



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:55 AM UTC

PDB ID : 6QY3 / pdb_00006qy3
EMDB ID : EMD-4671
Title : Segment of the Cas1-Cas2-Csn2-DNA filament complex from the Type II-A CRISPR-Cas system
Authors : Wilkinson, M.; Drabavicius, G.; Silanskas, A.; Gasiunas, G.; Siksnys, V.; Wigley, D.B.
Deposited on : 2019-03-08
Resolution : 9.10 Å (reported)
Based on initial models : 6QXF, 6XQF

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

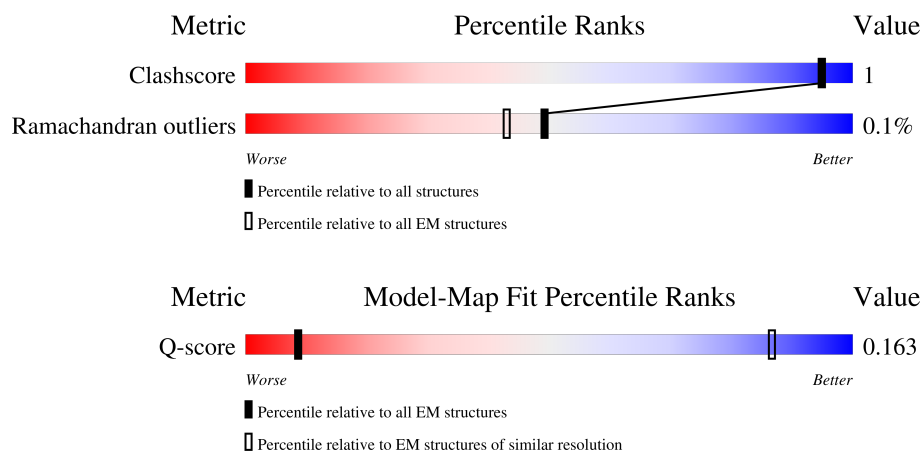
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 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.



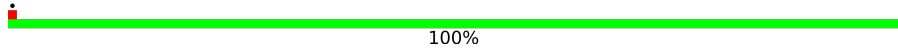
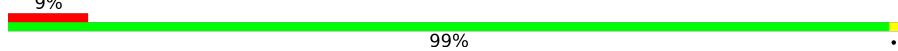
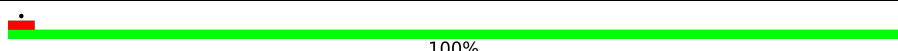
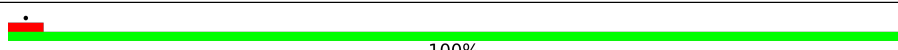
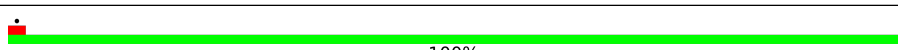
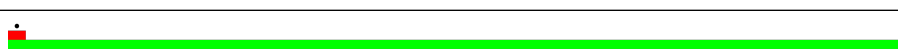
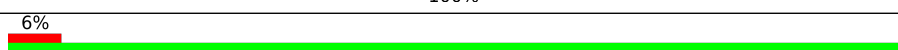
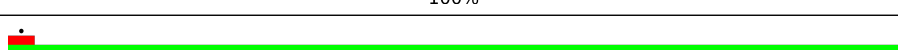
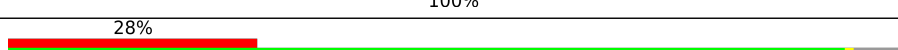
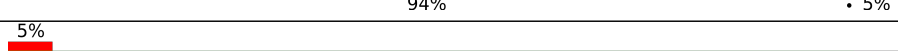
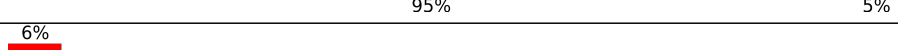
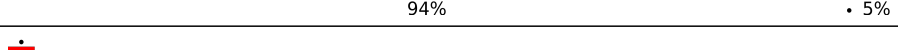
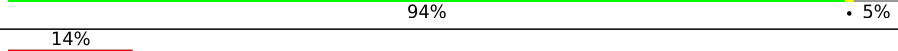
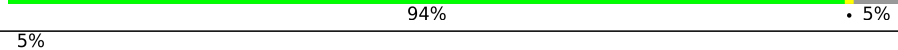
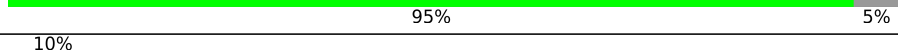
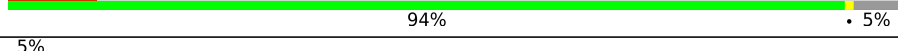
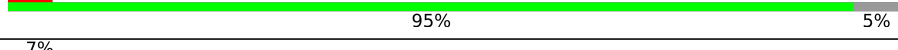
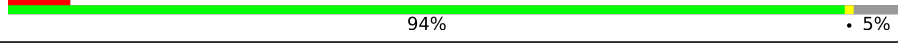
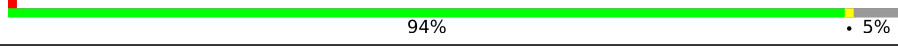
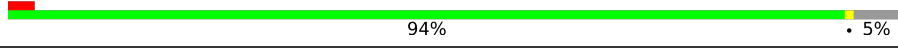
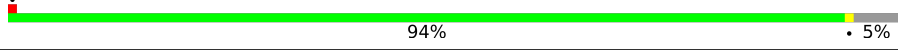
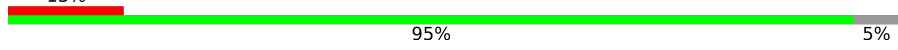
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	244 (8.60 - 9.60)

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	219	5% 100%
1	B	219	8% 100%
1	C	219	12% 100%
1	D	219	• 100%
1	E	219	5% 100%

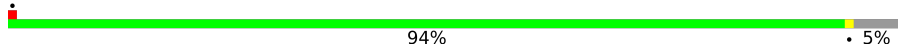
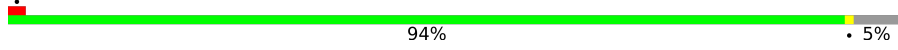
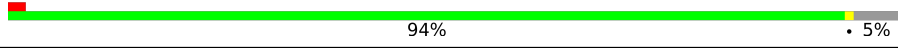
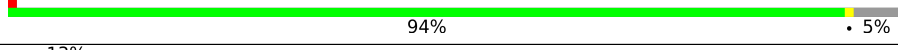
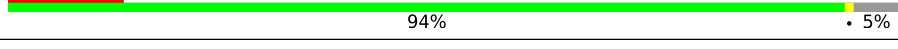
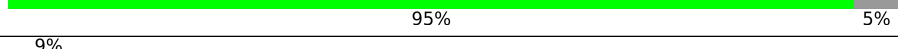
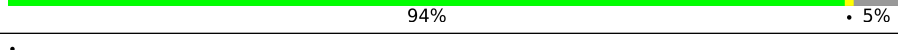
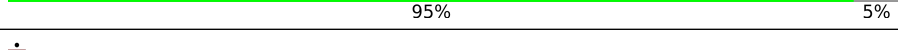
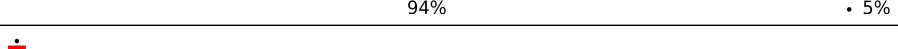
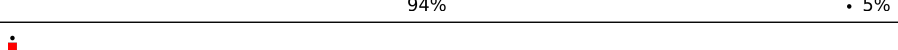
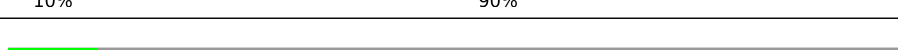
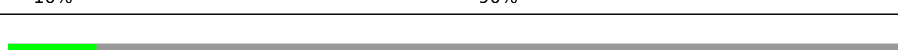
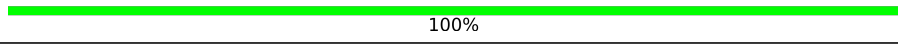
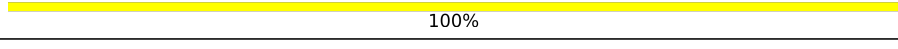
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Mol	Chain	Length	Quality of chain
1	F	219	
1	G	219	
1	H	219	
1	a	219	
1	b	219	
1	c	219	
1	d	219	
1	e	219	
1	f	219	
1	g	219	
1	h	219	
2	I	302	
2	J	302	
2	L	302	
2	M	302	
2	O	302	
2	P	302	
2	R	302	
2	S	302	
2	U	302	
2	V	302	
2	Y	302	
2	Z	302	
2	i	302	
2	j	302	

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Mol	Chain	Length	Quality of chain
2	l	302	
2	m	302	
2	o	302	
2	p	302	
2	r	302	
2	s	302	
2	u	302	
2	v	302	
2	y	302	
2	z	302	
3	K	114	
3	N	114	
3	Q	114	
3	T	114	
3	W	114	
3	X	114	
3	k	114	
3	n	114	
3	q	114	
3	t	114	
3	w	114	
3	x	114	
4	1	66	
5	2	66	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 54986 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 CRISPR-associated protein Csn2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	218	Total	C	N	O	0	0
			1086	650	218	218		
1	B	219	Total	C	N	O	0	0
			1091	653	219	219		
1	C	218	Total	C	N	O	0	0
			1086	650	218	218		
1	D	219	Total	C	N	O	0	0
			1091	653	219	219		
1	E	218	Total	C	N	O	0	0
			1086	650	218	218		
1	F	219	Total	C	N	O	0	0
			1091	653	219	219		
1	G	218	Total	C	N	O	0	0
			1086	650	218	218		
1	H	219	Total	C	N	O	0	0
			1091	653	219	219		
1	a	218	Total	C	N	O	0	0
			1086	650	218	218		
1	b	219	Total	C	N	O	0	0
			1091	653	219	219		
1	c	218	Total	C	N	O	0	0
			1086	650	218	218		
1	d	219	Total	C	N	O	0	0
			1091	653	219	219		
1	e	218	Total	C	N	O	0	0
			1086	650	218	218		
1	f	219	Total	C	N	O	0	0
			1091	653	219	219		
1	g	218	Total	C	N	O	0	0
			1086	650	218	218		
1	h	219	Total	C	N	O	0	0
			1091	653	219	219		

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	I	287	Total	C	N	O	0	0
			1425	851	287	287		
2	J	287	Total	C	N	O	0	0
			1425	851	287	287		
2	L	287	Total	C	N	O	0	0
			1425	851	287	287		
2	M	287	Total	C	N	O	0	0
			1425	851	287	287		
2	O	287	Total	C	N	O	0	0
			1425	851	287	287		
2	P	287	Total	C	N	O	0	0
			1425	851	287	287		
2	R	287	Total	C	N	O	0	0
			1425	851	287	287		
2	S	287	Total	C	N	O	0	0
			1425	851	287	287		
2	U	287	Total	C	N	O	0	0
			1425	851	287	287		
2	V	287	Total	C	N	O	0	0
			1425	851	287	287		
2	Y	287	Total	C	N	O	0	0
			1425	851	287	287		
2	Z	287	Total	C	N	O	0	0
			1425	851	287	287		
2	i	287	Total	C	N	O	0	0
			1425	851	287	287		
2	j	287	Total	C	N	O	0	0
			1425	851	287	287		
2	l	287	Total	C	N	O	0	0
			1425	851	287	287		
2	m	287	Total	C	N	O	0	0
			1425	851	287	287		
2	o	287	Total	C	N	O	0	0
			1425	851	287	287		
2	p	287	Total	C	N	O	0	0
			1425	851	287	287		
2	r	287	Total	C	N	O	0	0
			1425	851	287	287		
2	s	287	Total	C	N	O	0	0
			1425	851	287	287		
2	u	287	Total	C	N	O	0	0
			1425	851	287	287		
2	v	287	Total	C	N	O	0	0
			1425	851	287	287		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	y	287	Total	C	N	O	0	0
			1425	851	287	287		
2	z	287	Total	C	N	O	0	0
			1425	851	287	287		

