



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 5, 2022 – 04:31 PM EST

PDB ID : 7RIM  
Title : RNA polymerase II elongation complex with hairpin polyamide Py-Im 1, scaffold 1  
Authors : Oh, J.; Dervan, P.B.; Wang, D.  
Deposited on : 2021-07-20  
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.25  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.25

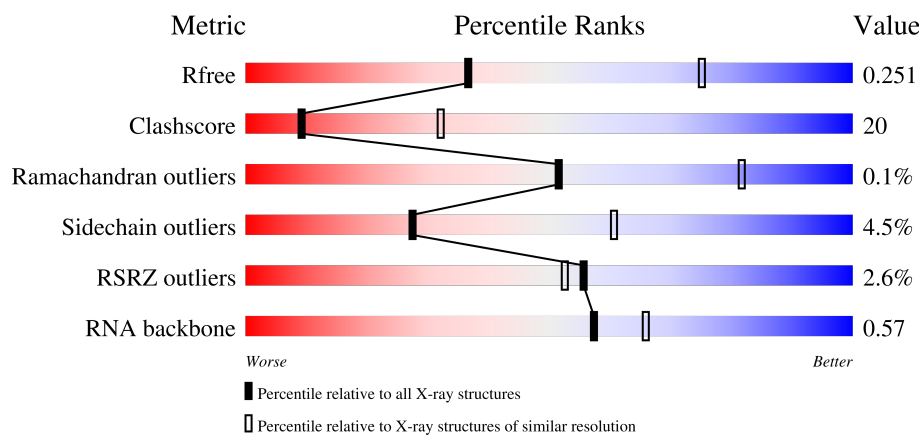
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	9	<div> <div>89%</div> <div>11%</div> </div>
2	T	30	<div> <div>20%</div> <div>63%</div> <div>13%</div> </div>
3	N	20	<div> <div>10%</div> <div>65%</div> <div>25%</div> </div>
4	A	1733	<div> <div>3%</div> <div>50%</div> <div>28%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
5	B	1224	<div><div></div><div>2%61%30%8%</div></div>
6	C	318	<div><div></div><div>52%30%16%</div></div>
7	E	215	<div><div></div><div>7%49%45%</div></div>
8	F	155	<div><div></div><div>%32%20%45%</div></div>
9	H	146	<div><div></div><div>8%42%46%9%</div></div>
10	I	122	<div><div></div><div>65%29%</div></div>
11	J	70	<div><div></div><div>60%30%7%</div></div>
12	K	120	<div><div></div><div>63%32%5%</div></div>
13	L	70	<div><div></div><div>%40%20%39%</div></div>

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29191 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			199	88	40	62	9			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	0	0
			525	252	84	163	26			

- Molecule 3 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	15	Total	C	N	O	P	0	0	0
			312	147	66	84	15			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1384	Total	C	N	O	S	0	0	0
			10828	6831	1896	2041	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1129	Total	C	N	O	S	0	0	0
			8899	5630	1561	1655	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	212	Total	C	N	O	S	0	0	0
			1731	1100	305	315	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			952	585	173	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

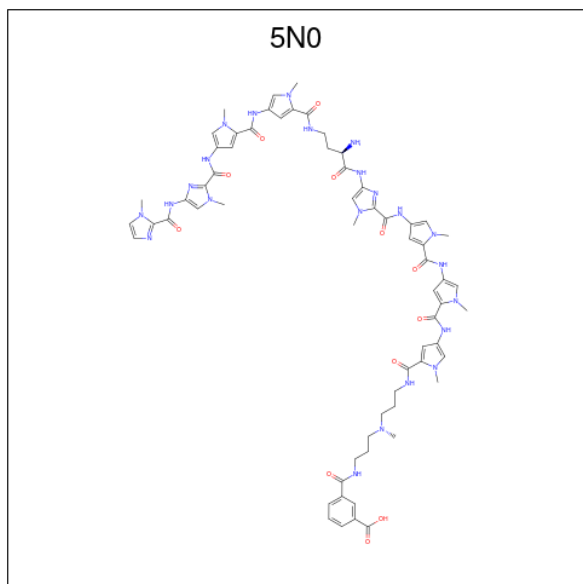
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

