WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Dec 19, 2022 – 01:12 pm GMT

PDB ID	:	7NT5
EMDB ID	:	EMD-12581
Title	:	CryoEM structure of the Nipah virus nucleocapsid single helical turn assembly
Authors	:	Ker, D.S.; Jenkins, H.T.; Greive, S.J.; Antson, A.A.
Deposited on	:	2021-03-09
Resolution	:	3.50 Å(reported)
Based on initial model	:	4CO6

The following versions of software and data (see references (i)) were used in the production of this report:
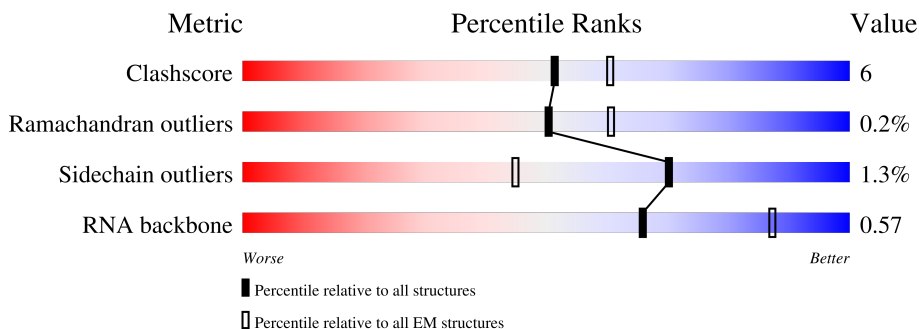
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.50 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.
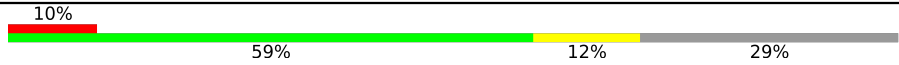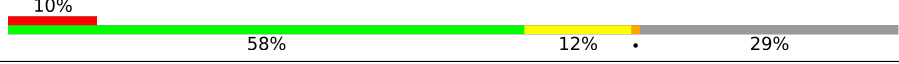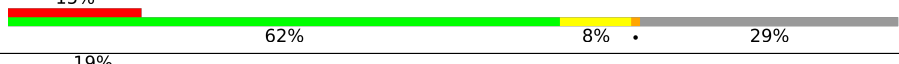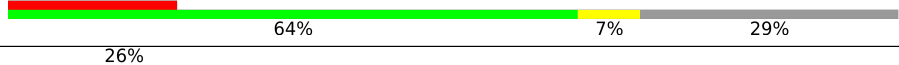
Metric	Percentile Ranks	Value
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		1.3%
RNA backbone		0.57

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
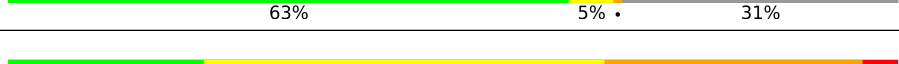
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	554	28% / 62% 8% • 29%
1	B	554	21% / 58% 12% 29%
1	C	554	17% / 60% 10% • 29%
1	D	554	16% / 63% 8% 29%
1	E	554	13% / 62% 8% • 29%
1	F	554	10% / 59% 11% • 29%
1	G	554	10% / 59% 12% 29%

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Mol	Chain	Length	Quality of chain
1	H	554	10% 59% 12% 29%
1	I	554	10% 58% 12% 29%
1	J	554	15% 62% 8% 29%
1	K	554	19% 64% 7% 29%
1	L	554	26% 64% 6% 29%
1	M	554	32% 63% 5% 31%
2	N	78	22% 45% 29%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 40200 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	394	Total	C	N	O	S	0	0
			2974	1891	511	557	15		
1	B	395	Total	C	N	O	S	0	0
			2979	1894	512	558	15		
1	C	394	Total	C	N	O	S	0	0
			2974	1891	511	557	15		
1	D	395	Total	C	N	O	S	0	0
			2979	1894	512	558	15		
1	E	395	Total	C	N	O	S	0	0
			2979	1894	512	558	15		
1	F	395	Total	C	N	O	S	0	0
			2979	1894	512	558	15		
1	G	395	Total	C	N	O	S	0	0
			2979	1894	512	558	15		
1	H	395	Total	C	N	O	S	0	0
			2979	1894	512	558	15		
1	I	395	Total	C	N	O	S	0	0
			2979	1894	512	558	15		
1	J	395	Total	C	N	O	S	0	0
			2979	1894	512	558	15		
1	K	395	Total	C	N	O	S	0	0
			2979	1894	512	558	15		
1	L	393	Total	C	N	O	S	0	0
			2969	1888	510	556	15		
1	M	382	Total	C	N	O	S	0	0
			2916	1857	499	545	15		

There are 286 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q9IK92
A	-20	GLY	-	expression tag	UNP Q9IK92
A	-19	SER	-	expression tag	UNP Q9IK92
A	-18	SER	-	expression tag	UNP Q9IK92

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	HIS	-	expression tag	UNP Q9IK92
A	-16	HIS	-	expression tag	UNP Q9IK92
A	-15	HIS	-	expression tag	UNP Q9IK92
A	-14	HIS	-	expression tag	UNP Q9IK92
A	-13	HIS	-	expression tag	UNP Q9IK92
A	-12	HIS	-	expression tag	UNP Q9IK92
A	-11	SER	-	expression tag	UNP Q9IK92
A	-10	SER	-	expression tag	UNP Q9IK92
A	-9	GLY	-	expression tag	UNP Q9IK92
A	-8	LEU	-	expression tag	UNP Q9IK92
A	-7	GLU	-	expression tag	UNP Q9IK92
A	-6	VAL	-	expression tag	UNP Q9IK92
A	-5	LEU	-	expression tag	UNP Q9IK92
A	-4	PHE	-	expression tag	UNP Q9IK92
A	-3	GLN	-	expression tag	UNP Q9IK92
A	-2	GLY	-	expression tag	UNP Q9IK92
A	-1	PRO	-	expression tag	UNP Q9IK92
A	0	ALA	-	expression tag	UNP Q9IK92
B	-21	MET	-	initiating methionine	UNP Q9IK92
B	-20	GLY	-	expression tag	UNP Q9IK92
B	-19	SER	-	expression tag	UNP Q9IK92
B	-18	SER	-	expression tag	UNP Q9IK92
B	-17	HIS	-	expression tag	UNP Q9IK92
B	-16	HIS	-	expression tag	UNP Q9IK92
B	-15	HIS	-	expression tag	UNP Q9IK92
B	-14	HIS	-	expression tag	UNP Q9IK92
B	-13	HIS	-	expression tag	UNP Q9IK92
B	-12	HIS	-	expression tag	UNP Q9IK92
B	-11	SER	-	expression tag	UNP Q9IK92
B	-10	SER	-	expression tag	UNP Q9IK92
B	-9	GLY	-	expression tag	UNP Q9IK92
B	-8	LEU	-	expression tag	UNP Q9IK92
B	-7	GLU	-	expression tag	UNP Q9IK92
B	-6	VAL	-	expression tag	UNP Q9IK92
B	-5	LEU	-	expression tag	UNP Q9IK92
B	-4	PHE	-	expression tag	UNP Q9IK92
B	-3	GLN	-	expression tag	UNP Q9IK92
B	-2	GLY	-	expression tag	UNP Q9IK92
B	-1	PRO	-	expression tag	UNP Q9IK92
B	0	ALA	-	expression tag	UNP Q9IK92
C	-21	MET	-	initiating methionine	UNP Q9IK92
C	-20	GLY	-	expression tag	UNP Q9IK92

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	SER	-	expression tag	UNP Q9IK92
C	-18	SER	-	expression tag	UNP Q9IK92
C	-17	HIS	-	expression tag	UNP Q9IK92
C	-16	HIS	-	expression tag	UNP Q9IK92
C	-15	HIS	-	expression tag	UNP Q9IK92
C	-14	HIS	-	expression tag	UNP Q9IK92
C	-13	HIS	-	expression tag	UNP Q9IK92
C	-12	HIS	-	expression tag	UNP Q9IK92
C	-11	SER	-	expression tag	UNP Q9IK92
C	-10	SER	-	expression tag	UNP Q9IK92
C	-9	GLY	-	expression tag	UNP Q9IK92
C	-8	LEU	-	expression tag	UNP Q9IK92
C	-7	GLU	-	expression tag	UNP Q9IK92
C	-6	VAL	-	expression tag	UNP Q9IK92
C	-5	LEU	-	expression tag	UNP Q9IK92
C	-4	PHE	-	expression tag	UNP Q9IK92
C	-3	GLN	-	expression tag	UNP Q9IK92
C	-2	GLY	-	expression tag	UNP Q9IK92
C	-1	PRO	-	expression tag	UNP Q9IK92
C	0	ALA	-	expression tag	UNP Q9IK92
D	-21	MET	-	initiating methionine	UNP Q9IK92
D	-20	GLY	-	expression tag	UNP Q9IK92
D	-19	SER	-	expression tag	UNP Q9IK92
D	-18	SER	-	expression tag	UNP Q9IK92
D	-17	HIS	-	expression tag	UNP Q9IK92
D	-16	HIS	-	expression tag	UNP Q9IK92
D	-15	HIS	-	expression tag	UNP Q9IK92
D	-14	HIS	-	expression tag	UNP Q9IK92
D	-13	HIS	-	expression tag	UNP Q9IK92
D	-12	HIS	-	expression tag	UNP Q9IK92
D	-11	SER	-	expression tag	UNP Q9IK92
D	-10	SER	-	expression tag	UNP Q9IK92
D	-9	GLY	-	expression tag	UNP Q9IK92
D	-8	LEU	-	expression tag	UNP Q9IK92
D	-7	GLU	-	expression tag	UNP Q9IK92
D	-6	VAL	-	expression tag	UNP Q9IK92
D	-5	LEU	-	expression tag	UNP Q9IK92
D	-4	PHE	-	expression tag	UNP Q9IK92
D	-3	GLN	-	expression tag	UNP Q9IK92
D	-2	GLY	-	expression tag	UNP Q9IK92
D	-1	PRO	-	expression tag	UNP Q9IK92
D	0	ALA	-	expression tag	UNP Q9IK92

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-21	MET	-	initiating methionine	UNP Q9IK92
E	-20	GLY	-	expression tag	UNP Q9IK92
E	-19	SER	-	expression tag	UNP Q9IK92
E	-18	SER	-	expression tag	UNP Q9IK92
E	-17	HIS	-	expression tag	UNP Q9IK92
E	-16	HIS	-	expression tag	UNP Q9IK92
E	-15	HIS	-	expression tag	UNP Q9IK92
E	-14	HIS	-	expression tag	UNP Q9IK92
E	-13	HIS	-	expression tag	UNP Q9IK92
E	-12	HIS	-	expression tag	UNP Q9IK92
E	-11	SER	-	expression tag	UNP Q9IK92
E	-10	SER	-	expression tag	UNP Q9IK92
E	-9	GLY	-	expression tag	UNP Q9IK92
E	-8	LEU	-	expression tag	UNP Q9IK92
E	-7	GLU	-	expression tag	UNP Q9IK92
E	-6	VAL	-	expression tag	UNP Q9IK92
E	-5	LEU	-	expression tag	UNP Q9IK92
E	-4	PHE	-	expression tag	UNP Q9IK92
E	-3	GLN	-	expression tag	UNP Q9IK92
E	-2	GLY	-	expression tag	UNP Q9IK92
E	-1	PRO	-	expression tag	UNP Q9IK92
E	0	ALA	-	expression tag	UNP Q9IK92
F	-21	MET	-	initiating methionine	UNP Q9IK92
F	-20	GLY	-	expression tag	UNP Q9IK92
F	-19	SER	-	expression tag	UNP Q9IK92
F	-18	SER	-	expression tag	UNP Q9IK92
F	-17	HIS	-	expression tag	UNP Q9IK92
F	-16	HIS	-	expression tag	UNP Q9IK92
F	-15	HIS	-	expression tag	UNP Q9IK92
F	-14	HIS	-	expression tag	UNP Q9IK92
F	-13	HIS	-	expression tag	UNP Q9IK92
F	-12	HIS	-	expression tag	UNP Q9IK92
F	-11	SER	-	expression tag	UNP Q9IK92
F	-10	SER	-	expression tag	UNP Q9IK92
F	-9	GLY	-	expression tag	UNP Q9IK92
F	-8	LEU	-	expression tag	UNP Q9IK92
F	-7	GLU	-	expression tag	UNP Q9IK92
F	-6	VAL	-	expression tag	UNP Q9IK92
F	-5	LEU	-	expression tag	UNP Q9IK92
F	-4	PHE	-	expression tag	UNP Q9IK92
F	-3	GLN	-	expression tag	UNP Q9IK92
F	-2	GLY	-	expression tag	UNP Q9IK92

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	PRO	-	expression tag	UNP Q9IK92
F	0	ALA	-	expression tag	UNP Q9IK92
G	-21	MET	-	initiating methionine	UNP Q9IK92
G	-20	GLY	-	expression tag	UNP Q9IK92
G	-19	SER	-	expression tag	UNP Q9IK92
G	-18	SER	-	expression tag	UNP Q9IK92
G	-17	HIS	-	expression tag	UNP Q9IK92
G	-16	HIS	-	expression tag	UNP Q9IK92
G	-15	HIS	-	expression tag	UNP Q9IK92
G	-14	HIS	-	expression tag	UNP Q9IK92
G	-13	HIS	-	expression tag	UNP Q9IK92
G	-12	HIS	-	expression tag	UNP Q9IK92
G	-11	SER	-	expression tag	UNP Q9IK92
G	-10	SER	-	expression tag	UNP Q9IK92
G	-9	GLY	-	expression tag	UNP Q9IK92
G	-8	LEU	-	expression tag	UNP Q9IK92
G	-7	GLU	-	expression tag	UNP Q9IK92
G	-6	VAL	-	expression tag	UNP Q9IK92
G	-5	LEU	-	expression tag	UNP Q9IK92
G	-4	PHE	-	expression tag	UNP Q9IK92
G	-3	GLN	-	expression tag	UNP Q9IK92
G	-2	GLY	-	expression tag	UNP Q9IK92
G	-1	PRO	-	expression tag	UNP Q9IK92
G	0	ALA	-	expression tag	UNP Q9IK92
H	-21	MET	-	initiating methionine	UNP Q9IK92
H	-20	GLY	-	expression tag	UNP Q9IK92
H	-19	SER	-	expression tag	UNP Q9IK92
H	-18	SER	-	expression tag	UNP Q9IK92
H	-17	HIS	-	expression tag	UNP Q9IK92
H	-16	HIS	-	expression tag	UNP Q9IK92
H	-15	HIS	-	expression tag	UNP Q9IK92
H	-14	HIS	-	expression tag	UNP Q9IK92
H	-13	HIS	-	expression tag	UNP Q9IK92
H	-12	HIS	-	expression tag	UNP Q9IK92
H	-11	SER	-	expression tag	UNP Q9IK92
H	-10	SER	-	expression tag	UNP Q9IK92
H	-9	GLY	-	expression tag	UNP Q9IK92
H	-8	LEU	-	expression tag	UNP Q9IK92
H	-7	GLU	-	expression tag	UNP Q9IK92
H	-6	VAL	-	expression tag	UNP Q9IK92
H	-5	LEU	-	expression tag	UNP Q9IK92
H	-4	PHE	-	expression tag	UNP Q9IK92

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	GLN	-	expression tag	UNP Q9IK92
H	-2	GLY	-	expression tag	UNP Q9IK92
H	-1	PRO	-	expression tag	UNP Q9IK92
H	0	ALA	-	expression tag	UNP Q9IK92
I	-21	MET	-	initiating methionine	UNP Q9IK92
I	-20	GLY	-	expression tag	UNP Q9IK92
I	-19	SER	-	expression tag	UNP Q9IK92
I	-18	SER	-	expression tag	UNP Q9IK92
I	-17	HIS	-	expression tag	UNP Q9IK92
I	-16	HIS	-	expression tag	UNP Q9IK92
I	-15	HIS	-	expression tag	UNP Q9IK92
I	-14	HIS	-	expression tag	UNP Q9IK92
I	-13	HIS	-	expression tag	UNP Q9IK92
I	-12	HIS	-	expression tag	UNP Q9IK92
I	-11	SER	-	expression tag	UNP Q9IK92
I	-10	SER	-	expression tag	UNP Q9IK92
I	-9	GLY	-	expression tag	UNP Q9IK92
I	-8	LEU	-	expression tag	UNP Q9IK92
I	-7	GLU	-	expression tag	UNP Q9IK92
I	-6	VAL	-	expression tag	UNP Q9IK92
I	-5	LEU	-	expression tag	UNP Q9IK92
I	-4	PHE	-	expression tag	UNP Q9IK92
I	-3	GLN	-	expression tag	UNP Q9IK92
I	-2	GLY	-	expression tag	UNP Q9IK92
I	-1	PRO	-	expression tag	UNP Q9IK92
I	0	ALA	-	expression tag	UNP Q9IK92
J	-21	MET	-	initiating methionine	UNP Q9IK92
J	-20	GLY	-	expression tag	UNP Q9IK92
J	-19	SER	-	expression tag	UNP Q9IK92
J	-18	SER	-	expression tag	UNP Q9IK92
J	-17	HIS	-	expression tag	UNP Q9IK92
J	-16	HIS	-	expression tag	UNP Q9IK92
J	-15	HIS	-	expression tag	UNP Q9IK92
J	-14	HIS	-	expression tag	UNP Q9IK92
J	-13	HIS	-	expression tag	UNP Q9IK92
J	-12	HIS	-	expression tag	UNP Q9IK92
J	-11	SER	-	expression tag	UNP Q9IK92
J	-10	SER	-	expression tag	UNP Q9IK92
J	-9	GLY	-	expression tag	UNP Q9IK92
J	-8	LEU	-	expression tag	UNP Q9IK92
J	-7	GLU	-	expression tag	UNP Q9IK92
J	-6	VAL	-	expression tag	UNP Q9IK92

