



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:58 AM UTC

PDB ID : 7NT5 / pdb_00007nt5
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

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
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

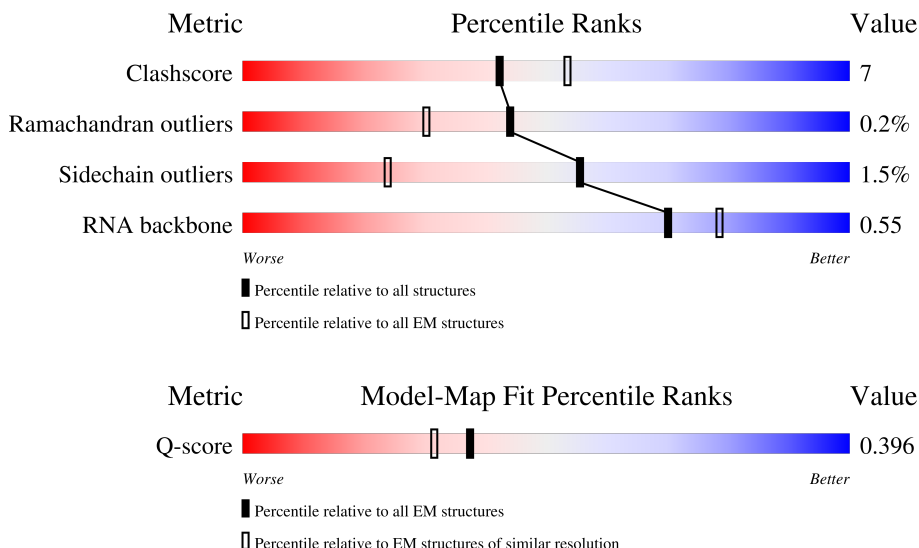
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	554	
1	B	554	
1	C	554	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	D	554	
1	E	554	
1	F	554	
1	G	554	
1	H	554	
1	I	554	
1	J	554	
1	K	554	
1	L	554	
1	M	554	
2	N	78	

2 Entry composition [i](#)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

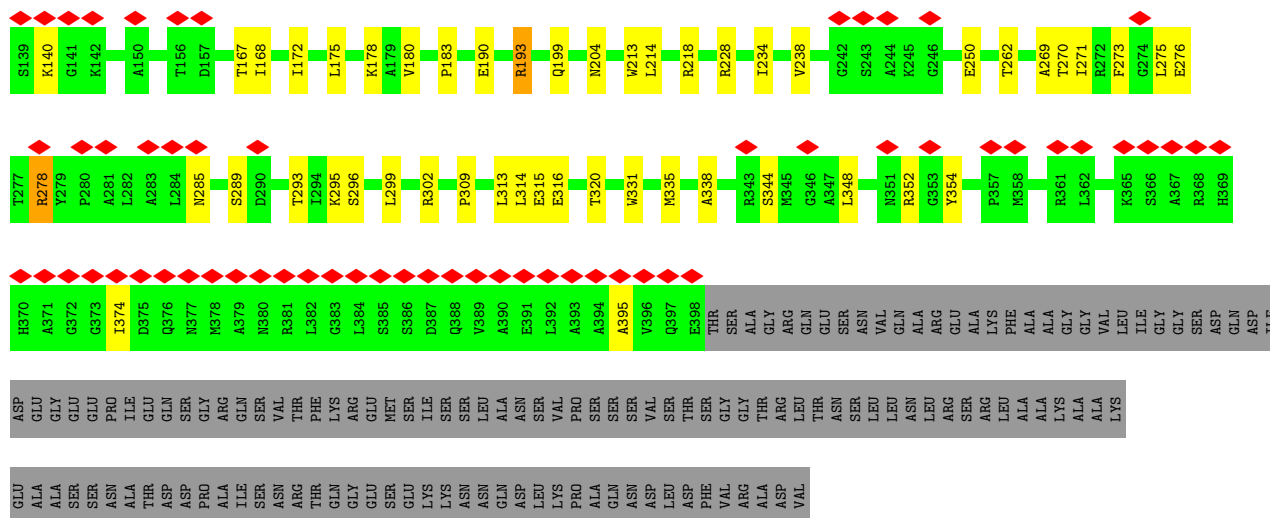
Continued on next page...

Continued from previous page...

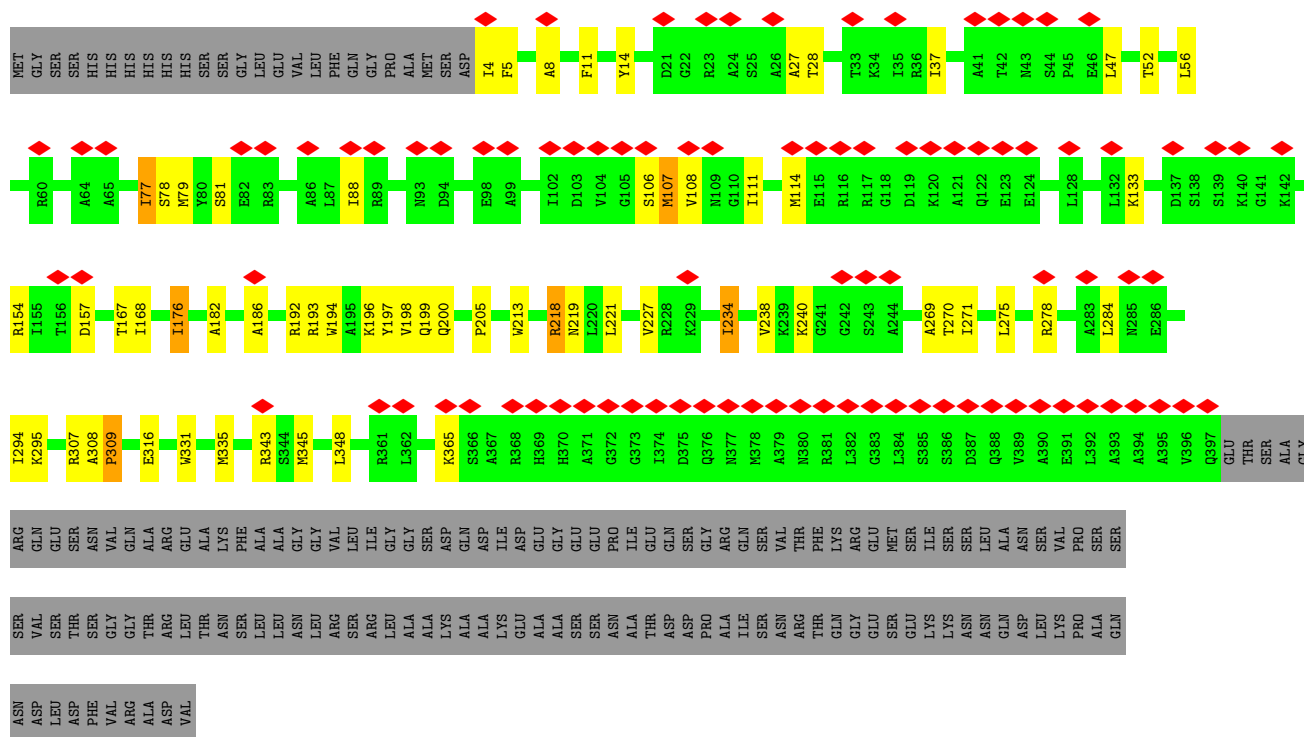
Chain	Residue	Modelled	Actual	Comment	Reference
L	-7	GLU	-	expression tag	UNP Q9IK92
L	-6	VAL	-	expression tag	UNP Q9IK92
L	-5	LEU	-	expression tag	UNP Q9IK92
L	-4	PHE	-	expression tag	UNP Q9IK92
L	-3	GLN	-	expression tag	UNP Q9IK92
L	-2	GLY	-	expression tag	UNP Q9IK92
L	-1	PRO	-	expression tag	UNP Q9IK92
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).

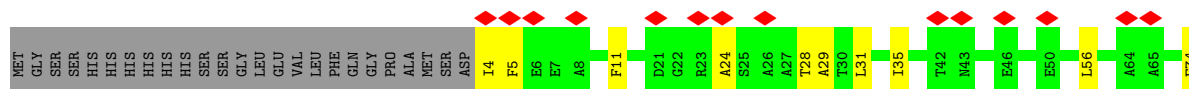
Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	78	Total	C	N	O	P	0	0
			1556	702	156	621	77		