There are 312 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	290	LEU	-	expression tag	UNP G3ECR2
I	291	GLU	-	expression tag	UNP G3ECR2
I	292	SER	-	expression tag	UNP G3ECR2
I	293	GLY	-	expression tag	UNP G3ECR2
I	294	TRP	-	expression tag	UNP G3ECR2
I	295	SER	-	expression tag	UNP G3ECR2
I	296	HIS	-	expression tag	UNP G3ECR2
I	297	PRO	-	expression tag	UNP G3ECR2
I	298	GLN	-	expression tag	UNP G3ECR2
I	299	PHE	-	expression tag	UNP G3ECR2
I	300	GLU	-	expression tag	UNP G3ECR2
I	301	LYS	-	expression tag	UNP G3ECR2
I	302	ALA	-	expression tag	UNP G3ECR2
J	290	LEU	-	expression tag	UNP G3ECR2
J	291	GLU	-	expression tag	UNP G3ECR2
J	292	SER	-	expression tag	UNP G3ECR2
J	293	GLY	-	expression tag	UNP G3ECR2
J	294	TRP	-	expression tag	UNP G3ECR2
J	295	SER	-	expression tag	UNP G3ECR2
J	296	HIS	-	expression tag	UNP G3ECR2
J	297	PRO	-	expression tag	UNP G3ECR2
J	298	GLN	-	expression tag	UNP G3ECR2
J	299	PHE	-	expression tag	UNP G3ECR2
J	300	GLU	-	expression tag	UNP G3ECR2
J	301	LYS	-	expression tag	UNP G3ECR2
J	302	ALA	-	expression tag	UNP G3ECR2
L	290	LEU	-	expression tag	UNP G3ECR2
L	291	GLU	-	expression tag	UNP G3ECR2
L	292	SER	-	expression tag	UNP G3ECR2
L	293	GLY	-	expression tag	UNP G3ECR2
L	294	TRP	-	expression tag	UNP G3ECR2
L	295	SER	-	expression tag	UNP G3ECR2
L	296	HIS	-	expression tag	UNP G3ECR2
L	297	PRO	-	expression tag	UNP G3ECR2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	298	GLN	-	expression tag	UNP G3ECR2
L	299	PHE	-	expression tag	UNP G3ECR2
L	300	GLU	-	expression tag	UNP G3ECR2
L	301	LYS	-	expression tag	UNP G3ECR2
L	302	ALA	-	expression tag	UNP G3ECR2
M	290	LEU	-	expression tag	UNP G3ECR2
M	291	GLU	-	expression tag	UNP G3ECR2
M	292	SER	-	expression tag	UNP G3ECR2
M	293	GLY	-	expression tag	UNP G3ECR2
M	294	TRP	-	expression tag	UNP G3ECR2
M	295	SER	-	expression tag	UNP G3ECR2
M	296	HIS	-	expression tag	UNP G3ECR2
M	297	PRO	-	expression tag	UNP G3ECR2
M	298	GLN	-	expression tag	UNP G3ECR2
M	299	PHE	-	expression tag	UNP G3ECR2
M	300	GLU	-	expression tag	UNP G3ECR2
M	301	LYS	-	expression tag	UNP G3ECR2
M	302	ALA	-	expression tag	UNP G3ECR2
O	290	LEU	-	expression tag	UNP G3ECR2
O	291	GLU	-	expression tag	UNP G3ECR2
O	292	SER	-	expression tag	UNP G3ECR2
O	293	GLY	-	expression tag	UNP G3ECR2
O	294	TRP	-	expression tag	UNP G3ECR2
O	295	SER	-	expression tag	UNP G3ECR2
O	296	HIS	-	expression tag	UNP G3ECR2
O	297	PRO	-	expression tag	UNP G3ECR2
O	298	GLN	-	expression tag	UNP G3ECR2
O	299	PHE	-	expression tag	UNP G3ECR2
O	300	GLU	-	expression tag	UNP G3ECR2
O	301	LYS	-	expression tag	UNP G3ECR2
O	302	ALA	-	expression tag	UNP G3ECR2
P	290	LEU	-	expression tag	UNP G3ECR2
P	291	GLU	-	expression tag	UNP G3ECR2
P	292	SER	-	expression tag	UNP G3ECR2
P	293	GLY	-	expression tag	UNP G3ECR2
P	294	TRP	-	expression tag	UNP G3ECR2
P	295	SER	-	expression tag	UNP G3ECR2
P	296	HIS	-	expression tag	UNP G3ECR2
P	297	PRO	-	expression tag	UNP G3ECR2
P	298	GLN	-	expression tag	UNP G3ECR2
P	299	PHE	-	expression tag	UNP G3ECR2
P	300	GLU	-	expression tag	UNP G3ECR2

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Chain	Residue	Modelled	Actual	Comment	Reference
P	301	LYS	-	expression tag	UNP G3ECR2
P	302	ALA	-	expression tag	UNP G3ECR2
R	290	LEU	-	expression tag	UNP G3ECR2
R	291	GLU	-	expression tag	UNP G3ECR2
R	292	SER	-	expression tag	UNP G3ECR2
R	293	GLY	-	expression tag	UNP G3ECR2
R	294	TRP	-	expression tag	UNP G3ECR2
R	295	SER	-	expression tag	UNP G3ECR2
R	296	HIS	-	expression tag	UNP G3ECR2
R	297	PRO	-	expression tag	UNP G3ECR2
R	298	GLN	-	expression tag	UNP G3ECR2
R	299	PHE	-	expression tag	UNP G3ECR2
R	300	GLU	-	expression tag	UNP G3ECR2
R	301	LYS	-	expression tag	UNP G3ECR2
R	302	ALA	-	expression tag	UNP G3ECR2
S	290	LEU	-	expression tag	UNP G3ECR2
S	291	GLU	-	expression tag	UNP G3ECR2
S	292	SER	-	expression tag	UNP G3ECR2
S	293	GLY	-	expression tag	UNP G3ECR2
S	294	TRP	-	expression tag	UNP G3ECR2
S	295	SER	-	expression tag	UNP G3ECR2
S	296	HIS	-	expression tag	UNP G3ECR2
S	297	PRO	-	expression tag	UNP G3ECR2
S	298	GLN	-	expression tag	UNP G3ECR2
S	299	PHE	-	expression tag	UNP G3ECR2
S	300	GLU	-	expression tag	UNP G3ECR2
S	301	LYS	-	expression tag	UNP G3ECR2
S	302	ALA	-	expression tag	UNP G3ECR2
U	290	LEU	-	expression tag	UNP G3ECR2
U	291	GLU	-	expression tag	UNP G3ECR2
U	292	SER	-	expression tag	UNP G3ECR2
U	293	GLY	-	expression tag	UNP G3ECR2
U	294	TRP	-	expression tag	UNP G3ECR2
U	295	SER	-	expression tag	UNP G3ECR2
U	296	HIS	-	expression tag	UNP G3ECR2
U	297	PRO	-	expression tag	UNP G3ECR2
U	298	GLN	-	expression tag	UNP G3ECR2
U	299	PHE	-	expression tag	UNP G3ECR2
U	300	GLU	-	expression tag	UNP G3ECR2
U	301	LYS	-	expression tag	UNP G3ECR2
U	302	ALA	-	expression tag	UNP G3ECR2
V	290	LEU	-	expression tag	UNP G3ECR2

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Chain	Residue	Modelled	Actual	Comment	Reference
V	291	GLU	-	expression tag	UNP G3ECR2
V	292	SER	-	expression tag	UNP G3ECR2
V	293	GLY	-	expression tag	UNP G3ECR2
V	294	TRP	-	expression tag	UNP G3ECR2
V	295	SER	-	expression tag	UNP G3ECR2
V	296	HIS	-	expression tag	UNP G3ECR2
V	297	PRO	-	expression tag	UNP G3ECR2
V	298	GLN	-	expression tag	UNP G3ECR2
V	299	PHE	-	expression tag	UNP G3ECR2
V	300	GLU	-	expression tag	UNP G3ECR2
V	301	LYS	-	expression tag	UNP G3ECR2
V	302	ALA	-	expression tag	UNP G3ECR2
Y	290	LEU	-	expression tag	UNP G3ECR2
Y	291	GLU	-	expression tag	UNP G3ECR2
Y	292	SER	-	expression tag	UNP G3ECR2
Y	293	GLY	-	expression tag	UNP G3ECR2
Y	294	TRP	-	expression tag	UNP G3ECR2
Y	295	SER	-	expression tag	UNP G3ECR2
Y	296	HIS	-	expression tag	UNP G3ECR2
Y	297	PRO	-	expression tag	UNP G3ECR2
Y	298	GLN	-	expression tag	UNP G3ECR2
Y	299	PHE	-	expression tag	UNP G3ECR2
Y	300	GLU	-	expression tag	UNP G3ECR2
Y	301	LYS	-	expression tag	UNP G3ECR2
Y	302	ALA	-	expression tag	UNP G3ECR2
Z	290	LEU	-	expression tag	UNP G3ECR2
Z	291	GLU	-	expression tag	UNP G3ECR2
Z	292	SER	-	expression tag	UNP G3ECR2
Z	293	GLY	-	expression tag	UNP G3ECR2
Z	294	TRP	-	expression tag	UNP G3ECR2
Z	295	SER	-	expression tag	UNP G3ECR2
Z	296	HIS	-	expression tag	UNP G3ECR2
Z	297	PRO	-	expression tag	UNP G3ECR2
Z	298	GLN	-	expression tag	UNP G3ECR2
Z	299	PHE	-	expression tag	UNP G3ECR2
Z	300	GLU	-	expression tag	UNP G3ECR2
Z	301	LYS	-	expression tag	UNP G3ECR2
Z	302	ALA	-	expression tag	UNP G3ECR2
i	290	LEU	-	expression tag	UNP G3ECR2
i	291	GLU	-	expression tag	UNP G3ECR2
i	292	SER	-	expression tag	UNP G3ECR2
i	293	GLY	-	expression tag	UNP G3ECR2

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Chain	Residue	Modelled	Actual	Comment	Reference
i	294	TRP	-	expression tag	UNP G3ECR2
i	295	SER	-	expression tag	UNP G3ECR2
i	296	HIS	-	expression tag	UNP G3ECR2
i	297	PRO	-	expression tag	UNP G3ECR2
i	298	GLN	-	expression tag	UNP G3ECR2
i	299	PHE	-	expression tag	UNP G3ECR2
i	300	GLU	-	expression tag	UNP G3ECR2
i	301	LYS	-	expression tag	UNP G3ECR2
i	302	ALA	-	expression tag	UNP G3ECR2
j	290	LEU	-	expression tag	UNP G3ECR2
j	291	GLU	-	expression tag	UNP G3ECR2
j	292	SER	-	expression tag	UNP G3ECR2
j	293	GLY	-	expression tag	UNP G3ECR2
j	294	TRP	-	expression tag	UNP G3ECR2
j	295	SER	-	expression tag	UNP G3ECR2
j	296	HIS	-	expression tag	UNP G3ECR2
j	297	PRO	-	expression tag	UNP G3ECR2
j	298	GLN	-	expression tag	UNP G3ECR2
j	299	PHE	-	expression tag	UNP G3ECR2
j	300	GLU	-	expression tag	UNP G3ECR2
j	301	LYS	-	expression tag	UNP G3ECR2
j	302	ALA	-	expression tag	UNP G3ECR2
l	290	LEU	-	expression tag	UNP G3ECR2
l	291	GLU	-	expression tag	UNP G3ECR2
l	292	SER	-	expression tag	UNP G3ECR2
l	293	GLY	-	expression tag	UNP G3ECR2
l	294	TRP	-	expression tag	UNP G3ECR2
l	295	SER	-	expression tag	UNP G3ECR2
l	296	HIS	-	expression tag	UNP G3ECR2
l	297	PRO	-	expression tag	UNP G3ECR2
l	298	GLN	-	expression tag	UNP G3ECR2
l	299	PHE	-	expression tag	UNP G3ECR2
l	300	GLU	-	expression tag	UNP G3ECR2
l	301	LYS	-	expression tag	UNP G3ECR2
l	302	ALA	-	expression tag	UNP G3ECR2
m	290	LEU	-	expression tag	UNP G3ECR2
m	291	GLU	-	expression tag	UNP G3ECR2
m	292	SER	-	expression tag	UNP G3ECR2
m	293	GLY	-	expression tag	UNP G3ECR2
m	294	TRP	-	expression tag	UNP G3ECR2
m	295	SER	-	expression tag	UNP G3ECR2
m	296	HIS	-	expression tag	UNP G3ECR2