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-5	LEU	-	expression tag	UNP Q9IK92
J	-4	PHE	-	expression tag	UNP Q9IK92
J	-3	GLN	-	expression tag	UNP Q9IK92
J	-2	GLY	-	expression tag	UNP Q9IK92
J	-1	PRO	-	expression tag	UNP Q9IK92
J	0	ALA	-	expression tag	UNP Q9IK92
K	-21	MET	-	initiating methionine	UNP Q9IK92
K	-20	GLY	-	expression tag	UNP Q9IK92
K	-19	SER	-	expression tag	UNP Q9IK92
K	-18	SER	-	expression tag	UNP Q9IK92
K	-17	HIS	-	expression tag	UNP Q9IK92
K	-16	HIS	-	expression tag	UNP Q9IK92
K	-15	HIS	-	expression tag	UNP Q9IK92
K	-14	HIS	-	expression tag	UNP Q9IK92
K	-13	HIS	-	expression tag	UNP Q9IK92
K	-12	HIS	-	expression tag	UNP Q9IK92
K	-11	SER	-	expression tag	UNP Q9IK92
K	-10	SER	-	expression tag	UNP Q9IK92
K	-9	GLY	-	expression tag	UNP Q9IK92
K	-8	LEU	-	expression tag	UNP Q9IK92
K	-7	GLU	-	expression tag	UNP Q9IK92
K	-6	VAL	-	expression tag	UNP Q9IK92
K	-5	LEU	-	expression tag	UNP Q9IK92
K	-4	PHE	-	expression tag	UNP Q9IK92
K	-3	GLN	-	expression tag	UNP Q9IK92
K	-2	GLY	-	expression tag	UNP Q9IK92
K	-1	PRO	-	expression tag	UNP Q9IK92
K	0	ALA	-	expression tag	UNP Q9IK92
L	-21	MET	-	initiating methionine	UNP Q9IK92
L	-20	GLY	-	expression tag	UNP Q9IK92
L	-19	SER	-	expression tag	UNP Q9IK92
L	-18	SER	-	expression tag	UNP Q9IK92
L	-17	HIS	-	expression tag	UNP Q9IK92
L	-16	HIS	-	expression tag	UNP Q9IK92
L	-15	HIS	-	expression tag	UNP Q9IK92
L	-14	HIS	-	expression tag	UNP Q9IK92
L	-13	HIS	-	expression tag	UNP Q9IK92
L	-12	HIS	-	expression tag	UNP Q9IK92
L	-11	SER	-	expression tag	UNP Q9IK92
L	-10	SER	-	expression tag	UNP Q9IK92
L	-9	GLY	-	expression tag	UNP Q9IK92
L	-8	LEU	-	expression tag	UNP Q9IK92

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-7	GLU	-	expression tag	UNP Q9IK92
L	-6	VAL	-	expression tag	UNP Q9IK92
L	-5	LEU	-	expression tag	UNP Q9IK92
L	-4	PHE	-	expression tag	UNP Q9IK92
L	-3	GLN	-	expression tag	UNP Q9IK92
L	-2	GLY	-	expression tag	UNP Q9IK92
L	-1	PRO	-	expression tag	UNP Q9IK92
L	0	ALA	-	expression tag	UNP Q9IK92
M	-21	MET	-	initiating methionine	UNP Q9IK92
M	-20	GLY	-	expression tag	UNP Q9IK92
M	-19	SER	-	expression tag	UNP Q9IK92
M	-18	SER	-	expression tag	UNP Q9IK92
M	-17	HIS	-	expression tag	UNP Q9IK92
M	-16	HIS	-	expression tag	UNP Q9IK92
M	-15	HIS	-	expression tag	UNP Q9IK92
M	-14	HIS	-	expression tag	UNP Q9IK92
M	-13	HIS	-	expression tag	UNP Q9IK92
M	-12	HIS	-	expression tag	UNP Q9IK92
M	-11	SER	-	expression tag	UNP Q9IK92
M	-10	SER	-	expression tag	UNP Q9IK92
M	-9	GLY	-	expression tag	UNP Q9IK92
M	-8	LEU	-	expression tag	UNP Q9IK92
M	-7	GLU	-	expression tag	UNP Q9IK92
M	-6	VAL	-	expression tag	UNP Q9IK92
M	-5	LEU	-	expression tag	UNP Q9IK92
M	-4	PHE	-	expression tag	UNP Q9IK92
M	-3	GLN	-	expression tag	UNP Q9IK92
M	-2	GLY	-	expression tag	UNP Q9IK92
M	-1	PRO	-	expression tag	UNP Q9IK92
M	0	ALA	-	expression tag	UNP Q9IK92

- Molecule 2 is a RNA chain called RNA (78-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	N	78	1556	702	156	621	77	0	0

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 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.
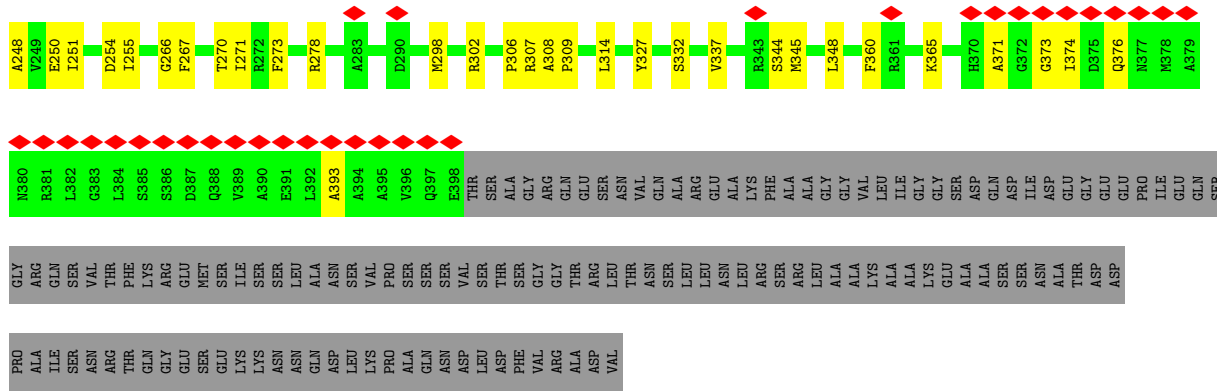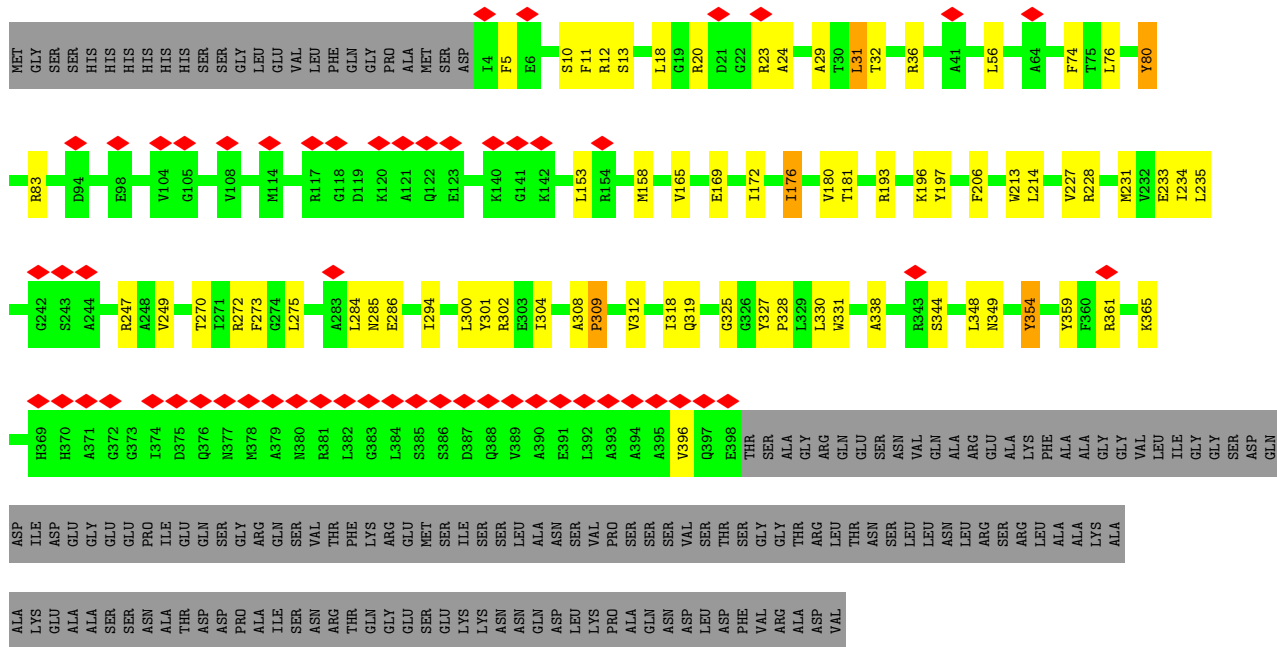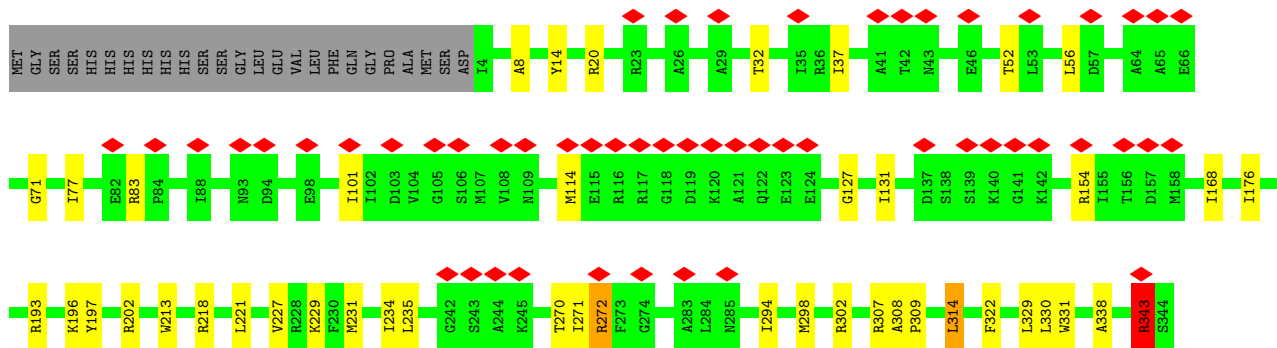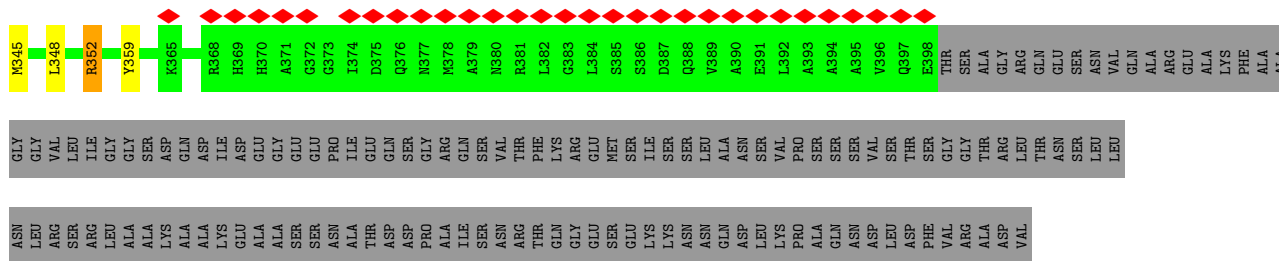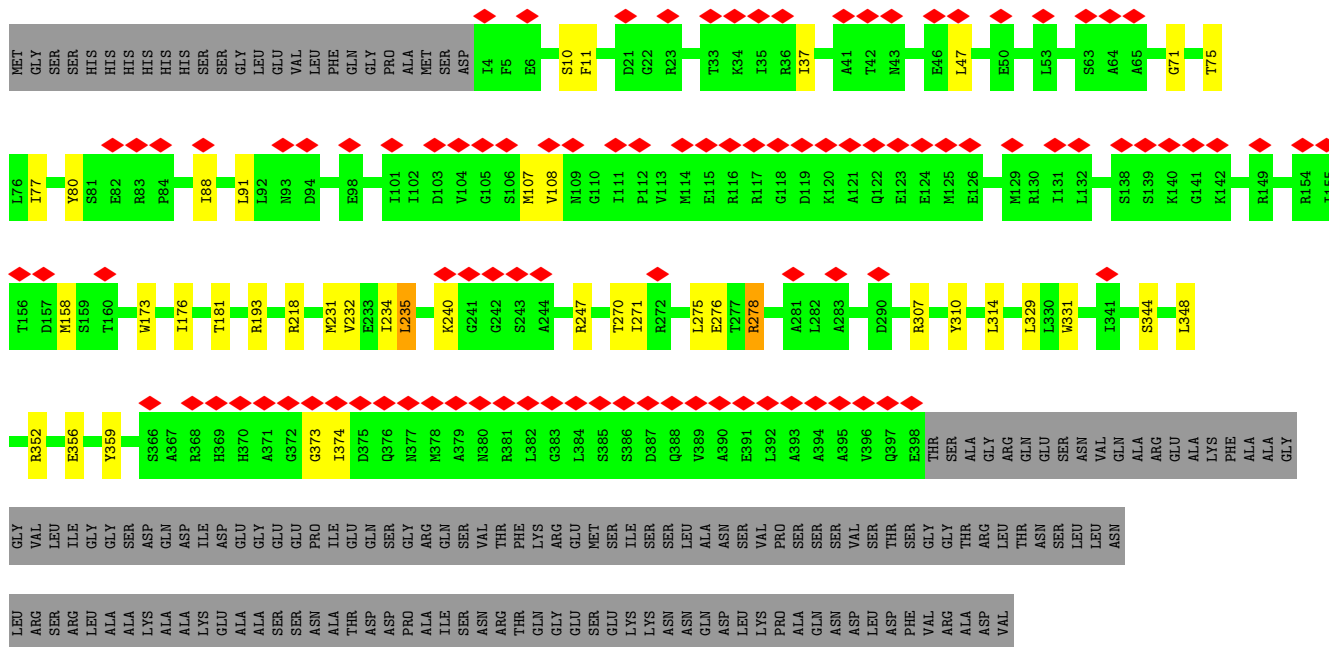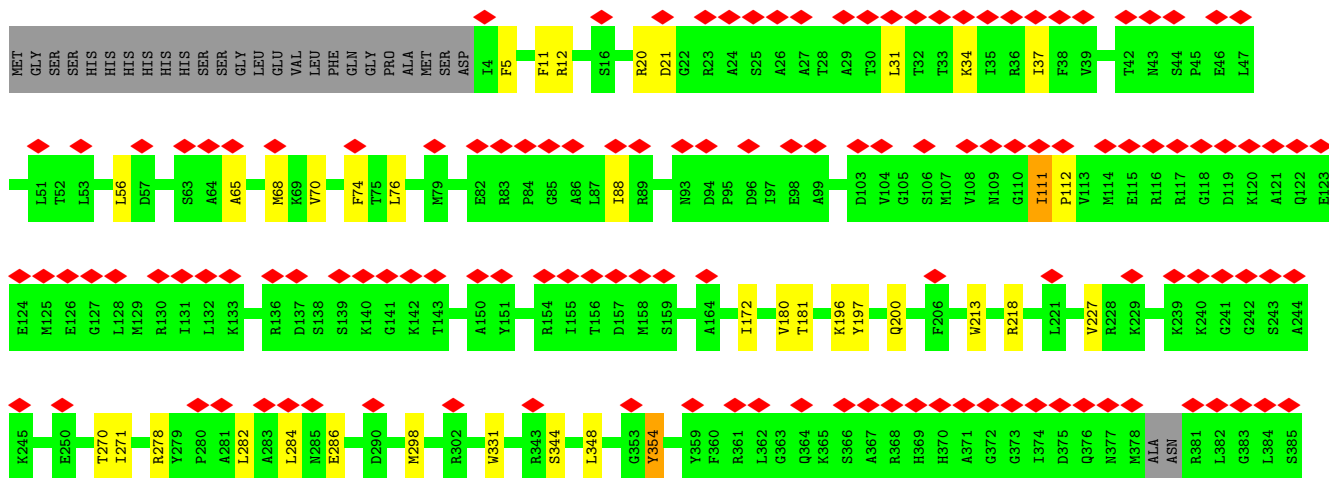
• Molecule 1: Nucleoprotein

• Molecule 1: Nucleoprotein

E46 L47 T52 L53 L56 A64 A65 E66 G71 L76 I77 Y80 S81 E82 R83 L87 I88 R89 N93 D94 E98 I101 I102 D103 V104 G105 S106 M107 V108 N109 G110 I111 P112 V113 M114 E115 R116 R117 G118 D119 K120 A121 Q122 E123 E126 I131 L132

D137 S138 S139 K140 G141 K142 A150 T156 D157 T167 I168 I172 L175 K178 A179 V180 P183 E190 R193 Q199 R202 V203 N204 W213 L214 R218 R228 V238 K239 G242 S243 A244 K245 G246 E250 T262 T270 R271 R272 F273 G274

