



wwPDB EM Validation Summary Report ⓘ

May 10, 2026 – 12:22 AM JST

PDB ID : 9K11 / pdb_00009k11
EMDB ID : EMD-61961
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 0U scaffold at 2.96 Angstrom
Authors : Xie, G.; Du, X.; Du, J.
Deposited on : 2024-10-16
Resolution : 2.96 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

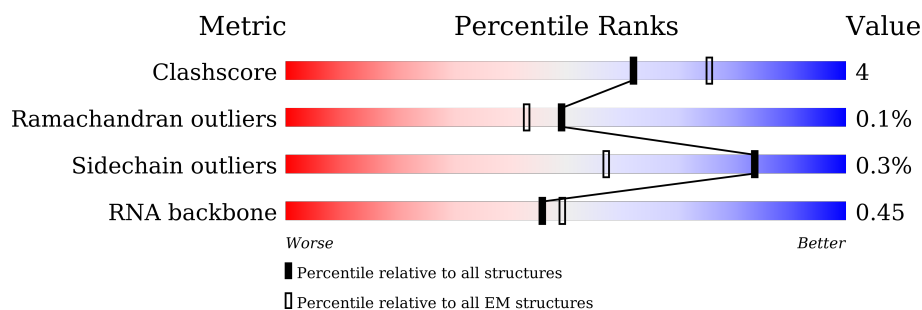
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	41% 32% 24%
2	N	34	41% 29% 6% 24%
3	P	20	15% 30% 10% 45%
4	A	2032	37% 58%
5	C	319	83% 7% 10%
6	F	144	53% 44%
7	J	71	86% 11%
8	K	116	86% 7% 7%

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Mol	Chain	Length	Quality of chain
9	L	51	 76% 12% 12%
10	H	146	 77% 20% •
11	I	114	 67% 18% 15%
12	E	230	 75% 16% 9%
13	B	1169	 77% 6% 17%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23916 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 0U template DNA (34-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	26	Total	C	N	O	P	0	0
			534	254	106	148	26		

- Molecule 2 is a DNA chain called 0U nontemplated DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	26	Total	C	N	O	P	0	0
			534	259	83	166	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	11	Total	C	N	O	P	0	0
			239	107	49	72	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	844	Total	C	N	O	S	0	0
			6608	4176	1136	1252	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	971	Total	C	N	O	S	0	0
			7694	4848	1364	1438	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

[illegible]

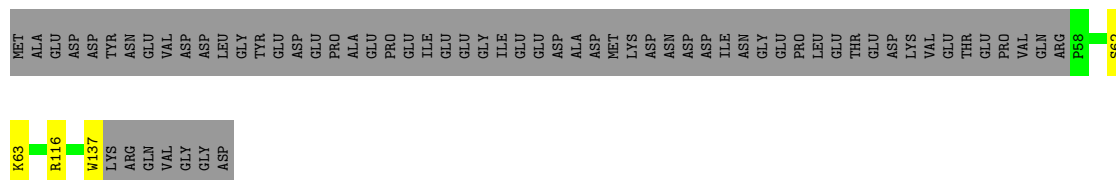
- Molecule 5: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein

Chain C:  83% 7% 10%



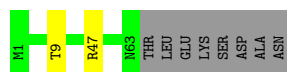
- Molecule 6: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein

Chain F:  53% 44%



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

Chain J:  86% 11%



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

Chain K:  86% 7% 7%



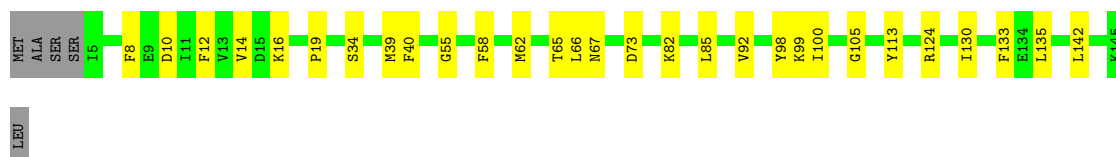
- Molecule 9: DNA-directed RNA polymerase II, IV and V subunit 12

