capsid protein

Chain Bg:  66% 22% 11%



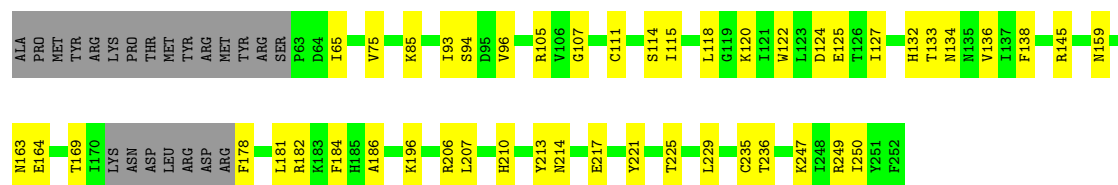
- Molecule 1: Capsid protein

Chain Bh:  66% 22% 11%



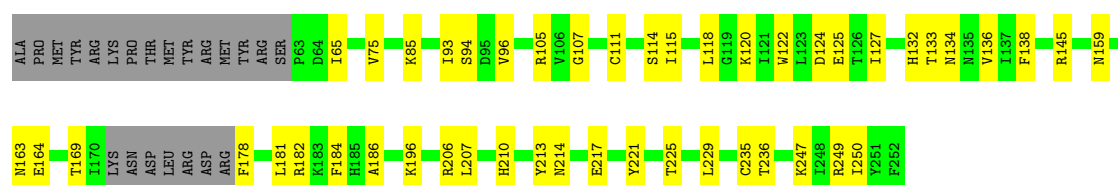
- Molecule 1: Capsid protein

Chain Bi:  66% 23% 11%



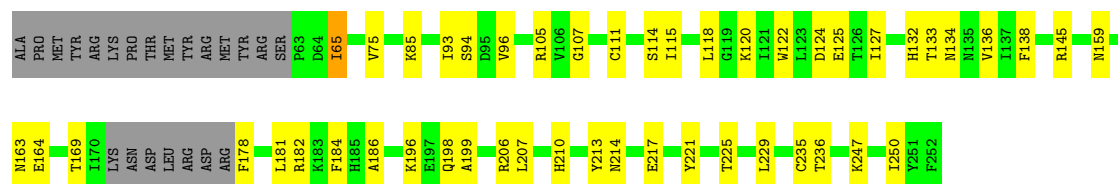
- Molecule 1: Capsid protein

Chain Bj:  66% 23% 11%



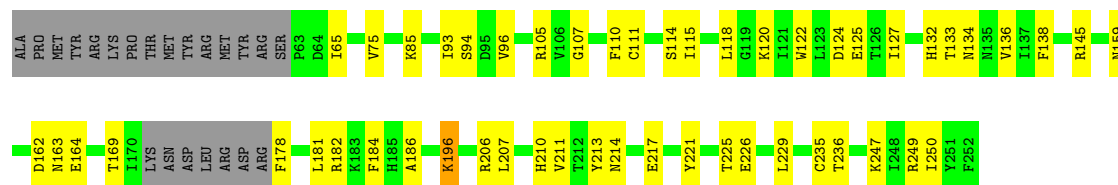
- Molecule 1: Capsid protein

Chain Bm:  66% 23% 11%



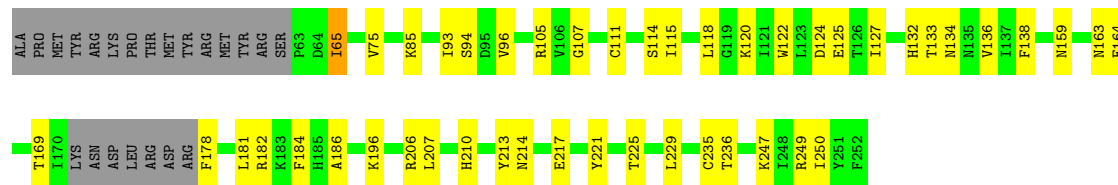
- Molecule 1: Capsid protein

Chain Bn:  64% 24% 11%

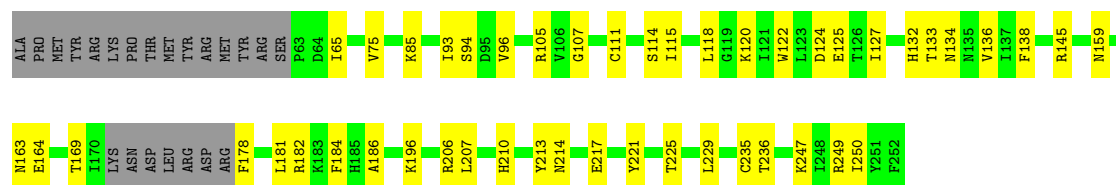


- Molecule 1: Capsid protein

