



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:41 PM UTC

PDB ID : 7CR8 / pdb_00007cr8
Title : Synechocystis Cas1-Cas2-prespacerL complex
Authors : Yu, Y.; Chen, Q.
Deposited on : 2020-08-12
Resolution : 3.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

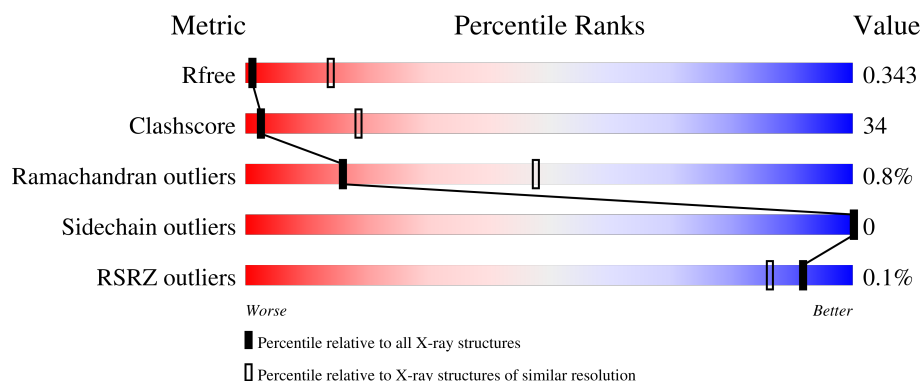
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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.



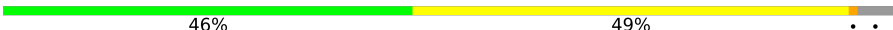
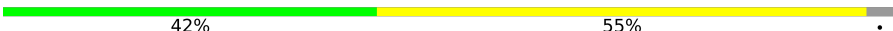
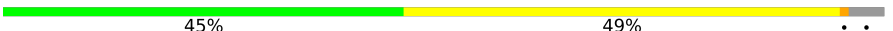
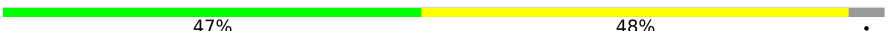
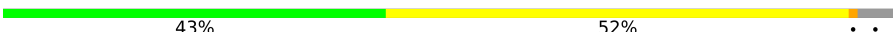
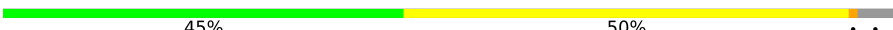
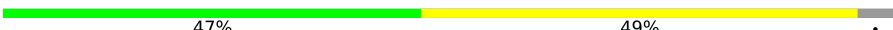
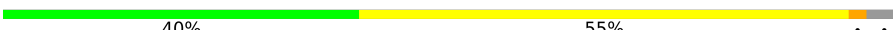
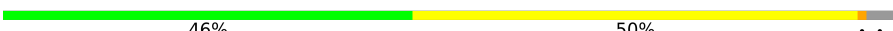
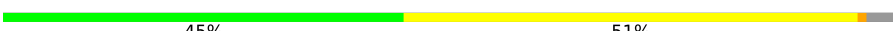
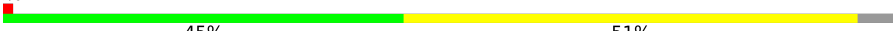
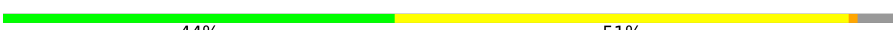
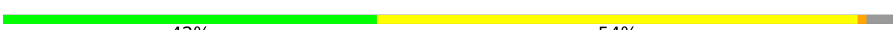
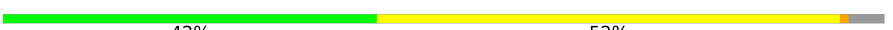
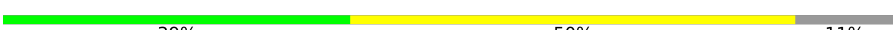
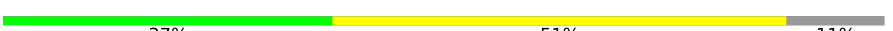
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	43% 53% .
1	B	336	38% 57% ..
1	C	336	41% 56% .
1	D	336	47% 47% ..
1	I	336	43% 53% .

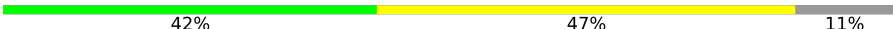
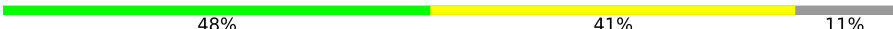
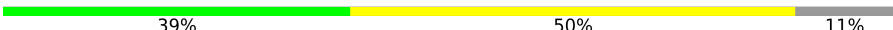
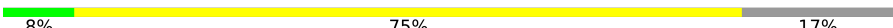
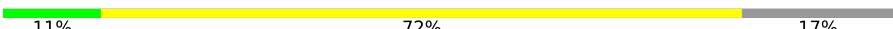
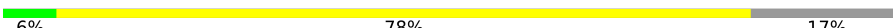
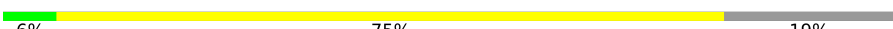
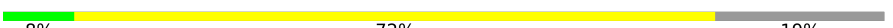
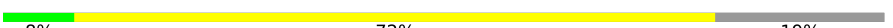
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Mol	Chain	Length	Quality of chain
1	J	336	 46% 49% . .
1	K	336	 42% 55% .
1	L	336	 45% 49% . .
1	Q	336	 47% 48% .
1	R	336	 43% 52% . .
1	S	336	 40% 57% .
1	T	336	 45% 50% . .
1	a	336	 47% 49% .
1	b	336	 40% 55% . .
1	c	336	 46% 50% . .
1	d	336	 48% 47% . .
1	i	336	 48% 48% .
1	j	336	 39% 57% . .
1	k	336	 45% 51% . .
1	l	336	 49% 46% . .
1	q	336	 % 45% 51% .
1	r	336	 44% 51% . .
1	s	336	 42% 54% . .
1	t	336	 42% 52% . .
2	E	105	 39% 50% 11%
2	F	105	 37% 51% 11%
2	M	105	 44% 45% 11%
2	N	105	 39% 50% 11%
2	U	105	 47% 42% 11%
2	V	105	 40% 49% 11%

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Mol	Chain	Length	Quality of chain
2	e	105	
2	f	105	
2	m	105	
2	n	105	
2	u	105	
2	v	105	
3	G	36	
3	O	36	
3	W	36	
3	g	36	
3	o	36	
3	w	36	
4	H	36	
4	P	36	
4	X	36	
4	h	36	
4	p	36	
4	x	36	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 146030 atoms, of which 67410 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 endonuclease Cas1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	I	322	Total	C	H	N	O	S	0	0	0
			5072	1661	2484	462	460	5			
1	J	324	Total	C	H	N	O	S	0	0	0
			5046	1668	2445	462	465	6			
1	K	325	Total	C	H	N	O	S	0	0	0
			4966	1674	2354	466	466	6			
1	L	322	Total	C	H	N	O	S	0	0	0
			5031	1657	2445	460	463	6			
1	Q	322	Total	C	H	N	O	S	0	0	0
			5072	1661	2484	462	460	5			
1	R	324	Total	C	H	N	O	S	0	0	0
			5046	1668	2445	462	465	6			
1	S	325	Total	C	H	N	O	S	0	0	0
			4966	1674	2354	466	466	6			
1	T	322	Total	C	H	N	O	S	0	0	0
			5031	1657	2445	460	463	6			
1	a	323	Total	C	H	N	O	S	0	0	0
			5080	1666	2484	463	461	6			
1	b	324	Total	C	H	N	O	S	0	0	0
			5046	1668	2445	462	465	6			
1	c	325	Total	C	H	N	O	S	0	0	0
			4966	1674	2354	466	466	6			
1	d	322	Total	C	H	N	O	S	0	0	0
			5031	1657	2445	460	463	6			
1	i	322	Total	C	H	N	O	S	0	0	0
			5072	1661	2484	462	460	5			
1	j	324	Total	C	H	N	O	S	0	0	0
			5046	1668	2445	462	465	6			
1	k	325	Total	C	H	N	O	S	0	0	0
			4966	1674	2354	466	466	6			
1	l	322	Total	C	H	N	O	S	0	0	0
			5031	1657	2445	460	463	6			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	q	322	Total	C	H	N	O	S	0	0	0
			5072	1661	2484	462	460	5			
1	r	324	Total	C	H	N	O	S	0	0	0
			5046	1668	2445	462	465	6			
1	s	325	Total	C	H	N	O	S	0	0	0
			4966	1674	2354	466	466	6			
1	t	322	Total	C	H	N	O	S	0	0	0
			5031	1657	2445	460	463	6			
1	A	322	Total	C	H	N	O	S	0	0	0
			5072	1661	2484	462	460	5			
1	B	324	Total	C	H	N	O	S	0	0	0
			5046	1668	2445	462	465	6			
1	C	325	Total	C	H	N	O	S	0	0	0
			4966	1674	2354	466	466	6			
1	D	322	Total	C	H	N	O	S	0	0	0
			5031	1657	2445	460	463	6			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-10	GLY	-	expression tag	UNP Q6ZEI2
I	-9	ALA	-	expression tag	UNP Q6ZEI2
I	-8	SER	-	expression tag	UNP Q6ZEI2
I	-7	GLY	-	expression tag	UNP Q6ZEI2
I	-6	SER	-	expression tag	UNP Q6ZEI2
I	-5	GLY	-	expression tag	UNP Q6ZEI2
I	-4	THR	-	expression tag	UNP Q6ZEI2
I	-3	GLY	-	expression tag	UNP Q6ZEI2
I	-2	SER	-	expression tag	UNP Q6ZEI2
I	-1	GLY	-	expression tag	UNP Q6ZEI2
I	0	SER	-	expression tag	UNP Q6ZEI2
J	-10	GLY	-	expression tag	UNP Q6ZEI2
J	-9	ALA	-	expression tag	UNP Q6ZEI2
J	-8	SER	-	expression tag	UNP Q6ZEI2
J	-7	GLY	-	expression tag	UNP Q6ZEI2
J	-6	SER	-	expression tag	UNP Q6ZEI2
J	-5	GLY	-	expression tag	UNP Q6ZEI2
J	-4	THR	-	expression tag	UNP Q6ZEI2
J	-3	GLY	-	expression tag	UNP Q6ZEI2
J	-2	SER	-	expression tag	UNP Q6ZEI2
J	-1	GLY	-	expression tag	UNP Q6ZEI2
J	0	SER	-	expression tag	UNP Q6ZEI2
K	-10	GLY	-	expression tag	UNP Q6ZEI2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	ALA	-	expression tag	UNP Q6ZEI2
K	-8	SER	-	expression tag	UNP Q6ZEI2
K	-7	GLY	-	expression tag	UNP Q6ZEI2
K	-6	SER	-	expression tag	UNP Q6ZEI2
K	-5	GLY	-	expression tag	UNP Q6ZEI2
K	-4	THR	-	expression tag	UNP Q6ZEI2
K	-3	GLY	-	expression tag	UNP Q6ZEI2
K	-2	SER	-	expression tag	UNP Q6ZEI2
K	-1	GLY	-	expression tag	UNP Q6ZEI2
K	0	SER	-	expression tag	UNP Q6ZEI2
L	-10	GLY	-	expression tag	UNP Q6ZEI2
L	-9	ALA	-	expression tag	UNP Q6ZEI2
L	-8	SER	-	expression tag	UNP Q6ZEI2
L	-7	GLY	-	expression tag	UNP Q6ZEI2
L	-6	SER	-	expression tag	UNP Q6ZEI2
L	-5	GLY	-	expression tag	UNP Q6ZEI2
L	-4	THR	-	expression tag	UNP Q6ZEI2
L	-3	GLY	-	expression tag	UNP Q6ZEI2
L	-2	SER	-	expression tag	UNP Q6ZEI2
L	-1	GLY	-	expression tag	UNP Q6ZEI2
L	0	SER	-	expression tag	UNP Q6ZEI2
Q	-10	GLY	-	expression tag	UNP Q6ZEI2
Q	-9	ALA	-	expression tag	UNP Q6ZEI2
Q	-8	SER	-	expression tag	UNP Q6ZEI2
Q	-7	GLY	-	expression tag	UNP Q6ZEI2
Q	-6	SER	-	expression tag	UNP Q6ZEI2
Q	-5	GLY	-	expression tag	UNP Q6ZEI2
Q	-4	THR	-	expression tag	UNP Q6ZEI2
Q	-3	GLY	-	expression tag	UNP Q6ZEI2
Q	-2	SER	-	expression tag	UNP Q6ZEI2
Q	-1	GLY	-	expression tag	UNP Q6ZEI2
Q	0	SER	-	expression tag	UNP Q6ZEI2
R	-10	GLY	-	expression tag	UNP Q6ZEI2
R	-9	ALA	-	expression tag	UNP Q6ZEI2
R	-8	SER	-	expression tag	UNP Q6ZEI2
R	-7	GLY	-	expression tag	UNP Q6ZEI2
R	-6	SER	-	expression tag	UNP Q6ZEI2
R	-5	GLY	-	expression tag	UNP Q6ZEI2
R	-4	THR	-	expression tag	UNP Q6ZEI2
R	-3	GLY	-	expression tag	UNP Q6ZEI2
R	-2	SER	-	expression tag	UNP Q6ZEI2
R	-1	GLY	-	expression tag	UNP Q6ZEI2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	0	SER	-	expression tag	UNP Q6ZEI2
S	-10	GLY	-	expression tag	UNP Q6ZEI2
S	-9	ALA	-	expression tag	UNP Q6ZEI2
S	-8	SER	-	expression tag	UNP Q6ZEI2
S	-7	GLY	-	expression tag	UNP Q6ZEI2
S	-6	SER	-	expression tag	UNP Q6ZEI2
S	-5	GLY	-	expression tag	UNP Q6ZEI2
S	-4	THR	-	expression tag	UNP Q6ZEI2
S	-3	GLY	-	expression tag	UNP Q6ZEI2
S	-2	SER	-	expression tag	UNP Q6ZEI2
S	-1	GLY	-	expression tag	UNP Q6ZEI2
S	0	SER	-	expression tag	UNP Q6ZEI2
T	-10	GLY	-	expression tag	UNP Q6ZEI2
T	-9	ALA	-	expression tag	UNP Q6ZEI2
T	-8	SER	-	expression tag	UNP Q6ZEI2
T	-7	GLY	-	expression tag	UNP Q6ZEI2
T	-6	SER	-	expression tag	UNP Q6ZEI2
T	-5	GLY	-	expression tag	UNP Q6ZEI2
T	-4	THR	-	expression tag	UNP Q6ZEI2
T	-3	GLY	-	expression tag	UNP Q6ZEI2
T	-2	SER	-	expression tag	UNP Q6ZEI2
T	-1	GLY	-	expression tag	UNP Q6ZEI2
T	0	SER	-	expression tag	UNP Q6ZEI2
a	-10	GLY	-	expression tag	UNP Q6ZEI2
a	-9	ALA	-	expression tag	UNP Q6ZEI2
a	-8	SER	-	expression tag	UNP Q6ZEI2
a	-7	GLY	-	expression tag	UNP Q6ZEI2
a	-6	SER	-	expression tag	UNP Q6ZEI2
a	-5	GLY	-	expression tag	UNP Q6ZEI2
a	-4	THR	-	expression tag	UNP Q6ZEI2
a	-3	GLY	-	expression tag	UNP Q6ZEI2
a	-2	SER	-	expression tag	UNP Q6ZEI2
a	-1	GLY	-	expression tag	UNP Q6ZEI2
a	0	SER	-	expression tag	UNP Q6ZEI2
b	-10	GLY	-	expression tag	UNP Q6ZEI2
b	-9	ALA	-	expression tag	UNP Q6ZEI2
b	-8	SER	-	expression tag	UNP Q6ZEI2
b	-7	GLY	-	expression tag	UNP Q6ZEI2
b	-6	SER	-	expression tag	UNP Q6ZEI2
b	-5	GLY	-	expression tag	UNP Q6ZEI2
b	-4	THR	-	expression tag	UNP Q6ZEI2
b	-3	GLY	-	expression tag	UNP Q6ZEI2