- Molecule 14 is 3-({3-[(3-{[4-({4-[(4-{[4-((2R)-2-amino-4-[(1-methyl-4-{[1-methyl-4-({1-met

hyl-4-[(1-methyl-1H-imidazole-2-carbonyl)amino]-1H-imidazole-2-carbonyl}amino)-1H-pyrrole-2-carbonyl]amino}-1H-pyrrole-2-carbonyl)amino]butanoyl}amino)-1-methyl-1H-imidazole-2-carbonyl]amino}-1-methyl-1H-pyrrole-2-carbonyl)amino]-1-methyl-1H-pyrrole-2-carbonyl}amino)-1-methyl-1H-pyrrole-2-carbonyl]amino}propyl)(methylamino)propyl}carbamoyl)benzoic acid (three-letter code: 5N0) (formula: C<sub>64</sub>H<sub>75</sub>N<sub>23</sub>O<sub>12</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	T	1	Total	C	N	O	0	0
			99	64	23	12		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		



- Molecule 1: RNA

- Molecule 2: Template strand DNA

- Molecule 3: Non-template DNA

- Molecule 4: DNA-directed RNA polymerase II subunit RPB1



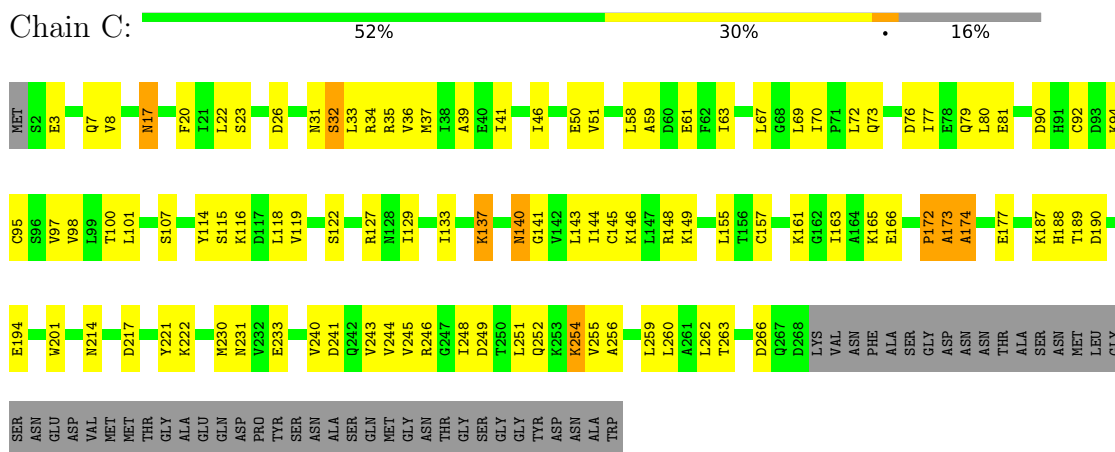
WORLD WIDE  
**PDB**  
PROTEIN DATA BANK