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Chain	Residue	Modelled	Actual	Comment	Reference
m	297	PRO	-	expression tag	UNP G3ECR2
m	298	GLN	-	expression tag	UNP G3ECR2
m	299	PHE	-	expression tag	UNP G3ECR2
m	300	GLU	-	expression tag	UNP G3ECR2
m	301	LYS	-	expression tag	UNP G3ECR2
m	302	ALA	-	expression tag	UNP G3ECR2
o	290	LEU	-	expression tag	UNP G3ECR2
o	291	GLU	-	expression tag	UNP G3ECR2
o	292	SER	-	expression tag	UNP G3ECR2
o	293	GLY	-	expression tag	UNP G3ECR2
o	294	TRP	-	expression tag	UNP G3ECR2
o	295	SER	-	expression tag	UNP G3ECR2
o	296	HIS	-	expression tag	UNP G3ECR2
o	297	PRO	-	expression tag	UNP G3ECR2
o	298	GLN	-	expression tag	UNP G3ECR2
o	299	PHE	-	expression tag	UNP G3ECR2
o	300	GLU	-	expression tag	UNP G3ECR2
o	301	LYS	-	expression tag	UNP G3ECR2
o	302	ALA	-	expression tag	UNP G3ECR2
p	290	LEU	-	expression tag	UNP G3ECR2
p	291	GLU	-	expression tag	UNP G3ECR2
p	292	SER	-	expression tag	UNP G3ECR2
p	293	GLY	-	expression tag	UNP G3ECR2
p	294	TRP	-	expression tag	UNP G3ECR2
p	295	SER	-	expression tag	UNP G3ECR2
p	296	HIS	-	expression tag	UNP G3ECR2
p	297	PRO	-	expression tag	UNP G3ECR2
p	298	GLN	-	expression tag	UNP G3ECR2
p	299	PHE	-	expression tag	UNP G3ECR2
p	300	GLU	-	expression tag	UNP G3ECR2
p	301	LYS	-	expression tag	UNP G3ECR2
p	302	ALA	-	expression tag	UNP G3ECR2
r	290	LEU	-	expression tag	UNP G3ECR2
r	291	GLU	-	expression tag	UNP G3ECR2
r	292	SER	-	expression tag	UNP G3ECR2
r	293	GLY	-	expression tag	UNP G3ECR2
r	294	TRP	-	expression tag	UNP G3ECR2
r	295	SER	-	expression tag	UNP G3ECR2
r	296	HIS	-	expression tag	UNP G3ECR2
r	297	PRO	-	expression tag	UNP G3ECR2
r	298	GLN	-	expression tag	UNP G3ECR2
r	299	PHE	-	expression tag	UNP G3ECR2

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Chain	Residue	Modelled	Actual	Comment	Reference
r	300	GLU	-	expression tag	UNP G3ECR2
r	301	LYS	-	expression tag	UNP G3ECR2
r	302	ALA	-	expression tag	UNP G3ECR2
s	290	LEU	-	expression tag	UNP G3ECR2
s	291	GLU	-	expression tag	UNP G3ECR2
s	292	SER	-	expression tag	UNP G3ECR2
s	293	GLY	-	expression tag	UNP G3ECR2
s	294	TRP	-	expression tag	UNP G3ECR2
s	295	SER	-	expression tag	UNP G3ECR2
s	296	HIS	-	expression tag	UNP G3ECR2
s	297	PRO	-	expression tag	UNP G3ECR2
s	298	GLN	-	expression tag	UNP G3ECR2
s	299	PHE	-	expression tag	UNP G3ECR2
s	300	GLU	-	expression tag	UNP G3ECR2
s	301	LYS	-	expression tag	UNP G3ECR2
s	302	ALA	-	expression tag	UNP G3ECR2
u	290	LEU	-	expression tag	UNP G3ECR2
u	291	GLU	-	expression tag	UNP G3ECR2
u	292	SER	-	expression tag	UNP G3ECR2
u	293	GLY	-	expression tag	UNP G3ECR2
u	294	TRP	-	expression tag	UNP G3ECR2
u	295	SER	-	expression tag	UNP G3ECR2
u	296	HIS	-	expression tag	UNP G3ECR2
u	297	PRO	-	expression tag	UNP G3ECR2
u	298	GLN	-	expression tag	UNP G3ECR2
u	299	PHE	-	expression tag	UNP G3ECR2
u	300	GLU	-	expression tag	UNP G3ECR2
u	301	LYS	-	expression tag	UNP G3ECR2
u	302	ALA	-	expression tag	UNP G3ECR2
v	290	LEU	-	expression tag	UNP G3ECR2
v	291	GLU	-	expression tag	UNP G3ECR2
v	292	SER	-	expression tag	UNP G3ECR2
v	293	GLY	-	expression tag	UNP G3ECR2
v	294	TRP	-	expression tag	UNP G3ECR2
v	295	SER	-	expression tag	UNP G3ECR2
v	296	HIS	-	expression tag	UNP G3ECR2
v	297	PRO	-	expression tag	UNP G3ECR2
v	298	GLN	-	expression tag	UNP G3ECR2
v	299	PHE	-	expression tag	UNP G3ECR2
v	300	GLU	-	expression tag	UNP G3ECR2
v	301	LYS	-	expression tag	UNP G3ECR2
v	302	ALA	-	expression tag	UNP G3ECR2

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Chain	Residue	Modelled	Actual	Comment	Reference
y	290	LEU	-	expression tag	UNP G3ECR2
y	291	GLU	-	expression tag	UNP G3ECR2
y	292	SER	-	expression tag	UNP G3ECR2
y	293	GLY	-	expression tag	UNP G3ECR2
y	294	TRP	-	expression tag	UNP G3ECR2
y	295	SER	-	expression tag	UNP G3ECR2
y	296	HIS	-	expression tag	UNP G3ECR2
y	297	PRO	-	expression tag	UNP G3ECR2
y	298	GLN	-	expression tag	UNP G3ECR2
y	299	PHE	-	expression tag	UNP G3ECR2
y	300	GLU	-	expression tag	UNP G3ECR2
y	301	LYS	-	expression tag	UNP G3ECR2
y	302	ALA	-	expression tag	UNP G3ECR2
z	290	LEU	-	expression tag	UNP G3ECR2
z	291	GLU	-	expression tag	UNP G3ECR2
z	292	SER	-	expression tag	UNP G3ECR2
z	293	GLY	-	expression tag	UNP G3ECR2
z	294	TRP	-	expression tag	UNP G3ECR2
z	295	SER	-	expression tag	UNP G3ECR2
z	296	HIS	-	expression tag	UNP G3ECR2
z	297	PRO	-	expression tag	UNP G3ECR2
z	298	GLN	-	expression tag	UNP G3ECR2
z	299	PHE	-	expression tag	UNP G3ECR2
z	300	GLU	-	expression tag	UNP G3ECR2
z	301	LYS	-	expression tag	UNP G3ECR2
z	302	ALA	-	expression tag	UNP G3ECR2

- Molecule 3 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	11	Total	C	N	O	0	0
			54	32	11	11		
3	N	11	Total	C	N	O	0	0
			54	32	11	11		
3	Q	11	Total	C	N	O	0	0
			54	32	11	11		
3	T	11	Total	C	N	O	0	0
			54	32	11	11		
3	W	11	Total	C	N	O	0	0
			54	32	11	11		
3	X	11	Total	C	N	O	0	0
			54	32	11	11		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	k	11	Total	C	N	O	0	0
			54	32	11	11		
3	n	11	Total	C	N	O	0	0
			54	32	11	11		
3	q	11	Total	C	N	O	0	0
			54	32	11	11		
3	t	11	Total	C	N	O	0	0
			54	32	11	11		
3	w	11	Total	C	N	O	0	0
			54	32	11	11		
3	x	11	Total	C	N	O	0	0
			54	32	11	11		

- Molecule 4 is a DNA chain called DNA (66-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	66	Total	C	N	O	P	0	0
			1320	660	132	462	66		

- Molecule 5 is a DNA chain called DNA (66-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	66	Total	C	N	O	P	0	0
			1386	660	330	330	66		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Ca	0
			2	2	
6	B	2	Total	Ca	0
			2	2	
6	E	2	Total	Ca	0
			2	2	
6	F	2	Total	Ca	0
			2	2	
6	a	2	Total	Ca	0
			2	2	
6	b	2	Total	Ca	0
			2	2	
6	e	2	Total	Ca	0
			2	2	

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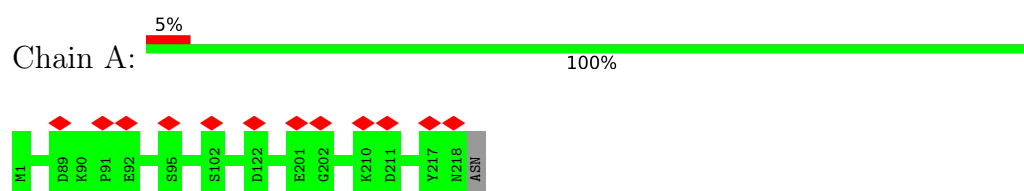
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Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
6	f	2	2	2	0

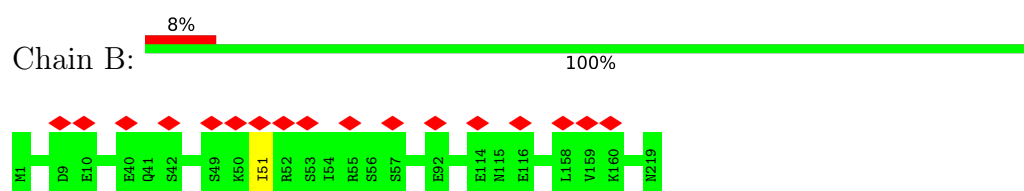
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

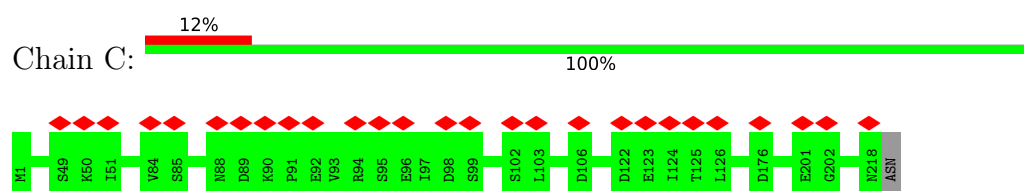
- Molecule 1: CRISPR-associated protein Csn2



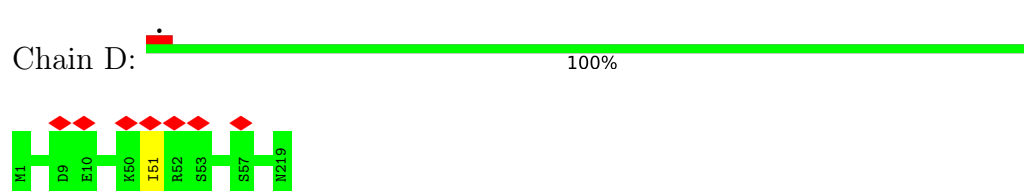
- Molecule 1: CRISPR-associated protein Csn2



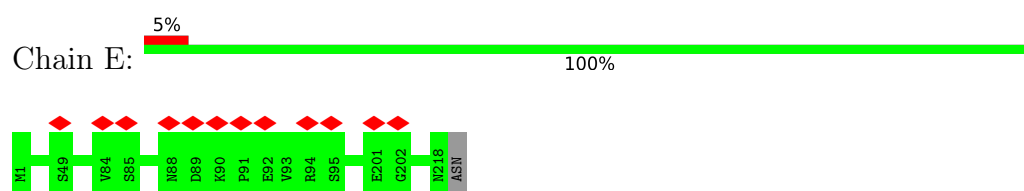
- Molecule 1: CRISPR-associated protein Csn2



- Molecule 1: CRISPR-associated protein Csn2



- Molecule 1: CRISPR-associated protein Csn2



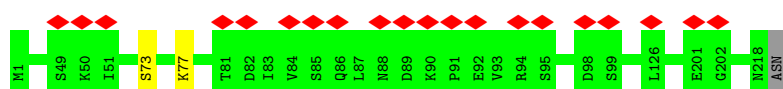
- Molecule 1: CRISPR-associated protein Csn2

Chain F:  100%



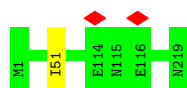
- Molecule 1: CRISPR-associated protein Csn2

Chain G:  9% 99%

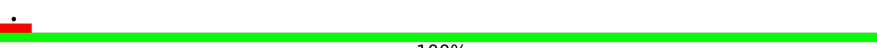


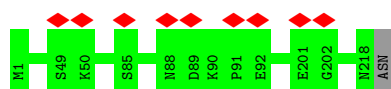
- Molecule 1: CRISPR-associated protein Csn2

Chain H:  100%



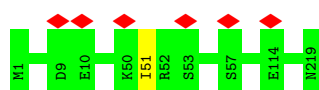
- Molecule 1: CRISPR-associated protein Csn2

