



wwPDB EM Validation Summary Report ⓘ

May 10, 2026 – 12:19 AM JST

PDB ID : 9K14 / pdb_00009k14
EMDB ID : EMD-61964
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 3U scaffold at 3.8 Angstrom
Authors : Xie, G.; Du, X.; Du, J.
Deposited on : 2024-10-16
Resolution : 3.80 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

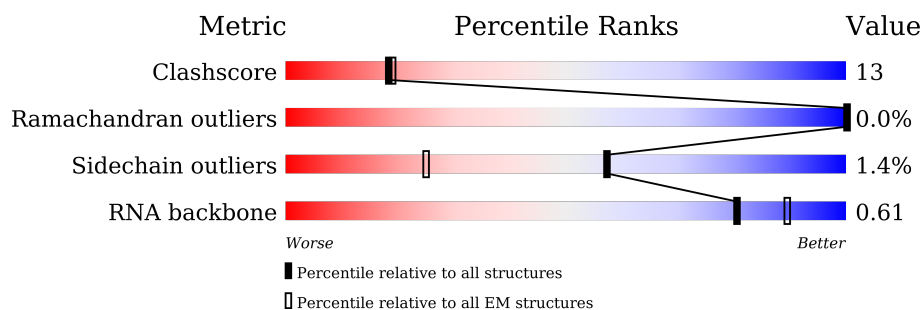
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	T	34	6% 29% . 62%
2	N	34	18% 24% 9% 50%
3	P	20	30% 5% 65%
4	A	2032	28% 12% 59%
5	C	319	68% 21% . 10%
6	F	144	38% 17% 44%
7	J	71	68% 21% 11%
8	K	116	68% 24% . 7%

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Mol	Chain	Length	Quality of chain
9	L	51	 73%16%12%
10	H	146	 58%38%. .
11	I	114	 51%31%.18%
12	E	230	 50%40%.9%
13	B	1169	 65%17%17%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23198 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	13	Total	C	N	O	P	0	0
			265	126	48	78	13		

- Molecule 2 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	17	Total	C	N	O	P	0	0
			349	166	62	104	17		

- Molecule 3 is a RNA chain called RNA (5'-R(*UP*AP*UP*AP*UP*GP*CP*AP*GP*AP*AP*AP*GP*CP*GP*AP*CP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	7	Total	C	N	O	P	0	0
			150	67	28	48	7		

- Molecule 4 is a protein called DNA-directed RNA polymerase V largest subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	832	Total	C	N	O	S	0	0
			6506	4113	1120	1229	44		

- Molecule 5 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	287	Total	C	N	O	S	0	0
			2256	1418	380	445	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	THR	SER	conflict	UNP A0A0D3D418

- Molecule 6 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	80	Total	C	N	O	S	0	0
			660	420	114	122	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	51	GLU	ASP	conflict	UNP A0A0D3BZZ8

- Molecule 7 is a protein called DNA-directed RNA polymerase II, IV and V subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	63	Total	C	N	O	S	0	0
			507	324	85	91	7		

- Molecule 8 is a protein called DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	108	Total	C	N	O	S	0	0
			890	565	156	167	2		

- Molecule 9 is a protein called DNA-directed RNA polymerase II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	45	Total	C	N	O	S	0	0
			365	224	70	67	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	18	GLU	LYS	conflict	UNP A0A0D2ZPP3
L	32	CYS	ARG	conflict	UNP A0A0D2ZPP3

- Molecule 10 is a protein called DNA-directed RNA polymerase II, IV and V subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	141	Total	C	N	O	S	0	0
			1129	729	183	208	9		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	94	Total	C	N	O	S	0	0
			763	467	145	139	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	20	ARG	LYS	conflict	UNP A0A0D3A7P5
I	40	ASP	ASN	conflict	UNP A0A0D3A7P5