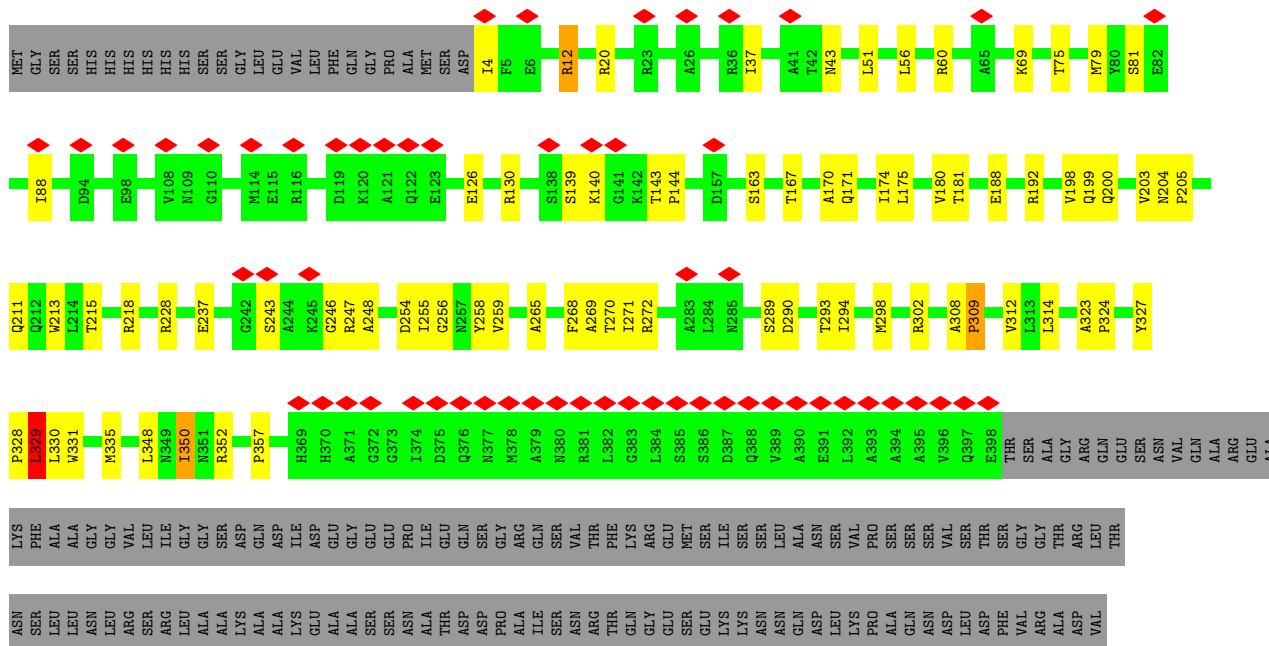
• Molecule 1: Nucleoprotein



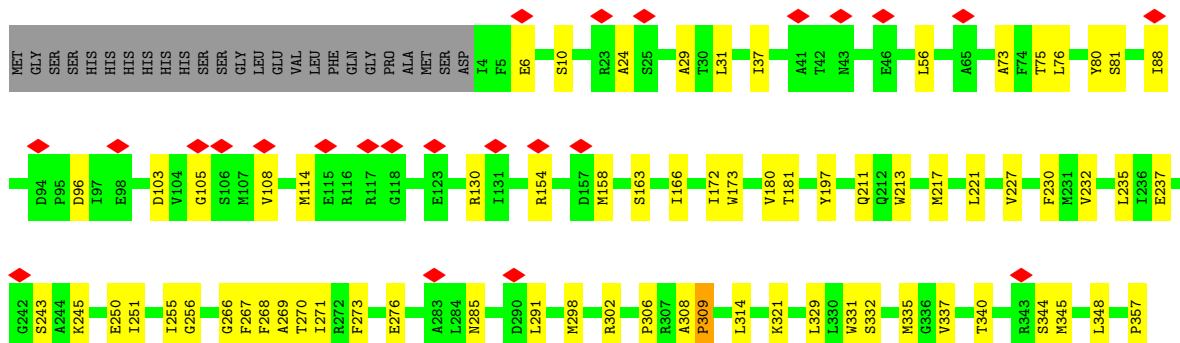
• Molecule 1: Nucleoprotein



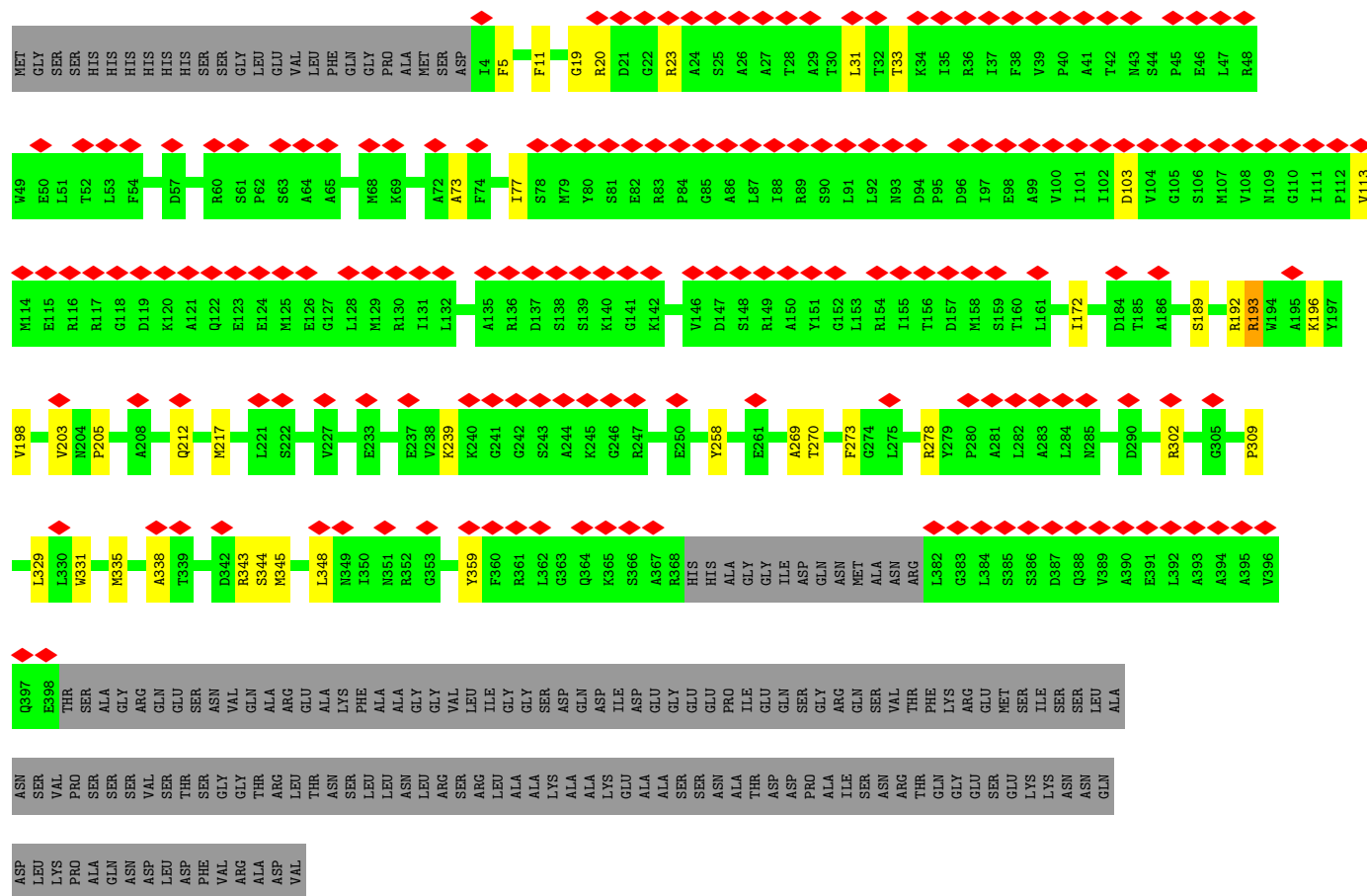
- Molecule 1: Nucleoprotein



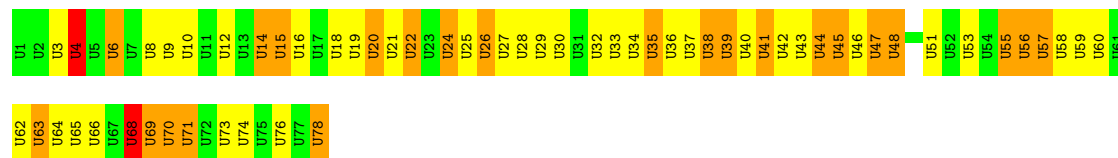
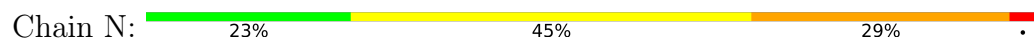
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



- Molecule 2: RNA (78-MER)



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 ($e^-/\text{\AA}^2$)	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	0.70	0/3025	1.38	15/4096 (0.4%)
1	B	0.75	0/3030	1.46	11/4103 (0.3%)
1	C	0.76	0/3025	1.47	17/4096 (0.4%)
1	D	0.79	1/3030 (0.0%)	1.48	14/4103 (0.3%)
1	E	0.83	1/3030 (0.0%)	1.49	14/4103 (0.3%)
1	F	0.88	2/3030 (0.1%)	1.54	24/4103 (0.6%)
1	G	0.89	0/3030	1.58	25/4103 (0.6%)
1	H	0.87	1/3030 (0.0%)	1.53	20/4103 (0.5%)
1	I	0.83	0/3030	1.56	31/4103 (0.8%)
1	J	0.78	0/3030	1.45	17/4103 (0.4%)
1	K	0.74	0/3030	1.42	11/4103 (0.3%)
1	L	0.69	0/3019	1.36	7/4086 (0.2%)
1	M	0.74	3/2966 (0.1%)	1.40	12/4013 (0.3%)
2	N	0.92	4/1711 (0.2%)	1.49	30/2643 (1.1%)
All	All	0.80	12/41016 (0.0%)	1.47	248/55861 (0.4%)

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	13.52	1.48	1.33
1	M	302	ARG	NE-CZ	6.62	1.40	1.33
1	F	323	ALA	CA-CB	-6.27	1.44	1.53
1	E	345	MET	CG-SD	6.22	1.96	1.80
1	H	345	MET	CG-SD	6.14	1.96	1.80
2	N	35	U	O3'-P	5.70	1.69	1.61
2	N	41	U	O3'-P	5.63	1.69	1.61
2	N	25	U	O3'-P	-5.54	1.52	1.61
1	F	319	GLN	C-O	5.47	1.30	1.24
1	M	278	ARG	NE-CZ	5.42	1.39	1.33
1	D	356	GLU	C-O	-5.30	1.21	1.23
2	N	26	U	O3'-P	5.10	1.68	1.61