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Chain	Residue	Modelled	Actual	Comment	Reference
b	-2	SER	-	expression tag	UNP Q6ZEI2
b	-1	GLY	-	expression tag	UNP Q6ZEI2
b	0	SER	-	expression tag	UNP Q6ZEI2
c	-10	GLY	-	expression tag	UNP Q6ZEI2
c	-9	ALA	-	expression tag	UNP Q6ZEI2
c	-8	SER	-	expression tag	UNP Q6ZEI2
c	-7	GLY	-	expression tag	UNP Q6ZEI2
c	-6	SER	-	expression tag	UNP Q6ZEI2
c	-5	GLY	-	expression tag	UNP Q6ZEI2
c	-4	THR	-	expression tag	UNP Q6ZEI2
c	-3	GLY	-	expression tag	UNP Q6ZEI2
c	-2	SER	-	expression tag	UNP Q6ZEI2
c	-1	GLY	-	expression tag	UNP Q6ZEI2
c	0	SER	-	expression tag	UNP Q6ZEI2
d	-10	GLY	-	expression tag	UNP Q6ZEI2
d	-9	ALA	-	expression tag	UNP Q6ZEI2
d	-8	SER	-	expression tag	UNP Q6ZEI2
d	-7	GLY	-	expression tag	UNP Q6ZEI2
d	-6	SER	-	expression tag	UNP Q6ZEI2
d	-5	GLY	-	expression tag	UNP Q6ZEI2
d	-4	THR	-	expression tag	UNP Q6ZEI2
d	-3	GLY	-	expression tag	UNP Q6ZEI2
d	-2	SER	-	expression tag	UNP Q6ZEI2
d	-1	GLY	-	expression tag	UNP Q6ZEI2
d	0	SER	-	expression tag	UNP Q6ZEI2
i	-10	GLY	-	expression tag	UNP Q6ZEI2
i	-9	ALA	-	expression tag	UNP Q6ZEI2
i	-8	SER	-	expression tag	UNP Q6ZEI2
i	-7	GLY	-	expression tag	UNP Q6ZEI2
i	-6	SER	-	expression tag	UNP Q6ZEI2
i	-5	GLY	-	expression tag	UNP Q6ZEI2
i	-4	THR	-	expression tag	UNP Q6ZEI2
i	-3	GLY	-	expression tag	UNP Q6ZEI2
i	-2	SER	-	expression tag	UNP Q6ZEI2
i	-1	GLY	-	expression tag	UNP Q6ZEI2
i	0	SER	-	expression tag	UNP Q6ZEI2
j	-10	GLY	-	expression tag	UNP Q6ZEI2
j	-9	ALA	-	expression tag	UNP Q6ZEI2
j	-8	SER	-	expression tag	UNP Q6ZEI2
j	-7	GLY	-	expression tag	UNP Q6ZEI2
j	-6	SER	-	expression tag	UNP Q6ZEI2
j	-5	GLY	-	expression tag	UNP Q6ZEI2

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Chain	Residue	Modelled	Actual	Comment	Reference
j	-4	THR	-	expression tag	UNP Q6ZEI2
j	-3	GLY	-	expression tag	UNP Q6ZEI2
j	-2	SER	-	expression tag	UNP Q6ZEI2
j	-1	GLY	-	expression tag	UNP Q6ZEI2
j	0	SER	-	expression tag	UNP Q6ZEI2
k	-10	GLY	-	expression tag	UNP Q6ZEI2
k	-9	ALA	-	expression tag	UNP Q6ZEI2
k	-8	SER	-	expression tag	UNP Q6ZEI2
k	-7	GLY	-	expression tag	UNP Q6ZEI2
k	-6	SER	-	expression tag	UNP Q6ZEI2
k	-5	GLY	-	expression tag	UNP Q6ZEI2
k	-4	THR	-	expression tag	UNP Q6ZEI2
k	-3	GLY	-	expression tag	UNP Q6ZEI2
k	-2	SER	-	expression tag	UNP Q6ZEI2
k	-1	GLY	-	expression tag	UNP Q6ZEI2
k	0	SER	-	expression tag	UNP Q6ZEI2
l	-10	GLY	-	expression tag	UNP Q6ZEI2
l	-9	ALA	-	expression tag	UNP Q6ZEI2
l	-8	SER	-	expression tag	UNP Q6ZEI2
l	-7	GLY	-	expression tag	UNP Q6ZEI2
l	-6	SER	-	expression tag	UNP Q6ZEI2
l	-5	GLY	-	expression tag	UNP Q6ZEI2
l	-4	THR	-	expression tag	UNP Q6ZEI2
l	-3	GLY	-	expression tag	UNP Q6ZEI2
l	-2	SER	-	expression tag	UNP Q6ZEI2
l	-1	GLY	-	expression tag	UNP Q6ZEI2
l	0	SER	-	expression tag	UNP Q6ZEI2
q	-10	GLY	-	expression tag	UNP Q6ZEI2
q	-9	ALA	-	expression tag	UNP Q6ZEI2
q	-8	SER	-	expression tag	UNP Q6ZEI2
q	-7	GLY	-	expression tag	UNP Q6ZEI2
q	-6	SER	-	expression tag	UNP Q6ZEI2
q	-5	GLY	-	expression tag	UNP Q6ZEI2
q	-4	THR	-	expression tag	UNP Q6ZEI2
q	-3	GLY	-	expression tag	UNP Q6ZEI2
q	-2	SER	-	expression tag	UNP Q6ZEI2
q	-1	GLY	-	expression tag	UNP Q6ZEI2
q	0	SER	-	expression tag	UNP Q6ZEI2
r	-10	GLY	-	expression tag	UNP Q6ZEI2
r	-9	ALA	-	expression tag	UNP Q6ZEI2
r	-8	SER	-	expression tag	UNP Q6ZEI2
r	-7	GLY	-	expression tag	UNP Q6ZEI2

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Chain	Residue	Modelled	Actual	Comment	Reference
r	-6	SER	-	expression tag	UNP Q6ZEI2
r	-5	GLY	-	expression tag	UNP Q6ZEI2
r	-4	THR	-	expression tag	UNP Q6ZEI2
r	-3	GLY	-	expression tag	UNP Q6ZEI2
r	-2	SER	-	expression tag	UNP Q6ZEI2
r	-1	GLY	-	expression tag	UNP Q6ZEI2
r	0	SER	-	expression tag	UNP Q6ZEI2
s	-10	GLY	-	expression tag	UNP Q6ZEI2
s	-9	ALA	-	expression tag	UNP Q6ZEI2
s	-8	SER	-	expression tag	UNP Q6ZEI2
s	-7	GLY	-	expression tag	UNP Q6ZEI2
s	-6	SER	-	expression tag	UNP Q6ZEI2
s	-5	GLY	-	expression tag	UNP Q6ZEI2
s	-4	THR	-	expression tag	UNP Q6ZEI2
s	-3	GLY	-	expression tag	UNP Q6ZEI2
s	-2	SER	-	expression tag	UNP Q6ZEI2
s	-1	GLY	-	expression tag	UNP Q6ZEI2
s	0	SER	-	expression tag	UNP Q6ZEI2
t	-10	GLY	-	expression tag	UNP Q6ZEI2
t	-9	ALA	-	expression tag	UNP Q6ZEI2
t	-8	SER	-	expression tag	UNP Q6ZEI2
t	-7	GLY	-	expression tag	UNP Q6ZEI2
t	-6	SER	-	expression tag	UNP Q6ZEI2
t	-5	GLY	-	expression tag	UNP Q6ZEI2
t	-4	THR	-	expression tag	UNP Q6ZEI2
t	-3	GLY	-	expression tag	UNP Q6ZEI2
t	-2	SER	-	expression tag	UNP Q6ZEI2
t	-1	GLY	-	expression tag	UNP Q6ZEI2
t	0	SER	-	expression tag	UNP Q6ZEI2
A	-10	GLY	-	expression tag	UNP Q6ZEI2
A	-9	ALA	-	expression tag	UNP Q6ZEI2
A	-8	SER	-	expression tag	UNP Q6ZEI2
A	-7	GLY	-	expression tag	UNP Q6ZEI2
A	-6	SER	-	expression tag	UNP Q6ZEI2
A	-5	GLY	-	expression tag	UNP Q6ZEI2
A	-4	THR	-	expression tag	UNP Q6ZEI2
A	-3	GLY	-	expression tag	UNP Q6ZEI2
A	-2	SER	-	expression tag	UNP Q6ZEI2
A	-1	GLY	-	expression tag	UNP Q6ZEI2
A	0	SER	-	expression tag	UNP Q6ZEI2
B	-10	GLY	-	expression tag	UNP Q6ZEI2
B	-9	ALA	-	expression tag	UNP Q6ZEI2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	SER	-	expression tag	UNP Q6ZEI2
B	-7	GLY	-	expression tag	UNP Q6ZEI2
B	-6	SER	-	expression tag	UNP Q6ZEI2
B	-5	GLY	-	expression tag	UNP Q6ZEI2
B	-4	THR	-	expression tag	UNP Q6ZEI2
B	-3	GLY	-	expression tag	UNP Q6ZEI2
B	-2	SER	-	expression tag	UNP Q6ZEI2
B	-1	GLY	-	expression tag	UNP Q6ZEI2
B	0	SER	-	expression tag	UNP Q6ZEI2
C	-10	GLY	-	expression tag	UNP Q6ZEI2
C	-9	ALA	-	expression tag	UNP Q6ZEI2
C	-8	SER	-	expression tag	UNP Q6ZEI2
C	-7	GLY	-	expression tag	UNP Q6ZEI2
C	-6	SER	-	expression tag	UNP Q6ZEI2
C	-5	GLY	-	expression tag	UNP Q6ZEI2
C	-4	THR	-	expression tag	UNP Q6ZEI2
C	-3	GLY	-	expression tag	UNP Q6ZEI2
C	-2	SER	-	expression tag	UNP Q6ZEI2
C	-1	GLY	-	expression tag	UNP Q6ZEI2
C	0	SER	-	expression tag	UNP Q6ZEI2
D	-10	GLY	-	expression tag	UNP Q6ZEI2
D	-9	ALA	-	expression tag	UNP Q6ZEI2
D	-8	SER	-	expression tag	UNP Q6ZEI2
D	-7	GLY	-	expression tag	UNP Q6ZEI2
D	-6	SER	-	expression tag	UNP Q6ZEI2
D	-5	GLY	-	expression tag	UNP Q6ZEI2
D	-4	THR	-	expression tag	UNP Q6ZEI2
D	-3	GLY	-	expression tag	UNP Q6ZEI2
D	-2	SER	-	expression tag	UNP Q6ZEI2
D	-1	GLY	-	expression tag	UNP Q6ZEI2
D	0	SER	-	expression tag	UNP Q6ZEI2

- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cas2 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	M	93	Total	C	H	N	O	S	0	0	0
			1502	490	748	124	136	4			
2	N	93	Total	C	H	N	O	S	0	0	0
			1513	490	759	124	136	4			
2	U	93	Total	C	H	N	O	S	0	0	0
			1502	490	748	124	136	4			
2	V	93	Total	C	H	N	O	S	0	0	0
			1513	490	759	124	136	4			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	e	93	Total 1502	C 490	H 748	N 124	O 136	S 4	0	0	0
2	f	93	Total 1513	C 490	H 759	N 124	O 136	S 4	0	0	0
2	m	93	Total 1502	C 490	H 748	N 124	O 136	S 4	0	0	0
2	n	93	Total 1513	C 490	H 759	N 124	O 136	S 4	0	0	0
2	u	93	Total 1502	C 490	H 748	N 124	O 136	S 4	0	0	0
2	v	93	Total 1513	C 490	H 759	N 124	O 136	S 4	0	0	0
2	E	93	Total 1502	C 490	H 748	N 124	O 136	S 4	0	0	0
2	F	93	Total 1513	C 490	H 759	N 124	O 136	S 4	0	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-10	GLY	-	expression tag	UNP Q6ZEI1
M	-9	ALA	-	expression tag	UNP Q6ZEI1
M	-8	SER	-	expression tag	UNP Q6ZEI1
M	-7	GLY	-	expression tag	UNP Q6ZEI1
M	-6	SER	-	expression tag	UNP Q6ZEI1
M	-5	GLY	-	expression tag	UNP Q6ZEI1
M	-4	THR	-	expression tag	UNP Q6ZEI1
M	-3	GLY	-	expression tag	UNP Q6ZEI1
M	-2	SER	-	expression tag	UNP Q6ZEI1
M	-1	GLY	-	expression tag	UNP Q6ZEI1
M	0	SER	-	expression tag	UNP Q6ZEI1
N	-10	GLY	-	expression tag	UNP Q6ZEI1
N	-9	ALA	-	expression tag	UNP Q6ZEI1
N	-8	SER	-	expression tag	UNP Q6ZEI1
N	-7	GLY	-	expression tag	UNP Q6ZEI1
N	-6	SER	-	expression tag	UNP Q6ZEI1
N	-5	GLY	-	expression tag	UNP Q6ZEI1
N	-4	THR	-	expression tag	UNP Q6ZEI1
N	-3	GLY	-	expression tag	UNP Q6ZEI1
N	-2	SER	-	expression tag	UNP Q6ZEI1
N	-1	GLY	-	expression tag	UNP Q6ZEI1
N	0	SER	-	expression tag	UNP Q6ZEI1
U	-10	GLY	-	expression tag	UNP Q6ZEI1

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-9	ALA	-	expression tag	UNP Q6ZEI1
U	-8	SER	-	expression tag	UNP Q6ZEI1
U	-7	GLY	-	expression tag	UNP Q6ZEI1
U	-6	SER	-	expression tag	UNP Q6ZEI1
U	-5	GLY	-	expression tag	UNP Q6ZEI1
U	-4	THR	-	expression tag	UNP Q6ZEI1
U	-3	GLY	-	expression tag	UNP Q6ZEI1
U	-2	SER	-	expression tag	UNP Q6ZEI1
U	-1	GLY	-	expression tag	UNP Q6ZEI1
U	0	SER	-	expression tag	UNP Q6ZEI1
V	-10	GLY	-	expression tag	UNP Q6ZEI1
V	-9	ALA	-	expression tag	UNP Q6ZEI1
V	-8	SER	-	expression tag	UNP Q6ZEI1
V	-7	GLY	-	expression tag	UNP Q6ZEI1
V	-6	SER	-	expression tag	UNP Q6ZEI1
V	-5	GLY	-	expression tag	UNP Q6ZEI1
V	-4	THR	-	expression tag	UNP Q6ZEI1
V	-3	GLY	-	expression tag	UNP Q6ZEI1
V	-2	SER	-	expression tag	UNP Q6ZEI1
V	-1	GLY	-	expression tag	UNP Q6ZEI1
V	0	SER	-	expression tag	UNP Q6ZEI1
e	-10	GLY	-	expression tag	UNP Q6ZEI1
e	-9	ALA	-	expression tag	UNP Q6ZEI1
e	-8	SER	-	expression tag	UNP Q6ZEI1
e	-7	GLY	-	expression tag	UNP Q6ZEI1
e	-6	SER	-	expression tag	UNP Q6ZEI1
e	-5	GLY	-	expression tag	UNP Q6ZEI1
e	-4	THR	-	expression tag	UNP Q6ZEI1
e	-3	GLY	-	expression tag	UNP Q6ZEI1
e	-2	SER	-	expression tag	UNP Q6ZEI1
e	-1	GLY	-	expression tag	UNP Q6ZEI1
e	0	SER	-	expression tag	UNP Q6ZEI1
f	-10	GLY	-	expression tag	UNP Q6ZEI1
f	-9	ALA	-	expression tag	UNP Q6ZEI1
f	-8	SER	-	expression tag	UNP Q6ZEI1
f	-7	GLY	-	expression tag	UNP Q6ZEI1
f	-6	SER	-	expression tag	UNP Q6ZEI1
f	-5	GLY	-	expression tag	UNP Q6ZEI1
f	-4	THR	-	expression tag	UNP Q6ZEI1
f	-3	GLY	-	expression tag	UNP Q6ZEI1
f	-2	SER	-	expression tag	UNP Q6ZEI1
f	-1	GLY	-	expression tag	UNP Q6ZEI1

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Chain	Residue	Modelled	Actual	Comment	Reference
f	0	SER	-	expression tag	UNP Q6ZEI1
m	-10	GLY	-	expression tag	UNP Q6ZEI1
m	-9	ALA	-	expression tag	UNP Q6ZEI1
m	-8	SER	-	expression tag	UNP Q6ZEI1
m	-7	GLY	-	expression tag	UNP Q6ZEI1
m	-6	SER	-	expression tag	UNP Q6ZEI1
m	-5	GLY	-	expression tag	UNP Q6ZEI1
m	-4	THR	-	expression tag	UNP Q6ZEI1
m	-3	GLY	-	expression tag	UNP Q6ZEI1
m	-2	SER	-	expression tag	UNP Q6ZEI1
m	-1	GLY	-	expression tag	UNP Q6ZEI1
m	0	SER	-	expression tag	UNP Q6ZEI1
n	-10	GLY	-	expression tag	UNP Q6ZEI1
n	-9	ALA	-	expression tag	UNP Q6ZEI1
n	-8	SER	-	expression tag	UNP Q6ZEI1
n	-7	GLY	-	expression tag	UNP Q6ZEI1
n	-6	SER	-	expression tag	UNP Q6ZEI1
n	-5	GLY	-	expression tag	UNP Q6ZEI1
n	-4	THR	-	expression tag	UNP Q6ZEI1
n	-3	GLY	-	expression tag	UNP Q6ZEI1
n	-2	SER	-	expression tag	UNP Q6ZEI1
n	-1	GLY	-	expression tag	UNP Q6ZEI1
n	0	SER	-	expression tag	UNP Q6ZEI1
u	-10	GLY	-	expression tag	UNP Q6ZEI1
u	-9	ALA	-	expression tag	UNP Q6ZEI1
u	-8	SER	-	expression tag	UNP Q6ZEI1
u	-7	GLY	-	expression tag	UNP Q6ZEI1
u	-6	SER	-	expression tag	UNP Q6ZEI1
u	-5	GLY	-	expression tag	UNP Q6ZEI1
u	-4	THR	-	expression tag	UNP Q6ZEI1
u	-3	GLY	-	expression tag	UNP Q6ZEI1
u	-2	SER	-	expression tag	UNP Q6ZEI1
u	-1	GLY	-	expression tag	UNP Q6ZEI1
u	0	SER	-	expression tag	UNP Q6ZEI1
v	-10	GLY	-	expression tag	UNP Q6ZEI1
v	-9	ALA	-	expression tag	UNP Q6ZEI1
v	-8	SER	-	expression tag	UNP Q6ZEI1
v	-7	GLY	-	expression tag	UNP Q6ZEI1
v	-6	SER	-	expression tag	UNP Q6ZEI1
v	-5	GLY	-	expression tag	UNP Q6ZEI1
v	-4	THR	-	expression tag	UNP Q6ZEI1
v	-3	GLY	-	expression tag	UNP Q6ZEI1

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Chain	Residue	Modelled	Actual	Comment	Reference
v	-2	SER	-	expression tag	UNP Q6ZEI1
v	-1	GLY	-	expression tag	UNP Q6ZEI1
v	0	SER	-	expression tag	UNP Q6ZEI1
E	-10	GLY	-	expression tag	UNP Q6ZEI1
E	-9	ALA	-	expression tag	UNP Q6ZEI1
E	-8	SER	-	expression tag	UNP Q6ZEI1
E	-7	GLY	-	expression tag	UNP Q6ZEI1
E	-6	SER	-	expression tag	UNP Q6ZEI1
E	-5	GLY	-	expression tag	UNP Q6ZEI1
E	-4	THR	-	expression tag	UNP Q6ZEI1
E	-3	GLY	-	expression tag	UNP Q6ZEI1
E	-2	SER	-	expression tag	UNP Q6ZEI1
E	-1	GLY	-	expression tag	UNP Q6ZEI1
E	0	SER	-	expression tag	UNP Q6ZEI1
F	-10	GLY	-	expression tag	UNP Q6ZEI1
F	-9	ALA	-	expression tag	UNP Q6ZEI1
F	-8	SER	-	expression tag	UNP Q6ZEI1
F	-7	GLY	-	expression tag	UNP Q6ZEI1
F	-6	SER	-	expression tag	UNP Q6ZEI1
F	-5	GLY	-	expression tag	UNP Q6ZEI1
F	-4	THR	-	expression tag	UNP Q6ZEI1
F	-3	GLY	-	expression tag	UNP Q6ZEI1
F	-2	SER	-	expression tag	UNP Q6ZEI1
F	-1	GLY	-	expression tag	UNP Q6ZEI1
F	0	SER	-	expression tag	UNP Q6ZEI1

- Molecule 3 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	30	Total	C	N	O	P	0	0	0
			610	292	98	190	30			
3	W	30	Total	C	N	O	P	0	0	0
			610	292	98	190	30			
3	g	30	Total	C	N	O	P	0	0	0
			610	292	98	190	30			
3	o	30	Total	C	N	O	P	0	0	0
			610	292	98	190	30			
3	w	30	Total	C	N	O	P	0	0	0
			610	292	98	190	30			
3	G	30	Total	C	N	O	P	0	0	0
			610	292	98	190	30			

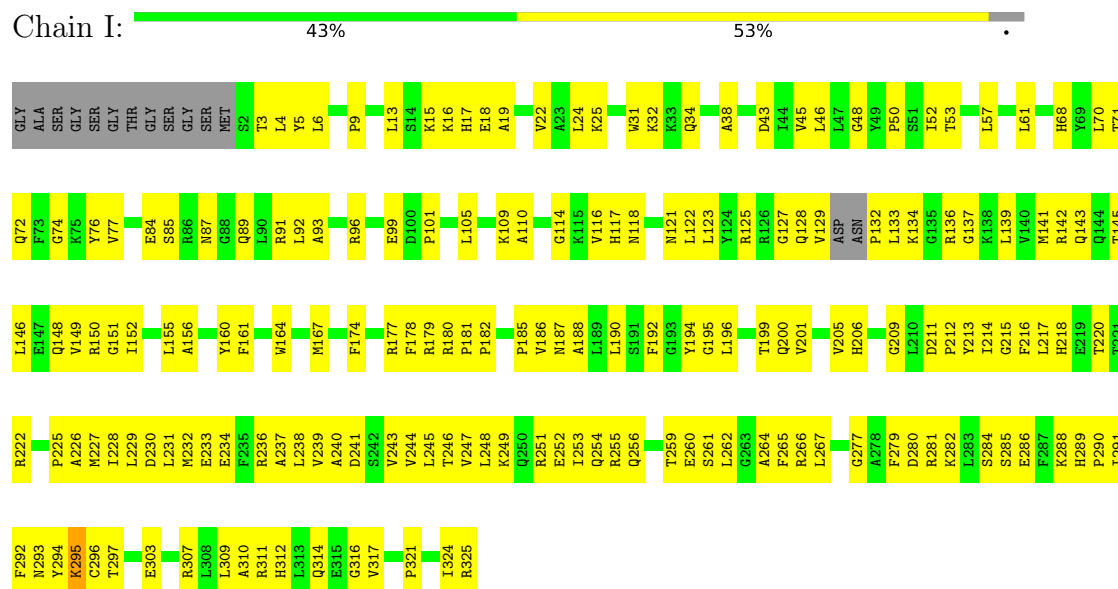
- Molecule 4 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	29	Total	C	N	O	P	0	0	0
			597	283	113	172	29			
4	X	29	Total	C	N	O	P	0	0	0
			597	283	113	172	29			
4	h	29	Total	C	N	O	P	0	0	0
			597	283	113	172	29			
4	p	29	Total	C	N	O	P	0	0	0
			597	283	113	172	29			
4	x	29	Total	C	N	O	P	0	0	0
			597	283	113	172	29			
4	H	29	Total	C	N	O	P	0	0	0
			597	283	113	172	29			

