



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:01 am GMT

PDB ID : 3LD0  
Title : Crystal structure of B.licheniformis Anti-TRAP protein, an antagonist of TRAP-RNA interactions  
Authors : Shevtsov, M.B.; Chen, Y.; Isupov, M.N.; Gollnick, P.; Antson, A.A.  
Deposited on : 2010-01-12  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

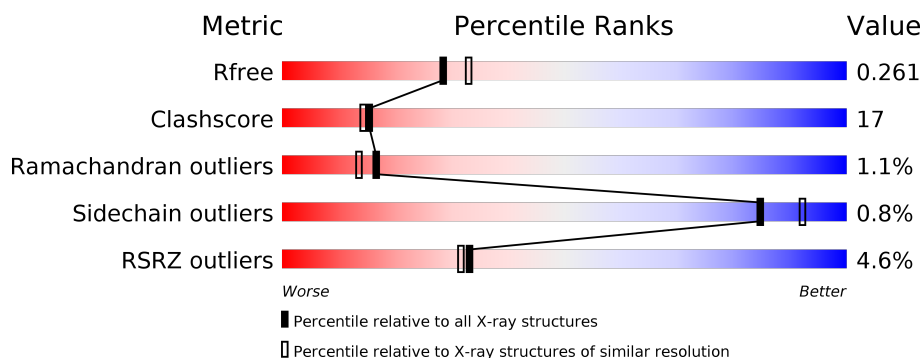
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	1	53	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>8%</div> </div> </div>
1	2	53	<div> <div>66%</div> <div>32%</div> <div></div> </div>
1	3	53	<div> <div>79%</div> <div>21%</div> </div>
1	4	53	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>25%</div> </div> </div>
1	5	53	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
1	6	53	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>26%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	7	53	 6% 77% 21% •
1	8	53	 2% 72% 28%
1	9	53	 4% 75% 25%
1	A	53	 81% 15% •
1	B	53	 4% 75% 25%
1	C	53	 6% 77% 21% •
1	D	53	 2% 77% 23%
1	E	53	 77% 23%
1	F	53	 4% 75% 25%
1	G	53	 85% 13% •
1	H	53	 2% 77% 21% •
1	I	53	 4% 75% 21% •
1	J	53	 21% 64% 32% •
1	K	53	 74% 26%
1	L	53	 4% 83% 15% •
1	M	53	 13% 79% 19% •
1	N	53	 79% 17% •
1	O	53	 4% 79% 21%
1	P	53	 13% 72% 26% •
1	Q	53	 2% 83% 15% •
1	R	53	 6% 79% 21%
1	S	53	 4% 81% 17% •
1	T	53	 8% 74% 26%
1	U	53	 4% 77% 21% •
1	V	53	 81% 17% •

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	W	53	
1	X	53	
1	Y	53	
1	Z	53	
1	a	53	
1	b	53	
1	c	53	
1	d	53	
1	e	53	
1	f	53	
1	g	53	
1	h	53	
1	i	53	
1	j	53	
1	k	53	
1	l	53	
1	m	53	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20524 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 Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	B	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	C	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	D	53	Total	C	N	O	S	0	1	0
			403	249	69	80	5			
1	E	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	F	53	Total	C	N	O	S	0	2	0
			406	252	70	79	5			
1	G	52	Total	C	N	O	S	0	1	0
			393	244	68	76	5			
1	H	52	Total	C	N	O	S	0	2	0
			398	247	69	77	5			
1	I	53	Total	C	N	O	S	0	1	0
			401	247	70	79	5			
1	J	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	K	53	Total	C	N	O	S	0	2	0
			406	250	70	81	5			
1	L	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	M	53	Total	C	N	O	S	0	1	0
			401	247	69	80	5			
1	N	52	Total	C	N	O	S	0	0	0
			388	241	68	74	5			
1	O	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	P	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	53	Total	C	N	O	S	3	1	0
			401	247	70	79	5			
1	R	53	Total	C	N	O	S	0	1	0
			401	247	70	79	5			
1	S	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	T	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	U	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	V	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	W	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	X	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	Y	53	Total	C	N	O	S	0	1	0
			399	246	69	79	5			
1	Z	52	Total	C	N	O	S	0	3	0
			399	250	69	75	5			
1	1	53	Total	C	N	O	S	0	1	0
			401	247	70	79	5			
1	2	52	Total	C	N	O	S	0	2	0
			396	247	68	76	5			
1	3	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	4	52	Total	C	N	O	S	0	1	0
			391	242	68	76	5			
1	5	53	Total	C	N	O	S	0	1	0
			401	247	70	79	5			
1	6	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	7	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	8	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	9	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	a	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	b	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	d	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	e	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	f	53	Total	C	N	O	S	0	1	0
			403	249	69	80	5			
1	g	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	h	53	Total	C	N	O	S	0	1	0
			401	247	70	79	5			
1	i	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	j	53	Total	C	N	O	S	0	1	0
			401	247	69	80	5			
1	k	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			
1	l	52	Total	C	N	O	S	0	1	0
			391	244	68	74	5			
1	m	53	Total	C	N	O	S	0	0	0
			398	246	69	78	5			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	LEU	SER	variant	UNP Q65NU7
A	51	ILE	LEU	variant	UNP Q65NU7
A	52	HIS	ASN	variant	UNP Q65NU7
B	130	LEU	SER	variant	UNP Q65NU7
B	151	ILE	LEU	variant	UNP Q65NU7
B	152	HIS	ASN	variant	UNP Q65NU7
C	230	LEU	SER	variant	UNP Q65NU7
C	251	ILE	LEU	variant	UNP Q65NU7
C	252	HIS	ASN	variant	UNP Q65NU7
D	30	LEU	SER	variant	UNP Q65NU7
D	51	ILE	LEU	variant	UNP Q65NU7
D	52	HIS	ASN	variant	UNP Q65NU7
E	130	LEU	SER	variant	UNP Q65NU7
E	151	ILE	LEU	variant	UNP Q65NU7
E	152	HIS	ASN	variant	UNP Q65NU7
F	230	LEU	SER	variant	UNP Q65NU7
F	251	ILE	LEU	variant	UNP Q65NU7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	252	HIS	ASN	variant	UNP Q65NU7
G	30	LEU	SER	variant	UNP Q65NU7
G	51	ILE	LEU	variant	UNP Q65NU7
G	52	HIS	ASN	variant	UNP Q65NU7
H	130	LEU	SER	variant	UNP Q65NU7
H	151	ILE	LEU	variant	UNP Q65NU7
H	152	HIS	ASN	variant	UNP Q65NU7
I	230	LEU	SER	variant	UNP Q65NU7
I	251	ILE	LEU	variant	UNP Q65NU7
I	252	HIS	ASN	variant	UNP Q65NU7
J	30	LEU	SER	variant	UNP Q65NU7
J	51	ILE	LEU	variant	UNP Q65NU7
J	52	HIS	ASN	variant	UNP Q65NU7
K	130	LEU	SER	variant	UNP Q65NU7
K	151	ILE	LEU	variant	UNP Q65NU7
K	152	HIS	ASN	variant	UNP Q65NU7
L	230	LEU	SER	variant	UNP Q65NU7
L	251	ILE	LEU	variant	UNP Q65NU7
L	252	HIS	ASN	variant	UNP Q65NU7
M	30	LEU	SER	variant	UNP Q65NU7
M	51	ILE	LEU	variant	UNP Q65NU7
M	52	HIS	ASN	variant	UNP Q65NU7
N	130	LEU	SER	variant	UNP Q65NU7
N	151	ILE	LEU	variant	UNP Q65NU7
N	152	HIS	ASN	variant	UNP Q65NU7
O	230	LEU	SER	variant	UNP Q65NU7
O	251	ILE	LEU	variant	UNP Q65NU7
O	252	HIS	ASN	variant	UNP Q65NU7
P	30	LEU	SER	variant	UNP Q65NU7
P	51	ILE	LEU	variant	UNP Q65NU7
P	52	HIS	ASN	variant	UNP Q65NU7
Q	130	LEU	SER	variant	UNP Q65NU7
Q	151	ILE	LEU	variant	UNP Q65NU7
Q	152	HIS	ASN	variant	UNP Q65NU7
R	230	LEU	SER	variant	UNP Q65NU7
R	251	ILE	LEU	variant	UNP Q65NU7
R	252	HIS	ASN	variant	UNP Q65NU7
S	30	LEU	SER	variant	UNP Q65NU7
S	51	ILE	LEU	variant	UNP Q65NU7
S	52	HIS	ASN	variant	UNP Q65NU7
T	130	LEU	SER	variant	UNP Q65NU7
T	151	ILE	LEU	variant	UNP Q65NU7

