wwPDB X-ray Structure Validation Summary Report (i)

Nov 20, 2023 – 04:15 PM JST

PDB ID	:	7CR8
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 (i) 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 (i)) were used in the production of this report:

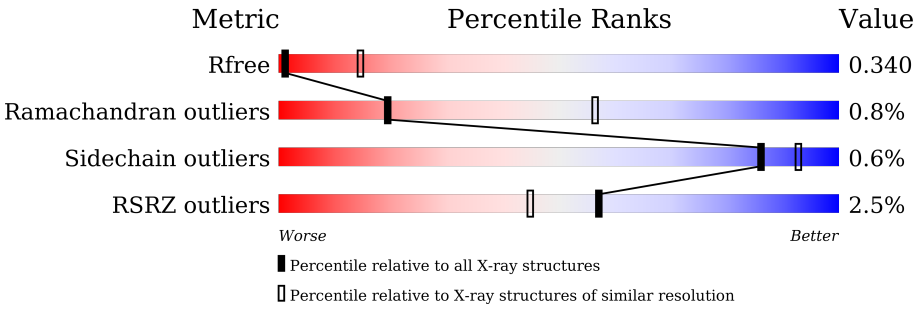
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1049 (3.88-3.52)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 <=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	94%
1	B	336	93%
1	C	336	96%
1	D	336	93%
1	I	336	95%
1	J	336	94%
1	K	336	95%

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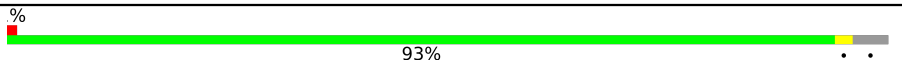
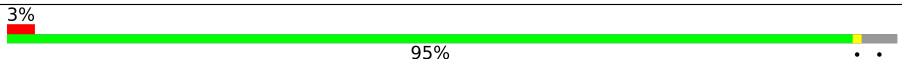
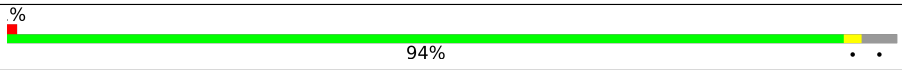
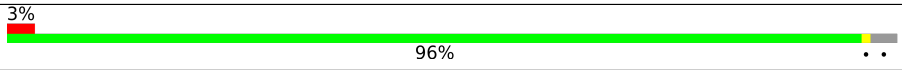
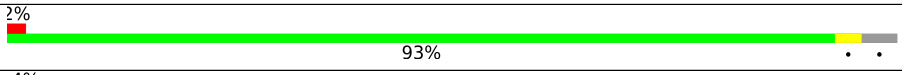
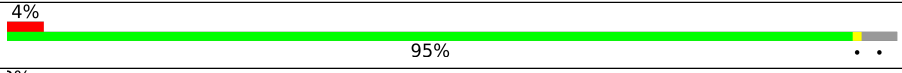
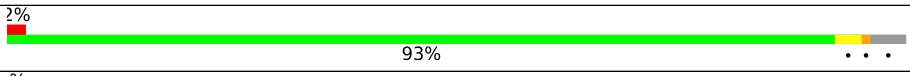
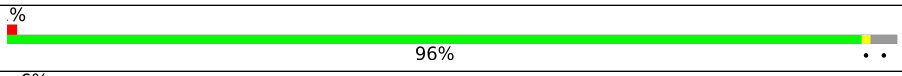
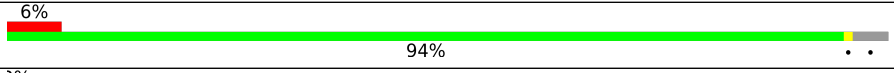
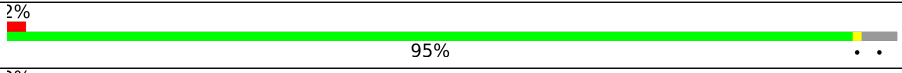
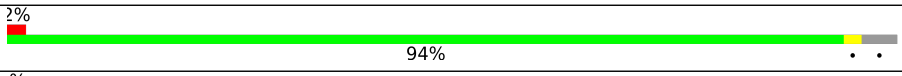
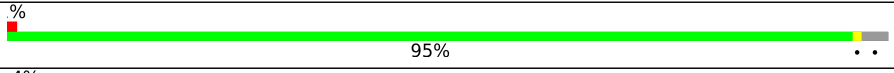
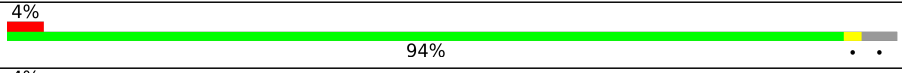
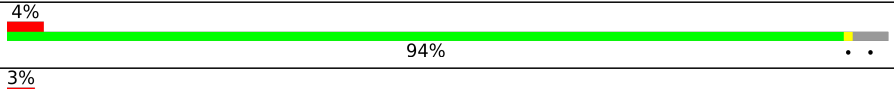
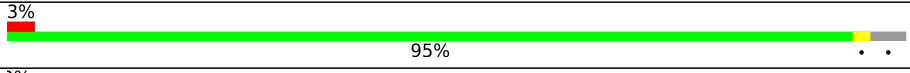
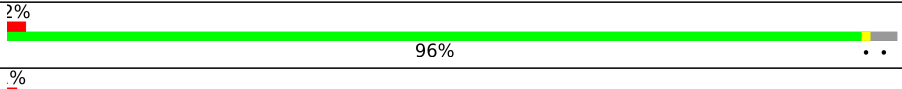
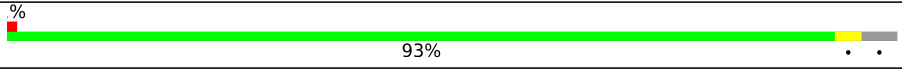
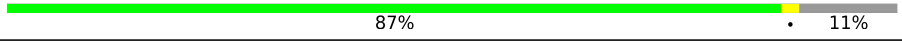
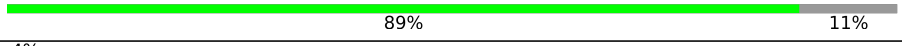
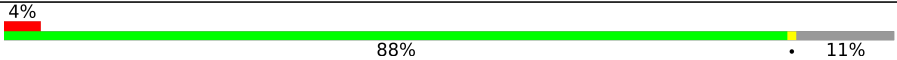
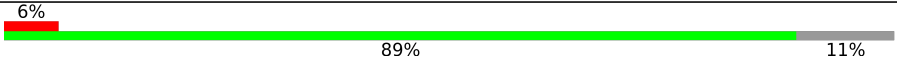
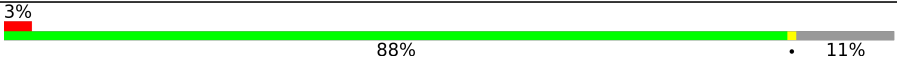
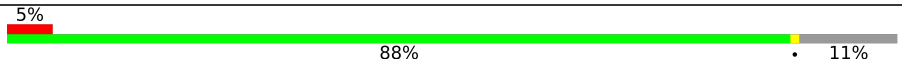
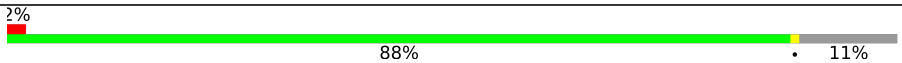
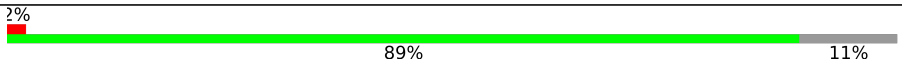
Mol	Chain	Length	Quality of chain
1	L	336	
1	Q	336	
1	R	336	
1	S	336	
1	T	336	
1	a	336	
1	b	336	
1	c	336	
1	d	336	
1	i	336	
1	j	336	
1	k	336	
1	l	336	
1	q	336	
1	r	336	
1	s	336	
1	t	336	
2	E	105	
2	F	105	
2	M	105	
2	N	105	
2	U	105	
2	V	105	
2	e	105	
2	f	105	