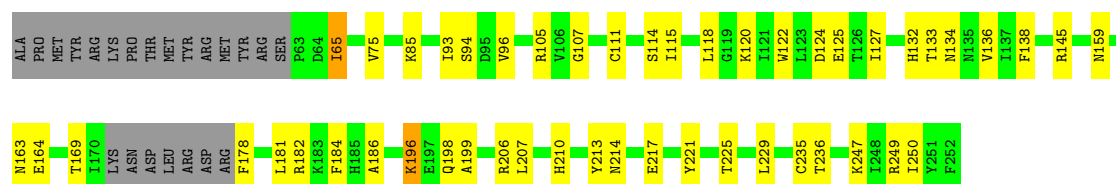
Chain Bo:  67% 22% 11%



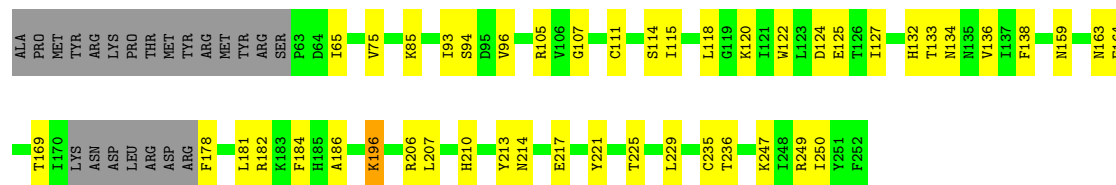
● Molecule 1: Capsid protein

Chain Bp:  66% 23% 11%

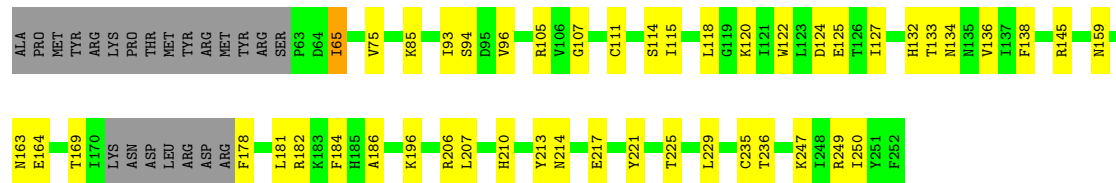
● Molecule 1: Capsid protein

Chain Bq:  65% 23% 11%

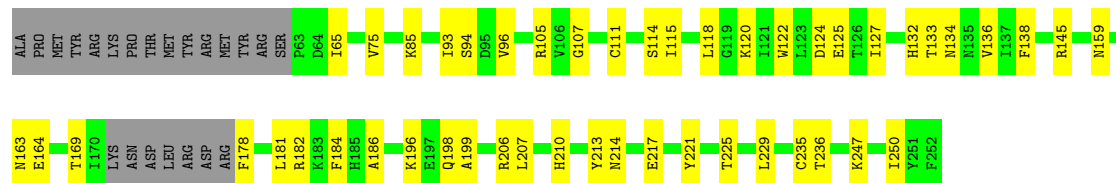
● Molecule 1: Capsid protein

Chain Br:  67% 22% 11%

● Molecule 1: Capsid protein

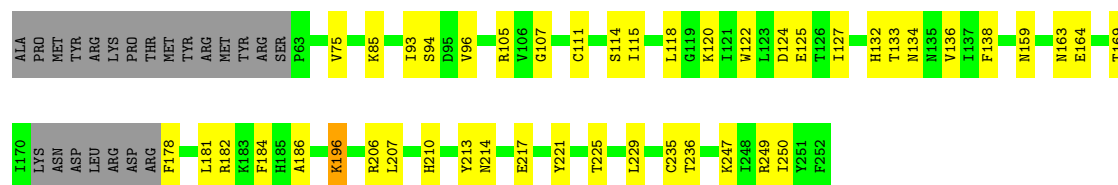
Chain Bs:  66% 22% 11%

● Molecule 1: Capsid protein

Chain Bt:  66% 23% 11%

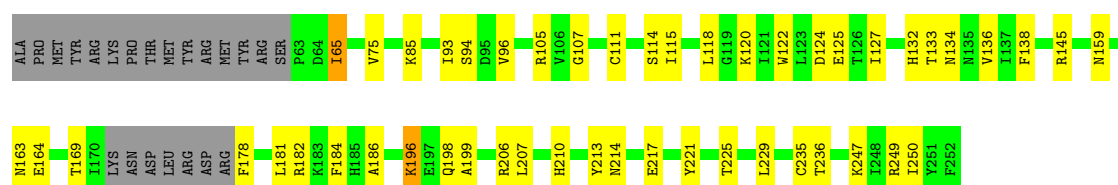
- Molecule 1: Capsid protein

