



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 07:22 AM EDT

PDB ID : 9QLR / pdb_00009qlr
Title : Nonamer crystal structure of the transcription factor MraZ from Mycoplasma genitalium
Authors : Reverter, D.; Sanchez-Alba, L.
Deposited on : 2025-03-21
Resolution : 3.85 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

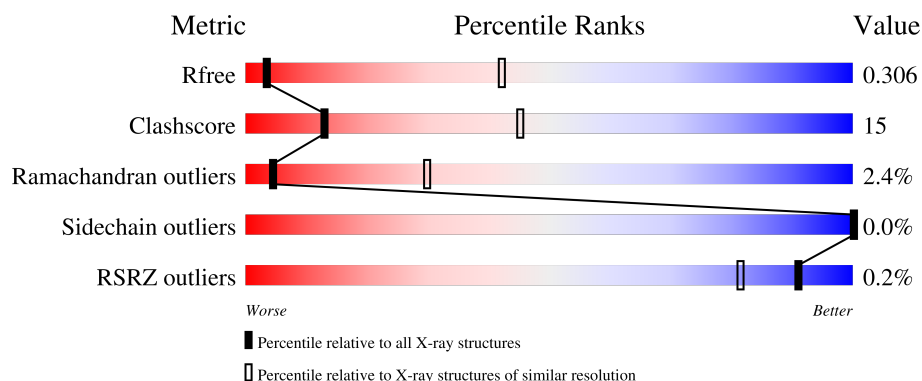
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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.



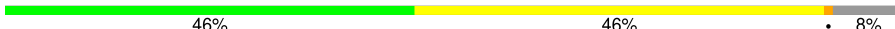
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

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	149	54% 38% 8%
1	B	149	62% 30% 8%
1	C	149	62% 30% 8%
1	D	149	52% 38% 8%
1	E	149	62% 30% 8%

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Mol	Chain	Length	Quality of chain
1	F	149	
1	G	149	
1	H	149	
1	I	149	
1	J	149	
1	K	149	
1	L	149	
1	M	149	
1	N	149	
1	O	149	
1	P	149	
1	Q	149	
1	R	149	
1	S	149	
1	T	149	
1	U	149	
1	V	149	
1	W	149	
1	X	149	
1	Y	149	
1	Z	149	
1	a	149	
1	b	149	
1	c	149	
1	d	149	

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Mol	Chain	Length	Quality of chain
1	e	149	% 50%40%8% ••
1	f	149	62%29%8% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 40248 atoms, of which 0 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 Transcriptional regulator MraZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	K	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	L	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	M	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	N	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	O	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	P	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	Q	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	R	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	A	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	B	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	C	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	D	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	E	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	F	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	G	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	I	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	S	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	T	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	U	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	V	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	W	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	X	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	Y	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	Z	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	a	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	b	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	c	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	d	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	e	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	f	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	g	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	h	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	i	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			
1	j	137	Total	C	N	O	S	0	0	0
			1118	712	190	213	3			

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	142	LEU	-	expression tag	UNP P47463
J	143	GLU	-	expression tag	UNP P47463
J	144	HIS	-	expression tag	UNP P47463
J	145	HIS	-	expression tag	UNP P47463
J	146	HIS	-	expression tag	UNP P47463
J	147	HIS	-	expression tag	UNP P47463
J	148	HIS	-	expression tag	UNP P47463
J	149	HIS	-	expression tag	UNP P47463
K	142	LEU	-	expression tag	UNP P47463
K	143	GLU	-	expression tag	UNP P47463
K	144	HIS	-	expression tag	UNP P47463
K	145	HIS	-	expression tag	UNP P47463
K	146	HIS	-	expression tag	UNP P47463
K	147	HIS	-	expression tag	UNP P47463
K	148	HIS	-	expression tag	UNP P47463
K	149	HIS	-	expression tag	UNP P47463
L	142	LEU	-	expression tag	UNP P47463
L	143	GLU	-	expression tag	UNP P47463
L	144	HIS	-	expression tag	UNP P47463
L	145	HIS	-	expression tag	UNP P47463
L	146	HIS	-	expression tag	UNP P47463
L	147	HIS	-	expression tag	UNP P47463
L	148	HIS	-	expression tag	UNP P47463
L	149	HIS	-	expression tag	UNP P47463
M	142	LEU	-	expression tag	UNP P47463
M	143	GLU	-	expression tag	UNP P47463
M	144	HIS	-	expression tag	UNP P47463
M	145	HIS	-	expression tag	UNP P47463
M	146	HIS	-	expression tag	UNP P47463
M	147	HIS	-	expression tag	UNP P47463
M	148	HIS	-	expression tag	UNP P47463
M	149	HIS	-	expression tag	UNP P47463
N	142	LEU	-	expression tag	UNP P47463
N	143	GLU	-	expression tag	UNP P47463
N	144	HIS	-	expression tag	UNP P47463
N	145	HIS	-	expression tag	UNP P47463
N	146	HIS	-	expression tag	UNP P47463
N	147	HIS	-	expression tag	UNP P47463
N	148	HIS	-	expression tag	UNP P47463
N	149	HIS	-	expression tag	UNP P47463
O	142	LEU	-	expression tag	UNP P47463
O	143	GLU	-	expression tag	UNP P47463
O	144	HIS	-	expression tag	UNP P47463

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Chain	Residue	Modelled	Actual	Comment	Reference
O	145	HIS	-	expression tag	UNP P47463
O	146	HIS	-	expression tag	UNP P47463
O	147	HIS	-	expression tag	UNP P47463
O	148	HIS	-	expression tag	UNP P47463
O	149	HIS	-	expression tag	UNP P47463
P	142	LEU	-	expression tag	UNP P47463
P	143	GLU	-	expression tag	UNP P47463
P	144	HIS	-	expression tag	UNP P47463
P	145	HIS	-	expression tag	UNP P47463
P	146	HIS	-	expression tag	UNP P47463
P	147	HIS	-	expression tag	UNP P47463
P	148	HIS	-	expression tag	UNP P47463
P	149	HIS	-	expression tag	UNP P47463
Q	142	LEU	-	expression tag	UNP P47463
Q	143	GLU	-	expression tag	UNP P47463
Q	144	HIS	-	expression tag	UNP P47463
Q	145	HIS	-	expression tag	UNP P47463
Q	146	HIS	-	expression tag	UNP P47463
Q	147	HIS	-	expression tag	UNP P47463
Q	148	HIS	-	expression tag	UNP P47463
Q	149	HIS	-	expression tag	UNP P47463
R	142	LEU	-	expression tag	UNP P47463
R	143	GLU	-	expression tag	UNP P47463
R	144	HIS	-	expression tag	UNP P47463
R	145	HIS	-	expression tag	UNP P47463
R	146	HIS	-	expression tag	UNP P47463
R	147	HIS	-	expression tag	UNP P47463
R	148	HIS	-	expression tag	UNP P47463
R	149	HIS	-	expression tag	UNP P47463
A	142	LEU	-	expression tag	UNP P47463
A	143	GLU	-	expression tag	UNP P47463
A	144	HIS	-	expression tag	UNP P47463
A	145	HIS	-	expression tag	UNP P47463
A	146	HIS	-	expression tag	UNP P47463
A	147	HIS	-	expression tag	UNP P47463
A	148	HIS	-	expression tag	UNP P47463
A	149	HIS	-	expression tag	UNP P47463
B	142	LEU	-	expression tag	UNP P47463
B	143	GLU	-	expression tag	UNP P47463
B	144	HIS	-	expression tag	UNP P47463
B	145	HIS	-	expression tag	UNP P47463
B	146	HIS	-	expression tag	UNP P47463