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Mol	Chain	Length	Quality of chain
2	m	105	88% 11%
2	n	105	89% 11%
2	u	105	3% 88% 11%
2	v	105	2% 89% 11%
3	G	36	83% 17%
3	O	36	83% 17%
3	W	36	6% 83% 17%
3	g	36	3% 83% 17%
3	o	36	3% 83% 17%
3	w	36	6% 83% 17%
4	H	36	81% 19%
4	P	36	81% 19%
4	X	36	81% 19%
4	h	36	81% 19%
4	p	36	3% 81% 19%
4	x	36	81% 19%

2 Entry composition (i)

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	C	H	N	O	S	0	0	0
			1502	490	748	124	136	4			
2	f	93	Total	C	H	N	O	S	0	0	0
			1513	490	759	124	136	4			
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			
2	E	93	Total	C	H	N	O	S	0	0	0
			1502	490	748	124	136	4			
2	F	93	Total	C	H	N	O	S	0	0	0
			1513	490	759	124	136	4			

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).

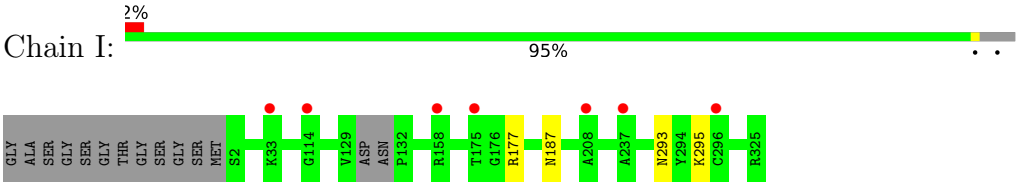
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	29	Total	C	N	O	P	0	0	0
			597	283	113	172	29			
4	X	29	Total	C	N	O	P	0	0	0
			597	283	113	172	29			
4	h	29	Total	C	N	O	P	0	0	0
			597	283	113	172	29			
4	p	29	Total	C	N	O	P	0	0	0
			597	283	113	172	29			
4	x	29	Total	C	N	O	P	0	0	0
			597	283	113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

3 Residue-property plots (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 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.

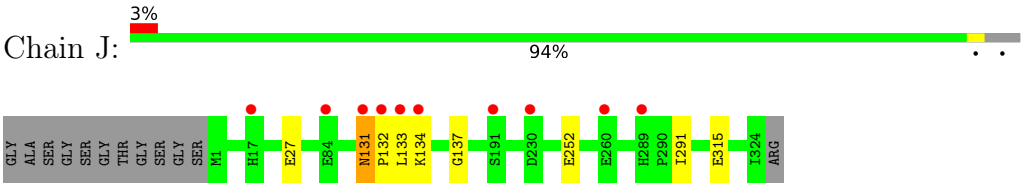
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain I:



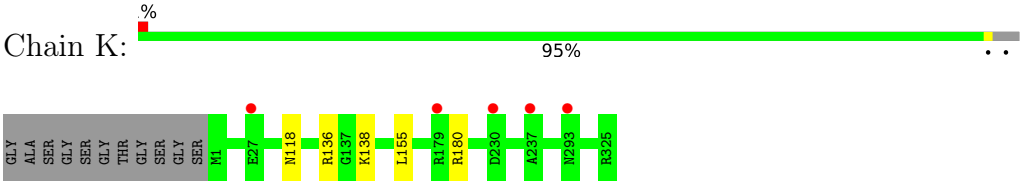
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain J:



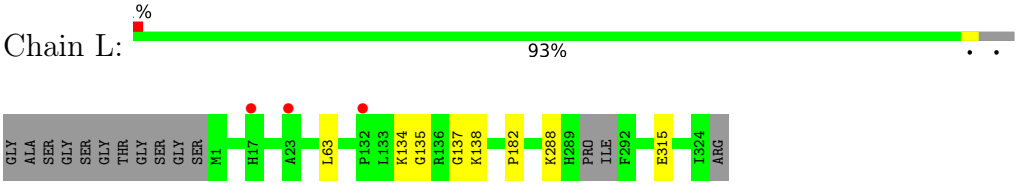
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain K:



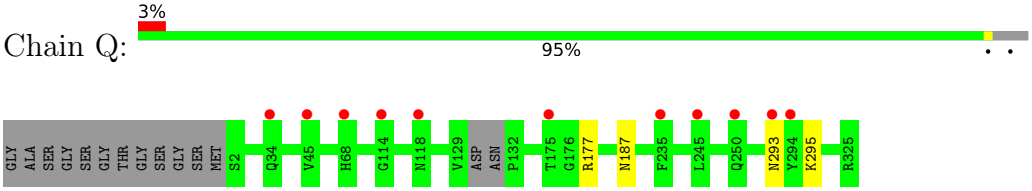
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain L:



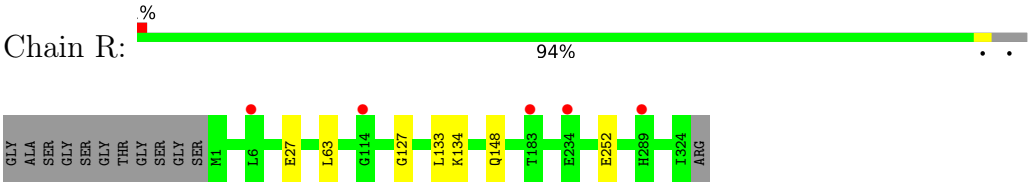
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain Q:



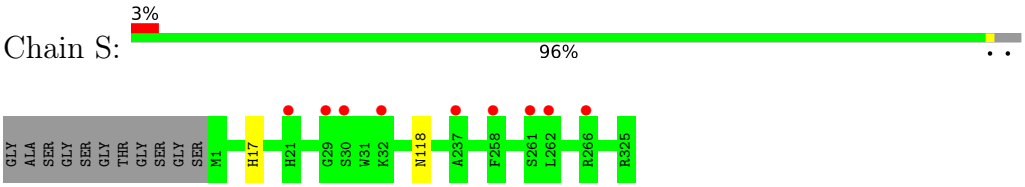
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain R:



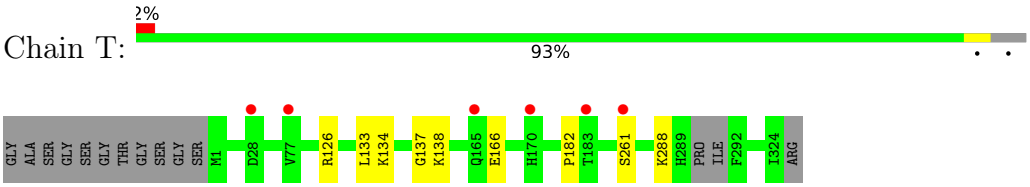
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain S:



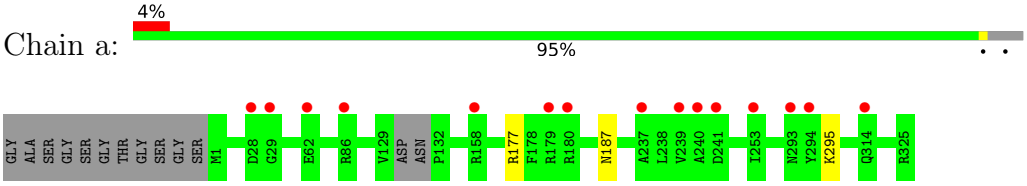
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain T:



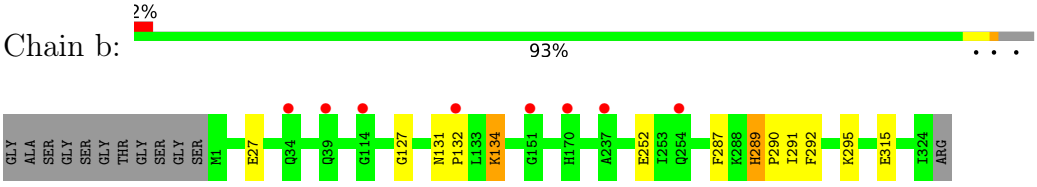
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain a:



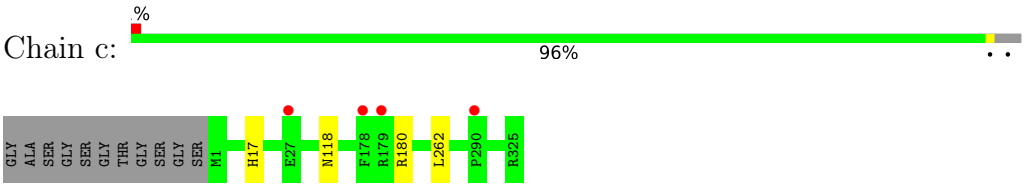
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain b:



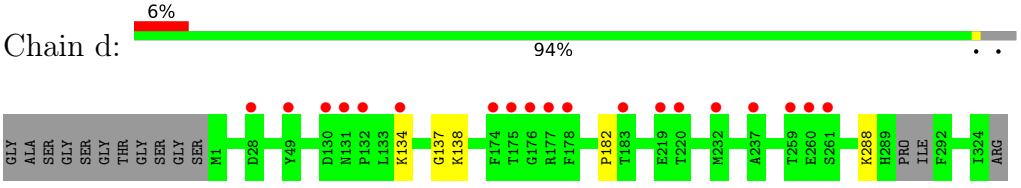
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain c:



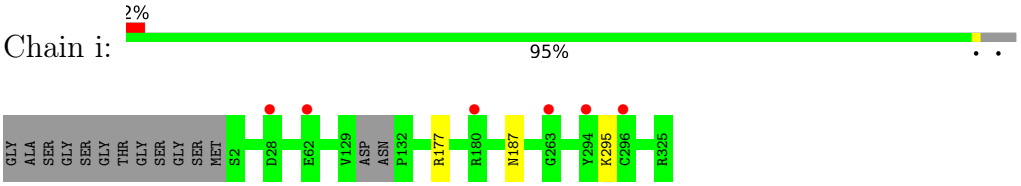
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain d:



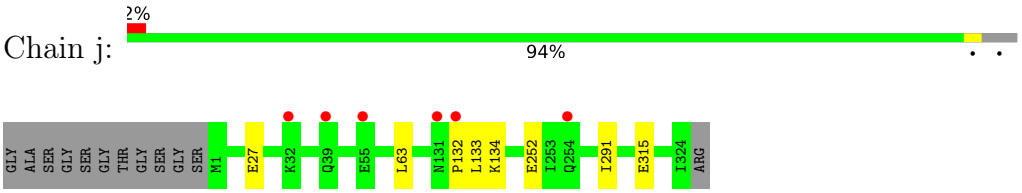
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain i:



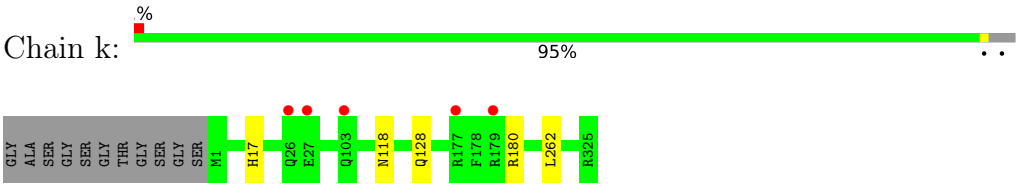
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain j:



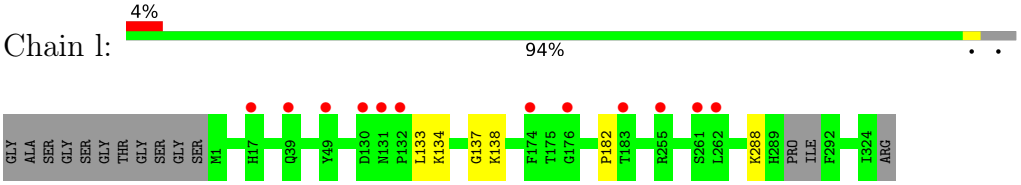
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain k:



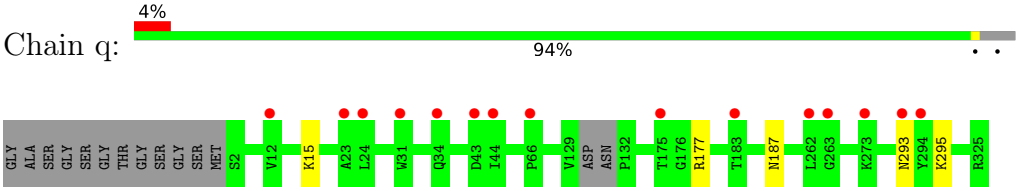
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain l:



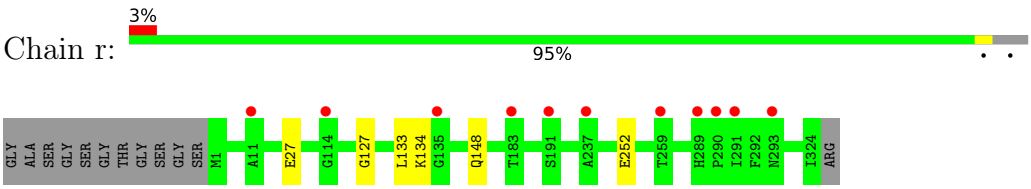
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain q:



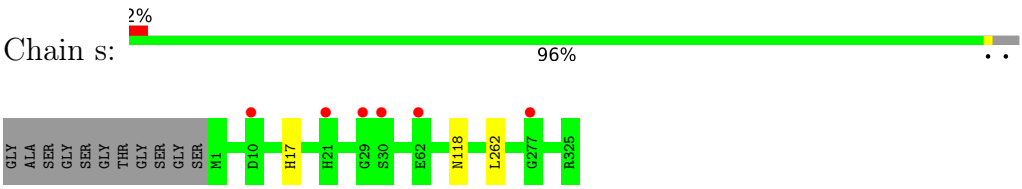
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain r:



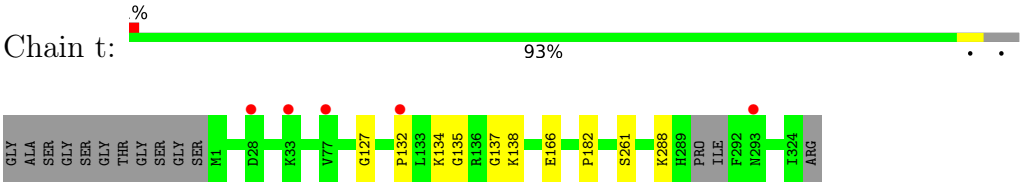
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain s:



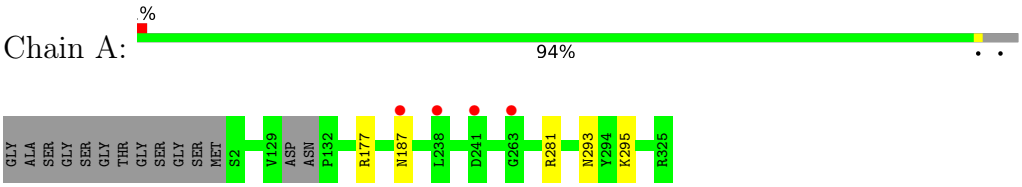
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain t:



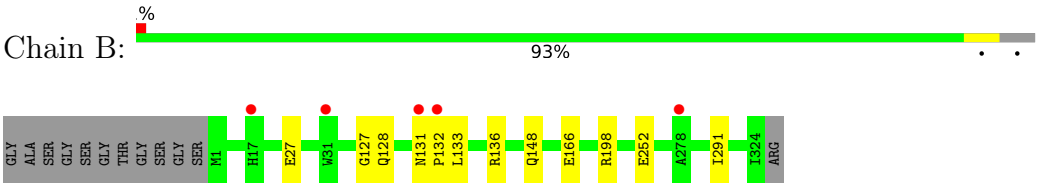
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain A:



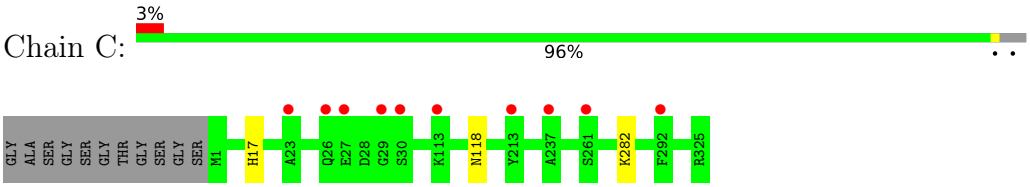
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain B:



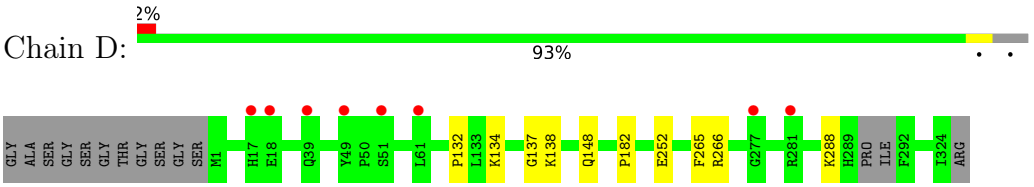
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain C:



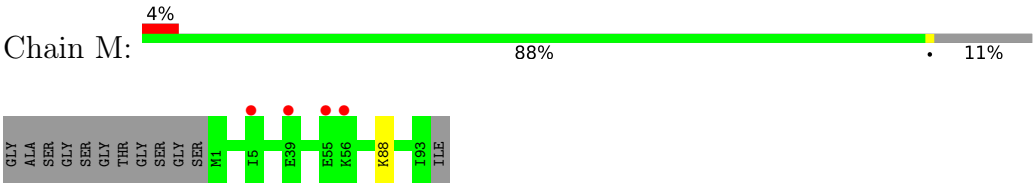
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain D:



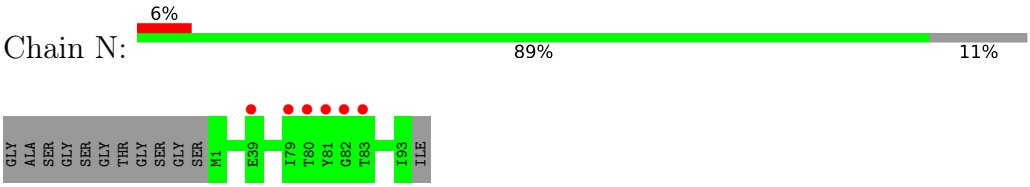
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain M:



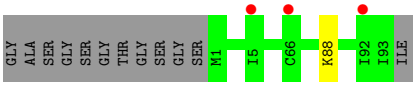
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain N:



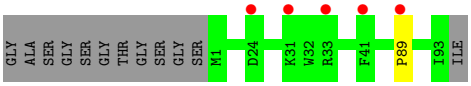
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain U:



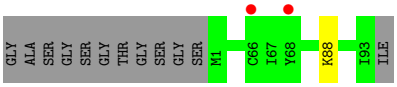
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain V:



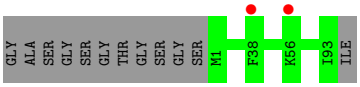
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain e:



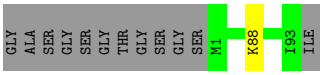
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain f:



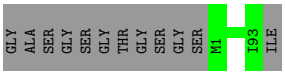
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain m:



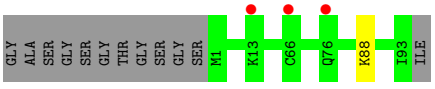
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain n:



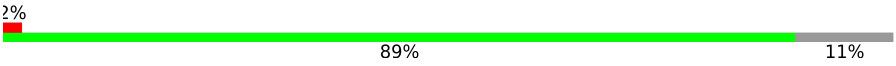
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

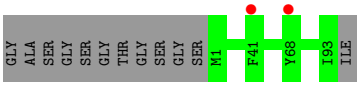
Chain u:



• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain v:



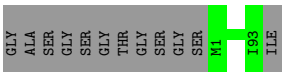


• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain E:

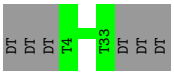
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

Chain F:



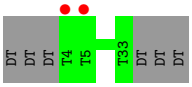
• Molecule 3: DNA (36-MER)

Chain O:



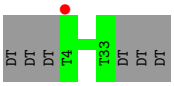
• Molecule 3: DNA (36-MER)

Chain W:



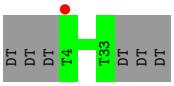
• Molecule 3: DNA (36-MER)

Chain g:



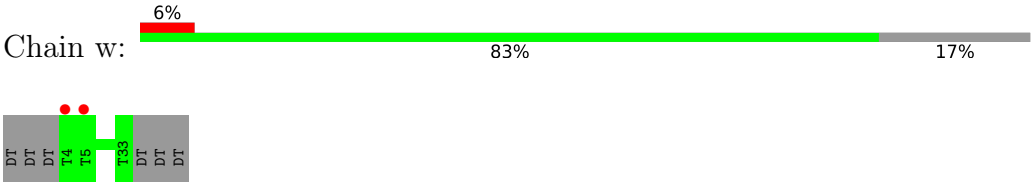
• Molecule 3: DNA (36-MER)

Chain o:



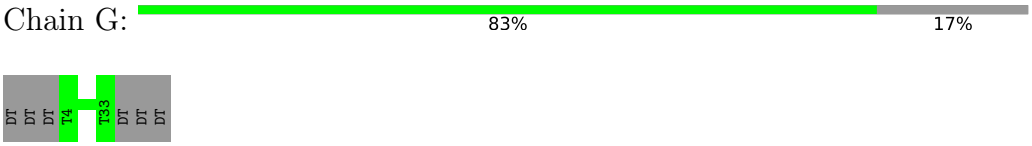
• Molecule 3: DNA (36-MER)

Chain w:



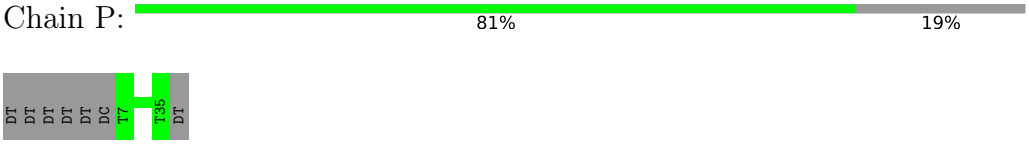
• Molecule 3: DNA (36-MER)

Chain G:



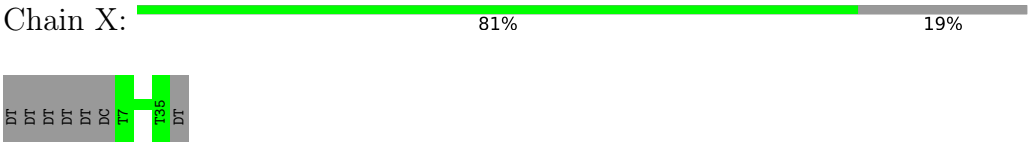
• Molecule 4: DNA (36-MER)

Chain P:



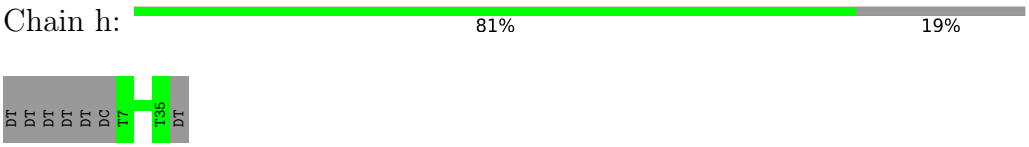
• Molecule 4: DNA (36-MER)

Chain X:



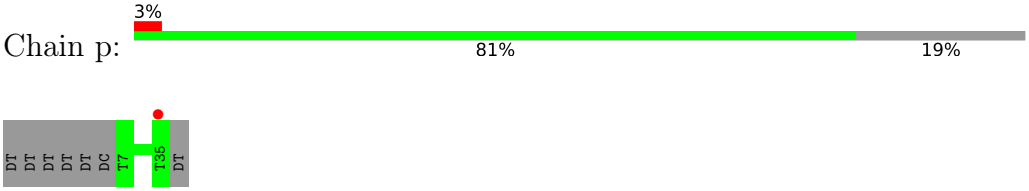
• Molecule 4: DNA (36-MER)

Chain h:



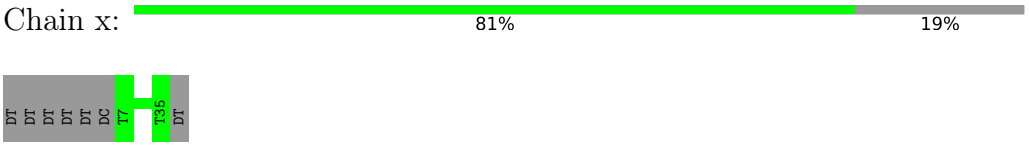
• Molecule 4: DNA (36-MER)

Chain p:



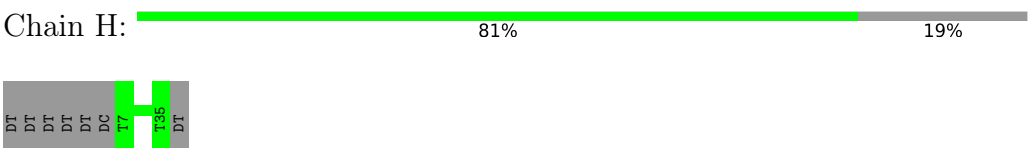
• Molecule 4: DNA (36-MER)

Chain x:



• Molecule 4: DNA (36-MER)

Chain H:



4 Data and refinement statistics (i)

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 49.36 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.56-3.70) 99.9 (49.36-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.295 , 0.341 0.295 , 0.340	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)	0.33 , 97.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	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	0.90	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.33	0/2646	0.60	1/3577 (0.0%)
1	B	0.31	0/2660	0.58	1/3599 (0.0%)
1	C	0.30	0/2671	0.55	0/3613
1	D	0.33	2/2643 (0.1%)	0.63	3/3573 (0.1%)
1	I	0.28	0/2646	0.57	0/3577
1	J	0.28	0/2660	0.55	0/3599
1	K	0.31	0/2671	0.59	2/3613 (0.1%)
1	L	0.28	0/2643	0.57	1/3573 (0.0%)
1	Q	0.28	0/2646	0.56	0/3577
1	R	0.28	0/2660	0.56	0/3599
1	S	0.28	0/2671	0.54	0/3613
1	T	0.29	0/2643	0.59	3/3573 (0.1%)
1	a	0.28	0/2654	0.55	0/3587
1	b	0.30	0/2660	0.61	0/3599
1	c	0.28	0/2671	0.52	0/3613
1	d	0.27	0/2643	0.54	0/3573
1	i	0.28	0/2646	0.54	0/3577
1	j	0.28	0/2660	0.57	0/3599
1	k	0.28	0/2671	0.54	0/3613
1	l	0.27	0/2643	0.55	1/3573 (0.0%)
1	q	0.28	0/2646	0.57	0/3577
1	r	0.28	0/2660	0.57	0/3599
1	s	0.28	0/2671	0.54	0/3613
1	t	0.29	0/2643	0.56	0/3573
2	E	0.33	0/769	0.53	0/1038
2	F	0.28	0/769	0.54	0/1038
2	M	0.26	0/769	0.49	0/1038
2	N	0.27	0/769	0.54	0/1038
2	U	0.27	0/769	0.53	0/1038
2	V	0.30	0/769	0.57	0/1038
2	e	0.28	0/769	0.55	0/1038
2	f	0.27	0/769	0.53	0/1038
2	m	0.26	0/769	0.53	0/1038
2	n	0.27	0/769	0.54	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	u	0.27	0/769	0.53	0/1038
2	v	0.26	0/769	0.55	0/1038
3	G	0.59	0/679	1.01	0/1046
3	O	0.51	0/679	0.99	0/1046
3	W	0.53	0/679	1.01	0/1046
3	g	0.55	0/679	1.00	0/1046
3	o	0.57	0/679	1.00	0/1046
3	w	0.51	0/679	1.00	0/1046
4	H	0.54	0/670	0.89	0/1032
4	P	0.54	0/670	0.90	0/1032
4	X	0.53	0/670	0.90	0/1032
4	h	0.55	0/670	0.91	0/1032
4	p	0.54	0/670	0.89	0/1032
4	x	0.51	0/670	0.90	0/1032
All	All	0.32	2/81050 (0.0%)	0.62	12/111106 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	252	GLU	CD-OE1	-5.58	1.19	1.25
1	D	252	GLU	CD-OE2	-5.04	1.20	1.25