L275 E276 T277 R278 Y279 P280 A281 L282 A283 L284 N285 S289 D290 T293 I294 K295 S296 L299 L300 Y301 R302 R307 L313 W331 A338 R343 G346 A347 L348 N351 R352 G353 Y354 P357 M358 R361 L362 K365 S366 A367 R368 H369 H370 A371 G372 G373 I374

D375 Q376 N377 M378 A379 N380 R381 L382 G383 L384 S385 S386 D387 Q388 V389 A390 E391 L392 A393 A394 A395 V396 Q397 E398 THR SER GLY ARG GLU GLU SER ASN VAL GLN ALA ARG ALA LYS PHE ALA ALA GLY VAL ILE GLY SER ASP ASP ILE ASP GLU GLY GLU GLU

PRO ILE GLU SER GLY ARG GLN SER VAL THR PHE LYS ARG GLU MET SER ILE SER LEU ALA ASN VAL PRO SER SER VAL SER THR SER GLY THR LEU THR ASN LEU LEU ASN LEU ARG ALA ARG LEU ALA ALA LYS ALA ALA LYS GLU ALA ALA SER

ASN ALA THR ASP PRO ALA ILE SER ARG THR GLN GLY GLU SER GLU LYS LYS ASN ASN GLN ASP LEU LYS PRO ALA GLN ASN ASP LEU ASP PHE VAL ARG ALA ASP VAL

● Molecule 1: Nucleoprotein

Chain C:

17%

60%   10% ·   29%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU GLU VAL LEU PHE GLN GLY PRO ALA MET SER ASP I4 F5 A8 F11 Y14 D21 G22 R23 A24 S25 A26 A27 T28 T33 K34 I35 R36 I37 A41 T42 N43 S44 P45 E46 L47 T52 L56

R60 A64 A65 I77 S78 S81 E82 R83 A86 L87 I88 R89 N93 D94 E98 A99 I102 D103 V104 G105 S106 M107 V108 N109 I111 M114 E115 R116 R117 G118 D119 K120 A121 Q122 E123 E124 L128 L132 K133 D137 S138 S139 K140 G141 K142 R154

I155 T156 D157 T167 I168 I176 A182 A186 R192 R193 W194 A195 K196 Y197 V198 Q199 Q200 P205 W213 R218 L221 V227 R228 K229 I234 V238 K239 K240 G241 G242 S243 A244 T270 I271 L275 E276 T277 R278 A283 L284 N285 E286 I294 K295

R307 A308 P309 W331 R343 S344 M345 L348 R361 L362 K365 S366 A367 R368 H369 H370 A371 G372 G373 I374 D375 Q376 N377 M378 A379 N380 R381 L382 G383 L384 S385 S386 D387 Q388 V389 A390 E391 L392 A393 A394 A395 V396 Q397 GLU THR SER ALA GLY ARG GLU GLU SER ASN VAL

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

GLY THR ARG LEU THR ASN SER LEU LEU ASN LEU ARG ALA SER ARG LEU ALA ALA LYS ALA ALA LYS GLU ALA ALA SER ASN ALA THR ASP PRO ALA ILE SER ASN ARG GLN GLY GLU SER GLU LYS LYS ASN ASN GLN ASP LEU LYS PRO ALA GLN ASN ASP LEU ASP PHE VAL

ARG ALA ASP VAL

● Molecule 1: Nucleoprotein

Chain D:

16%

63%   8%   29%

• Molecule 1: Nucleoprotein

Chain E:

13%

62% 8% • 29%

• Molecule 1: Nucleoprotein

Chain F:

10%

59% 11% • 29%

• Molecule 1: Nucleoprotein

Chain G:

10%

59%　　12%　　29%

• Molecule 1: Nucleoprotein

Chain H:

10%

59%　　12%　　29%

• Molecule 1: Nucleoprotein

Chain I:

10%
58%   12%   •   29%

• Molecule 1: Nucleoprotein

Chain J:

15%
62%   8%   •   29%

• Molecule 1: Nucleoprotein

Chain K:

19%

64%   7%   29%

• Molecule 1: Nucleoprotein

Chain L:

26%

64%   6%   29%

S386 D387 Q388 V389 A390 E391 L392 A393 A394 A395 V396 Q397 E398 THR SER ALA GLY ARG GLN GLU SER ASN VAL GLN ALA ARG GLU ALA LYS PHE ALA ALA GLY GLY VAL LEU ILE GLY GLY SER ASP GLN ASP ILE ASP GLU GLU GLY GLU PRO ILE GLU GLN SER GLY ARG GLN SER VAL THR

PHE LYS ARG GLU MET SER ILE SER SER LEU ALA ASN VAL SER PRO SER SER VAL SER THR SER GLY THR ARG LEU THR ASN SER LEU LEU ASN LEU ARG SER ARG LEU ALA ALA LYS ALA ALA LYS GLU ALA ALA SER SER ASN ALA THR ASP ASP PRO ALA ILE SER ASN ARG

THR GLN GLY GLU SER GLU LYS LYS ASN ASN GLN ASP LEU LYS PRO ALA GLN ASN ASP PHE VAL ARG ALA ASP VAL

• Molecule 1: Nucleoprotein

Chain M:

32%

63%　　　　　5% •　　　　　31%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL LEU PHE GLN GLY PRO ALA MET SER ASP I4 F5 F11 G19 R20 D21 G22 R23 A24 S25 A26 A27 T28 A29 T30 L31 T32 T33 K34 I35 R36 I37 F38 V39 P40 A41 T42 N43 S44 P45 E46 L47 R48

W49 E50 L51 T52 L53 F54 D57 R60 S61 P62 S63 A64 A65 M68 K69 A72 A73 F74 I77 S78 M79 Y80 S81 E82 R83 P84 G85 A86 L87 I88 R89 S90 L91 L92 N93 D94 P95 D96 I97 E98 A99 V100 I101 I102 D103 V104 G105 S106 M107 V108 N109 G110 I111 P112 V113

M114 E115 R116 R117 G118 D119 K120 A121 Q122 E123 E124 M125 E126 G127 L128 M129 R130 I131 L132 A135 R136 D137 S138 S139 K140 G141 K142 V146 D147 S148 R149 A150 Y151 G152 L153 R154 I155 T156 D157 M158 S159 T160 L161 I172 K178 D184 T185 A186 S189 R192 R193 W194 A195

V198 R202 V203 N204 P205 A208 Q212 L221 S222 V227 E233 E237 V238 K239 K240 Q241 G242 S243 A244 K245 G246 R247 E250 Y258 E261 T270 F273 G274 L275 P280 A281 L282 A283 L284 N285 D290 R302 G305 L313 Q319

L329 L330 W331 A338 T339 D342 R343 S344 M345 L348 N349 I350 N351 R352 G353 Y359 F360 R361 L362 G363 Q364 K365 S366 A367 R368 HIS HIS ALA GLY GLY ILE ASP GLN ASN MET ALA ASN ARG L382 G383 L384 S385 D386 D387 Q388 V389 A390 E391 L392 A393 A394 A395 V396 Q397 E398 THR SER ALA GLY ARG GLN GLU MET SER ILE SER SER LEU ALA ASN SER VAL

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

PRO SER SER SER VAL SER THR SER GLY THR GLY ARG LEU THR ASN SER LEU LEU ASN LEU ARG SER ARG LEU ALA ALA LYS ALA ALA LYS GLU ALA ALA SER SER ASN ALA THR ASP ASP PRO ALA ILE SER ASN ARG THR GLN GLY GLU SER GLU LYS LYS ASN ASN GLN ASP LEU LYS

PRO ALA GLN ASN ASP LEU ASP PHE VAL ARG ALA ALA ASP VAL

• Molecule 2: RNA (78-MER)

Chain N:

22%　　　　　45%　　　　　29%　　　　　•

U1 U2 U3 U4 U5 U6 U7 U8 U9 U10 U11 U12 U13 U14 U15 U16 U17 U18 U19 U20 U21 U22 U23 U24 U25 U26 U27 U28 U29 U30 U33 U34 U35 U36 U37 U38 U39 U40 U41 U42 U43 U44 U45 U46 U47 U48 U49 U50 U51 U52 U53 U54 U55 U56 U57 U58 U59 U60

U63 U64 U65 U68 U69 U70 U71 U72 U73 U74 U75 U76 U77 U78

4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124891	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 $(e^-/\text{Å}^2)$	41	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	251.51999, 251.51999, 251.51999	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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	A	0.52	0/3025	1.04	9/4096 (0.2%)
1	B	0.57	0/3030	1.12	11/4103 (0.3%)
1	C	0.59	1/3025 (0.0%)	1.12	8/4096 (0.2%)
1	D	0.60	0/3030	1.17	13/4103 (0.3%)
1	E	0.64	1/3030 (0.0%)	1.15	12/4103 (0.3%)
1	F	0.68	1/3030 (0.0%)	1.21	16/4103 (0.4%)
1	G	0.68	0/3030	1.28	23/4103 (0.6%)
1	H	0.70	2/3030 (0.1%)	1.22	18/4103 (0.4%)
1	I	0.65	1/3030 (0.0%)	1.23	19/4103 (0.5%)
1	J	0.61	0/3030	1.14	11/4103 (0.3%)
1	K	0.55	0/3030	1.07	6/4103 (0.1%)
1	L	0.50	0/3019	1.00	1/4086 (0.0%)
1	M	0.55	2/2966 (0.1%)	1.16	12/4013 (0.3%)
2	N	1.18	4/1711 (0.2%)	1.53	33/2643 (1.2%)
All	All	0.64	12/41016 (0.0%)	1.17	192/55861 (0.3%)

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	A	0	1
1	C	0	1
1	F	0	2
1	I	0	3
1	K	0	2
2	N	0	5
All	All	0	14

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	343	ARG	NE-CZ	11.44	1.48	1.33
2	N	35	U	O3'-P	7.12	1.69	1.61
2	N	41	U	O3'-P	7.03	1.69	1.61
2	N	25	U	O3'-P	-6.93	1.52	1.61
2	N	26	U	O3'-P	6.38	1.68	1.61
1	E	345	MET	CG-SD	5.83	1.96	1.81
1	H	345	MET	CG-SD	5.75	1.96	1.81
1	M	302	ARG	NE-CZ	5.60	1.40	1.33
1	H	169	GLU	CD-OE2	-5.52	1.19	1.25
1	F	169	GLU	CD-OE1	-5.25	1.19	1.25
1	I	169	GLU	CD-OE1	-5.22	1.20	1.25
1	C	276	GLU	CD-OE2	5.01	1.31	1.25

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	343	ARG	NE-CZ-NH1	-24.90	107.85	120.30
1	M	343	ARG	NE-CZ-NH2	19.31	129.96	120.30
1	M	302	ARG	CD-NE-CZ	10.56	138.39	123.60
1	M	343	ARG	CD-NE-CZ	10.28	137.99	123.60
1	E	193	ARG	NE-CZ-NH2	10.25	125.42	120.30
1	D	228	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	I	12	ARG	NE-CZ-NH1	-9.34	115.63	120.30
1	H	307	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	J	322	PHE	CB-CG-CD2	-9.15	114.39	120.80
1	I	12	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	G	259	VAL	CG1-CB-CG2	-8.83	96.77	110.90
1	F	176	ILE	CG1-CB-CG2	-8.77	92.11	111.40
2	N	55	U	C5'-C4'-O4'	8.62	119.44	109.10
1	F	12	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	D	228	ARG	CD-NE-CZ	8.38	135.33	123.60
1	B	83	ARG	CG-CD-NE	8.24	129.10	111.80
1	F	272	ARG	NE-CZ-NH2	8.23	124.41	120.30
1	C	307	ARG	CG-CD-NE	8.20	129.01	111.80
1	G	352	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	M	302	ARG	CG-CD-NE	7.87	128.32	111.80
1	D	343	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	F	75	THR	CA-CB-CG2	7.52	122.93	112.40
1	M	302	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	F	248	ALA	N-CA-CB	-7.08	100.19	110.10
1	E	258	TYR	CB-CG-CD2	-7.08	116.75	121.00
1	D	302	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	I	193	ARG	CG-CD-NE	7.01	126.53	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	302	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	B	278	ARG	NE-CZ-NH1	-6.97	116.82	120.30
2	N	17	U	O5'-P-OP2	-6.87	99.51	105.70
1	E	261	GLU	CB-CA-C	6.85	124.09	110.40
1	I	12	ARG	CB-CG-CD	6.84	129.39	111.60
1	H	230	PHE	CB-CG-CD2	-6.83	116.02	120.80
1	J	352	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	307	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	J	343	ARG	NE-CZ-NH2	6.73	123.67	120.30
1	E	272	ARG	NE-CZ-NH2	6.73	123.67	120.30
1	I	214	LEU	CB-CG-CD1	-6.70	99.61	111.00
1	C	182	ALA	CB-CA-C	6.70	120.15	110.10
1	C	176	ILE	CG1-CB-CG2	-6.70	96.67	111.40
1	G	80	TYR	CG-CD2-CE2	-6.68	115.96	121.30
1	H	154	ARG	CB-CG-CD	6.67	128.95	111.60
2	N	20	U	O5'-P-OP2	6.60	118.62	110.70
1	I	83	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	D	247	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	J	218	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	H	247	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	G	247	ARG	NE-CZ-NH1	6.47	123.54	120.30
2	N	36	U	O4'-C1'-N1	6.45	113.36	108.20
1	H	230	PHE	CB-CG-CD1	6.44	125.31	120.80
2	N	45	U	N1-C1'-C2'	6.43	122.36	114.00
2	N	33	U	O4'-C1'-N1	6.43	113.35	108.20
2	N	34	U	O5'-P-OP1	6.42	118.40	110.70
2	N	69	U	O5'-P-OP1	-6.41	99.93	105.70
2	N	12	U	O4'-C1'-N1	6.37	113.30	108.20
1	G	234	ILE	CG1-CB-CG2	-6.37	97.39	111.40
2	N	70	U	O4'-C1'-N1	6.37	113.30	108.20
1	H	130	ARG	CG-CD-NE	6.37	125.17	111.80
1	C	228	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	196	LYS	CB-CA-C	6.33	123.06	110.40
2	N	57	U	O4'-C1'-N1	6.30	113.24	108.20
1	F	295	LYS	CB-CG-CD	6.25	127.86	111.60
1	D	343	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	H	307	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	258	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	K	235	LEU	CB-CG-CD1	-6.18	100.49	111.00
1	K	307	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	N	9	U	O4'-C1'-N1	6.16	113.12	108.20
1	K	307	ARG	CG-CD-NE	-6.14	98.92	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	307	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	247	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	F	172	ILE	CA-CB-CG2	6.11	123.13	110.90
2	N	41	U	C5'-C4'-C3'	-6.08	106.28	116.00
1	E	193	ARG	N-CA-CB	6.05	121.50	110.60
2	N	71	U	O4'-C1'-N1	6.05	113.04	108.20
1	E	218	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	I	233	GLU	CB-CA-C	5.99	122.37	110.40
1	J	202	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	N	23	U	C5'-C4'-O4'	5.94	116.22	109.10
1	G	230	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	F	80	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	G	176	ILE	CG1-CB-CG2	-5.88	98.47	111.40
1	G	290	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	G	60	ARG	CG-CD-NE	5.85	124.08	111.80
1	G	171	GLN	CB-CA-C	5.83	122.07	110.40
1	C	309	PRO	CB-CA-C	-5.83	97.42	112.00
1	J	352	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	G	248	ALA	CB-CA-C	5.81	118.81	110.10
2	N	51	U	C3'-C2'-C1'	-5.79	96.87	101.50
2	N	41	U	N1-C1'-C2'	5.78	121.51	114.00
1	E	352	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	E	278	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	B	89	ARG	CG-CD-NE	5.76	123.90	111.80
2	N	45	U	O4'-C1'-N1	5.76	112.81	108.20
1	K	352	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	N	49	U	C5'-C4'-O4'	5.75	116.00	109.10
1	H	278	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	I	247	ARG	CB-CG-CD	5.72	126.47	111.60
2	N	7	U	C5'-C4'-O4'	5.71	115.95	109.10
1	G	60	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	F	154	ARG	CG-CD-NE	5.70	123.76	111.80
1	G	218	ARG	CB-CG-CD	-5.69	96.81	111.60
2	N	45	U	C3'-C2'-C1'	-5.69	96.95	101.50
1	C	218	ARG	CG-CD-NE	-5.67	99.90	111.80
1	B	278	ARG	CD-NE-CZ	5.66	131.52	123.60
1	A	182	ALA	CB-CA-C	5.64	118.56	110.10
2	N	40	U	P-O5'-C5'	-5.64	111.88	120.90
1	K	247	ARG	NE-CZ-NH1	5.63	123.11	120.30
2	N	74	U	C5'-C4'-C3'	-5.63	107.00	116.00
2	N	30	U	O4'-C1'-N1	5.62	112.69	108.20
1	G	149	ARG	NE-CZ-NH2	-5.61	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	272	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	M	302	ARG	CB-CA-C	5.58	121.55	110.40
1	B	80	TYR	CG-CD2-CE2	-5.57	116.84	121.30
2	N	55	U	C5'-C4'-C3'	-5.57	107.09	116.00
1	E	176	ILE	CG1-CB-CG2	-5.56	99.16	111.40
1	J	20	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	G	272	ARG	CB-CG-CD	-5.54	97.19	111.60
1	H	218	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	202	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	193	ARG	CG-CD-NE	-5.52	100.21	111.80
1	B	202	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	H	365	LYS	CB-CG-CD	5.51	125.94	111.60
1	E	193	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	D	206	PHE	CB-CG-CD1	5.49	124.64	120.80
1	G	43	ASN	CB-CA-C	5.49	121.37	110.40
1	A	352	ARG	CB-CG-CD	5.46	125.80	111.60
1	H	194	TRP	CB-CG-CD1	-5.46	119.91	127.00
1	E	60	ARG	CG-CD-NE	5.45	123.25	111.80
1	G	230	PHE	CB-CG-CD1	5.45	124.61	120.80
1	H	136	ARG	NE-CZ-NH2	-5.44	117.58	120.30
2	N	42	U	O4'-C1'-N1	5.44	112.55	108.20
1	A	202	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	K	218	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	F	258	TYR	CB-CA-C	5.41	121.22	110.40
1	H	248	ALA	CB-CA-C	5.39	118.19	110.10
1	M	193	ARG	CB-CG-CD	5.39	125.62	111.60
1	I	165	VAL	CG1-CB-CG2	5.39	119.52	110.90
1	M	193	ARG	CG-CD-NE	-5.39	100.48	111.80
1	H	75	THR	CA-CB-CG2	5.38	119.93	112.40
1	F	272	ARG	CD-NE-CZ	5.38	131.13	123.60
1	B	190	GLU	CB-CA-C	5.37	121.14	110.40
2	N	22	U	P-O5'-C5'	-5.36	112.32	120.90
2	N	33	U	C3'-C2'-C1'	-5.36	97.22	101.50
1	I	272	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	F	206	PHE	CB-CG-CD1	5.33	124.53	120.80
1	M	23	ARG	CG-CD-NE	5.32	122.97	111.80
1	G	249	VAL	CA-CB-CG2	5.32	118.87	110.90
2	N	27	U	O4'-C1'-N1	5.29	112.44	108.20
1	A	282	LEU	CB-CG-CD1	5.28	119.98	111.00
1	I	249	VAL	CA-CB-CG1	5.26	118.79	110.90
1	M	313	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	D	228	ARG	NE-CZ-NH2	-5.25	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	343	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	D	343	ARG	CG-CD-NE	5.25	122.82	111.80
1	F	309	PRO	CB-CA-C	-5.25	98.88	112.00
1	G	218	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	J	154	ARG	CB-CG-CD	5.23	125.19	111.60
1	H	254	ASP	CB-CG-OD1	5.22	122.99	118.30
1	G	247	ARG	CB-CG-CD	5.21	125.14	111.60
2	N	35	U	C2'-C3'-O3'	5.20	122.01	113.70
1	B	307	ARG	CB-CA-C	-5.19	100.02	110.40
1	D	178	LYS	N-CA-CB	-5.18	101.28	110.60
1	F	202	ARG	CB-CA-C	5.17	120.75	110.40
2	N	4	U	C5'-C4'-C3'	-5.17	107.74	116.00
1	F	75	THR	OG1-CB-CG2	-5.15	98.16	110.00
1	I	301	TYR	CB-CA-C	5.14	120.69	110.40
1	B	278	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	I	36	ARG	NE-CZ-NH2	5.13	122.87	120.30
2	N	30	U	O5'-P-OP2	-5.12	101.09	105.70
1	G	199	GLN	CB-CA-C	5.12	120.64	110.40
1	J	314	LEU	N-CA-CB	-5.12	100.17	110.40
1	G	149	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	I	354	TYR	CB-CG-CD1	5.11	124.07	121.00
1	B	300	LEU	CB-CG-CD1	5.11	119.68	111.00
1	I	80	TYR	CG-CD2-CE2	-5.10	117.22	121.30
1	C	228	ARG	CD-NE-CZ	5.08	130.72	123.60
1	I	80	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	H	218	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	H	89	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	E	341	ILE	CG1-CB-CG2	5.06	122.54	111.40
1	H	211	GLN	N-CA-CB	5.06	119.71	110.60
1	I	309	PRO	CB-CA-C	-5.05	99.38	112.00
2	N	60	U	O4'-C1'-N1	5.04	112.23	108.20
1	J	272	ARG	CB-CG-CD	5.04	124.69	111.60
1	L	218	ARG	CG-CD-NE	-5.03	101.23	111.80
1	D	322	PHE	CB-CG-CD2	-5.02	117.28	120.80
1	J	83	ARG	N-CA-CB	-5.01	101.57	110.60
1	M	202	ARG	CB-CA-C	5.01	120.43	110.40
1	D	83	ARG	CG-CD-NE	5.01	122.33	111.80
1	I	83	ARG	CG-CD-NE	5.01	122.33	111.80
1	G	75	THR	CA-CB-CG2	5.01	119.41	112.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	LEU	Peptide
1	C	154	ARG	Peptide
1	F	283	ALA	Peptide
1	F	80	TYR	Peptide
1	I	13	SER	Mainchain
1	I	359	TYR	Sidechain
1	I	80	TYR	Peptide
1	K	359	TYR	Sidechain
1	K	80	TYR	Peptide
2	N	24	U	Sidechain
2	N	47	U	Sidechain
2	N	48	U	Sidechain
2	N	68	U	Sidechain
2	N	70	U	Sidechain