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Chain	Residue	Modelled	Actual	Comment	Reference
B	147	HIS	-	expression tag	UNP P47463
B	148	HIS	-	expression tag	UNP P47463
B	149	HIS	-	expression tag	UNP P47463
C	142	LEU	-	expression tag	UNP P47463
C	143	GLU	-	expression tag	UNP P47463
C	144	HIS	-	expression tag	UNP P47463
C	145	HIS	-	expression tag	UNP P47463
C	146	HIS	-	expression tag	UNP P47463
C	147	HIS	-	expression tag	UNP P47463
C	148	HIS	-	expression tag	UNP P47463
C	149	HIS	-	expression tag	UNP P47463
D	142	LEU	-	expression tag	UNP P47463
D	143	GLU	-	expression tag	UNP P47463
D	144	HIS	-	expression tag	UNP P47463
D	145	HIS	-	expression tag	UNP P47463
D	146	HIS	-	expression tag	UNP P47463
D	147	HIS	-	expression tag	UNP P47463
D	148	HIS	-	expression tag	UNP P47463
D	149	HIS	-	expression tag	UNP P47463
E	142	LEU	-	expression tag	UNP P47463
E	143	GLU	-	expression tag	UNP P47463
E	144	HIS	-	expression tag	UNP P47463
E	145	HIS	-	expression tag	UNP P47463
E	146	HIS	-	expression tag	UNP P47463
E	147	HIS	-	expression tag	UNP P47463
E	148	HIS	-	expression tag	UNP P47463
E	149	HIS	-	expression tag	UNP P47463
F	142	LEU	-	expression tag	UNP P47463
F	143	GLU	-	expression tag	UNP P47463
F	144	HIS	-	expression tag	UNP P47463
F	145	HIS	-	expression tag	UNP P47463
F	146	HIS	-	expression tag	UNP P47463
F	147	HIS	-	expression tag	UNP P47463
F	148	HIS	-	expression tag	UNP P47463
F	149	HIS	-	expression tag	UNP P47463
G	142	LEU	-	expression tag	UNP P47463
G	143	GLU	-	expression tag	UNP P47463
G	144	HIS	-	expression tag	UNP P47463
G	145	HIS	-	expression tag	UNP P47463
G	146	HIS	-	expression tag	UNP P47463
G	147	HIS	-	expression tag	UNP P47463
G	148	HIS	-	expression tag	UNP P47463

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Chain	Residue	Modelled	Actual	Comment	Reference
G	149	HIS	-	expression tag	UNP P47463
H	142	LEU	-	expression tag	UNP P47463
H	143	GLU	-	expression tag	UNP P47463
H	144	HIS	-	expression tag	UNP P47463
H	145	HIS	-	expression tag	UNP P47463
H	146	HIS	-	expression tag	UNP P47463
H	147	HIS	-	expression tag	UNP P47463
H	148	HIS	-	expression tag	UNP P47463
H	149	HIS	-	expression tag	UNP P47463
I	142	LEU	-	expression tag	UNP P47463
I	143	GLU	-	expression tag	UNP P47463
I	144	HIS	-	expression tag	UNP P47463
I	145	HIS	-	expression tag	UNP P47463
I	146	HIS	-	expression tag	UNP P47463
I	147	HIS	-	expression tag	UNP P47463
I	148	HIS	-	expression tag	UNP P47463
I	149	HIS	-	expression tag	UNP P47463
S	142	LEU	-	expression tag	UNP P47463
S	143	GLU	-	expression tag	UNP P47463
S	144	HIS	-	expression tag	UNP P47463
S	145	HIS	-	expression tag	UNP P47463
S	146	HIS	-	expression tag	UNP P47463
S	147	HIS	-	expression tag	UNP P47463
S	148	HIS	-	expression tag	UNP P47463
S	149	HIS	-	expression tag	UNP P47463
T	142	LEU	-	expression tag	UNP P47463
T	143	GLU	-	expression tag	UNP P47463
T	144	HIS	-	expression tag	UNP P47463
T	145	HIS	-	expression tag	UNP P47463
T	146	HIS	-	expression tag	UNP P47463
T	147	HIS	-	expression tag	UNP P47463
T	148	HIS	-	expression tag	UNP P47463
T	149	HIS	-	expression tag	UNP P47463
U	142	LEU	-	expression tag	UNP P47463
U	143	GLU	-	expression tag	UNP P47463
U	144	HIS	-	expression tag	UNP P47463
U	145	HIS	-	expression tag	UNP P47463
U	146	HIS	-	expression tag	UNP P47463
U	147	HIS	-	expression tag	UNP P47463
U	148	HIS	-	expression tag	UNP P47463
U	149	HIS	-	expression tag	UNP P47463
V	142	LEU	-	expression tag	UNP P47463

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Chain	Residue	Modelled	Actual	Comment	Reference
V	143	GLU	-	expression tag	UNP P47463
V	144	HIS	-	expression tag	UNP P47463
V	145	HIS	-	expression tag	UNP P47463
V	146	HIS	-	expression tag	UNP P47463
V	147	HIS	-	expression tag	UNP P47463
V	148	HIS	-	expression tag	UNP P47463
V	149	HIS	-	expression tag	UNP P47463
W	142	LEU	-	expression tag	UNP P47463
W	143	GLU	-	expression tag	UNP P47463
W	144	HIS	-	expression tag	UNP P47463
W	145	HIS	-	expression tag	UNP P47463
W	146	HIS	-	expression tag	UNP P47463
W	147	HIS	-	expression tag	UNP P47463
W	148	HIS	-	expression tag	UNP P47463
W	149	HIS	-	expression tag	UNP P47463
X	142	LEU	-	expression tag	UNP P47463
X	143	GLU	-	expression tag	UNP P47463
X	144	HIS	-	expression tag	UNP P47463
X	145	HIS	-	expression tag	UNP P47463
X	146	HIS	-	expression tag	UNP P47463
X	147	HIS	-	expression tag	UNP P47463
X	148	HIS	-	expression tag	UNP P47463
X	149	HIS	-	expression tag	UNP P47463
Y	142	LEU	-	expression tag	UNP P47463
Y	143	GLU	-	expression tag	UNP P47463
Y	144	HIS	-	expression tag	UNP P47463
Y	145	HIS	-	expression tag	UNP P47463
Y	146	HIS	-	expression tag	UNP P47463
Y	147	HIS	-	expression tag	UNP P47463
Y	148	HIS	-	expression tag	UNP P47463
Y	149	HIS	-	expression tag	UNP P47463
Z	142	LEU	-	expression tag	UNP P47463
Z	143	GLU	-	expression tag	UNP P47463
Z	144	HIS	-	expression tag	UNP P47463
Z	145	HIS	-	expression tag	UNP P47463
Z	146	HIS	-	expression tag	UNP P47463
Z	147	HIS	-	expression tag	UNP P47463
Z	148	HIS	-	expression tag	UNP P47463
Z	149	HIS	-	expression tag	UNP P47463
a	142	LEU	-	expression tag	UNP P47463
a	143	GLU	-	expression tag	UNP P47463
a	144	HIS	-	expression tag	UNP P47463