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	266	ARG	CB-CG-CD	8.69	134.20	111.60
1	D	266	ARG	CA-CB-CG	8.09	131.19	113.40
1	T	126	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	T	133	LEU	N-CA-C	6.80	129.37	111.00
1	A	281	ARG	NE-CZ-NH1	6.73	123.67	120.30

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 (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	41 74
1	B	322/336 (96%)	273 (85%)	44 (14%)	5 (2%)	9 43
1	C	323/336 (96%)	281 (87%)	41 (13%)	1 (0%)	41 74
1	D	318/336 (95%)	283 (89%)	30 (9%)	5 (2%)	9 43
1	I	318/336 (95%)	279 (88%)	38 (12%)	1 (0%)	41 74
1	J	322/336 (96%)	274 (85%)	43 (13%)	5 (2%)	9 43
1	K	323/336 (96%)	278 (86%)	45 (14%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	318/336 (95%)	278 (87%)	34 (11%)	6 (2%)	8 40
1	Q	318/336 (95%)	278 (87%)	39 (12%)	1 (0%)	41 74
1	R	322/336 (96%)	273 (85%)	46 (14%)	3 (1%)	17 54
1	S	323/336 (96%)	278 (86%)	44 (14%)	1 (0%)	41 74
1	T	318/336 (95%)	283 (89%)	30 (9%)	5 (2%)	9 43
1	a	319/336 (95%)	276 (86%)	42 (13%)	1 (0%)	41 74
1	b	322/336 (96%)	278 (86%)	36 (11%)	8 (2%)	5 35
1	c	323/336 (96%)	284 (88%)	38 (12%)	1 (0%)	41 74
1	d	318/336 (95%)	281 (88%)	32 (10%)	5 (2%)	9 43
1	i	318/336 (95%)	275 (86%)	42 (13%)	1 (0%)	41 74
1	j	322/336 (96%)	272 (84%)	46 (14%)	4 (1%)	13 48
1	k	323/336 (96%)	282 (87%)	40 (12%)	1 (0%)	41 74
1	l	318/336 (95%)	283 (89%)	30 (9%)	5 (2%)	9 43
1	q	318/336 (95%)	278 (87%)	39 (12%)	1 (0%)	41 74
1	r	322/336 (96%)	273 (85%)	46 (14%)	3 (1%)	17 54
1	s	323/336 (96%)	275 (85%)	47 (15%)	1 (0%)	41 74
1	t	318/336 (95%)	282 (89%)	30 (9%)	6 (2%)	8 40
2	E	91/105 (87%)	86 (94%)	4 (4%)	1 (1%)	14 50
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%)	14 50
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%)	19 56

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 (i)

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%)	269 (99%)	3 (1%)	73 85
1	B	274/280 (98%)	273 (100%)	1 (0%)	91 95
1	C	275/280 (98%)	273 (99%)	2 (1%)	84 91
1	D	272/280 (97%)	272 (100%)	0	100 100
1	I	272/280 (97%)	269 (99%)	3 (1%)	73 85
1	J	274/280 (98%)	272 (99%)	2 (1%)	84 91
1	K	275/280 (98%)	273 (99%)	2 (1%)	84 91
1	L	272/280 (97%)	272 (100%)	0	100 100
1	Q	272/280 (97%)	269 (99%)	3 (1%)	73 85
1	R	274/280 (98%)	271 (99%)	3 (1%)	73 85
1	S	275/280 (98%)	274 (100%)	1 (0%)	91 95
1	T	272/280 (97%)	272 (100%)	0	100 100
1	a	273/280 (98%)	271 (99%)	2 (1%)	84 91
1	b	274/280 (98%)	269 (98%)	5 (2%)	59 77
1	c	275/280 (98%)	274 (100%)	1 (0%)	91 95
1	d	272/280 (97%)	272 (100%)	0	100 100
1	i	272/280 (97%)	270 (99%)	2 (1%)	84 91
1	j	274/280 (98%)	271 (99%)	3 (1%)	73 85
1	k	275/280 (98%)	273 (99%)	2 (1%)	84 91
1	l	272/280 (97%)	272 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	q	272/280 (97%)	268 (98%)	4 (2%)	65 81
1	r	274/280 (98%)	272 (99%)	2 (1%)	84 91
1	s	275/280 (98%)	274 (100%)	1 (0%)	91 95
1	t	272/280 (97%)	272 (100%)	0	100 100
2	E	83/89 (93%)	82 (99%)	1 (1%)	71 84
2	F	83/89 (93%)	83 (100%)	0	100 100
2	M	83/89 (93%)	82 (99%)	1 (1%)	71 84
2	N	83/89 (93%)	83 (100%)	0	100 100
2	U	83/89 (93%)	82 (99%)	1 (1%)	71 84
2	V	83/89 (93%)	83 (100%)	0	100 100
2	e	83/89 (93%)	82 (99%)	1 (1%)	71 84
2	f	83/89 (93%)	83 (100%)	0	100 100
2	m	83/89 (93%)	82 (99%)	1 (1%)	71 84
2	n	83/89 (93%)	83 (100%)	0	100 100
2	u	83/89 (93%)	82 (99%)	1 (1%)	71 84
2	v	83/89 (93%)	83 (100%)	0	100 100
All	All	7555/7788 (97%)	7507 (99%)	48 (1%)	86 93