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	343	ARG	NE-CZ-NH1	-13.65	107.85	121.50
1	M	343	ARG	NE-CZ-NH2	11.95	129.96	119.20
1	M	302	ARG	CD-NE-CZ	9.99	138.39	124.40
1	M	343	ARG	CD-NE-CZ	9.71	137.99	124.40
2	N	44	U	C4'-C3'-O3'	-8.86	99.71	113.00
2	N	68	U	C4'-C3'-O3'	-8.57	100.14	113.00
1	C	309	PRO	CB-CA-C	-8.06	97.42	111.21
1	B	314	LEU	CA-C-O	-7.90	112.95	121.56
1	E	261	GLU	CB-CA-C	7.89	124.09	111.23
1	I	12	ARG	CB-CG-CD	7.86	129.39	111.30
1	D	228	ARG	CD-NE-CZ	7.81	135.33	124.40
1	B	83	ARG	CG-CD-NE	7.77	129.10	112.00
1	A	196	LYS	CB-CA-C	7.76	123.06	110.88
1	D	356	GLU	CB-CA-C	7.75	116.71	111.20
1	C	307	ARG	CG-CD-NE	7.73	129.01	112.00
2	N	57	U	C1'-C2'-O2'	7.69	123.34	111.80
1	H	154	ARG	CB-CG-CD	7.67	128.95	111.30
1	G	43	ASN	CB-CA-C	7.65	121.37	111.50
1	G	314	LEU	N-CA-C	-7.65	98.96	110.28
1	J	6	GLU	CB-CG-CD	7.64	125.59	112.60
1	C	79	MET	CA-C-N	7.47	130.51	120.65
1	C	79	MET	C-N-CA	7.47	130.51	120.65
1	I	350	ILE	N-CA-CB	7.47	122.01	112.22
1	F	172	ILE	CA-CB-CG2	7.43	123.13	110.50
1	M	302	ARG	CG-CD-NE	7.42	128.32	112.00
1	I	233	GLU	CB-CG-CD	7.35	125.10	112.60
1	D	178	LYS	N-CA-CB	-7.35	101.28	110.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	75	THR	CA-CB-CG2	7.31	122.93	110.50
1	B	309	PRO	CB-CA-C	-7.30	100.41	111.44
2	N	20	U	C4'-C3'-O3'	-7.26	102.11	113.00
1	F	309	PRO	CB-CA-C	-7.21	98.88	111.21
1	I	157	ASP	CA-CB-CG	7.20	119.80	112.60
1	F	295	LYS	CB-CG-CD	7.20	127.86	111.30
1	D	210	THR	CA-CB-OG1	-7.08	98.98	109.60
1	I	233	GLU	CB-CA-C	6.98	122.37	110.79
1	I	309	PRO	CB-CA-C	-6.92	99.38	111.21
1	E	193	ARG	NE-CZ-NH2	6.92	125.42	119.20
1	F	276	GLU	CB-CG-CD	6.91	124.35	112.60
1	F	258	TYR	CB-CA-C	6.84	121.22	109.24
1	J	314	LEU	N-CA-CB	-6.83	100.17	110.35
2	N	39	U	C1'-C2'-O2'	6.77	121.95	111.80
1	E	157	ASP	CA-CB-CG	6.76	119.36	112.60
1	F	321	LYS	O-C-N	6.74	129.27	122.12
1	E	309	PRO	CB-CA-C	-6.71	99.73	111.21
1	B	315	GLU	CB-CA-C	6.69	119.45	111.22
1	C	182	ALA	CB-CA-C	6.67	120.15	110.87
1	F	248	ALA	N-CA-CB	-6.66	100.19	109.91
2	N	63	U	C1'-C2'-O2'	6.66	121.79	111.80
1	I	193	ARG	CG-CD-NE	6.60	126.53	112.00
1	E	268	PHE	CA-CB-CG	-6.60	107.20	113.80
1	I	247	ARG	CB-CG-CD	6.60	126.47	111.30
2	N	32	U	C4'-C3'-O3'	-6.56	103.16	113.00
1	I	237	GLU	CB-CG-CD	6.55	123.73	112.60
1	C	176	ILE	CB-CA-C	6.52	121.57	112.05
1	G	309	PRO	CB-CA-C	-6.51	100.07	111.21
1	E	193	ARG	N-CA-CB	6.51	121.50	110.49
1	J	276	GLU	CB-CG-CD	6.51	123.67	112.60
1	H	103	ASP	CB-CA-C	6.48	120.26	109.89
2	N	41	U	C5'-C4'-C3'	-6.48	106.28	116.00
2	N	55	U	C5'-C4'-O4'	6.43	119.44	109.80
2	N	69	U	C1'-C2'-O2'	6.42	121.44	111.80
1	E	321	LYS	O-C-N	6.42	128.92	122.12
1	G	268	PHE	CA-CB-CG	-6.40	107.40	113.80
1	G	259	VAL	CG1-CB-CG2	-6.38	96.77	110.80
2	N	14	U	C4'-C3'-O3'	-6.37	103.45	113.00
1	H	365	LYS	CB-CG-CD	6.36	125.94	111.30
2	N	62	U	C4'-C3'-O3'	-6.35	103.47	113.00
2	N	41	U	N1-C1'-C2'	6.34	121.51	112.00
1	I	354	TYR	CA-C-N	6.33	129.74	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	354	TYR	C-N-CA	6.33	129.74	120.82
1	I	171	GLN	OE1-CD-NE2	-6.31	116.29	122.60
1	A	352	ARG	CB-CG-CD	6.30	125.80	111.30
1	G	218	ARG	CB-CG-CD	-6.30	96.81	111.30
2	N	74	U	C4'-C3'-O3'	-6.30	103.55	113.00
1	H	268	PHE	CA-CB-CG	-6.25	107.55	113.80
1	B	190	GLU	CB-CA-C	6.23	121.14	110.79
1	F	188	GLU	CB-CG-CD	6.23	123.19	112.60
1	M	193	ARG	CB-CG-CD	6.22	125.62	111.30
1	A	309	PRO	CB-CA-C	-6.22	102.05	111.44
1	J	285	ASN	CA-CB-CG	6.22	118.82	112.60
1	I	256	GLY	CA-C-O	-6.21	114.72	120.80
1	F	176	ILE	CG1-CB-CG2	-6.20	92.11	110.70
1	I	12	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	J	250	GLU	CB-CG-CD	6.19	123.12	112.60
1	M	103	ASP	CB-CA-C	6.19	119.54	110.26
1	G	171	GLN	CB-CA-C	6.18	122.07	110.63
1	I	301	TYR	CB-CA-C	6.17	120.69	110.81
1	H	211	GLN	N-CA-CB	6.17	119.71	110.22
1	J	321	LYS	O-C-N	6.14	128.63	122.12
1	G	272	ARG	CB-CG-CD	-6.13	97.19	111.30
1	I	245	LYS	CA-C-N	6.11	126.15	120.34
1	I	245	LYS	C-N-CA	6.11	126.15	120.34
1	G	314	LEU	CA-C-N	-6.11	114.05	122.30
1	G	314	LEU	C-N-CA	-6.11	114.05	122.30
2	N	56	U	C4'-C3'-O3'	-6.05	103.92	113.00
1	J	154	ARG	CB-CG-CD	6.04	125.19	111.30
2	N	15	U	C1'-C2'-O2'	6.03	120.85	111.80
1	G	247	ARG	CB-CG-CD	6.02	125.14	111.30
2	N	40	U	P-O5'-C5'	-6.02	111.88	120.90
1	E	286	GLU	CB-CG-CD	6.00	122.81	112.60
2	N	74	U	C5'-C4'-C3'	-6.00	107.00	116.00
2	N	38	U	C4'-C3'-O3'	-5.99	104.01	113.00
1	H	130	ARG	CG-CD-NE	5.99	125.17	112.00
1	G	329	LEU	N-CA-CB	5.98	118.74	110.07
2	N	34	U	C3'-C2'-O2'	5.96	119.65	110.70
1	J	83	ARG	N-CA-CB	-5.96	101.57	110.99
1	K	307	ARG	CG-CD-NE	-5.95	98.92	112.00
1	F	194	TRP	O-C-N	5.95	128.19	122.07
2	N	55	U	C5'-C4'-C3'	-5.94	107.09	116.00
1	G	199	GLN	CB-CA-C	5.93	120.64	110.79
1	F	196	LYS	CB-CA-C	5.91	120.06	110.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ASN	CA-CB-CG	5.91	118.51	112.60
1	I	12	ARG	NE-CZ-NH1	-5.87	115.63	121.50
1	G	314	LEU	CA-C-O	-5.85	114.61	121.16
1	A	6	GLU	CB-CG-CD	5.84	122.54	112.60
1	D	276	GLU	CB-CG-CD	5.84	122.54	112.60
1	I	196	LYS	CB-CA-C	5.83	120.03	110.88
1	J	272	ARG	CB-CG-CD	5.82	124.69	111.30
1	F	272	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	C	193	ARG	CB-CG-CD	5.78	124.59	111.30
2	N	22	U	P-O5'-C5'	-5.72	112.32	120.90
1	G	357	PRO	CB-CA-C	5.71	120.45	112.11
1	K	157	ASP	CA-CB-CG	5.71	118.31	112.60
1	H	276	GLU	CB-CG-CD	5.71	122.31	112.60
1	B	320	THR	CB-CA-C	5.68	121.14	110.63
1	J	303	GLU	CB-CG-CD	5.68	122.25	112.60
1	M	302	ARG	CB-CA-C	5.67	121.55	110.67
1	E	182	ALA	CB-CA-C	5.66	115.22	111.20
1	H	309	PRO	CB-CA-C	-5.66	101.53	111.21
1	G	12	ARG	CB-CG-CD	5.65	124.30	111.30
1	K	309	PRO	CB-CA-C	-5.65	101.55	111.21
1	H	96	ASP	CA-CB-CG	5.65	118.25	112.60
1	K	233	GLU	CB-CG-CD	5.62	122.16	112.60
1	J	79	MET	CA-C-N	5.59	129.21	120.82
1	J	79	MET	C-N-CA	5.59	129.21	120.82
1	H	256	GLY	CA-C-O	-5.58	115.33	120.80
2	N	45	U	N1-C1'-C2'	5.58	122.36	114.00
1	D	343	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	F	75	THR	OG1-CB-CG2	-5.57	98.16	109.30
1	K	250	GLU	CB-CG-CD	5.57	122.07	112.60
1	D	268	PHE	CA-CB-CG	-5.56	108.24	113.80
1	K	268	PHE	CA-CB-CG	-5.55	108.25	113.80
1	H	75	THR	CA-CB-CG2	5.55	119.93	110.50
1	H	285	ASN	CA-CB-CG	5.55	118.15	112.60
1	A	196	LYS	CB-CG-CD	5.54	124.05	111.30
1	J	314	LEU	N-CA-C	-5.54	98.23	107.99
2	N	35	U	C2'-C3'-O3'	5.54	122.01	113.70
1	F	324	PRO	CB-CA-C	5.54	119.58	111.22
1	C	234	ILE	CB-CG1-CD1	-5.54	102.18	113.80
1	D	309	PRO	CB-CA-C	-5.54	103.08	111.44
1	B	193	ARG	CB-CG-CD	5.53	124.02	111.30
1	H	321	LYS	O-C-N	5.52	127.97	122.12
1	L	309	PRO	CB-CA-C	-5.52	103.11	111.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	4	U	C5'-C4'-C3'	-5.51	107.74	116.00
1	I	13	SER	CA-C-O	-5.51	113.64	119.97
1	C	218	ARG	CG-CD-NE	-5.50	99.90	112.00
1	C	219	ASN	CA-CB-CG	-5.50	107.10	112.60
1	F	258	TYR	N-CA-C	-5.49	106.71	113.41
1	G	60	ARG	CG-CD-NE	5.49	124.08	112.00
1	H	357	PRO	CB-CA-C	5.48	120.12	112.11
1	D	357	PRO	N-CA-CB	5.48	108.56	103.41
1	I	21	ASP	N-CA-C	5.47	117.05	111.14
1	A	377	ASN	CA-C-N	5.47	128.06	120.29
1	A	377	ASN	C-N-CA	5.47	128.06	120.29
1	F	12	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	I	234	ILE	CB-CG1-CD1	-5.45	102.36	113.80
1	F	315	GLU	CB-CG-CD	5.43	121.83	112.60
1	E	180	VAL	CA-C-O	-5.43	114.99	120.69
1	K	342	ASP	CA-C-N	5.42	127.81	120.38
1	K	342	ASP	C-N-CA	5.42	127.81	120.38
1	L	306	PRO	CB-CA-C	-5.42	103.75	112.21
1	M	309	PRO	CB-CA-C	-5.42	101.95	111.21
1	B	89	ARG	CG-CD-NE	5.41	123.90	112.00
1	I	268	PHE	CA-CB-CG	-5.41	108.39	113.80
2	N	44	U	C3'-C2'-O2'	5.40	118.80	110.70
1	F	264	MET	CA-C-N	5.40	129.77	121.19
1	F	264	MET	C-N-CA	5.40	129.77	121.19
1	H	180	VAL	CA-C-O	-5.39	114.76	119.29
1	A	5	PHE	CA-C-N	5.38	127.80	120.54
1	A	5	PHE	C-N-CA	5.38	127.80	120.54
1	I	77	ILE	CA-C-N	-5.36	115.74	125.66
1	I	77	ILE	C-N-CA	-5.36	115.74	125.66
1	C	193	ARG	CG-CD-NE	-5.36	100.21	112.00
1	H	103	ASP	CA-CB-CG	5.35	117.95	112.60
1	I	79	MET	CA-C-N	5.35	128.85	120.82
1	I	79	MET	C-N-CA	5.35	128.85	120.82
1	F	154	ARG	CG-CD-NE	5.35	123.76	112.00
1	I	5	PHE	CA-CB-CG	5.33	119.13	113.80
1	E	315	GLU	CB-CG-CD	5.33	121.66	112.60
1	G	175	LEU	O-C-N	5.31	127.82	122.09
1	E	192	ARG	N-CA-C	-5.30	103.14	110.35
1	D	80	TYR	CB-CA-C	-5.29	102.35	110.81
1	C	77	ILE	CA-C-N	-5.28	115.89	125.66
1	C	77	ILE	C-N-CA	-5.28	115.89	125.66
1	A	43	ASN	CA-C-N	5.28	128.38	120.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ASN	C-N-CA	5.28	128.38	120.83
1	K	261	GLU	CB-CA-C	5.28	119.96	111.36
1	G	75	THR	CA-CB-CG2	5.24	119.41	110.50
1	G	254	ASP	CB-CA-C	5.24	119.11	110.88
1	M	212	GLN	CA-C-O	-5.24	115.00	120.55
1	M	193	ARG	CG-CD-NE	-5.24	100.48	112.00
1	C	218	ARG	N-CA-CB	5.22	117.80	110.12
2	N	4	U	O5'-C5'-C4'	5.21	119.31	111.50
1	B	314	LEU	N-CA-C	-5.20	103.17	110.50
2	N	66	U	C5'-C4'-C3'	-5.19	108.22	116.00
1	C	157	ASP	CA-CB-CG	5.17	117.77	112.60
1	I	154	ARG	CB-CG-CD	5.17	123.19	111.30
1	K	359	TYR	CB-CA-C	5.16	119.62	110.85
1	L	187	GLU	CB-CG-CD	5.15	121.36	112.60
2	N	24	U	N1-C1'-C2'	5.15	119.72	112.00
1	K	103	ASP	CA-CB-CG	5.14	117.74	112.60
1	L	352	ARG	CA-C-N	5.14	125.69	119.98
1	L	352	ARG	C-N-CA	5.14	125.69	119.98
1	A	187	GLU	CB-CG-CD	5.12	121.31	112.60
1	C	316	GLU	CA-C-N	5.12	127.86	120.38
1	C	316	GLU	C-N-CA	5.12	127.86	120.38
1	E	60	ARG	CG-CD-NE	5.11	123.25	112.00
1	J	231	MET	N-CA-CB	5.11	117.59	109.82
2	N	14	U	C3'-C2'-O2'	5.10	118.35	110.70
1	G	248	ALA	CB-CA-C	5.10	118.81	110.96
1	D	342	ASP	CB-CA-C	5.09	118.44	110.19
1	H	230	PHE	CB-CA-C	-5.09	102.89	110.88
1	B	278	ARG	CD-NE-CZ	5.09	131.52	124.40
1	D	154	ARG	CA-C-N	5.08	127.31	120.50
1	D	154	ARG	C-N-CA	5.08	127.31	120.50
1	F	202	ARG	CB-CA-C	5.08	120.75	110.38
1	J	268	PHE	CA-CB-CG	-5.08	108.72	113.80
1	G	290	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	131	ILE	CB-CG1-CD1	5.07	124.44	113.80
1	D	211	GLN	N-CA-CB	5.07	118.15	110.14
1	F	319	GLN	O-C-N	5.05	127.92	122.11
1	I	365	LYS	CB-CG-CD	5.05	122.92	111.30
1	E	196	LYS	N-CA-C	-5.05	103.82	110.43
1	G	246	GLY	CA-C-O	-5.04	116.46	121.90
1	A	250	GLU	CB-CG-CD	5.03	121.16	112.60
1	M	196	LYS	CB-CA-C	5.03	118.86	110.81
1	B	316	GLU	CB-CG-CD	5.03	121.14	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	52	THR	N-CA-CB	5.03	117.60	110.16
1	L	347	ALA	CA-C-N	5.02	127.97	120.95
1	L	347	ALA	C-N-CA	5.02	127.97	120.95
1	G	350	ILE	CB-CG1-CD1	-5.01	103.27	113.80
1	H	163	SER	CA-C-N	5.01	127.26	120.65
1	H	163	SER	C-N-CA	5.01	127.26	120.65
1	I	285	ASN	CA-CB-CG	5.01	117.61	112.60
1	G	258	TYR	CB-CA-C	5.00	118.00	109.24
1	H	340	THR	CA-CB-CG2	5.00	119.00	110.50
1	J	277	THR	CA-C-N	5.00	131.09	121.54
1	J	277	THR	C-N-CA	5.00	131.09	121.54