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Chain	Residue	Modelled	Actual	Comment	Reference
a	145	HIS	-	expression tag	UNP P47463
a	146	HIS	-	expression tag	UNP P47463
a	147	HIS	-	expression tag	UNP P47463
a	148	HIS	-	expression tag	UNP P47463
a	149	HIS	-	expression tag	UNP P47463
b	142	LEU	-	expression tag	UNP P47463
b	143	GLU	-	expression tag	UNP P47463
b	144	HIS	-	expression tag	UNP P47463
b	145	HIS	-	expression tag	UNP P47463
b	146	HIS	-	expression tag	UNP P47463
b	147	HIS	-	expression tag	UNP P47463
b	148	HIS	-	expression tag	UNP P47463
b	149	HIS	-	expression tag	UNP P47463
c	142	LEU	-	expression tag	UNP P47463
c	143	GLU	-	expression tag	UNP P47463
c	144	HIS	-	expression tag	UNP P47463
c	145	HIS	-	expression tag	UNP P47463
c	146	HIS	-	expression tag	UNP P47463
c	147	HIS	-	expression tag	UNP P47463
c	148	HIS	-	expression tag	UNP P47463
c	149	HIS	-	expression tag	UNP P47463
d	142	LEU	-	expression tag	UNP P47463
d	143	GLU	-	expression tag	UNP P47463
d	144	HIS	-	expression tag	UNP P47463
d	145	HIS	-	expression tag	UNP P47463
d	146	HIS	-	expression tag	UNP P47463
d	147	HIS	-	expression tag	UNP P47463
d	148	HIS	-	expression tag	UNP P47463
d	149	HIS	-	expression tag	UNP P47463
e	142	LEU	-	expression tag	UNP P47463
e	143	GLU	-	expression tag	UNP P47463
e	144	HIS	-	expression tag	UNP P47463
e	145	HIS	-	expression tag	UNP P47463
e	146	HIS	-	expression tag	UNP P47463
e	147	HIS	-	expression tag	UNP P47463
e	148	HIS	-	expression tag	UNP P47463
e	149	HIS	-	expression tag	UNP P47463
f	142	LEU	-	expression tag	UNP P47463
f	143	GLU	-	expression tag	UNP P47463
f	144	HIS	-	expression tag	UNP P47463
f	145	HIS	-	expression tag	UNP P47463
f	146	HIS	-	expression tag	UNP P47463

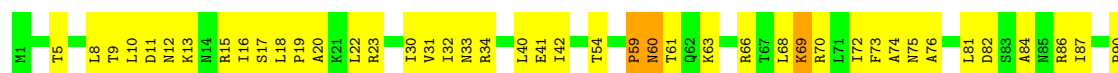
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Chain	Residue	Modelled	Actual	Comment	Reference
f	147	HIS	-	expression tag	UNP P47463
f	148	HIS	-	expression tag	UNP P47463
f	149	HIS	-	expression tag	UNP P47463
g	142	LEU	-	expression tag	UNP P47463
g	143	GLU	-	expression tag	UNP P47463
g	144	HIS	-	expression tag	UNP P47463
g	145	HIS	-	expression tag	UNP P47463
g	146	HIS	-	expression tag	UNP P47463
g	147	HIS	-	expression tag	UNP P47463
g	148	HIS	-	expression tag	UNP P47463
g	149	HIS	-	expression tag	UNP P47463
h	142	LEU	-	expression tag	UNP P47463
h	143	GLU	-	expression tag	UNP P47463
h	144	HIS	-	expression tag	UNP P47463
h	145	HIS	-	expression tag	UNP P47463
h	146	HIS	-	expression tag	UNP P47463
h	147	HIS	-	expression tag	UNP P47463
h	148	HIS	-	expression tag	UNP P47463
h	149	HIS	-	expression tag	UNP P47463
i	142	LEU	-	expression tag	UNP P47463
i	143	GLU	-	expression tag	UNP P47463
i	144	HIS	-	expression tag	UNP P47463
i	145	HIS	-	expression tag	UNP P47463
i	146	HIS	-	expression tag	UNP P47463
i	147	HIS	-	expression tag	UNP P47463
i	148	HIS	-	expression tag	UNP P47463
i	149	HIS	-	expression tag	UNP P47463
j	142	LEU	-	expression tag	UNP P47463
j	143	GLU	-	expression tag	UNP P47463
j	144	HIS	-	expression tag	UNP P47463
j	145	HIS	-	expression tag	UNP P47463
j	146	HIS	-	expression tag	UNP P47463
j	147	HIS	-	expression tag	UNP P47463
j	148	HIS	-	expression tag	UNP P47463
j	149	HIS	-	expression tag	UNP P47463

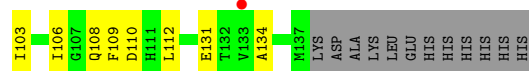
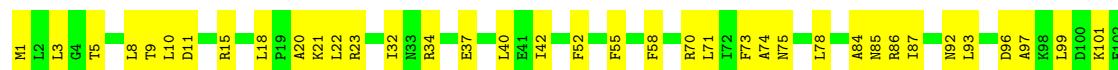
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