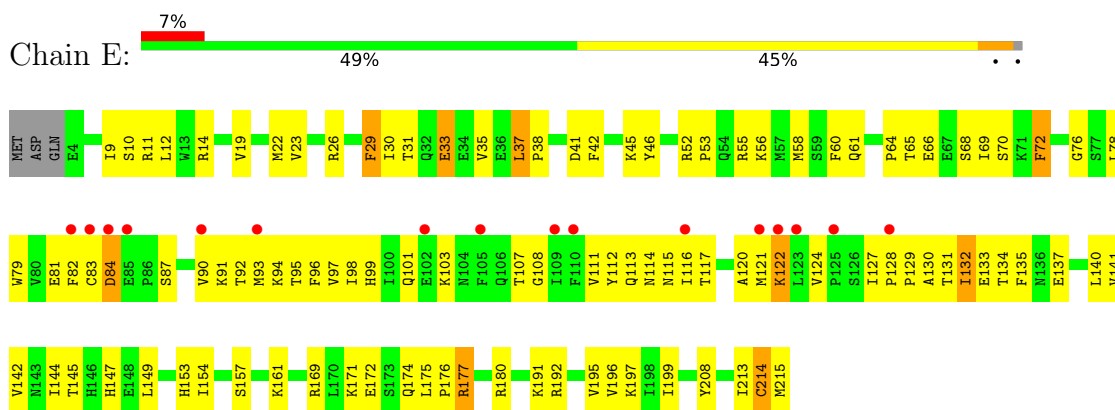




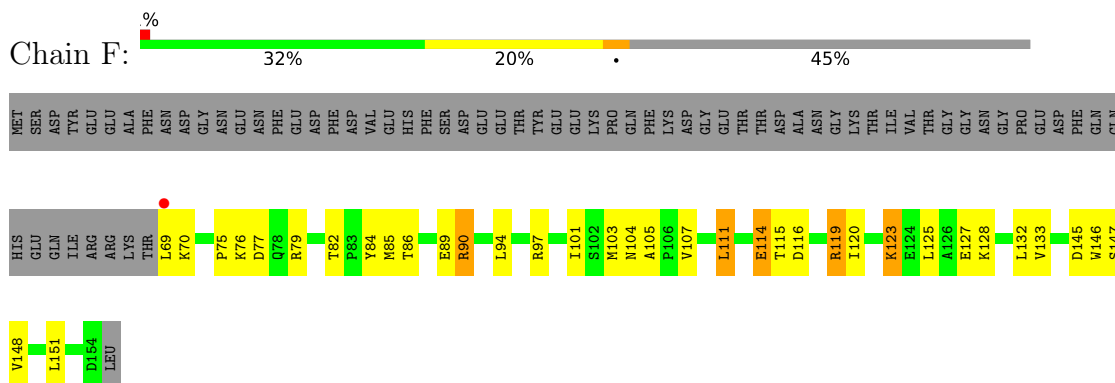
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3



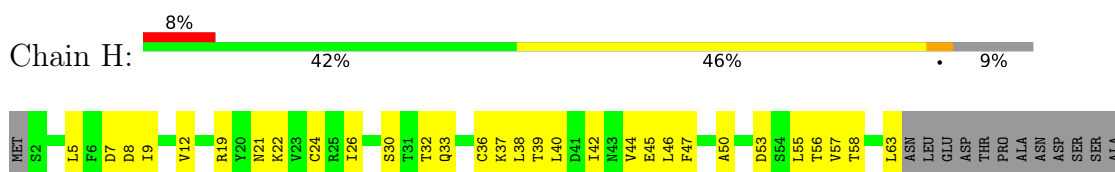
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