Chain a:  100%

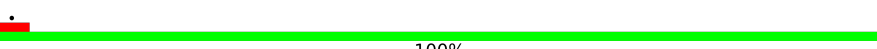


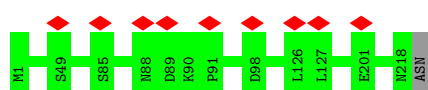
- Molecule 1: CRISPR-associated protein Csn2

Chain b:  100%



- Molecule 1: CRISPR-associated protein Csn2

Chain c:  100%

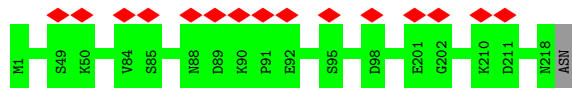


- Molecule 1: CRISPR-associated protein Csn2

Chain d:  100%



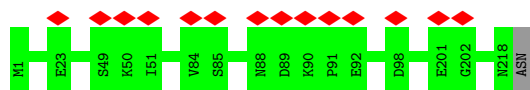
- Molecule 1: CRISPR-associated protein Csn2



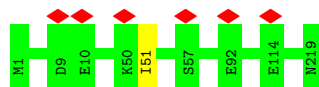
- Molecule 1: CRISPR-associated protein Csn2



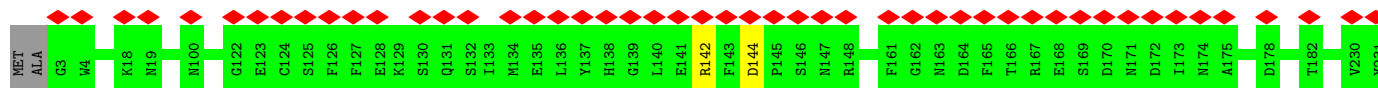
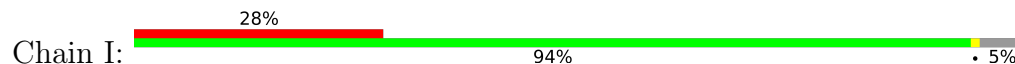
- Molecule 1: CRISPR-associated protein Csn2



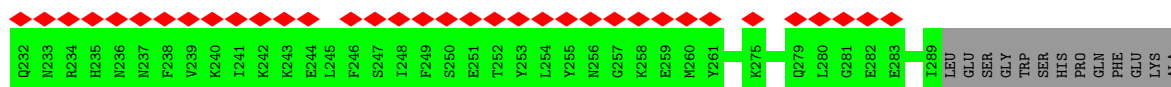
- Molecule 1: CRISPR-associated protein Csn2

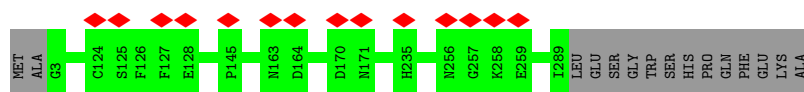


- Molecule 2: CRISPR-associated endonuclease Cas1

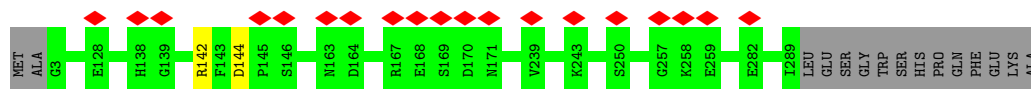


- Molecule 2: CRISPR-associated endonuclease Cas1

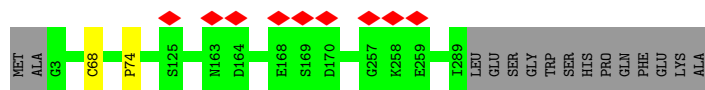




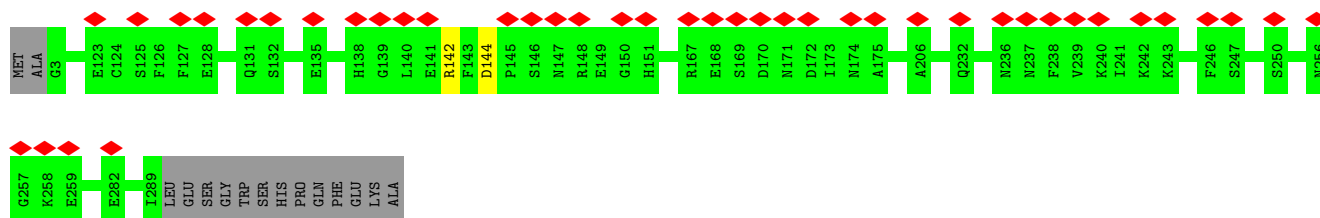
- Molecule 2: CRISPR-associated endonuclease Cas1



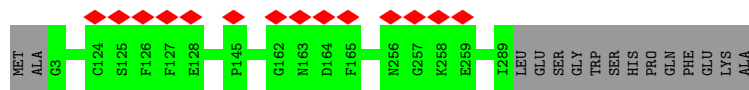
- Molecule 2: CRISPR-associated endonuclease Cas1



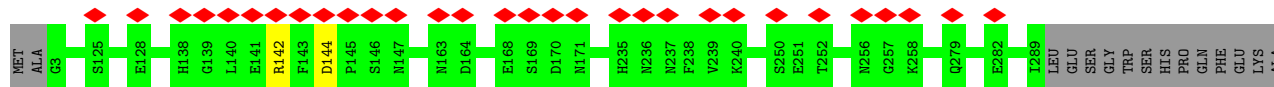
- Molecule 2: CRISPR-associated endonuclease Cas1



- Molecule 2: CRISPR-associated endonuclease Cas1

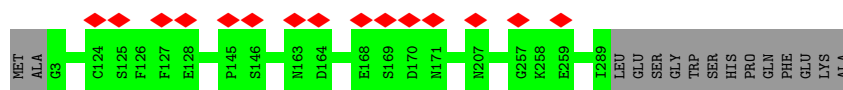


- Molecule 2: CRISPR-associated endonuclease Cas1

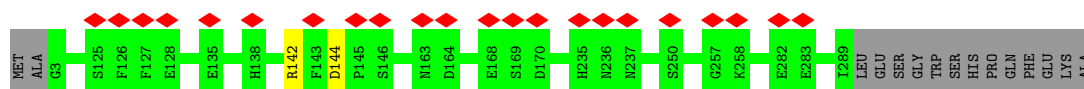


- Molecule 2: CRISPR-associated endonuclease Cas1

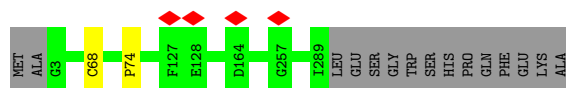




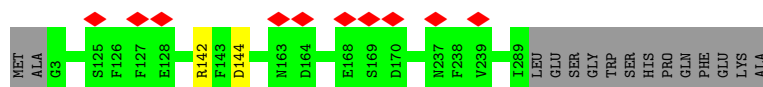
- Molecule 2: CRISPR-associated endonuclease Cas1



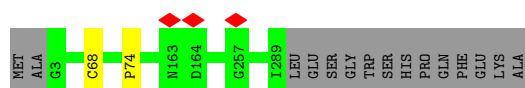
- Molecule 2: CRISPR-associated endonuclease Cas1



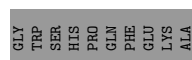
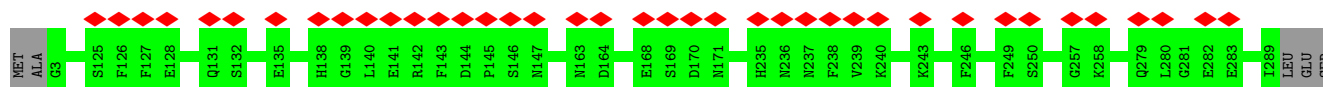
- Molecule 2: CRISPR-associated endonuclease Cas1



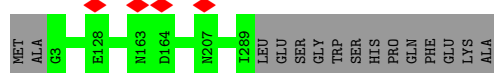
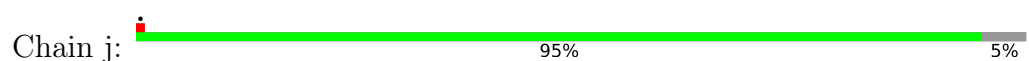
- Molecule 2: CRISPR-associated endonuclease Cas1



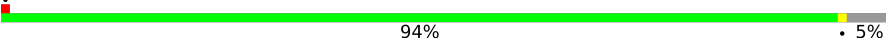
- Molecule 2: CRISPR-associated endonuclease Cas1

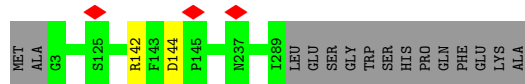


- Molecule 2: CRISPR-associated endonuclease Cas1

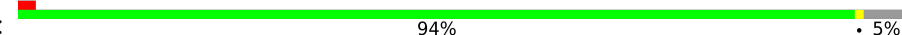


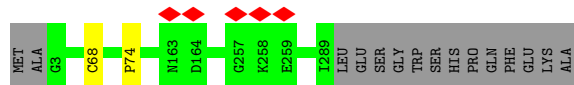
- Molecule 2: CRISPR-associated endonuclease Cas1

Chain l:  94% • 5%

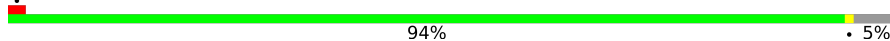


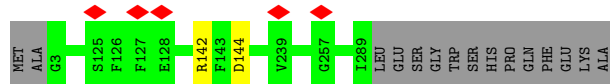
- Molecule 2: CRISPR-associated endonuclease Cas1

Chain m:  94% • 5%

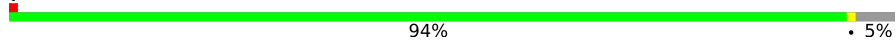


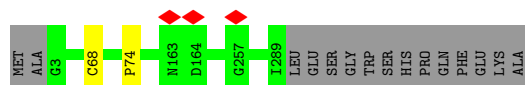
- Molecule 2: CRISPR-associated endonuclease Cas1

Chain o:  94% • 5%

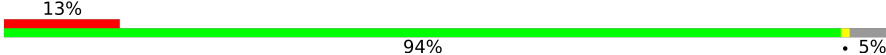


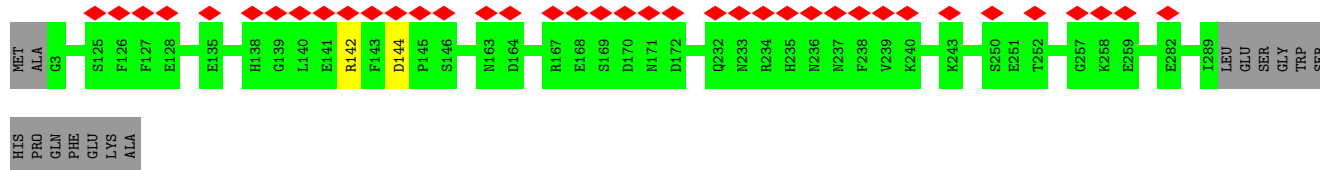
- Molecule 2: CRISPR-associated endonuclease Cas1

Chain p:  94% • 5%

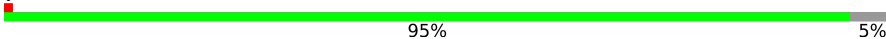


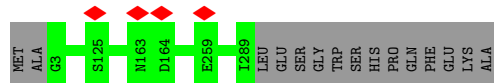
- Molecule 2: CRISPR-associated endonuclease Cas1

Chain r:  13% 94% • 5%

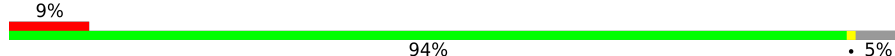


- Molecule 2: CRISPR-associated endonuclease Cas1

Chain s:  95% 5%



- Molecule 2: CRISPR-associated endonuclease Cas1

Chain u:  9% 94% • 5%

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

ARG LEU LYS ALA ASN PRO LYS GLY MET ASN ILE THR ILE LEU THR VAL THR THR GLU GLN PHE ARG LYS ALA ARG MET ILE TYR LEU PHE ARG LYS GLY ASP PHE LEU ASN THR SER GLU ILE ALA ASN SER E100 Y110 CYS ASP ASP

• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain T: 10% 90%

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

ARG LEU LYS ALA ASN PRO LYS GLY MET ASN ILE THR ILE LEU THR VAL THR THR GLU GLN PHE ARG LYS ALA ARG MET ILE TYR LEU PHE ARG LYS GLY ASP PHE LEU ASN THR SER GLU ILE ALA ASN SER E100 Y110 CYS ASP GLU ASP

• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain W: 10% 90%

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

ARG LEU LYS ALA ASN PRO LYS GLY MET ASN ILE THR ILE LEU THR VAL THR THR GLU GLN PHE ARG LYS ALA ARG MET ILE TYR LEU PHE ARG LYS GLY ASP PHE LEU ASN THR SER GLU ILE ALA ASN SER E100 Y110 CYS ASP GLU ASP

• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain X: 10% 90%

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

ARG LEU LYS ALA ASN PRO LYS GLY MET ASN ILE THR ILE LEU THR VAL THR THR GLU GLN PHE ARG LYS ALA ARG MET ILE TYR LEU PHE ARG LYS GLY ASP PHE LEU ASN THR SER GLU ILE ALA ASN SER E100 Y110 CYS ASP GLU ASP

• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain k: 10% 90%

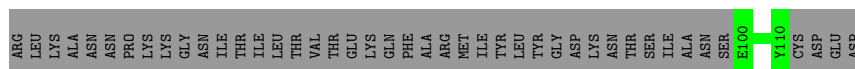
MET SER TYR ARG TYR MET ARG MET ILE LEU MET MET PHE ASP MET PRO THR ASP THR ALA GLU GLU ARG LYS LYS ALA ARG TYR ARG PHE LEU LEU PHE LEU MET HIS GLN PHE SER VAL TYR SER LYS LEU LEU LEU ASN HIS THR ALA ALA THR THR ALA MET VAL VAL GLY

ARG LEU LYS ALA ASN PRO LYS GLY MET ASN ILE THR ILE LEU THR VAL THR THR GLU GLN PHE ARG LYS ALA ARG MET ILE TYR LEU PHE ARG LYS GLY ASP PHE LEU ASN THR SER GLU ILE ALA ASN SER E100 Y110 CYS ASP GLU ASP

• Molecule 3: CRISPR-associated endoribonuclease Cas2

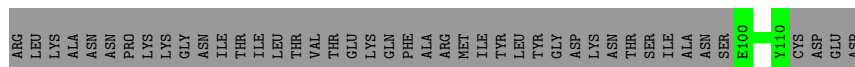
Chain n: 10% 90%

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



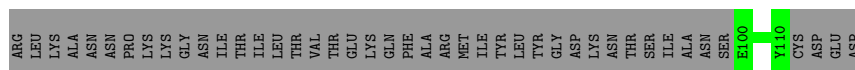
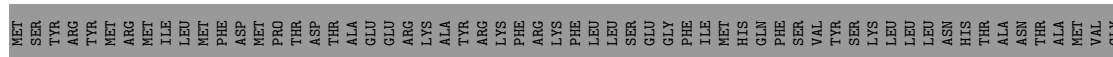
- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain q: 10% 90%



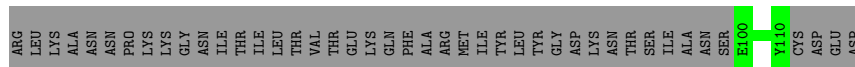
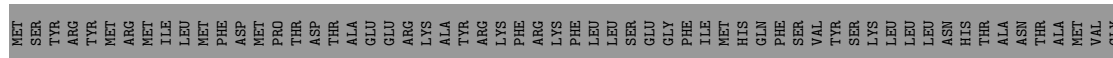
- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain t: 10% 90%



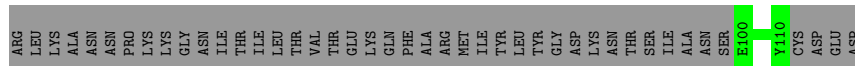
- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain w: 10% 90%



- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain x: 10% 90%



- Molecule 4: DNA (66-MER)

Chain 1: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: DNA (66-MER)

Chain 2: 100%

A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13	A14	A15	A16	A17	A18	A19	A20	A21	A22	A23	A24	A25	A26	A27	A28	A29	A30	A31	A32	A33	A34	A35	A36	A37	A38	A39	A40	A41	A42	A43	A44	A45	A46	A47	A48	A49	A50	A51	A52	A53	A54	A55	A56	A57	A58	A59	A60
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A61	A62	A63	A64	A65	A66
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66576	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 ($e^-/\text{\AA}^2$)	92.8	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	129032	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.015	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	355.88, 355.88, 355.88	wwPDB
Map dimensions	328, 328, 328	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.07	0/1085	0.24	0/1515
1	B	0.07	0/1090	0.27	0/1522
1	C	0.07	0/1085	0.24	0/1515
1	D	0.07	0/1090	0.27	0/1522
1	E	0.07	0/1085	0.24	0/1515
1	F	0.07	0/1090	0.27	0/1522
1	G	0.18	0/1085	0.31	0/1515
1	H	0.07	0/1090	0.27	0/1522
1	a	0.07	0/1085	0.23	0/1515
1	b	0.07	0/1090	0.27	0/1522
1	c	0.07	0/1085	0.24	0/1515
1	d	0.07	0/1090	0.27	0/1522
1	e	0.07	0/1085	0.24	0/1515
1	f	0.07	0/1090	0.27	0/1522
1	g	0.07	0/1085	0.24	0/1515
1	h	0.07	0/1090	0.27	0/1522
2	I	0.08	0/1424	0.29	0/1986
2	J	0.08	0/1424	0.26	0/1986
2	L	0.08	0/1424	0.29	0/1986
2	M	0.08	0/1424	0.26	0/1986
2	O	0.08	0/1424	0.29	0/1986
2	P	0.08	0/1424	0.26	0/1986
2	R	0.08	0/1424	0.29	0/1986
2	S	0.08	0/1424	0.26	0/1986
2	U	0.08	0/1424	0.29	0/1986
2	V	0.08	0/1424	0.26	0/1986
2	Y	0.08	0/1424	0.29	0/1986
2	Z	0.08	0/1424	0.26	0/1986
2	i	0.08	0/1424	0.29	0/1986
2	j	0.08	0/1424	0.26	0/1986
2	l	0.08	0/1424	0.29	0/1986
2	m	0.08	0/1424	0.26	0/1986

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	o	0.08	0/1424	0.29	0/1986
2	p	0.08	0/1424	0.26	0/1986
2	r	0.08	0/1424	0.29	0/1986
2	s	0.08	0/1424	0.26	0/1986
2	u	0.08	0/1424	0.29	0/1986
2	v	0.08	0/1424	0.26	0/1986
2	y	0.08	0/1424	0.29	0/1986
2	z	0.08	0/1424	0.26	0/1986
3	K	0.10	0/53	0.27	0/72
3	N	0.11	0/53	0.27	0/72
3	Q	0.10	0/53	0.27	0/72
3	T	0.10	0/53	0.27	0/72
3	W	0.11	0/53	0.28	0/72
3	X	0.11	0/53	0.27	0/72
3	k	0.10	0/53	0.27	0/72
3	n	0.10	0/53	0.27	0/72
3	q	0.10	0/53	0.27	0/72
3	t	0.10	0/53	0.27	0/72
3	w	0.10	0/53	0.28	0/72
3	x	0.10	0/53	0.27	0/72
4	1	0.25	0/1451	0.61	0/2240
5	2	0.17	0/1583	0.36	0/2438
All	All	0.09	0/55246	0.29	0/77502

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1086	0	450	0	0
1	B	1091	0	452	0	0
1	C	1086	0	450	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1091	0	452	0	0
1	E	1086	0	450	0	0
1	F	1091	0	452	0	0
1	G	1086	0	450	1	0
1	H	1091	0	452	0	0
1	a	1086	0	450	0	0
1	b	1091	0	452	0	0
1	c	1086	0	450	0	0
1	d	1091	0	452	0	0
1	e	1086	0	450	0	0
1	f	1091	0	452	0	0
1	g	1086	0	450	0	0
1	h	1091	0	452	0	0
2	I	1425	0	616	1	0
2	J	1425	0	616	0	0
2	L	1425	0	616	1	0
2	M	1425	0	616	1	0
2	O	1425	0	616	1	0
2	P	1425	0	616	0	0
2	R	1425	0	616	1	0
2	S	1425	0	616	0	0
2	U	1425	0	616	1	0
2	V	1425	0	616	1	0
2	Y	1425	0	616	1	0
2	Z	1425	0	616	1	0
2	i	1425	0	616	0	0
2	j	1425	0	616	0	0
2	l	1425	0	616	1	0
2	m	1425	0	616	1	0
2	o	1425	0	616	1	0
2	p	1425	0	616	1	0
2	r	1425	0	616	1	0
2	s	1425	0	616	0	0
2	u	1425	0	616	1	0
2	v	1425	0	616	0	0
2	y	1425	0	616	1	0
2	z	1425	0	616	1	0
3	K	54	0	22	0	0
3	N	54	0	22	0	0
3	Q	54	0	22	0	0
3	T	54	0	22	0	0
3	W	54	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	54	0	22	0	0
3	k	54	0	22	0	0
3	n	54	0	22	0	0
3	q	54	0	22	0	0
3	t	54	0	22	0	0
3	w	54	0	22	0	0
3	x	54	0	22	0	0
4	1	1320	0	793	0	0
5	2	1386	0	727	65	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	a	2	0	0	0	0
6	b	2	0	0	0	0
6	e	2	0	0	0	0
6	f	2	0	0	0	0
All	All	54986	0	23784	83	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 1.

