



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 04:01 PM UTC

PDB ID : 9EK2 / pdb_00009ek2
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 : 2LYB, 7TBP

This is a Full wwPDB EM Validation Report for a publicly released PDB 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:

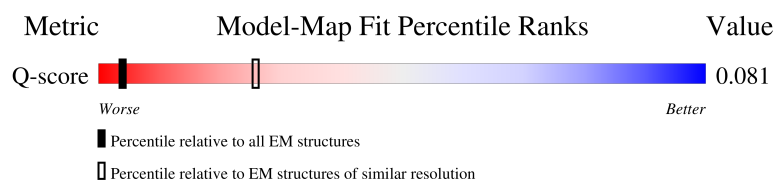
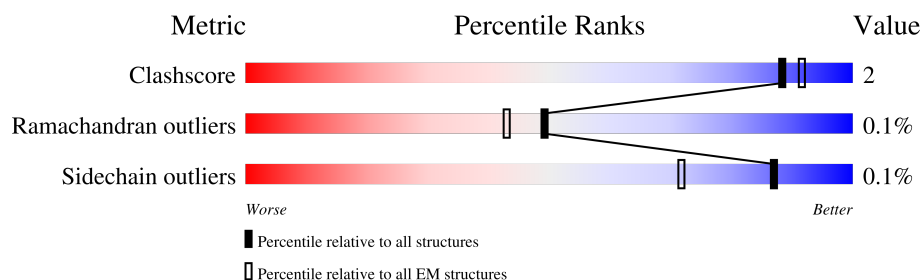
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	280 (7.82 - 8.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	13% 92% 8%
1	B	115	9% 97% .
1	C	115	9% 87% 13%
1	D	115	14% 89% 11%

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Mol	Chain	Length	Quality of chain
1	E	115	
1	F	115	
1	G	115	
1	H	115	
1	I	115	
1	J	115	
1	K	115	
1	L	115	
1	M	115	
1	N	115	
1	O	115	
1	P	115	
1	Q	115	
1	R	115	
1	S	115	
1	T	115	
1	U	115	
1	V	115	
1	W	115	
1	X	115	
1	Y	115	
1	Z	115	
1	a	115	
1	b	115	
1	c	115	

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Mol	Chain	Length	Quality of chain
1	d	115	100% 96% .
1	e	115	31% 93% 7%
1	f	115	86% 92% 8%
1	g	115	93% 97% .
1	h	115	63% 94% 6%
1	i	115	100% 91% 9%
1	j	115	100% 95% 5%
1	k	115	95% 96% .
1	l	115	36% 97% .
1	m	115	87% 94% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MYR	c	201	-	-	X	-
2	MYR	e	201	-	-	X	-

2 Entry composition

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

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

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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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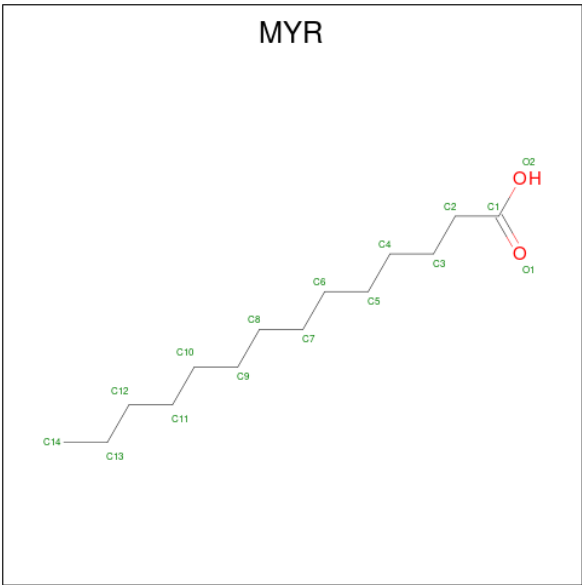
Chain	Residue	Modelled	Actual	Comment	Reference
b	20	LYS	LEU	engineered mutation	UNP P12497
b	73	LYS	GLU	engineered mutation	UNP P12497
b	82	THR	ALA	engineered mutation	UNP P12497
B	20	LYS	LEU	engineered mutation	UNP P12497
B	73	LYS	GLU	engineered mutation	UNP P12497
B	82	THR	ALA	engineered mutation	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 (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



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

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

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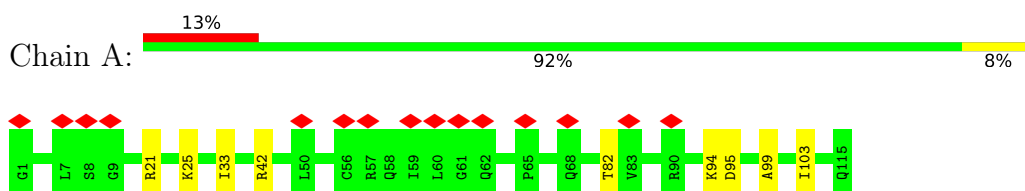
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Mol	Chain	Residues	Atoms			AltConf
2	U	1	Total	C	O	0
			15	14	1	
2	X	1	Total	C	O	0
			15	14	1	
2	a	1	Total	C	O	0
			15	14	1	
2	d	1	Total	C	O	0
			15	14	1	

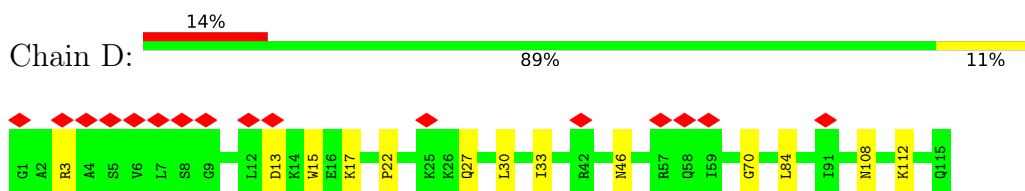
3 Residue-property plots [i](#)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

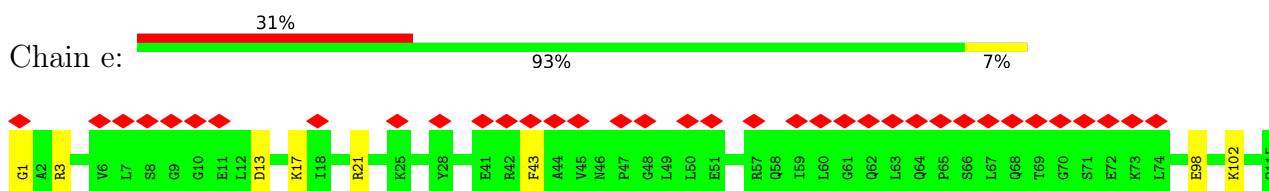
- Molecule 1: Matrix protein p17



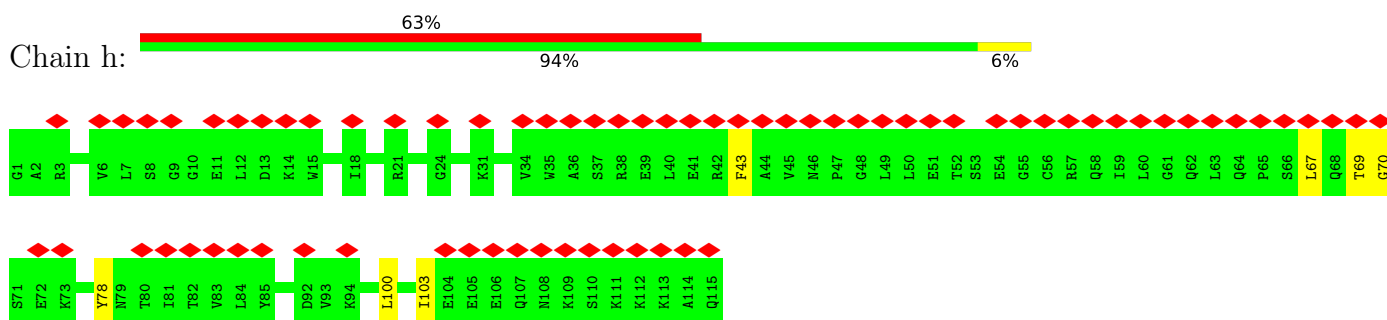
- Molecule 1: Matrix protein p17



- Molecule 1: Matrix protein p17

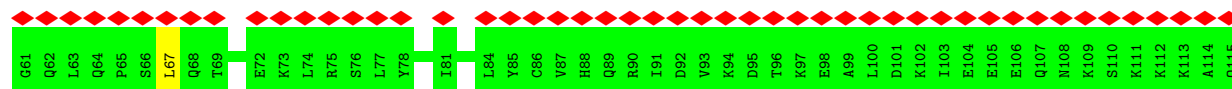
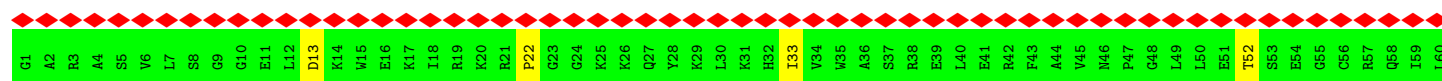


- Molecule 1: Matrix protein p17

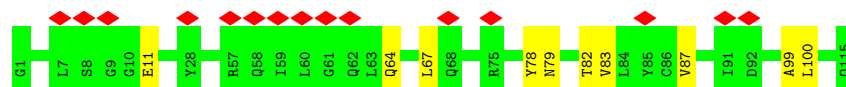
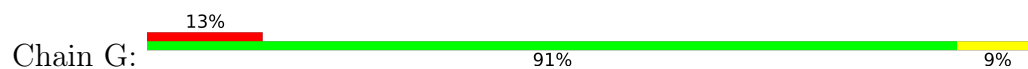


- Molecule 1: Matrix protein p17

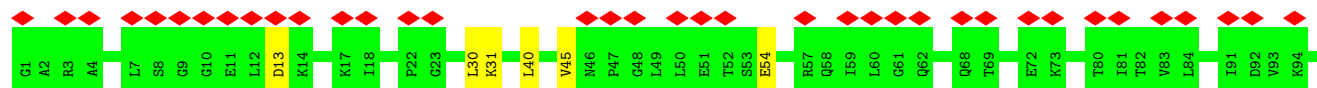




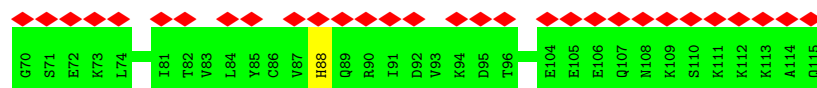
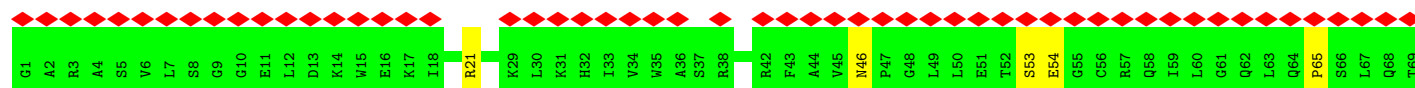
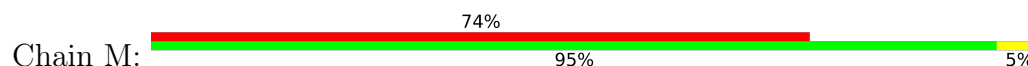
• Molecule 1: Matrix protein p17



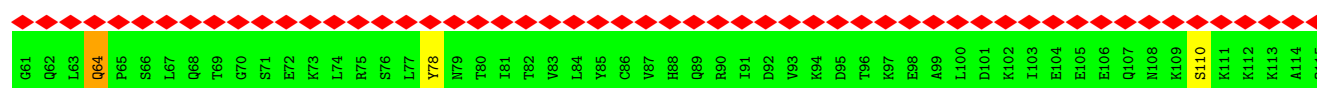
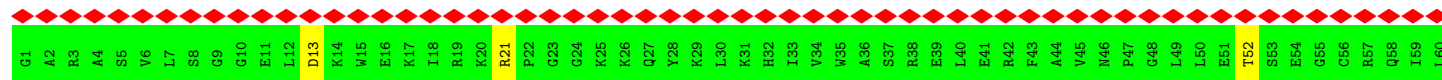
• Molecule 1: Matrix protein p17



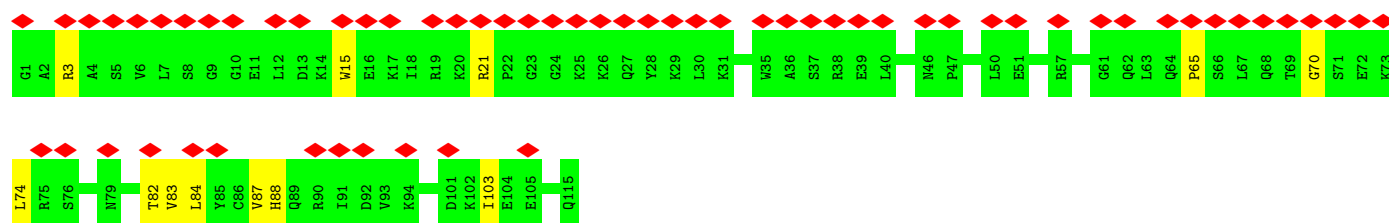
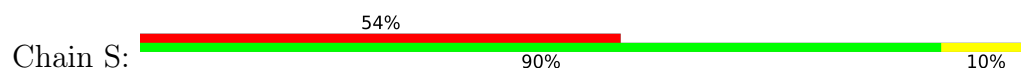
• Molecule 1: Matrix protein p17



• Molecule 1: Matrix protein p17



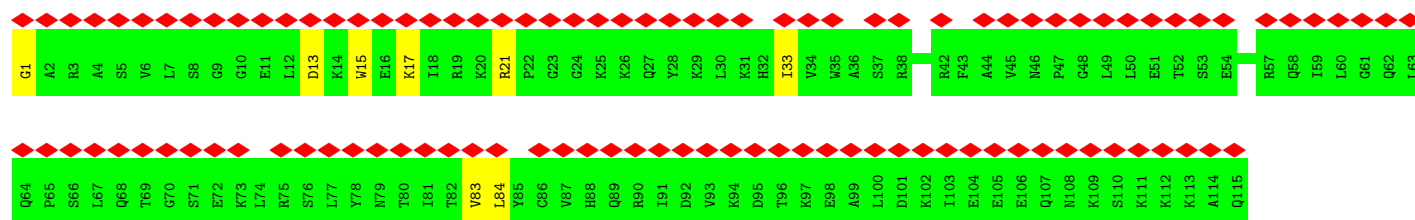
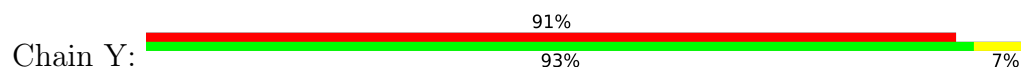
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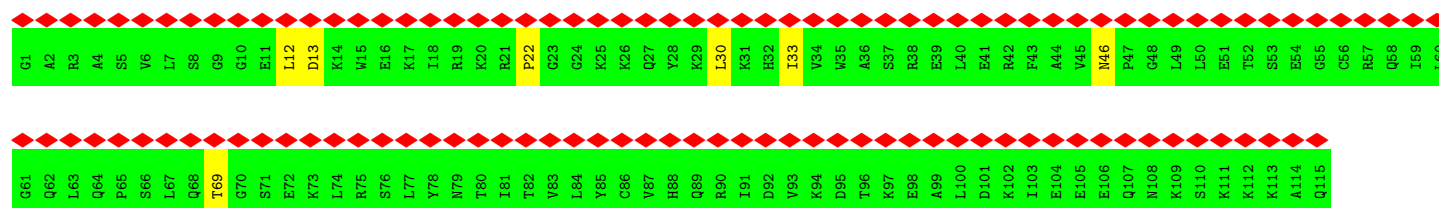
- Molecule 1: Matrix protein p17