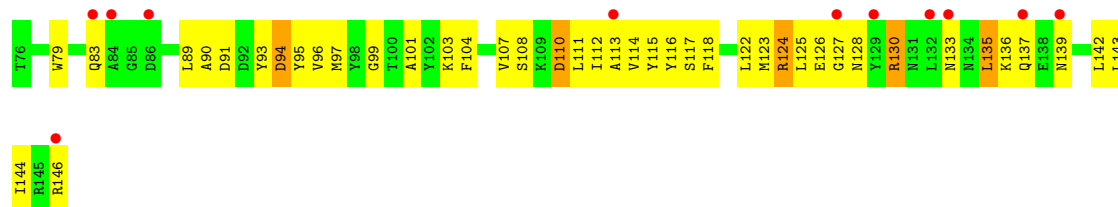


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

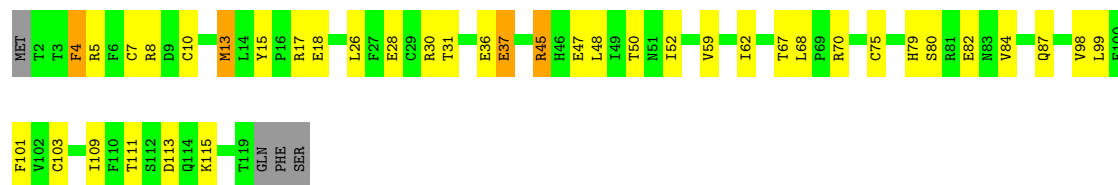


• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3





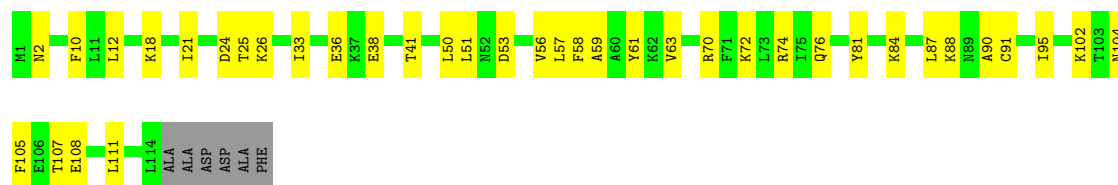
- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 12: DNA-directed RNA polymerase II subunit RPB11



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.22Å 221.93Å 193.71Å 90.00° 99.63° 90.00°	Depositor
Resolution (Å)	82.43 – 2.90 95.49 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (82.43-2.90) 100.0 (95.49-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, $R_{free}$	0.215 , 0.251 0.215 , 0.251	Depositor DCC
$R_{free}$ test set	7776 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.3	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 71.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	29191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 5N0, 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	R	0.86	1/223 (0.4%)	1.04	0/345
2	T	0.78	0/584	1.21	2/898 (0.2%)
3	N	0.76	0/352	1.00	0/541
4	A	0.35	0/11020	0.59	5/14907 (0.0%)
5	B	0.32	1/9071 (0.0%)	0.54	2/12242 (0.0%)
6	C	0.32	0/2139	0.56	0/2899
7	E	0.36	0/1767	0.60	2/2378 (0.1%)
8	F	0.33	0/696	0.61	2/943 (0.2%)
9	H	0.44	0/1082	0.77	3/1466 (0.2%)
10	I	0.43	0/970	0.58	0/1308
11	J	0.28	0/541	0.51	0/727
12	K	0.33	0/937	0.55	0/1265
13	L	0.37	0/339	0.69	0/450
All	All	0.37	2/29721 (0.0%)	0.61	16/40369 (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	5
6	C	0	2
9	H	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1	A	OP3-P	-10.91	1.48	1.61
5	B	278	GLN	CG-CD	5.12	1.62	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	179	LEU	CB-CG-CD1	-8.51	96.53	111.00
2	T	22	DT	O4'-C4'-C3'	-8.40	100.96	106.00
5	B	90	ILE	CG1-CB-CG2	-6.57	96.94	111.40
7	E	37	LEU	CA-CB-CG	6.31	129.81	115.30
9	H	130	ARG	NE-CZ-NH1	-5.92	117.34	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1106	ASN	Peptide
4	A	4	GLN	Peptide
4	A	524	VAL	Peptide
4	A	55	ASP	Peptide
4	A	592	ASP	Peptide

## 5.2 Too-close contacts [i](#)

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	R	199	0	98	9	0
2	T	525	0	297	25	0
3	N	312	0	167	15	0
4	A	10828	0	10876	478	1
5	B	8899	0	8853	329	0
6	C	2101	0	2056	87	1
7	E	1731	0	1758	97	0
8	F	684	0	692	40	0
9	H	1064	0	1029	81	0
10	I	952	0	897	43	0
11	J	532	0	542	18	0
12	K	919	0	929	37	0
13	L	337	0	352	15	0
14	T	99	0	0	2	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
16	A	1	0	0	0	0
All	All	29191	0	28546	1147	1

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 20.