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
T	152	HIS	ASN	variant	UNP Q65NU7
U	230	LEU	SER	variant	UNP Q65NU7
U	251	ILE	LEU	variant	UNP Q65NU7
U	252	HIS	ASN	variant	UNP Q65NU7
V	30	LEU	SER	variant	UNP Q65NU7
V	51	ILE	LEU	variant	UNP Q65NU7
V	52	HIS	ASN	variant	UNP Q65NU7
W	130	LEU	SER	variant	UNP Q65NU7
W	151	ILE	LEU	variant	UNP Q65NU7
W	152	HIS	ASN	variant	UNP Q65NU7
X	230	LEU	SER	variant	UNP Q65NU7
X	251	ILE	LEU	variant	UNP Q65NU7
X	252	HIS	ASN	variant	UNP Q65NU7
Y	30	LEU	SER	variant	UNP Q65NU7
Y	51	ILE	LEU	variant	UNP Q65NU7
Y	52	HIS	ASN	variant	UNP Q65NU7
Z	130	LEU	SER	variant	UNP Q65NU7
Z	151	ILE	LEU	variant	UNP Q65NU7
Z	152	HIS	ASN	variant	UNP Q65NU7
1	230	LEU	SER	variant	UNP Q65NU7
1	251	ILE	LEU	variant	UNP Q65NU7
1	252	HIS	ASN	variant	UNP Q65NU7
2	30	LEU	SER	variant	UNP Q65NU7
2	51	ILE	LEU	variant	UNP Q65NU7
2	52	HIS	ASN	variant	UNP Q65NU7
3	130	LEU	SER	variant	UNP Q65NU7
3	151	ILE	LEU	variant	UNP Q65NU7
3	152	HIS	ASN	variant	UNP Q65NU7
4	230	LEU	SER	variant	UNP Q65NU7
4	251	ILE	LEU	variant	UNP Q65NU7
4	252	HIS	ASN	variant	UNP Q65NU7
5	30	LEU	SER	variant	UNP Q65NU7
5	51	ILE	LEU	variant	UNP Q65NU7
5	52	HIS	ASN	variant	UNP Q65NU7
6	130	LEU	SER	variant	UNP Q65NU7
6	151	ILE	LEU	variant	UNP Q65NU7
6	152	HIS	ASN	variant	UNP Q65NU7
7	230	LEU	SER	variant	UNP Q65NU7
7	251	ILE	LEU	variant	UNP Q65NU7
7	252	HIS	ASN	variant	UNP Q65NU7
8	30	LEU	SER	variant	UNP Q65NU7
8	51	ILE	LEU	variant	UNP Q65NU7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
8	52	HIS	ASN	variant	UNP Q65NU7
9	130	LEU	SER	variant	UNP Q65NU7
9	151	ILE	LEU	variant	UNP Q65NU7
9	152	HIS	ASN	variant	UNP Q65NU7
a	230	LEU	SER	variant	UNP Q65NU7
a	251	ILE	LEU	variant	UNP Q65NU7
a	252	HIS	ASN	variant	UNP Q65NU7
b	30	LEU	SER	variant	UNP Q65NU7
b	51	ILE	LEU	variant	UNP Q65NU7
b	52	HIS	ASN	variant	UNP Q65NU7
c	130	LEU	SER	variant	UNP Q65NU7
c	151	ILE	LEU	variant	UNP Q65NU7
c	152	HIS	ASN	variant	UNP Q65NU7
d	230	LEU	SER	variant	UNP Q65NU7
d	251	ILE	LEU	variant	UNP Q65NU7
d	252	HIS	ASN	variant	UNP Q65NU7
e	30	LEU	SER	variant	UNP Q65NU7
e	51	ILE	LEU	variant	UNP Q65NU7
e	52	HIS	ASN	variant	UNP Q65NU7
f	130	LEU	SER	variant	UNP Q65NU7
f	151	ILE	LEU	variant	UNP Q65NU7
f	152	HIS	ASN	variant	UNP Q65NU7
g	230	LEU	SER	variant	UNP Q65NU7
g	251	ILE	LEU	variant	UNP Q65NU7
g	252	HIS	ASN	variant	UNP Q65NU7
h	30	LEU	SER	variant	UNP Q65NU7
h	51	ILE	LEU	variant	UNP Q65NU7
h	52	HIS	ASN	variant	UNP Q65NU7
i	130	LEU	SER	variant	UNP Q65NU7
i	151	ILE	LEU	variant	UNP Q65NU7
i	152	HIS	ASN	variant	UNP Q65NU7
j	230	LEU	SER	variant	UNP Q65NU7
j	251	ILE	LEU	variant	UNP Q65NU7
j	252	HIS	ASN	variant	UNP Q65NU7
k	30	LEU	SER	variant	UNP Q65NU7
k	51	ILE	LEU	variant	UNP Q65NU7
k	52	HIS	ASN	variant	UNP Q65NU7
l	130	LEU	SER	variant	UNP Q65NU7
l	151	ILE	LEU	variant	UNP Q65NU7
l	152	HIS	ASN	variant	UNP Q65NU7
m	230	LEU	SER	variant	UNP Q65NU7
m	251	ILE	LEU	variant	UNP Q65NU7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
m	252	HIS	ASN	variant	UNP Q65NU7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Zn 1 1	0	0