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	34	0
1	B	2979	0	2957	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2974	0	2955	54	0
1	D	2979	0	2957	55	0
1	E	2979	0	2957	62	0
1	F	2979	0	2957	60	0
1	G	2979	0	2957	55	0
1	H	2979	0	2957	47	0
1	I	2979	0	2957	48	0
1	J	2979	0	2957	47	0
1	K	2979	0	2957	41	0
1	L	2969	0	2949	42	0
1	M	2916	0	2922	27	0
2	N	1556	0	779	114	0
All	All	40200	0	39173	529	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 7.

All (529) 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:D:275:LEU:HD21	1:E:8:ALA:HB2	1.62	0.81
1:H:158:MET:HE3	1:I:31:LEU:HD13	1.64	0.80
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:G:51:LEU:HD23	1:G:79:MET:HE1	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:MET:HE1	1:F:32:THR:O	1.89	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:L:298:MET:HE2	1:M:11:PHE:CD2	2.27	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
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:K:269:ALA:CB	1:K:335:MET:HE1	2.27	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:M:269:ALA:CB	1:M:335:MET:HE1	2.28	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:H:331:TRP:CD1	1:H:335:MET:HE3	2.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:271:ILE:HD13	1:G:298:MET:HE2	1.82	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:F:269:ALA:CB	1:F:335:MET:HE1	2.32	0.60
1:L:181:THR:HB	2:N:69:U:H5'	1.84	0.60
1:L:298:MET:HE2	1:M:11:PHE:HD2	1.67	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
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:E:178:LYS:NZ	2:N:29:U:OP2	2.28	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:269:ALA:CB	1:G:335:MET:HE1	2.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:269:ALA:CB	1:E:335:MET:HE1	2.35	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: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:H:269:ALA:HB3	1:H:335:MET:HE1	1.86	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:K:269:ALA:HB3	1:K:335:MET:HE1	1.88	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
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:302:ARG:HH22	1:E:10:SER:C	2.14	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:F:73:ALA:CB	1:F:217:MET:HE1	2.37	0.55
1:M:269:ALA:HB1	1:M:335:MET:HE1	1.89	0.55
1:C:199:GLN:HG3	2:N:19:U:H3	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:269:ALA:CB	1:D:335:MET:HE1	2.37	0.54
1:G:265:ALA:CB	2:N:39:U:OP1	2.55	0.54
1:K:269:ALA:HB1	1:K:335:MET:HE1	1.91	0.53
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:L:269:ALA:CB	1:L:335:MET:HE1	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:M:269:ALA:HB3	1:M:335:MET:HE1	1.91	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: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:H:269:ALA:CB	1:H:335:MET:HE1	2.40	0.52
1:J:269:ALA:CB	1:J:335:MET:HE1	2.40	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ALA:HB3	1:C:218:ARG:HH22	1.76	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:C:77:ILE:O	1:C:78:SER:HB3	2.09	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:E:344:SER:O	2:N:28:U:O2'	2.26	0.49
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:F:269:ALA:HB1	1:F:335:MET:HE1	1.94	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: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
1:F:340:THR:HG21	1:F:367:ALA:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:269:ALA:CB	1:A:335:MET:HE1	2.43	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:G:269:ALA:HB1	1:G:335:MET:HE1	1.95	0.48
1:E:341:ILE:HG13	1:F:286:GLU:CD	2.39	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:I:269:ALA:CB	1:I:335:MET:HE1	2.42	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:F:269:ALA:HB3	1:F:335:MET:HE1	1.95	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:J:271:ILE:HD13	1:J:298:MET:HE2	1.95	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:E:181:THR:OG1	2:N:26:U:O2'	2.23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:269:ALA:HB1	1:L:335:MET:HE1	1.95	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:J:302:ARG:NH2	1:K:10:SER:C	2.72	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
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:J:227:VAL:HG12	1:J:231:MET:HE3	1.97	0.47
1:K:176:ILE:HD11	1:K:231:MET:SD	2.55	0.47
1:C:269:ALA:CB	1:C:335:MET:HE1	2.44	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:B:11:PHE:O	1:B:12:ARG:C	2.58	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:J:335:MET:HE2	1:J:335:MET:N	2.31	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:ARG:HH11	2:N:42:U:P	2.39	0.46
1:L:271:ILE:HG12	1:L:298:MET:HE3	1.96	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:E:269:ALA:HB1	1:E:335:MET:HE1	1.97	0.46
1:G:51:LEU:CD2	1:G:79:MET:HE1	2.42	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
1:E:269:ALA:HB3	1:E:335:MET:HE1	1.98	0.46
1:I:298:MET:HE2	1:J:11:PHE:CD2	2.51	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
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:E:181:THR:HG1	2:N:26:U:HO2'	1.51	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:M:335:MET:N	1:M:335:MET:HE2	2.32	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:B:269:ALA:CB	1:B:335:MET:HE1	2.47	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:K:276:GLU:CD	1:L:12:ARG:HE	2.25	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLU:CD	1:B:124:GLU:H	2.25	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:H:344:SER:O	2:N:46:U:O2'	2.28	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:G:302:ARG:NH2	1:H:10:SER:C	2.75	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:J:227:VAL:CG1	1:J:231:MET:HE3	2.47	0.44
1:C:294:ILE:HD12	1:C:294:ILE:C	2.42	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:K:158:MET:HE2	1:L:31:LEU:HD13	1.98	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
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:311:MET:HE1	1:E:322:PHE:CE2	2.53	0.44
1:I:153:LEU:HD11	1:I:206:PHE:HE2	1.83	0.44
1:B:344:SER:O	2:N:10:U:O2'	2.35	0.43
1:F:73:ALA:HB1	1:F:217:MET:HE1	1.98	0.43
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:269:ALA:HB3	1:G:335:MET:HE1	1.98	0.43
1:E:92:LEU:HD11	1:E:97:ILE:HD11	1.99	0.43
1:E:275:LEU:HD23	1:E:275:LEU:C	2.43	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:J:235:LEU:HD23	1:J:235:LEU:C	2.44	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:D:335:MET:N	1:D:335:MET:HE2	2.33	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:A:19:GLY:C	1:A:21:ASP:H	2.26	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: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:J:269:ALA:HB1	1:J:335:MET:HE1	2.00	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:J:298:MET:HE2	1:K:11:PHE:CD2	2.54	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:269:ALA:HB1	1:D:335:MET:HE1	2.00	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:L:311:MET:HE1	1:L:322:PHE:CE2	2.55	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:F:73:ALA:HB2	1:F:217:MET:HE1	2.02	0.42
1:F:263:GLY:C	1:F:312:VAL:HG21	2.45	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:J:311:MET:HE1	1:J:322:PHE:CE2	2.55	0.42
1:K:91:LEU:CD1	1:K:234:ILE:HG22	2.49	0.42
1:L:335:MET:HE2	1:L:335:MET:N	2.35	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:F:172:ILE:HA	1:F:175:LEU:HD12	2.01	0.42
1:H:73:ALA:HB1	1:H:217:MET:HE1	2.00	0.42
1:H:197:TYR:CD1	1:H:251:ILE:CD1	3.02	0.42
1:I:335:MET:N	1:I:335:MET:HE2	2.34	0.42
1:J:158:MET:HE1	1:K:34:LYS:HG2	2.01	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:I:255:ILE:O	1:I:256:GLY:C	2.62	0.41
1:I:298:MET:HE2	1:J:11:PHE:HD2	1.85	0.41
1:K:240:LYS:HD3	1:L:21:ASP:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:344:SER:O	2:N:64:U:O2'	2.35	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:A:264:MET:HE1	1:A:308:ALA:O	2.19	0.41
1:D:269:ALA:HB3	1:D:335:MET:HE1	2.01	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:A:335:MET:N	1:A:335:MET:HE2	2.36	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:M:73:ALA:HB1	1:M:217:MET:HE1	2.02	0.41
1:A:295:LYS:HE2	1:B:4:ILE:HA	2.03	0.41
1:D:311:MET:HE1	1:D:322:PHE:CE2	2.55	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:MET:N	1:B:335:MET:HE2	2.36	0.41
1:C:133:LYS:HB2	1:C:133:LYS:HE3	1.98	0.41
1:G:302:ARG:HH22	1:H:10:SER:C	2.30	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:M:19:GLY:O	1:M:20:ARG:CB	2.68	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:G:255:ILE:O	1:G:256:GLY:C	2.64	0.40
1:I:73:ALA:CB	1:I:217:MET:HE1	2.52	0.40
1:I:300:LEU:O	1:I:304:ILE:HG13	2.21	0.40
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%)	24	57
1	C	392/554 (71%)	377 (96%)	14 (4%)	1 (0%)	36	67
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%)	36	67
1	G	393/554 (71%)	385 (98%)	8 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	393/554 (71%)	382 (97%)	10 (2%)	1 (0%)	36	67
1	I	393/554 (71%)	380 (97%)	12 (3%)	1 (0%)	36	67
1	J	393/554 (71%)	380 (97%)	13 (3%)	0	100	100
1	K	393/554 (71%)	381 (97%)	11 (3%)	1 (0%)	36	67
1	L	389/554 (70%)	377 (97%)	11 (3%)	1 (0%)	36	67
1	M	378/554 (68%)	365 (97%)	12 (3%)	1 (0%)	36	67
All	All	5088/7202 (71%)	4910 (96%)	169 (3%)	9 (0%)	44	74