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	2974	0	2955	30	0
1	B	2979	0	2957	53	0
1	C	2974	0	2955	52	0
1	D	2979	0	2957	50	0
1	E	2979	0	2957	55	0
1	F	2979	0	2957	53	0
1	G	2979	0	2957	47	0
1	H	2979	0	2957	40	0
1	I	2979	0	2957	42	0
1	J	2979	0	2957	36	0
1	K	2979	0	2957	33	0
1	L	2969	0	2949	34	0
1	M	2916	0	2922	20	0
2	N	1556	0	779	110	0
All	All	40200	0	39173	456	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 6.

All (456) 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:F:295:LYS:NZ	1:G:4:ILE:O	1.89	1.05
1:D:348:LEU:HD12	2:N:21:U:C2'	2.00	0.92
1:D:348:LEU:HD12	2:N:21:U:H2'	1.57	0.86
1:D:352:ARG:HH22	2:N:20:U:H5"	1.39	0.85
1:C:199:GLN:NE2	2:N:20:U:O2	2.09	0.85
1:K:232:VAL:HG11	1:K:314:LEU:HD23	1.58	0.84
1:I:181:THR:HB	2:N:51:U:H5'	1.59	0.84
1:C:278:ARG:HG3	1:D:5:PHE:CE1	2.14	0.82
1:M:193:ARG:HH11	2:N:78:U:H5"	1.45	0.82
1:H:158:MET:HE3	1:I:31:LEU:HD13	1.62	0.81
1:D:275:LEU:HD21	1:E:8:ALA:HB2	1.62	0.81
1:E:181:THR:OG1	2:N:27:U:H5'	1.82	0.80
1:L:348:LEU:HA	2:N:70:U:H5'	1.64	0.80
1:G:188:GLU:HG3	1:G:192:ARG:HH21	1.45	0.79
1:D:348:LEU:CD1	2:N:21:U:H2'	2.14	0.78
1:B:278:ARG:NH1	1:C:5:PHE:HB3	1.99	0.77
1:E:376:GLN:O	1:F:285:ASN:OD1	2.01	0.77
1:J:37:ILE:HD11	1:J:101:ILE:HG22	1.66	0.77
1:A:232:VAL:CG2	1:A:313:LEU:HD23	2.16	0.76
1:D:352:ARG:NH2	2:N:20:U:H5"	2.00	0.75
1:K:181:THR:HB	2:N:63:U:H5'	1.68	0.75
1:D:348:LEU:HD12	2:N:21:U:O2'	1.86	0.74
1:B:295:LYS:HE3	1:C:4:ILE:O	1.89	0.73
1:C:343:ARG:NH1	1:D:353:GLY:O	2.20	0.73
1:L:76:LEU:HD21	1:L:172:ILE:HD11	1.69	0.73
1:G:167:THR:HG21	1:G:204:ASN:H	1.53	0.72
1:E:302:ARG:NH1	1:F:14:TYR:HB2	2.05	0.72
1:B:302:ARG:NH1	1:C:14:TYR:HB2	2.07	0.70
1:M:193:ARG:NH1	2:N:78:U:OP2	2.25	0.69
1:E:348:LEU:HD12	2:N:27:U:C2'	2.22	0.69
1:G:163:SER:O	1:G:167:THR:HG23	1.92	0.69
1:F:239:LYS:O	1:G:20:ARG:NH1	2.27	0.68
1:E:265:ALA:CB	2:N:27:U:OP1	2.42	0.68
1:H:374:ILE:HA	1:I:284:LEU:HD22	1.75	0.67
1:A:176:ILE:HD12	1:A:231:MET:HG3	1.76	0.67
1:M:77:ILE:HD11	1:M:172:ILE:HG21	1.75	0.67
1:E:271:ILE:HD13	1:F:11:PHE:CE2	2.29	0.66
1:C:37:ILE:HD11	1:C:88:ILE:HG21	1.76	0.66
1:F:180:VAL:HG21	1:F:228:ARG:HD3	1.76	0.66
1:G:350:ILE:HD12	1:G:350:ILE:O	1.96	0.66
1:E:348:LEU:HD12	2:N:27:U:O2'	1.96	0.66
1:F:341:ILE:HD12	1:G:329:LEU:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:343:ARG:NH2	1:K:356:GLU:OE1	2.28	0.66
1:B:348:LEU:HD12	2:N:9:U:O2'	1.96	0.65
1:F:193:ARG:NH1	2:N:36:U:OP2	2.26	0.65
1:A:180:VAL:CG1	1:A:228:ARG:HD3	2.27	0.65
1:J:348:LEU:HB2	2:N:58:U:O4'	1.97	0.64
1:K:348:LEU:HD12	2:N:63:U:O2'	1.97	0.64
1:H:181:THR:HB	2:N:45:U:H5'	1.80	0.64
1:B:352:ARG:NH1	2:N:8:U:OP2	2.30	0.64
1:E:348:LEU:HB2	2:N:28:U:O4'	1.97	0.64
1:E:302:ARG:NH2	1:F:7:GLU:OE2	2.28	0.64
1:F:180:VAL:CG2	1:F:228:ARG:HD3	2.28	0.64
1:C:271:ILE:CD1	1:D:11:PHE:CE2	2.81	0.63
1:G:265:ALA:HB2	2:N:39:U:OP1	1.97	0.63
1:E:180:VAL:CG2	1:E:228:ARG:HD3	2.28	0.63
1:B:193:ARG:NH1	2:N:12:U:OP2	2.32	0.63
1:G:198:VAL:CG2	1:G:205:PRO:HG3	2.29	0.62
1:E:352:ARG:HH12	2:N:27:U:H5	1.47	0.62
1:B:348:LEU:HD12	2:N:9:U:C2'	2.29	0.62
1:E:271:ILE:HD13	1:F:11:PHE:HE2	1.65	0.62
1:B:123:GLU:HA	1:B:126:GLU:HG2	1.82	0.62
1:D:167:THR:HG23	1:D:194:TRP:HH2	1.64	0.62
1:C:106:SER:OG	1:C:108:VAL:HG23	2.00	0.62
1:B:37:ILE:HG22	1:B:71:GLY:HA2	1.82	0.62
1:D:372:GLY:CA	1:E:286:GLU:OE2	2.49	0.61
1:J:352:ARG:NH1	2:N:56:U:OP2	2.22	0.61
1:C:47:LEU:HD22	1:C:107:MET:HB3	1.83	0.61
1:F:308:ALA:N	1:F:309:PRO:CD	2.63	0.61
1:L:70:VAL:HG23	1:L:227:VAL:HG13	1.81	0.61
1:G:192:ARG:NH1	2:N:42:U:OP2	2.31	0.61
1:B:111:ILE:H	1:B:112:PRO:HD2	1.65	0.61
1:J:196:LYS:HE3	1:J:197:TYR:CE1	2.36	0.60
1:B:348:LEU:HB2	2:N:10:U:O4'	2.02	0.60
1:E:81:SER:HA	1:F:29:ALA:O	2.01	0.60
1:G:198:VAL:HG21	1:G:205:PRO:HG3	1.83	0.60
2:N:47:U:C5	2:N:48:U:C5	2.90	0.60
1:C:198:VAL:HG21	1:C:205:PRO:HG3	1.84	0.60
1:E:265:ALA:HB2	2:N:27:U:OP1	2.02	0.60
1:L:181:THR:HB	2:N:69:U:H5'	1.84	0.60
1:D:372:GLY:HA2	1:E:286:GLU:OE2	2.02	0.59
1:K:348:LEU:HB2	2:N:64:U:O4'	2.02	0.59
1:G:188:GLU:HG3	1:G:192:ARG:NH2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:338:ALA:HB1	1:J:345:MET:HG3	1.84	0.59
1:H:76:LEU:HD21	1:H:172:ILE:HD11	1.84	0.59
1:J:307:ARG:HD3	1:J:314:LEU:HD21	1.85	0.59
1:M:345:MET:SD	2:N:76:U:C2	2.96	0.59
1:E:265:ALA:HB3	2:N:27:U:OP1	2.03	0.58
1:A:278:ARG:HA	1:A:282:LEU:HD21	1.84	0.58
1:B:275:LEU:HD21	1:C:8:ALA:HB2	1.84	0.58
1:G:170:ALA:O	1:G:174:ILE:HG23	2.03	0.58
1:G:139:SER:O	1:G:140:LYS:HG2	2.04	0.58
1:J:294:ILE:HG13	1:J:330:LEU:CD2	2.34	0.58
1:D:270:THR:HG22	1:D:331:TRP:HA	1.86	0.58
1:E:348:LEU:HD12	2:N:27:U:H2'	1.84	0.58
1:E:271:ILE:CD1	1:F:11:PHE:HE2	2.17	0.57
1:M:258:TYR:HD1	2:N:78:U:C5	2.20	0.57
1:C:238:VAL:HG12	1:D:28:THR:HG21	1.85	0.57
1:J:271:ILE:HD13	1:J:298:MET:HE2	1.85	0.57
1:B:395:ALA:HB1	1:C:365:LYS:HD3	1.85	0.57
1:G:181:THR:HB	2:N:39:U:H5'	1.85	0.57
1:C:271:ILE:HD13	1:D:11:PHE:CD2	2.39	0.57
1:H:37:ILE:HD13	1:H:88:ILE:HG21	1.87	0.57
1:L:354:TYR:OH	2:N:68:U:OP2	2.23	0.57
1:D:302:ARG:NH2	1:E:10:SER:OG	2.38	0.57
1:B:87:LEU:HA	1:C:27:ALA:HB1	1.87	0.57
1:B:374:ILE:HA	1:C:284:LEU:HD23	1.87	0.57
1:E:178:LYS:NZ	2:N:29:U:OP2	2.28	0.57
1:K:270:THR:HG22	1:K:331:TRP:HA	1.87	0.57
1:E:278:ARG:CZ	1:F:5:PHE:HB3	2.35	0.57
1:M:348:LEU:HB2	2:N:76:U:O4'	2.04	0.57
1:G:192:ARG:HH12	2:N:41:U:H5'	1.71	0.56
1:G:56:LEU:HD23	1:G:213:TRP:CZ2	2.40	0.56
1:H:181:THR:HB	2:N:45:U:C5'	2.34	0.56
1:H:348:LEU:HD12	2:N:45:U:O2'	2.05	0.56
1:B:37:ILE:HD11	1:B:101:ILE:HG22	1.88	0.56
2:N:44:U:O2'	2:N:45:U:H5'	2.06	0.56
1:F:200:GLN:NE2	2:N:37:U:H1'	2.20	0.56
1:D:76:LEU:HD21	1:D:172:ILE:HD11	1.87	0.56
1:G:200:GLN:NE2	2:N:43:U:H1'	2.21	0.56
1:D:348:LEU:CD1	2:N:21:U:C2'	2.77	0.55
1:J:37:ILE:HG22	1:J:71:GLY:HA2	1.86	0.55
1:J:235:LEU:HD23	1:J:235:LEU:O	2.05	0.55
1:A:278:ARG:HA	1:A:282:LEU:CD2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:LYS:HD3	2:N:37:U:C6	2.41	0.55
1:K:71:GLY:O	1:K:75:THR:HG23	2.06	0.55
1:D:198:VAL:HG21	1:D:205:PRO:HG3	1.89	0.55
1:H:158:MET:CE	1:I:31:LEU:HD13	2.35	0.55
1:C:199:GLN:HG3	2:N:19:U:H3	1.72	0.54
1:C:271:ILE:CD1	1:D:11:PHE:HE2	2.18	0.54
1:K:374:ILE:HA	1:L:284:LEU:CD2	2.37	0.54
1:F:198:VAL:HG21	1:F:205:PRO:HG3	1.90	0.54
2:N:38:U:O2'	2:N:39:U:H5'	2.07	0.54
1:E:345:MET:SD	2:N:28:U:O2	2.66	0.54
1:J:52:THR:HG23	1:J:168:ILE:HD11	1.88	0.54
1:J:270:THR:HG22	1:J:331:TRP:HA	1.89	0.54
1:M:77:ILE:HD11	1:M:172:ILE:CG2	2.38	0.54
1:G:265:ALA:CB	2:N:39:U:OP1	2.55	0.54
1:J:308:ALA:N	1:J:309:PRO:CD	2.71	0.53
1:L:70:VAL:HG23	1:L:227:VAL:CG1	2.38	0.53
1:A:275:LEU:CD2	1:B:8:ALA:HB2	2.37	0.53
1:H:371:ALA:HB1	1:H:393:ALA:HB1	1.91	0.53
1:M:258:TYR:CD1	2:N:78:U:C5	2.97	0.53
1:A:81:SER:HA	1:B:29:ALA:O	2.09	0.53
1:J:348:LEU:HD12	2:N:57:U:O2'	2.08	0.53
1:G:308:ALA:N	1:G:309:PRO:CD	2.72	0.53
1:I:294:ILE:HG13	1:I:330:LEU:CD2	2.38	0.53
1:L:270:THR:HG22	1:L:331:TRP:HA	1.89	0.53
1:C:198:VAL:CG2	1:C:205:PRO:HG3	2.39	0.53
1:M:270:THR:HG22	1:M:331:TRP:HA	1.91	0.52
2:N:8:U:O2'	2:N:9:U:H5'	2.10	0.52
1:F:76:LEU:HD13	1:F:172:ILE:HD11	1.91	0.52
1:K:91:LEU:HD12	1:K:234:ILE:HG22	1.91	0.52
1:H:273:PHE:HB3	1:H:337:VAL:HG23	1.92	0.52
1:C:196:LYS:HE2	1:C:197:TYR:CE1	2.44	0.52
1:B:302:ARG:HH11	1:C:14:TYR:HB2	1.75	0.52
1:C:77:ILE:O	1:C:78:SER:HB3	2.09	0.52
1:C:271:ILE:HD13	1:D:11:PHE:CE2	2.45	0.52
1:F:171:GLN:O	1:F:174:ILE:HG12	2.10	0.52
1:F:318:ILE:O	1:F:318:ILE:HG22	2.09	0.52
1:B:289:SER:O	1:B:293:THR:HG23	2.10	0.51
1:C:167:THR:HG23	1:C:194:TRP:HH2	1.75	0.51
1:I:158:MET:SD	1:J:32:THR:O	2.68	0.51
1:L:278:ARG:HA	1:L:282:LEU:HD12	1.91	0.51
1:I:275:LEU:HD21	1:J:8:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:271:ILE:CD1	1:L:298:MET:HE2	2.40	0.51
1:C:186:ALA:HB3	1:C:218:ARG:HH22	1.76	0.51
1:G:271:ILE:HD13	1:G:298:MET:HE2	1.91	0.51
1:L:200:GLN:OE1	2:N:73:U:H1'	2.11	0.51
1:D:35:ILE:CD1	1:D:97:ILE:HD12	2.41	0.51
1:F:196:LYS:HG2	2:N:37:U:C5	2.46	0.51
1:H:348:LEU:HD12	2:N:45:U:C2'	2.41	0.51
1:I:76:LEU:HD21	1:I:172:ILE:HD11	1.93	0.51
1:J:329:LEU:HD11	1:J:359:TYR:CG	2.45	0.51
1:L:348:LEU:CA	2:N:70:U:H5'	2.38	0.51
1:I:325:GLY:HA3	2:N:48:U:O2'	2.10	0.51
1:K:232:VAL:CG1	1:K:314:LEU:HD23	2.36	0.51
1:B:354:TYR:HE1	2:N:6:U:H4'	1.76	0.51
1:E:302:ARG:NH1	1:F:14:TYR:CB	2.72	0.51
1:B:302:ARG:NH1	1:C:14:TYR:CB	2.74	0.50
1:I:270:THR:HG22	1:I:331:TRP:HA	1.94	0.50
1:I:349:ASN:ND2	2:N:51:U:C4	2.79	0.50
1:A:275:LEU:HD21	1:B:8:ALA:HB2	1.93	0.50
1:D:302:ARG:HH22	1:E:10:SER:C	2.14	0.50
1:G:237:GLU:O	1:H:24:ALA:HB2	2.12	0.50
1:K:108:VAL:HG12	1:K:108:VAL:O	2.11	0.50
1:E:270:THR:HG22	1:E:331:TRP:HA	1.93	0.50
1:L:111:ILE:H	1:L:112:PRO:CD	2.24	0.50
1:C:294:ILE:HD12	1:C:295:LYS:N	2.26	0.50
1:A:373:GLY:HA2	1:B:285:ASN:H	1.77	0.50
1:D:372:GLY:HA3	1:E:286:GLU:OE2	2.11	0.50
1:D:167:THR:HG23	1:D:194:TRP:CH2	2.45	0.50
1:G:352:ARG:NH2	2:N:39:U:C5	2.80	0.50
1:A:348:LEU:HB2	2:N:4:U:O4'	2.12	0.50
1:B:271:ILE:HG22	1:B:276:GLU:OE2	2.12	0.50
1:C:176:ILE:HB	1:C:221:LEU:HD21	1.93	0.50
1:H:56:LEU:HD23	1:H:213:TRP:CZ2	2.46	0.49
1:I:275:LEU:HD21	1:J:8:ALA:CB	2.41	0.49
1:H:302:ARG:NH2	1:I:10:SER:O	2.46	0.49
1:K:373:GLY:HA3	1:L:286:GLU:OE2	2.13	0.49
1:L:344:SER:OG	2:N:71:U:H4'	2.12	0.49
1:E:180:VAL:HG23	1:E:228:ARG:HD3	1.93	0.49
1:B:178:LYS:NZ	2:N:10:U:OP1	2.43	0.49
1:C:192:ARG:NH1	2:N:18:U:OP2	2.42	0.49
1:C:345:MET:SD	2:N:16:U:O2	2.71	0.49
1:D:345:MET:SD	2:N:22:U:C2	3.06	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:THR:HG21	1:F:367:ALA:HB3	1.95	0.49
1:H:373:GLY:HA3	1:I:286:GLU:OE2	2.12	0.49
1:G:192:ARG:NH1	2:N:41:U:H5'	2.27	0.49
1:B:122:GLN:O	1:B:123:GLU:HB3	2.11	0.49
1:C:275:LEU:HD11	1:C:294:ILE:HD13	1.95	0.49
1:C:345:MET:SD	2:N:16:U:C2	3.06	0.49
1:H:332:SER:O	1:H:360:PHE:HA	2.12	0.49
1:J:271:ILE:CD1	1:K:11:PHE:HE2	2.25	0.49
1:A:166:ILE:CG2	1:A:251:ILE:CD1	2.90	0.49
1:F:215:THR:HG22	1:F:218:ARG:HH12	1.78	0.49
1:H:308:ALA:N	1:H:309:PRO:CD	2.76	0.49
1:I:196:LYS:HE3	1:I:197:TYR:CE1	2.48	0.49
1:K:271:ILE:CD1	1:L:11:PHE:HE2	2.26	0.49
1:E:181:THR:OG1	2:N:26:U:O2'	2.23	0.48
1:I:181:THR:HB	2:N:51:U:C5'	2.35	0.48
1:D:301:TYR:CD1	1:E:11:PHE:HE1	2.31	0.48
1:F:170:ALA:O	1:F:174:ILE:HG23	2.13	0.48
1:K:278:ARG:HB2	1:L:5:PHE:CE1	2.48	0.48
1:D:348:LEU:HB2	2:N:22:U:O4'	2.12	0.48
1:A:273:PHE:HD1	1:A:341:ILE:HD11	1.79	0.48
1:C:81:SER:HA	1:D:29:ALA:O	2.14	0.48
1:J:196:LYS:HE3	1:J:197:TYR:CZ	2.49	0.48
1:F:167:THR:HG23	1:F:194:TRP:HH2	1.79	0.48
1:H:306:PRO:HA	1:I:18:LEU:HD11	1.96	0.48
1:I:56:LEU:HD23	1:I:213:TRP:CZ2	2.48	0.48
1:L:74:PHE:HE1	1:L:227:VAL:HA	1.78	0.48