2	g	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0
2	h	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	c	1	Total Zn 1 1	0	0
2	6	1	Total Zn 1 1	0	0
2	W	1	Total Zn 1 1	0	0
2	N	1	Total Zn 1 1	0	0
2	X	1	Total Zn 1 1	0	0
2	2	1	Total Zn 1 1	0	0
2	S	1	Total Zn 1 1	0	0
2	f	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	k	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	b	1	Total Zn 1 1	0	0
2	V	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	5	1	Total 1	Zn 1	0	0
2	R	1	Total 1	Zn 1	0	0
2	M	1	Total 1	Zn 1	0	0
2	j	1	Total 1	Zn 1	0	0
2	1	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	e	1	Total 1	Zn 1	0	0
2	I	1	Total 1	Zn 1	0	0
2	Z	1	Total 1	Zn 1	0	0
2	a	1	Total 1	Zn 1	0	0
2	4	1	Total 1	Zn 1	0	0
2	U	1	Total 1	Zn 1	0	0
2	9	1	Total 1	Zn 1	0	0
2	L	1	Total 1	Zn 1	0	0
2	m	1	Total 1	Zn 1	0	0
2	G	1	Total 1	Zn 1	0	0
2	Q	1	Total 1	Zn 1	0	0
2	d	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0
2	i	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	7	1	Total 1	Zn 1	0	0
2	T	1	Total 1	Zn 1	0	0
2	8	1	Total 1	Zn 1	0	0
2	O	1	Total 1	Zn 1	0	0
2	Y	1	Total 1	Zn 1	0	0
2	1	1	Total 1	Zn 1	0	0
2	3	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	g	1	Total 1	Mg 1	0	0
3	J	1	Total 1	Mg 1	0	0
3	1	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	k	1	Total 1	Mg 1	0	0
3	b	1	Total 1	Mg 1	0	0
3	h	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	I	1	Total 1	Mg 1	0	0
3	V	1	Total 1	Mg 1	0	0
3	3	1	Total 1	Mg 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	5	1	Total 1	Mg 1	0	0
3	8	1	Total 1	Mg 1	0	0
3	O	1	Total 1	Mg 1	0	0
3	R	1	Total 1	Mg 1	0	0
3	S	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total 26	O 26	0	0
4	B	36	Total 36	O 36	0	0
4	C	32	Total 32	O 32	0	0
4	D	42	Total 42	O 42	0	0
4	E	47	Total 47	O 47	0	0
4	F	44	Total 44	O 44	0	0
4	G	39	Total 39	O 39	0	0
4	H	31	Total 31	O 31	0	0
4	I	21	Total 21	O 21	0	0
4	J	20	Total 20	O 20	0	0
4	K	39	Total 39	O 39	0	0
4	L	38	Total 38	O 38	0	0
4	M	15	Total 15	O 15	0	0
4	N	25	Total 25	O 25	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	23	Total 23	O 23	0	0
4	P	35	Total 35	O 35	0	0
4	Q	32	Total 32	O 32	0	0
4	R	27	Total 27	O 27	0	0
4	S	29	Total 29	O 29	0	0
4	T	22	Total 22	O 22	0	0
4	U	30	Total 30	O 30	0	0
4	V	20	Total 20	O 20	0	0
4	W	22	Total 22	O 22	0	0
4	X	14	Total 14	O 14	0	0
4	Y	30	Total 30	O 30	0	0
4	Z	37	Total 37	O 37	0	0
4	1	19	Total 19	O 19	0	0
4	2	37	Total 37	O 37	0	0
4	3	40	Total 40	O 40	0	0
4	4	30	Total 30	O 30	0	0
4	5	34	Total 34	O 34	0	0
4	6	17	Total 17	O 17	0	0
4	7	10	Total 10	O 10	0	0
4	8	30	Total 30	O 30	0	0
4	9	17	Total 17	O 17	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	a	35	Total 35	O 35	0	0
4	b	15	Total 15	O 15	0	0
4	c	25	Total 25	O 25	0	0
4	d	29	Total 29	O 29	0	0
4	e	22	Total 22	O 22	0	0
4	f	47	Total 47	O 47	0	0
4	g	30	Total 30	O 30	0	0
4	h	28	Total 28	O 28	0	0
4	i	21	Total 21	O 21	0	0
4	j	15	Total 15	O 15	0	0
4	k	11	Total 11	O 11	0	0
4	l	28	Total 28	O 28	0	0
4	m	19	Total 19	O 19	0	0



### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain A: 




- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain B: 




- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain C: 




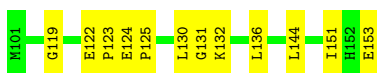
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain D: 




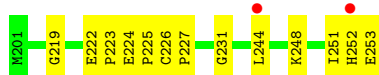
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain E: 



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain F: 



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain G: 85% 13% .



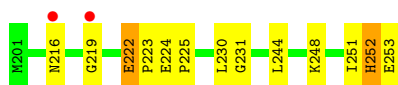
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain H: 77% 21% .



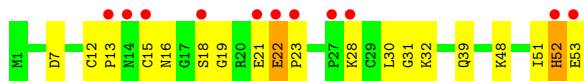
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain I: 75% 21% .



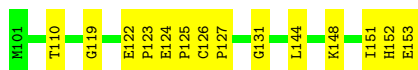
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain J: 64% 32% .



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain K: 74% 26%



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain L: 83% 15% .



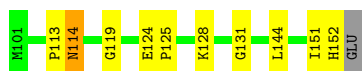
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain M: 79% 19% .



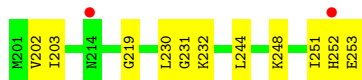
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain N: 79% 17% . .



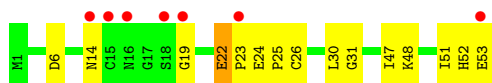
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain O: 4% 79% 21%



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain P: 13% 72% 26% .



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain Q: 2% 83% 15% .



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain R: 6% 79% 21%



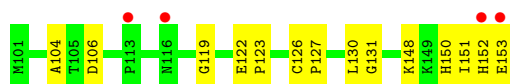
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

Chain S: 4% 81% 17% .

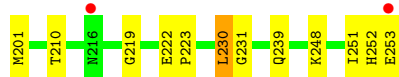
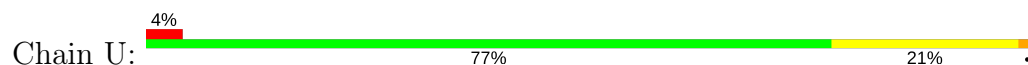


- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

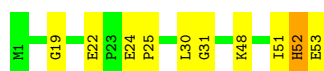
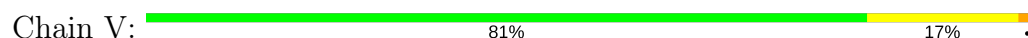
Chain T: 8% 74% 26%



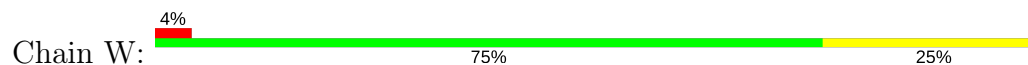
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



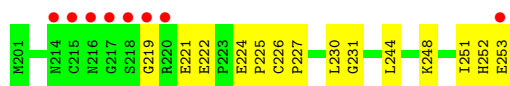
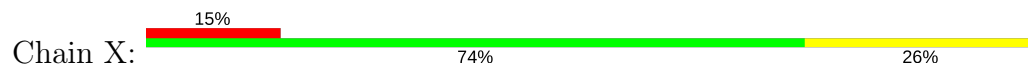
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



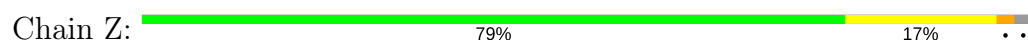
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



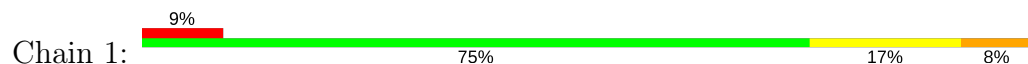
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

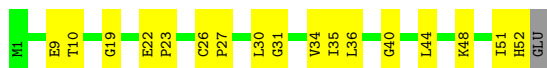


- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

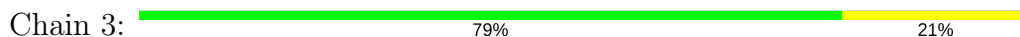




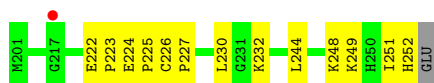
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



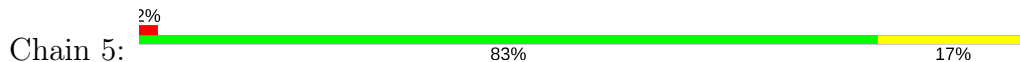
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



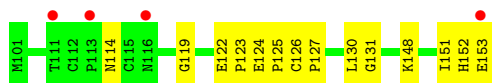
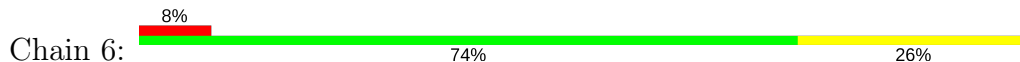
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



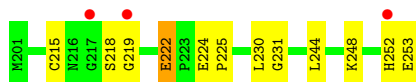
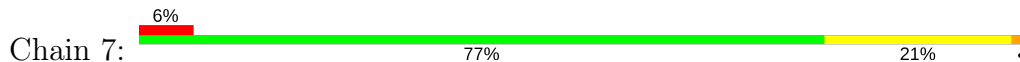
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

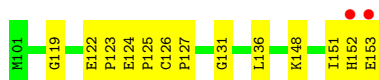
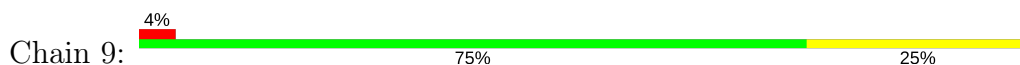


- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

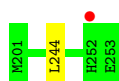




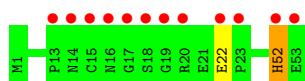
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



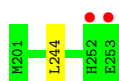
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



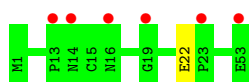
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

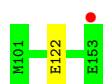


- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

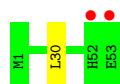




- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



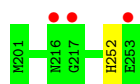
- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA

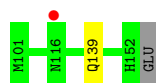


- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



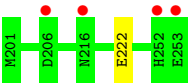
There are no outlier residues recorded for this chain.

- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA



- Molecule 1: Inhibitor of TRAP, regulated by T-BOX (Trp) sequence RtpA







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.54Å 99.86Å 123.18Å 90.00° 117.61° 90.00°	Depositor
Resolution (Å)	29.27 – 2.20 29.27 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.27-2.20) 99.7 (29.27-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, $R_{free}$	0.194 , 0.259 0.197 , 0.261	Depositor DCC
$R_{free}$ test set	1300 reflections (1.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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 44.10 % 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 1.6027e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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

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	1	0.38	0/413	0.56	0/557
1	2	0.42	0/411	0.56	0/556
1	3	0.47	0/405	0.59	0/546
1	4	0.43	0/403	0.60	0/545
1	5	0.43	0/413	0.57	0/557
1	6	0.37	0/405	0.55	0/546
1	7	0.38	0/405	0.59	0/546
1	8	0.40	0/405	0.56	0/546
1	9	0.42	0/405	0.59	0/546
1	A	0.41	0/405	0.57	0/546
1	B	0.46	0/405	0.58	0/546
1	C	0.41	0/405	0.58	0/546
1	D	0.45	0/413	0.62	0/557
1	E	0.50	0/405	0.61	0/546
1	F	0.39	0/421	0.57	0/568
1	G	0.42	0/403	0.57	0/545
1	H	0.43	0/411	0.56	0/556
1	I	0.42	0/413	0.57	0/557
1	J	0.37	0/405	0.52	0/546
1	K	0.42	0/421	0.58	0/568
1	L	0.47	0/405	0.60	0/546
1	M	0.38	0/413	0.53	0/557
1	N	0.39	0/395	0.54	0/534
1	O	0.36	0/405	0.54	0/546
1	P	0.40	0/405	0.55	0/546
1	Q	0.43	0/413	0.60	0/557
1	R	0.43	0/413	0.57	0/557
1	S	0.39	0/405	0.54	0/546
1	T	0.42	0/405	0.54	0/546
1	U	0.41	0/405	0.52	0/546
1	V	0.37	0/405	0.54	0/546
1	W	0.41	0/405	0.56	0/546

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	X	0.40	0/405	0.57	0/546
1	Y	0.47	0/411	0.55	0/554
1	Z	0.39	0/419	0.55	0/567
1	a	0.44	0/405	0.57	0/546
1	b	0.34	0/405	0.51	0/546
1	c	0.38	0/405	0.59	0/546
1	d	0.36	0/405	0.55	0/546
1	e	0.39	0/405	0.54	0/546
1	f	0.48	0/413	0.58	0/557
1	g	0.43	0/405	0.59	0/546
1	h	0.40	0/413	0.58	0/557
1	i	0.38	0/405	0.53	0/546
1	j	0.43	0/413	0.53	0/557
1	k	0.36	0/405	0.55	0/546
1	l	0.43	0/403	0.55	0/545
1	m	0.38	0/405	0.53	0/546
All	All	0.41	0/19568	0.56	0/26396

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	1	401	0	394	17	0
1	2	396	0	400	28	0
1	3	398	0	392	22	0
1	4	391	0	386	16	0
1	5	401	0	397	13	0
1	6	398	0	392	12	0
1	7	398	0	392	12	0
1	8	398	0	395	20	0
1	9	398	0	392	15	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	398	0	395	14	0
1	B	398	0	392	25	0
1	C	398	0	392	14	0
1	D	403	0	399	15	0
1	E	398	0	392	10	0
1	F	406	0	405	16	0
1	G	393	0	393	6	0
1	H	398	0	396	10	0
1	I	401	0	394	21	0
1	J	398	0	395	18	0
1	K	406	0	398	16	0
1	L	398	0	392	7	0
1	M	401	0	395	20	0
1	N	388	0	386	8	0
1	O	398	0	392	16	0
1	P	398	0	395	18	0
1	Q	401	0	394	13	0
1	R	401	0	394	24	0
1	S	398	0	395	19	0
1	T	398	0	392	13	0
1	U	398	0	392	14	0
1	V	398	0	395	14	0
1	W	398	0	392	16	0
1	X	398	0	392	14	0
1	Y	399	0	396	18	0
1	Z	399	0	406	12	0
1	a	398	0	392	0	0
1	b	398	0	395	0	0
1	c	398	0	392	0	0
1	d	398	0	392	0	0
1	e	398	0	395	0	0
1	f	403	0	396	0	0
1	g	398	0	392	0	0
1	h	401	0	397	0	0
1	i	398	0	392	0	0
1	j	401	0	392	0	0
1	k	398	0	395	0	0
1	l	391	0	393	0	0
1	m	398	0	392	0	0
2	1	1	0	0	0	0
2	2	1	0	0	0	0
2	3	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4	1	0	0	0	0
2	5	1	0	0	0	0
2	6	1	0	0	0	0
2	7	1	0	0	0	0
2	8	1	0	0	0	0
2	9	1	0	0	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	1	0	0	0	0
2	Z	1	0	0	0	0
2	a	1	0	0	0	0
2	b	1	0	0	0	0
2	c	1	0	0	0	0
2	d	1	0	0	0	0
2	e	1	0	0	0	0
2	f	1	0	0	0	0
2	g	1	0	0	0	0
2	h	1	0	0	0	0
2	i	1	0	0	0	0
2	j	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	k	1	0	0	0	0
2	l	1	0	0	0	0
2	m	1	0	0	0	0
3	1	1	0	0	0	0
3	3	1	0	0	0	0
3	5	1	0	0	0	0
3	8	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	O	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	V	1	0	0	0	0
3	b	1	0	0	0	0
3	g	1	0	0	0	0
3	h	1	0	0	0	0
3	k	1	0	0	0	0
4	1	19	0	0	1	0
4	2	37	0	0	2	0
4	3	40	0	0	1	0
4	4	30	0	0	7	0
4	5	34	0	0	1	0
4	6	17	0	0	0	0
4	7	10	0	0	0	0
4	8	30	0	0	3	0
4	9	17	0	0	1	0
4	A	26	0	0	2	0
4	B	36	0	0	4	0
4	C	32	0	0	1	0
4	D	42	0	0	3	1
4	E	47	0	0	2	0
4	F	44	0	0	1	0
4	G	39	0	0	0	0
4	H	31	0	0	2	0
4	I	21	0	0	1	0
4	J	20	0	0	3	0
4	K	39	0	0	1	2
4	L	38	0	0	1	1
4	M	15	0	0	1	0
4	N	25	0	0	1	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	23	0	0	2	0
4	P	35	0	0	4	0
4	Q	32	0	0	0	0
4	R	27	0	0	0	0
4	S	29	0	0	2	0
4	T	22	0	0	0	1
4	U	30	0	0	4	0
4	V	20	0	0	0	0
4	W	22	0	0	6	0
4	X	14	0	0	0	0
4	Y	30	0	0	0	0
4	Z	37	0	0	1	0
4	a	35	0	0	0	0
4	b	15	0	0	0	0
4	c	25	0	0	0	1
4	d	29	0	0	0	0
4	e	22	0	0	0	0
4	f	47	0	0	0	0
4	g	30	0	0	0	0
4	h	28	0	0	0	0
4	i	21	0	0	0	1
4	j	15	0	0	0	0
4	k	11	0	0	0	0
4	l	28	0	0	0	0
4	m	19	0	0	0	0
All	All	20524	0	18914	451	4

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 17.