- Molecule 12 is a protein called RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	209	Total	C	N	O	S	0	0
			1706	1085	303	316	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	101	GLY	SER	conflict	UNP A0A0D3DTU3
E	182	GLN	HIS	conflict	UNP A0A0D3DTU3
E	210	ILE	VAL	conflict	UNP A0A0D3DTU3

- Molecule 13 is a protein called DNA-directed RNA polymerase IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	965	Total	C	N	O	S	0	0
			7645	4816	1355	1430	44		

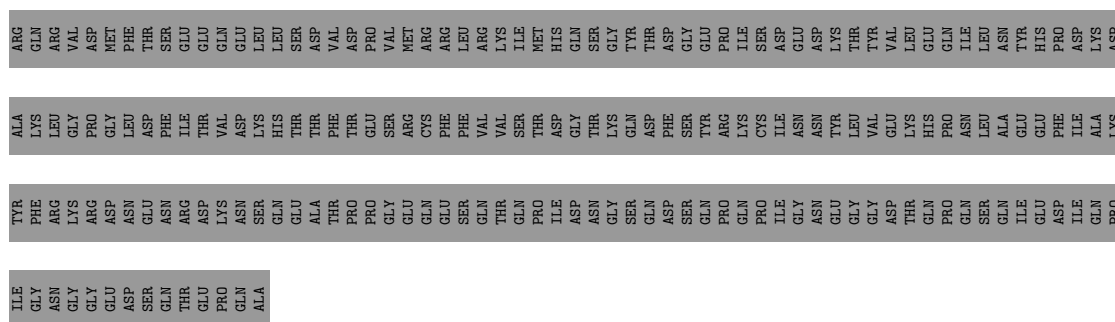
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Mg	0
			1	1	

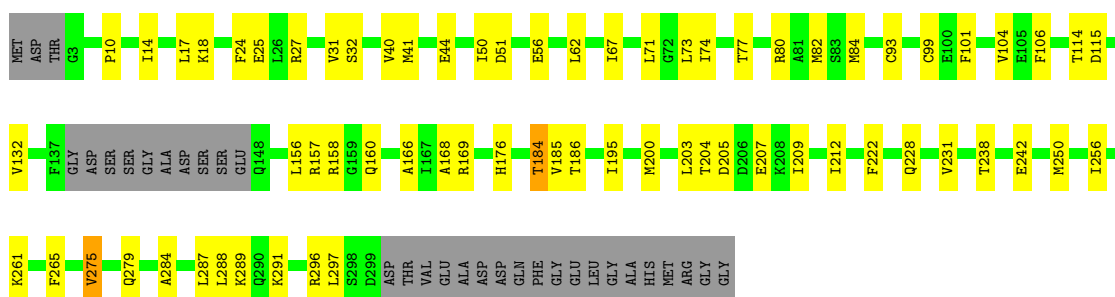
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total 1	Zn 1	0
15	C	1	Total 1	Zn 1	0
15	J	1	Total 1	Zn 1	0
15	L	1	Total 1	Zn 1	0
15	I	2	Total 2	Zn 2	0

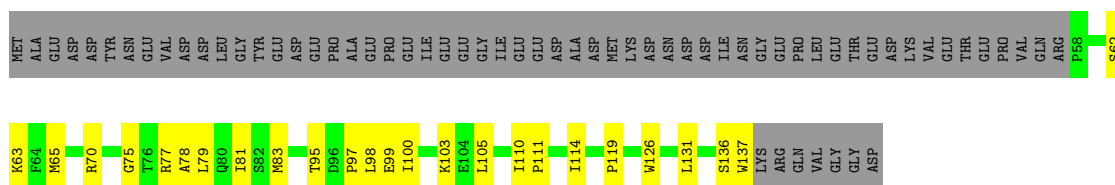
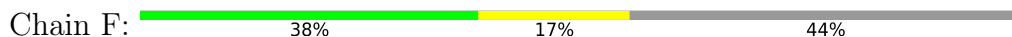