Chain L:  76% 12% 12%



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

Chain H:  77% 20% 3%



- | | | | | | |
|-----|-----|------|------|------|------|
| VAL | ARG | Q766 | I435 | ASP | MET |
| ALA | GLN | Q782 | M464 | GLU | THR |
| SER | PRO | S783 | S783 | TYR | ASP |
| GLY | VAL | I784 | R487 | GLU | ILE |
| ARG | ASP | E799 | V483 | LYS | ASP |
| ARG | ARG | LYS | I494 | GLN | GLU |
| ILE | LYS | Y804 | I496 | LEU | GLU |
| ARG | ARG | Y804 | I496 | SER | ILE |
| GLY | PHE | G437 | R488 | LYS | ALA |
| PRO | GLY | S810 | V499 | LYS | ALA |
| TYR | GLY | LYS | G500 | T162 | GLY |
| CYS | ILE | ASP | V499 | E183 | GLY |
| ARG | LYS | GLU | G500 | LYS | V15 |
| LEU | PHE | GLU | S531 | GLY | V15 |
| CYS | GLY | ARG | M531 | GLY | R18 |
| CYS | GLU | LYS | M531 | LYS | D19 |
| SER | MET | LYS | D559 | ASN | L20 |
| PRO | GLU | LYS | T560 | GLY | F53 |
| ASP | GLU | MET | S561 | GLU | F53 |
| VAL | ASP | GLU | T562 | SER | Q59 |
| VAL | LEU | V822 | G578 | Y191 | Q59 |
| VAL | ILE | ALA | R596 | N251 | P72 |
| VAL | ALA | K831 | R596 | SER | P72 |
| ASN | HIS | V835 | E604 | ASP | PHE |
| VAL | GLY | L884 | I605 | ALA | ASP |
| PRO | ALA | S885 | K606 | GLU | PR0 |
| TYR | SER | S886 | R625 | ASP | THR |
| GLY | ALA | L898 | K637 | PHE | ASN |
| ALA | ASN | S886 | E662 | K258 | ASN |
| LYS | LEU | L898 | E663 | R258 | LVS |
| LEU | HIS | L898 | E664 | ASP | ASP |
| LEU | GLU | R902 | E670 | K260 | HIS |
| TYR | ARG | R902 | L675 | Y267 | GLU |
| GLN | LEU | P942 | K677 | S286 | TRP |
| GLU | PHE | THR | E686 | ARG | ARG |
| LEU | THR | THR | E686 | E289 | Y86 |
| PHE | LEU | P948 | E686 | D320 | V04 |
| SER | SER | S949 | E664 | Y267 | Y86 |
| MET | ASP | R950 | E664 | D320 | V04 |
| MET | ASP | S950 | E664 | N326 | V130 |
| GLY | SER | S962 | L675 | Y267 | V130 |
| ILE | GLN | S962 | K677 | S286 | V134 |
| CYS | GLN | I965 | E686 | T362 | PHE |
| LEU | MET | THR | E686 | G400 | VAL |
| LEU | HIS | ILE | E686 | R416 | VAL |
| ASN | ASN | THR | E686 | T417 | VAL |
| PHE | THR | THR | E686 | M418 | ARG |
| GLU | ARG | CYS | E686 | T419 | LVS |
| THR | ASN | CYS | E686 | K420 | ASP |
| ASN | ASN | CYS | E686 | A421 | PHE |
| LEU | LEU | CYS | E686 | Q423 | THR |
| LEU | LEU | CYS | E686 | T427 | THR |
| CYS | CYS | CYS | E686 | G724 | CYS |
| | LVS | ASN | E686 | R710 | |
| | LVS | ASN | E686 | G724 | |
| | LVS | ASN | E686 | L741 | |
| | LVS | ASN | E686 | L748 | |
| | LVS | ASN | E686 | N764 | |
| | LVS | ASN | E686 | G726 | |