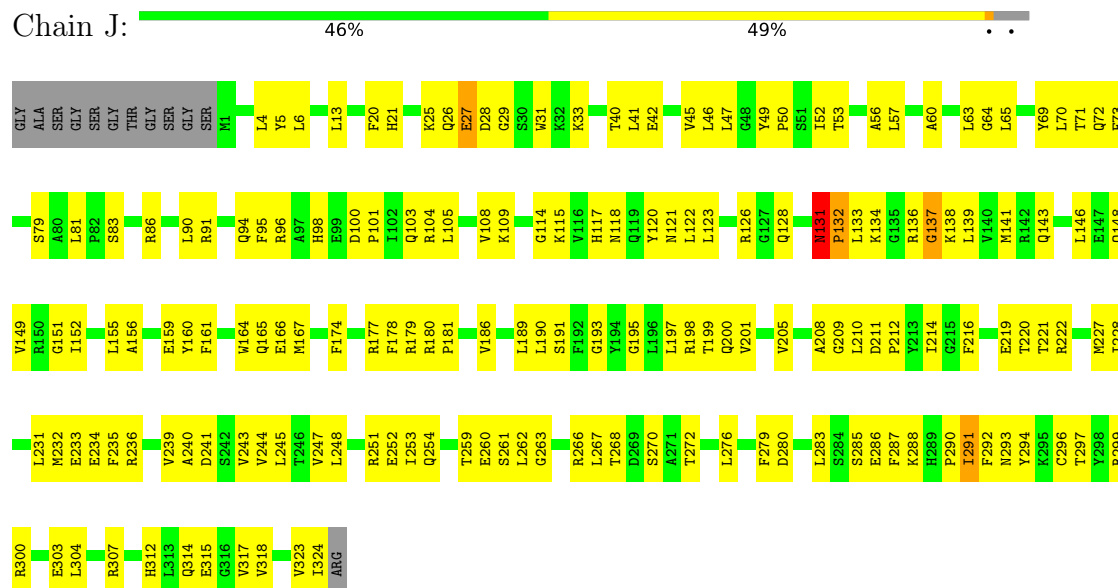
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

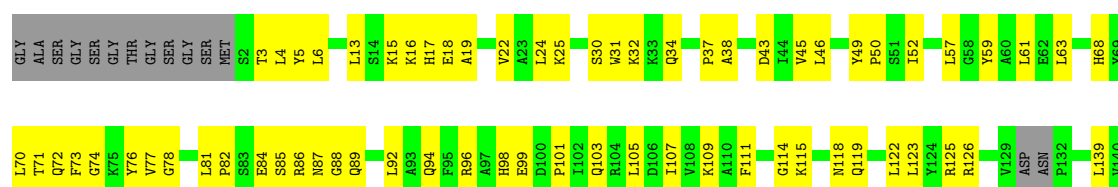
• Molecule 1: CRISPR-associated endonuclease Cas1

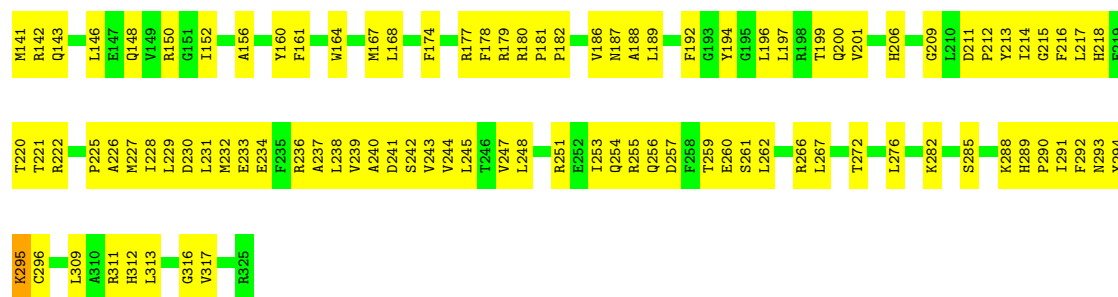


• Molecule 1: CRISPR-associated endonuclease Cas1

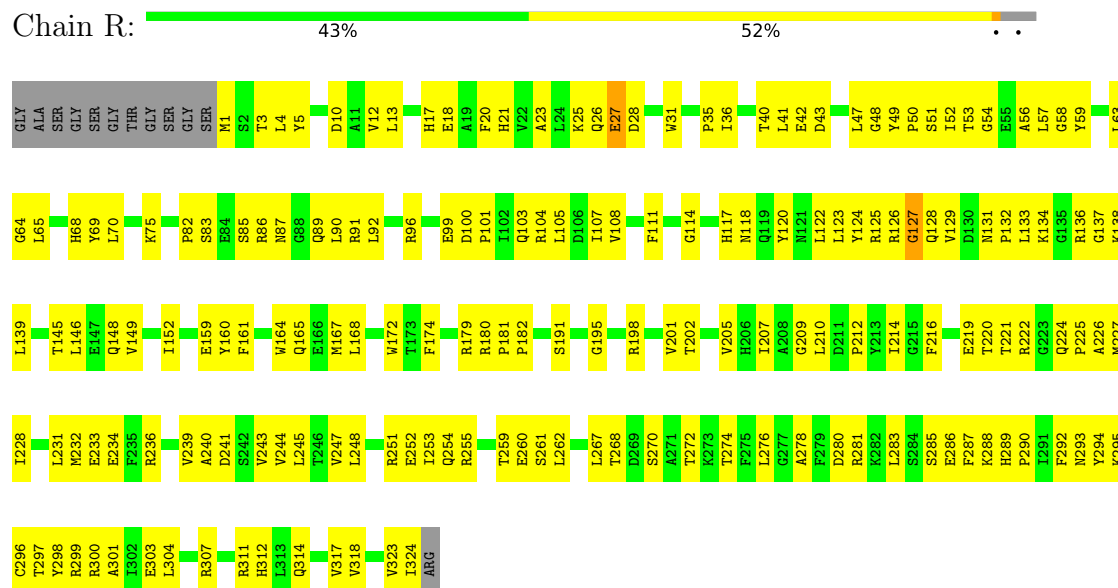


Chain K: 42% 55% .

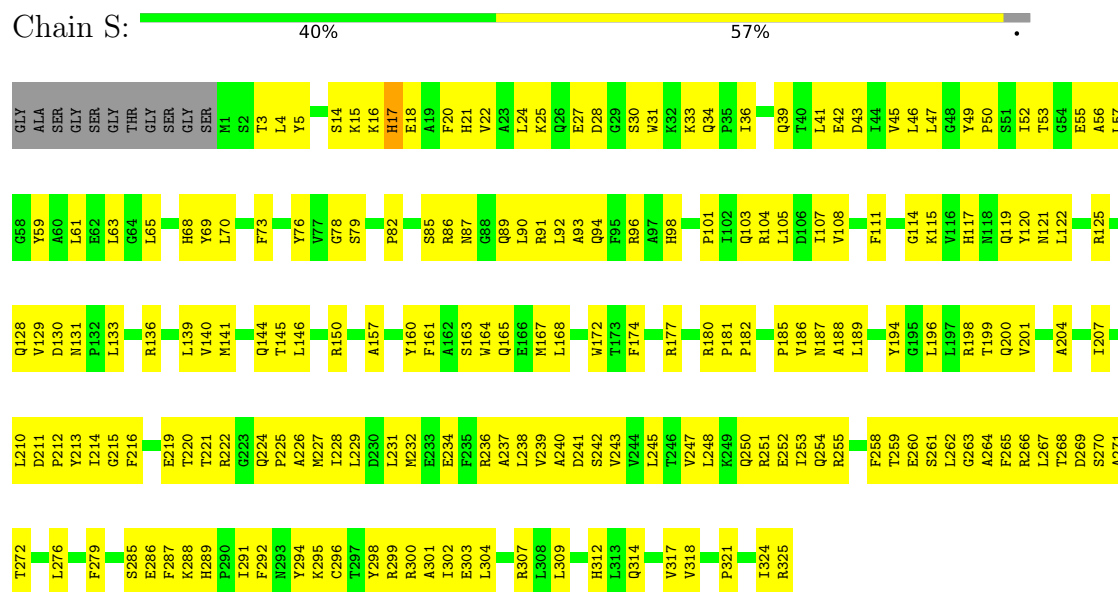




• Molecule 1: CRISPR-associated endonuclease Cas1



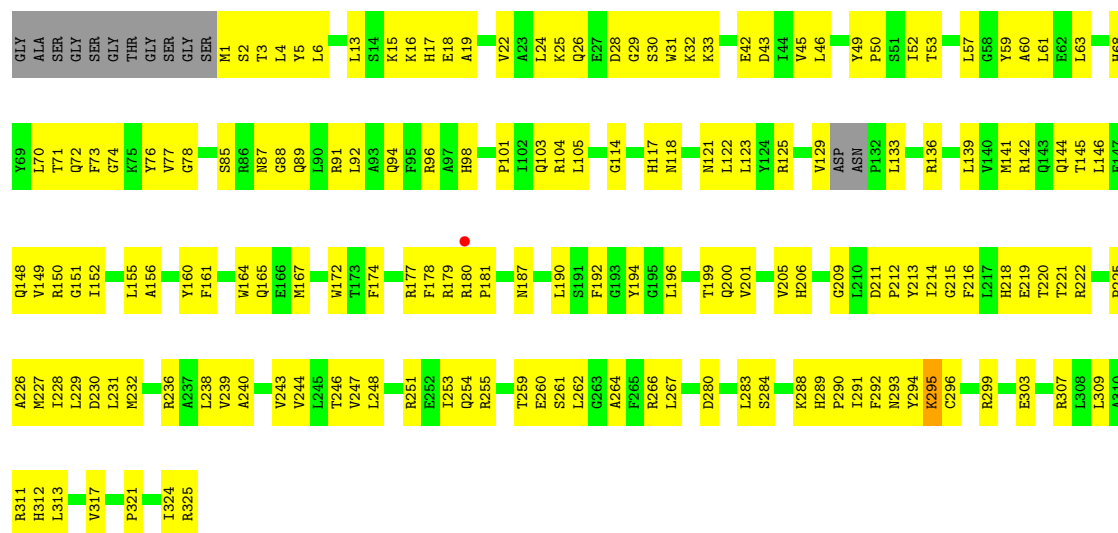
• Molecule 1: CRISPR-associated endonuclease Cas1



• Molecule 1: CRISPR-associated endonuclease Cas1

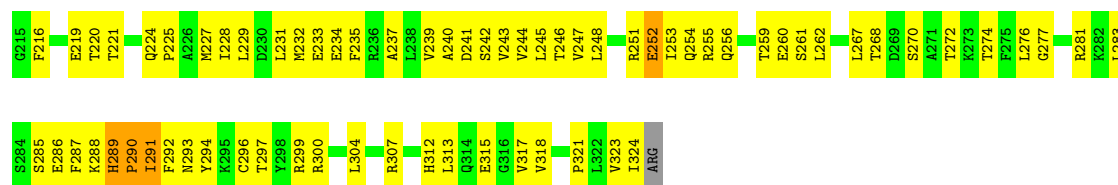
ILE	A226	V149	T71	GLY
	F292	R150	Q72	ALA
	N293	G151		SER
	N284	I152	P82	GLY
	F295		S83	SER
	C286	L155	E84	GLY
		A156	S85	THR
		E159	R86	GLY
	E303		N87	SER
	L304	Y160		GLY
R307	F235		R91	SER
	R236	S163	L92	M1
	A237	W164	A93	
	L238	Q165		L4
	V239	Q166	R96	Y5
	A240	E166		L6
	D241	M167		T7
	S242		D100	Q8
	V243	F174	P101	P9
	V244		I102	D10
V317	L245	F178	Q103	A11
	T246	R179	R104	L12
	V247	R180	L105	V11
	L248	F181	D106	
	K249	P182	I107	K15
	Q250	T183	V108	
	R251	D184	K109	E18
	E252	P185	A110	
	T253	V186	F111	H21
	Q254	N187		V22
V323			G114	A23
	D257	F192	K115	L24
	F258		V116	K25
	T259	G195	H117	Q26
	E260	L196	N118	
	S261	L197	Q119	
	L262	R198	Y120	V31
	G263		N121	K32
	A264	V201	K33	K33
	F265	T202	L122	Q94
C286	R266	A203	L123	P35
	L267	R204	Y124	I36
	T268	A204	R125	P37
	D269	V205	R126	A38
	S270	H206	G127	Q39
	A271	I207	Q128	T40
	T272	A208		L41
	K273	G209	P132	E42
	T274		L133	D43
	L275	P212	K134	I44
ARG	L276	Y213	G135	V45
		L214	R136	L46
		G215	G137	L47
	F279	F216	K138	
		L217	L139	S51
	L283		V140	I52
		T220	M141	T53
	E286	T221		G54
	F287	R222	T145	E55
	K288	G223	L146	
P80	H289	Q224	F147	Y69
	D80	R225	G149	L70

Chain a: 47% 49% .