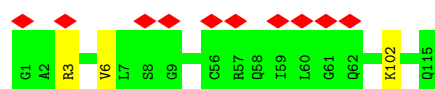
- Molecule 1: Matrix protein p17



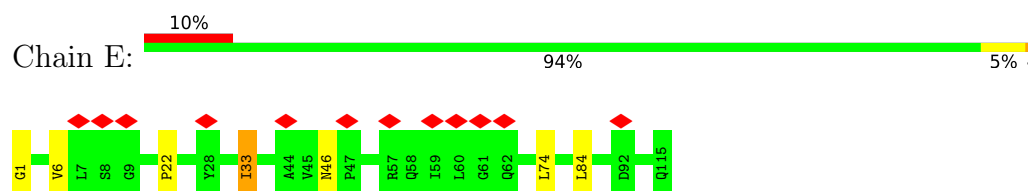
- Molecule 1: Matrix protein p17



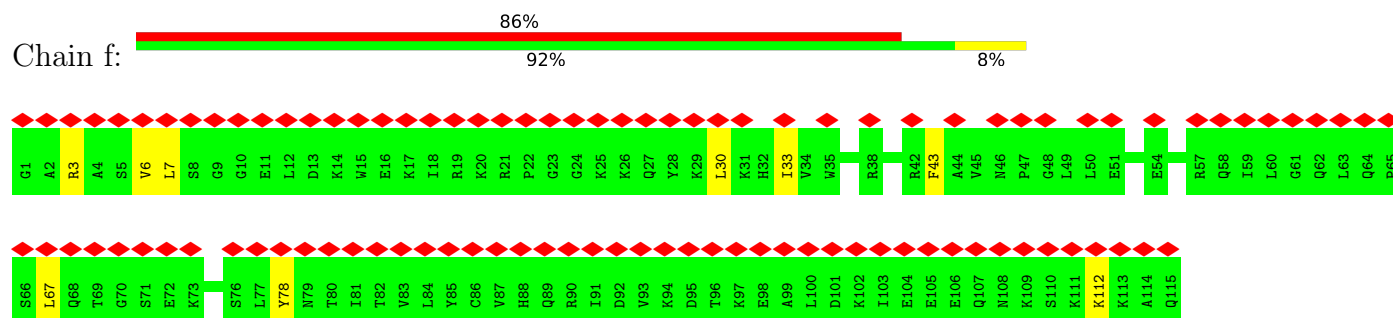
- Molecule 1: Matrix protein p17



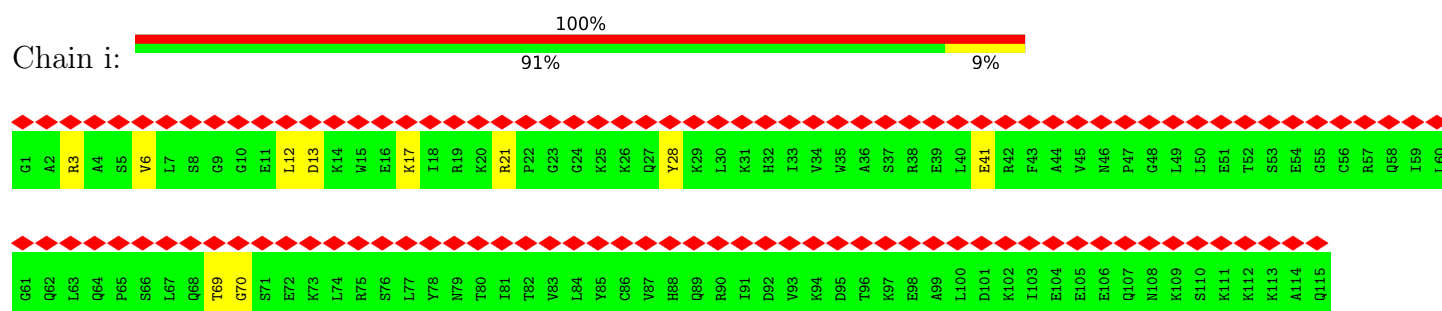
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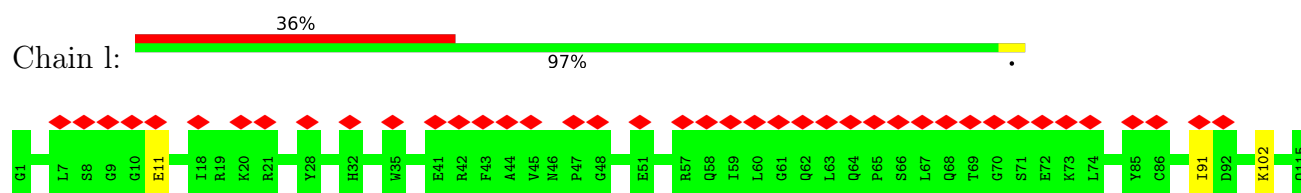
- Molecule 1: Matrix protein p17



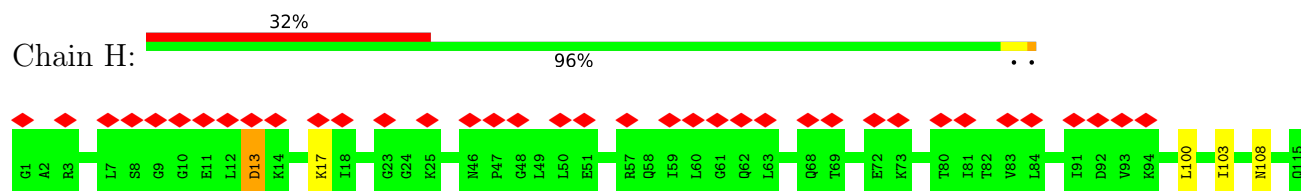
- Molecule 1: Matrix protein p17



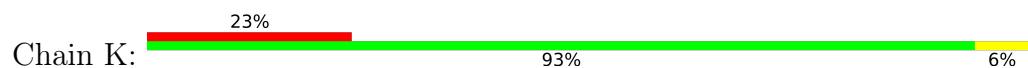
- Molecule 1: Matrix protein p17

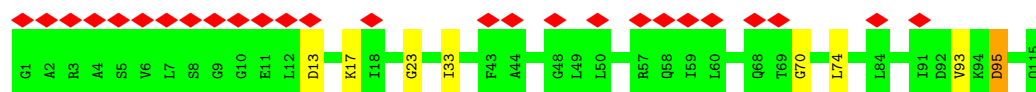


- Molecule 1: Matrix protein p17

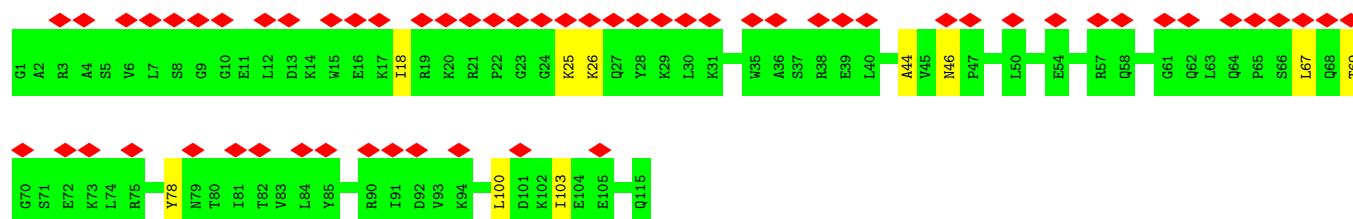
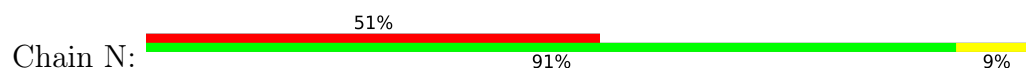


- Molecule 1: Matrix protein p17

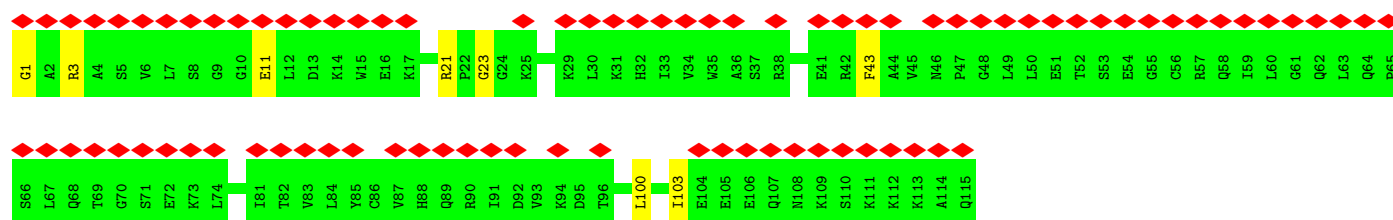
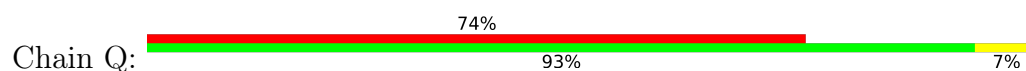




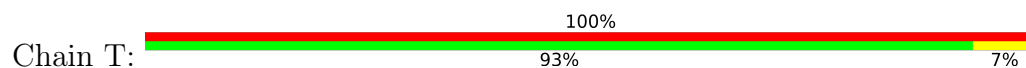
- Molecule 1: Matrix protein p17



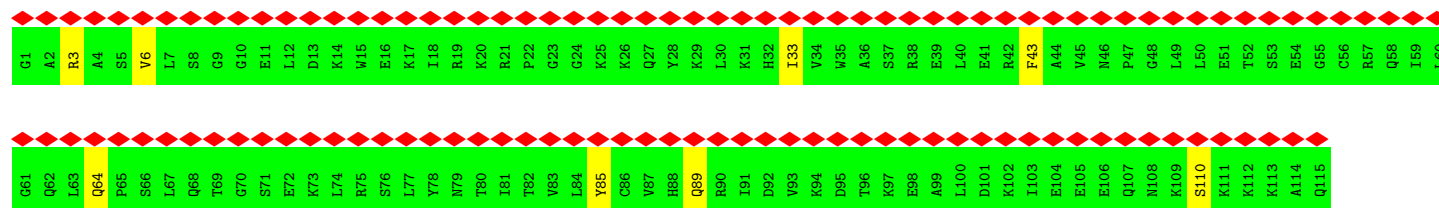
- Molecule 1: Matrix protein p17



- Molecule 1: Matrix protein p17



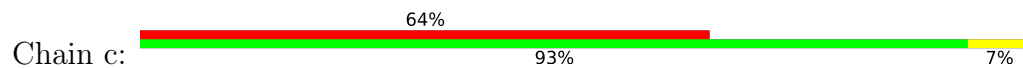
- Molecule 1: Matrix protein p17



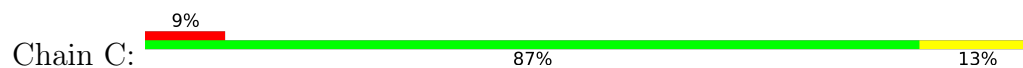
- Molecule 1: Matrix protein p17



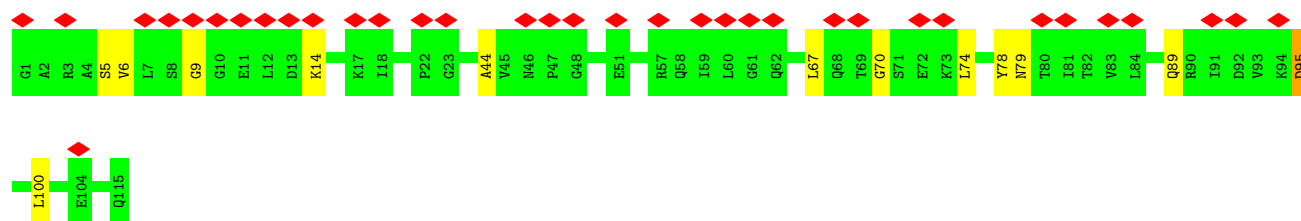
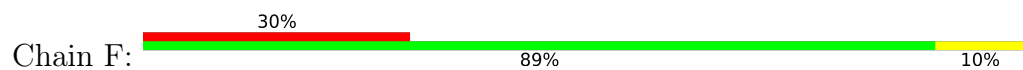
• Molecule 1: Matrix protein p17



• Molecule 1: Matrix protein p17



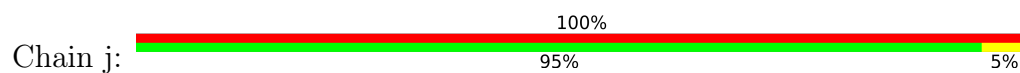
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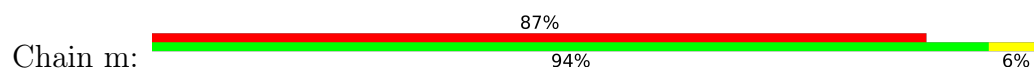
• Molecule 1: Matrix protein p17



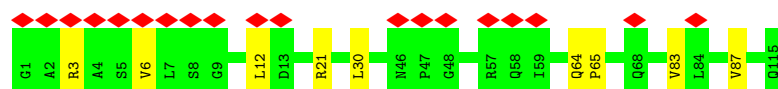
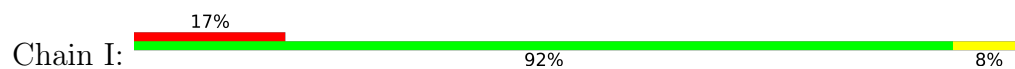
• Molecule 1: Matrix protein p17