Chain J: 58% 34% 8%

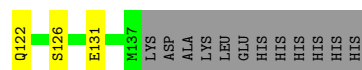




- Molecule 1: Transcriptional regulator MraZ



- Molecule 1: Transcriptional regulator MraZ



- Molecule 1: Transcriptional regulator MraZ

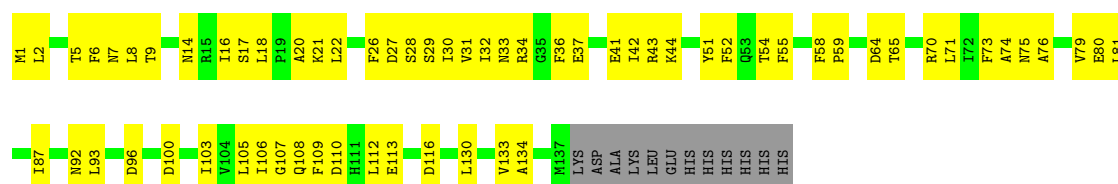


- Molecule 1: Transcriptional regulator MraZ

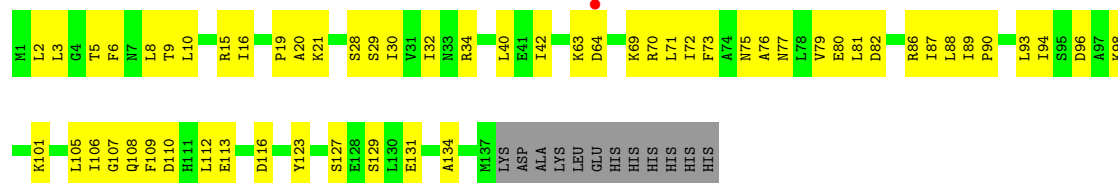


- Molecule 1: Transcriptional regulator MraZ

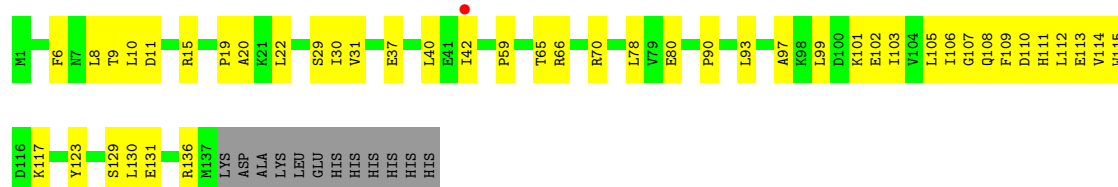




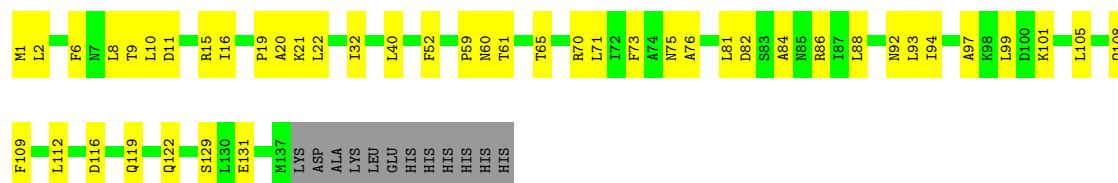
- Molecule 1: Transcriptional regulator MraZ



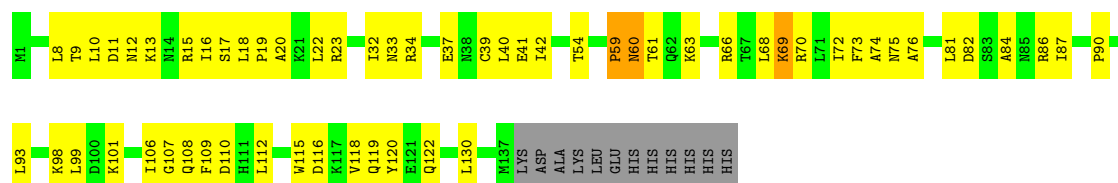
- Molecule 1: Transcriptional regulator MraZ



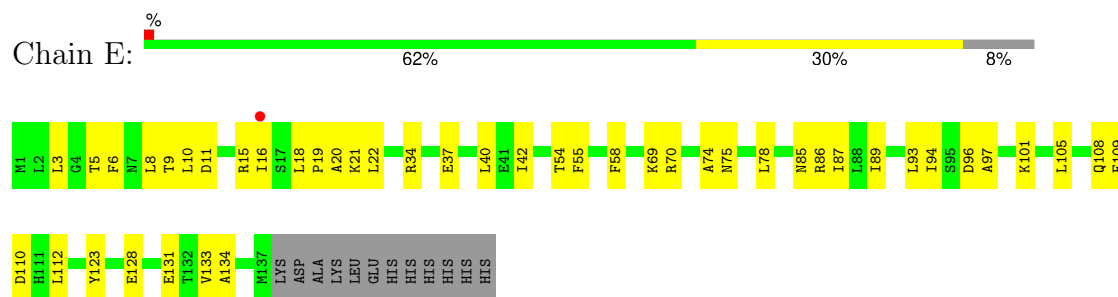
- Molecule 1: Transcriptional regulator MraZ



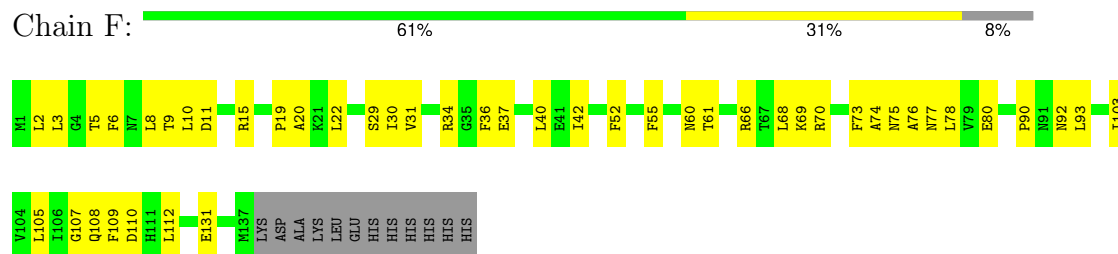
- Molecule 1: Transcriptional regulator MraZ



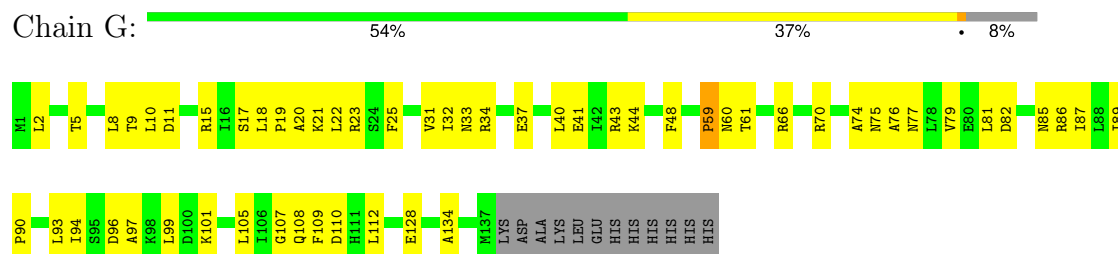
- Molecule 1: Transcriptional regulator MraZ