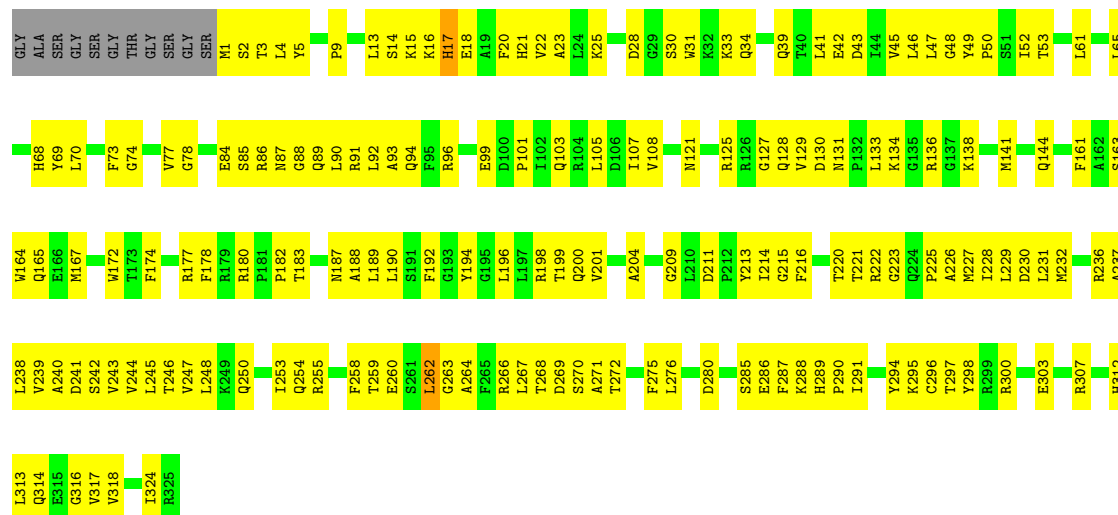
Chain b: 40% 55% .





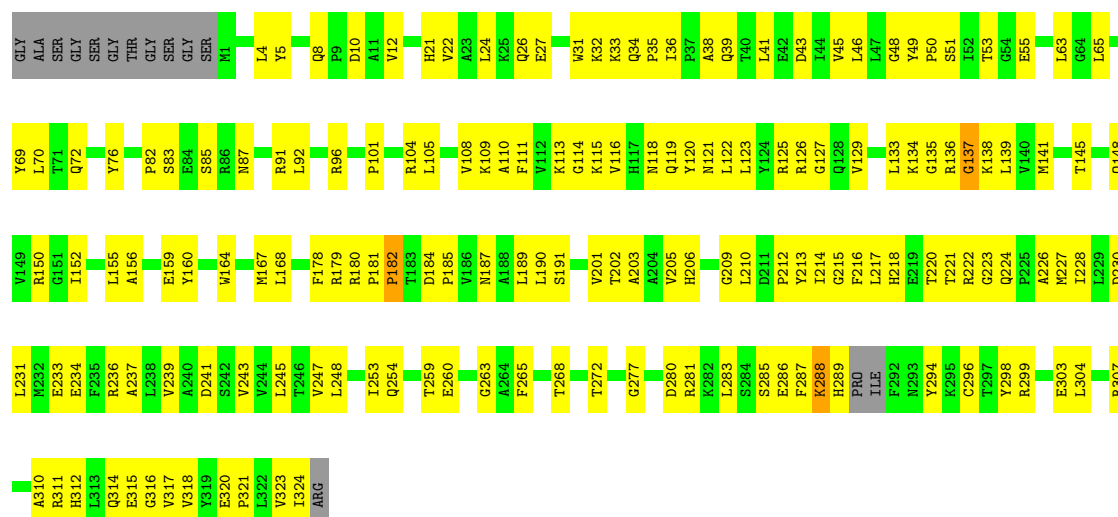
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain c: 46% 50%



• Molecule 1: CRISPR-associated endonuclease Cas1

Chain d: 48% 47%



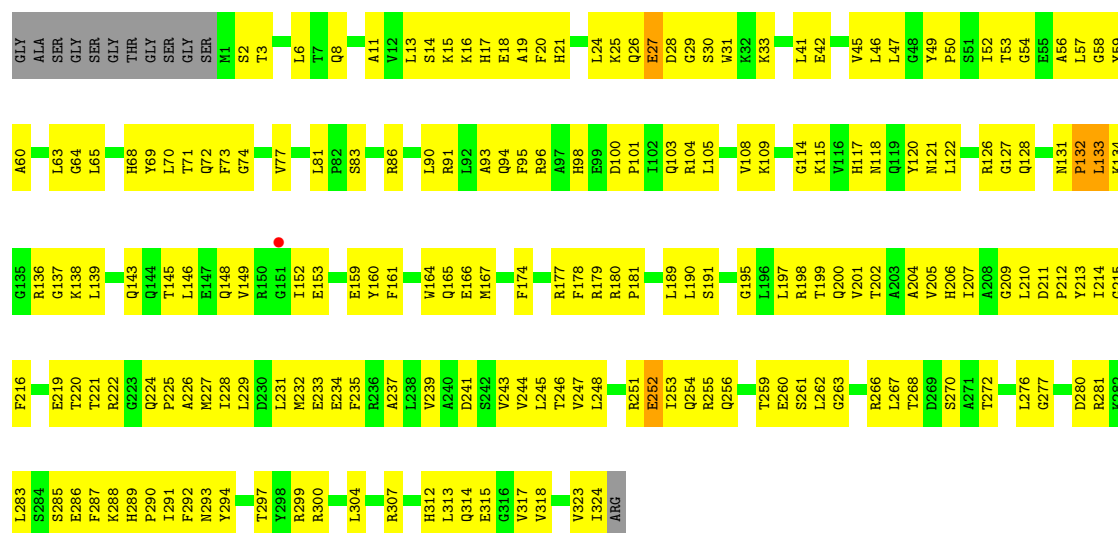
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain i: 48% 48%