Chain B1:  67% 21% 11%



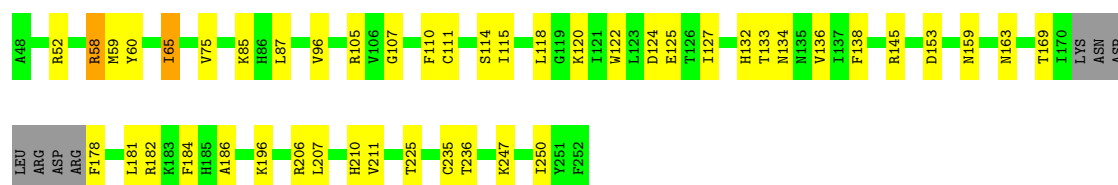
- Molecule 1: Capsid protein

Chain B2:  65% 23% 11%



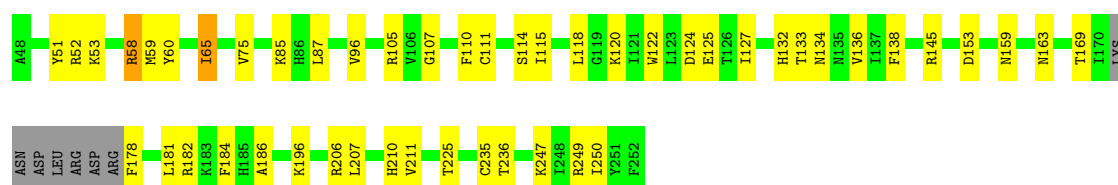
- Molecule 1: Capsid protein

Chain Bw:  74% 21% 5%



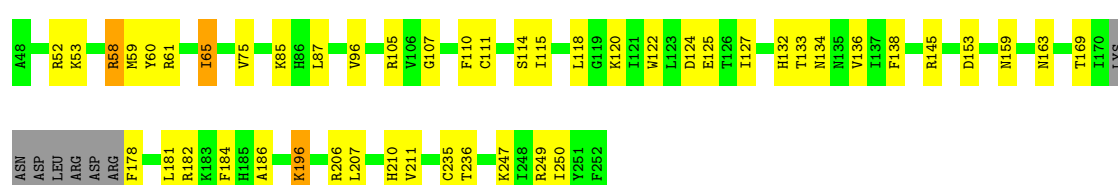
- Molecule 1: Capsid protein

Chain BH:  73% 23% 4%



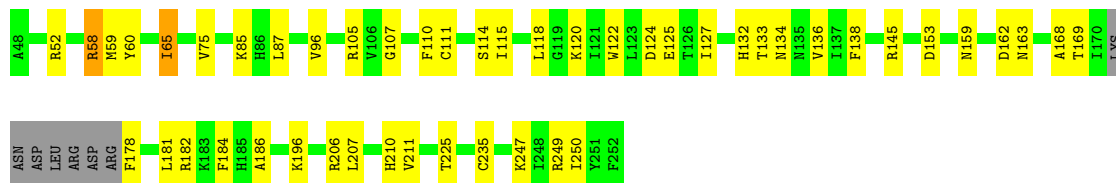
- Molecule 1: Capsid protein

Chain BQ:  73% 22% 5%



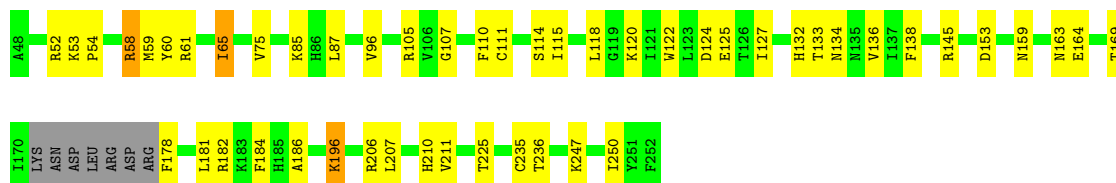
- Molecule 1: Capsid protein

Chain BV:  73% 22% ..



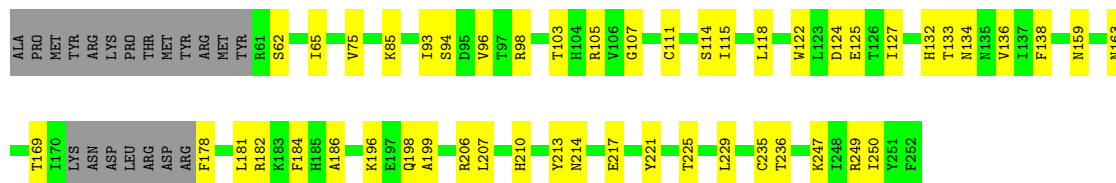
- Molecule 1: Capsid protein

Chain Bk:  72% 23% ..