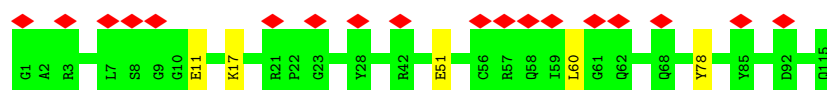
• Molecule 1: Matrix protein p17



• Molecule 1: Matrix protein p17



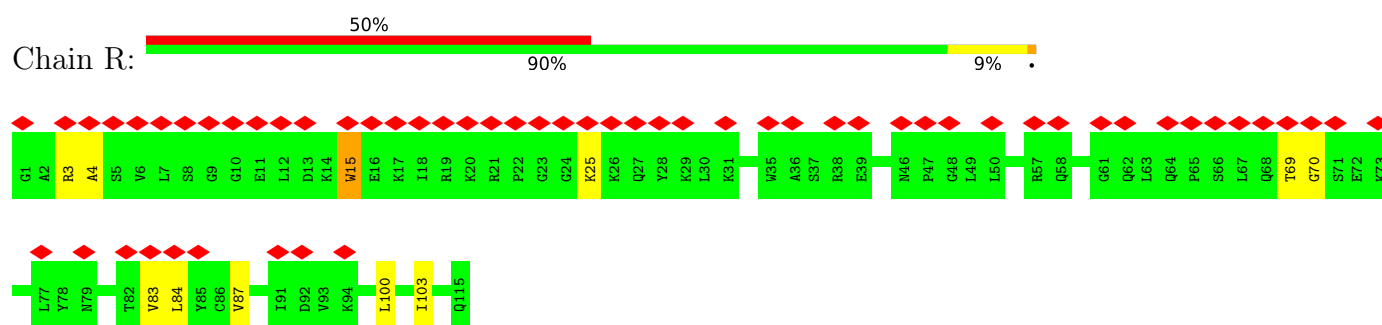
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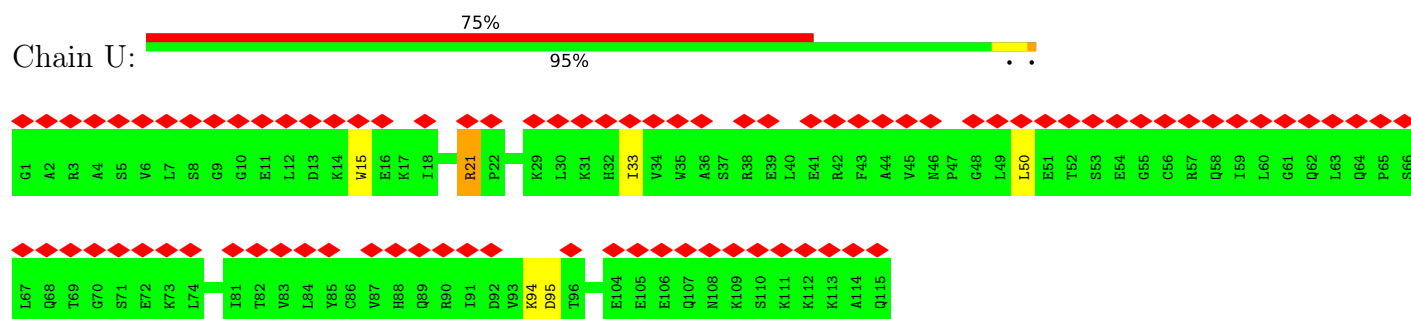
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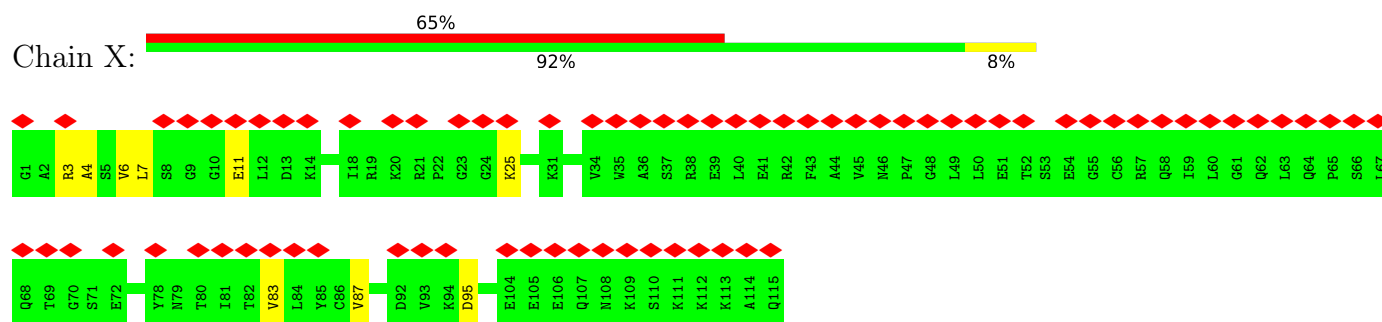
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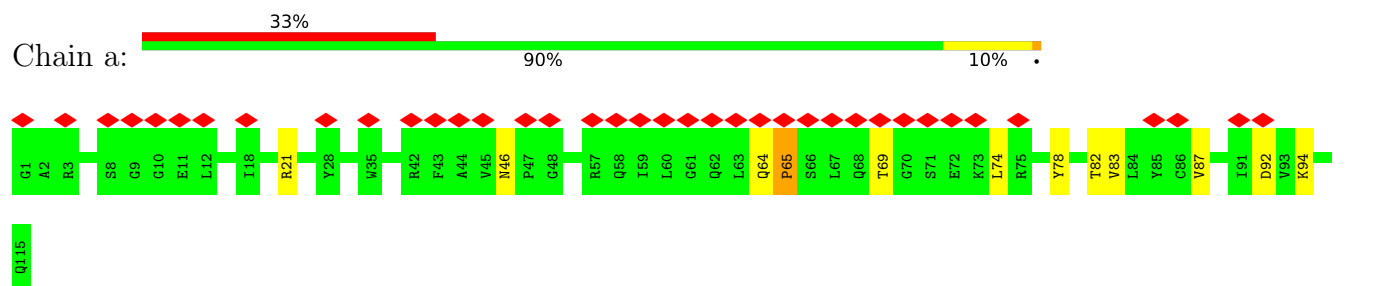
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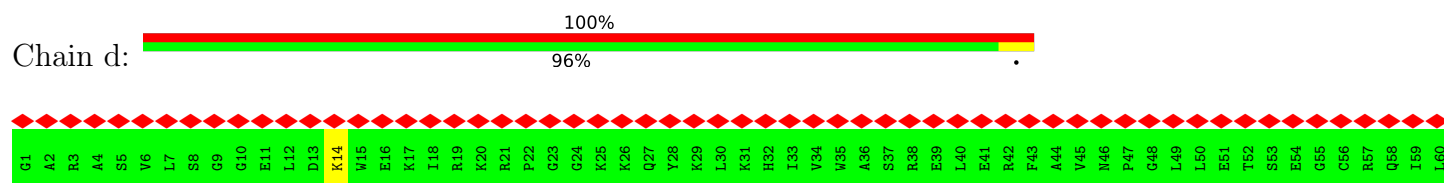
- Molecule 1: Matrix protein p17



- Molecule 1: Matrix protein p17



- Molecule 1: Matrix protein p17



G61	Q62	L63	Q64	P65	S66	L67	Q68	T69	G70	S71	E72	K73	L74	R75	S76	L77	Y78	N79	T80	I81	T82	V83	L84	Y85	C86	V87	H88	Q89	R90	I91	D92	V93	K94	D95	T96	K97	E98	A99	L100	D101	K102	I103	E104	E105	E106	Q107	N108	K109	S110	K111	K112	K113	A114	Q115
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4 Experimental information

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 ($e^-/\text{\AA}^2$)	123	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	87.058	Depositor
Minimum map value	-23.201	Depositor
Average map value	0.981	Depositor
Map value standard deviation	5.676	Depositor
Recommended contour level	20	Depositor
Map size (Å)	300.0, 300.0, 300.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.0, 3.0, 3.0	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.96	1/933 (0.1%)	1.22	4/1247 (0.3%)
1	B	0.83	0/933	1.28	1/1247 (0.1%)
1	C	0.87	2/933 (0.2%)	1.23	4/1247 (0.3%)
1	D	0.89	0/933	1.40	8/1247 (0.6%)
1	E	0.84	1/933 (0.1%)	1.30	7/1247 (0.6%)
1	F	0.85	0/933	1.25	3/1247 (0.2%)
1	G	0.85	0/933	1.30	5/1247 (0.4%)
1	H	0.82	0/933	1.31	3/1247 (0.2%)
1	I	0.88	0/933	1.29	2/1247 (0.2%)
1	J	0.83	0/933	1.24	3/1247 (0.2%)
1	K	0.92	0/933	1.28	4/1247 (0.3%)
1	L	0.86	0/933	1.26	3/1247 (0.2%)
1	M	0.84	1/933 (0.1%)	1.39	9/1247 (0.7%)
1	N	0.85	0/933	1.29	6/1247 (0.5%)
1	O	0.87	1/933 (0.1%)	1.33	6/1247 (0.5%)
1	P	0.82	0/933	1.39	7/1247 (0.6%)
1	Q	0.90	0/933	1.32	8/1247 (0.6%)
1	R	0.81	1/933 (0.1%)	1.30	6/1247 (0.5%)
1	S	0.83	1/933 (0.1%)	1.29	2/1247 (0.2%)
1	T	0.87	0/933	1.27	6/1247 (0.5%)
1	U	0.87	1/933 (0.1%)	1.28	5/1247 (0.4%)
1	V	0.86	1/933 (0.1%)	1.33	3/1247 (0.2%)
1	W	0.89	0/933	1.33	7/1247 (0.6%)
1	X	0.85	0/933	1.35	3/1247 (0.2%)
1	Y	0.83	0/933	1.32	3/1247 (0.2%)
1	Z	0.79	0/933	1.27	5/1247 (0.4%)
1	a	0.89	2/933 (0.2%)	1.33	6/1247 (0.5%)
1	b	0.86	1/933 (0.1%)	1.27	5/1247 (0.4%)
1	c	0.88	0/933	1.33	5/1247 (0.4%)
1	d	0.83	0/933	1.29	4/1247 (0.3%)
1	e	0.85	0/933	1.26	2/1247 (0.2%)
1	f	0.87	0/933	1.30	4/1247 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	g	0.88	1/933 (0.1%)	1.20	0/1247
1	h	0.84	0/933	1.28	5/1247 (0.4%)
1	i	0.88	0/933	1.34	8/1247 (0.6%)
1	j	0.86	0/933	1.35	10/1247 (0.8%)
1	k	0.86	1/933 (0.1%)	1.34	3/1247 (0.2%)
1	l	0.87	0/933	1.35	3/1247 (0.2%)
1	m	0.87	1/933 (0.1%)	1.30	3/1247 (0.2%)
All	All	0.86	16/36387 (0.0%)	1.30	181/48633 (0.4%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	22	PRO	N-CD	-6.75	1.38	1.47
1	S	65	PRO	N-CD	-6.24	1.39	1.47
1	g	22	PRO	N-CD	-5.96	1.39	1.47
1	b	22	PRO	N-CD	-5.78	1.39	1.47
1	O	74	LEU	CB-CG	5.64	1.64	1.53
1	M	65	PRO	N-CD	-5.39	1.40	1.47
1	U	15	TRP	NE1-CE2	-5.38	1.31	1.37
1	C	22	PRO	N-CD	-5.35	1.40	1.47
1	k	22	PRO	N-CD	-5.33	1.40	1.47
1	a	74	LEU	CB-CG	5.31	1.64	1.53
1	A	42	ARG	NE-CZ	5.30	1.38	1.33
1	V	22	PRO	N-CD	-5.28	1.40	1.47
1	a	65	PRO	N-CD	-5.19	1.40	1.47
1	m	47	PRO	N-CD	-5.18	1.40	1.47
1	C	47	PRO	N-CD	-5.11	1.40	1.47
1	R	15	TRP	NE1-CE2	-5.10	1.31	1.37