• Molecule 1: CRISPR-associated endonuclease Cas1

Chain j: 39% 57%

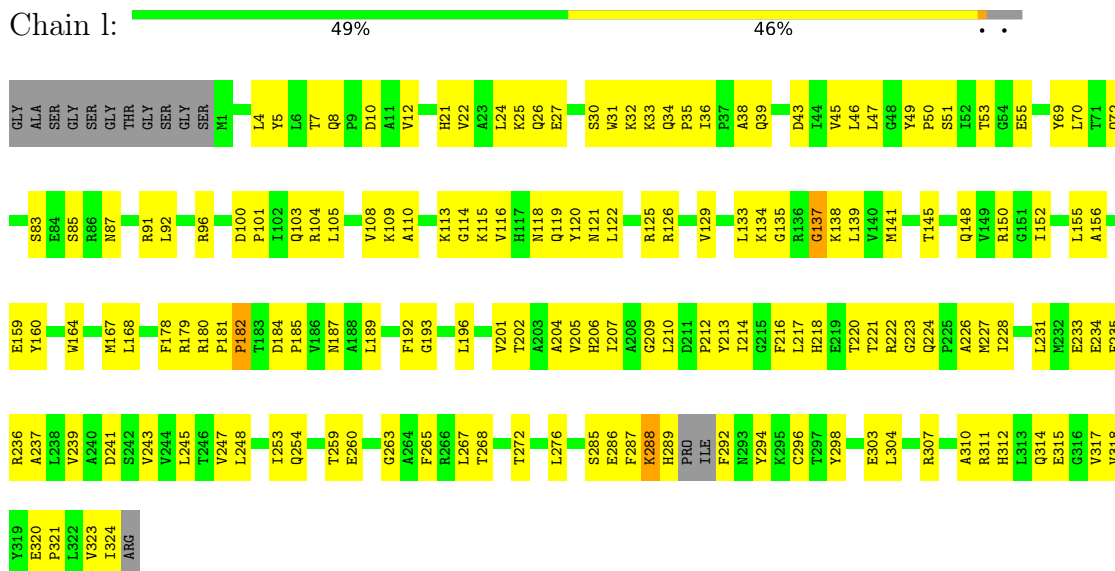


• Molecule 1: CRISPR-associated endonuclease Cas1

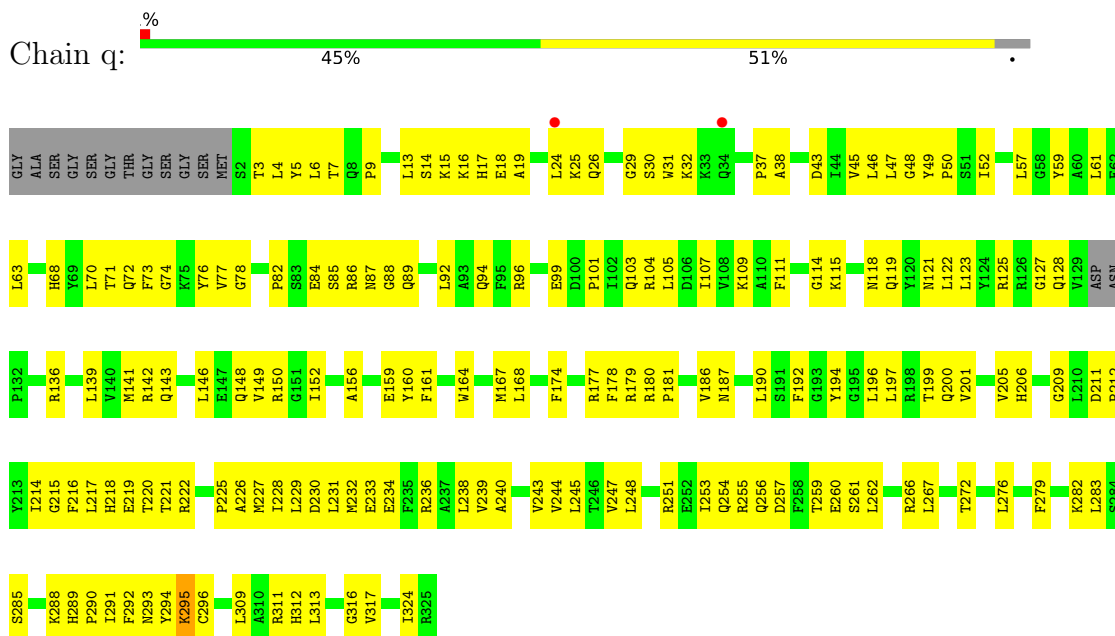
Chain k: 45% 51%



- Molecule 1: CRISPR-associated endonuclease Cas1

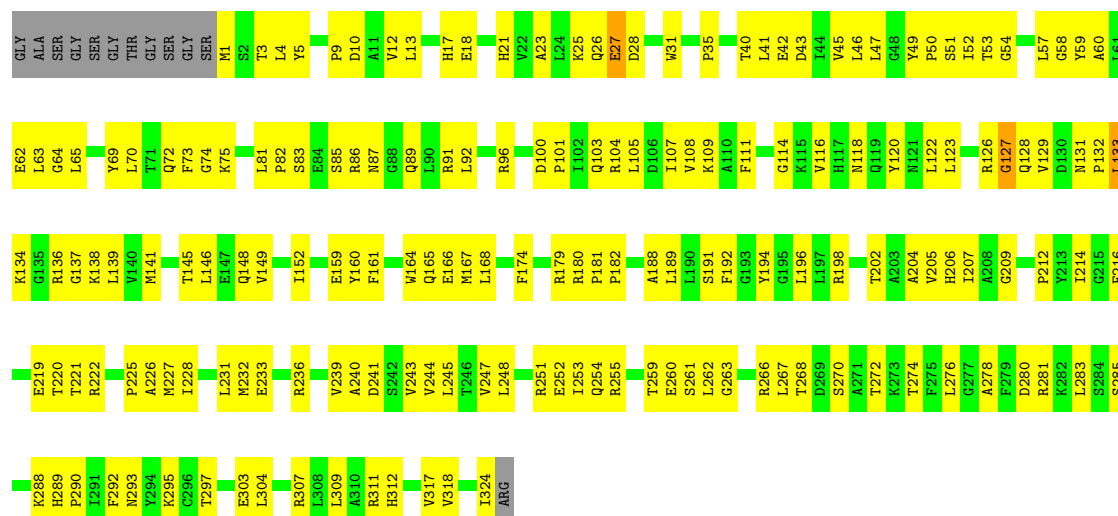


- Molecule 1: CRISPR-associated endonuclease Cas1



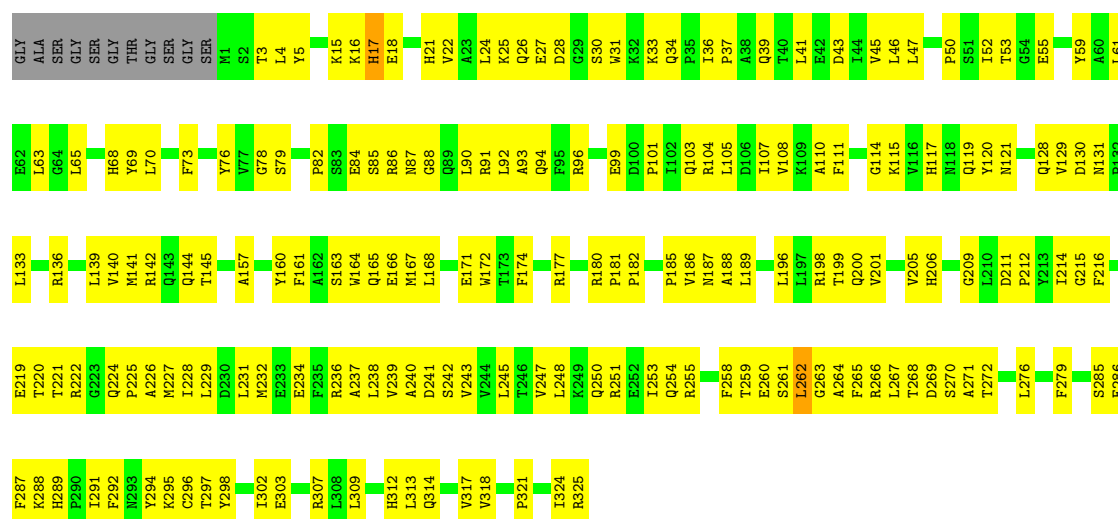
- Molecule 1: CRISPR-associated endonuclease Cas1





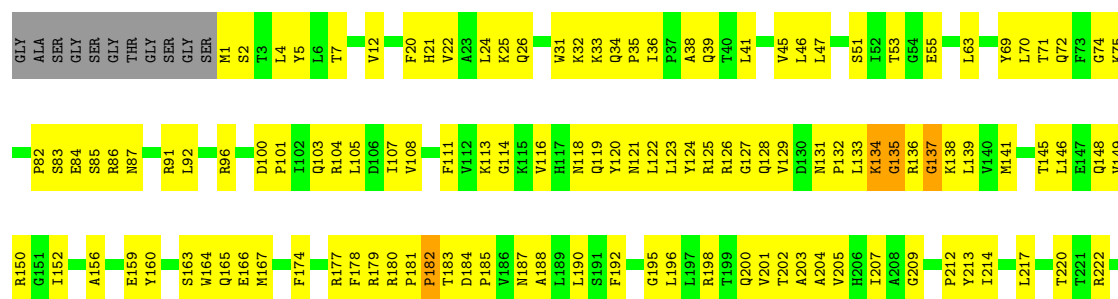
• Molecule 1: CRISPR-associated endonuclease Cas1

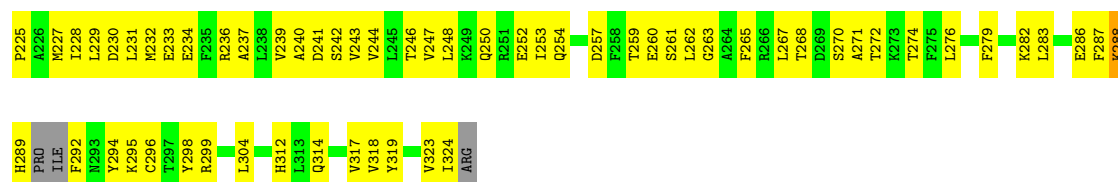
Chain s: 42% 54%



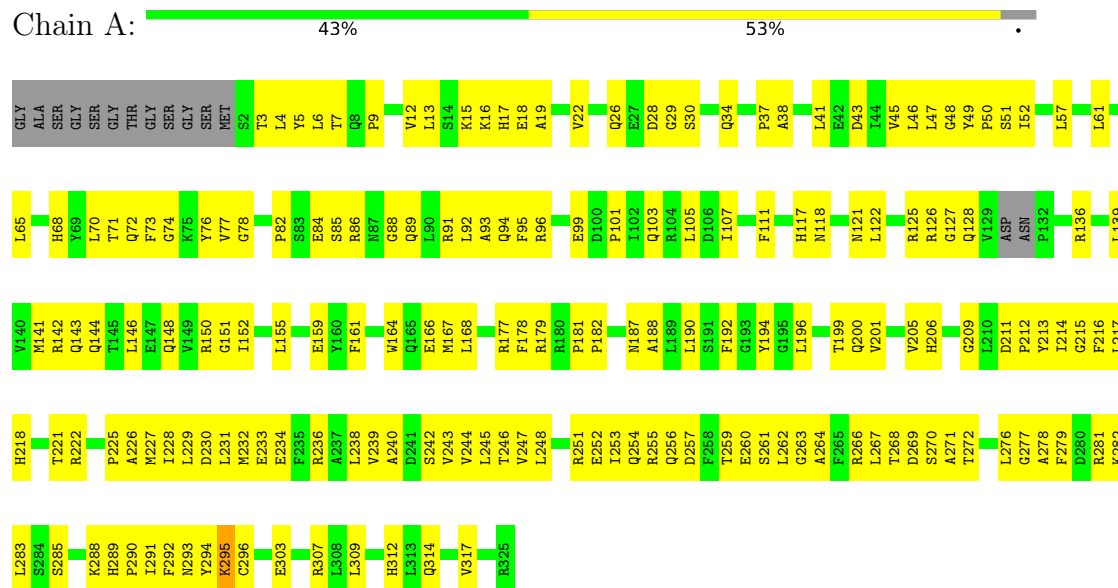
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain t: 42% 52%

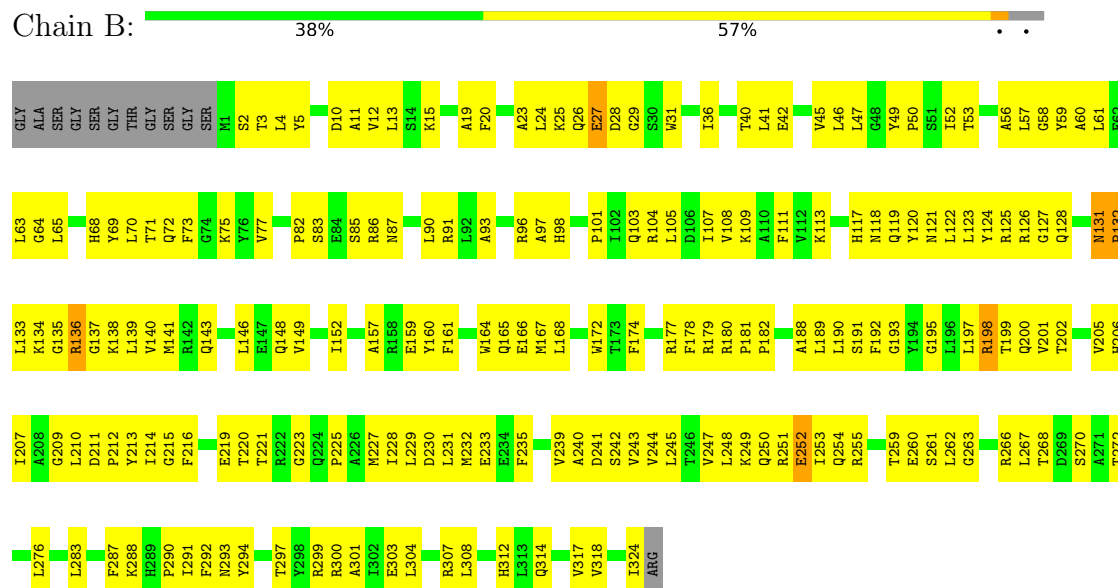




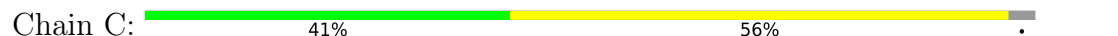
• Molecule 1: CRISPR-associated endonuclease Cas1

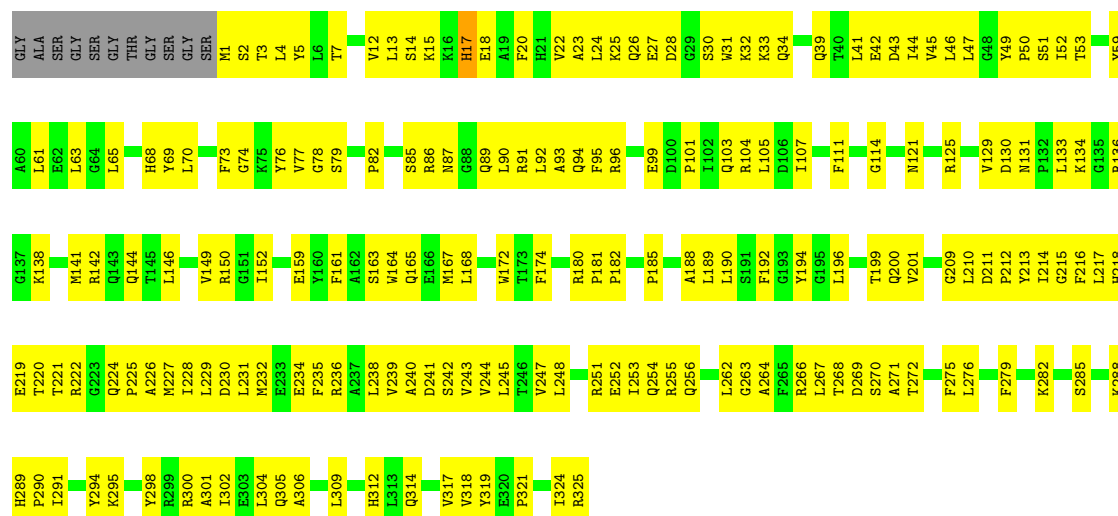


• Molecule 1: CRISPR-associated endonuclease Cas1



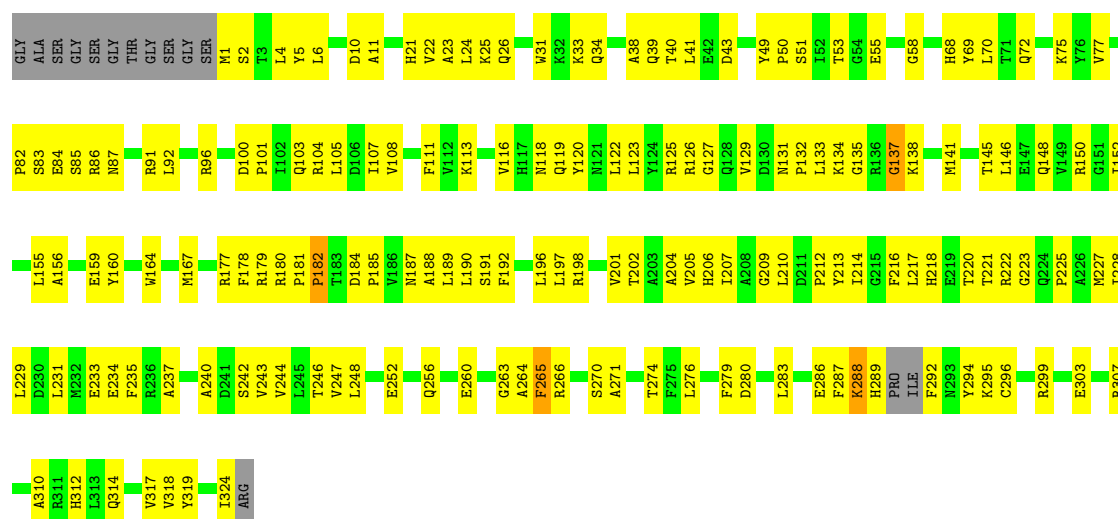
• Molecule 1: CRISPR-associated endonuclease Cas1





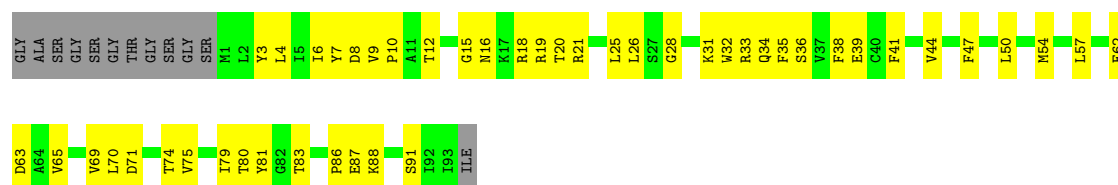
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain D: 47% 47% . .