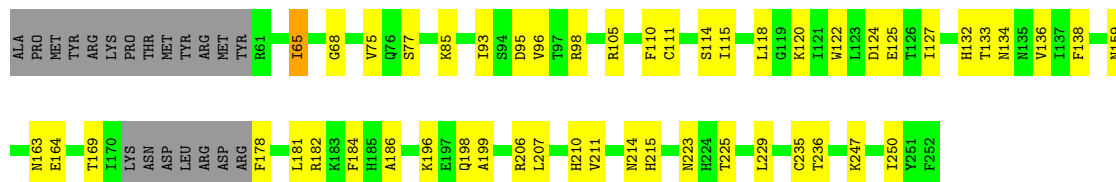
- Molecule 1: Capsid protein

Chain Bv:  66% 24% 10%



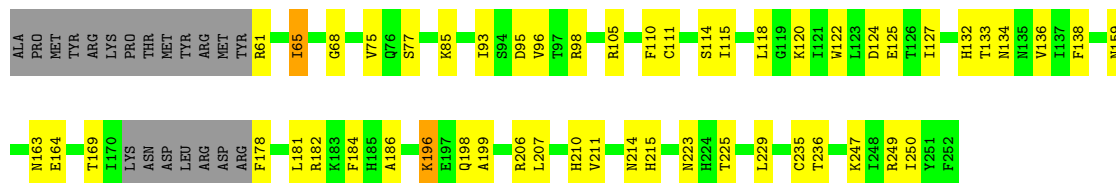
- Molecule 1: Capsid protein

Chain BI:  66% 24% 10%



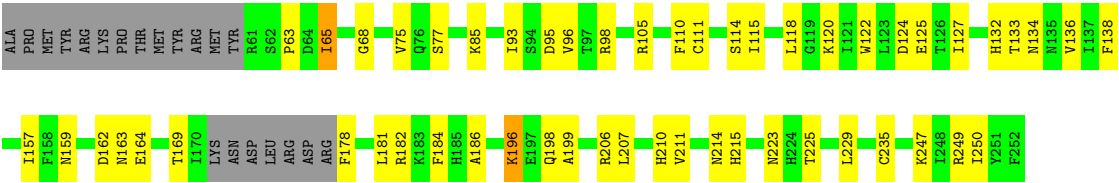
- Molecule 1: Capsid protein

Chain BR:  65% 24% 10%

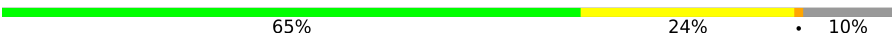


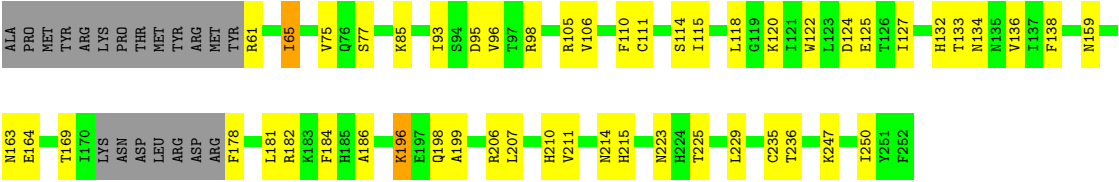
● Molecule 1: Capsid protein

Chain BW:  64% 25% 10%



● Molecule 1: Capsid protein

Chain Bl:  65% 24% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	24451	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)	780	Depositor
Maximum defocus (nm)	5600	Depositor
Magnification	94000	Depositor
Image detector	FEI FALCON II (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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.21	0/1532	0.69	0/2067
1	2	0.22	0/1532	0.70	0/2067
1	3	0.21	0/1532	0.69	0/2067
1	A	0.23	0/1532	0.71	0/2067
1	B	0.22	0/1532	0.69	0/2067
1	B1	0.21	0/1532	0.69	0/2067
1	B2	0.21	0/1532	0.69	0/2067
1	B3	0.21	0/1532	0.69	0/2067
1	BA	0.21	0/1532	0.69	0/2067
1	BB	0.22	0/1532	0.69	0/2067
1	BC	0.30	0/1532	0.78	0/2067
1	BD	0.21	0/1532	0.69	0/2067
1	BE	0.21	0/1532	0.69	0/2067
1	BF	0.22	0/1532	0.70	0/2067
1	BG	0.22	0/1532	0.70	0/2067
1	BH	0.30	0/1671	0.80	2/2254 (0.1%)
1	BI	0.30	0/1549	0.79	0/2090
1	BJ	0.22	0/1532	0.69	0/2067
1	BK	0.21	0/1532	0.69	0/2067
1	BL	0.21	0/1532	0.69	0/2067
1	BM	0.21	0/1532	0.69	0/2067
1	BN	0.21	0/1532	0.69	0/2067
1	BO	0.21	0/1532	0.69	0/2067
1	BP	0.68	4/1532 (0.3%)	0.90	7/2067 (0.3%)
1	BQ	0.32	0/1671	0.81	2/2254 (0.1%)
1	BR	0.29	0/1549	0.79	0/2090
1	BS	0.23	0/1532	0.70	0/2067
1	BT	0.25	0/1532	0.71	0/2067
1	BU	0.22	0/1532	0.69	0/2067
1	BV	0.30	0/1671	0.80	2/2254 (0.1%)
1	BW	0.39	1/1549 (0.1%)	0.82	0/2090
1	BX	0.22	0/1532	0.69	0/2067
1	BY	0.22	0/1532	0.71	0/2067
1	BZ	0.21	0/1532	0.69	0/2067