The worst 5 of 451 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)
1:2:44[B]:LEU:HD21	1:3:146:PHE:CE2	1.37	1.55
1:2:44[B]:LEU:CD2	1:3:146:PHE:CE2	2.08	1.36
1:B:116:ASN:ND2	1:R:214[B]:ASN:HD21	1.50	1.08
1:2:44[B]:LEU:CD2	1:3:146:PHE:HE2	1.55	1.08
1:P:48:LYS:NZ	1:P:53:GLU:OE1	1.88	1.06

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:1069:HOH:O	4:T:1217:HOH:O[2_446]	2.02	0.18
4:c:352:HOH:O	4:i:964:HOH:O[2_546]	2.05	0.15
4:K:1162:HOH:O	4:L:1085:HOH:O[2_445]	2.14	0.06
4:D:741:HOH:O	4:K:1164:HOH:O[2_455]	2.16	0.04

## 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	1	52/53 (98%)	49 (94%)	1 (2%)	2 (4%)	4	1
1	2	52/53 (98%)	50 (96%)	2 (4%)	0	100	100
1	3	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
1	4	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
1	5	52/53 (98%)	50 (96%)	2 (4%)	0	100	100
1	6	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
1	7	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	9	5
1	8	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
1	9	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
1	A	51/53 (96%)	48 (94%)	1 (2%)	2 (4%)	3	1
1	B	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
1	C	51/53 (96%)	48 (94%)	1 (2%)	2 (4%)	3	1
1	D	52/53 (98%)	49 (94%)	3 (6%)	0	100	100
1	E	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
1	F	53/53 (100%)	50 (94%)	3 (6%)	0	100	100
1	G	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
1	H	52/53 (98%)	50 (96%)	2 (4%)	0	100	100
1	I	52/53 (98%)	49 (94%)	1 (2%)	2 (4%)	4	1
1	J	51/53 (96%)	48 (94%)	1 (2%)	2 (4%)	3	1

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	53/53 (100%)	49 (92%)	4 (8%)	0	100	100
1	L	51/53 (96%)	48 (94%)	2 (4%)	1 (2%)	9	5
1	M	52/53 (98%)	49 (94%)	2 (4%)	1 (2%)	9	6
1	N	50/53 (94%)	48 (96%)	2 (4%)	0	100	100
1	O	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
1	P	51/53 (96%)	48 (94%)	2 (4%)	1 (2%)	9	5
1	Q	52/53 (98%)	50 (96%)	1 (2%)	1 (2%)	9	6
1	R	52/53 (98%)	49 (94%)	3 (6%)	0	100	100
1	S	51/53 (96%)	48 (94%)	2 (4%)	1 (2%)	9	5
1	T	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
1	U	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
1	V	51/53 (96%)	48 (94%)	2 (4%)	1 (2%)	9	5
1	W	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
1	X	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
1	Y	52/53 (98%)	49 (94%)	3 (6%)	0	100	100
1	Z	53/53 (100%)	51 (96%)	1 (2%)	1 (2%)	9	6
1	a	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
1	b	51/53 (96%)	45 (88%)	4 (8%)	2 (4%)	3	1
1	c	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
1	d	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
1	e	51/53 (96%)	48 (94%)	2 (4%)	1 (2%)	9	5
1	f	52/53 (98%)	49 (94%)	2 (4%)	1 (2%)	9	6
1	g	51/53 (96%)	48 (94%)	2 (4%)	1 (2%)	9	5
1	h	52/53 (98%)	48 (92%)	4 (8%)	0	100	100
1	i	51/53 (96%)	48 (94%)	2 (4%)	1 (2%)	9	5
1	j	52/53 (98%)	49 (94%)	2 (4%)	1 (2%)	9	6
1	k	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
1	l	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
1	m	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	9	5
All	All	2466/2544 (97%)	2320 (94%)	120 (5%)	26 (1%)	17	13

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	52	HIS
1	1	252	HIS
1	b	52	HIS
1	e	22	GLU
1	P	22	GLU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	47/46 (102%)	45 (96%)	2 (4%)	33	41
1	2	47/46 (102%)	47 (100%)	0	100	100
1	3	46/46 (100%)	45 (98%)	1 (2%)	57	70
1	4	46/46 (100%)	46 (100%)	0	100	100
1	5	47/46 (102%)	47 (100%)	0	100	100
1	6	46/46 (100%)	46 (100%)	0	100	100
1	7	46/46 (100%)	46 (100%)	0	100	100
1	8	46/46 (100%)	46 (100%)	0	100	100
1	9	46/46 (100%)	46 (100%)	0	100	100
1	A	46/46 (100%)	46 (100%)	0	100	100
1	B	46/46 (100%)	46 (100%)	0	100	100
1	C	46/46 (100%)	45 (98%)	1 (2%)	57	70
1	D	47/46 (102%)	47 (100%)	0	100	100
1	E	46/46 (100%)	45 (98%)	1 (2%)	57	70
1	F	48/46 (104%)	48 (100%)	0	100	100
1	G	46/46 (100%)	46 (100%)	0	100	100
1	H	47/46 (102%)	46 (98%)	1 (2%)	59	72
1	I	47/46 (102%)	47 (100%)	0	100	100
1	J	46/46 (100%)	45 (98%)	1 (2%)	57	70
1	K	48/46 (104%)	48 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	46/46 (100%)	46 (100%)	0	100	100
1	M	47/46 (102%)	47 (100%)	0	100	100
1	N	45/46 (98%)	44 (98%)	1 (2%)	57	70
1	O	46/46 (100%)	46 (100%)	0	100	100
1	P	46/46 (100%)	46 (100%)	0	100	100
1	Q	47/46 (102%)	47 (100%)	0	100	100
1	R	47/46 (102%)	47 (100%)	0	100	100
1	S	46/46 (100%)	46 (100%)	0	100	100
1	T	46/46 (100%)	46 (100%)	0	100	100
1	U	46/46 (100%)	44 (96%)	2 (4%)	33	41
1	V	46/46 (100%)	46 (100%)	0	100	100
1	W	46/46 (100%)	46 (100%)	0	100	100
1	X	46/46 (100%)	46 (100%)	0	100	100
1	Y	47/46 (102%)	47 (100%)	0	100	100
1	Z	48/46 (104%)	48 (100%)	0	100	100
1	a	46/46 (100%)	45 (98%)	1 (2%)	57	70
1	b	46/46 (100%)	45 (98%)	1 (2%)	57	70
1	c	46/46 (100%)	44 (96%)	2 (4%)	33	41
1	d	46/46 (100%)	45 (98%)	1 (2%)	57	70
1	e	46/46 (100%)	46 (100%)	0	100	100
1	f	47/46 (102%)	47 (100%)	0	100	100
1	g	46/46 (100%)	45 (98%)	1 (2%)	57	70
1	h	47/46 (102%)	46 (98%)	1 (2%)	59	72
1	i	46/46 (100%)	46 (100%)	0	100	100
1	j	47/46 (102%)	47 (100%)	0	100	100
1	k	46/46 (100%)	46 (100%)	0	100	100
1	l	46/46 (100%)	45 (98%)	1 (2%)	57	70
1	m	46/46 (100%)	46 (100%)	0	100	100
All	All	2226/2208 (101%)	2208 (99%)	18 (1%)	85	92