• Molecule 2: CRISPR-associated endonuclease Cas2 1

Chain M: 44% 45% 11%



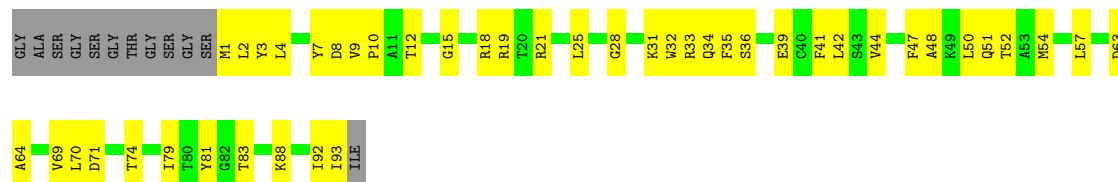
• Molecule 2: CRISPR-associated endonuclease Cas2 1

Chain N: 39% 50% 11%



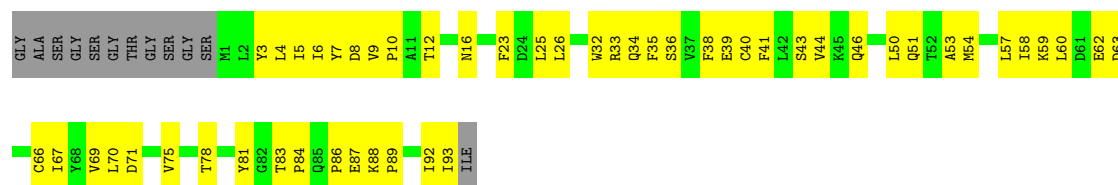
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain U: 47% 42% 11%



• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain V: 40% 49% 11%



• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain e: 48% 41% 11%



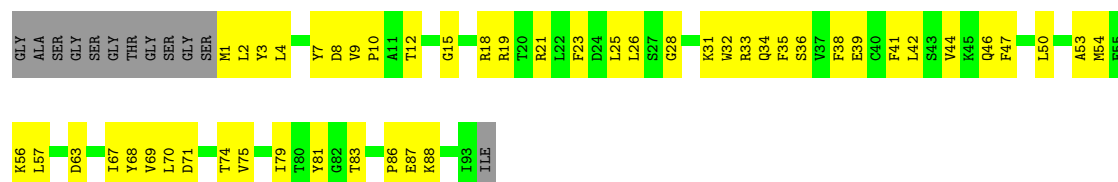
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain f: 49% 40% 11%

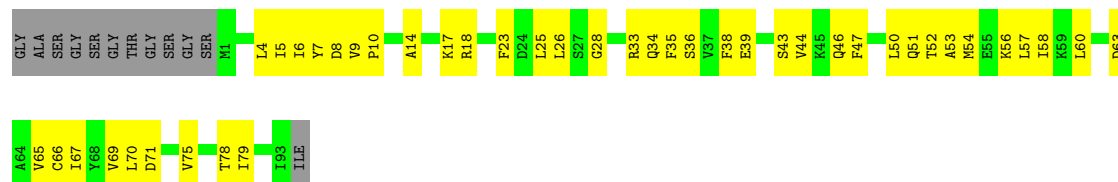


• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

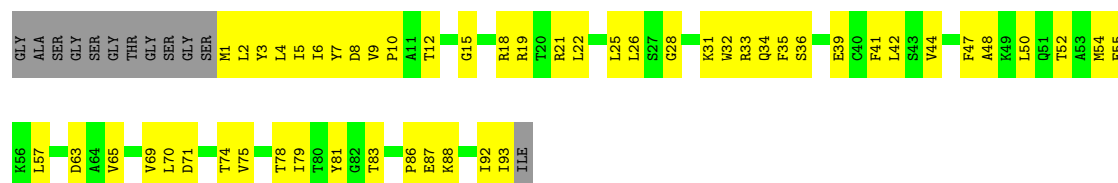
Chain m: 42% 47% 11%



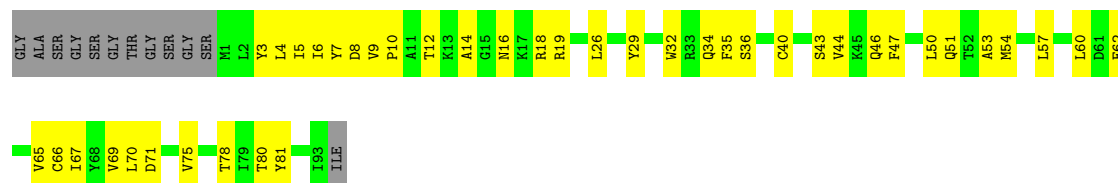
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1



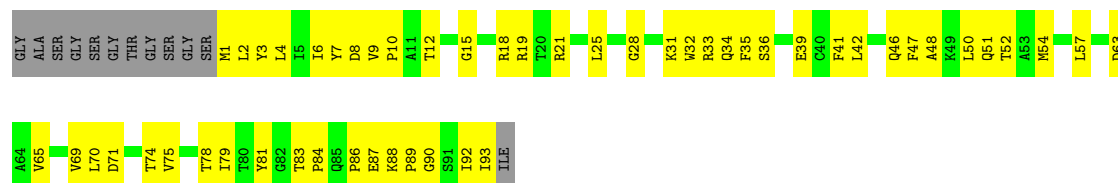
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1



• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

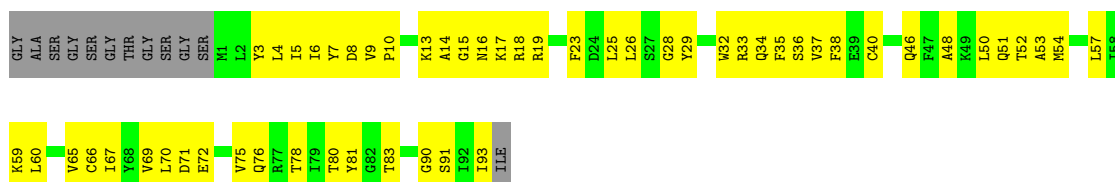


• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

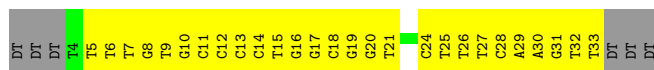


• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

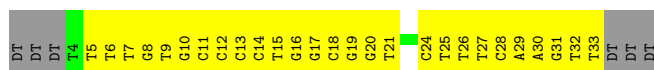




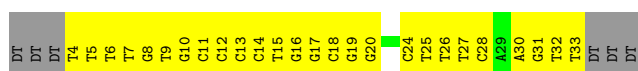
• Molecule 3: DNA (36-MER)



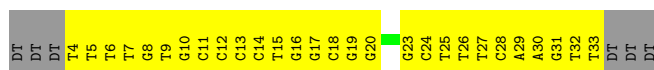
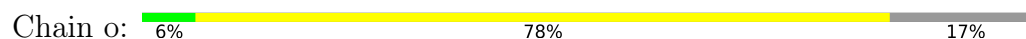
• Molecule 3: DNA (36-MER)



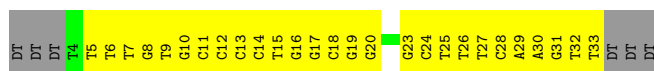
• Molecule 3: DNA (36-MER)



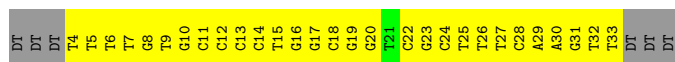
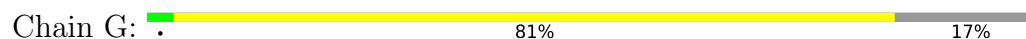
• Molecule 3: DNA (36-MER)



• Molecule 3: DNA (36-MER)

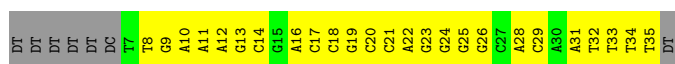


• Molecule 3: DNA (36-MER)



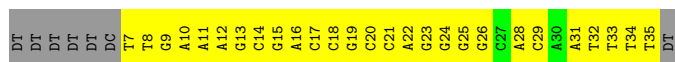
• Molecule 4: DNA (36-MER)

Chain P: 11% 69% 19%



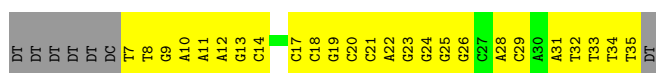
- Molecule 4: DNA (36-MER)

Chain X: 6% 75% 19%



- Molecule 4: DNA (36-MER)

Chain h: 11% 69% 19%



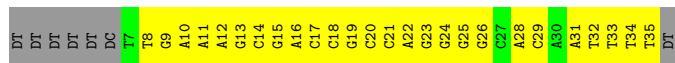
- Molecule 4: DNA (36-MER)

Chain p: 8% 72% 19%



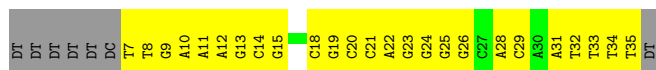
- Molecule 4: DNA (36-MER)

Chain x: 8% 72% 19%



- Molecule 4: DNA (36-MER)

Chain H: 11% 69% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	185.40Å 185.40Å 382.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.56 – 3.70 47.56 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.56-3.70) 99.9 (47.56-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.295 , 0.341 0.297 , 0.343	Depositor DCC
R_{free} test set	1573 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	129.3	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 220.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l 0.398 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	146030	wwPDB-VP
Average B, all atoms (Å ²)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.27	0/2646	0.57	0/3577
1	B	0.24	0/2660	0.60	2/3599 (0.1%)
1	C	0.24	0/2671	0.57	0/3613
1	D	0.22	0/2643	0.64	3/3573 (0.1%)
1	I	0.20	0/2646	0.58	0/3577
1	J	0.19	0/2660	0.56	0/3599
1	K	0.24	0/2671	0.57	0/3613
1	L	0.19	0/2643	0.58	1/3573 (0.0%)
1	Q	0.19	0/2646	0.54	0/3577
1	R	0.19	0/2660	0.57	0/3599
1	S	0.21	0/2671	0.55	0/3613
1	T	0.22	0/2643	0.61	3/3573 (0.1%)
1	a	0.19	0/2654	0.53	0/3587
1	b	0.22	0/2660	0.65	0/3599
1	c	0.20	0/2671	0.53	0/3613
1	d	0.17	0/2643	0.52	0/3573
1	i	0.20	0/2646	0.52	0/3577
1	j	0.19	0/2660	0.59	1/3599 (0.0%)
1	k	0.20	0/2671	0.55	0/3613
1	l	0.18	0/2643	0.53	0/3573
1	q	0.19	0/2646	0.56	0/3577
1	r	0.19	0/2660	0.57	1/3599 (0.0%)
1	s	0.19	0/2671	0.55	0/3613
1	t	0.20	0/2643	0.58	0/3573
2	E	0.27	0/769	0.50	0/1038
2	F	0.16	0/769	0.50	0/1038
2	M	0.15	0/769	0.45	0/1038
2	N	0.16	0/769	0.50	0/1038
2	U	0.15	0/769	0.46	0/1038
2	V	0.23	0/769	0.55	0/1038
2	e	0.16	0/769	0.48	0/1038
2	f	0.16	0/769	0.50	0/1038
2	m	0.14	0/769	0.45	0/1038
2	n	0.17	0/769	0.53	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	u	0.14	0/769	0.45	0/1038
2	v	0.15	0/769	0.51	0/1038
3	G	0.25	0/679	0.44	0/1046
3	O	0.20	0/679	0.42	0/1046
3	W	0.21	0/679	0.43	0/1046
3	g	0.22	0/679	0.43	0/1046
3	o	0.23	0/679	0.43	0/1046
3	w	0.20	0/679	0.42	0/1046
4	H	0.23	0/670	0.41	0/1032
4	P	0.23	0/670	0.44	0/1032
4	X	0.22	0/670	0.41	0/1032
4	h	0.22	0/670	0.42	0/1032
4	p	0.22	0/670	0.42	0/1032
4	x	0.20	0/670	0.41	0/1032
All	All	0.20	0/81050	0.55	11/111106 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
1	J	0	2
1	T	0	1
1	b	0	1
1	c	0	1
1	k	0	1
1	s	0	1
1	t	0	2
All	All	0	12

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	266	ARG	CB-CG-CD	9.96	134.20	111.30
1	T	133	LEU	N-CA-C	8.72	129.37	110.80
1	D	266	ARG	CA-CB-CG	8.54	131.19	114.10
1	r	133	LEU	N-CA-C	5.89	123.34	110.80
1	L	33	LYS	N-CA-C	5.82	117.81	110.24

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	131	ASN	Peptide
1	J	137	GLY	Peptide
1	T	261	SER	Peptide
1	b	290	PRO	Peptide
1	c	262	LEU	Peptide

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	2588	2484	2621	206	0
1	B	2601	2445	2630	229	6
1	C	2612	2354	2643	226	0
1	D	2586	2445	2611	156	2
1	I	2588	2484	2621	182	0
1	J	2601	2445	2630	182	2
1	K	2612	2354	2643	221	4
1	L	2586	2445	2611	169	2
1	Q	2588	2484	2621	177	0
1	R	2601	2445	2630	195	1
1	S	2612	2354	2643	193	0
1	T	2586	2445	2611	172	2
1	a	2596	2484	2633	184	0
1	b	2601	2445	2630	204	1
1	c	2612	2354	2643	190	2
1	d	2586	2445	2611	169	0
1	i	2588	2484	2621	168	0
1	j	2601	2445	2630	207	1
1	k	2612	2354	2643	195	2
1	l	2586	2445	2611	159	0
1	q	2588	2484	2621	175	0
1	r	2601	2445	2630	187	1
1	s	2612	2354	2643	180	0
1	t	2586	2445	2611	181	2
2	E	754	748	779	74	0
2	F	754	759	779	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	754	748	779	55	0
2	N	754	759	779	64	0
2	U	754	748	779	52	0
2	V	754	759	779	58	0
2	e	754	748	779	54	0
2	f	754	759	779	56	0
2	m	754	748	779	58	0
2	n	754	759	779	52	0
2	u	754	748	779	58	0
2	v	754	759	779	51	0
3	G	610	0	343	86	0
3	O	610	0	343	84	0
3	W	610	0	343	72	0
3	g	610	0	343	83	0
3	o	610	0	343	81	0
3	w	610	0	343	75	0
4	H	597	0	326	59	0
4	P	597	0	326	66	0
4	X	597	0	326	61	0
4	h	597	0	326	52	0
4	p	597	0	326	55	0
4	x	597	0	326	61	0
All	All	78620	67410	76404	5303	14

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 34.

