



wwPDB EM Validation Summary Report ⓘ

May 10, 2026 – 12:13 AM JST

PDB ID : 9K12 / pdb_00009k12
EMDB ID : EMD-61962
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 1U scaffold at 3.5 Angstrom
Authors : Xie, G.; Du, X.; Du, J.
Deposited on : 2024-10-16
Resolution : 3.46 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

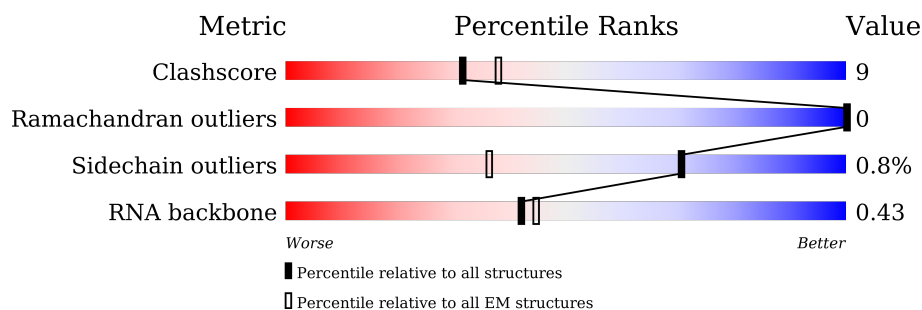
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 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	15% 53% 32%
2	N	34	29% 47% 24%
3	P	20	10% 20% 20% 5% 45%
4	A	2032	32% 9% 58%
5	C	319	79% 11% 10%
6	F	144	38% 18% 44%
7	J	71	77% 11% 11%
8	K	116	77% 16% 7%

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Mol	Chain	Length	Quality of chain
9	L	51	 75% 14% 12%
10	H	146	 68% 27% • •
11	I	114	 68% 17% 15%
12	E	230	 70% 20% • 9%
13	B	1169	 69% 13% 17%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23813 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	23	Total	C	N	O	P	0	0
			465	223	80	139	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	26	Total	C	N	O	P	0	0
			537	255	102	154	26		

- 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*GP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	11	Total	C	N	O	P	0	0
			237	106	46	74	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	845	Total	C	N	O	S	0	0
			6615	4180	1137	1254	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	97	Total	C	N	O	S	0	0
			787	482	150	143	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	966	Total	C	N	O	S	0	0
			7652	4821	1356	1431	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

GLU	SER	GLU	ASP	GLU	ASN	LYS	GLN	ALA	ALA	VAL	ALA	GLY	ALA	LEU	F1227	T1156	GLN	M836	E660	F541	LYS	SER
SER	ILE	LEU	GLY	ASP	SER	SER	LYS	LEU	ASN	GLU	ALA	PRO	ASN	GLU	E1228	M1161	ALA	M661	F542	GLY	SER	
GLY	GLY	GLY	GLY	ASN	GLY	GLY	LYS	GLY	VAL	GLU	VAL	SER	GLY	PRO	L1229	F1164	GLY	I663	Q543	HIS	SER	
PRO	PRO	PRO	TRP	SER	ASN	SER	ASN	ASP	ASN	ASP	ASN	ASP	GLY	LYS	N1232	F1164	LYS	V666	L545	P396	LYS	
MET	MET	TRP	ASP	ASP	GLY	TYR	GLY	ASP	GLY	ASP	GLY	ASP	GLY	ASP	LYS	Y1169	LYS	L546	L547	TRP		
PHE	PHE	VAL	VAL	TRP	VAL	LYS	LYS	TRP	ASP	ASP	ASP	ASP	GLY	ASP	GLY	GLY	ASP	A548	I399	THR		
THR	THR	GLY	GLY	GLY	GLY	LYS	LYS	GLY	ALA	GLY	ALA	SER	GLY	SER	THR	T1173	ALA	V400	GLU			
ALA	ALA	GLY	LYS	LYS	PRO	ASN	PRO	GLY	SER	GLY	SER	GLY	ALA	GLY	GLY	ARG	LYS	H401	LYS			
ARG	ARG	ALA	GLY	GLY	TRP	ALA	ALA	GLY	SER	GLY	TRP	GLY	SER	GLY	GLY	LEU	ASN	R402	MET			
GLN	GLN	THR	THR	THR	THR	THR	THR	THR	TRP	GLY	TRP	GLN	ASN	ASP	ASN	ILE	GLN	S554	ARG			
GLY	GLY	ARG	GLY	GLY	GLY	GLY	GLY	GLY	ASN	ASP	ASN	ASN	ASN	ASP	ASP	ILE	GLY	C555	THR			
LYS	LYS	THR	THR	THR	THR	THR	THR	THR	SER	ASP	SER	SER	SER	LEU	ASP	LYS	GLY	V562	LEU			
ASN	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS	GLY	F411	PHE			
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS	GLY	L567	ILE			
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	LYS	GLY	L577	ARG			
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS	GLY	A578	GLY			
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	LYS	GLY	D449	SER			
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	GLY	L441	F322			
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	GLY	GLY	M442	S323			
SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	GLY	GLY	L457	T329			
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	GLY	F458	G330			
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY	A465	D331			
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLY	GLY	A468	N335			
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	V469	E338			
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	GLY	E468	V339			
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	GLY	GLY	L472	G340			
SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	GLY	GLY	S474	I341			
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	GLY	L607	P342			
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	GLY	M609	M343			
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY	L477	E344			
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L479	I345			
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	GLY	L467	E352			
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	GLY	V857	S356			
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	GLY	GLY	V806	H358			
SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	GLY	GLY	S512	N359			
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	GLY	L516	I360			
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY	R822	C372			
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Y375	Y375			
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	GLY	P527	I376			
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	GLY	A528	Q377			
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY	V529	Y382			
SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	GLY	GLY	V630	A385			
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY	GLY	A538	ASP			
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	GLY	M539	GLY			
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY	T540	SER			
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	GLY	GLY					