- Molecule 5: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein



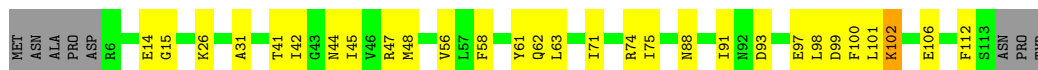
- Molecule 6: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein



- Molecule 7: DNA-directed RNA polymerase II, IV and V subunit 10

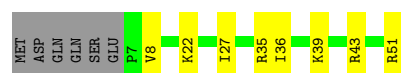


- Molecule 8: DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein



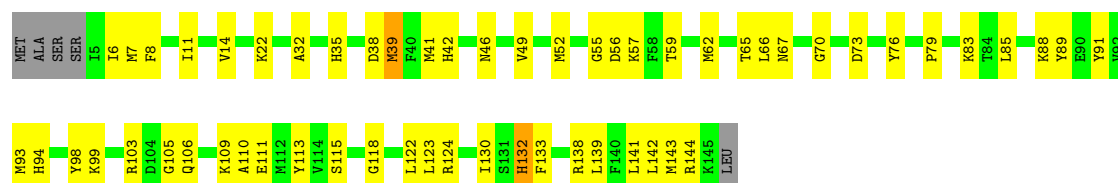
- Molecule 9: DNA-directed RNA polymerase II, IV and V subunit 12

Chain L:  73% 16% 12%



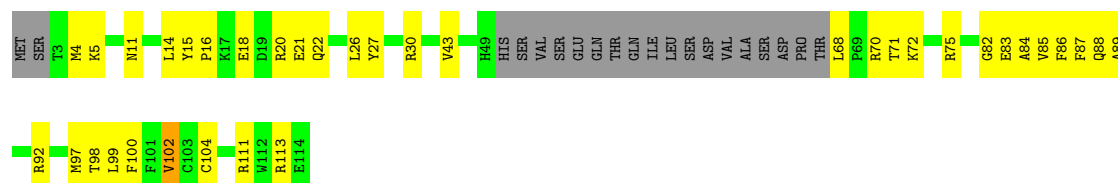
- Molecule 10: DNA-directed RNA polymerase II, IV and V subunit 8

Chain H:  58% 38% ..



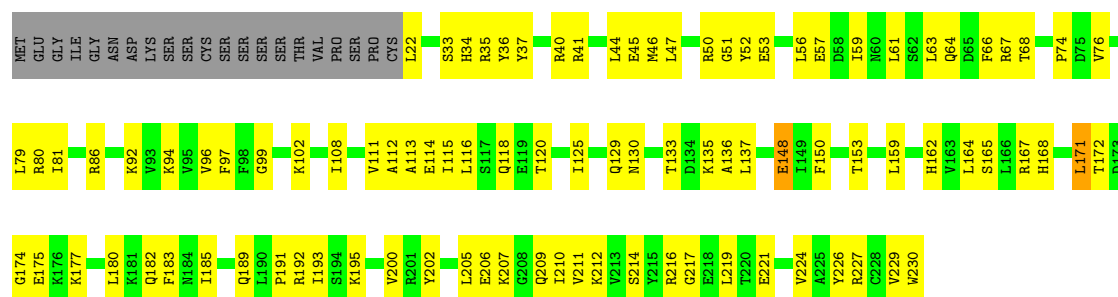
- Molecule 11: DNA-directed RNA polymerase subunit

Chain I:  51% 31% . 18%



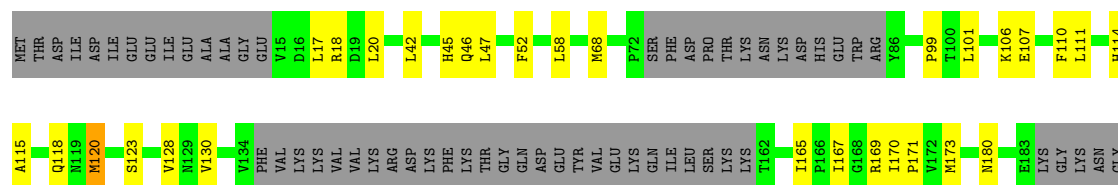
- Molecule 12: RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein

Chain E:  50% 40% . 9%



- Molecule 13: DNA-directed RNA polymerase IV and V subunit 2

Chain B:  65% 17% 17%



ARG	ARG	ASP	F929	ASP	SER	P626	GLU	SER	C318	GLU	SER	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
ARG	ARG	ASP	I936	ASP	GLU	L633	LYS	LYS	F321	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
ILE	ILE	ARG	P937	ARG	LYS	L633	ARG	LYS	R322	GLU	SER	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
GLY	GLY	PHE	P938	PHE	ARG	K637	ARG	LYS	R322	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
PRO	PRO	GLY	D939	GLY	LYS	K640	LYS	LYS	R322	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
TYR	TYR	GLY	I940	GLY	LYS	K640	GLY	MET	N326	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
CYS	CYS	ILE	V941	ILE	MET	V941	MET	ASP	N326	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
ARG	ARG	PHE	I942	PHE	ASP	E656	ASP	GLU	A327	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
LEU	LEU	PHE	N943	PHE	GLU	E656	GLU	GLU	A327	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
CYS	CYS	GLY	P948	GLY	V822	E663	GLY	V822	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
GLU	GLU	GLU	P948	GLU	V822	E663	GLU	V822	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
SER	SER	MET	Q951	MET	K827	C666	MET	K827	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
PRO	PRO	GLU	Q951	GLU	K827	C666	GLU	K827	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
ASP	ASP	ARG	L961	ASP	R834	V835	ARG	R834	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
TYR	TYR	VAL	L961	TYR	V835	V835	CYS	V835	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
VAL	VAL	CYS	I965	CYS	L838	L675	ILE	L838	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
VAL	VAL	ALA	P968	ALA	M850	Q678	ALA	M850	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
ASN	ASN	HIS	R969	HIS	M850	Q678	HIS	M850	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
VAL	VAL	GLY	Q970	GLY	D654	H718	GLY	D654	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
PRO	PRO	ALA	K971	ALA	R859	H718	ALA	R859	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
TYR	TYR	SER	K972	SER	C860	C960	SER	C860	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
GLY	GLY	ALA	K973	ALA	T861	T861	ALA	T861	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
ALA	ALA	ASN	G974	ASN	T861	T861	ASN	T861	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
LEU	LEU	LEU	K975	LEU	D866	P744	LEU	D866	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
LEU	LEU	HIS	Y979	HIS	H867	L748	HIS	H867	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
LEU	LEU	GLU	Y979	GLU	H867	L748	GLU	H867	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
TYR	TYR	ARG	R1003	ARG	K872	F749	ARG	K872	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
GLN	GLN	LEU	R1003	LEU	K872	F749	LEU	K872	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
GLU	GLU	PHE	R1003	PHE	H873	T751	PHE	H873	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279	V284	K288	E289	A290	I294	T304	V307	V308	I311	D315
LEU	LEU	THR	S1007	THR	G877	M752	THR	G877	V470	GLU	GLU	Y191	A215	Q216	E217	W225	S229	P230	R236	T239	R240	R241	F244	I245	Q252	LYS	ALA	GLU	ASP	PHE	K258	R259	K260	V266	Y267	I273	P274	V275	W276	V277	L278	F279										