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	21	ARG	CA-C-N	8.84	130.89	119.84
1	Q	21	ARG	C-N-CA	8.84	130.89	119.84
1	L	51	GLU	N-CA-C	-7.93	101.94	111.69
1	U	21	ARG	CA-C-N	7.91	127.57	119.82
1	U	21	ARG	C-N-CA	7.91	127.57	119.82
1	P	13	ASP	N-CA-C	-7.75	102.16	111.69
1	H	108	ASN	CA-C-N	7.34	129.99	120.44
1	H	108	ASN	C-N-CA	7.34	129.99	120.44
1	N	25	LYS	N-CA-C	7.27	119.20	111.28
1	V	14	LYS	N-CA-C	7.22	119.23	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	46	ASN	CA-C-N	7.17	126.87	119.56
1	c	46	ASN	C-N-CA	7.17	126.87	119.56
1	a	21	ARG	CA-C-N	7.13	126.83	119.56
1	a	21	ARG	C-N-CA	7.13	126.83	119.56
1	f	33	ILE	N-CA-C	-7.02	104.14	111.58
1	S	21	ARG	CA-C-N	7.00	126.52	119.24
1	S	21	ARG	C-N-CA	7.00	126.52	119.24
1	k	13	ASP	N-CA-C	-6.94	102.94	111.40
1	c	17	LYS	N-CA-C	-6.94	106.01	114.75
1	f	7	LEU	N-CA-C	-6.87	100.31	110.48
1	f	43	PHE	CA-CB-CG	6.85	120.65	113.80
1	a	69	THR	CA-C-N	6.83	126.48	119.92
1	a	69	THR	C-N-CA	6.83	126.48	119.92
1	A	25	LYS	N-CA-C	6.82	120.23	109.39
1	b	13	ASP	N-CA-C	-6.82	103.30	111.69
1	i	28	TYR	N-CA-C	-6.79	100.23	110.28
1	M	21	ARG	CA-C-N	6.78	128.31	119.84
1	M	21	ARG	C-N-CA	6.78	128.31	119.84
1	A	21	ARG	CA-C-N	6.75	126.45	119.56
1	A	21	ARG	C-N-CA	6.75	126.45	119.56
1	D	70	GLY	N-CA-C	6.75	121.17	112.54
1	L	11	GLU	N-CA-C	6.74	118.71	111.36
1	i	70	GLY	N-CA-C	6.71	119.64	111.93
1	T	102	LYS	N-CA-C	6.66	118.62	111.36
1	C	108	ASN	CA-C-N	6.63	129.17	120.28
1	C	108	ASN	C-N-CA	6.63	129.17	120.28
1	T	14	LYS	N-CA-C	6.59	118.26	111.14
1	P	21	ARG	CA-C-N	6.57	126.26	119.56
1	P	21	ARG	C-N-CA	6.57	126.26	119.56
1	H	13	ASP	N-CA-C	-6.35	103.88	111.69
1	Z	11	GLU	N-CA-C	6.34	117.86	111.07
1	j	69	THR	CA-C-N	6.34	126.12	120.10
1	j	69	THR	C-N-CA	6.34	126.12	120.10
1	T	108	ASN	CA-C-N	6.16	128.54	120.28
1	T	108	ASN	C-N-CA	6.16	128.54	120.28
1	W	110	SER	CA-C-N	6.15	128.52	120.28
1	W	110	SER	C-N-CA	6.15	128.52	120.28
1	j	21	ARG	CA-C-N	6.15	125.64	119.24
1	j	21	ARG	C-N-CA	6.15	125.64	119.24
1	E	33	ILE	N-CA-C	-6.13	104.32	111.00
1	d	14	LYS	N-CA-C	6.08	117.99	111.36
1	W	33	ILE	N-CA-C	-6.08	104.37	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	i	69	THR	CA-C-N	6.05	125.85	120.10
1	i	69	THR	C-N-CA	6.05	125.85	120.10
1	A	33	ILE	N-CA-C	-6.01	104.45	111.00
1	N	46	ASN	CA-C-N	5.94	126.05	119.87
1	N	46	ASN	C-N-CA	5.94	126.05	119.87
1	Y	1	GLY	CA-C-N	5.93	129.04	120.38
1	Y	1	GLY	C-N-CA	5.93	129.04	120.38
1	h	43	PHE	CA-C-N	5.87	130.47	122.19
1	h	43	PHE	C-N-CA	5.87	130.47	122.19
1	W	64	GLN	CA-C-N	5.86	125.53	119.56
1	W	64	GLN	C-N-CA	5.86	125.53	119.56
1	k	33	ILE	N-CA-C	-5.84	104.63	111.00
1	b	69	THR	CA-C-N	5.82	125.63	120.10
1	b	69	THR	C-N-CA	5.82	125.63	120.10
1	O	68	GLN	N-CA-C	5.81	117.28	111.07
1	b	46	ASN	CA-C-N	5.78	126.54	120.12
1	b	46	ASN	C-N-CA	5.78	126.54	120.12
1	P	110	SER	CA-C-N	5.75	127.98	120.28
1	P	110	SER	C-N-CA	5.75	127.98	120.28
1	X	95	ASP	CA-CB-CG	5.73	118.33	112.60
1	a	46	ASN	CA-C-N	5.72	125.34	119.56
1	a	46	ASN	C-N-CA	5.72	125.34	119.56
1	B	102	LYS	N-CA-C	5.67	117.47	111.28
1	R	70	GLY	N-CA-C	5.67	118.44	111.93
1	G	11	GLU	N-CA-C	5.65	117.52	111.36
1	l	102	LYS	N-CA-C	5.64	117.43	111.28
1	e	43	PHE	CA-C-N	5.61	130.54	122.35
1	e	43	PHE	C-N-CA	5.61	130.54	122.35
1	j	46	ASN	CA-C-N	5.59	125.68	119.87
1	j	46	ASN	C-N-CA	5.59	125.68	119.87
1	D	27	GLN	N-CA-C	5.58	118.18	109.52
1	E	1	GLY	CA-C-N	5.58	129.54	120.60
1	E	1	GLY	C-N-CA	5.58	129.54	120.60
1	R	25	LYS	N-CA-C	5.58	117.36	111.28
1	i	41	GLU	CA-C-N	5.54	127.70	120.28
1	i	41	GLU	C-N-CA	5.54	127.70	120.28
1	d	95	ASP	CA-CB-CG	5.54	118.14	112.60
1	C	54	GLU	CA-C-N	5.53	126.11	119.98
1	C	54	GLU	C-N-CA	5.53	126.11	119.98
1	D	46	ASN	CA-C-N	5.51	125.87	119.47
1	D	46	ASN	C-N-CA	5.51	125.87	119.47
1	K	23	GLY	CA-C-N	5.50	125.33	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	23	GLY	C-N-CA	5.50	125.33	120.10
1	E	6	VAL	CA-C-N	5.44	128.57	120.90
1	E	6	VAL	C-N-CA	5.44	128.57	120.90
1	X	11	GLU	N-CA-C	5.42	116.87	111.07
1	Q	23	GLY	N-CA-C	-5.40	106.25	112.73
1	c	69	THR	CA-C-N	5.39	125.22	120.10
1	c	69	THR	C-N-CA	5.39	125.22	120.10
1	G	64	GLN	CA-C-N	5.39	125.06	119.56
1	G	64	GLN	C-N-CA	5.39	125.06	119.56
1	M	88	HIS	CA-CB-CG	5.38	119.17	113.80
1	O	20	LYS	N-CA-C	5.37	117.13	111.28
1	R	69	THR	CA-C-N	5.36	125.19	120.10
1	R	69	THR	C-N-CA	5.36	125.19	120.10
1	L	17	LYS	N-CA-C	5.34	118.02	111.82
1	m	4	ALA	CA-C-N	5.33	128.16	120.38
1	m	4	ALA	C-N-CA	5.33	128.16	120.38
1	W	43	PHE	CA-C-N	5.30	129.67	122.19
1	W	43	PHE	C-N-CA	5.30	129.67	122.19
1	Y	21	ARG	N-CA-C	-5.30	103.45	108.22
1	Z	46	ASN	CA-C-N	5.29	125.37	119.87
1	Z	46	ASN	C-N-CA	5.29	125.37	119.87
1	F	95	ASP	N-CA-C	5.28	116.03	108.74
1	K	33	ILE	N-CA-C	-5.27	105.25	111.00
1	k	67	LEU	N-CA-C	5.27	117.02	111.28
1	h	69	THR	CA-C-N	5.27	125.10	120.10
1	h	69	THR	C-N-CA	5.27	125.10	120.10
1	j	43	PHE	CA-CB-CG	5.26	119.06	113.80
1	Q	1	GLY	CA-C-N	5.26	129.02	120.60
1	Q	1	GLY	C-N-CA	5.26	129.02	120.60
1	d	64	GLN	CA-C-N	5.26	124.92	119.56
1	d	64	GLN	C-N-CA	5.26	124.92	119.56
1	I	21	ARG	CA-C-N	5.25	125.56	119.47
1	I	21	ARG	C-N-CA	5.25	125.56	119.47
1	R	4	ALA	CA-C-N	5.25	127.84	120.28
1	R	4	ALA	C-N-CA	5.25	127.84	120.28
1	F	89	GLN	CA-C-N	5.23	129.61	122.34
1	F	89	GLN	C-N-CA	5.23	129.61	122.34
1	Q	11	GLU	N-CA-C	5.23	116.67	111.07
1	G	100	LEU	CA-C-N	5.23	127.28	120.28
1	G	100	LEU	C-N-CA	5.23	127.28	120.28
1	K	95	ASP	CA-CB-CG	5.21	117.81	112.60
1	M	46	ASN	CA-C-N	5.17	125.25	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	46	ASN	C-N-CA	5.17	125.25	119.87
1	f	112	LYS	N-CA-C	5.17	116.91	111.28
1	M	53	SER	CA-C-N	5.16	127.19	120.28
1	M	53	SER	C-N-CA	5.16	127.19	120.28
1	J	13	ASP	CA-CB-CG	5.16	117.76	112.60
1	j	102	LYS	N-CA-C	5.16	116.90	111.28
1	O	46	ASN	CA-C-N	5.15	124.81	119.56
1	O	46	ASN	C-N-CA	5.15	124.81	119.56
1	h	70	GLY	N-CA-C	5.13	117.83	111.93
1	D	112	LYS	N-CA-C	5.12	116.86	111.28
1	P	64	GLN	CA-C-N	5.12	124.78	119.56
1	P	64	GLN	C-N-CA	5.12	124.78	119.56
1	U	33	ILE	N-CA-C	-5.12	105.42	111.00
1	M	54	GLU	CA-C-N	5.11	125.61	119.94
1	M	54	GLU	C-N-CA	5.11	125.61	119.94
1	D	22	PRO	N-CA-C	-5.10	102.69	110.95
1	N	26	LYS	N-CA-C	5.09	117.68	110.10
1	U	50	LEU	CA-C-N	5.08	127.09	120.28
1	U	50	LEU	C-N-CA	5.08	127.09	120.28
1	i	21	ARG	CA-C-N	5.07	126.17	119.84
1	i	21	ARG	C-N-CA	5.07	126.17	119.84
1	m	25	LYS	N-CA-C	5.07	118.76	112.58
1	V	4	ALA	CA-C-N	5.06	127.48	120.29
1	V	4	ALA	C-N-CA	5.06	127.48	120.29
1	l	91	ILE	CA-C-N	-5.05	115.47	122.30
1	l	91	ILE	C-N-CA	-5.05	115.47	122.30
1	T	64	GLN	N-CA-C	5.05	120.97	109.81
1	O	89	GLN	CA-C-N	5.05	129.35	122.34
1	O	89	GLN	C-N-CA	5.05	129.35	122.34
1	X	25	LYS	N-CA-C	5.04	116.47	111.07
1	T	111	LYS	N-CA-C	5.04	116.78	111.28
1	J	54	GLU	CA-C-N	5.03	125.53	119.94
1	J	54	GLU	C-N-CA	5.03	125.53	119.94
1	Z	23	GLY	CA-C-N	5.03	125.44	120.31
1	Z	23	GLY	C-N-CA	5.03	125.44	120.31
1	Q	43	PHE	CA-C-N	5.03	129.28	122.19
1	Q	43	PHE	C-N-CA	5.03	129.28	122.19
1	N	18	ILE	N-CA-C	5.02	115.58	109.30
1	j	63	LEU	CA-C-N	5.02	126.36	120.09
1	j	63	LEU	C-N-CA	5.02	126.36	120.09
1	E	46	ASN	CA-C-N	5.00	125.07	119.87
1	E	46	ASN	C-N-CA	5.00	125.07	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	44	ALA	N-CA-C	5.00	118.50	111.74
1	D	108	ASN	CA-C-N	5.00	126.94	120.44
1	D	108	ASN	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	959	3	0
1	B	921	0	959	1	0
1	C	921	0	959	8	0
1	D	921	0	959	11	0
1	E	921	0	958	2	0
1	F	921	0	959	9	0
1	G	921	0	958	4	0
1	H	921	0	959	2	0
1	I	921	0	958	7	0
1	J	921	0	959	3	0
1	K	921	0	959	3	0
1	L	921	0	959	1	0
1	M	921	0	958	0	0
1	N	921	0	959	3	0
1	O	921	0	959	1	0
1	P	921	0	959	1	0
1	Q	921	0	959	2	0
1	R	921	0	959	7	0
1	S	921	0	959	11	0
1	T	921	0	958	2	0
1	U	921	0	958	1	0
1	V	921	0	959	1	0
1	W	921	0	958	2	0
1	X	921	0	959	3	0
1	Y	921	0	959	6	0
1	Z	921	0	958	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	921	0	959	4	0
1	b	921	0	958	2	0
1	c	921	0	959	13	0
1	d	921	0	958	3	0
1	e	921	0	959	9	0
1	f	921	0	958	9	0
1	g	921	0	959	1	0
1	h	921	0	959	2	0
1	i	921	0	958	3	0
1	j	921	0	958	0	0
1	k	921	0	959	0	0
1	l	921	0	958	0	0
1	m	921	0	959	2	0
2	A	15	0	27	0	0
2	B	15	0	27	0	0
2	C	15	0	27	0	0
2	D	15	0	27	2	0
2	E	15	0	27	0	0
2	F	15	0	27	0	0
2	G	15	0	27	0	0
2	H	15	0	27	0	0
2	I	15	0	27	0	0
2	J	15	0	27	0	0
2	K	15	0	27	0	0
2	L	15	0	27	0	0
2	M	15	0	27	0	0
2	N	15	0	27	0	0
2	O	15	0	27	0	0
2	P	15	0	27	0	0
2	Q	15	0	27	2	0
2	R	15	0	27	8	0
2	S	15	0	27	7	0
2	T	15	0	27	0	0
2	U	15	0	27	0	0
2	V	15	0	27	0	0
2	W	15	0	27	0	0
2	X	15	0	27	1	0
2	Y	15	0	27	0	0
2	Z	15	0	27	0	0
2	a	15	0	27	0	0
2	b	15	0	27	0	0
2	c	15	0	27	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	15	0	27	0	0
2	e	15	0	27	9	0
2	f	15	0	27	0	0
2	g	15	0	27	0	0
2	h	15	0	27	0	0
2	i	15	0	27	0	0
2	j	15	0	27	0	0
2	k	15	0	27	0	0
2	l	15	0	27	0	0
2	m	15	0	27	0	0
All	All	36504	0	38440	141	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 2.