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ba	0.21	0/1532	0.69	0/2067
1	Bb	0.21	0/1532	0.69	0/2067
1	Bc	0.21	0/1532	0.69	0/2067
1	Bd	0.21	0/1532	0.69	0/2067
1	Be	0.21	0/1532	0.69	0/2067
1	Bf	0.21	0/1532	0.70	0/2067
1	Bg	0.21	0/1532	0.69	0/2067
1	Bh	0.21	0/1532	0.69	0/2067
1	Bi	0.21	0/1532	0.69	0/2067
1	Bj	0.21	0/1532	0.69	0/2067
1	Bk	0.31	0/1671	0.80	2/2254 (0.1%)
1	Bl	0.30	0/1549	0.79	0/2090
1	Bm	0.21	0/1532	0.69	0/2067
1	Bn	0.22	0/1532	0.70	0/2067
1	Bo	0.21	0/1532	0.69	0/2067
1	Bp	0.21	0/1532	0.69	0/2067
1	Bq	0.21	0/1532	0.69	0/2067
1	Br	0.21	0/1532	0.69	0/2067
1	Bs	0.22	0/1531	0.70	0/2065
1	Bt	0.22	0/1532	0.69	0/2067
1	Bu	0.22	0/1532	0.70	0/2067
1	Bv	0.27	0/1549	0.81	4/2090 (0.2%)
1	Bw	0.30	0/1671	0.80	2/2254 (0.1%)
1	Bx	0.21	0/1532	0.69	0/2067
1	By	0.21	0/1532	0.69	0/2067
1	Bz	0.22	0/1532	0.69	0/2067
1	C	0.31	0/1532	0.78	0/2067
1	D	0.21	0/1532	0.69	0/2067
1	E	0.21	0/1532	0.69	0/2067
1	F	0.22	0/1532	0.70	0/2067
1	G	0.23	0/1532	0.70	0/2067
1	H	0.30	0/1671	0.80	2/2254 (0.1%)
1	I	0.29	0/1549	0.79	0/2090
1	J	0.24	0/1532	0.69	0/2067
1	K	0.21	0/1532	0.69	0/2067
1	L	0.21	0/1532	0.69	0/2067
1	M	0.21	0/1532	0.69	0/2067
1	N	0.21	0/1532	0.69	0/2067
1	O	0.21	0/1532	0.69	0/2067
1	P	0.22	0/1532	0.76	3/2067 (0.1%)
1	Q	0.30	0/1671	0.80	2/2254 (0.1%)
1	R	0.29	0/1549	0.83	2/2090 (0.1%)
1	S	0.22	0/1532	0.69	0/2067