All (83) 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)
5:2:35:DA:H2''	5:2:36:DA:C8	2.36	0.61
5:2:15:DA:H2''	5:2:16:DA:C8	2.37	0.60
5:2:34:DA:H2''	5:2:35:DA:C8	2.37	0.59
5:2:44:DA:H2''	5:2:45:DA:C8	2.38	0.59
5:2:45:DA:H2''	5:2:46:DA:C8	2.39	0.58
5:2:27:DA:H2''	5:2:28:DA:C8	2.38	0.57
5:2:24:DA:H2''	5:2:25:DA:C8	2.39	0.57
5:2:25:DA:H2''	5:2:26:DA:C8	2.40	0.57
5:2:32:DA:H2''	5:2:33:DA:C8	2.40	0.56
5:2:33:DA:H2''	5:2:34:DA:C8	2.39	0.56
5:2:11:DA:H2''	5:2:12:DA:C8	2.40	0.56
5:2:28:DA:H2''	5:2:29:DA:C8	2.39	0.56
5:2:43:DA:H2''	5:2:44:DA:C8	2.41	0.56
5:2:56:DA:H2''	5:2:57:DA:C8	2.41	0.56
5:2:8:DA:H2''	5:2:9:DA:C8	2.41	0.56
5:2:7:DA:H2''	5:2:8:DA:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:52:DA:H2''	5:2:53:DA:C8	2.40	0.56
5:2:9:DA:H2''	5:2:10:DA:C8	2.41	0.56
5:2:57:DA:H2''	5:2:58:DA:C8	2.41	0.56
5:2:61:DA:H2''	5:2:62:DA:C8	2.41	0.56
5:2:51:DA:H2''	5:2:52:DA:C8	2.41	0.56
5:2:38:DA:H2''	5:2:39:DA:C8	2.40	0.55
5:2:10:DA:H2''	5:2:11:DA:C8	2.42	0.55
5:2:39:DA:H2''	5:2:40:DA:C8	2.41	0.55
5:2:49:DA:H2''	5:2:50:DA:C8	2.41	0.55
5:2:29:DA:H2''	5:2:30:DA:C8	2.41	0.55
5:2:40:DA:H2''	5:2:41:DA:C8	2.41	0.55
5:2:18:DA:H2''	5:2:19:DA:C8	2.41	0.55
5:2:21:DA:H2''	5:2:22:DA:C8	2.41	0.55
5:2:31:DA:H2''	5:2:32:DA:C8	2.41	0.55
5:2:50:DA:H2''	5:2:51:DA:C8	2.42	0.55
5:2:53:DA:H2''	5:2:54:DA:C8	2.41	0.55
5:2:60:DA:H2''	5:2:61:DA:C8	2.41	0.55
5:2:59:DA:H2''	5:2:60:DA:C8	2.42	0.55
5:2:22:DA:H2''	5:2:23:DA:C8	2.41	0.54
5:2:5:DA:H2''	5:2:6:DA:C8	2.42	0.54
5:2:23:DA:H2''	5:2:24:DA:C8	2.42	0.54
5:2:4:DA:H2''	5:2:5:DA:C8	2.42	0.54
5:2:58:DA:H2''	5:2:59:DA:C8	2.42	0.54
5:2:6:DA:H2''	5:2:7:DA:C8	2.42	0.54
5:2:54:DA:H2''	5:2:55:DA:C8	2.42	0.54
5:2:55:DA:H2''	5:2:56:DA:C8	2.43	0.54
5:2:62:DA:H2''	5:2:63:DA:C8	2.42	0.54
5:2:3:DA:H2''	5:2:4:DA:C8	2.43	0.54
5:2:19:DA:H2''	5:2:20:DA:C8	2.43	0.54
5:2:30:DA:H2''	5:2:31:DA:C8	2.42	0.54
5:2:20:DA:H2''	5:2:21:DA:C8	2.43	0.54
5:2:12:DA:H2''	5:2:13:DA:C8	2.43	0.54
5:2:48:DA:H2''	5:2:49:DA:C8	2.42	0.53
5:2:41:DA:H2''	5:2:42:DA:C8	2.43	0.53
5:2:42:DA:H2''	5:2:43:DA:C8	2.44	0.52
5:2:2:DA:H2''	5:2:3:DA:C8	2.45	0.52
5:2:37:DA:H2''	5:2:38:DA:C8	2.45	0.51
5:2:46:DA:H2''	5:2:47:DA:C8	2.45	0.51
5:2:13:DA:H2''	5:2:14:DA:C8	2.46	0.51
5:2:36:DA:H2''	5:2:37:DA:C8	2.47	0.50
5:2:14:DA:H2''	5:2:15:DA:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:47:DA:H2''	5:2:48:DA:C8	2.47	0.50
5:2:63:DA:H2''	5:2:64:DA:C8	2.47	0.49
5:2:26:DA:H2''	5:2:27:DA:C8	2.48	0.49
5:2:65:DA:H2''	5:2:66:DA:C8	2.49	0.47
5:2:1:DA:H2''	5:2:2:DA:C8	2.50	0.47
5:2:64:DA:H2''	5:2:65:DA:C8	2.50	0.46
5:2:16:DA:H2''	5:2:17:DA:C8	2.50	0.46
5:2:17:DA:H2''	5:2:18:DA:C8	2.54	0.43
2:U:142:ARG:C	2:U:144:ASP:H	2.28	0.42
2:R:142:ARG:C	2:R:144:ASP:H	2.28	0.42
2:u:142:ARG:C	2:u:144:ASP:H	2.28	0.42
2:r:142:ARG:C	2:r:144:ASP:H	2.28	0.41
2:L:142:ARG:C	2:L:144:ASP:H	2.28	0.41
2:l:142:ARG:C	2:l:144:ASP:H	2.28	0.41
2:Y:142:ARG:C	2:Y:144:ASP:H	2.28	0.41
1:G:73:SER:O	1:G:77:LYS:CB	2.69	0.41
2:y:142:ARG:C	2:y:144:ASP:H	2.28	0.41
2:M:68:CYS:HA	2:M:74:PRO:HA	2.03	0.41
2:O:142:ARG:C	2:O:144:ASP:H	2.28	0.41
2:m:68:CYS:HA	2:m:74:PRO:HA	2.03	0.41
2:I:142:ARG:C	2:I:144:ASP:H	2.28	0.41
2:o:142:ARG:C	2:o:144:ASP:H	2.28	0.40
2:Z:68:CYS:HA	2:Z:74:PRO:HA	2.03	0.40
2:V:68:CYS:HA	2:V:74:PRO:HA	2.03	0.40
2:z:68:CYS:HA	2:z:74:PRO:HA	2.03	0.40
2:p:68:CYS:HA	2:p:74:PRO:HA	2.03	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	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	B	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	24	63
1	C	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	D	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	24	63
1	E	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	F	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	24	63
1	G	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	H	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	24	63
1	a	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	b	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	24	63
1	c	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	d	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	24	63
1	e	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	f	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	24	63
1	g	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	h	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	24	63
2	I	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	J	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
2	L	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	M	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	O	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	P	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	R	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	S	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	U	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	V	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
2	Y	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	Z	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	i	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	j	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	l	285/302 (94%)	277 (97%)	8 (3%)	0	100	100
2	m	285/302 (94%)	280 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	o	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	p	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
2	r	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	s	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	u	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	v	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
2	y	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	z	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
3	K	9/114 (8%)	9 (100%)	0	0	100	100
3	N	9/114 (8%)	9 (100%)	0	0	100	100
3	Q	9/114 (8%)	9 (100%)	0	0	100	100
3	T	9/114 (8%)	9 (100%)	0	0	100	100
3	W	9/114 (8%)	9 (100%)	0	0	100	100
3	X	9/114 (8%)	9 (100%)	0	0	100	100
3	k	9/114 (8%)	9 (100%)	0	0	100	100
3	n	9/114 (8%)	9 (100%)	0	0	100	100
3	q	9/114 (8%)	9 (100%)	0	0	100	100
3	t	9/114 (8%)	9 (100%)	0	0	100	100
3	w	9/114 (8%)	9 (100%)	0	0	100	100
3	x	9/114 (8%)	9 (100%)	0	0	100	100
All	All	10412/12120 (86%)	10162 (98%)	242 (2%)	8 (0%)	49	83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	ILE
1	D	51	ILE
1	F	51	ILE
1	H	51	ILE
1	b	51	ILE
1	d	51	ILE
1	f	51	ILE
1	h	51	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

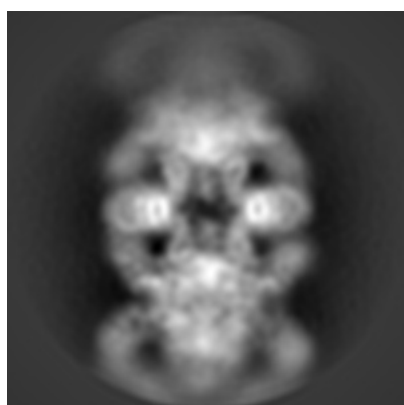
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4671. These allow visual inspection of the internal detail of the map and identification of artifacts.

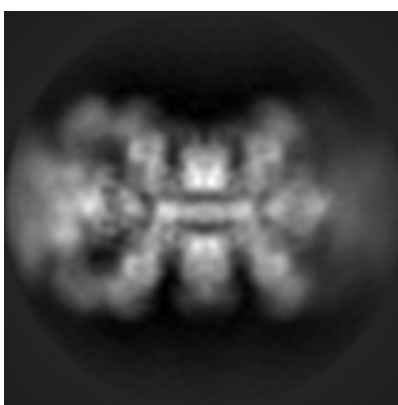
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

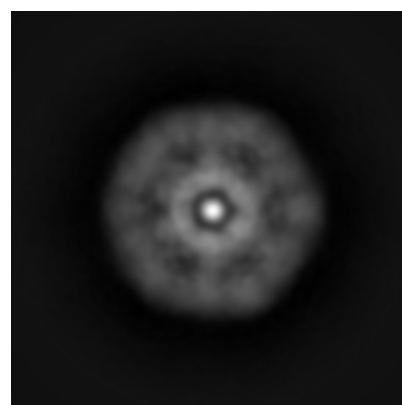
6.1.1 Primary map



X



Y

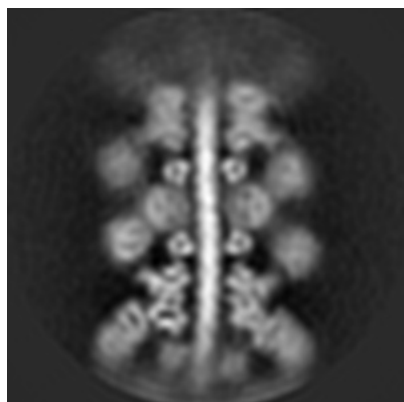


Z

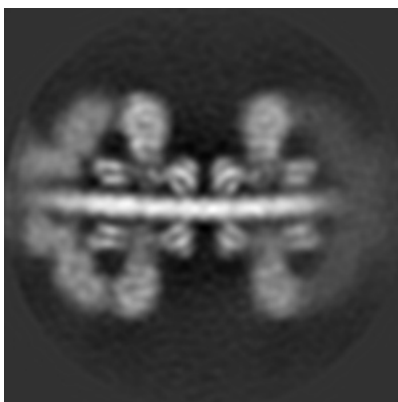
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

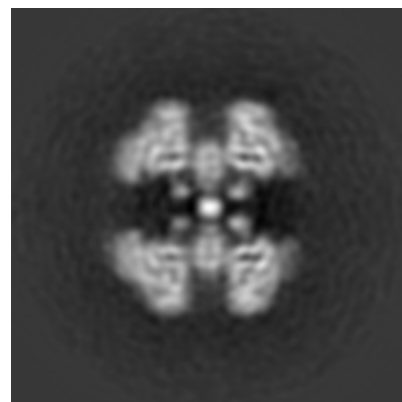
6.2.1 Primary map



X Index: 164



Y Index: 164

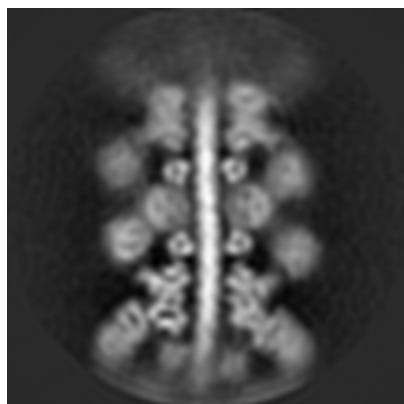


Z Index: 164

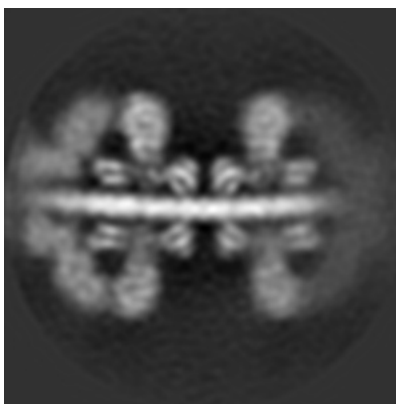
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

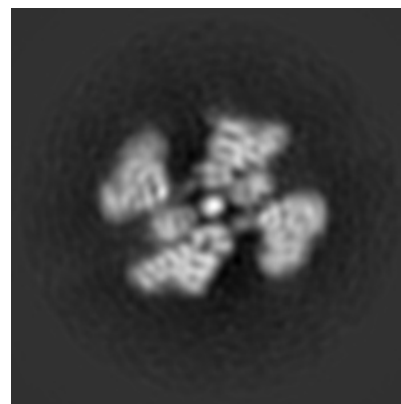
6.3.1 Primary map



X Index: 164



Y Index: 164

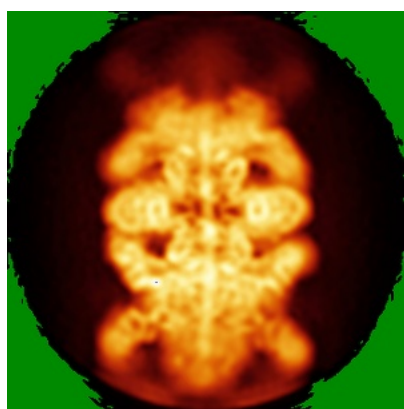


Z Index: 106

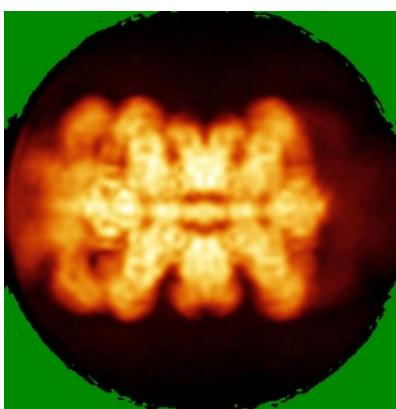
The images above show the largest variance slices of the map in three orthogonal directions.