All (141) 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:S:82:THR:HG23	1:S:103:ILE:HG13	1.58	0.86
1:S:82:THR:HG23	1:S:103:ILE:CG1	2.05	0.85
1:S:3:ARG:HH12	2:S:201:MYR:C5	1.92	0.82
1:d:82:THR:HG23	1:d:103:ILE:CG1	2.14	0.78
1:Y:15:TRP:CZ3	1:Y:83:VAL:HG12	2.22	0.74
1:S:3:ARG:HH12	2:S:201:MYR:H51	1.52	0.73
1:d:82:THR:HG23	1:d:103:ILE:HG13	1.70	0.72
1:f:30:LEU:HD13	2:c:201:MYR:H31	1.75	0.69
1:f:30:LEU:HD22	2:c:201:MYR:H31	1.73	0.69
1:c:3:ARG:HH12	2:c:201:MYR:C4	2.05	0.68
1:G:82:THR:HG22	1:G:99:ALA:HB1	1.75	0.68
1:e:3:ARG:NH1	2:e:201:MYR:O1	2.28	0.67
1:e:1:GLY:C	2:e:201:MYR:O1	2.35	0.66
1:c:3:ARG:HH12	2:c:201:MYR:H42	1.61	0.65
1:A:99:ALA:O	1:A:103:ILE:HD13	1.96	0.65
1:c:3:ARG:HH12	2:c:201:MYR:C3	2.10	0.64
1:D:30:LEU:HD11	2:R:201:MYR:C2	2.28	0.64
1:e:3:ARG:HG3	2:e:201:MYR:O1	1.98	0.64
1:N:69:THR:OG1	1:O:62:GLN:NE2	2.30	0.64
1:f:67:LEU:HD11	1:f:78:TYR:CE1	2.36	0.61
1:D:30:LEU:HD11	2:R:201:MYR:H21	1.83	0.61
1:P:64:GLN:NE2	1:P:78:TYR:OH	2.34	0.61
1:Y:13:ASP:OD1	1:Y:17:LYS:NZ	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:82:THR:HG23	1:d:103:ILE:HG12	1.83	0.60
1:e:3:ARG:NH1	2:e:201:MYR:C1	2.65	0.60
1:S:82:THR:HG23	1:S:103:ILE:HG12	1.84	0.59
1:E:33:ILE:HG12	1:E:84:LEU:HD21	1.85	0.58
1:c:3:ARG:NH2	2:c:201:MYR:H41	2.19	0.58
1:J:30:LEU:HD12	1:J:30:LEU:C	2.28	0.58
1:c:3:ARG:HH22	2:c:201:MYR:H41	1.68	0.58
1:c:12:LEU:HD22	1:c:30:LEU:HD22	1.85	0.57
1:D:15:TRP:CZ3	1:D:84:LEU:HD23	2.40	0.57
1:Y:15:TRP:CZ3	1:Y:84:LEU:HD23	2.39	0.57
1:S:3:ARG:NH1	2:S:201:MYR:H31	2.19	0.57
1:h:100:LEU:O	1:h:103:ILE:HG22	2.05	0.57
1:L:60:LEU:HD22	1:L:78:TYR:CE1	2.40	0.57
1:J:40:LEU:HD22	1:J:45:VAL:CG1	2.36	0.56
1:F:70:GLY:HA3	1:F:74:LEU:HD23	1.87	0.56
1:I:64:GLN:HB3	1:I:65:PRO:HD3	1.88	0.56
1:R:100:LEU:O	1:R:103:ILE:HG22	2.06	0.55
1:S:70:GLY:HA3	1:S:74:LEU:HD23	1.88	0.55
1:c:3:ARG:HH12	2:c:201:MYR:C2	2.20	0.55
1:Y:15:TRP:CZ3	1:Y:83:VAL:CG1	2.90	0.55
1:c:3:ARG:NH1	2:c:201:MYR:C3	2.69	0.55
1:i:3:ARG:O	1:i:6:VAL:HG12	2.08	0.54
1:W:3:ARG:O	1:W:6:VAL:HG22	2.06	0.54
1:R:3:ARG:HH12	2:R:201:MYR:H62	1.71	0.54
1:I:3:ARG:O	1:I:6:VAL:HG22	2.08	0.53
1:c:3:ARG:HH22	2:c:201:MYR:C4	2.22	0.53
1:a:78:TYR:O	1:a:82:THR:HG23	2.09	0.53
1:Z:100:LEU:O	1:Z:103:ILE:HG22	2.09	0.52
1:W:85:TYR:CE2	1:W:89:GLN:HG3	2.45	0.52
1:I:83:VAL:O	1:I:87:VAL:HG23	2.09	0.52
1:Q:100:LEU:O	1:Q:103:ILE:HG22	2.10	0.52
1:A:94:LYS:NZ	1:A:95:ASP:OD2	2.40	0.51
1:S:3:ARG:HH12	2:S:201:MYR:C6	2.23	0.51
1:e:13:ASP:OD1	1:e:17:LYS:NZ	2.44	0.50
1:D:15:TRP:CZ3	1:D:84:LEU:CD2	2.95	0.50
1:D:13:ASP:OD1	1:D:17:LYS:NZ	2.44	0.50
1:C:59:ILE:HG22	1:C:63:LEU:HD12	1.93	0.50
1:K:93:VAL:CG1	1:K:95:ASP:O	2.60	0.50
1:c:85:TYR:O	1:c:89:GLN:HG2	2.12	0.50
1:R:3:ARG:CZ	2:R:201:MYR:H41	2.41	0.50
1:b:30:LEU:HD12	1:b:33:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:201:MYR:C2	1:F:5:SER:OG	2.61	0.49
1:D:30:LEU:HD21	2:R:201:MYR:C5	2.43	0.49
1:c:3:ARG:NH1	2:c:201:MYR:C2	2.76	0.49
1:S:83:VAL:O	1:S:87:VAL:HG23	2.14	0.48
1:R:3:ARG:HH12	2:R:201:MYR:C6	2.26	0.48
1:c:3:ARG:NH1	2:c:201:MYR:C4	2.74	0.48
1:X:3:ARG:O	1:X:6:VAL:HG22	2.13	0.48
1:a:83:VAL:O	1:a:87:VAL:HG23	2.14	0.48
1:H:100:LEU:O	1:H:103:ILE:HG22	2.14	0.48
1:B:3:ARG:O	1:B:6:VAL:HG22	2.14	0.47
1:C:67:LEU:HD11	1:C:78:TYR:CG	2.49	0.47
1:R:15:TRP:CZ3	1:R:84:LEU:HD23	2.49	0.47
1:C:59:ILE:HG22	1:C:63:LEU:CD1	2.45	0.47
1:a:64:GLN:N	1:a:65:PRO:HD2	2.30	0.47
1:h:67:LEU:HD11	1:h:78:TYR:CD1	2.49	0.47
1:G:79:ASN:O	1:G:83:VAL:HG23	2.14	0.47
1:A:82:THR:HG23	1:A:103:ILE:HG12	1.97	0.47
1:e:3:ARG:HG2	2:e:201:MYR:C3	2.45	0.47
1:D:3:ARG:HH12	2:D:201:MYR:H31	1.80	0.46
1:f:67:LEU:HD11	1:f:78:TYR:CD1	2.50	0.46
1:D:30:LEU:HD12	1:D:33:ILE:HD12	1.97	0.46
1:C:67:LEU:HD22	1:C:75:ARG:HA	1.97	0.46
2:e:201:MYR:H21	1:F:5:SER:OG	2.16	0.46
1:f:30:LEU:HD13	2:c:201:MYR:C5	2.45	0.46
1:i:13:ASP:OD1	1:i:17:LYS:NZ	2.50	0.45
1:f:30:LEU:HD13	2:c:201:MYR:C3	2.45	0.45
1:T:70:GLY:HA3	1:T:74:LEU:HD23	1.99	0.45
1:C:59:ILE:O	1:C:63:LEU:HG	2.17	0.45
1:m:82:THR:HG23	1:m:103:ILE:CG1	2.47	0.45
1:S:15:TRP:CE3	1:S:84:LEU:HD23	2.52	0.45
1:Y:15:TRP:CZ3	1:Y:84:LEU:CD2	3.01	0.44
1:F:6:VAL:O	1:F:6:VAL:HG12	2.17	0.44
1:e:3:ARG:HG3	2:e:201:MYR:C1	2.47	0.44
1:f:3:ARG:O	1:f:6:VAL:HG22	2.17	0.44
1:N:100:LEU:O	1:N:103:ILE:HG22	2.18	0.44
1:i:12:LEU:HD21	2:Q:201:MYR:C2	2.48	0.44
1:g:60:LEU:HD22	1:g:78:TYR:CE1	2.53	0.44
1:J:30:LEU:HD12	1:J:31:LYS:N	2.33	0.44
1:C:3:ARG:O	1:C:6:VAL:HG22	2.19	0.43
1:X:4:ALA:HA	1:X:7:LEU:HG	2.00	0.43
1:N:67:LEU:HD22	1:N:78:TYR:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:VAL:O	1:C:87:VAL:HG23	2.19	0.43
1:Y:33:ILE:HG22	2:X:201:MYR:H22	2.00	0.43
1:F:67:LEU:HD11	1:F:78:TYR:CD1	2.53	0.43
1:e:3:ARG:HG2	2:e:201:MYR:H31	1.99	0.43
1:K:13:ASP:OD1	1:K:17:LYS:NZ	2.52	0.43
1:a:92:ASP:OD2	1:a:94:LYS:NZ	2.52	0.43
1:c:85:TYR:CE2	1:c:89:GLN:HG3	2.54	0.42
2:S:201:MYR:H72	1:I:6:VAL:HG11	2.00	0.42
1:R:83:VAL:O	1:R:87:VAL:HG23	2.19	0.42
1:D:30:LEU:CD1	2:R:201:MYR:H21	2.48	0.42
1:f:30:LEU:CB	2:c:201:MYR:H51	2.48	0.42
1:F:95:ASP:OD1	1:F:95:ASP:C	2.61	0.42
1:H:13:ASP:OD1	1:H:17:LYS:NZ	2.53	0.42
1:F:9:GLY:O	1:F:14:LYS:NZ	2.51	0.42
1:F:79:ASN:OD1	1:F:100:LEU:HD21	2.20	0.42
1:D:3:ARG:NH1	2:D:201:MYR:C1	2.82	0.42
1:X:83:VAL:O	1:X:87:VAL:HG23	2.20	0.41
1:G:83:VAL:O	1:G:87:VAL:HG23	2.20	0.41
1:I:64:GLN:HB3	1:I:65:PRO:CD	2.50	0.41
1:D:30:LEU:HD11	2:R:201:MYR:H22	2.00	0.41
1:G:67:LEU:HD21	1:G:78:TYR:HB2	2.02	0.41
2:S:201:MYR:C5	1:I:12:LEU:HD13	2.50	0.41
1:Q:3:ARG:CZ	2:Q:201:MYR:H41	2.51	0.41
1:U:94:LYS:NZ	1:U:95:ASP:OD2	2.52	0.41
2:S:201:MYR:H32	1:I:30:LEU:HD22	2.02	0.41
1:K:70:GLY:HA3	1:K:74:LEU:HD23	2.03	0.41
1:e:98:GLU:OE2	1:e:102:LYS:HE2	2.21	0.41
1:E:74:LEU:HD23	1:F:44:ALA:HB1	2.03	0.41
1:V:9:GLY:O	1:V:14:LYS:NZ	2.55	0.40
1:T:63:LEU:HD22	1:T:74:LEU:HD11	2.03	0.40
1:C:93:VAL:HA	1:C:98:GLU:CD	2.46	0.40
1:b:12:LEU:HD22	1:b:30:LEU:HD13	2.03	0.40
1:f:30:LEU:HD13	2:c:201:MYR:C4	2.51	0.40
1:m:83:VAL:O	1:m:87:VAL:HG23	2.21	0.40
1:S:84:LEU:O	1:S:88:HIS:CD2	2.75	0.40
1:R:15:TRP:CZ3	1:R:84:LEU:CD2	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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	51
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
1	e	113/115 (98%)	112 (99%)	0	1 (1%)	14	51
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	51
1	m	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
All	All	4407/4485 (98%)	4392 (100%)	12 (0%)	3 (0%)	49	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 ⓘ

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	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%)	68	78
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%)	100 (100%)	0	100	100
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%)	99 (99%)	1 (1%)	68	78
1	l	100/100 (100%)	100 (100%)	0	100	100
1	m	100/100 (100%)	100 (100%)	0	100	100
All	All	3900/3900 (100%)	3898 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	k	52	THR
1	P	52	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	k	32	HIS
1	k	64	GLN
1	J	68	GLN
1	J	88	HIS
1	J	89	GLN
1	M	27	GLN
1	M	64	GLN
1	P	64	GLN
1	P	89	GLN
1	S	88	HIS
1	V	58	GLN
1	Y	88	HIS
1	b	88	HIS
1	H	27	GLN
1	H	62	GLN
1	K	88	HIS
1	Q	88	HIS
1	T	58	GLN
1	T	89	GLN
1	T	115	GLN
1	c	32	HIS
1	F	58	GLN
1	O	89	GLN

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Mol	Chain	Res	Type
1	O	107	GLN
1	a	89	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	X	201	1	13,14,15	0.57	0	12,13,15	0.54	0
2	MYR	e	201	1	13,14,15	0.51	0	12,13,15	0.43	0
2	MYR	Z	201	1	13,14,15	0.53	0	12,13,15	0.33	0
2	MYR	I	201	1	13,14,15	0.51	0	12,13,15	0.30	0
2	MYR	E	201	1	13,14,15	0.51	0	12,13,15	0.33	0
2	MYR	J	201	1	13,14,15	0.51	0	12,13,15	0.33	0
2	MYR	A	201	1	13,14,15	0.49	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	g	201	1	13,14,15	0.50	0	12,13,15	0.33	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	0.50	0	12,13,15	0.39	0
2	MYR	W	201	1	13,14,15	0.50	0	12,13,15	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MYR	j	201	1	13,14,15	0.52	0	12,13,15	0.25	0
2	MYR	R	201	1	13,14,15	0.55	0	12,13,15	1.13	1 (8%)
2	MYR	U	201	1	13,14,15	0.52	0	12,13,15	0.31	0
2	MYR	V	201	1	13,14,15	0.51	0	12,13,15	0.26	0
2	MYR	O	201	1	13,14,15	0.51	0	12,13,15	0.33	0
2	MYR	Y	201	1	13,14,15	0.50	0	12,13,15	0.32	0
2	MYR	L	201	1	13,14,15	0.49	0	12,13,15	0.23	0
2	MYR	f	201	1	13,14,15	0.51	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	c	201	1	13,14,15	0.91	1 (7%)	12,13,15	1.35	1 (8%)
2	MYR	C	201	1	13,14,15	0.47	0	12,13,15	0.42	0
2	MYR	B	201	1	13,14,15	0.53	0	12,13,15	0.33	0
2	MYR	b	201	1	13,14,15	0.51	0	12,13,15	0.33	0
2	MYR	k	201	1	13,14,15	0.49	0	12,13,15	0.34	0
2	MYR	h	201	1	13,14,15	0.49	0	12,13,15	0.35	0
2	MYR	d	201	1	13,14,15	0.47	0	12,13,15	0.48	0
2	MYR	T	201	1	13,14,15	0.52	0	12,13,15	0.35	0
2	MYR	P	201	1	13,14,15	0.53	0	12,13,15	0.31	0
2	MYR	H	201	1	13,14,15	0.52	0	12,13,15	0.40	0
2	MYR	M	201	1	13,14,15	0.54	0	12,13,15	0.27	0
2	MYR	l	201	1	13,14,15	0.52	0	12,13,15	0.37	0
2	MYR	K	201	1	13,14,15	0.50	0	12,13,15	0.32	0
2	MYR	S	201	1	13,14,15	0.77	0	12,13,15	0.73	0
2	MYR	D	201	1	13,14,15	0.57	0	12,13,15	0.43	0
2	MYR	G	201	1	13,14,15	0.53	0	12,13,15	0.34	0
2	MYR	F	201	1	13,14,15	0.50	0	12,13,15	0.38	0
2	MYR	N	201	1	13,14,15	0.51	0	12,13,15	0.33	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	X	201	1	-	1/12/12/13	-
2	MYR	e	201	1	-	2/12/12/13	-
2	MYR	Z	201	1	-	0/12/12/13	-
2	MYR	I	201	1	-	1/12/12/13	-
2	MYR	E	201	1	-	0/12/12/13	-
2	MYR	J	201	1	-	2/12/12/13	-
2	MYR	A	201	1	-	0/12/12/13	-
2	MYR	i	201	1	-	4/12/12/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	g	201	1	-	1/12/12/13	-
2	MYR	a	201	1	-	0/12/12/13	-
2	MYR	m	201	1	-	0/12/12/13	-
2	MYR	W	201	1	-	0/12/12/13	-
2	MYR	j	201	1	-	1/12/12/13	-
2	MYR	R	201	1	-	5/12/12/13	-
2	MYR	U	201	1	-	0/12/12/13	-
2	MYR	V	201	1	-	2/12/12/13	-
2	MYR	O	201	1	-	0/12/12/13	-
2	MYR	Y	201	1	-	1/12/12/13	-
2	MYR	L	201	1	-	3/12/12/13	-
2	MYR	f	201	1	-	0/12/12/13	-
2	MYR	Q	201	1	-	2/12/12/13	-
2	MYR	c	201	1	-	2/12/12/13	-
2	MYR	C	201	1	-	4/12/12/13	-
2	MYR	B	201	1	-	2/12/12/13	-
2	MYR	b	201	1	-	0/12/12/13	-
2	MYR	k	201	1	-	1/12/12/13	-
2	MYR	h	201	1	-	1/12/12/13	-
2	MYR	d	201	1	-	2/12/12/13	-
2	MYR	T	201	1	-	0/12/12/13	-
2	MYR	P	201	1	-	0/12/12/13	-
2	MYR	H	201	1	-	2/12/12/13	-
2	MYR	M	201	1	-	2/12/12/13	-
2	MYR	l	201	1	-	1/12/12/13	-
2	MYR	K	201	1	-	1/12/12/13	-
2	MYR	S	201	1	-	5/12/12/13	-
2	MYR	D	201	1	-	1/12/12/13	-
2	MYR	G	201	1	-	1/12/12/13	-
2	MYR	F	201	1	-	0/12/12/13	-
2	MYR	N	201	1	-	3/12/12/13	-

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(°)	Ideal(°)
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.