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77772	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	0.51	0/601	0.69	4/924 (0.4%)
2	N	0.42	0/595	1.03	6/918 (0.7%)
3	P	0.55	1/268 (0.4%)	0.51	1/416 (0.2%)
4	A	0.33	0/6722	0.62	1/9076 (0.0%)
5	C	0.39	0/2286	0.63	0/3087
6	F	0.30	0/673	0.55	0/905
7	J	0.41	0/515	0.58	0/696
8	K	0.38	0/908	0.59	0/1224
9	L	0.34	0/369	0.53	0/493
10	H	0.30	0/1155	0.70	0/1557
11	I	0.31	0/804	0.61	0/1081
12	E	0.26	0/1732	0.63	2/2332 (0.1%)
13	B	0.40	0/7845	0.61	2/10574 (0.0%)
All	All	0.36	1/24473 (0.0%)	0.63	16/33283 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1
10	H	0	1
11	I	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	18	G	C1'-N9	-7.04	1.37	1.48

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	20	DA	P-O3'-C3'	-16.07	96.10	120.20
2	N	20	DA	O3'-P-O5'	-12.59	85.12	104.00
2	N	20	DA	OP1-P-O3'	9.74	137.23	108.00
1	T	28	DA	P-O3'-C3'	-6.76	110.06	120.20
2	N	18	DT	P-O3'-C3'	-6.08	111.08	120.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1050	TRP	Peptide
10	H	105	GLY	Peptide
11	I	68	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	534	0	291	22	0
2	N	534	0	302	33	0
3	P	239	0	122	8	0
4	A	6608	0	6662	51	0
5	C	2256	0	2270	13	0
6	F	660	0	669	3	0
7	J	507	0	512	1	0
8	K	890	0	883	4	0
9	L	365	0	365	5	0
10	H	1129	0	1128	16	0
11	I	787	0	739	11	0
12	E	1706	0	1759	19	0
13	B	7694	0	7633	49	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L	1	0	0	0	0
All	All	23916	0	23335	198	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 4.

The worst 5 of 198 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:29:DC:N4	2:N:6:DG:H1	1.07	1.41
1:T:29:DC:N4	2:N:6:DG:N1	1.66	1.34
2:N:21:DT:H1'	2:N:22:DT:H72	1.43	0.98
1:T:29:DC:H41	2:N:6:DG:H1	1.25	0.79
2:N:21:DT:H1'	2:N:22:DT:C7	2.14	0.78

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	836/2032 (41%)	789 (94%)	47 (6%)	0	100	100
5	C	283/319 (89%)	276 (98%)	7 (2%)	0	100	100
6	F	78/144 (54%)	72 (92%)	6 (8%)	0	100	100
7	J	61/71 (86%)	57 (93%)	4 (7%)	0	100	100
8	K	106/116 (91%)	99 (93%)	7 (7%)	0	100	100
9	L	43/51 (84%)	38 (88%)	5 (12%)	0	100	100
10	H	139/146 (95%)	122 (88%)	17 (12%)	0	100	100
11	I	93/114 (82%)	88 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	E	207/230 (90%)	196 (95%)	11 (5%)	0	100	100
13	B	959/1169 (82%)	907 (95%)	50 (5%)	2 (0%)	43	66
All	All	2805/4392 (64%)	2644 (94%)	159 (6%)	2 (0%)	49	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	B	499	VAL
13	B	500	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	749/1709 (44%)	748 (100%)	1 (0%)	88	95
5	C	253/276 (92%)	253 (100%)	0	100	100
6	F	72/128 (56%)	72 (100%)	0	100	100
7	J	56/63 (89%)	56 (100%)	0	100	100
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%)	123 (100%)	0	100	100
11	I	85/101 (84%)	85 (100%)	0	100	100
12	E	190/209 (91%)	189 (100%)	1 (0%)	81	90
13	B	849/1026 (83%)	844 (99%)	5 (1%)	78	89
All	All	2515/3790 (66%)	2508 (100%)	7 (0%)	84	92

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	B	494	LEU
13	B	496	THR

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Mol	Chain	Res	Type
13	B	499	VAL
13	B	498	ARG
13	B	493	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
13	B	602	GLN
13	B	1000	GLN
13	B	705	HIS
13	B	764	ASN
8	K	65	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	10/20 (50%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	12	A
3	P	14	A

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.