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

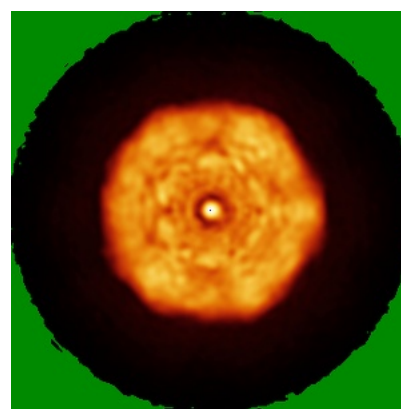
6.4.1 Primary map



X



Y



Z

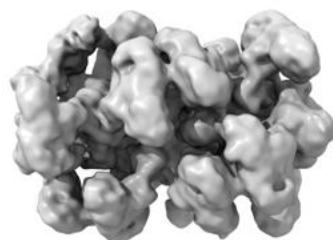
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

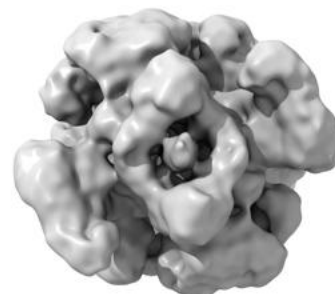
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

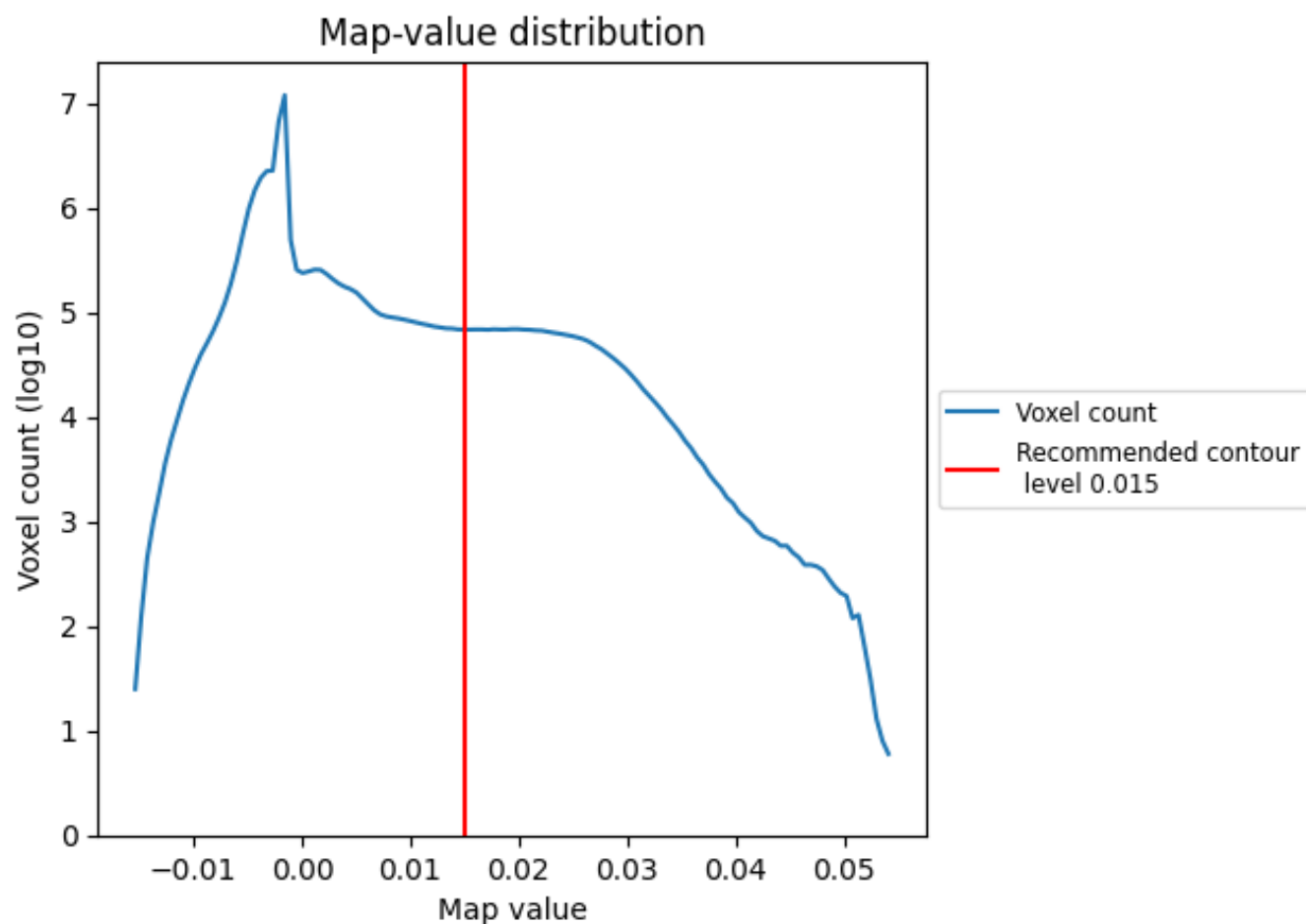
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

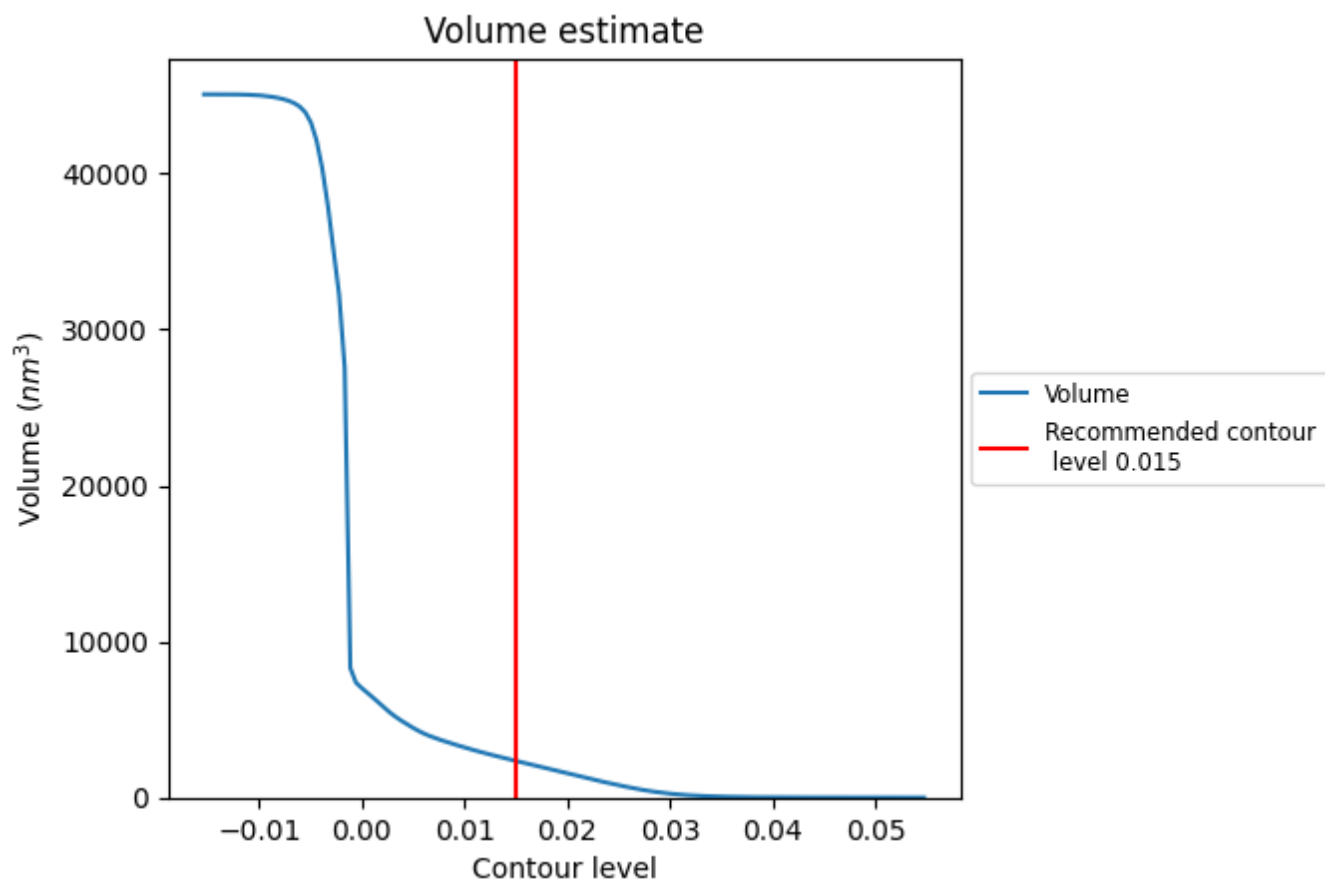
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

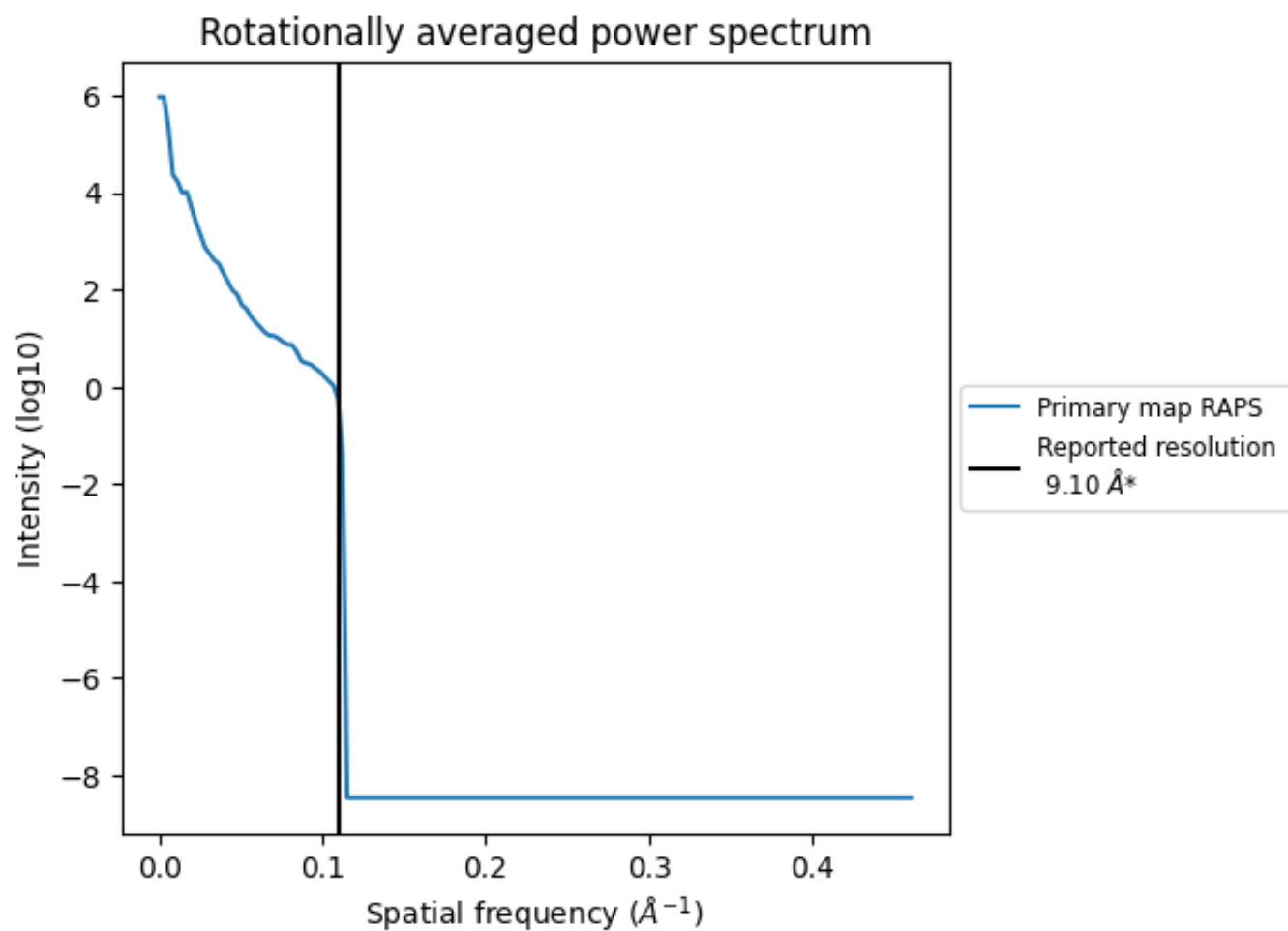
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2345 nm^3 ; this corresponds to an approximate mass of 2118 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 ⓘ