All (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
2	H	201	MYR	O1-C1-C2-C3
2	Q	201	MYR	O1-C1-C2-C3
2	c	201	MYR	C1-C2-C3-C4
2	C	201	MYR	O1-C1-C2-C3
2	g	201	MYR	O1-C1-C2-C3
2	R	201	MYR	O1-C1-C2-C3
2	R	201	MYR	C1-C2-C3-C4
2	d	201	MYR	O1-C1-C2-C3
2	d	201	MYR	C1-C2-C3-C4
2	R	201	MYR	C2-C3-C4-C5
2	c	201	MYR	C2-C3-C4-C5
2	i	201	MYR	C11-C10-C9-C8
2	e	201	MYR	C7-C8-C9-C10
2	Y	201	MYR	C6-C7-C8-C9
2	C	201	MYR	C5-C6-C7-C8
2	S	201	MYR	C5-C6-C7-C8
2	S	201	MYR	C3-C4-C5-C6
2	j	201	MYR	C5-C6-C7-C8
2	C	201	MYR	C7-C8-C9-C10
2	B	201	MYR	C5-C6-C7-C8
2	R	201	MYR	C3-C4-C5-C6
2	i	201	MYR	C11-C12-C13-C14
2	N	201	MYR	C6-C7-C8-C9
2	L	201	MYR	C6-C7-C8-C9
2	S	201	MYR	C4-C5-C6-C7
2	C	201	MYR	C11-C10-C9-C8
2	e	201	MYR	C2-C3-C4-C5
2	L	201	MYR	C9-C10-C11-C12
2	D	201	MYR	C1-C2-C3-C4
2	S	201	MYR	C1-C2-C3-C4
2	Q	201	MYR	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	L	201	MYR	C4-C5-C6-C7
2	N	201	MYR	C4-C5-C6-C7
2	G	201	MYR	C3-C4-C5-C6
2	I	201	MYR	C2-C3-C4-C5
2	B	201	MYR	C11-C10-C9-C8
2	M	201	MYR	C4-C5-C6-C7
2	S	201	MYR	C6-C7-C8-C9
2	M	201	MYR	C6-C7-C8-C9
2	X	201	MYR	C2-C3-C4-C5
2	V	201	MYR	C6-C7-C8-C9
2	J	201	MYR	C4-C5-C6-C7
2	H	201	MYR	C11-C10-C9-C8
2	K	201	MYR	C3-C4-C5-C6
2	I	201	MYR	C6-C7-C8-C9
2	i	201	MYR	C1-C2-C3-C4
2	N	201	MYR	C5-C6-C7-C8
2	R	201	MYR	C9-C10-C11-C12

There are no ring outliers.

7 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	201	MYR	1	0
2	e	201	MYR	9	0
2	R	201	MYR	8	0
2	Q	201	MYR	2	0
2	c	201	MYR	16	0
2	S	201	MYR	7	0
2	D	201	MYR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

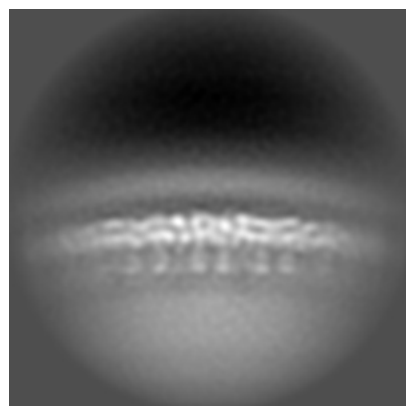
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52059. These allow visual inspection of the internal detail of the map and identification of artifacts.

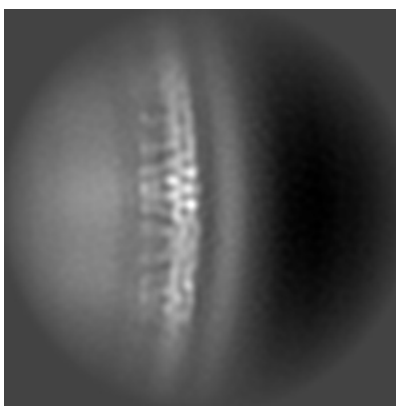
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

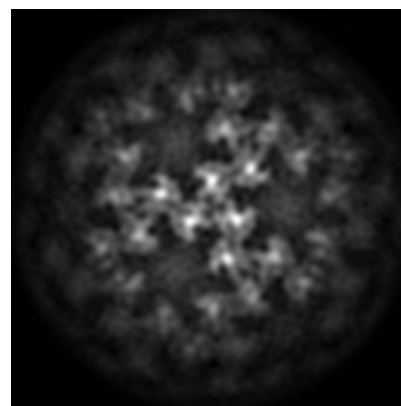
6.1.1 Primary map



X

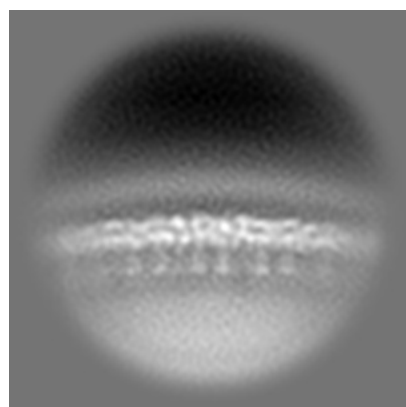


Y

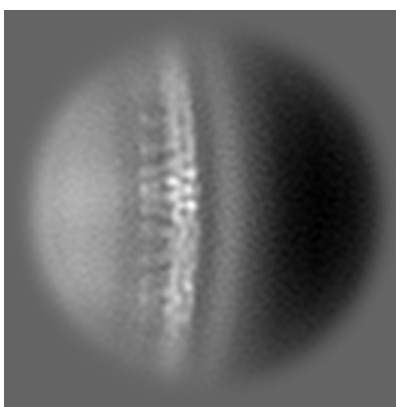


Z

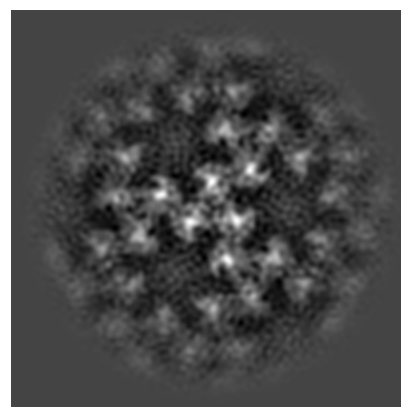
6.1.2 Raw map



X



Y

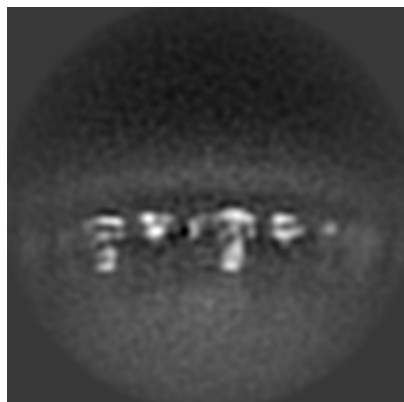


Z

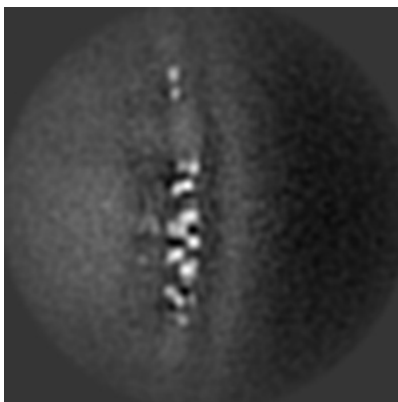
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

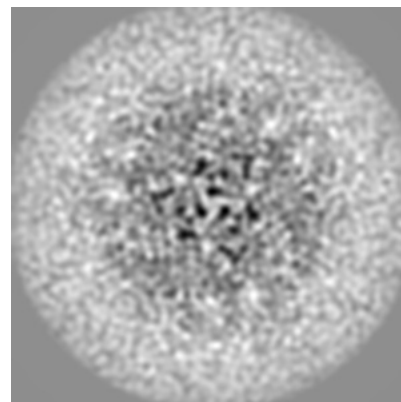
6.2.1 Primary map



X Index: 50



Y Index: 50

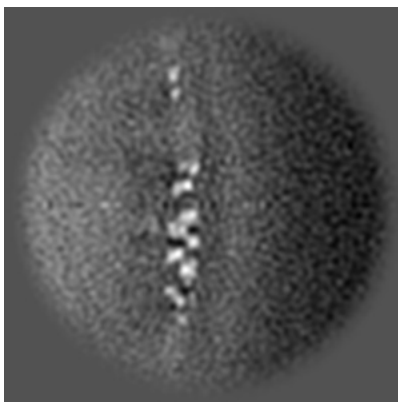


Z Index: 50

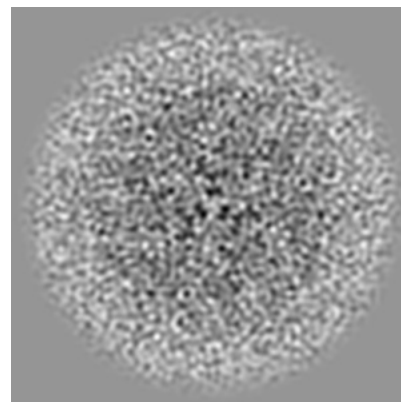
6.2.2 Raw map



X Index: 50



Y Index: 50

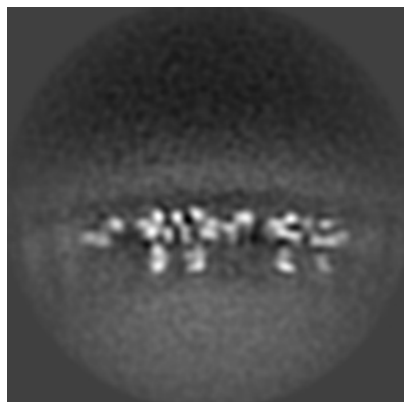


Z Index: 50

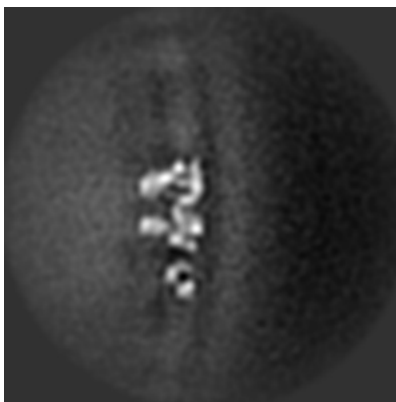
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

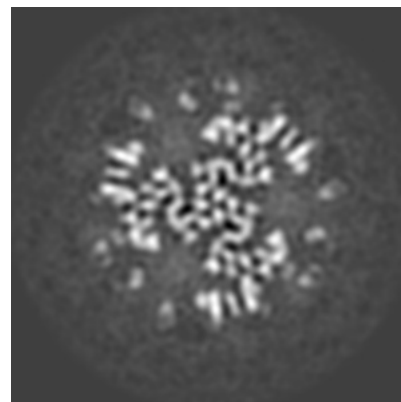
6.3.1 Primary map



X Index: 54

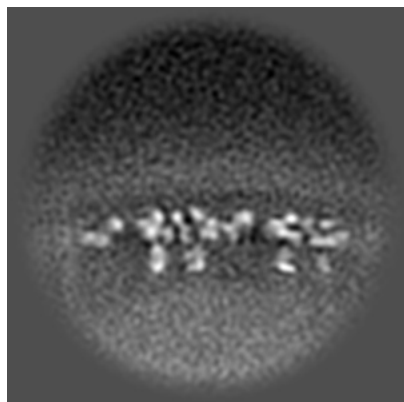


Y Index: 47

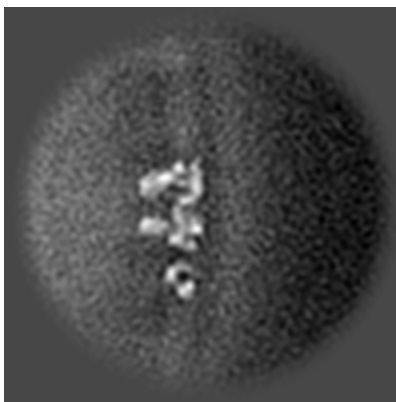


Z Index: 46

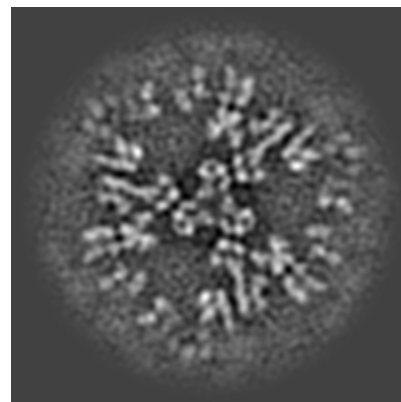
6.3.2 Raw map



X Index: 54



Y Index: 47

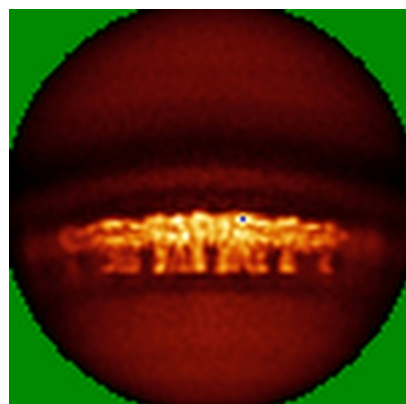


Z Index: 42

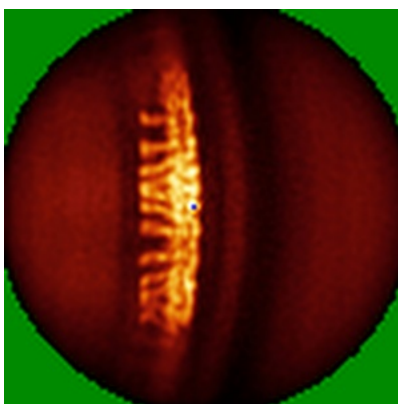
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