1:B:270:THR:HG22	1:B:331:TRP:HA	1.95	0.48
1:G:81:SER:HA	1:H:29:ALA:O	2.14	0.48
1:J:329:LEU:CD1	1:J:359:TYR:CG	2.96	0.48
1:C:199:GLN:CG	2:N:19:U:H3	2.27	0.48
1:E:302:ARG:HH12	1:F:14:TYR:HB2	1.77	0.48
1:H:235:LEU:HD23	1:H:235:LEU:O	2.14	0.48
1:I:74:PHE:HE1	1:I:227:VAL:HA	1.79	0.48
1:I:180:VAL:HG13	1:I:228:ARG:HD3	1.96	0.48
1:K:276:GLU:OE2	1:L:12:ARG:HG3	2.13	0.48
1:L:65:ALA:HB3	1:L:68:MET:HG2	1.96	0.48
1:G:270:THR:HG22	1:G:331:TRP:HA	1.96	0.47
1:H:371:ALA:CB	1:H:393:ALA:HB1	2.44	0.47
1:J:229:LYS:HG2	1:J:314:LEU:HD12	1.96	0.47
1:A:270:THR:HG22	1:A:331:TRP:HA	1.95	0.47
1:B:52:THR:CG2	1:B:168:ILE:HD11	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LEU:HD12	2:N:9:U:H2'	1.94	0.47
1:G:271:ILE:HD13	1:G:298:MET:CE	2.44	0.47
1:L:180:VAL:HG23	1:L:181:THR:HG23	1.96	0.47
1:C:240:LYS:HB2	1:D:24:ALA:HB2	1.95	0.47
1:J:127:GLY:O	1:J:131:ILE:HD13	2.14	0.47
1:K:37:ILE:HD12	1:K:88:ILE:HG21	1.97	0.47
1:M:345:MET:SD	2:N:76:U:O2	2.73	0.47
1:A:312:VAL:HG22	1:A:319:GLN:HG3	1.96	0.47
1:H:245:LYS:HB3	1:H:250:GLU:HG2	1.97	0.47
1:I:176:ILE:HD12	1:I:231:MET:HB3	1.97	0.47
1:E:235:LEU:HD11	1:E:256:GLY:HA3	1.96	0.47
1:G:327:TYR:N	1:G:328:PRO:CD	2.77	0.47
1:A:133:LYS:HG2	1:A:137:ASP:OD2	2.14	0.47
1:K:176:ILE:HD11	1:K:231:MET:SD	2.55	0.47
1:H:348:LEU:HB2	2:N:46:U:O4'	2.14	0.47
1:J:52:THR:CG2	1:J:168:ILE:HD11	2.45	0.47
1:E:278:ARG:NH1	1:F:5:PHE:HB3	2.30	0.47
1:A:56:LEU:HD23	1:A:213:TRP:CZ2	2.50	0.47
1:H:81:SER:HA	1:I:29:ALA:O	2.15	0.47
1:C:295:LYS:NZ	1:D:4:ILE:O	2.37	0.46
1:I:180:VAL:CG1	1:I:228:ARG:HD3	2.45	0.46
1:K:271:ILE:HD13	1:L:11:PHE:CE2	2.50	0.46
1:K:314:LEU:HD12	1:K:314:LEU:O	2.15	0.46
1:M:198:VAL:HG22	1:M:203:VAL:HG23	1.95	0.46
1:D:198:VAL:CG2	1:D:205:PRO:HG3	2.45	0.46
1:F:198:VAL:CG2	1:F:205:PRO:HG3	2.45	0.46
1:L:37:ILE:O	1:L:37:ILE:HG13	2.14	0.46
1:B:167:THR:HG21	1:B:204:ASN:H	1.79	0.46
1:B:180:VAL:CG2	1:B:228:ARG:HD3	2.46	0.46
1:F:172:ILE:O	1:F:175:LEU:HB2	2.16	0.46
1:G:192:ARG:HH11	2:N:42:U:P	2.39	0.46
1:F:232:VAL:HG11	1:F:314:LEU:HD11	1.98	0.46
1:G:237:GLU:OE2	1:H:24:ALA:HA	2.16	0.46
1:A:76:LEU:HD21	1:A:172:ILE:HD11	1.96	0.46
1:H:344:SER:HB2	2:N:47:U:O4'	2.14	0.46
1:B:52:THR:HG23	1:B:168:ILE:HD11	1.98	0.46
2:N:41:U:C4	2:N:42:U:C4	3.04	0.46
1:C:221:LEU:HD12	1:C:227:VAL:HG13	1.97	0.45
1:F:176:ILE:HD11	1:F:228:ARG:HG2	1.98	0.45
1:F:232:VAL:HB	1:F:314:LEU:HD21	1.97	0.45
1:I:76:LEU:CD2	1:I:172:ILE:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:344:SER:O	2:N:76:U:O2'	2.25	0.45
1:A:232:VAL:HG21	1:A:313:LEU:HD23	1.97	0.45
1:F:276:GLU:OE1	1:G:12:ARG:HD3	2.16	0.45
1:C:52:THR:HG23	1:C:168:ILE:HD11	1.98	0.45
1:C:56:LEU:HD23	1:C:213:TRP:CZ2	2.50	0.45
1:E:80:TYR:HE2	1:E:252:ILE:HD11	1.82	0.45
1:H:108:VAL:H	1:H:114:MET:HB3	1.82	0.45
1:I:348:LEU:HD12	2:N:51:U:O2'	2.16	0.45
1:A:237:GLU:OE2	1:B:25:SER:HB3	2.17	0.45
1:E:56:LEU:HD23	1:E:213:TRP:CZ2	2.52	0.45
1:H:266:GLY:O	1:H:270:THR:HG23	2.17	0.45
2:N:59:U:C5	2:N:60:U:C5	3.04	0.45
1:E:271:ILE:CD1	1:F:11:PHE:CE2	2.96	0.45
1:I:273:PHE:CD2	1:I:338:ALA:HB2	2.52	0.45
1:K:173:TRP:HA	1:K:176:ILE:HD12	1.98	0.45
1:K:235:LEU:HD23	1:K:235:LEU:O	2.16	0.45
1:A:273:PHE:CD1	1:A:341:ILE:HD11	2.52	0.45
1:G:126:GLU:HG3	1:G:130:ARG:HE	1.82	0.45
2:N:29:U:C5	2:N:30:U:C5	3.04	0.45
1:G:294:ILE:HG13	1:G:330:LEU:HD21	1.99	0.45
1:J:294:ILE:HG13	1:J:330:LEU:HD21	1.98	0.45
1:C:278:ARG:HD2	1:D:5:PHE:CD1	2.52	0.45
1:E:180:VAL:CG2	1:E:228:ARG:CD	2.94	0.45
1:E:302:ARG:HH11	1:F:14:TYR:HB2	1.79	0.45
1:H:232:VAL:HB	1:H:314:LEU:HD21	2.00	0.44
1:K:344:SER:HB2	2:N:65:U:C4'	2.48	0.44
1:B:238:VAL:HG12	1:C:28:THR:HG21	1.99	0.44
1:J:234:ILE:HD13	1:J:234:ILE:HG21	1.73	0.44
1:B:278:ARG:NH1	1:C:5:PHE:CB	2.77	0.44
1:F:173:TRP:HB3	1:F:255:ILE:HG21	2.00	0.44
1:F:371:ALA:CB	1:F:393:ALA:HB1	2.48	0.44
1:D:302:ARG:NH2	1:E:7:GLU:OE2	2.50	0.44
1:M:189:SER:HA	1:M:192:ARG:HE	1.83	0.44
1:B:56:LEU:HD23	1:B:213:TRP:CZ2	2.52	0.44
1:F:181:THR:HB	2:N:33:U:H5'	1.99	0.44
1:G:180:VAL:CG1	1:G:228:ARG:HD3	2.48	0.44
1:E:261:GLU:HB2	1:E:268:PHE:CE2	2.52	0.44
1:J:56:LEU:HD23	1:J:213:TRP:CZ2	2.53	0.44
1:B:123:GLU:HG3	1:B:126:GLU:HB2	1.98	0.44
1:D:308:ALA:N	1:D:309:PRO:CD	2.80	0.44
1:D:327:TYR:N	1:D:328:PRO:HD3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:ILE:HD12	1:F:286:GLU:HG2	2.00	0.44
1:G:348:LEU:HD12	2:N:39:U:O2'	2.18	0.44
1:I:354:TYR:CE1	2:N:48:U:H4'	2.53	0.44
1:E:341:ILE:HG13	1:F:286:GLU:CD	2.39	0.44
1:I:153:LEU:HD11	1:I:206:PHE:HE2	1.83	0.44
1:G:167:THR:HG22	1:G:203:VAL:HB	1.98	0.43
1:I:354:TYR:HE1	2:N:48:U:H4'	1.83	0.43
1:B:183:PRO:O	1:B:218:ARG:HD2	2.18	0.43
1:F:56:LEU:HD23	1:F:213:TRP:CZ2	2.52	0.43
1:K:348:LEU:HD12	2:N:63:U:C2'	2.47	0.43
1:B:175:LEU:HD21	1:B:214:LEU:HG	2.01	0.43
1:D:140:LYS:HE2	1:D:140:LYS:HB2	1.89	0.43
1:E:341:ILE:HG23	1:F:329:LEU:HD11	2.00	0.43
1:F:168:ILE:HA	1:F:171:GLN:HE21	1.83	0.43
1:G:37:ILE:HD13	1:G:88:ILE:HG12	1.99	0.43
1:E:92:LEU:HD11	1:E:97:ILE:HD11	1.99	0.43
1:G:181:THR:HB	2:N:39:U:C5'	2.48	0.43
1:J:176:ILE:HG13	1:J:221:LEU:HD13	2.01	0.43
1:B:262:THR:HG21	1:B:313:LEU:HD11	2.00	0.43
1:C:77:ILE:O	1:C:78:SER:CB	2.66	0.43
1:I:308:ALA:N	1:I:309:PRO:CD	2.82	0.43
1:G:289:SER:O	1:G:293:THR:HG23	2.19	0.43
1:B:108:VAL:H	1:B:114:MET:HB2	1.84	0.43
1:D:348:LEU:HD11	2:N:21:U:H2'	1.97	0.43
1:E:308:ALA:N	1:E:309:PRO:CD	2.81	0.43
1:F:259:VAL:O	1:F:262:THR:HB	2.18	0.43
1:H:173:TRP:HB3	1:H:255:ILE:HG21	1.99	0.43
1:J:302:ARG:NH2	1:K:10:SER:C	2.72	0.43
1:C:348:LEU:HD12	2:N:15:U:O2'	2.18	0.43
1:D:82:GLU:HG2	1:E:31:LEU:HD23	1.99	0.43
1:F:270:THR:HG22	1:F:331:TRP:HA	1.99	0.43
1:G:211:GLN:O	1:G:215:THR:HG23	2.18	0.43
1:H:37:ILE:CD1	1:H:88:ILE:HG21	2.48	0.43
1:I:20:ARG:NH2	1:I:318:ILE:HD11	2.34	0.43
1:K:193:ARG:HA	1:K:193:ARG:HD3	1.92	0.43
1:L:37:ILE:CD1	1:L:88:ILE:HG21	2.49	0.43
1:L:56:LEU:HD23	1:L:213:TRP:CZ2	2.53	0.43
1:B:271:ILE:CD1	1:C:11:PHE:HE2	2.32	0.43
1:L:271:ILE:HD13	1:M:11:PHE:CE2	2.54	0.43
1:L:348:LEU:HD12	2:N:69:U:O2'	2.19	0.43
1:A:120:LYS:CB	1:A:124:GLU:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:THR:HG22	1:C:331:TRP:HA	2.01	0.42
1:E:302:ARG:HH11	1:F:14:TYR:CB	2.32	0.42
1:C:308:ALA:N	1:C:309:PRO:CD	2.82	0.42
1:D:345:MET:SD	2:N:22:U:O2	2.77	0.42
1:J:37:ILE:CD1	1:J:101:ILE:HG22	2.41	0.42
1:L:278:ARG:HB2	1:M:5:PHE:CE1	2.53	0.42
1:M:198:VAL:HG11	1:M:205:PRO:HG3	2.01	0.42
1:D:327:TYR:N	1:D:328:PRO:CD	2.82	0.42
1:I:235:LEU:O	1:I:235:LEU:HD23	2.19	0.42
1:J:181:THR:HB	2:N:57:U:H5'	2.00	0.42
1:C:114:MET:O	1:C:114:MET:HG3	2.20	0.42
1:D:74:PHE:HE1	1:D:227:VAL:HA	1.84	0.42
1:I:327:TYR:N	1:I:328:PRO:CD	2.82	0.42
1:J:227:VAL:O	1:J:231:MET:HG2	2.20	0.42
1:B:354:TYR:CE1	2:N:6:U:H4'	2.54	0.42
1:C:200:GLN:NE2	2:N:19:U:H1'	2.34	0.42
1:E:192:ARG:O	1:E:193:ARG:HB2	2.20	0.42
1:H:76:LEU:CD2	1:H:172:ILE:HD11	2.48	0.42
1:C:343:ARG:HH11	1:D:356:GLU:H	1.67	0.42
1:E:37:ILE:N	1:E:37:ILE:HD12	2.34	0.42
1:E:181:THR:OG1	2:N:27:U:C5'	2.60	0.42
1:H:298:MET:SD	1:I:11:PHE:CD2	3.13	0.42
1:B:199:GLN:NE2	2:N:14:U:O2	2.50	0.42
1:D:318:ILE:O	1:D:321:LYS:HB2	2.20	0.42
1:I:302:ARG:NH2	1:J:14:TYR:HB2	2.34	0.42
1:K:91:LEU:CD1	1:K:234:ILE:HG22	2.49	0.42
1:M:329:LEU:HD22	1:M:359:TYR:CD2	2.55	0.42
1:B:101:ILE:O	1:B:101:ILE:HG13	2.18	0.42
1:G:180:VAL:HG13	1:G:228:ARG:HD3	2.01	0.42
1:A:237:GLU:OE2	1:B:25:SER:CB	2.68	0.42
1:B:11:PHE:O	1:B:12:ARG:C	2.58	0.42
1:F:172:ILE:HA	1:F:175:LEU:HD12	2.01	0.42
1:H:197:TYR:CD1	1:H:251:ILE:CD1	3.02	0.42
1:A:348:LEU:HD12	2:N:3:U:H3'	2.02	0.41
1:B:273:PHE:CD2	1:B:338:ALA:HB2	2.55	0.41
1:D:35:ILE:HD12	1:D:97:ILE:HD12	2.02	0.41
1:G:352:ARG:NH2	2:N:39:U:C6	2.88	0.41
1:K:240:LYS:HD3	1:L:21:ASP:O	2.20	0.41
1:J:77:ILE:CD1	1:J:231:MET:SD	3.08	0.41
1:D:167:THR:CG2	1:D:194:TRP:HH2	2.29	0.41
1:H:80:TYR:CE1	1:H:166:ILE:HG22	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:19:GLY:O	1:M:20:ARG:CB	2.68	0.41
1:A:47:LEU:O	1:A:51:LEU:HB2	2.21	0.41
1:A:265:ALA:HB3	2:N:3:U:OP1	2.20	0.41
1:D:56:LEU:HD23	1:D:213:TRP:CZ2	2.56	0.41
1:D:302:ARG:NH2	1:E:11:PHE:N	2.68	0.41
1:G:352:ARG:NH2	2:N:39:U:H5	2.19	0.41
1:A:87:LEU:HA	1:B:27:ALA:HB1	2.02	0.41
1:A:127:GLY:O	1:A:131:ILE:HD13	2.20	0.41
1:D:311:MET:O	1:D:314:LEU:O	2.39	0.41
1:G:69:LYS:HB3	1:G:69:LYS:HE2	1.89	0.41
1:G:327:TYR:N	1:G:328:PRO:HD3	2.36	0.41
1:K:47:LEU:HD22	1:K:107:MET:HB3	2.02	0.41
1:K:158:MET:SD	1:L:34:LYS:HE3	2.60	0.41
1:L:196:LYS:HE2	1:L:197:TYR:CE1	2.56	0.41
1:M:273:PHE:CD2	1:M:338:ALA:HB2	2.55	0.41
1:F:167:THR:CG2	1:F:194:TRP:HH2	2.33	0.41
1:H:237:GLU:O	1:I:24:ALA:HB2	2.20	0.41
1:I:361:ARG:O	1:I:365:LYS:HG2	2.20	0.41
1:K:271:ILE:CD1	1:L:11:PHE:CE2	3.03	0.41
1:B:76:LEU:HD22	1:B:172:ILE:HG13	2.02	0.41
1:E:324:PRO:HA	1:E:327:TYR:CZ	2.56	0.41
1:H:267:PHE:CE1	1:H:271:ILE:HD11	2.56	0.41
1:A:286:GLU:HB3	1:A:329:LEU:CD2	2.51	0.41
1:E:158:MET:CE	1:F:32:THR:O	2.69	0.41
1:E:169:GLU:O	1:E:173:TRP:HD1	2.04	0.41
1:G:143:THR:HB	1:G:144:PRO:CD	2.51	0.41
1:H:221:LEU:HD23	1:H:227:VAL:HG11	2.03	0.41
1:J:193:ARG:NH1	2:N:60:U:OP2	2.49	0.41
1:A:295:LYS:HE2	1:B:4:ILE:HA	2.03	0.41
1:F:327:TYR:N	1:F:328:PRO:CD	2.84	0.41
1:G:323:ALA:HA	1:G:324:PRO:HD3	1.90	0.41
1:I:312:VAL:HG22	1:I:319:GLN:HG3	2.03	0.41
1:I:344:SER:OG	2:N:53:U:O4'	2.34	0.41
1:L:76:LEU:HD21	1:L:172:ILE:CD1	2.45	0.41
1:C:133:LYS:HB2	1:C:133:LYS:HE3	1.98	0.41
1:H:243:SER:OG	1:I:23:ARG:HD3	2.20	0.41
1:K:310:TYR:O	1:K:314:LEU:HG	2.20	0.41
1:B:296:SER:O	1:B:299:LEU:HG	2.21	0.40
1:K:234:ILE:HD13	1:K:234:ILE:HG21	1.67	0.40
1:M:77:ILE:O	1:M:77:ILE:CG2	2.69	0.40
1:I:300:LEU:O	1:I:304:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:282:LEU:HD23	1:L:282:LEU:HA	1.87	0.40
1:A:166:ILE:HG23	1:A:251:ILE:CD1	2.52	0.40
1:F:265:ALA:CB	2:N:33:U:OP1	2.69	0.40
1:H:376:GLN:CB	1:I:285:ASN:OD1	2.69	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	392/554 (71%)	374 (95%)	18 (5%)	0	100	100
1	B	393/554 (71%)	380 (97%)	11 (3%)	2 (0%)	29	68
1	C	392/554 (71%)	377 (96%)	14 (4%)	1 (0%)	41	75
1	D	393/554 (71%)	377 (96%)	16 (4%)	0	100	100
1	E	393/554 (71%)	373 (95%)	20 (5%)	0	100	100
1	F	393/554 (71%)	379 (96%)	13 (3%)	1 (0%)	41	75
1	G	393/554 (71%)	385 (98%)	8 (2%)	0	100	100
1	H	393/554 (71%)	382 (97%)	10 (2%)	1 (0%)	41	75
1	I	393/554 (71%)	380 (97%)	12 (3%)	1 (0%)	41	75
1	J	393/554 (71%)	380 (97%)	13 (3%)	0	100	100
1	K	393/554 (71%)	381 (97%)	11 (3%)	1 (0%)	41	75
1	L	389/554 (70%)	377 (97%)	11 (3%)	1 (0%)	41	75
1	M	378/554 (68%)	365 (97%)	12 (3%)	1 (0%)	41	75
All	All	5088/7202 (71%)	4910 (96%)	169 (3%)	9 (0%)	50	81