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28375	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5625	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	T	0.35	0/295	0.57	1/450 (0.2%)
2	N	0.32	0/389	0.65	3/596 (0.5%)
3	P	0.09	0/167	0.20	0/258
4	A	0.23	0/6616	0.52	1/8931 (0.0%)
5	C	0.22	0/2286	0.47	0/3087
6	F	0.20	0/673	0.47	0/905
7	J	0.25	0/515	0.50	0/696
8	K	0.22	0/908	0.48	0/1224
9	L	0.22	0/369	0.50	0/493
10	H	0.20	0/1155	0.51	0/1557
11	I	0.18	0/778	0.44	0/1045
12	E	0.17	0/1732	0.44	0/2332
13	B	0.22	0/7794	0.46	4/10503 (0.0%)
All	All	0.22	0/23677	0.48	9/32077 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
13	B	942	ILE	CA-C-N	8.13	132.03	120.49
13	B	942	ILE	C-N-CA	8.13	132.03	120.49
2	N	24	DT	P-O3'-C3'	-7.77	108.55	120.20
13	B	781	GLU	CA-CB-CG	6.35	126.81	114.10
2	N	26	DC	P-O3'-C3'	-5.93	111.31	120.20

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	T	265	0	148	17	0
2	N	349	0	194	17	0
3	P	150	0	77	7	0
4	A	6506	0	6559	213	0
5	C	2256	0	2269	49	0
6	F	660	0	669	25	0
7	J	507	0	512	12	0
8	K	890	0	883	29	0
9	L	365	0	364	12	0
10	H	1129	0	1128	50	0
11	I	763	0	714	28	0
12	E	1706	0	1759	79	0
13	B	7645	0	7580	156	0
14	A	1	0	0	0	0
15	A	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	23198	0	22856	600	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 13.

The worst 5 of 600 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)
8:K:45:ILE:HA	8:K:48:MET:HE3	1.47	0.95
4:A:1096:LEU:HD22	12:E:35:ARG:HE	1.35	0.89
9:L:35:ARG:HH21	13:B:118:GLN:HB3	1.38	0.89
4:A:1096:LEU:HB2	12:E:35:ARG:HH21	1.37	0.88
4:A:529:VAL:HG22	10:H:93:MET:HE1	1.54	0.88

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	818/2032 (40%)	771 (94%)	47 (6%)	0	100	100
5	C	283/319 (89%)	269 (95%)	14 (5%)	0	100	100
6	F	78/144 (54%)	69 (88%)	9 (12%)	0	100	100
7	J	61/71 (86%)	57 (93%)	4 (7%)	0	100	100
8	K	106/116 (91%)	97 (92%)	9 (8%)	0	100	100
9	L	43/51 (84%)	39 (91%)	4 (9%)	0	100	100
10	H	139/146 (95%)	119 (86%)	20 (14%)	0	100	100
11	I	90/114 (79%)	82 (91%)	8 (9%)	0	100	100
12	E	207/230 (90%)	194 (94%)	13 (6%)	0	100	100
13	B	951/1169 (81%)	896 (94%)	54 (6%)	1 (0%)	48	79
All	All	2776/4392 (63%)	2593 (93%)	182 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	B	781	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 PDB entries followed by that with respect to all EM entries.

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	
4	A	737/1709 (43%)	725 (98%)	12 (2%)	55	68
5	C	253/276 (92%)	247 (98%)	6 (2%)	43	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	72/128 (56%)	72 (100%)	0	100	100
7	J	56/63 (89%)	55 (98%)	1 (2%)	51	67
8	K	98/105 (93%)	97 (99%)	1 (1%)	68	74
9	L	40/46 (87%)	40 (100%)	0	100	100
10	H	123/127 (97%)	121 (98%)	2 (2%)	55	68
11	I	82/101 (81%)	80 (98%)	2 (2%)	43	62
12	E	190/209 (91%)	187 (98%)	3 (2%)	55	68
13	B	844/1026 (82%)	836 (99%)	8 (1%)	70	74
All	All	2495/3790 (66%)	2460 (99%)	35 (1%)	57	70

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	B	130	VAL
13	B	170	ILE
13	B	752	MET
5	C	67	ILE
4	A	1169	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
13	B	602	GLN
13	B	824	GLN
13	B	780	GLN
13	B	390	ASN
13	B	539	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	6/20 (30%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	13	G

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Mol	Chain	Res	Type
3	P	14	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.