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	j	133	LEU
1	q	187	ASN
1	j	134	LYS
2	m	88	LYS
1	r	133	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	i	143	GLN
1	k	314	GLN
1	D	314	GLN
1	B	224	GLN
1	i	200	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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(Å^2)	Q<0.9
1	A	322/336 (95%)	0.03	4 (1%)	79	69	78, 124, 182, 218	0
1	B	324/336 (96%)	0.03	5 (1%)	73	63	88, 134, 188, 210	0
1	C	325/336 (96%)	0.10	10 (3%)	49	36	78, 120, 185, 220	0
1	D	322/336 (95%)	0.04	8 (2%)	57	45	90, 130, 187, 233	0
1	I	322/336 (95%)	0.05	7 (2%)	62	50	92, 135, 191, 217	0
1	J	324/336 (96%)	0.22	10 (3%)	49	36	98, 136, 190, 229	0
1	K	325/336 (96%)	0.09	5 (1%)	73	63	92, 131, 190, 219	0
1	L	322/336 (95%)	0.14	3 (0%)	84	76	92, 132, 187, 238	0
1	Q	322/336 (95%)	0.11	11 (3%)	45	34	99, 141, 191, 215	0
1	R	324/336 (96%)	0.12	5 (1%)	73	63	106, 147, 193, 213	0
1	S	325/336 (96%)	0.19	9 (2%)	53	40	82, 123, 185, 214	0
1	T	322/336 (95%)	0.06	6 (1%)	66	55	85, 131, 193, 234	0
1	a	323/336 (96%)	0.15	15 (4%)	32	24	84, 137, 191, 219	0
1	b	324/336 (96%)	0.09	8 (2%)	57	45	101, 140, 192, 221	0
1	c	325/336 (96%)	0.07	4 (1%)	79	69	98, 131, 186, 223	0
1	d	322/336 (95%)	0.16	19 (5%)	22	15	103, 143, 196, 236	0
1	i	322/336 (95%)	0.08	6 (1%)	66	55	93, 138, 191, 215	0
1	j	324/336 (96%)	0.10	6 (1%)	66	55	101, 140, 190, 230	0
1	k	325/336 (96%)	0.08	5 (1%)	73	63	98, 131, 187, 225	0
1	l	322/336 (95%)	0.11	12 (3%)	41	30	103, 144, 194, 235	0
1	q	322/336 (95%)	0.17	15 (4%)	31	23	96, 142, 189, 218	0
1	r	324/336 (96%)	0.12	11 (3%)	45	34	100, 147, 194, 211	0
1	s	325/336 (96%)	0.17	6 (1%)	68	57	84, 122, 183, 214	0
1	t	322/336 (95%)	0.09	5 (1%)	72	61	85, 131, 191, 232	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	E	93/105 (88%)	-0.05	0 100 100	104, 140, 172, 214	0
2	F	93/105 (88%)	0.04	0 100 100	101, 143, 180, 207	0
2	M	93/105 (88%)	0.15	4 (4%) 35 26	109, 145, 172, 207	0
2	N	93/105 (88%)	0.23	6 (6%) 18 12	106, 148, 176, 195	0
2	U	93/105 (88%)	0.20	3 (3%) 47 35	112, 149, 179, 208	0
2	V	93/105 (88%)	0.20	5 (5%) 25 19	98, 148, 181, 200	0
2	e	93/105 (88%)	-0.01	2 (2%) 62 50	113, 146, 177, 213	0
2	f	93/105 (88%)	0.20	2 (2%) 62 50	108, 149, 180, 198	0
2	m	93/105 (88%)	0.02	0 100 100	112, 144, 179, 209	0
2	n	93/105 (88%)	0.17	0 100 100	105, 149, 181, 198	0
2	u	93/105 (88%)	0.12	3 (3%) 47 35	115, 147, 176, 208	0
2	v	93/105 (88%)	0.21	2 (2%) 62 50	97, 147, 182, 203	0
3	G	30/36 (83%)	-0.20	0 100 100	154, 212, 242, 265	0
3	O	30/36 (83%)	-0.09	0 100 100	152, 216, 249, 269	0
3	W	30/36 (83%)	0.06	2 (6%) 17 12	156, 221, 244, 272	0
3	g	30/36 (83%)	0.12	1 (3%) 46 35	153, 219, 248, 264	0
3	o	30/36 (83%)	0.17	1 (3%) 46 35	153, 218, 247, 264	0
3	w	30/36 (83%)	0.06	2 (6%) 17 12	157, 220, 241, 270	0
4	H	29/36 (80%)	-0.27	0 100 100	187, 208, 232, 237	0
4	P	29/36 (80%)	-0.08	0 100 100	188, 209, 234, 238	0
4	X	29/36 (80%)	-0.29	0 100 100	193, 214, 237, 241	0
4	h	29/36 (80%)	-0.16	0 100 100	193, 214, 237, 242	0
4	p	29/36 (80%)	-0.01	1 (3%) 45 34	194, 215, 236, 242	0
4	x	29/36 (80%)	-0.27	0 100 100	191, 215, 239, 242	0
All	All	9229/9756 (94%)	0.10	229 (2%) 57 45	78, 139, 201, 272	0

The worst 5 of 229 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	132	PRO	11.2
1	l	130	ASP	8.9
3	g	4	DT	8.6
3	o	4	DT	8.0
1	L	132	PRO	7.2

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 monosaccharides 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.