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	ILE
1	L	111	ILE
1	B	77	ILE
1	M	31	LEU
1	C	111	ILE
1	K	77	ILE
1	F	77	ILE
1	H	105	GLY
1	I	396	VAL

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	299/454 (66%)	294 (98%)	5 (2%)	60	82
1	B	299/454 (66%)	292 (98%)	7 (2%)	50	77
1	C	299/454 (66%)	296 (99%)	3 (1%)	76	88
1	D	299/454 (66%)	298 (100%)	1 (0%)	92	97
1	E	299/454 (66%)	293 (98%)	6 (2%)	55	79
1	F	299/454 (66%)	297 (99%)	2 (1%)	84	93
1	G	299/454 (66%)	296 (99%)	3 (1%)	76	88
1	H	299/454 (66%)	297 (99%)	2 (1%)	84	93
1	I	299/454 (66%)	294 (98%)	5 (2%)	60	82
1	J	299/454 (66%)	296 (99%)	3 (1%)	76	88
1	K	299/454 (66%)	296 (99%)	3 (1%)	76	88
1	L	299/454 (66%)	296 (99%)	3 (1%)	76	88
1	M	299/454 (66%)	293 (98%)	6 (2%)	55	79
All	All	3887/5902 (66%)	3838 (99%)	49 (1%)	70	86

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG

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Mol	Chain	Res	Type
1	A	31	LEU
1	A	47	LEU
1	A	51	LEU
1	A	131	ILE
1	B	20	ARG
1	B	31	LEU
1	B	111	ILE
1	B	122	GLN
1	B	140	LYS
1	B	239	LYS
1	B	250	GLU
1	C	5	PHE
1	C	107	MET
1	C	234	ILE
1	D	31	LEU
1	E	31	LEU
1	E	166	ILE
1	E	171	GLN
1	E	193	ARG
1	E	200	GLN
1	E	251	ILE
1	F	31	LEU
1	F	223	GLN
1	G	193	ARG
1	G	329	LEU
1	G	364	GLN
1	H	6	GLU
1	H	327	TYR
1	I	5	PHE
1	I	31	LEU
1	I	32	THR
1	I	176	ILE
1	I	234	ILE
1	J	114	MET
1	J	272	ARG
1	J	343	ARG
1	K	275	LEU
1	K	278	ARG
1	K	329	LEU
1	L	20	ARG
1	L	31	LEU
1	L	354	TYR

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Mol	Chain	Res	Type
1	M	20	ARG
1	M	23	ARG
1	M	178	LYS
1	M	239	LYS
1	M	319	GLN
1	M	364	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	C	199	GLN
1	D	288	GLN
1	E	257	ASN
1	F	223	GLN
1	H	288	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	N	77/78 (98%)	5 (6%)	1 (1%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	N	4	U
2	N	6	U
2	N	55	U
2	N	71	U
2	N	78	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	N	35	U

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-12581. 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 ⓘ
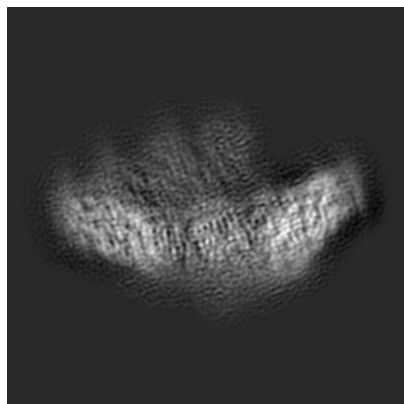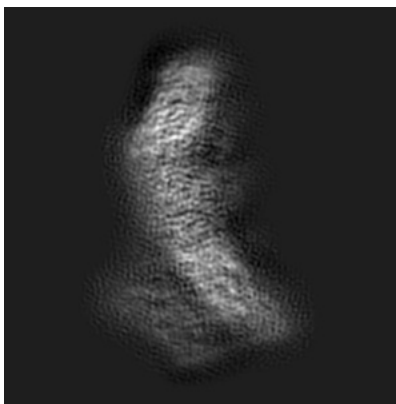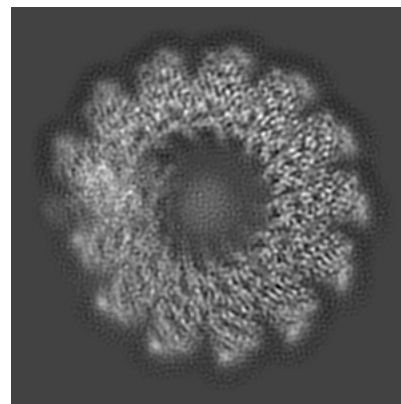
6.1.1 Primary map

X   Y   Z

6.1.2 Raw map

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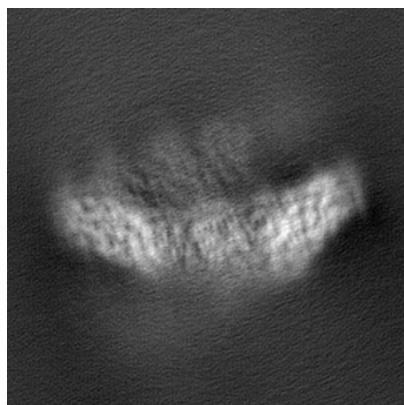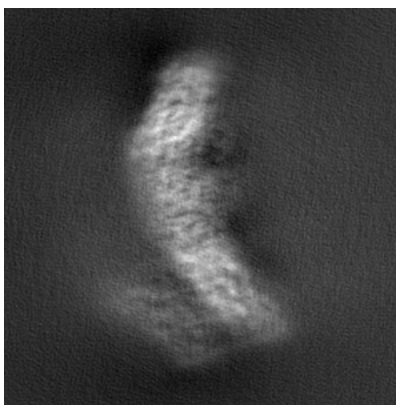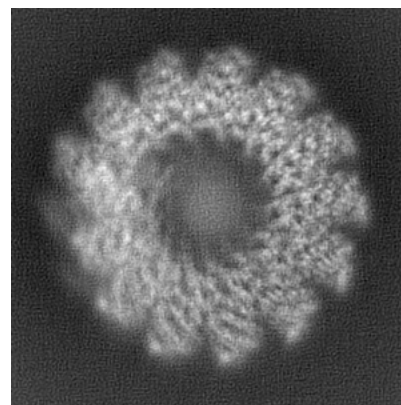
The images above show the map projected in three orthogonal directions.