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	T	0.26	0/1532	0.70	0/2067
1	U	0.21	0/1532	0.69	0/2067
1	V	0.31	0/1671	0.81	2/2254 (0.1%)
1	W	0.38	0/1549	0.80	0/2090
1	X	0.22	0/1532	0.69	0/2067
1	Y	0.23	0/1532	0.70	0/2067
1	Z	0.21	0/1532	0.69	0/2067
1	a	0.21	0/1532	0.69	0/2067
1	b	0.21	0/1532	0.69	0/2067
1	c	0.21	0/1532	0.69	0/2067
1	d	0.21	0/1532	0.70	0/2067
1	e	0.21	0/1532	0.69	0/2067
1	f	0.21	0/1532	0.69	0/2067
1	g	0.21	0/1532	0.69	0/2067
1	h	0.21	0/1532	0.69	0/2067
1	i	0.21	0/1532	0.69	0/2067
1	j	0.21	0/1532	0.69	0/2067
1	k	0.33	0/1671	0.81	2/2254 (0.1%)
1	l	0.30	0/1549	0.79	0/2090
1	m	0.21	0/1532	0.69	0/2067
1	n	0.24	0/1532	0.69	0/2067
1	o	0.21	0/1532	0.69	0/2067
1	p	0.22	0/1532	0.69	0/2067
1	q	0.21	0/1532	0.69	0/2067
1	r	0.21	0/1532	0.70	0/2067
1	s	0.21	0/1532	0.69	0/2067
1	t	0.21	0/1532	0.69	0/2067
1	u	0.22	0/1532	0.70	0/2067
1	v	0.27	0/1549	0.75	2/2090 (0.1%)
1	w	0.30	0/1671	0.80	2/2254 (0.1%)
1	x	0.21	0/1532	0.69	0/2067
1	y	0.21	0/1532	0.69	0/2067
1	z	0.22	0/1532	0.69	0/2067
All	All	0.25	5/170079 (0.0%)	0.72	38/229468 (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
1	1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	1
1	3	0	1
1	A	0	1
1	B	0	1
1	B1	0	1
1	B2	0	1
1	B3	0	1
1	BA	0	1
1	BB	0	1
1	BC	0	1
1	BD	0	1
1	BE	0	1
1	BF	0	1
1	BG	0	1
1	BH	0	2
1	BI	0	1
1	BJ	0	1
1	BK	0	1
1	BL	0	1
1	BM	0	1
1	BN	0	1
1	BO	0	1
1	BP	0	2
1	BQ	0	2
1	BR	0	1
1	BS	0	1
1	BT	0	1
1	BU	0	1
1	BV	0	2
1	BW	0	1
1	BX	0	1
1	BY	0	1
1	BZ	0	1
1	Ba	0	1
1	Bb	0	1
1	Bc	0	1
1	Bd	0	1
1	Be	0	1
1	Bf	0	1
1	Bg	0	1
1	Bh	0	1
1	Bi	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Bj	0	1
1	Bk	0	2
1	Bl	0	1
1	Bm	0	1
1	Bn	0	1
1	Bo	0	1
1	Bp	0	1
1	Bq	0	1
1	Br	0	1
1	Bs	0	1
1	Bt	0	1
1	Bu	0	1
1	Bv	0	1
1	Bw	0	2
1	Bx	0	1
1	By	0	1
1	Bz	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	2
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	1
1	Q	0	2
1	R	0	2
1	S	0	1
1	T	0	1
1	U	0	1
1	V	0	2
1	W	0	1
1	X	0	1
1	Y	0	1
1	Z	0	1
1	a	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	b	0	1
1	c	0	1
1	d	0	1
1	e	0	1
1	f	0	1
1	g	0	1
1	h	0	1
1	i	0	1
1	j	0	1
1	k	0	2
1	l	0	1
1	m	0	1
1	n	0	1
1	o	0	1
1	p	0	1
1	q	0	1
1	r	0	1
1	s	0	1
1	t	0	1
1	u	0	1
1	v	0	1
1	w	0	2
1	x	0	1
1	y	0	1
1	z	0	1
All	All	0	122

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BP	91	LYS	C-N	17.97	1.54	1.33
1	BP	144	ARG	C-N	11.08	1.47	1.33
1	BP	110	PHE	C-N	11.07	1.51	1.33
1	BW	157	ILE	C-N	6.55	1.42	1.33
1	BP	211	VAL	C-N	6.45	1.42	1.33

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BP	157	ILE	O-C-N	-12.34	109.00	122.83
1	Bv	62	SER	C-N-CD	-11.97	94.26	120.60
1	BP	157	ILE	CA-C-N	11.09	138.82	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BP	157	ILE	C-N-CA	11.09	138.82	121.19
1	BP	144	ARG	O-C-N	9.88	135.60	122.36

There are no chirality outliers.