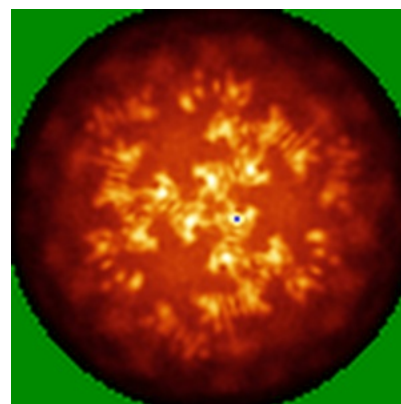
6.4.1 Primary map



X

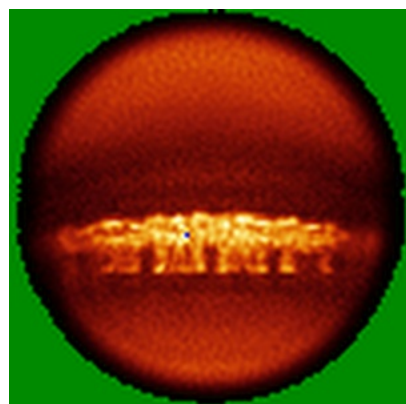


Y

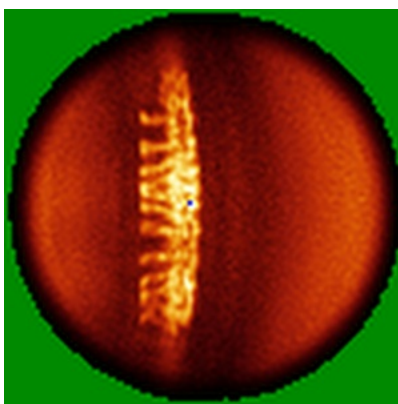


Z

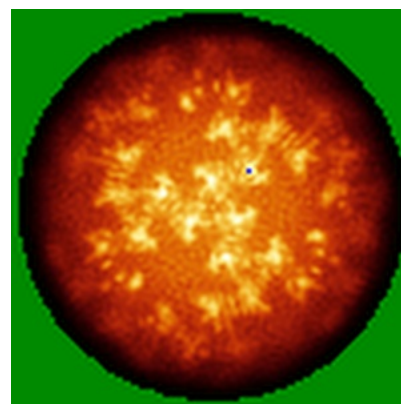
6.4.2 Raw map



X



Y

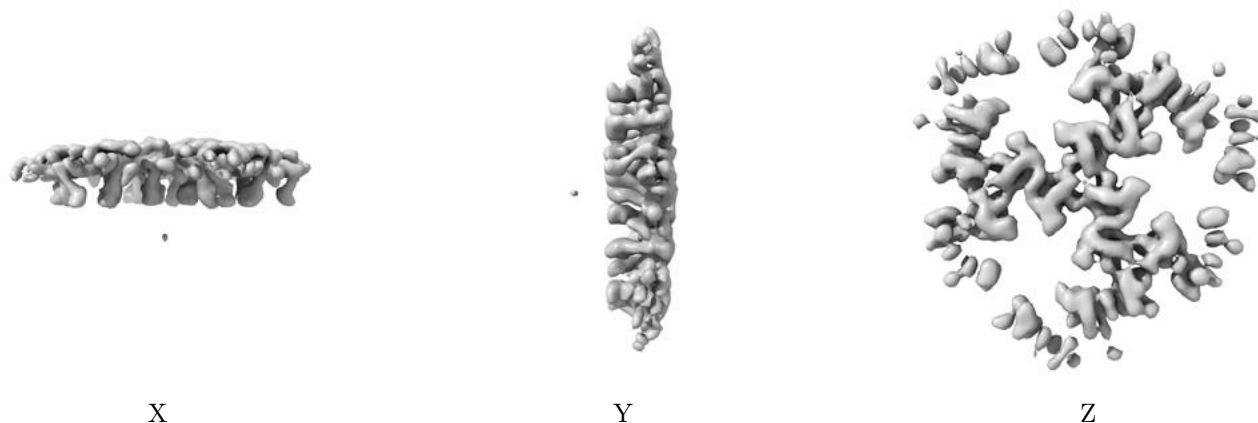


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 20.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

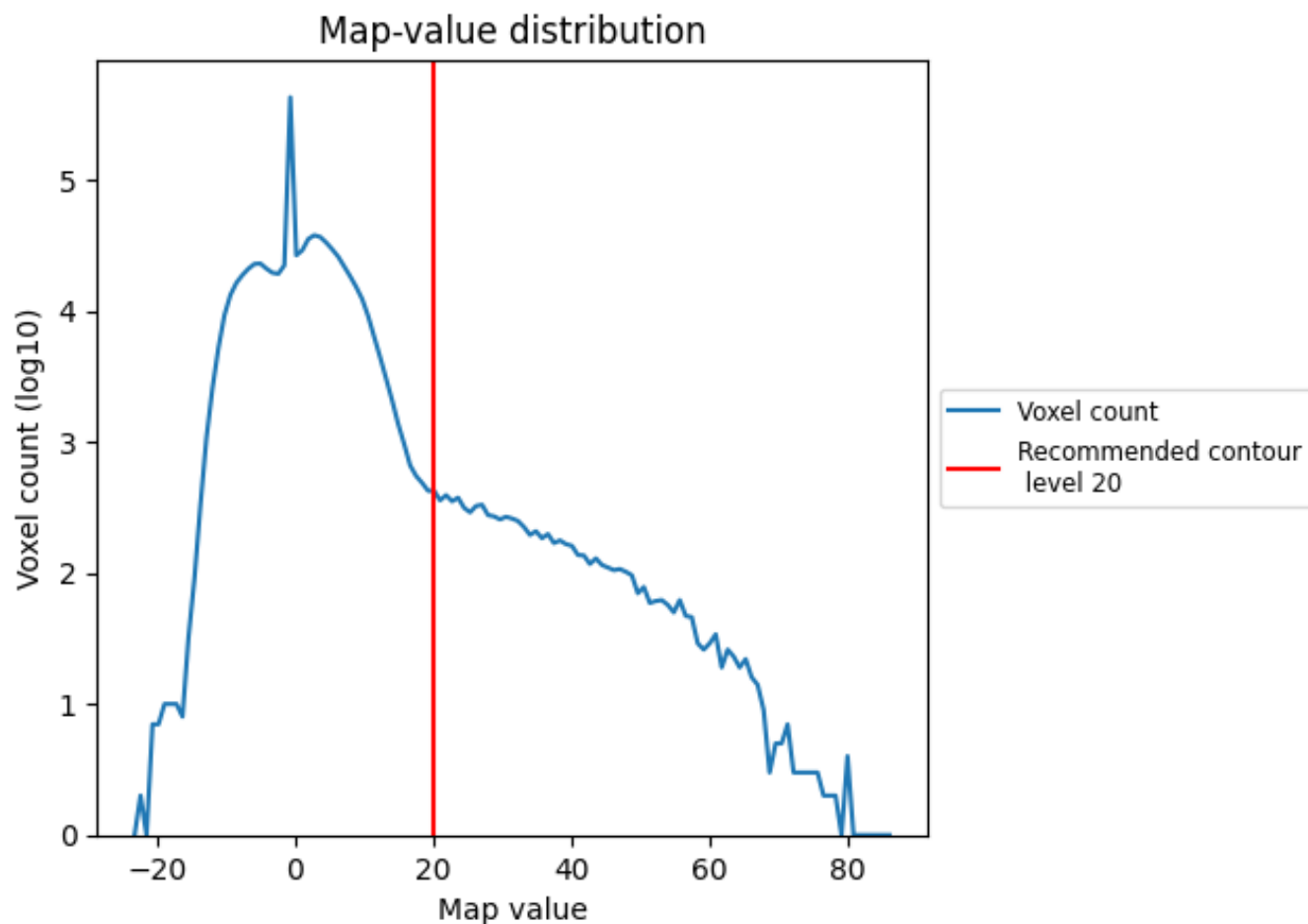
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

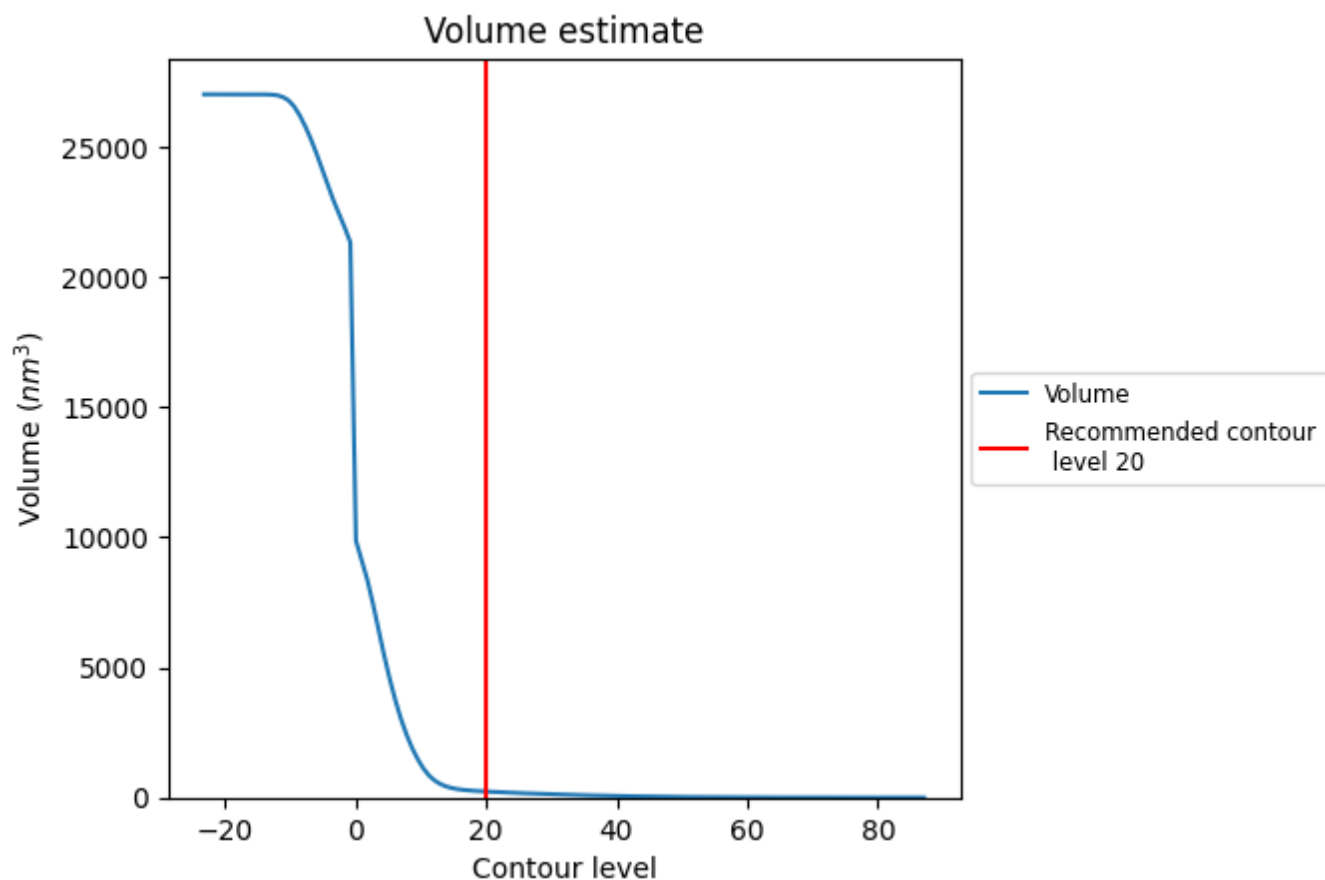
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

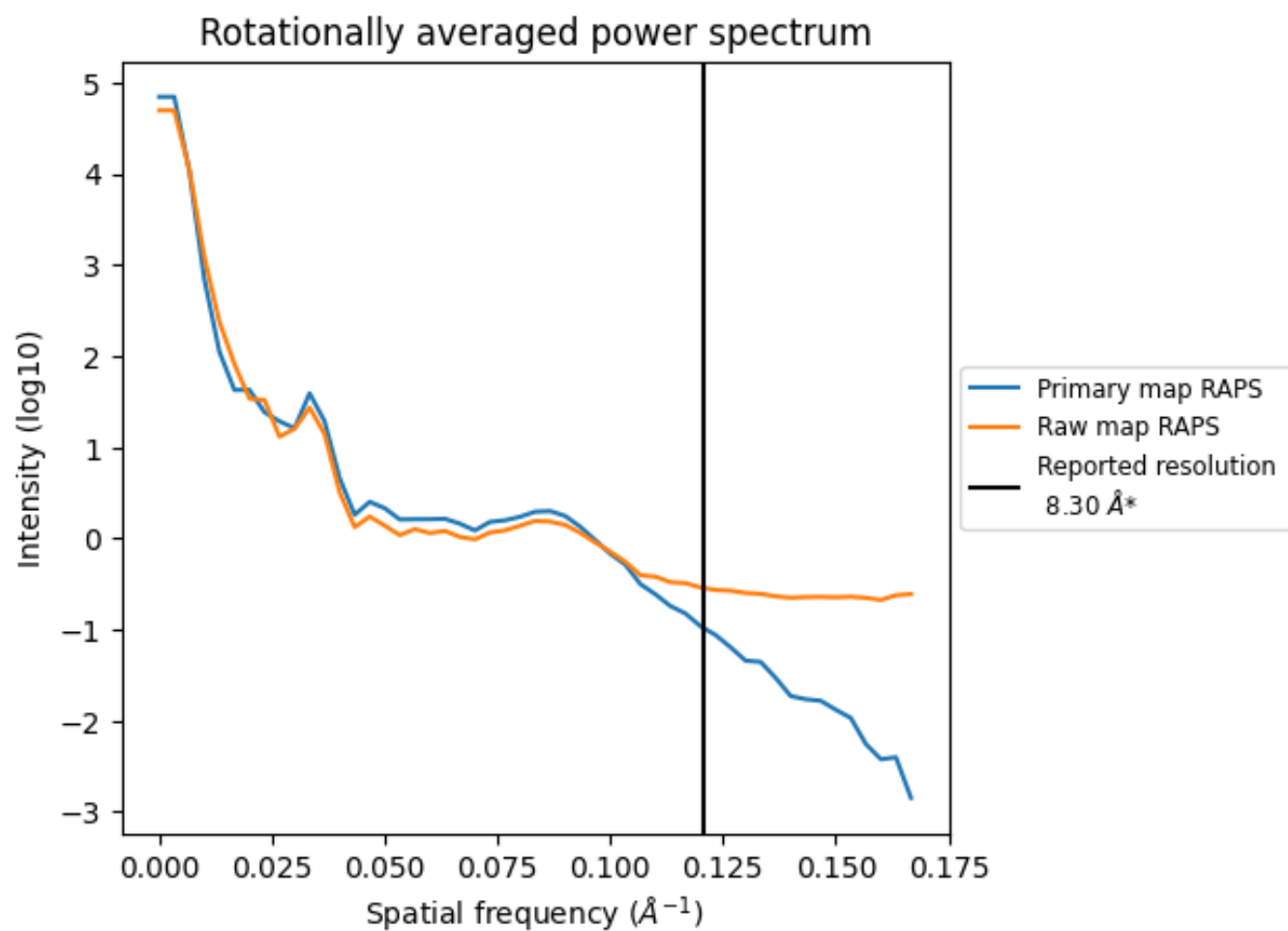
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 232 nm^3 ; this corresponds to an approximate mass of 209 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