GLU	PHE	I1027
LEU	THR	F1028
PHE	LEU	M1029
SER	SER	
MET	ASP	R1036
GLY	SER	L1037
ILE	SER	I1038
CYS	GLN	H1039
LEU	LEU	M1040
ASN	HIS	
PHE	ILE	K1044
GLU	CYS	V1045
THR	ARG	K1046
ASN	ASN	F1047
LEU	CYS	R1048
CYS	LYS	ASN
	SER	THR
	ALA	GLY
	ALA	PRO
	ASN	VAL
	VAL	HIS
	ILE	PRO
	GLU	LEU
	ARG	THR
	VAL	ARG
	ALA	GLN
	SER	PRO
	SER	VAL
	GLY	ALA
	ARG	ASP
	ARG	ARG
	ILE	LYS
	ARG	ARG
	GLY	PHE
	PRO	GLY
	TYR	GLY
	CYS	ILE
	ARG	LYS
	LEU	PHE
	CYS	GLY
	GLU	GLU
	SER	MET
	PRO	ARG
	ASP	ASP
	TYR	CYS
	VAL	LEU
	VAL	ILE
	MET	ALA
	VAL	ALA
	ASN	HIS
	VAL	GLY
	PRO	ALA
	TYR	SER
	GLY	ALA
	LYS	ASN
	LEU	LEU
	LEU	HIS
	TYR	GLU
	GLN	ARG
	GLN	LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79987	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	0.37	0/518	0.44	0/793
2	N	0.37	0/603	0.43	0/929
3	P	0.79	4/265 (1.5%)	0.21	0/411
4	A	0.14	0/6729	0.42	1/9086 (0.0%)
5	C	0.14	0/2286	0.39	0/3087
6	F	0.17	0/673	0.49	0/905
7	J	0.15	0/515	0.41	0/696
8	K	0.15	0/908	0.35	0/1224
9	L	0.13	0/369	0.34	0/493
10	H	0.16	0/1155	0.49	0/1557
11	I	0.14	0/804	0.36	0/1081
12	E	0.12	0/1732	0.36	0/2332
13	B	0.13	0/7801	0.37	0/10513
All	All	0.18	4/24358 (0.0%)	0.40	1/33107 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	15	G	C1'-N9	-6.07	1.38	1.48
3	P	14	C	C1'-N1	6.03	1.57	1.48
3	P	17	C	C1'-N1	5.69	1.56	1.48
3	P	19	C	C1'-N1	5.33	1.56	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	MET	CB-CA-C	5.23	115.81	109.85

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	465	0	262	39	0
2	N	537	0	293	25	0
3	P	237	0	121	10	0
4	A	6615	0	6668	130	0
5	C	2256	0	2269	25	0
6	F	660	0	669	20	0
7	J	507	0	512	6	0
8	K	890	0	883	15	0
9	L	365	0	364	5	0
10	H	1129	0	1128	30	0
11	I	787	0	736	14	0
12	E	1706	0	1759	27	0
13	B	7652	0	7589	105	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	23813	0	23253	407	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 9.

The worst 5 of 407 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:T:15:DA:C2	2:N:21:DA:C2	2.32	1.17
1:T:12:DC:C2'	1:T:13:DT:H72	1.94	0.98
1:T:15:DA:H2	2:N:21:DA:C2	1.76	0.95
1:T:12:DC:H2'	1:T:13:DT:H72	1.52	0.91
1:T:12:DC:H2'	1:T:13:DT:C7	2.04	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	837/2032 (41%)	798 (95%)	39 (5%)	0	100	100
5	C	283/319 (89%)	276 (98%)	7 (2%)	0	100	100
6	F	78/144 (54%)	71 (91%)	7 (9%)	0	100	100
7	J	61/71 (86%)	60 (98%)	1 (2%)	0	100	100
8	K	106/116 (91%)	102 (96%)	4 (4%)	0	100	100
9	L	43/51 (84%)	40 (93%)	3 (7%)	0	100	100
10	H	139/146 (95%)	124 (89%)	15 (11%)	0	100	100
11	I	93/114 (82%)	88 (95%)	5 (5%)	0	100	100
12	E	207/230 (90%)	198 (96%)	9 (4%)	0	100	100
13	B	952/1169 (81%)	921 (97%)	31 (3%)	0	100	100
All	All	2799/4392 (64%)	2678 (96%)	121 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	750/1709 (44%)	744 (99%)	6 (1%)	73	77
5	C	253/276 (92%)	251 (99%)	2 (1%)	73	77
6	F	72/128 (56%)	71 (99%)	1 (1%)	59	72
7	J	56/63 (89%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	98/105 (93%)	98 (100%)	0	100	100
9	L	40/46 (87%)	40 (100%)	0	100	100
10	H	123/127 (97%)	121 (98%)	2 (2%)	55	71
11	I	85/101 (84%)	85 (100%)	0	100	100
12	E	190/209 (91%)	186 (98%)	4 (2%)	47	66
13	B	845/1026 (82%)	839 (99%)	6 (1%)	76	78
All	All	2512/3790 (66%)	2491 (99%)	21 (1%)	70	77

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	E	127	VAL
13	B	245	ILE
13	B	913	MET
13	B	312	GLN
13	B	225	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
12	E	182	GLN
13	B	873	HIS
13	B	481	GLN
13	B	951	GLN
13	B	773	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	10/20 (50%)	3 (30%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	11	A
3	P	13	G
3	P	14	C

There are no RNA pucker outliers to report.

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 ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.