5 of 122 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	LYS	Peptide
1	B	196	LYS	Peptide
1	C	196	LYS	Peptide
1	D	196	LYS	Peptide
1	E	196	LYS	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	1	1495	0	1488	35	0
1	2	1495	0	1488	34	0
1	3	1495	0	1488	38	0
1	A	1495	0	1488	43	0
1	B	1495	0	1488	41	0
1	B1	1495	0	1488	35	0
1	B2	1495	0	1488	37	0
1	B3	1495	0	1488	37	0
1	BA	1495	0	1488	37	0
1	BB	1495	0	1488	37	0
1	BC	1495	0	1488	40	0
1	BD	1495	0	1488	35	0
1	BE	1495	0	1488	35	0
1	BF	1495	0	1488	36	0
1	BG	1495	0	1488	38	0
1	BH	1629	0	1624	37	0
1	BI	1512	0	1505	38	0
1	BJ	1495	0	1488	37	0
1	BK	1495	0	1488	37	0
1	BL	1495	0	1488	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BM	1495	0	1488	35	0
1	BN	1495	0	1488	33	0
1	BO	1495	0	1488	35	0
1	BP	1495	0	1488	51	0
1	BQ	1629	0	1624	38	0
1	BR	1512	0	1505	49	0
1	BS	1495	0	1488	45	0
1	BT	1495	0	1488	43	0
1	BU	1495	0	1488	36	0
1	BV	1629	0	1624	34	0
1	BW	1512	0	1505	44	0
1	BX	1495	0	1488	36	0
1	BY	1495	0	1488	43	0
1	BZ	1495	0	1488	34	0
1	Ba	1495	0	1488	35	0
1	Bb	1495	0	1488	37	0
1	Bc	1495	0	1488	35	0
1	Bd	1495	0	1488	37	0
1	Be	1495	0	1488	37	0
1	Bf	1495	0	1488	36	0
1	Bg	1495	0	1488	37	0
1	Bh	1495	0	1488	40	0
1	Bi	1495	0	1488	35	0
1	Bj	1495	0	1488	35	0
1	Bk	1629	0	1624	40	0
1	Bl	1512	0	1505	40	0
1	Bm	1495	0	1488	37	0
1	Bn	1495	0	1488	39	0
1	Bo	1495	0	1488	34	0
1	Bp	1495	0	1488	34	0
1	Bq	1495	0	1488	38	0
1	Br	1495	0	1488	34	0
1	Bs	1494	0	1484	34	0
1	Bt	1495	0	1488	35	0
1	Bu	1495	0	1488	37	0
1	Bv	1512	0	1505	38	0
1	Bw	1629	0	1624	34	0
1	Bx	1495	0	1488	35	0
1	By	1495	0	1488	36	0
1	Bz	1495	0	1488	37	0
1	C	1495	0	1488	44	0
1	D	1495	0	1488	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1495	0	1488	35	0
1	F	1495	0	1488	39	0
1	G	1495	0	1488	43	0
1	H	1629	0	1624	38	0
1	I	1512	0	1505	44	0
1	J	1495	0	1488	38	0
1	K	1495	0	1488	35	0
1	L	1495	0	1488	34	0
1	M	1495	0	1488	35	0
1	N	1495	0	1488	35	0
1	O	1495	0	1488	35	0
1	P	1495	0	1488	42	0
1	Q	1629	0	1624	41	0
1	R	1512	0	1505	43	0
1	S	1495	0	1488	37	0
1	T	1495	0	1488	42	0
1	U	1495	0	1488	40	0
1	V	1629	0	1624	40	0
1	W	1512	0	1505	45	0
1	X	1495	0	1488	40	0
1	Y	1495	0	1488	45	0
1	Z	1495	0	1488	36	0
1	a	1495	0	1488	38	0
1	b	1495	0	1488	37	0
1	c	1495	0	1488	35	0
1	d	1495	0	1488	37	0
1	e	1495	0	1488	34	0
1	f	1495	0	1488	36	0
1	g	1495	0	1488	38	0
1	h	1495	0	1488	38	0
1	i	1495	0	1488	34	0
1	j	1495	0	1488	37	0
1	k	1629	0	1624	43	0
1	l	1512	0	1505	41	0
1	m	1495	0	1488	36	0
1	n	1495	0	1488	41	0
1	o	1495	0	1488	38	0
1	p	1495	0	1488	36	0
1	q	1495	0	1488	37	0
1	r	1495	0	1488	39	0
1	s	1495	0	1488	36	0
1	t	1495	0	1488	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	u	1495	0	1488	38	0
1	v	1512	0	1505	42	0
1	w	1629	0	1624	37	0
1	x	1495	0	1488	35	0
1	y	1495	0	1488	35	0
1	z	1495	0	1488	34	0
All	All	165959	0	165206	3622	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 11.

The worst 5 of 3622 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:THR:HB	1:C:120:LYS:NZ	1.92	0.85
1:BA:105:ARG:NH1	1:BA:107:GLY:O	2.10	0.84
1:q:105:ARG:NH1	1:q:107:GLY:O	2.10	0.84
1:t:105:ARG:NH1	1:t:107:GLY:O	2.10	0.84
1:BE:105:ARG:NH1	1:BE:107:GLY:O	2.10	0.84

There are no symmetry-related clashes.