6.2　Central slices ⓘ
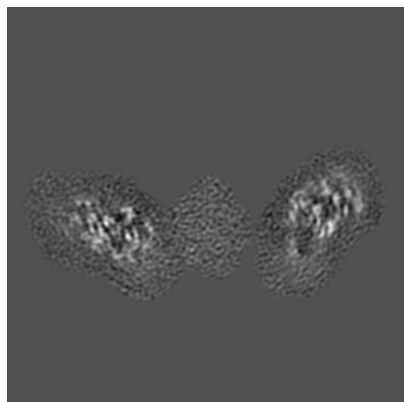
6.2.1　Primary map
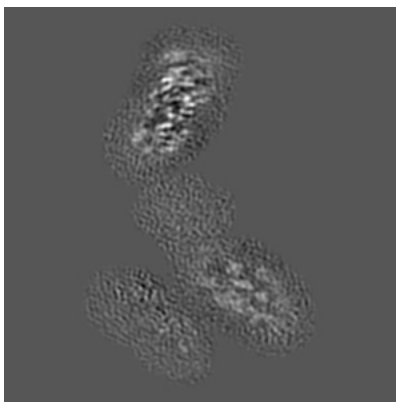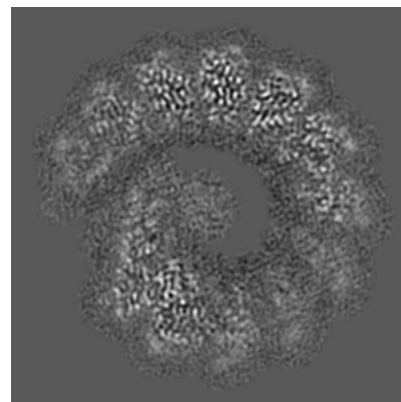
X Index: 120　　　　　Y Index: 120　　　　　Z Index: 120

6.2.2　Raw map
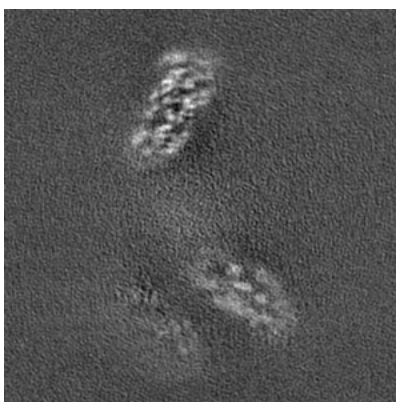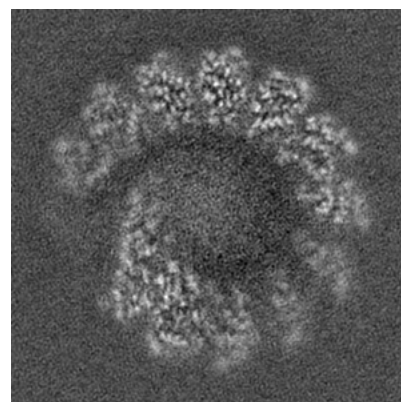
X Index: 120　　　　　Y Index: 120　　　　　Z Index: 120

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

6.3 Largest variance slices ⓘ
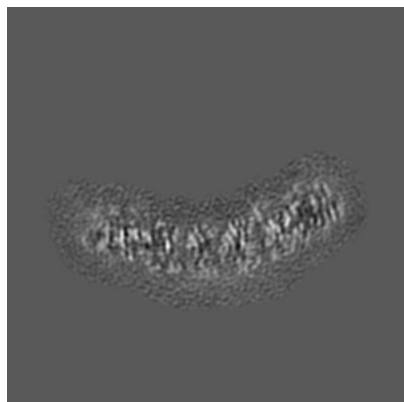
6.3.1 Primary map
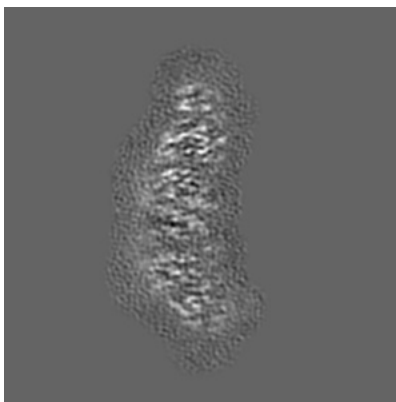
| X Index: 161 | Y Index: 172 | Z Index: 105 |
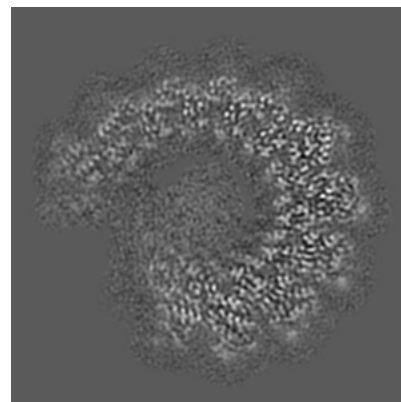
6.3.2 Raw map
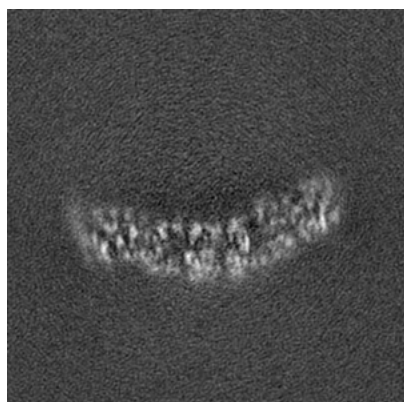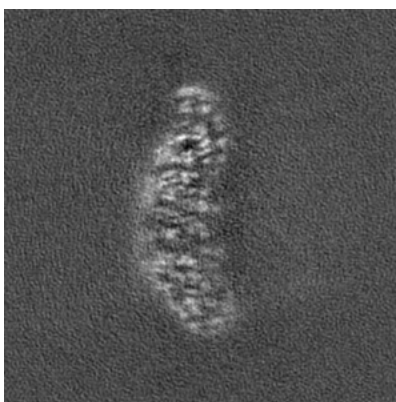
| X Index: 165 | Y Index: 173 | Z Index: 104 |
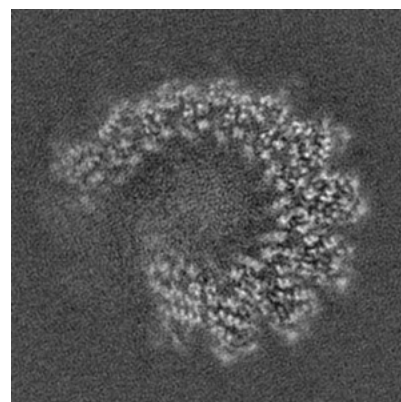
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

| X | Y | Z |
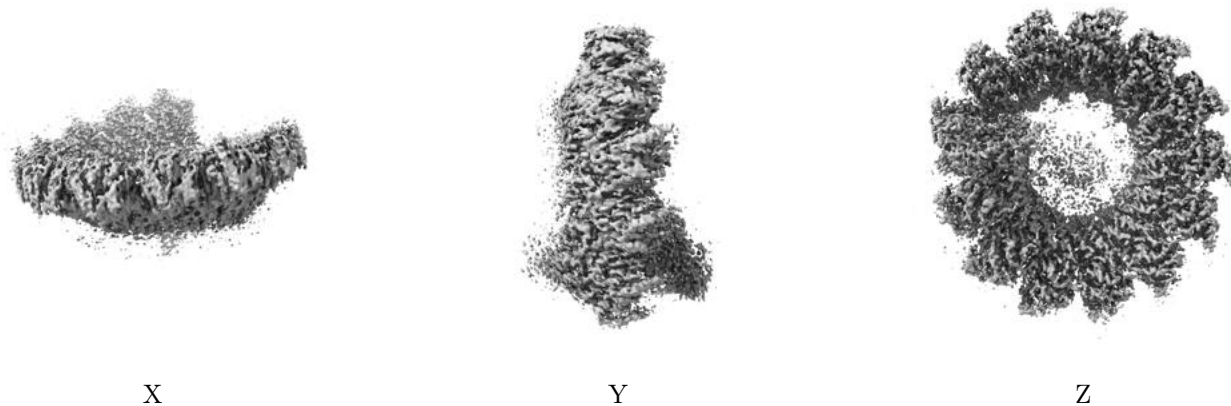
The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

| X | Y | Z |
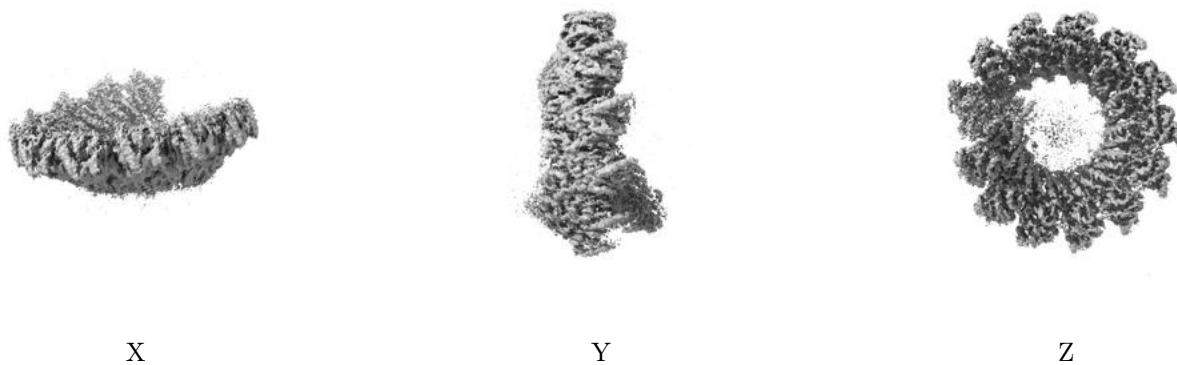
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.5.1 emd_12581_msk_1.map ⓘ
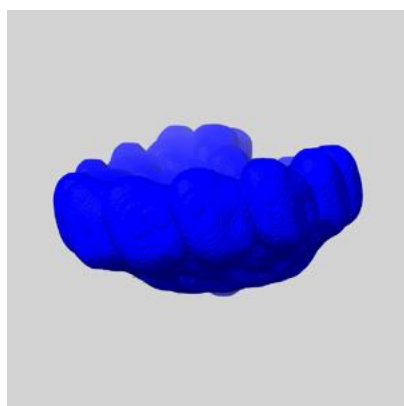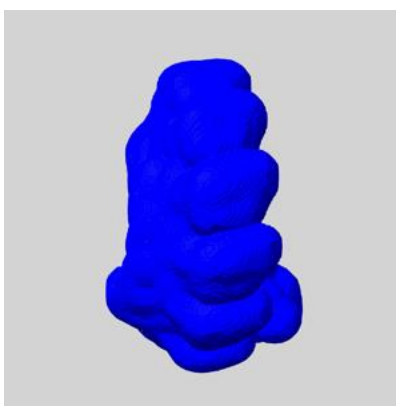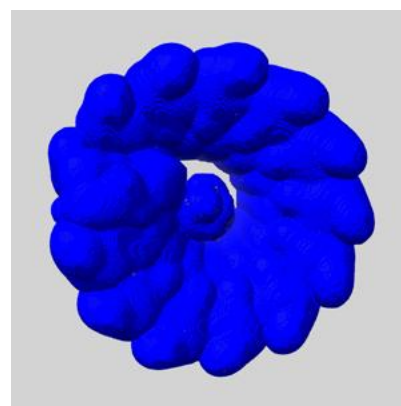
X Y Z

7 Map analysis (i)

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

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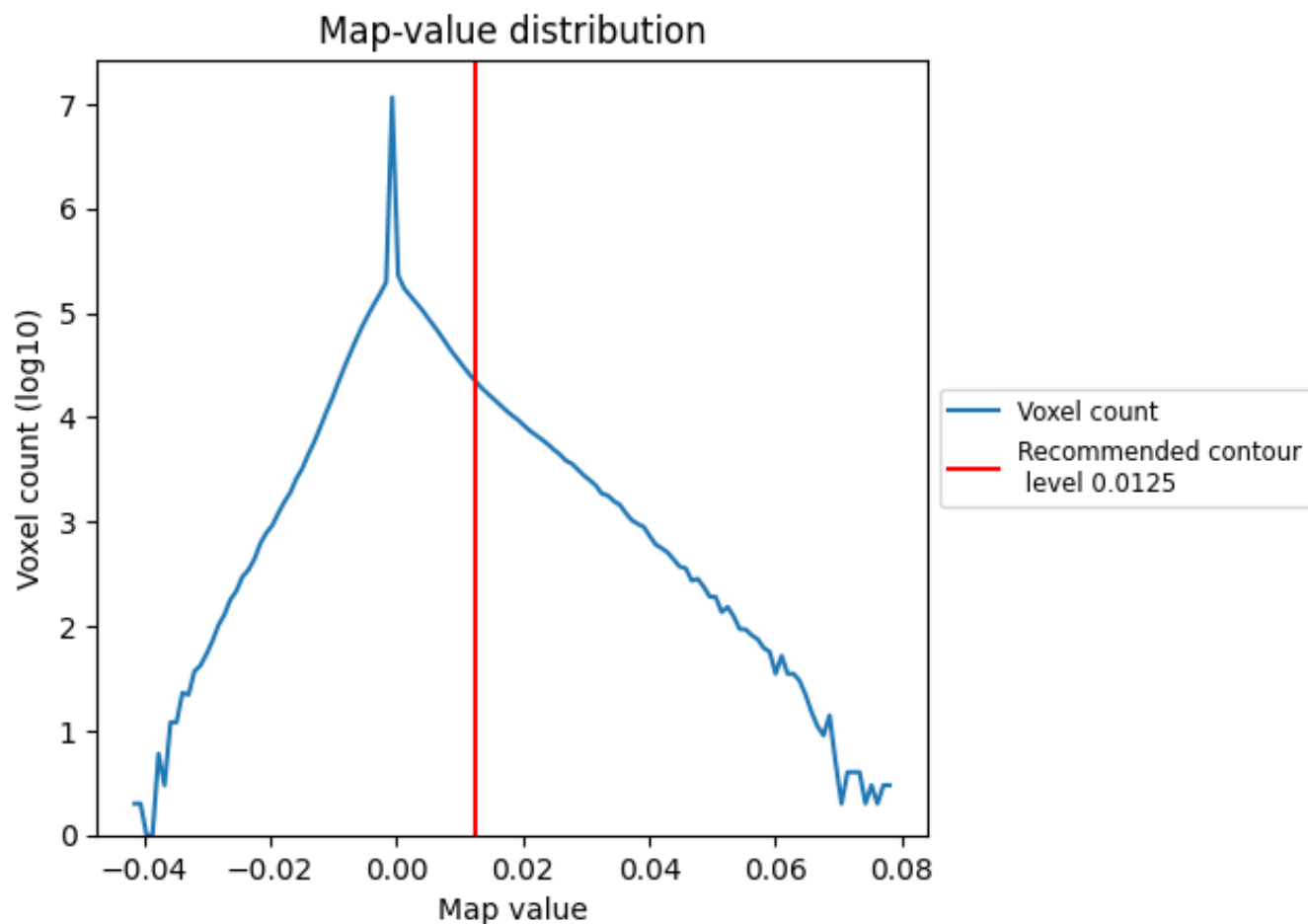
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
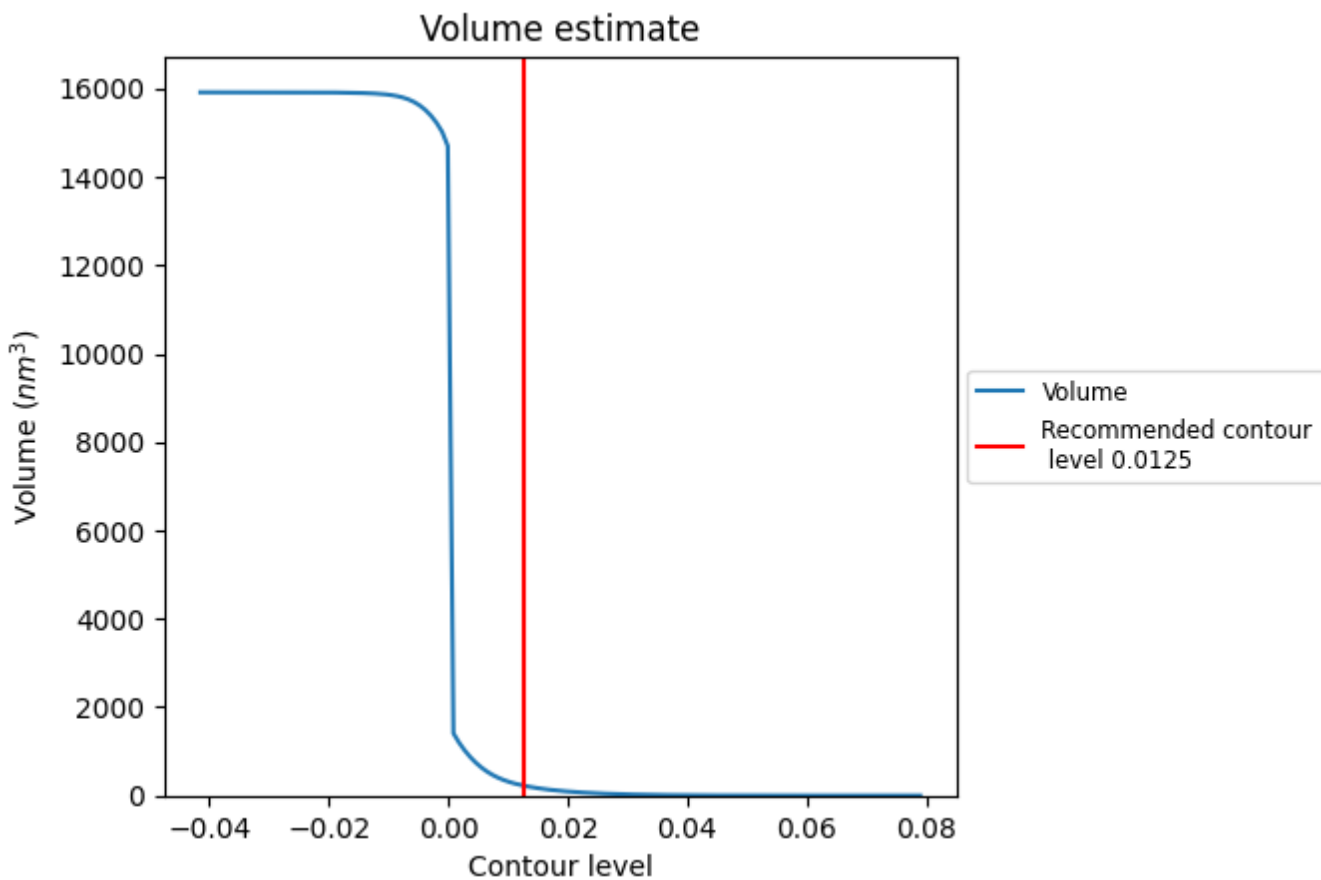
Volume estimate