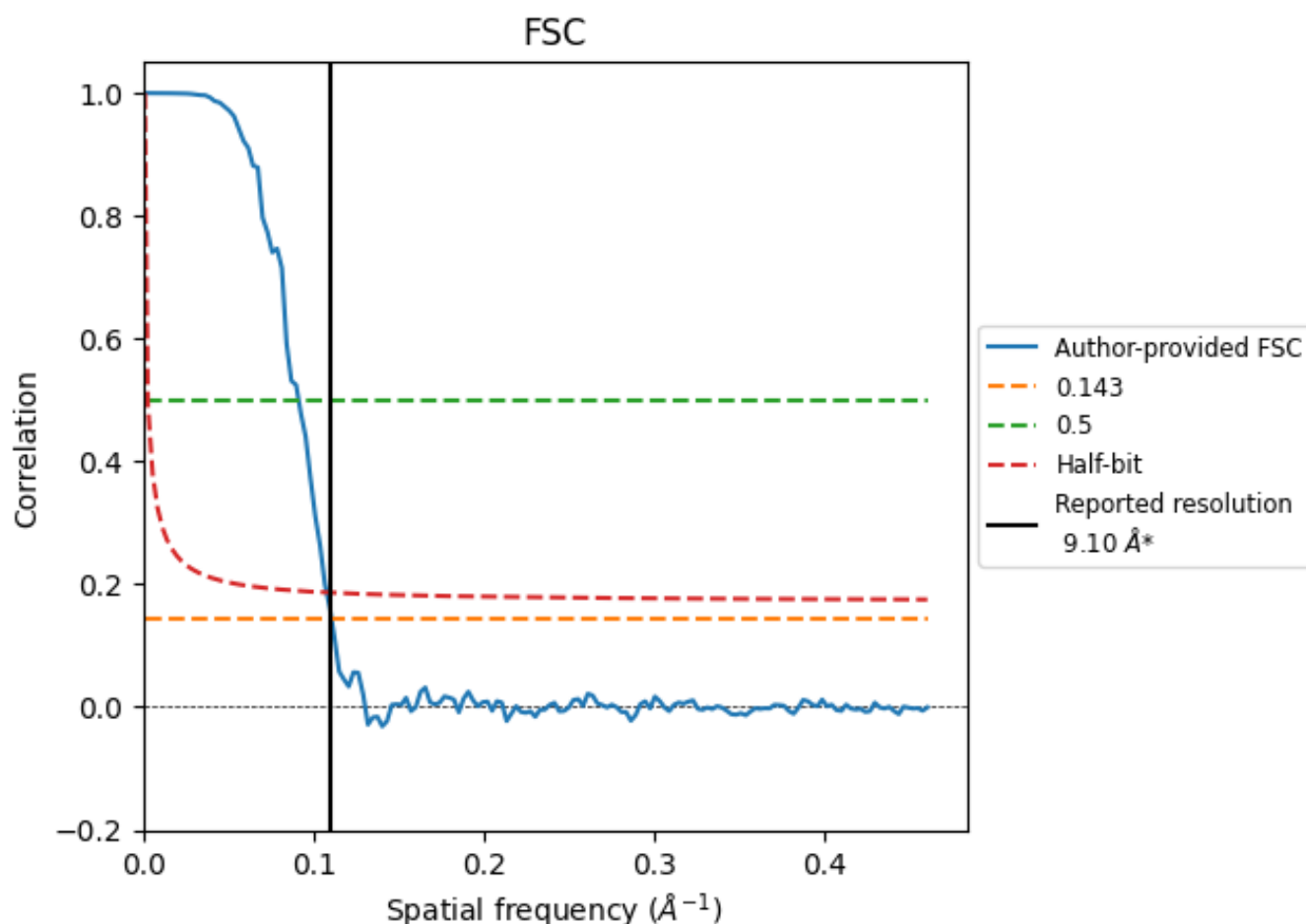


*Reported resolution corresponds to spatial frequency of 0.110 Å⁻¹

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 0.110 Å⁻¹

8.2 Resolution estimates [i](#)

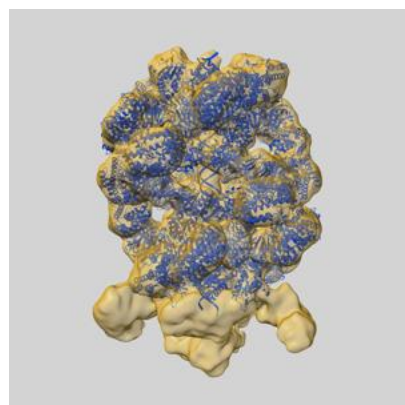
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	9.03	10.94	9.28
Unmasked-calculated*	-	-	-

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

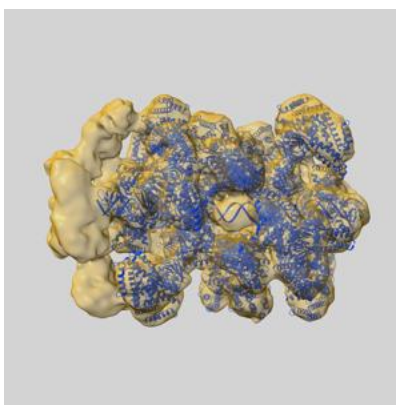
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4671 and PDB model 6QY3. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

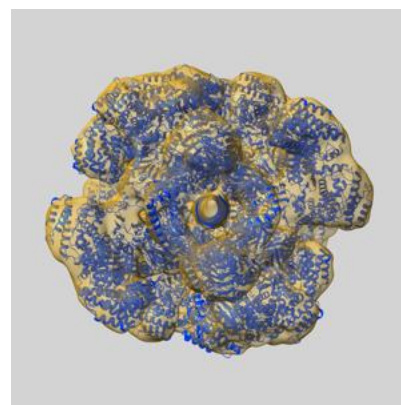
9.1 Map-model overlay [i](#)



X



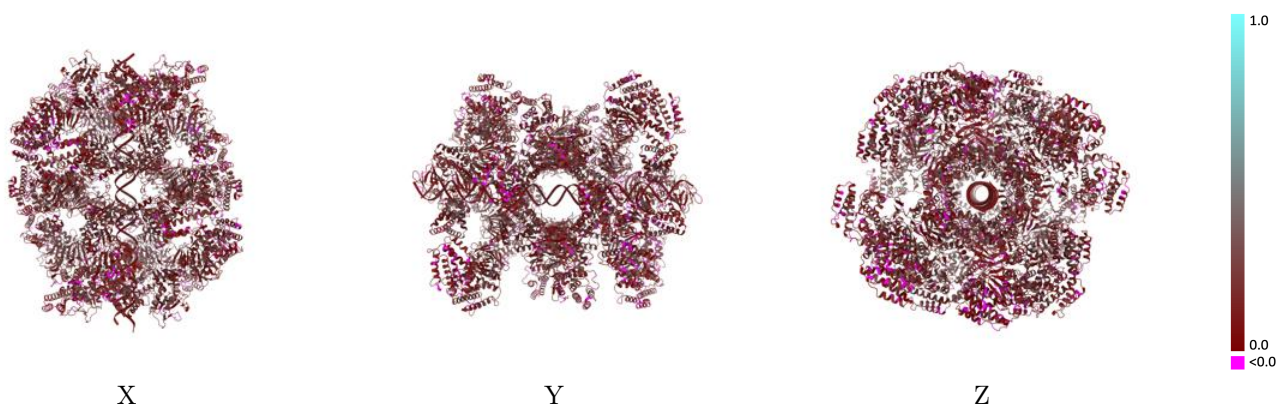
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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](#)

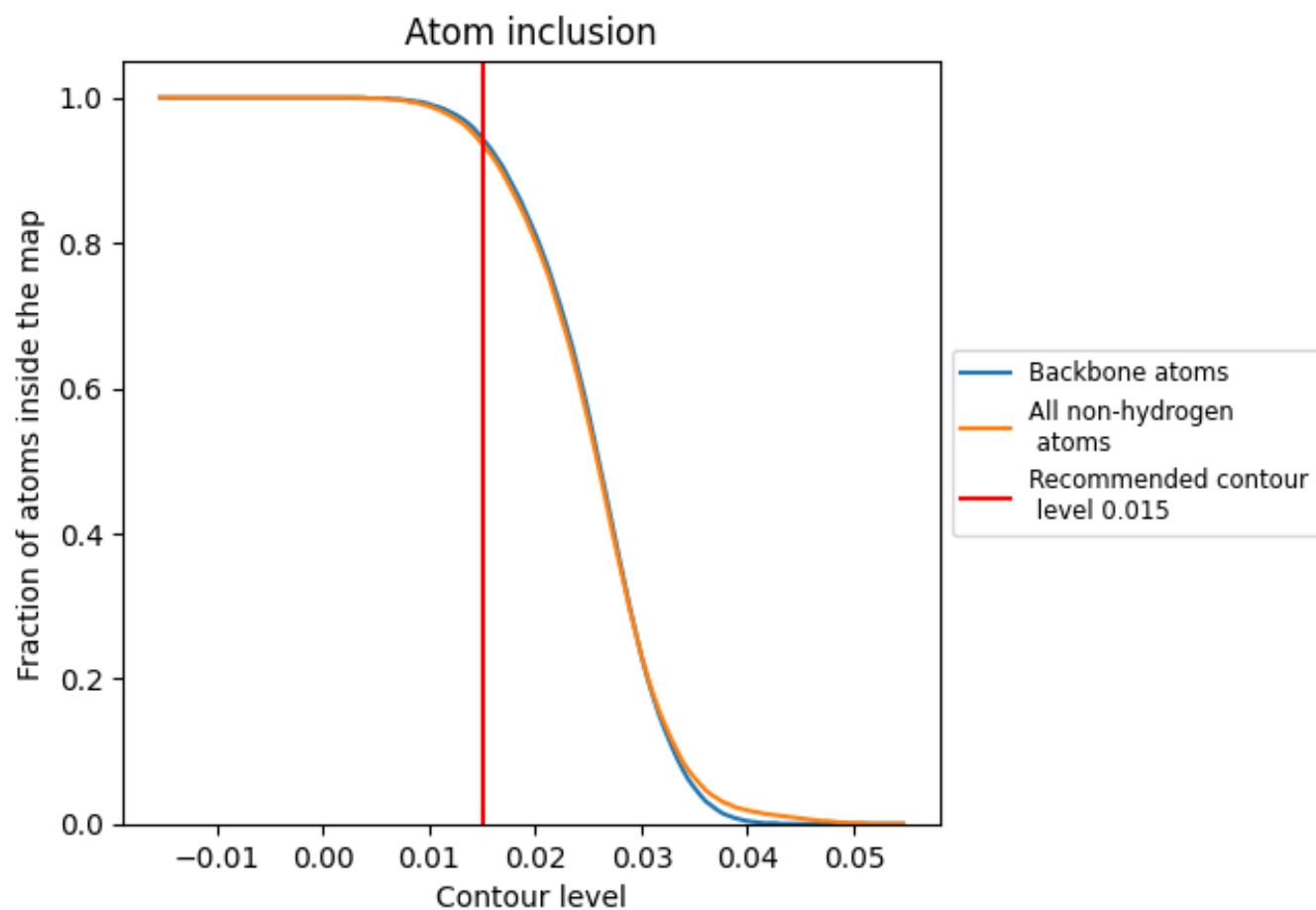


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9360	 0.1630
1	 0.9490	 0.1400
2	 0.9130	 0.1470
A	 0.9370	 0.1490
B	 0.9130	 0.1390
C	 0.8830	 0.1400
D	 0.9610	 0.1620
E	 0.9260	 0.1840
F	 0.9750	 0.1910
G	 0.9070	 0.1770
H	 0.9780	 0.2030
I	 0.7050	 0.0810
J	 0.9350	 0.1560
K	 0.9260	 0.0960
L	 0.9210	 0.1470
M	 0.9620	 0.1550
N	 0.9820	 0.1160
O	 0.8600	 0.1270
P	 0.9430	 0.1520
Q	 1.0000	 0.1230
R	 0.8950	 0.1250
S	 0.9410	 0.1580
T	 1.0000	 0.1390
U	 0.9090	 0.1650
V	 0.9780	 0.1720
W	 0.9630	 0.1080
X	 1.0000	 0.1770
Y	 0.9590	 0.1760
Z	 0.9830	 0.1840
a	 0.9450	 0.1720
b	 0.9550	 0.1970
c	 0.9350	 0.1760
d	 0.9670	 0.2000
e	 0.9240	 0.1690
f	 0.9650	 0.1940



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Chain	Atom inclusion	Q-score
g	 0.9240	 0.1820
h	 0.9660	 0.1920
i	 0.8530	 0.1180
j	 0.9810	 0.1870
k	 1.0000	 0.1440
l	 0.9780	 0.1720
m	 0.9750	 0.1620
n	 1.0000	 0.1770
o	 0.9780	 0.1790
p	 0.9850	 0.1880
q	 1.0000	 0.1640
r	 0.8560	 0.1290
s	 0.9790	 0.1740
t	 0.9630	 0.1430
u	 0.9020	 0.1640
v	 0.9810	 0.1830
w	 0.9820	 0.1350
x	 1.0000	 0.1100
y	 0.9680	 0.1650
z	 0.9750	 0.1790