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	1	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	2	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	3	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	A	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	B	179/205 (87%)	144 (80%)	35 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B1	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	B2	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	B3	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	BA	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	BB	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	BC	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	BD	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	BE	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	BF	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	BG	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	BH	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	24	62
1	BI	181/205 (88%)	145 (80%)	36 (20%)	0	100	100
1	BJ	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	BK	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	BL	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	BM	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	BN	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	BO	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	BP	179/205 (87%)	146 (82%)	33 (18%)	0	100	100
1	BQ	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	24	62
1	BR	181/205 (88%)	145 (80%)	36 (20%)	0	100	100
1	BS	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	BT	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	BU	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	BV	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	24	62
1	BW	181/205 (88%)	143 (79%)	37 (20%)	1 (1%)	21	58
1	BX	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	BY	179/205 (87%)	146 (82%)	33 (18%)	0	100	100
1	BZ	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Ba	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bb	179/205 (87%)	144 (80%)	35 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bc	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bd	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Be	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bf	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bg	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bh	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bi	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bj	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bk	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	24	62
1	Bl	181/205 (88%)	145 (80%)	36 (20%)	0	100	100
1	Bm	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	Bn	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	Bo	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bp	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bq	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Br	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bs	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bt	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bu	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bv	181/205 (88%)	145 (80%)	36 (20%)	0	100	100
1	Bw	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	24	62
1	Bx	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	By	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Bz	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	C	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	D	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	E	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	F	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	G	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	H	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	24	62
1	I	181/205 (88%)	145 (80%)	36 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	K	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	L	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	M	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	N	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	O	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	P	179/205 (87%)	146 (82%)	33 (18%)	0	100	100
1	Q	194/205 (95%)	154 (79%)	39 (20%)	1 (0%)	24	62
1	R	181/205 (88%)	145 (80%)	35 (19%)	1 (1%)	21	58
1	S	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	T	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	U	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	V	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	24	62
1	W	181/205 (88%)	145 (80%)	36 (20%)	0	100	100
1	X	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Y	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	Z	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	a	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	b	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	c	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	d	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	e	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	f	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	g	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	h	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	i	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	j	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	k	194/205 (95%)	154 (79%)	39 (20%)	1 (0%)	24	62
1	l	181/205 (88%)	145 (80%)	36 (20%)	0	100	100
1	m	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	n	179/205 (87%)	145 (81%)	34 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	o	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	p	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	q	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	r	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	s	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	t	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	u	179/205 (87%)	144 (80%)	35 (20%)	0	100	100
1	v	181/205 (88%)	146 (81%)	35 (19%)	0	100	100
1	w	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	24	62
1	x	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	y	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
1	z	179/205 (87%)	145 (81%)	34 (19%)	0	100	100
All	All	19860/22550 (88%)	16012 (81%)	3836 (19%)	12 (0%)	49	82

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BW	63	PRO
1	H	59	MET
1	Q	59	MET
1	V	59	MET
1	k	59	MET

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	1	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	2	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	3	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	A	162/183 (88%)	161 (99%)	1 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	B1	162/183 (88%)	162 (100%)	0	100	100
1	B2	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	B3	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BA	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BB	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BC	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BD	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BE	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BF	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BG	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BH	176/183 (96%)	175 (99%)	1 (1%)	78	80
1	BI	164/183 (90%)	163 (99%)	1 (1%)	78	80
1	BJ	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BK	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BL	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BM	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BN	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BO	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BP	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BQ	176/183 (96%)	175 (99%)	1 (1%)	78	80
1	BR	164/183 (90%)	163 (99%)	1 (1%)	78	80
1	BS	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BT	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BU	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BV	176/183 (96%)	175 (99%)	1 (1%)	78	80
1	BW	164/183 (90%)	163 (99%)	1 (1%)	78	80
1	BX	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BY	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	BZ	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Ba	162/183 (88%)	161 (99%)	1 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bb	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bc	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bd	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Be	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bf	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bg	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bh	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bi	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bj	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bk	176/183 (96%)	175 (99%)	1 (1%)	78	80
1	Bl	164/183 (90%)	163 (99%)	1 (1%)	78	80
1	Bm	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bn	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bo	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bp	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bq	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Br	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bs	161/183 (88%)	160 (99%)	1 (1%)	78	80
1	Bt	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bu	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bv	164/183 (90%)	163 (99%)	1 (1%)	78	80
1	Bw	176/183 (96%)	175 (99%)	1 (1%)	78	80
1	Bx	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	By	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Bz	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	C	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	D	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	E	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	F	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	G	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	H	176/183 (96%)	175 (99%)	1 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	164/183 (90%)	163 (99%)	1 (1%)	78	80
1	J	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	K	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	L	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	M	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	N	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	O	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	P	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Q	176/183 (96%)	175 (99%)	1 (1%)	78	80
1	R	164/183 (90%)	163 (99%)	1 (1%)	78	80
1	S	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	T	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	U	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	V	176/183 (96%)	175 (99%)	1 (1%)	78	80
1	W	164/183 (90%)	163 (99%)	1 (1%)	78	80
1	X	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Y	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	Z	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	a	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	b	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	c	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	d	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	e	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	f	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	g	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	h	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	i	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	j	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	k	176/183 (96%)	175 (99%)	1 (1%)	78	80
1	l	164/183 (90%)	163 (99%)	1 (1%)	78	80
1	m	162/183 (88%)	161 (99%)	1 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	n	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	o	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	p	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	q	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	r	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	s	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	t	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	u	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	v	164/183 (90%)	163 (99%)	1 (1%)	78	80
1	w	176/183 (96%)	175 (99%)	1 (1%)	78	80
1	x	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	y	162/183 (88%)	161 (99%)	1 (1%)	78	80
1	z	162/183 (88%)	161 (99%)	1 (1%)	78	80
All	All	17979/20130 (89%)	17870 (99%)	109 (1%)	76	80

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	l	65	ILE
1	Bb	65	ILE
1	Bw	65	ILE
1	BE	65	ILE
1	BT	65	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
1	Bh	132	HIS
1	BH	185	HIS
1	Bm	185	HIS
1	Bt	185	HIS
1	Bv	132	HIS

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.