The volume at the recommended contour level is 228 nm^3; this corresponds to an approximate mass of 206 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 ⓘ
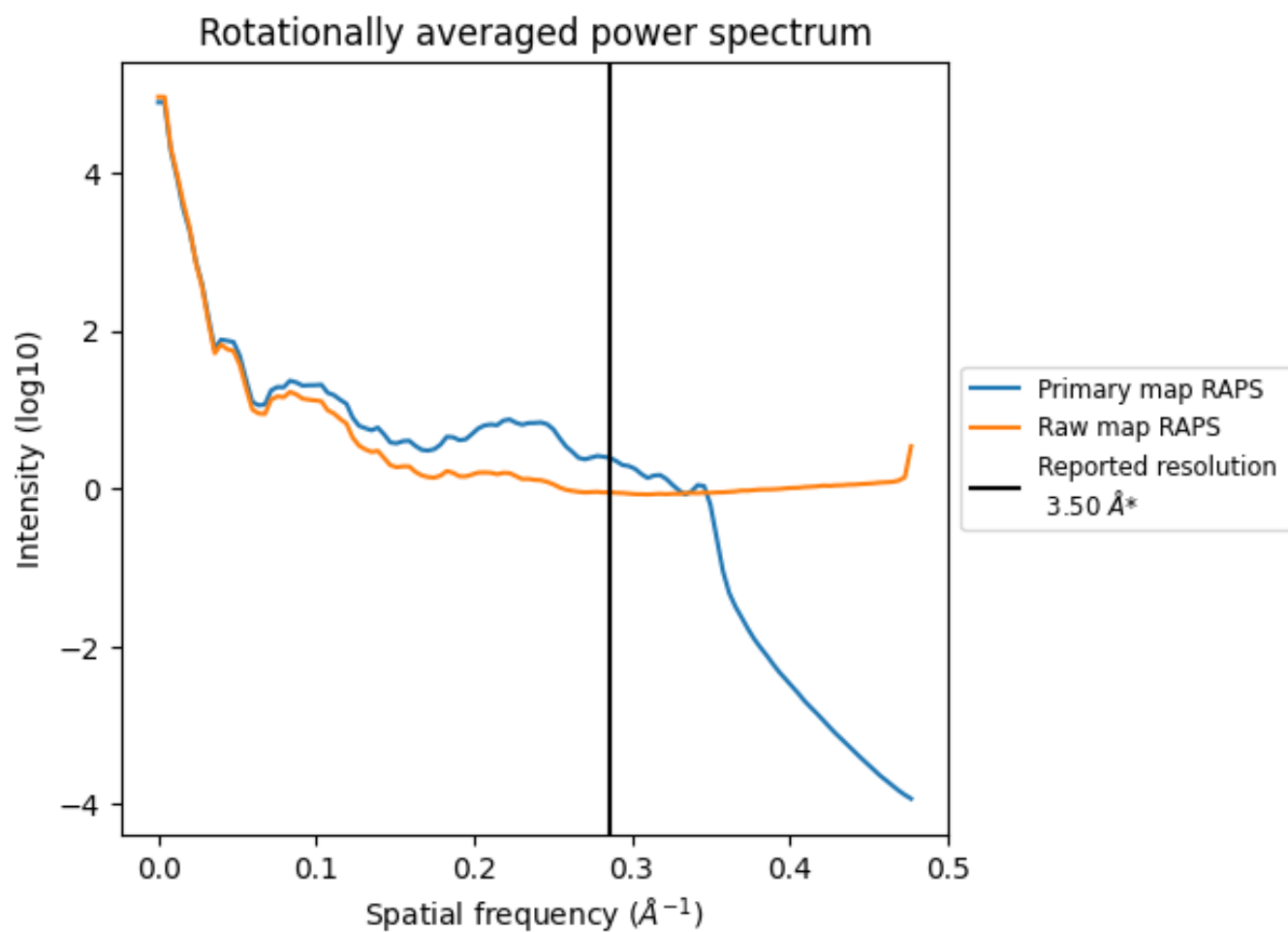
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ
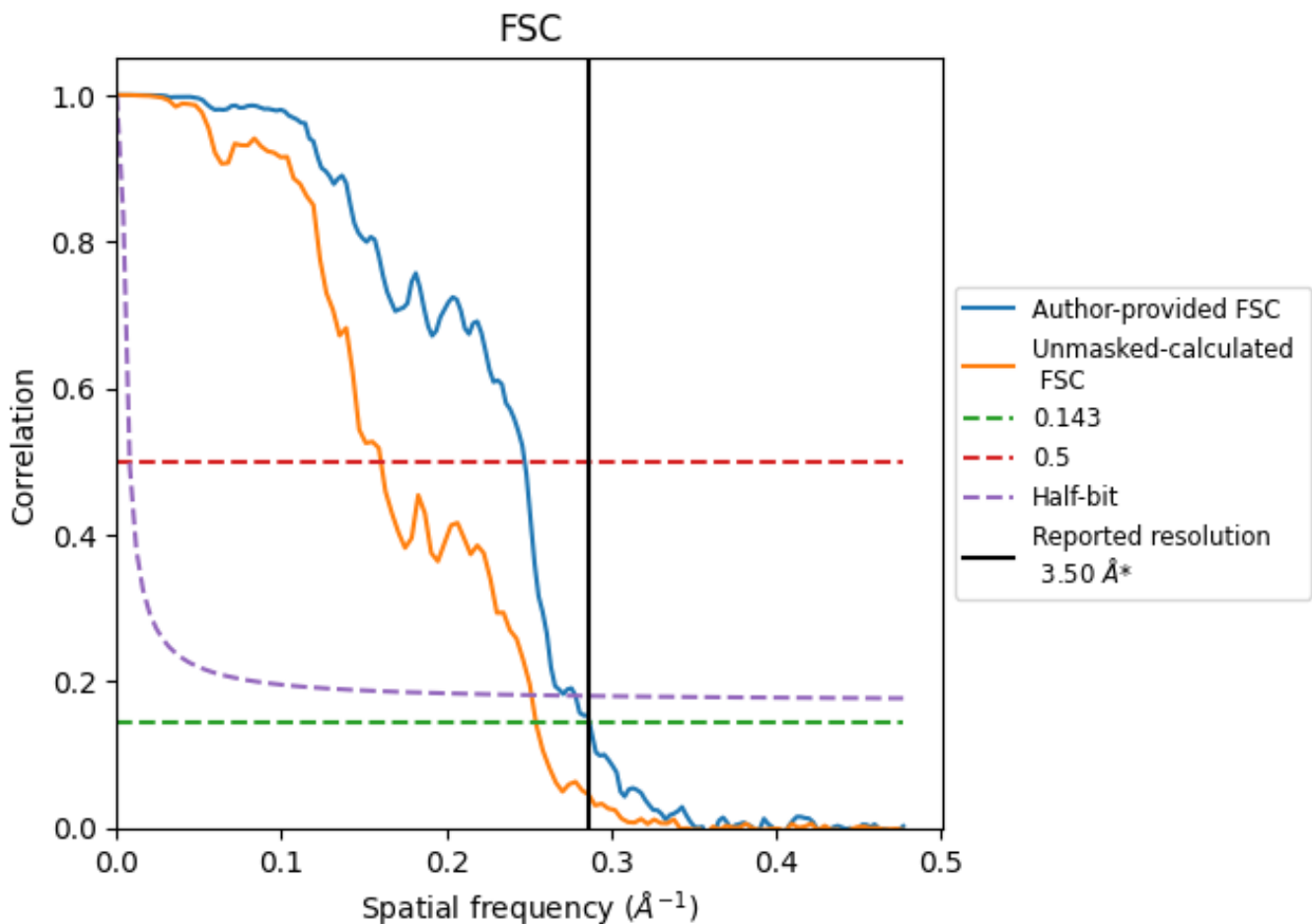
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.04	3.59
Unmasked-calculated*	3.93	6.24	3.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 3.5 by more than 10 %

9   Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12581 and PDB model 7NT5. Per-residue inclusion information can be found in section 3 on page 12.

9.1   Map-model overlay (i)
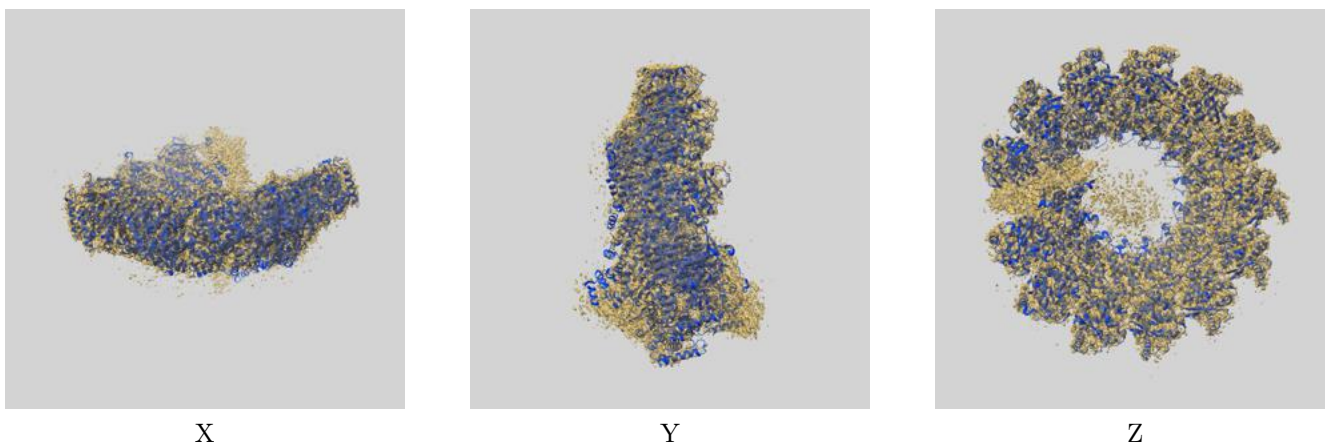
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0125 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　ⓘ

X　　　　　　　　　　Y　　　　　　　　　　Z
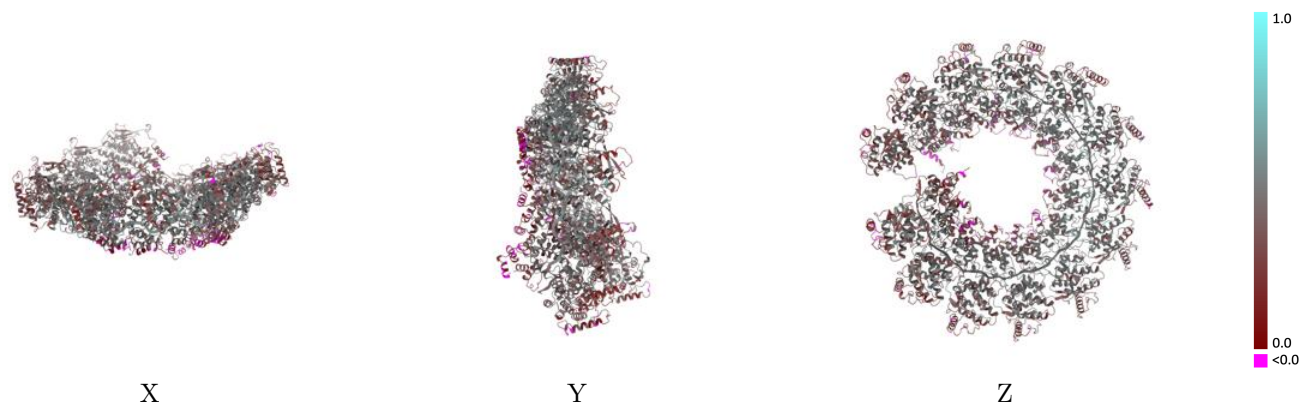
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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　ⓘ

X　　　　　　　　　　Y　　　　　　　　　　Z
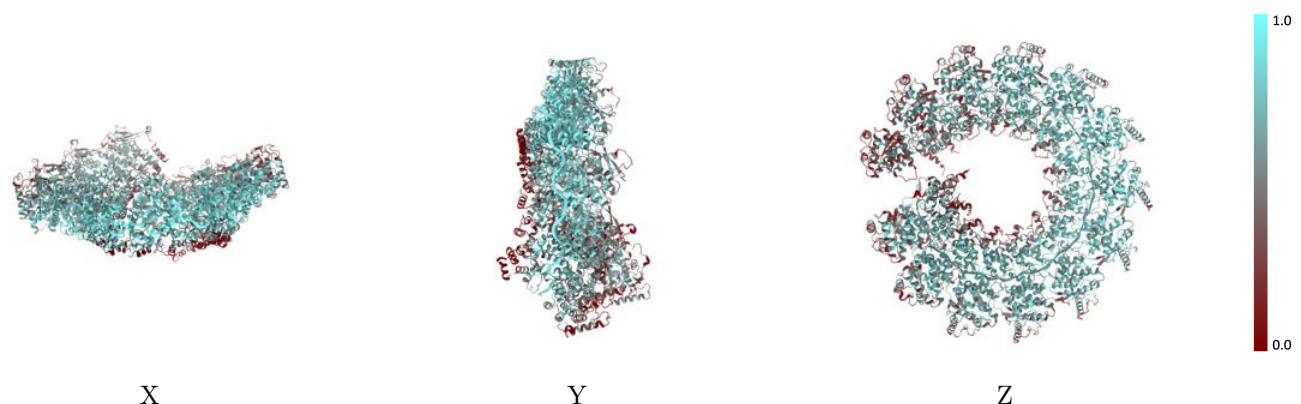
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0125).

## 9.4 Atom inclusion (i)
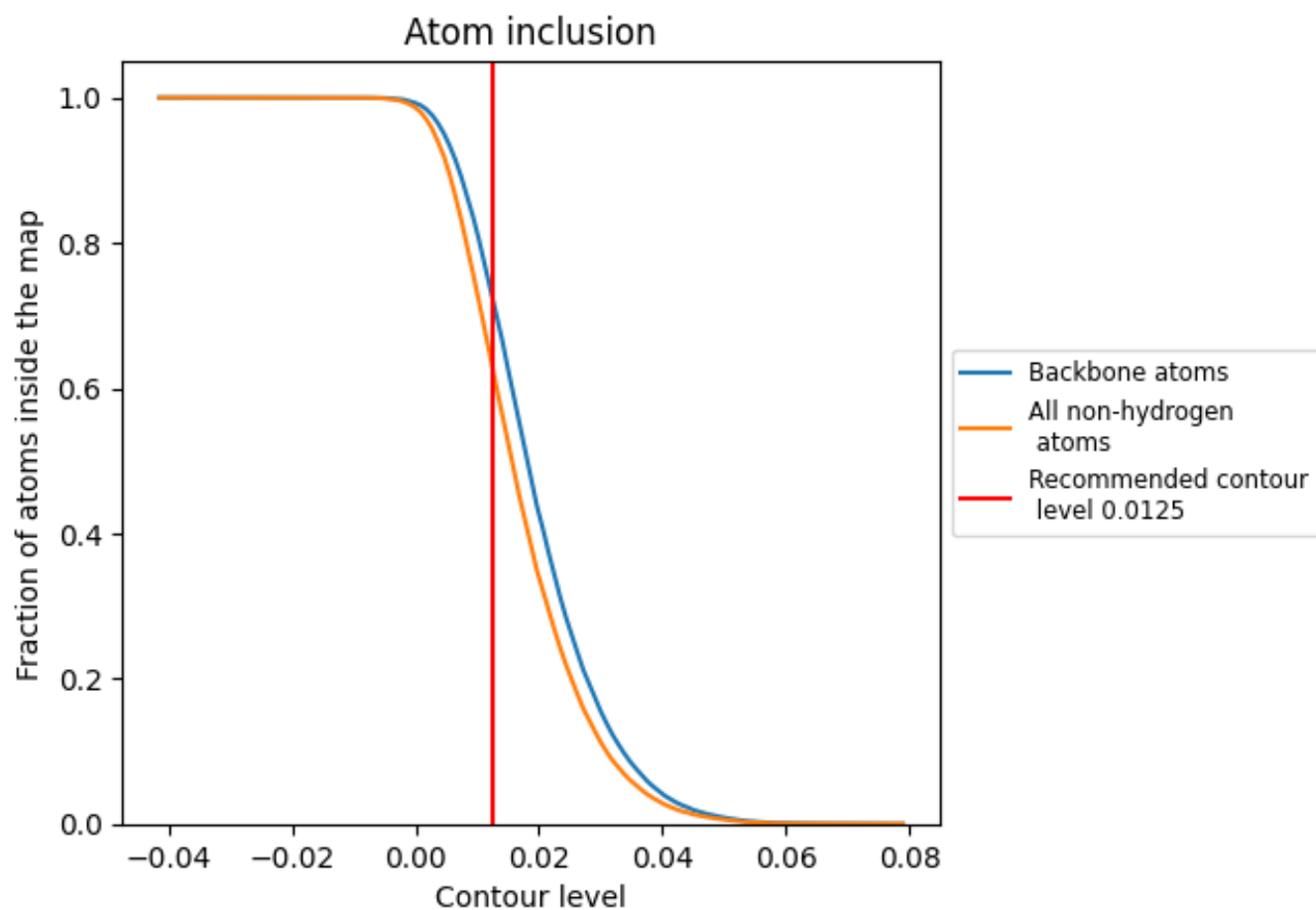
At the recommended contour level, 73% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0125) and Q-score
for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6282	0.3960
A	0.4921	0.3510
B	0.5781	0.3770
C	0.6183	0.3880
D	0.6344	0.4020
E	0.6677	0.4130
F	0.7103	0.4230
G	0.7188	0.4200
H	0.7233	0.4230
I	0.6989	0.4170
J	0.6433	0.4020
K	0.5898	0.3950
L	0.5109	0.3650
M	0.4361	0.3370
N	0.8888	0.4710

1.0

0.0
<0.0