The worst 5 of 5303 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:D:247:VAL:HB	1:D:252:GLU:OE2	1.29	1.27
1:s:262:LEU:HB3	1:s:264:ALA:HB2	1.15	1.12
1:C:15:LYS:NZ	3:G:9:DT:OP1	1.82	1.11
4:H:13:DG:H2''	4:H:14:DC:H5''	1.31	1.11
4:x:13:DG:H2''	4:x:14:DC:H5''	1.30	1.09

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:166:GLU:OE2	1:c:180:ARG:N[3_644]	1.87	0.33
1:k:180:ARG:N	1:t:166:GLU:OE2[3_754]	1.94	0.26
1:K:180:ARG:NH1	1:B:128:GLN:OE1[3_654]	1.98	0.22
1:K:180:ARG:H	1:B:166:GLU:OE2[3_654]	1.45	0.15
1:K:180:ARG:NH2	1:B:127:GLY:O[3_654]	2.06	0.14

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 X-ray entries followed by that with respect to entries of similar resolution.

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	318/336 (95%)	277 (87%)	40 (13%)	1 (0%)	36	65
1	B	322/336 (96%)	273 (85%)	44 (14%)	5 (2%)	7	35
1	C	323/336 (96%)	281 (87%)	41 (13%)	1 (0%)	36	65
1	D	318/336 (95%)	283 (89%)	30 (9%)	5 (2%)	7	35
1	I	318/336 (95%)	279 (88%)	38 (12%)	1 (0%)	36	65
1	J	322/336 (96%)	274 (85%)	43 (13%)	5 (2%)	7	35
1	K	323/336 (96%)	278 (86%)	45 (14%)	0	100	100
1	L	318/336 (95%)	278 (87%)	34 (11%)	6 (2%)	6	33
1	Q	318/336 (95%)	278 (87%)	39 (12%)	1 (0%)	36	65
1	R	322/336 (96%)	273 (85%)	46 (14%)	3 (1%)	14	45
1	S	323/336 (96%)	278 (86%)	44 (14%)	1 (0%)	36	65
1	T	318/336 (95%)	283 (89%)	30 (9%)	5 (2%)	7	35
1	a	319/336 (95%)	276 (86%)	42 (13%)	1 (0%)	36	65
1	b	322/336 (96%)	278 (86%)	36 (11%)	8 (2%)	4	29
1	c	323/336 (96%)	284 (88%)	38 (12%)	1 (0%)	36	65
1	d	318/336 (95%)	281 (88%)	32 (10%)	5 (2%)	7	35
1	i	318/336 (95%)	275 (86%)	42 (13%)	1 (0%)	36	65
1	j	322/336 (96%)	272 (84%)	46 (14%)	4 (1%)	10	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	k	323/336 (96%)	282 (87%)	40 (12%)	1 (0%)	36	65
1	l	318/336 (95%)	283 (89%)	30 (9%)	5 (2%)	7	35
1	q	318/336 (95%)	278 (87%)	39 (12%)	1 (0%)	36	65
1	r	322/336 (96%)	273 (85%)	46 (14%)	3 (1%)	14	45
1	s	323/336 (96%)	275 (85%)	47 (15%)	1 (0%)	36	65
1	t	318/336 (95%)	282 (89%)	30 (9%)	6 (2%)	6	33
2	E	91/105 (87%)	86 (94%)	4 (4%)	1 (1%)	11	42
2	F	91/105 (87%)	83 (91%)	8 (9%)	0	100	100
2	M	91/105 (87%)	86 (94%)	5 (6%)	0	100	100
2	N	91/105 (87%)	85 (93%)	6 (7%)	0	100	100
2	U	91/105 (87%)	87 (96%)	4 (4%)	0	100	100
2	V	91/105 (87%)	85 (93%)	5 (6%)	1 (1%)	11	42
2	e	91/105 (87%)	85 (93%)	6 (7%)	0	100	100
2	f	91/105 (87%)	86 (94%)	5 (6%)	0	100	100
2	m	91/105 (87%)	87 (96%)	4 (4%)	0	100	100
2	n	91/105 (87%)	86 (94%)	5 (6%)	0	100	100
2	u	91/105 (87%)	86 (94%)	5 (6%)	0	100	100
2	v	91/105 (87%)	85 (93%)	6 (7%)	0	100	100
All	All	8779/9324 (94%)	7701 (88%)	1005 (11%)	73 (1%)	16	48

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	134	LYS
1	b	132	PRO
1	l	138	LYS
1	I	295	LYS
1	J	27	GLU

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 X-ray entries followed by that with respect to entries of similar resolution.

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	272/280 (97%)	272 (100%)	0	100	100
1	B	274/280 (98%)	274 (100%)	0	100	100
1	C	275/280 (98%)	275 (100%)	0	100	100
1	D	272/280 (97%)	272 (100%)	0	100	100
1	I	272/280 (97%)	272 (100%)	0	100	100
1	J	274/280 (98%)	274 (100%)	0	100	100
1	K	275/280 (98%)	275 (100%)	0	100	100
1	L	272/280 (97%)	272 (100%)	0	100	100
1	Q	272/280 (97%)	272 (100%)	0	100	100
1	R	274/280 (98%)	274 (100%)	0	100	100
1	S	275/280 (98%)	275 (100%)	0	100	100
1	T	272/280 (97%)	272 (100%)	0	100	100
1	a	273/280 (98%)	273 (100%)	0	100	100
1	b	274/280 (98%)	274 (100%)	0	100	100
1	c	275/280 (98%)	275 (100%)	0	100	100
1	d	272/280 (97%)	272 (100%)	0	100	100
1	i	272/280 (97%)	272 (100%)	0	100	100
1	j	274/280 (98%)	274 (100%)	0	100	100
1	k	275/280 (98%)	275 (100%)	0	100	100
1	l	272/280 (97%)	272 (100%)	0	100	100
1	q	272/280 (97%)	272 (100%)	0	100	100
1	r	274/280 (98%)	274 (100%)	0	100	100
1	s	275/280 (98%)	275 (100%)	0	100	100
1	t	272/280 (97%)	272 (100%)	0	100	100
2	E	83/89 (93%)	83 (100%)	0	100	100
2	F	83/89 (93%)	83 (100%)	0	100	100
2	M	83/89 (93%)	83 (100%)	0	100	100
2	N	83/89 (93%)	83 (100%)	0	100	100
2	U	83/89 (93%)	83 (100%)	0	100	100
2	V	83/89 (93%)	83 (100%)	0	100	100
2	e	83/89 (93%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	f	83/89 (93%)	83 (100%)	0	100	100
2	m	83/89 (93%)	83 (100%)	0	100	100
2	n	83/89 (93%)	83 (100%)	0	100	100
2	u	83/89 (93%)	83 (100%)	0	100	100
2	v	83/89 (93%)	83 (100%)	0	100	100
All	All	7555/7788 (97%)	7555 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	k	314	GLN
1	s	128	GLN
1	l	98	HIS
1	r	94	GLN
1	s	314	GLN

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](#)

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	322/336 (95%)	-1.15	0	100	100	85, 136, 195, 232	0
1	B	324/336 (96%)	-1.09	0	100	100	97, 147, 198, 240	0
1	C	325/336 (96%)	-1.07	0	100	100	81, 130, 194, 221	0
1	D	322/336 (95%)	-1.07	0	100	100	93, 143, 198, 238	0
1	I	322/336 (95%)	-0.99	0	100	100	99, 146, 203, 232	0
1	J	324/336 (96%)	-1.05	0	100	100	105, 149, 203, 251	0
1	K	325/336 (96%)	-0.98	0	100	100	99, 143, 199, 227	0
1	L	322/336 (95%)	-1.04	0	100	100	97, 145, 203, 238	0
1	Q	322/336 (95%)	-1.07	0	100	100	102, 156, 204, 237	0
1	R	324/336 (96%)	-1.02	0	100	100	115, 161, 206, 245	0
1	S	325/336 (96%)	-0.99	0	100	100	89, 134, 195, 236	0
1	T	322/336 (95%)	-1.06	0	100	100	92, 144, 206, 239	0
1	a	323/336 (96%)	-0.99	1 (0%)	90	76	84, 150, 203, 241	0
1	b	324/336 (96%)	-0.98	1 (0%)	90	76	107, 153, 202, 243	0
1	c	325/336 (96%)	-1.06	0	100	100	106, 143, 195, 227	0
1	d	322/336 (95%)	-1.07	0	100	100	110, 156, 212, 236	0
1	i	322/336 (95%)	-1.08	0	100	100	100, 151, 203, 237	0
1	j	324/336 (96%)	-1.01	1 (0%)	90	76	107, 154, 199, 251	0
1	k	325/336 (96%)	-0.99	0	100	100	104, 143, 195, 226	0
1	l	322/336 (95%)	-1.14	0	100	100	110, 156, 209, 235	0
1	q	322/336 (95%)	-1.06	2 (0%)	85	66	100, 155, 201, 240	0
1	r	324/336 (96%)	-1.08	0	100	100	107, 161, 206, 243	0
1	s	325/336 (96%)	-1.00	0	100	100	90, 134, 196, 237	0
1	t	322/336 (95%)	-1.04	0	100	100	93, 145, 207, 240	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	E	93/105 (88%)	-1.10	0 100 100	109, 152, 192, 230	0
2	F	93/105 (88%)	-1.08	0 100 100	110, 156, 205, 219	0
2	M	93/105 (88%)	-1.11	0 100 100	116, 160, 193, 219	0
2	N	93/105 (88%)	-1.04	0 100 100	112, 162, 201, 215	0
2	U	93/105 (88%)	-0.96	0 100 100	122, 162, 195, 221	0
2	V	93/105 (88%)	-1.00	0 100 100	106, 160, 204, 219	0
2	e	93/105 (88%)	-1.09	0 100 100	122, 159, 198, 228	0
2	f	93/105 (88%)	-1.07	0 100 100	118, 160, 203, 220	0
2	m	93/105 (88%)	-1.09	0 100 100	122, 160, 199, 222	0
2	n	93/105 (88%)	-1.12	0 100 100	110, 160, 204, 218	0
2	u	93/105 (88%)	-1.03	0 100 100	126, 161, 196, 221	0
2	v	93/105 (88%)	-0.92	0 100 100	103, 163, 209, 218	0
3	G	30/36 (83%)	-0.74	0 100 100	154, 212, 242, 265	0
3	O	30/36 (83%)	-0.66	0 100 100	152, 216, 249, 269	0
3	W	30/36 (83%)	-0.56	0 100 100	156, 221, 244, 272	0
3	g	30/36 (83%)	-0.70	0 100 100	153, 219, 248, 264	0
3	o	30/36 (83%)	-0.60	0 100 100	153, 218, 247, 264	0
3	w	30/36 (83%)	-0.55	0 100 100	157, 220, 241, 270	0
4	H	29/36 (80%)	-0.73	0 100 100	187, 208, 232, 237	0
4	P	29/36 (80%)	-0.71	0 100 100	188, 209, 234, 238	0
4	X	29/36 (80%)	-0.68	0 100 100	193, 214, 237, 241	0
4	h	29/36 (80%)	-0.64	0 100 100	193, 214, 237, 242	0
4	p	29/36 (80%)	-0.60	0 100 100	194, 215, 236, 242	0
4	x	29/36 (80%)	-0.65	0 100 100	191, 215, 239, 242	0
All	All	9229/9756 (94%)	-1.03	5 (0%) 92 86	81, 151, 210, 272	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	b	154	GLY	3.2
1	j	151	GLY	3.2
1	a	180	ARG	3.2
1	q	34	GLN	2.4
1	q	24	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.