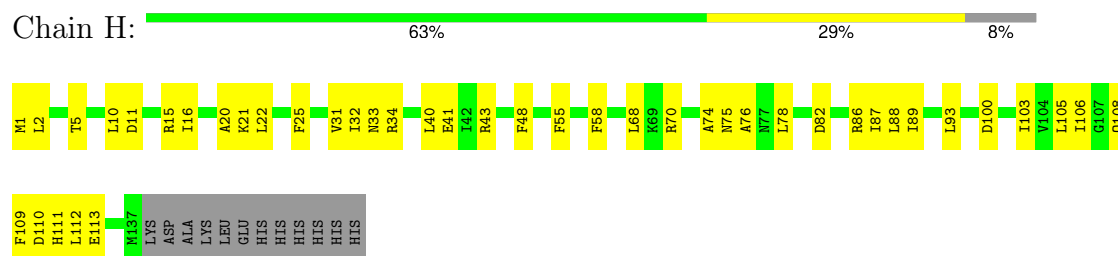
- Molecule 1: Transcriptional regulator MraZ



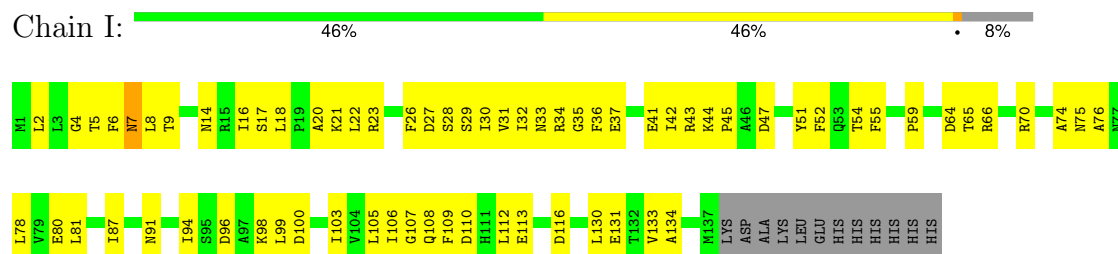
- Molecule 1: Transcriptional regulator MraZ



- Molecule 1: Transcriptional regulator MraZ

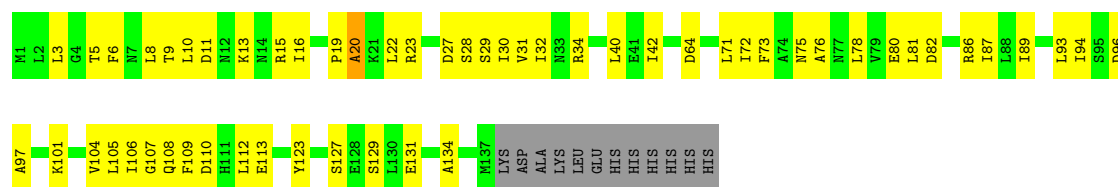


- Molecule 1: Transcriptional regulator MraZ



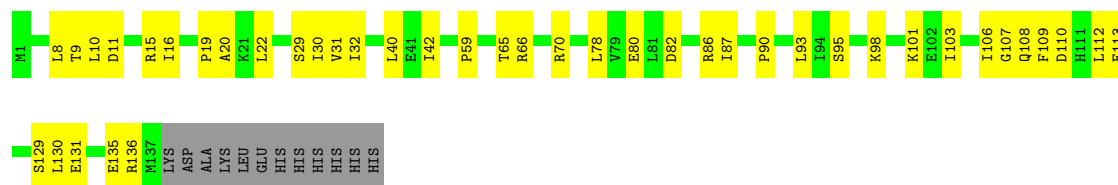
- Molecule 1: Transcriptional regulator MraZ

Chain S: 



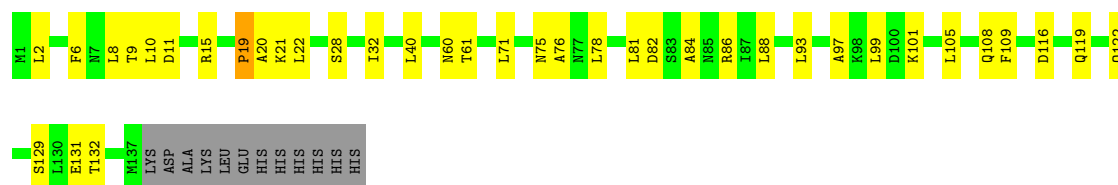
- Molecule 1: Transcriptional regulator MraZ

Chain T: 



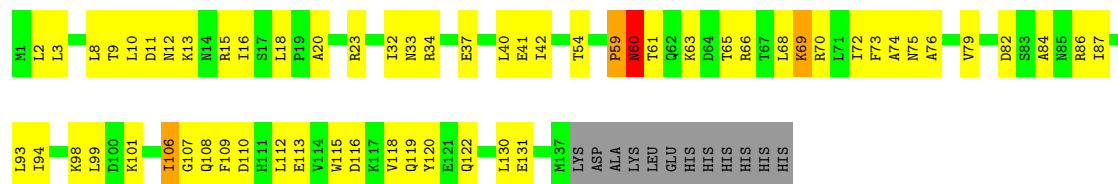
- Molecule 1: Transcriptional regulator MraZ

Chain U: 



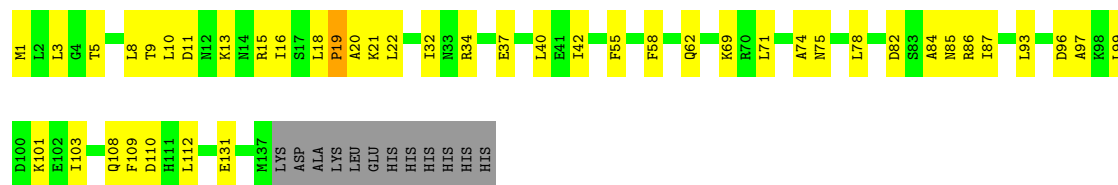
- Molecule 1: Transcriptional regulator MraZ

Chain V: 



- Molecule 1: Transcriptional regulator MraZ

Chain W: 



- Molecule 1: Transcriptional regulator MraZ

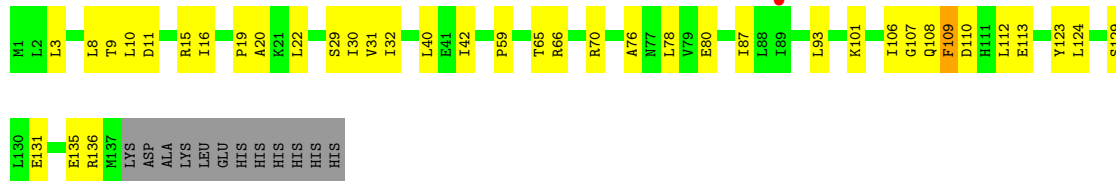
- Molecule 1: Transcriptional regulator MraZ