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%)	296 (99%)	3 (1%)	68	75
1	B	299/454 (66%)	292 (98%)	7 (2%)	44	64
1	C	299/454 (66%)	297 (99%)	2 (1%)	76	78
1	D	299/454 (66%)	296 (99%)	3 (1%)	68	75
1	E	299/454 (66%)	292 (98%)	7 (2%)	44	64
1	F	299/454 (66%)	295 (99%)	4 (1%)	61	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	299/454 (66%)	296 (99%)	3 (1%)	68	75
1	H	299/454 (66%)	295 (99%)	4 (1%)	61	72
1	I	299/454 (66%)	290 (97%)	9 (3%)	36	60
1	J	299/454 (66%)	293 (98%)	6 (2%)	48	67
1	K	299/454 (66%)	296 (99%)	3 (1%)	68	75
1	L	299/454 (66%)	297 (99%)	2 (1%)	76	78
1	M	299/454 (66%)	295 (99%)	4 (1%)	61	72
All	All	3887/5902 (66%)	3830 (98%)	57 (2%)	55	71

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	51	LEU
1	A	131	ILE
1	B	31	LEU
1	B	111	ILE
1	B	122	GLN
1	B	140	LYS
1	B	178	LYS
1	B	234	ILE
1	B	250	GLU
1	C	107	MET
1	C	234	ILE
1	D	31	LEU
1	D	178	LYS
1	D	329	LEU
1	E	31	LEU
1	E	158	MET
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	34	LYS
1	F	223	GLN
1	F	247	ARG
1	G	243	SER
1	G	312	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	329	LEU
1	H	6	GLU
1	H	31	LEU
1	H	291	LEU
1	H	329	LEU
1	I	5	PHE
1	I	12	ARG
1	I	31	LEU
1	I	32	THR
1	I	165	VAL
1	I	176	ILE
1	I	234	ILE
1	I	249	VAL
1	I	350	ILE
1	J	114	MET
1	J	165	VAL
1	J	171	GLN
1	J	272	ARG
1	J	276	GLU
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	M	23	ARG
1	M	33	THR
1	M	113	VAL
1	M	239	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	B	319	GLN
1	B	364	GLN
1	C	199	GLN
1	C	364	GLN
1	D	288	GLN
1	E	93	ASN
1	E	257	ASN
1	E	285	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	288	GLN
1	E	292	ASN
1	F	223	GLN
1	F	364	GLN
1	G	109	ASN
1	H	257	ASN
1	H	285	ASN
1	H	319	GLN
1	H	364	GLN
1	J	257	ASN
1	J	285	ASN
1	K	43	ASN
1	K	257	ASN
1	K	292	ASN
1	L	109	ASN
1	M	43	ASN
1	M	288	GLN
1	M	319	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

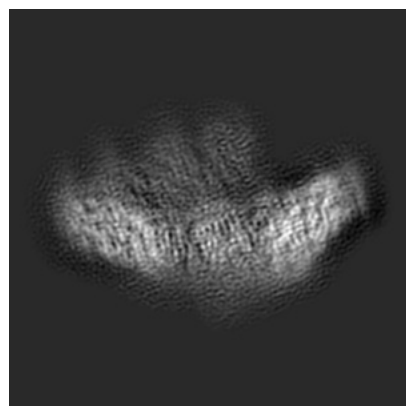
6 Map visualisation [i](#)

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.

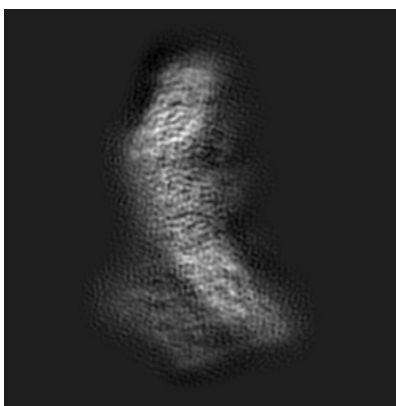
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

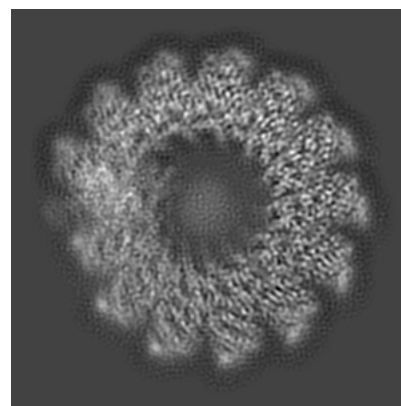
6.1.1 Primary map



X

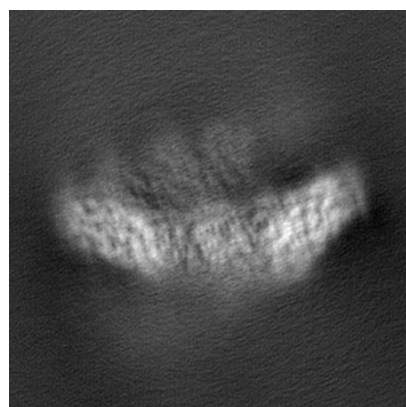


Y

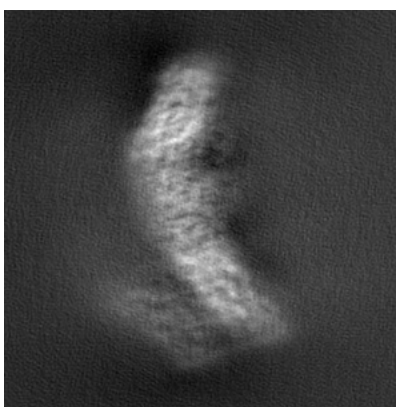


Z

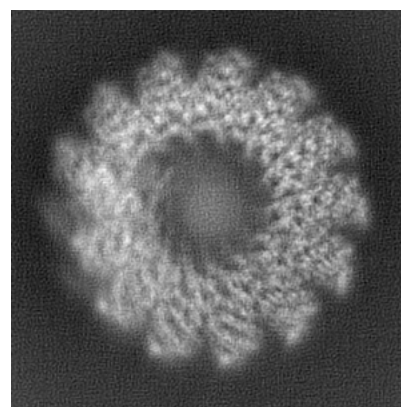
6.1.2 Raw map



X



Y

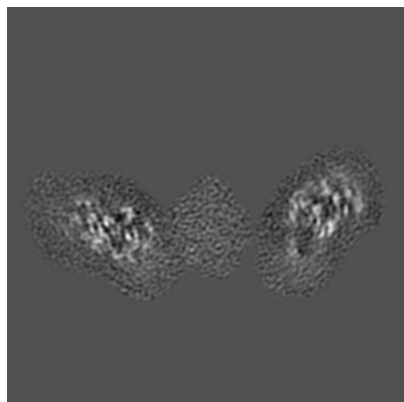


Z

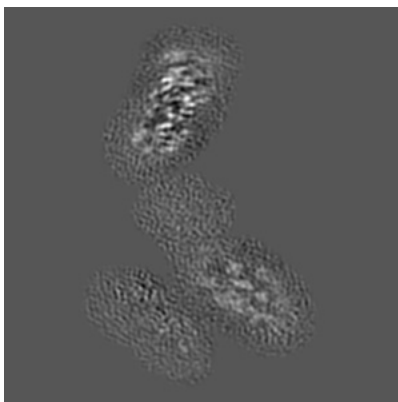
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

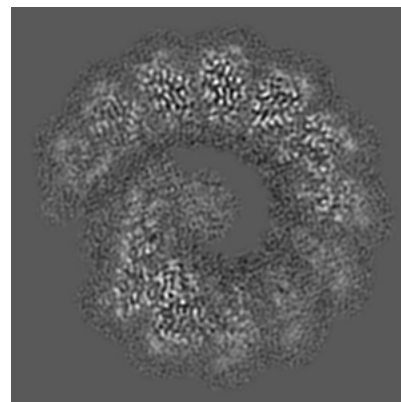
6.2.1 Primary map



X Index: 120



Y Index: 120

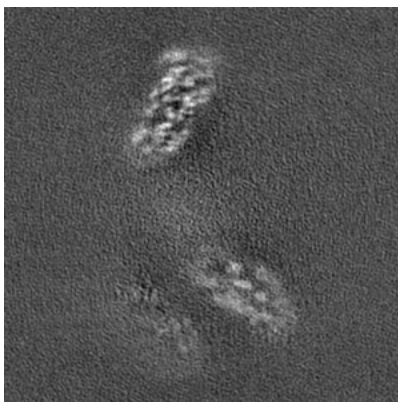


Z Index: 120

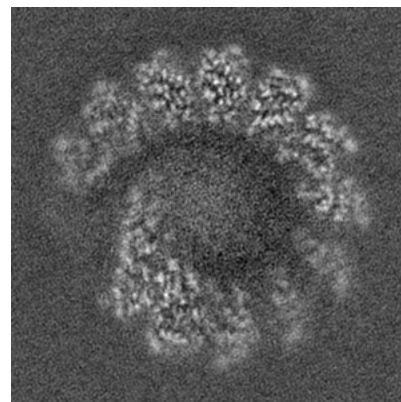
6.2.2 Raw map



X Index: 120



Y Index: 120

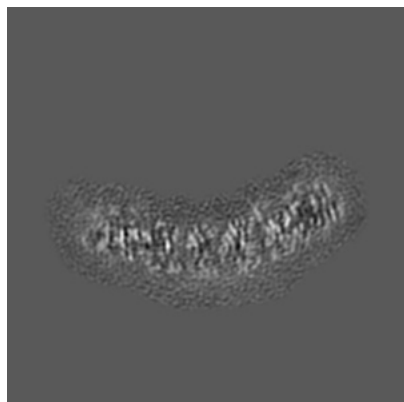


Z Index: 120

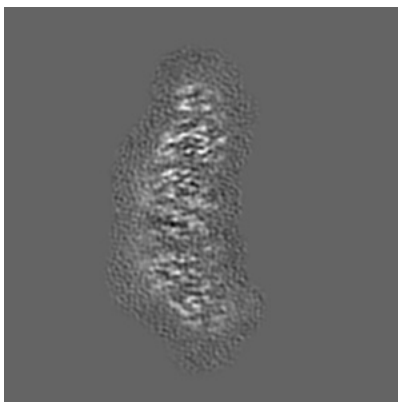
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