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	253	GLU
1	3	144	LEU
1	d	244	LEU
1	U	239	GLN
1	1	230	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	52	HIS
1	X	214	ASN
1	j	214	ASN
1	T	114	ASN
1	V	52	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 64 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1	53/53 (100%)	0.38	5 (9%) 9 8	14, 28, 43, 55	0
1	2	52/53 (98%)	-0.22	0 100 100	12, 21, 33, 56	0
1	3	53/53 (100%)	-0.24	0 100 100	10, 18, 32, 56	0
1	4	52/53 (98%)	-0.06	1 (1%) 67 65	14, 23, 36, 60	0
1	5	53/53 (100%)	-0.22	1 (1%) 67 65	13, 20, 30, 64	0
1	6	53/53 (100%)	0.33	4 (7%) 15 14	11, 29, 43, 61	0
1	7	53/53 (100%)	0.28	3 (5%) 24 24	14, 27, 41, 57	0
1	8	53/53 (100%)	0.01	1 (1%) 67 65	10, 25, 38, 55	0
1	9	53/53 (100%)	-0.23	2 (3%) 41 39	13, 21, 32, 54	0
1	A	53/53 (100%)	-0.27	0 100 100	12, 20, 33, 66	0
1	B	53/53 (100%)	-0.21	2 (3%) 41 39	11, 19, 32, 58	0
1	C	53/53 (100%)	0.17	3 (5%) 24 24	12, 23, 39, 55	0
1	D	53/53 (100%)	-0.16	1 (1%) 67 65	10, 18, 32, 56	0
1	E	53/53 (100%)	-0.27	0 100 100	11, 18, 34, 54	0
1	F	53/53 (100%)	-0.22	2 (3%) 41 39	10, 22, 35, 59	0
1	G	52/53 (98%)	-0.33	0 100 100	12, 20, 31, 54	0
1	H	52/53 (98%)	-0.36	1 (1%) 67 65	11, 19, 32, 58	0
1	I	53/53 (100%)	0.03	2 (3%) 41 39	12, 23, 38, 56	0
1	J	53/53 (100%)	0.74	11 (20%) 1 1	10, 33, 55, 57	0
1	K	53/53 (100%)	-0.20	0 100 100	13, 20, 32, 52	0
1	L	53/53 (100%)	-0.20	2 (3%) 41 39	10, 18, 34, 57	0
1	M	53/53 (100%)	0.42	7 (13%) 4 3	13, 28, 50, 55	0
1	N	52/53 (98%)	-0.19	0 100 100	14, 22, 32, 58	0
1	O	53/53 (100%)	-0.14	2 (3%) 41 39	12, 23, 40, 53	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	P	53/53 (100%)	0.52	7 (13%) 4 3	12, 28, 42, 66	0
1	Q	53/53 (100%)	-0.15	1 (1%) 67 65	13, 20, 36, 64	0
1	R	53/53 (100%)	-0.12	3 (5%) 24 24	11, 20, 34, 65	0
1	S	53/53 (100%)	0.08	2 (3%) 41 39	13, 23, 37, 58	0
1	T	53/53 (100%)	0.25	4 (7%) 15 14	12, 26, 41, 55	0
1	U	53/53 (100%)	-0.01	2 (3%) 41 39	14, 25, 38, 54	0
1	V	53/53 (100%)	-0.25	0 100 100	12, 22, 36, 52	0
1	W	53/53 (100%)	0.25	2 (3%) 41 39	12, 28, 39, 58	0
1	X	53/53 (100%)	0.71	8 (15%) 3 2	13, 27, 44, 53	0
1	Y	53/53 (100%)	-0.34	1 (1%) 67 65	12, 18, 31, 55	0
1	Z	52/53 (98%)	-0.22	0 100 100	11, 23, 34, 50	0
1	a	53/53 (100%)	-0.36	1 (1%) 67 65	10, 18, 30, 59	0
1	b	53/53 (100%)	0.88	12 (22%) 1 1	16, 35, 58, 62	0
1	c	53/53 (100%)	-0.03	1 (1%) 67 65	16, 23, 36, 60	0
1	d	53/53 (100%)	0.04	2 (3%) 41 39	13, 25, 37, 57	0
1	e	53/53 (100%)	0.42	6 (11%) 6 5	11, 27, 55, 58	0
1	f	53/53 (100%)	-0.21	1 (1%) 67 65	10, 19, 30, 60	0
1	g	53/53 (100%)	0.03	1 (1%) 67 65	10, 23, 36, 67	0
1	h	53/53 (100%)	-0.13	2 (3%) 41 39	10, 22, 31, 64	0
1	i	53/53 (100%)	0.08	2 (3%) 41 39	11, 25, 42, 66	0
1	j	53/53 (100%)	0.17	3 (5%) 24 24	14, 25, 39, 61	0
1	k	53/53 (100%)	0.10	0 100 100	14, 28, 37, 52	0
1	l	52/53 (98%)	0.20	1 (1%) 67 65	12, 27, 40, 49	0
1	m	53/53 (100%)	0.39	4 (7%) 15 14	12, 28, 40, 56	0
All	All	2537/2544 (99%)	0.02	116 (4%) 33 32	10, 23, 48, 67	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	13	PRO	6.9
1	X	216	ASN	6.6
1	b	16	ASN	6.1
1	B	152	HIS	6.0
1	C	253	GLU	5.7