- Molecule 1: Transcriptional regulator MraZ

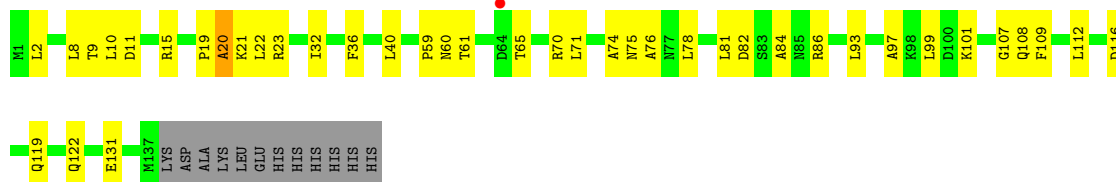
- Molecule 1: Transcriptional regulator MraZ

- Molecule 1: Transcriptional regulator MraZ

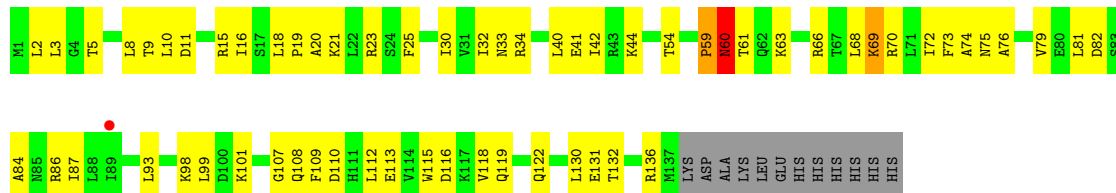
- Molecule 1: Transcriptional regulator MraZ



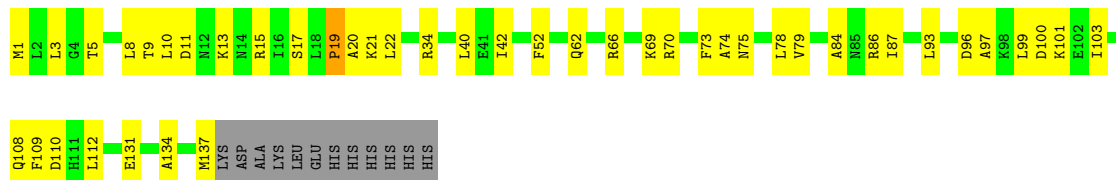
- Molecule 1: Transcriptional regulator MraZ



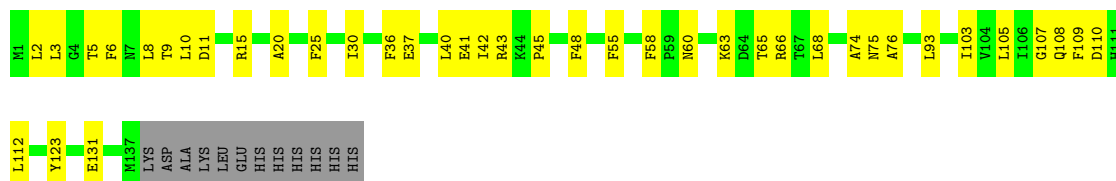
- Molecule 1: Transcriptional regulator MraZ



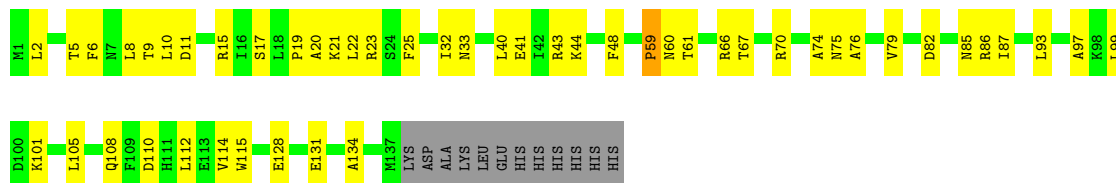
- Molecule 1: Transcriptional regulator MraZ



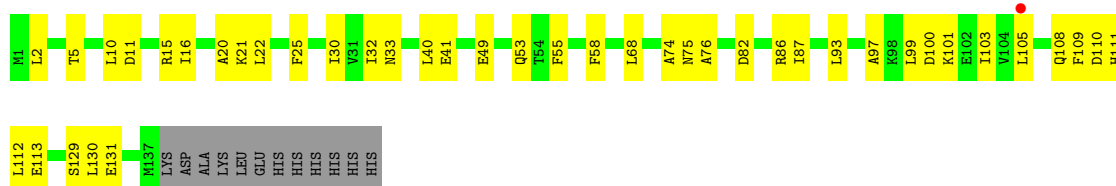
- Molecule 1: Transcriptional regulator MraZ



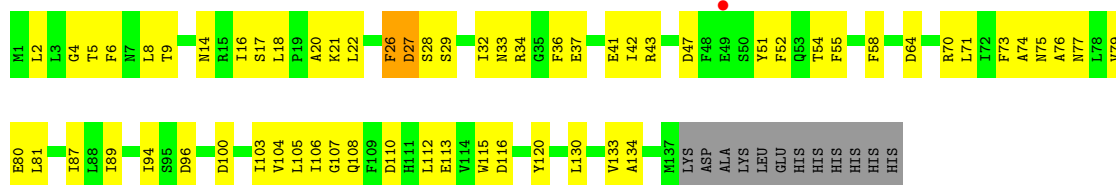
• Molecule 1: Transcriptional regulator MraZ