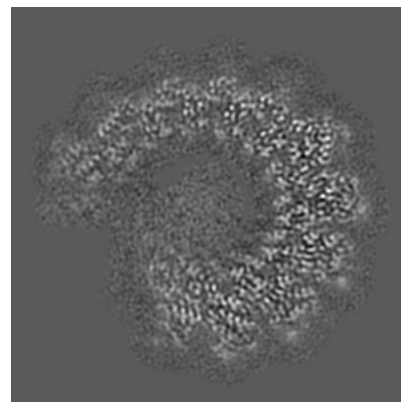
6.3.1 Primary map



X Index: 161

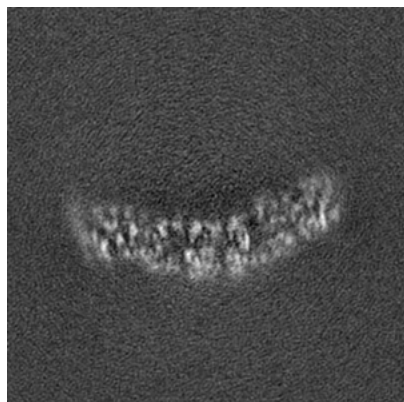


Y Index: 172

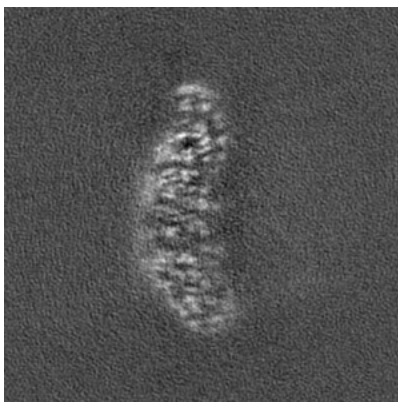


Z Index: 105

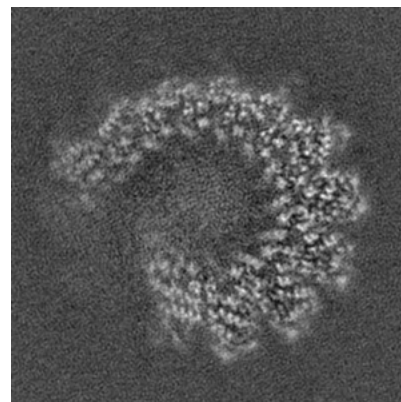
6.3.2 Raw map



X Index: 165



Y Index: 173

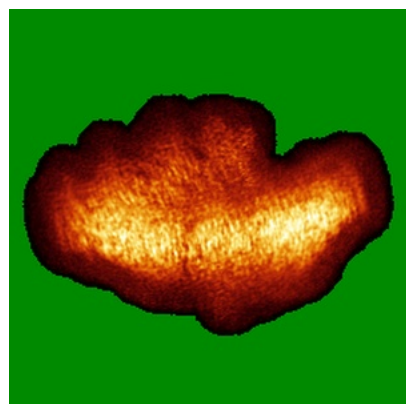


Z Index: 104

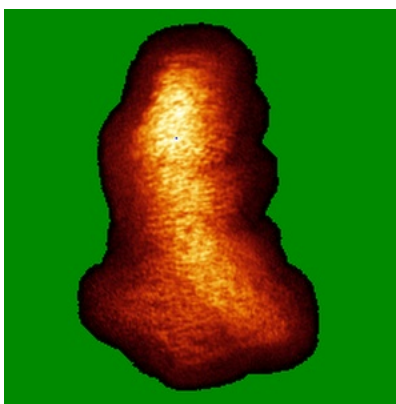
The images above show the largest variance slices of the map in three orthogonal directions.

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

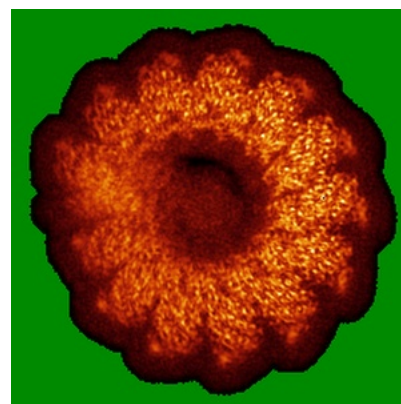
6.4.1 Primary map



X

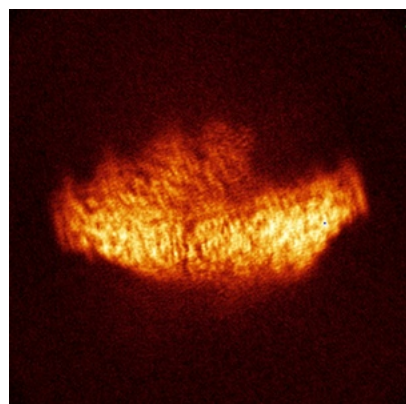


Y

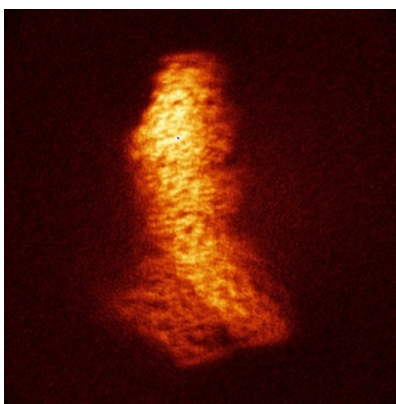


Z

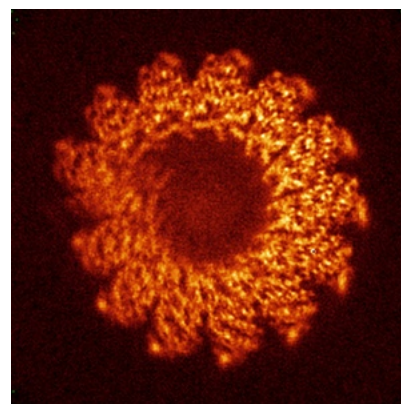
6.4.2 Raw map



X



Y

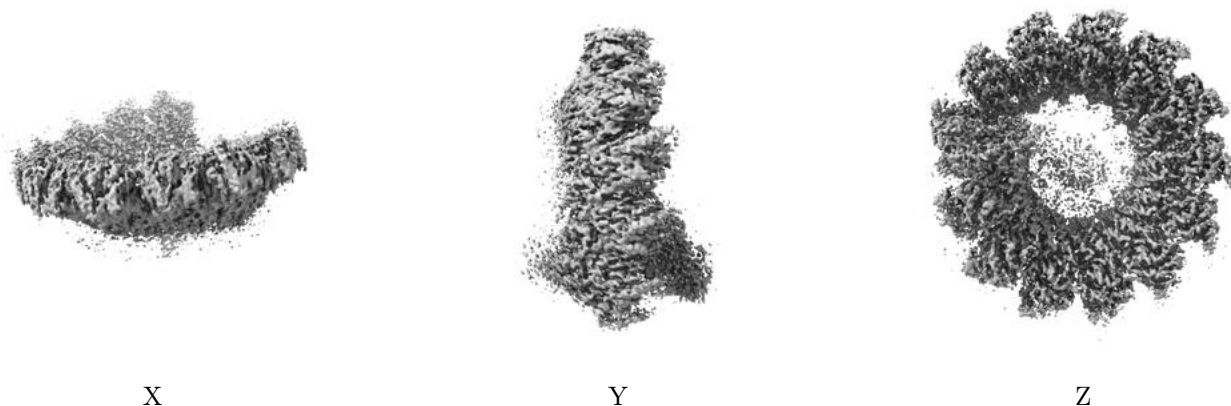


Z

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.

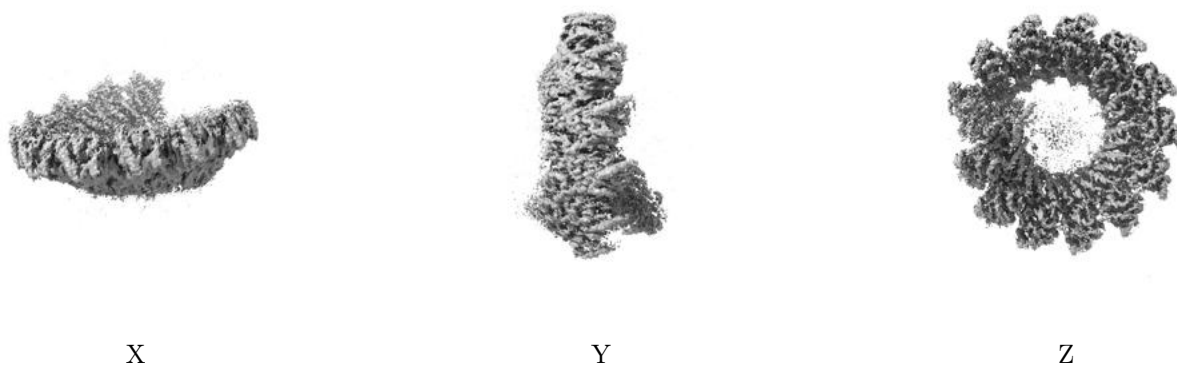
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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.

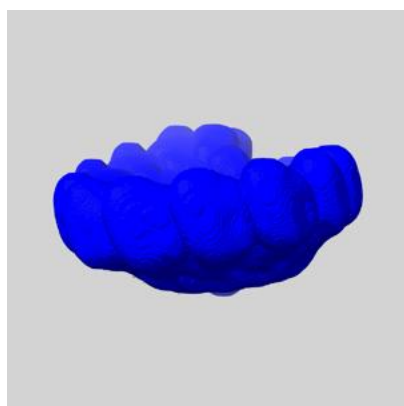
6.6 Mask visualisation [i](#)

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

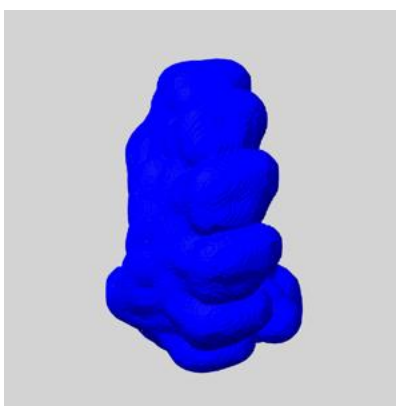
A mask typically either:

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

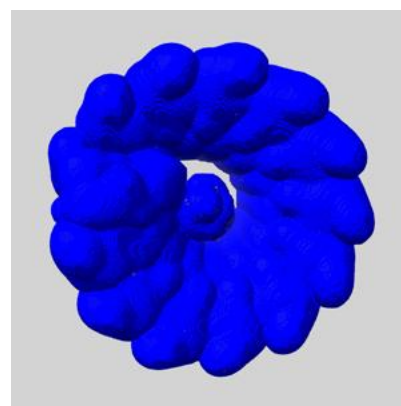
6.6.1 emd_12581_msk_1.map [i](#)