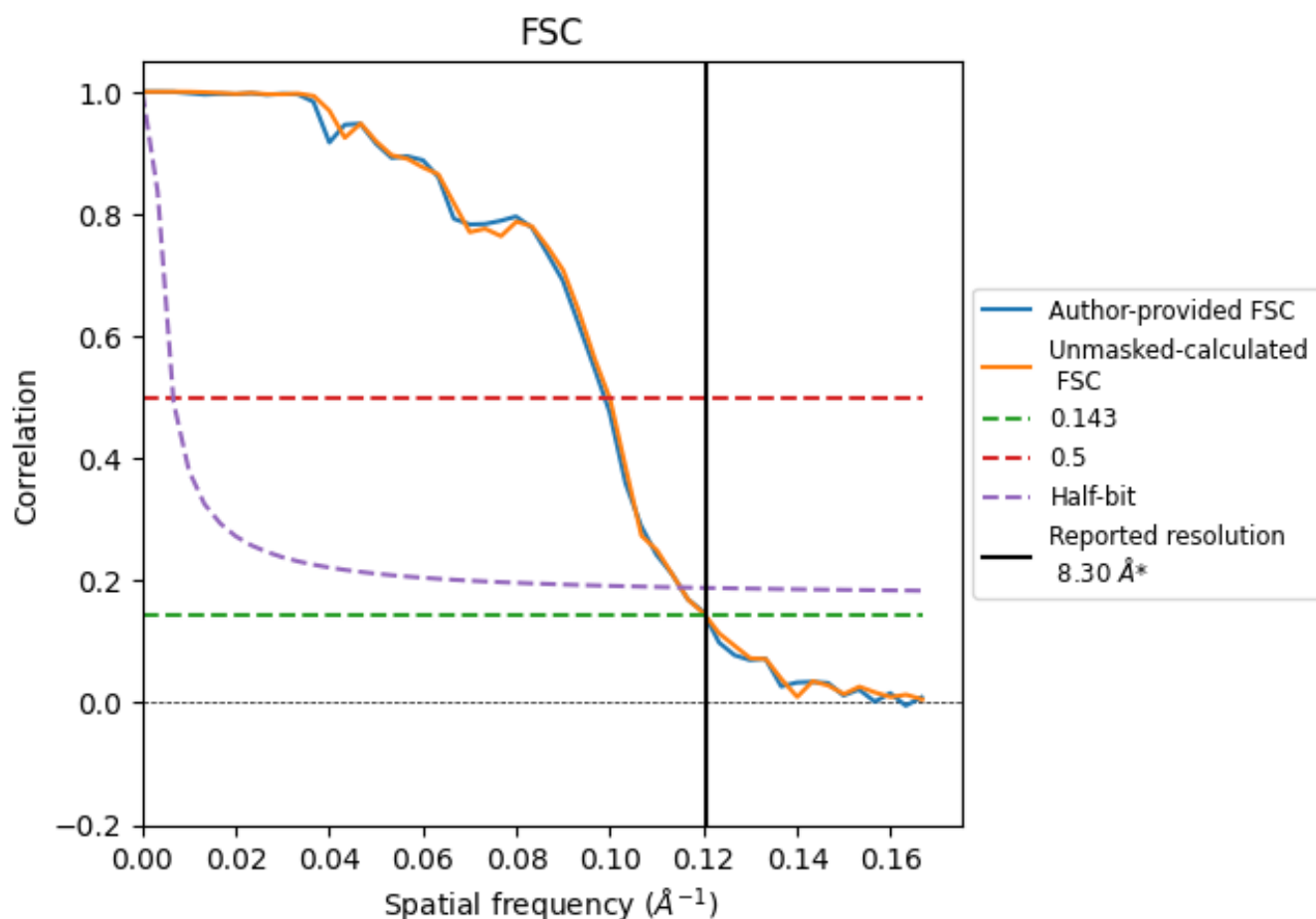


*Reported resolution corresponds to spatial frequency of 0.120 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.120 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

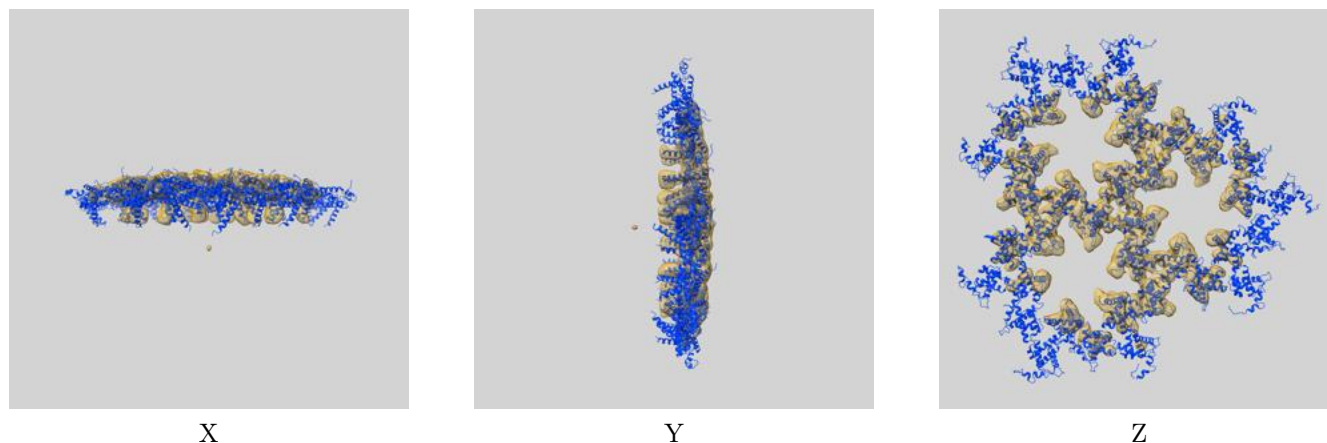
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.30	-	-
Author-provided FSC curve	8.31	10.12	8.70
Unmasked-calculated*	8.31	10.02	8.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

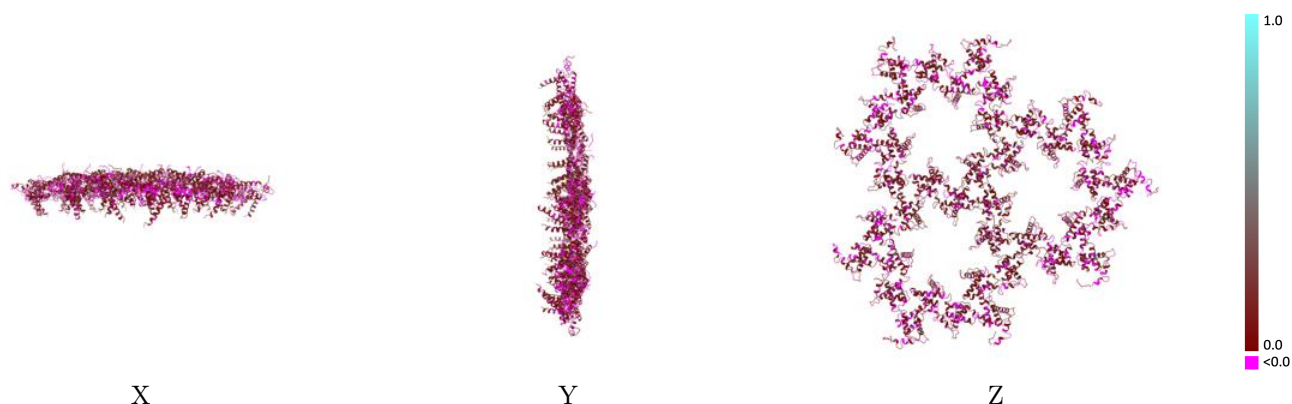
This section contains information regarding the fit between EMDB map EMD-52059 and PDB model 9EK2. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



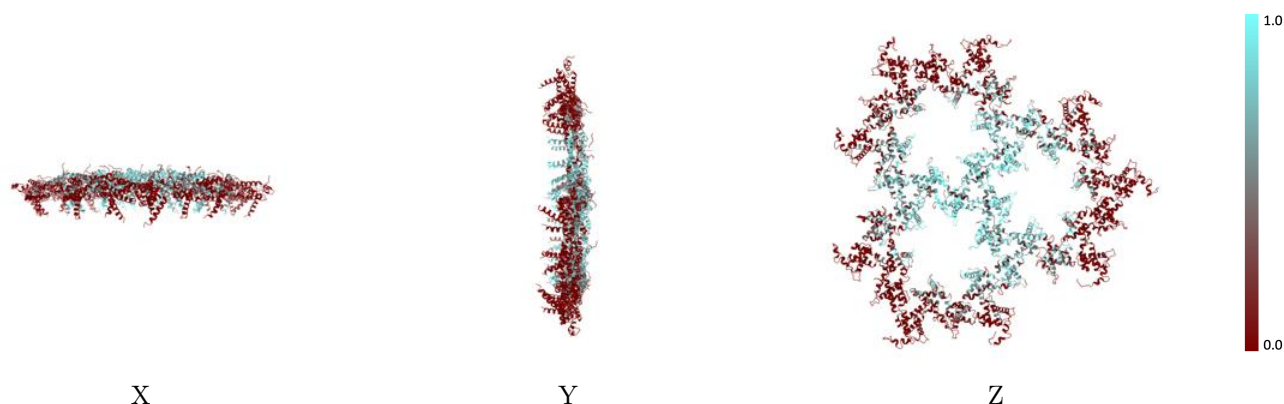
The images above show the 3D surface view of the map at the recommended contour level 20.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



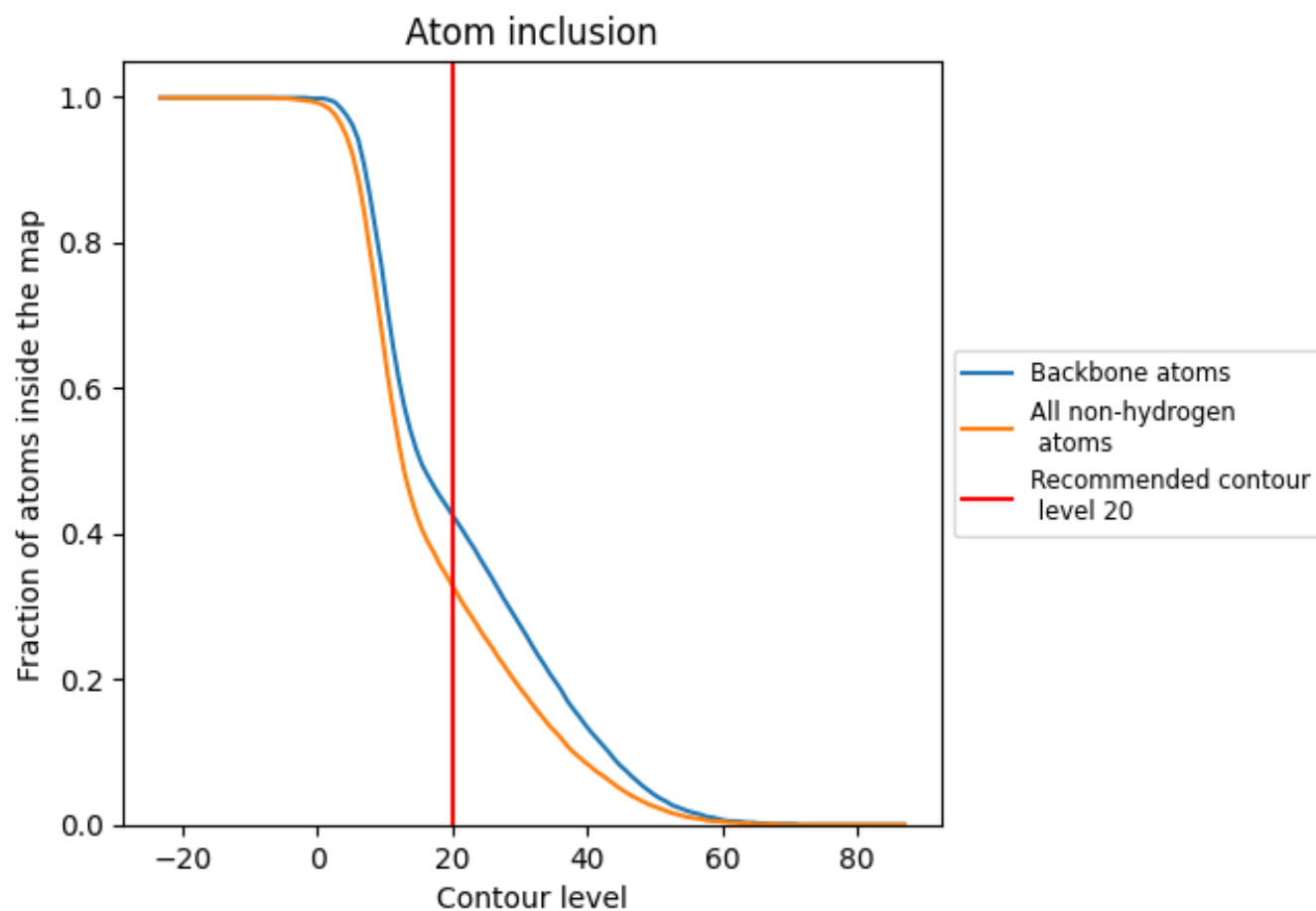
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (20).

9.4 Atom inclusion [i](#)



At the recommended contour level, 43% of all backbone atoms, 33% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (20) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3290	 0.0810
A	 0.7570	 0.1260
B	 0.7380	 0.1160
C	 0.7500	 0.1250
D	 0.6470	 0.1140
E	 0.7290	 0.1200
F	 0.5670	 0.0920
G	 0.7240	 0.1240
H	 0.5580	 0.0870
I	 0.6280	 0.1010
J	 0.5720	 0.0980
K	 0.6220	 0.1110
L	 0.7310	 0.1110
M	 0.2280	 0.0540
N	 0.3890	 0.0730
O	 0.0000	 0.0790
P	 0.0000	 0.0680
Q	 0.2310	 0.0650
R	 0.3860	 0.0760
S	 0.3780	 0.0740
T	 0.0000	 0.0750
U	 0.2320	 0.0500
V	 0.0000	 0.0520
W	 0.0000	 0.0500
X	 0.2950	 0.0850
Y	 0.1130	 0.0540
Z	 0.0390	 0.0610
a	 0.5410	 0.0870
b	 0.0000	 0.0490
c	 0.2950	 0.0810
d	 0.0000	 0.0560
e	 0.5410	 0.1040
f	 0.1230	 0.0740
g	 0.0420	 0.0650
h	 0.2950	 0.0830



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Chain	Atom inclusion	Q-score
i	 0.0000	 0.0640
j	 0.0000	 0.0380
k	 0.0360	 0.0740
l	 0.5210	 0.0910
m	 0.1210	 0.0590