Chain h:  59% 32% 8%

• Molecule 1: Transcriptional regulator MraZ

Chain i:  64% 28% 8%

• Molecule 1: Transcriptional regulator MraZ

Chain j:  50% 40% 8%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.62Å 203.82Å 149.30Å 90.00° 111.76° 90.00°	Depositor
Resolution (Å)	82.12 – 3.85 82.12 – 3.85	Depositor EDS
% Data completeness (in resolution range)	47.5 (82.12-3.85) 47.7 (82.12-3.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.89Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.248 , 0.308 0.254 , 0.306	Depositor DCC
R_{free} test set	1549 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å ²)	91.8	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	40248	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6126e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.21	0/1137	0.45	0/1536
1	B	0.18	0/1137	0.45	0/1536
1	C	0.21	0/1137	0.42	0/1536
1	D	0.22	0/1137	0.51	0/1536
1	E	0.20	0/1137	0.46	0/1536
1	F	0.20	0/1137	0.45	0/1536
1	G	0.19	0/1137	0.49	0/1536
1	H	0.20	0/1137	0.46	0/1536
1	I	0.33	0/1137	0.56	0/1536
1	J	0.21	0/1137	0.45	0/1536
1	K	0.19	0/1137	0.46	0/1536
1	L	0.19	0/1137	0.43	0/1536
1	M	0.21	0/1137	0.50	1/1536 (0.1%)
1	N	0.21	0/1137	0.46	0/1536
1	O	0.19	0/1137	0.44	0/1536
1	P	0.22	0/1137	0.51	0/1536
1	Q	0.19	0/1137	0.49	0/1536
1	R	0.21	0/1137	0.49	0/1536
1	S	0.19	0/1137	0.42	0/1536
1	T	0.17	0/1137	0.44	0/1536
1	U	0.27	1/1137 (0.1%)	0.45	0/1536
1	V	0.28	1/1137 (0.1%)	0.51	1/1536 (0.1%)
1	W	0.20	0/1137	0.45	0/1536
1	X	0.19	0/1137	0.43	0/1536
1	Y	0.20	0/1137	0.51	0/1536
1	Z	0.19	0/1137	0.47	0/1536
1	a	0.26	0/1137	0.55	0/1536
1	b	0.21	0/1137	0.42	0/1536
1	c	0.17	0/1137	0.43	0/1536
1	d	0.20	0/1137	0.42	0/1536
1	e	0.20	0/1137	0.50	1/1536 (0.1%)
1	f	0.20	0/1137	0.44	0/1536
1	g	0.20	0/1137	0.44	0/1536
1	h	0.22	0/1137	0.48	0/1536

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.19	0/1137	0.47	0/1536
1	j	0.21	0/1137	0.50	0/1536
All	All	0.21	2/40932 (0.0%)	0.47	3/55296 (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	I	0	1
1	R	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	19	PRO	CA-CB	-6.41	1.49	1.53
1	V	106	ILE	C-N	-5.47	1.30	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	60	ASN	N-CA-C	5.21	121.89	110.80
1	e	60	ASN	N-CA-C	5.13	121.74	110.80
1	V	60	ASN	N-CA-C	5.04	121.52	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	76	ALA	Peptide
1	R	76	ALA	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	1118	0	1119	38	0
1	B	1118	0	1119	32	0
1	C	1118	0	1119	34	0
1	D	1118	0	1119	51	0
1	E	1118	0	1119	38	0
1	F	1118	0	1119	38	0
1	G	1118	0	1119	40	0
1	H	1118	0	1119	35	0
1	I	1118	0	1119	55	0
1	J	1118	0	1119	38	0
1	K	1118	0	1119	30	0
1	L	1118	0	1119	41	0
1	M	1118	0	1119	65	0
1	N	1118	0	1119	34	0
1	O	1118	0	1119	29	0
1	P	1118	0	1119	31	0
1	Q	1118	0	1119	34	0
1	R	1118	0	1119	64	0
1	S	1118	0	1119	38	0
1	T	1118	0	1119	31	0
1	U	1118	0	1119	31	0
1	V	1118	0	1119	54	0
1	W	1118	0	1119	35	0
1	X	1118	0	1119	29	0
1	Y	1118	0	1119	30	0
1	Z	1118	0	1119	42	0
1	a	1118	0	1119	47	0
1	b	1118	0	1119	35	0
1	c	1118	0	1119	30	0
1	d	1118	0	1119	32	0
1	e	1118	0	1119	57	0
1	f	1118	0	1119	31	0
1	g	1118	0	1119	28	0
1	h	1118	0	1119	36	0
1	i	1118	0	1119	32	0
1	j	1118	0	1119	54	0
All	All	40248	0	40284	1208	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 1208 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:V:32:ILE:O	1:V:76:ALA:HA	1.52	1.08
1:D:32:ILE:O	1:D:76:ALA:HA	1.61	0.99
1:e:32:ILE:O	1:e:76:ALA:HA	1.63	0.98
1:M:32:ILE:O	1:M:76:ALA:HA	1.74	0.88
1:M:73:PHE:CD2	1:R:108:GLN:OE1	2.30	0.85

There are no symmetry-related clashes.

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	135/149 (91%)	124 (92%)	9 (7%)	2 (2%)	8	37
1	B	135/149 (91%)	122 (90%)	11 (8%)	2 (2%)	8	37
1	C	135/149 (91%)	125 (93%)	8 (6%)	2 (2%)	8	37
1	D	135/149 (91%)	120 (89%)	9 (7%)	6 (4%)	2	20
1	E	135/149 (91%)	123 (91%)	10 (7%)	2 (2%)	8	37
1	F	135/149 (91%)	122 (90%)	11 (8%)	2 (2%)	8	37
1	G	135/149 (91%)	121 (90%)	9 (7%)	5 (4%)	2	22
1	H	135/149 (91%)	120 (89%)	13 (10%)	2 (2%)	8	37
1	I	135/149 (91%)	110 (82%)	18 (13%)	7 (5%)	1	18
1	J	135/149 (91%)	124 (92%)	9 (7%)	2 (2%)	8	37
1	K	135/149 (91%)	122 (90%)	11 (8%)	2 (2%)	8	37
1	L	135/149 (91%)	125 (93%)	8 (6%)	2 (2%)	8	37
1	M	135/149 (91%)	120 (89%)	9 (7%)	6 (4%)	2	20
1	N	135/149 (91%)	124 (92%)	9 (7%)	2 (2%)	8	37
1	O	135/149 (91%)	120 (89%)	13 (10%)	2 (2%)	8	37
1	P	135/149 (91%)	120 (89%)	10 (7%)	5 (4%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	135/149 (91%)	120 (89%)	13 (10%)	2 (2%)	8	37
1	R	135/149 (91%)	111 (82%)	19 (14%)	5 (4%)	2	22
1	S	135/149 (91%)	124 (92%)	8 (6%)	3 (2%)	5	31
1	T	135/149 (91%)	122 (90%)	11 (8%)	2 (2%)	8	37
1	U	135/149 (91%)	126 (93%)	7 (5%)	2 (2%)	8	37
1	V	135/149 (91%)	121 (90%)	9 (7%)	5 (4%)	2	22
1	W	135/149 (91%)	123 (91%)	9 (7%)	3 (2%)	5	31
1	X	135/149 (91%)	123 (91%)	9 (7%)	3 (2%)	5	31
1	Y	135/149 (91%)	119 (88%)	13 (10%)	3 (2%)	5	31
1	Z	135/149 (91%)	119 (88%)	14 (10%)	2 (2%)	8	37
1	a	135/149 (91%)	111 (82%)	16 (12%)	8 (6%)	1	16
1	b	135/149 (91%)	123 (91%)	10 (7%)	2 (2%)	8	37
1	c	135/149 (91%)	123 (91%)	10 (7%)	2 (2%)	8	37
1	d	135/149 (91%)	126 (93%)	7 (5%)	2 (2%)	8	37
1	e	135/149 (91%)	119 (88%)	11 (8%)	5 (4%)	2	22
1	f	135/149 (91%)	124 (92%)	7 (5%)	4 (3%)	3	26
1	g	135/149 (91%)	122 (90%)	11 (8%)	2 (2%)	8	37
1	h	135/149 (91%)	122 (90%)	9 (7%)	4 (3%)	3	26
1	i	135/149 (91%)	119 (88%)	14 (10%)	2 (2%)	8	37
1	j	135/149 (91%)	110 (82%)	20 (15%)	5 (4%)	2	22
All	All	4860/5364 (91%)	4349 (90%)	394 (8%)	117 (2%)	4	30