X



Y

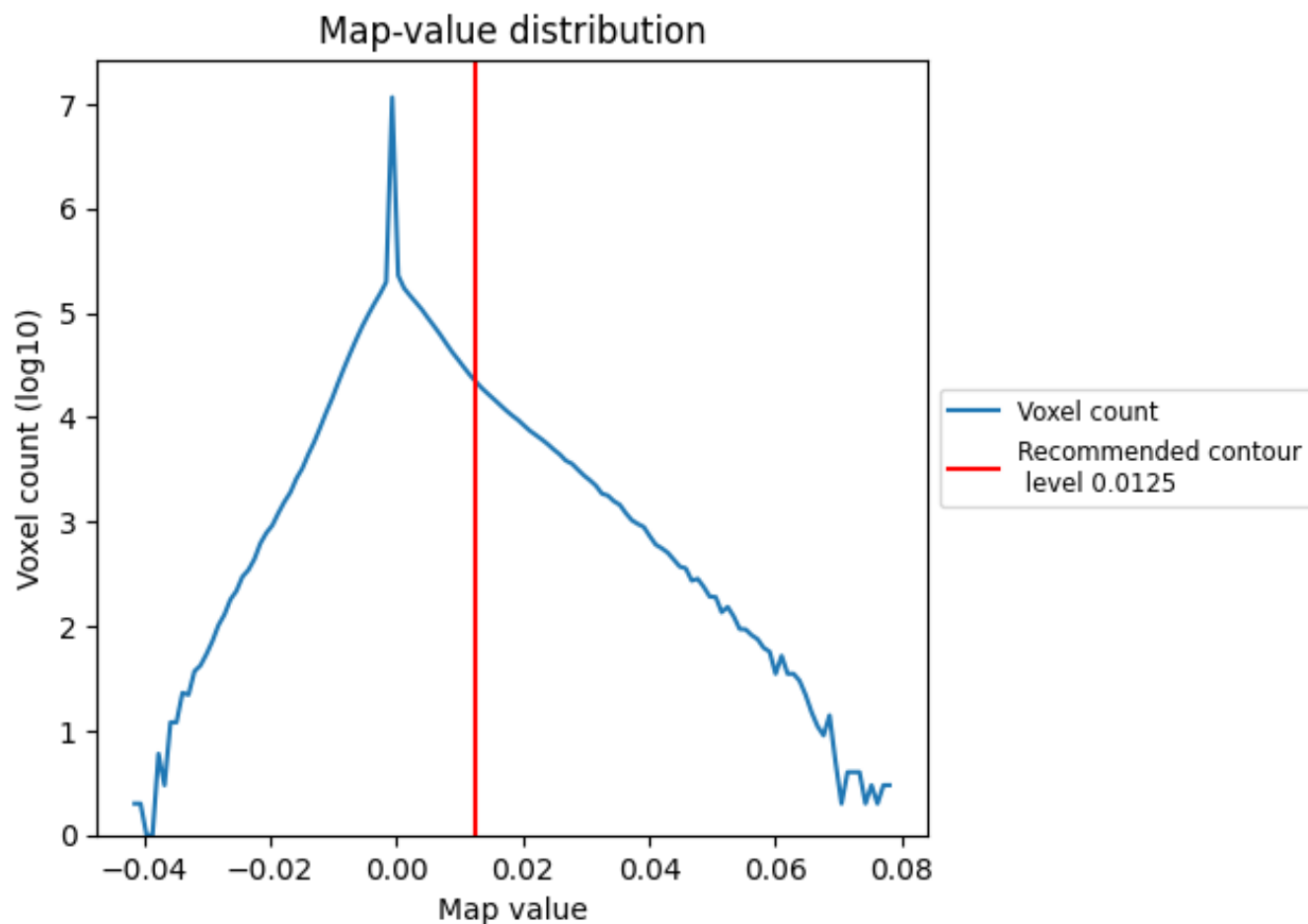


Z

7 Map analysis [i](#)

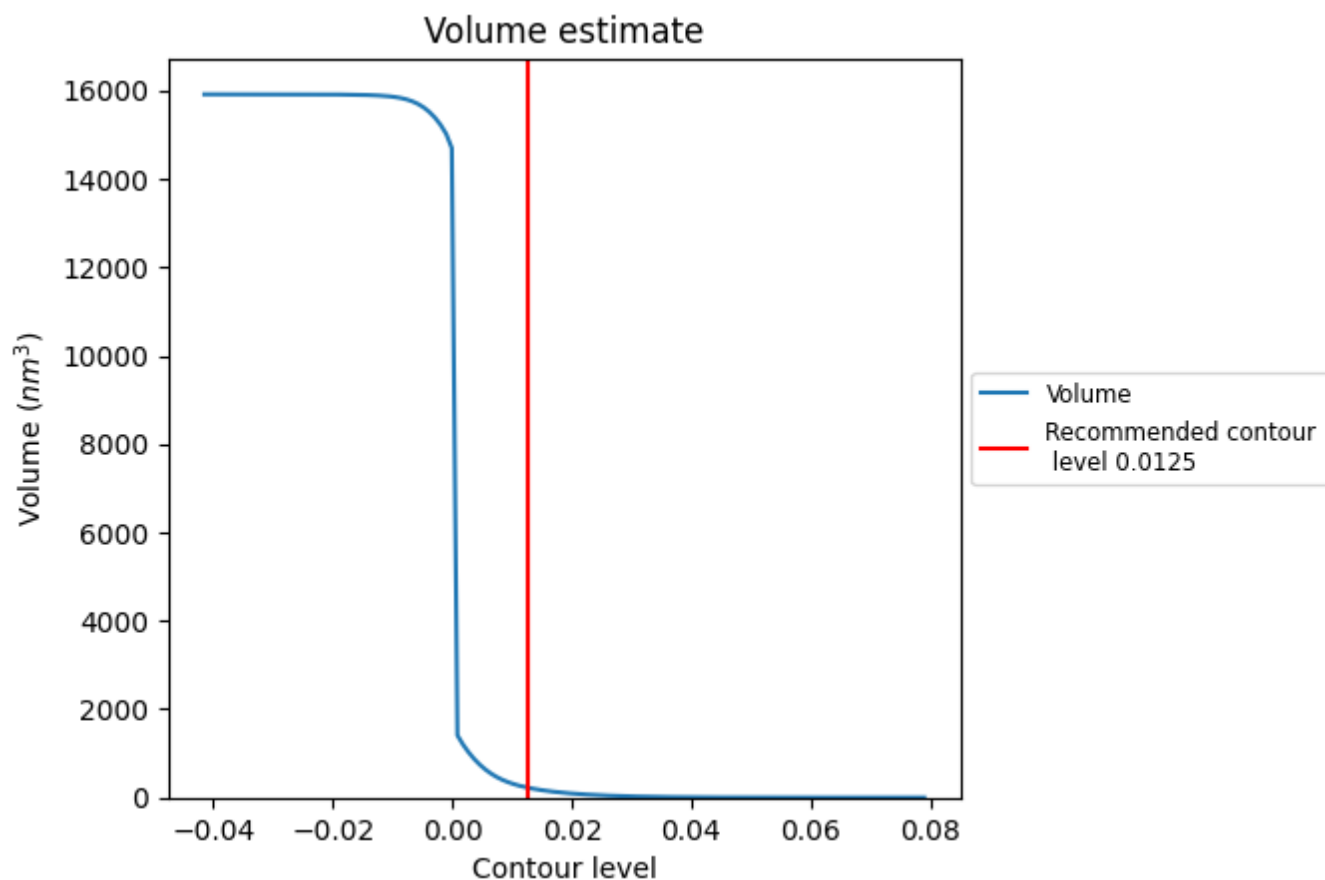
This section contains the results of statistical analysis of the map.

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.

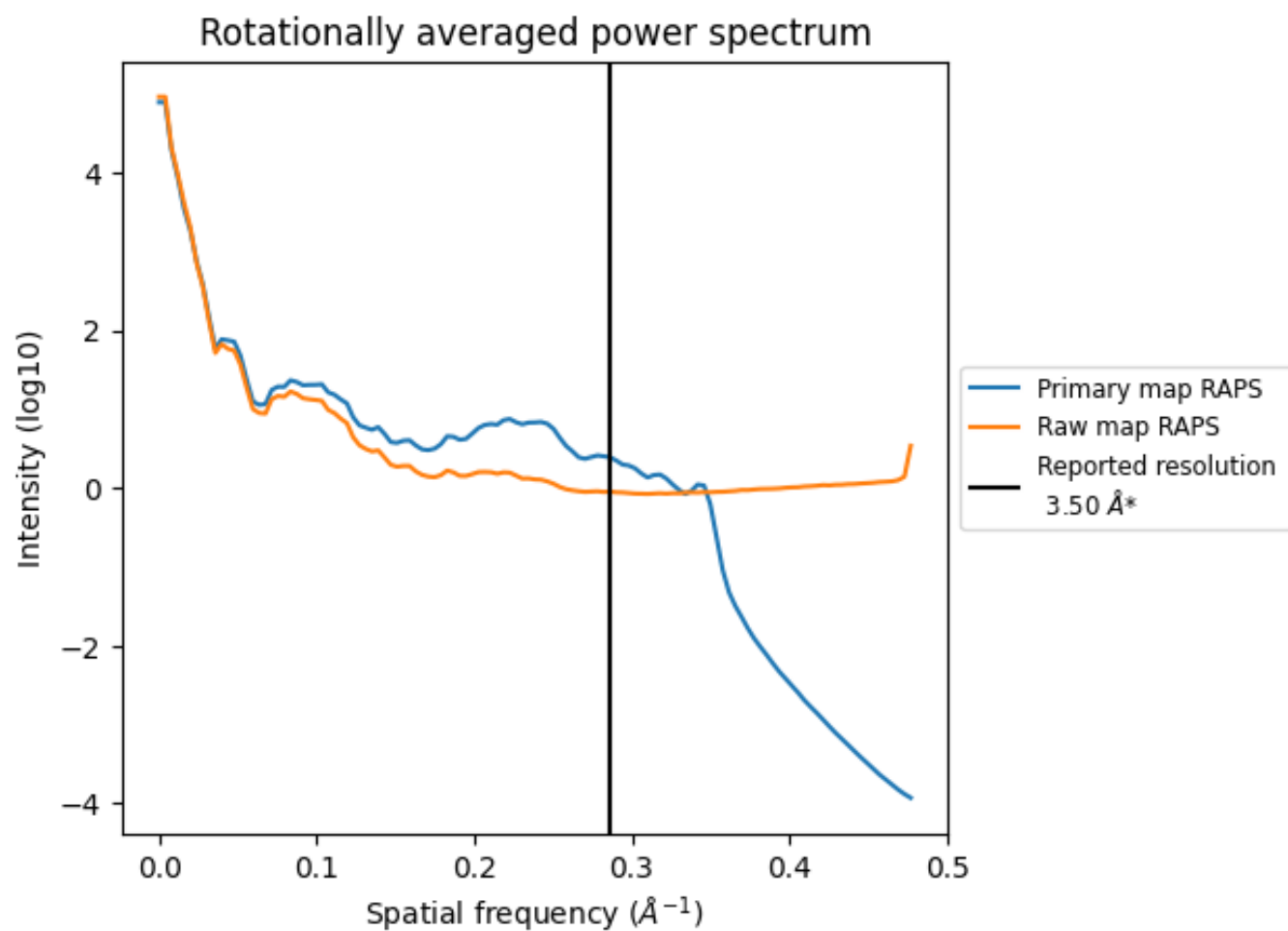
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 228 nm³; 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 ⓘ