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	V	54	1/1	0.84	0.23	-0.23	33,33,33,33	0
2	ZN	J	60	1/1	0.93	0.17	-0.63	46,46,46,46	0
3	MG	D	54	1/1	0.92	0.17	-0.64	26,26,26,26	0
2	ZN	e	60	1/1	0.97	0.12	-0.89	40,40,40,40	0
2	ZN	b	60	1/1	0.95	0.17	-0.94	40,40,40,40	0
3	MG	h	54	1/1	0.87	0.17	-0.98	50,50,50,50	0
3	MG	J	54	1/1	0.97	0.18	-0.99	34,34,34,34	0
3	MG	1	9	1/1	0.98	0.16	-1.07	22,22,22,22	0
3	MG	5	54	1/1	0.96	0.14	-1.07	45,45,45,45	0
2	ZN	M	60	1/1	0.98	0.10	-1.13	28,28,28,28	0
2	ZN	X	260	1/1	0.99	0.10	-1.15	26,26,26,26	0
3	MG	R	6	1/1	0.51	0.20	-1.20	56,56,56,56	0
2	ZN	l	160	1/1	0.97	0.10	-1.22	28,28,28,28	0
2	ZN	1	260	1/1	0.98	0.10	-1.24	29,29,29,29	0
2	ZN	O	260	1/1	0.99	0.05	-1.32	21,21,21,21	0
3	MG	S	54	1/1	0.86	0.14	-1.35	35,35,35,35	0
3	MG	k	54	1/1	0.88	0.11	-1.37	26,26,26,26	0
2	ZN	P	60	1/1	0.99	0.09	-1.41	26,26,26,26	0
3	MG	8	54	1/1	0.93	0.13	-1.42	26,26,26,26	0
2	ZN	g	260	1/1	0.96	0.04	-1.42	19,19,19,19	0
3	MG	g	14	1/1	0.84	0.17	-1.43	48,48,48,48	0
3	MG	B	1	1/1	0.93	0.07	-1.47	20,20,20,20	0
3	MG	b	54	1/1	0.91	0.13	-1.47	47,47,47,47	0
2	ZN	i	160	1/1	0.96	0.06	-1.48	21,21,21,21	0
2	ZN	C	260	1/1	0.99	0.06	-1.54	21,21,21,21	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	7	260	1/1	0.94	0.07	-1.59	23,23,23,23	0
2	ZN	d	260	1/1	0.97	0.06	-1.61	21,21,21,21	0
3	MG	I	3	1/1	0.95	0.15	-1.65	21,21,21,21	0
2	ZN	S	60	1/1	0.98	0.06	-1.80	18,18,18,18	0
2	ZN	T	160	1/1	0.99	0.07	-1.86	25,25,25,25	0
2	ZN	a	260	1/1	1.00	0.03	-1.98	15,15,15,15	0
2	ZN	m	260	1/1	0.99	0.07	-2.01	26,26,26,26	0
2	ZN	I	260	1/1	0.99	0.04	-2.11	20,20,20,20	0
2	ZN	k	60	1/1	0.98	0.07	-2.13	23,23,23,23	0
2	ZN	6	160	1/1	0.97	0.09	-2.13	33,33,33,33	0
2	ZN	h	60	1/1	0.99	0.04	-2.21	14,14,14,14	0
2	ZN	c	160	1/1	0.99	0.04	-2.31	19,19,19,19	0
2	ZN	R	260	1/1	0.99	0.02	-2.33	14,14,14,14	0
2	ZN	W	160	1/1	0.92	0.10	-2.37	24,24,24,24	0
2	ZN	U	260	1/1	0.99	0.06	-2.38	21,21,21,21	0
2	ZN	G	60	1/1	1.00	0.03	-2.45	16,16,16,16	0
2	ZN	8	60	1/1	0.98	0.05	-2.48	29,29,29,29	0
2	ZN	Y	60	1/1	0.99	0.03	-2.57	14,14,14,14	0
2	ZN	N	160	1/1	0.99	0.03	-2.71	14,14,14,14	0
2	ZN	5	60	1/1	1.00	0.05	-2.72	14,14,14,14	0
2	ZN	L	260	1/1	1.00	0.04	-2.76	14,14,14,14	0
2	ZN	F	260	1/1	0.99	0.02	-2.84	18,18,18,18	0
2	ZN	B	160	1/1	0.97	0.03	-2.88	14,14,14,14	0
2	ZN	V	60	1/1	0.99	0.02	-2.94	16,16,16,16	0
2	ZN	Z	160	1/1	0.98	0.04	-2.97	17,17,17,17	0
2	ZN	4	260	1/1	0.98	0.03	-3.08	17,17,17,17	0
2	ZN	3	160	1/1	1.00	0.05	-3.14	13,13,13,13	0
2	ZN	2	60	1/1	1.00	0.01	-3.15	16,16,16,16	0
2	ZN	H	160	1/1	0.99	0.02	-3.22	14,14,14,14	0
2	ZN	Q	160	1/1	0.99	0.04	-3.31	14,14,14,14	0
2	ZN	E	160	1/1	1.00	0.05	-3.33	14,14,14,14	0
2	ZN	j	260	1/1	0.95	0.07	-3.33	21,21,21,21	0
2	ZN	A	60	1/1	1.00	0.01	-3.49	14,14,14,14	0
2	ZN	D	60	1/1	1.00	0.03	-3.58	12,12,12,12	0
2	ZN	K	160	1/1	0.99	0.03	-4.12	15,15,15,15	0
2	ZN	f	160	1/1	0.99	0.02	-4.86	14,14,14,14	0
2	ZN	9	160	1/1	0.99	0.02	-6.09	16,16,16,16	0
3	MG	O	5	1/1	0.97	0.12	-	21,21,21,21	0
3	MG	3	10	1/1	0.97	0.16	-	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.