5 of 117 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	109	PHE
1	M	59	PRO
1	M	60	ASN
1	M	109	PHE
1	N	109	PHE

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	126/137 (92%)	126 (100%)	0	100	100
1	B	126/137 (92%)	126 (100%)	0	100	100
1	C	126/137 (92%)	126 (100%)	0	100	100
1	D	126/137 (92%)	126 (100%)	0	100	100
1	E	126/137 (92%)	126 (100%)	0	100	100
1	F	126/137 (92%)	126 (100%)	0	100	100
1	G	126/137 (92%)	126 (100%)	0	100	100
1	H	126/137 (92%)	126 (100%)	0	100	100
1	I	126/137 (92%)	126 (100%)	0	100	100
1	J	126/137 (92%)	126 (100%)	0	100	100
1	K	126/137 (92%)	126 (100%)	0	100	100
1	L	126/137 (92%)	126 (100%)	0	100	100
1	M	126/137 (92%)	126 (100%)	0	100	100
1	N	126/137 (92%)	126 (100%)	0	100	100
1	O	126/137 (92%)	126 (100%)	0	100	100
1	P	126/137 (92%)	126 (100%)	0	100	100
1	Q	126/137 (92%)	126 (100%)	0	100	100
1	R	126/137 (92%)	126 (100%)	0	100	100
1	S	126/137 (92%)	126 (100%)	0	100	100
1	T	126/137 (92%)	126 (100%)	0	100	100
1	U	126/137 (92%)	126 (100%)	0	100	100
1	V	126/137 (92%)	126 (100%)	0	100	100
1	W	126/137 (92%)	126 (100%)	0	100	100
1	X	126/137 (92%)	126 (100%)	0	100	100
1	Y	126/137 (92%)	126 (100%)	0	100	100
1	Z	126/137 (92%)	125 (99%)	1 (1%)	73	77
1	a	126/137 (92%)	126 (100%)	0	100	100
1	b	126/137 (92%)	126 (100%)	0	100	100
1	c	126/137 (92%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	126/137 (92%)	126 (100%)	0	100	100
1	e	126/137 (92%)	126 (100%)	0	100	100
1	f	126/137 (92%)	126 (100%)	0	100	100
1	g	126/137 (92%)	126 (100%)	0	100	100
1	h	126/137 (92%)	126 (100%)	0	100	100
1	i	126/137 (92%)	126 (100%)	0	100	100
1	j	126/137 (92%)	126 (100%)	0	100	100
All	All	4536/4932 (92%)	4535 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	72	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	62	GLN
1	i	111	HIS
1	I	108	GLN
1	h	62	GLN
1	b	108	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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, 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(Å ²)	Q<0.9
1	A	137/149 (91%)	-0.60	1 (0%) 84 66	80, 112, 146, 169	0
1	B	137/149 (91%)	-0.67	1 (0%) 84 66	80, 114, 153, 177	0
1	C	137/149 (91%)	-0.67	0 100 100	81, 110, 148, 174	0
1	D	137/149 (91%)	-0.63	0 100 100	75, 97, 133, 165	0
1	E	137/149 (91%)	-0.60	1 (0%) 84 66	71, 107, 159, 187	0
1	F	137/149 (91%)	-0.65	0 100 100	74, 96, 138, 178	0
1	G	137/149 (91%)	-0.67	0 100 100	72, 97, 129, 151	0
1	H	137/149 (91%)	-0.58	0 100 100	68, 96, 142, 163	0
1	I	137/149 (91%)	-0.53	0 100 100	71, 96, 148, 195	0
1	J	137/149 (91%)	-0.51	0 100 100	78, 109, 149, 174	0
1	K	137/149 (91%)	-0.54	0 100 100	77, 113, 157, 177	0
1	L	137/149 (91%)	-0.52	0 100 100	73, 106, 148, 174	0
1	M	137/149 (91%)	-0.50	0 100 100	71, 96, 130, 167	0
1	N	137/149 (91%)	-0.56	1 (0%) 84 66	74, 104, 161, 188	0
1	O	137/149 (91%)	-0.54	0 100 100	73, 93, 135, 171	0
1	P	137/149 (91%)	-0.61	0 100 100	69, 95, 133, 157	0
1	Q	137/149 (91%)	-0.50	0 100 100	67, 95, 141, 165	0
1	R	137/149 (91%)	-0.42	0 100 100	69, 97, 145, 195	0
1	S	137/149 (91%)	-0.51	0 100 100	79, 113, 150, 181	0
1	T	137/149 (91%)	-0.58	0 100 100	82, 116, 158, 183	0
1	U	137/149 (91%)	-0.66	0 100 100	84, 114, 152, 172	0
1	V	137/149 (91%)	-0.55	0 100 100	74, 100, 134, 161	0
1	W	137/149 (91%)	-0.47	0 100 100	81, 106, 165, 189	0
1	X	137/149 (91%)	-0.61	0 100 100	74, 101, 148, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	137/149 (91%)	-0.53	0 100 100	76, 100, 138, 162	0
1	Z	137/149 (91%)	-0.54	0 100 100	69, 100, 150, 171	0
1	a	137/149 (91%)	-0.60	0 100 100	75, 101, 152, 194	0
1	b	137/149 (91%)	-0.47	0 100 100	82, 111, 149, 180	0
1	c	137/149 (91%)	-0.48	1 (0%) 84 66	79, 117, 161, 184	0
1	d	137/149 (91%)	-0.49	1 (0%) 84 66	82, 109, 152, 172	0
1	e	137/149 (91%)	-0.44	1 (0%) 84 66	71, 101, 132, 167	0
1	f	137/149 (91%)	-0.52	0 100 100	79, 105, 164, 189	0
1	g	137/149 (91%)	-0.46	0 100 100	73, 98, 148, 172	0
1	h	137/149 (91%)	-0.55	0 100 100	73, 97, 134, 164	0
1	i	137/149 (91%)	-0.50	1 (0%) 84 66	68, 96, 147, 171	0
1	j	137/149 (91%)	-0.46	1 (0%) 84 66	70, 99, 150, 193	0
All	All	4932/5364 (91%)	-0.55	9 (0%) 91 81	67, 104, 149, 195	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	16	ILE	2.8
1	j	49	GLU	2.3
1	i	105	LEU	2.3
1	N	133	VAL	2.1
1	B	42	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.