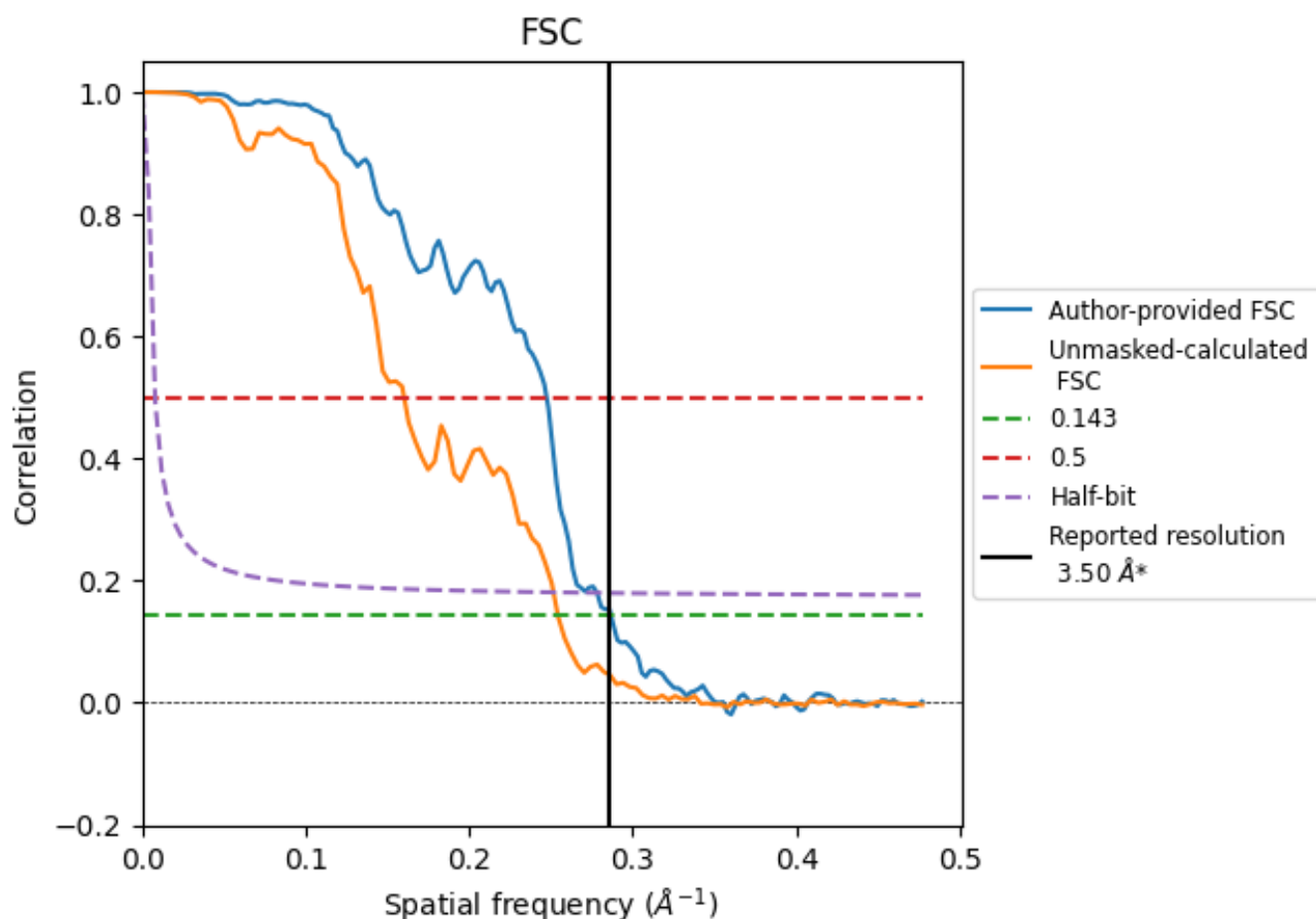


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

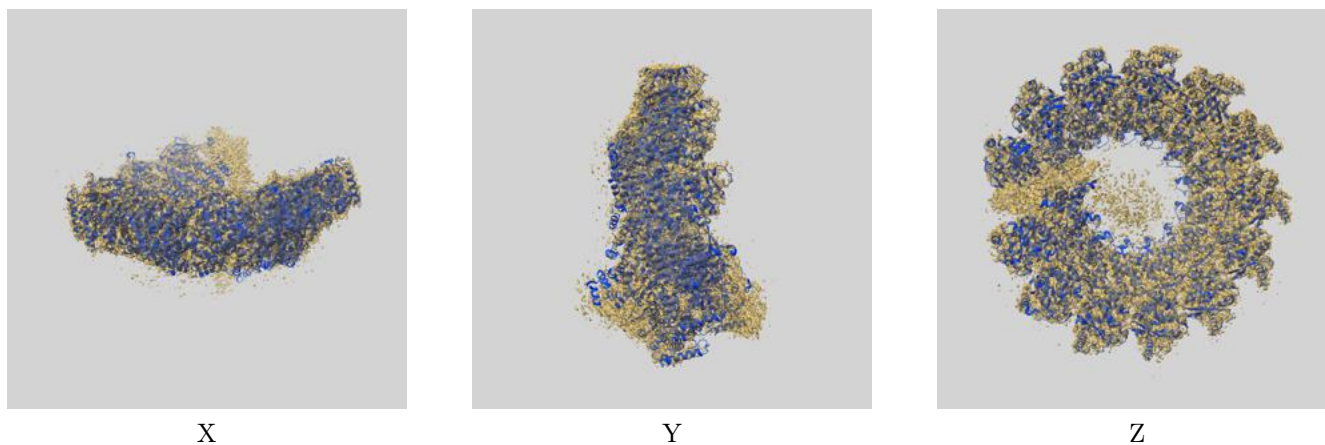
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.04	3.59
Unmasked-calculated*	3.93	6.24	3.97

*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](#)

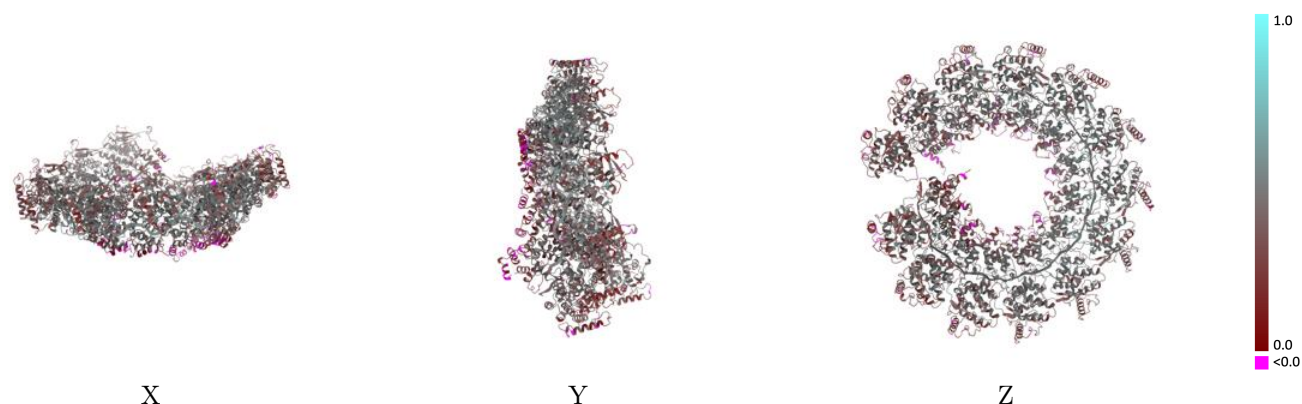
This section contains information regarding the fit between EMDB map EMD-12581 and PDB model 7NT5. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



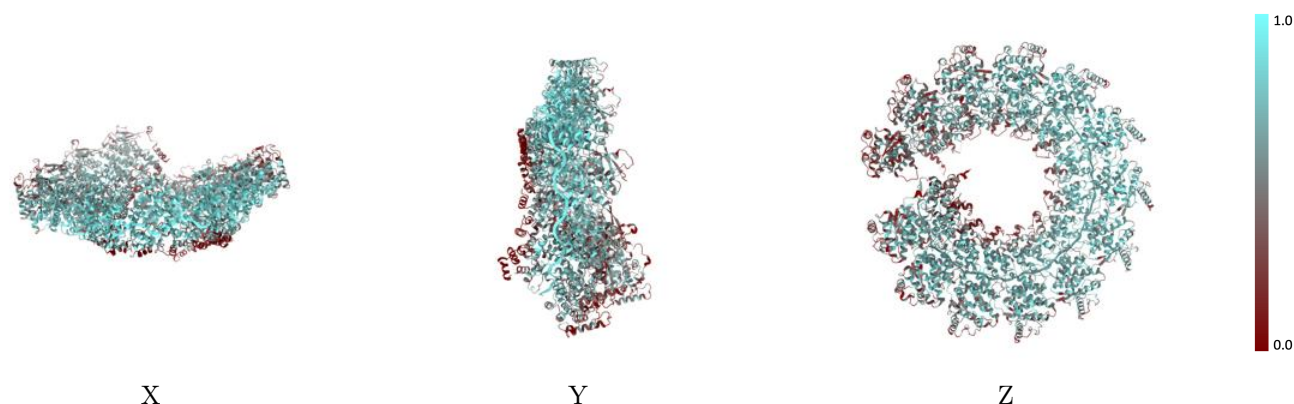
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



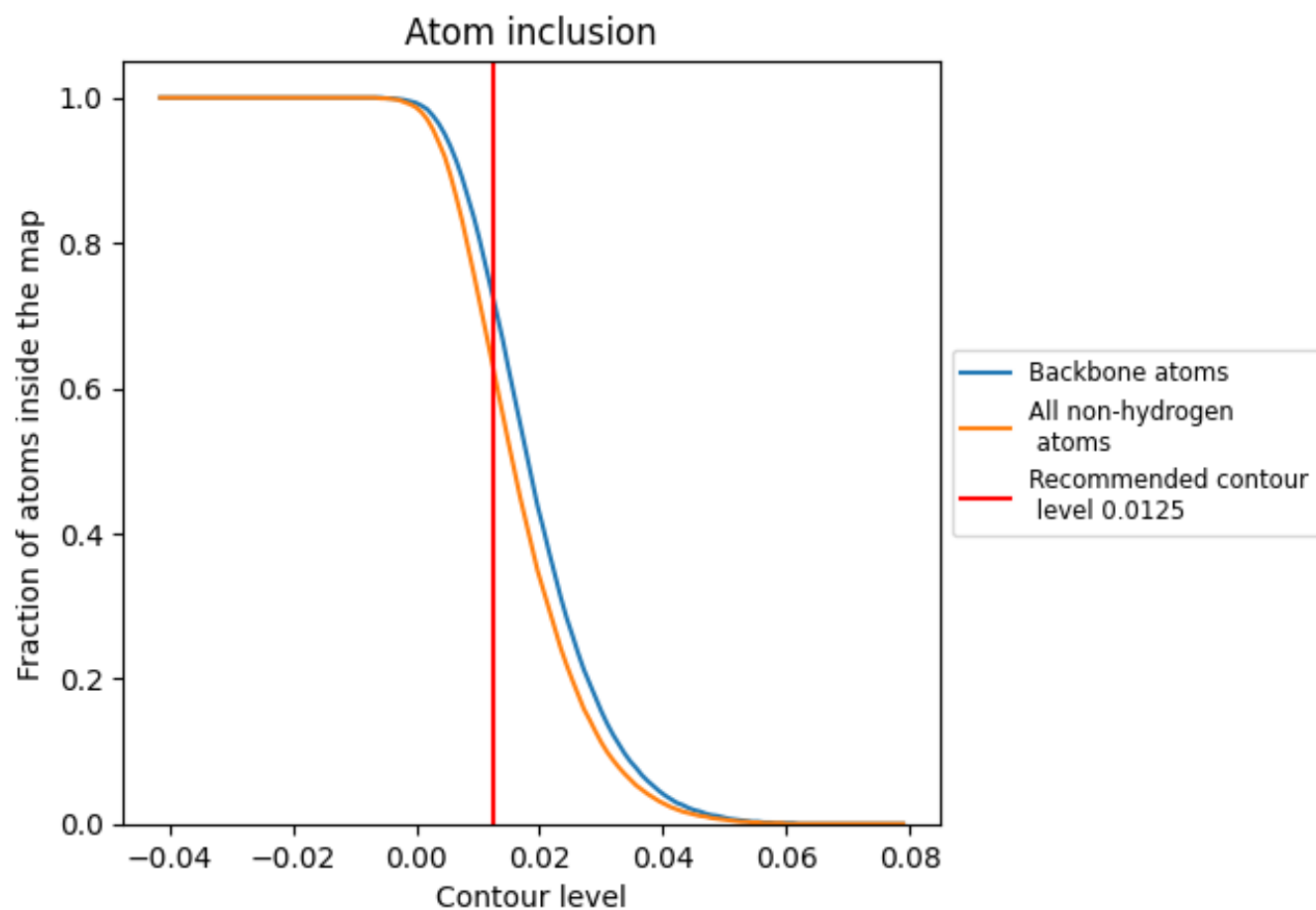
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% 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	 0.6280	 0.3960
A	 0.4920	 0.3510
B	 0.5780	 0.3770
C	 0.6180	 0.3880
D	 0.6340	 0.4020
E	 0.6680	 0.4130
F	 0.7100	 0.4230
G	 0.7190	 0.4200
H	 0.7230	 0.4230
I	 0.6990	 0.4170
J	 0.6430	 0.4020
K	 0.5900	 0.3950
L	 0.5110	 0.3650
M	 0.4360	 0.3370
N	 0.8890	 0.4710