The worst 5 of 1147 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)
12:K:107:THR:O	12:K:111:LEU:HD12	1.29	1.30
5:B:1165:ILE:HD12	5:B:1166:CYS:N	1.50	1.27
9:H:89:LEU:HD13	9:H:91:ASP:O	1.07	1.20
5:B:1101:ASP:O	5:B:1122:ARG:NH2	1.76	1.18
5:B:118:ARG:NH2	5:B:194:GLU:OE2	1.79	1.16

All (1) 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:A:419:LYS:NZ	6:C:90:ASP:O[2_555]	2.14	0.06

## 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 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
4	A	1370/1733 (79%)	1299 (95%)	68 (5%)	3 (0%)	47 78
5	B	1111/1224 (91%)	1068 (96%)	43 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	265/318 (83%)	256 (97%)	7 (3%)	2 (1%)	19	51
7	E	210/215 (98%)	201 (96%)	9 (4%)	0	100	100
8	F	84/155 (54%)	79 (94%)	5 (6%)	0	100	100
9	H	129/146 (88%)	118 (92%)	11 (8%)	0	100	100
10	I	116/122 (95%)	111 (96%)	5 (4%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100
12	K	112/120 (93%)	108 (96%)	4 (4%)	0	100	100
13	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
All	All	3501/4173 (84%)	3343 (96%)	153 (4%)	5 (0%)	51	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
6	C	173	ALA
6	C	174	ALA
4	A	1107	VAL
4	A	567	LYS

### 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	
4	A	1194/1520 (79%)	1137 (95%)	57 (5%)	25	58
5	B	958/1061 (90%)	925 (97%)	33 (3%)	37	71
6	C	235/274 (86%)	225 (96%)	10 (4%)	29	62
7	E	193/197 (98%)	180 (93%)	13 (7%)	16	43
8	F	73/137 (53%)	69 (94%)	4 (6%)	21	53
9	H	116/128 (91%)	110 (95%)	6 (5%)	23	55
10	I	110/116 (95%)	103 (94%)	7 (6%)	17	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	J	60/65 (92%)	56 (93%)	4 (7%)	16	43
12	K	99/102 (97%)	98 (99%)	1 (1%)	76	92
13	L	37/57 (65%)	34 (92%)	3 (8%)	11	33
All	All	3075/3657 (84%)	2937 (96%)	138 (4%)	27	61

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	F	114	GLU
9	H	94	ASP
11	J	7	CYS
4	A	1262	LYS
4	A	1224	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	822	ASN
5	B	1177	HIS
9	H	139	ASN
7	E	174	GLN
5	B	951	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/9 (88%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	9	G

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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
14	5N0	T	101	-	91,107,107	2.55	28 (30%)	91,153,153	1.57	10 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	5N0	T	101	-	-	13/47/92/92	0/9/9/9

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	101	5N0	C59-C63	7.28	1.54	1.47
14	T	101	5N0	C49-N23	6.65	1.48	1.33
14	T	101	5N0	C56-N25	6.18	1.47	1.33
14	T	101	5N0	C30-C31	6.02	1.58	1.53
14	T	101	5N0	C22-N10	5.95	1.46	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	101	5N0	C30-C31-N17	7.45	121.78	113.69
14	T	101	5N0	C6-C10-N6	6.59	120.85	113.69
14	T	101	5N0	C4-C5-N3	3.76	117.78	113.69
14	T	101	5N0	C29-N14-C26	-3.24	122.96	127.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	101	5N0	O3-C16-N8	-2.51	117.98	123.71

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

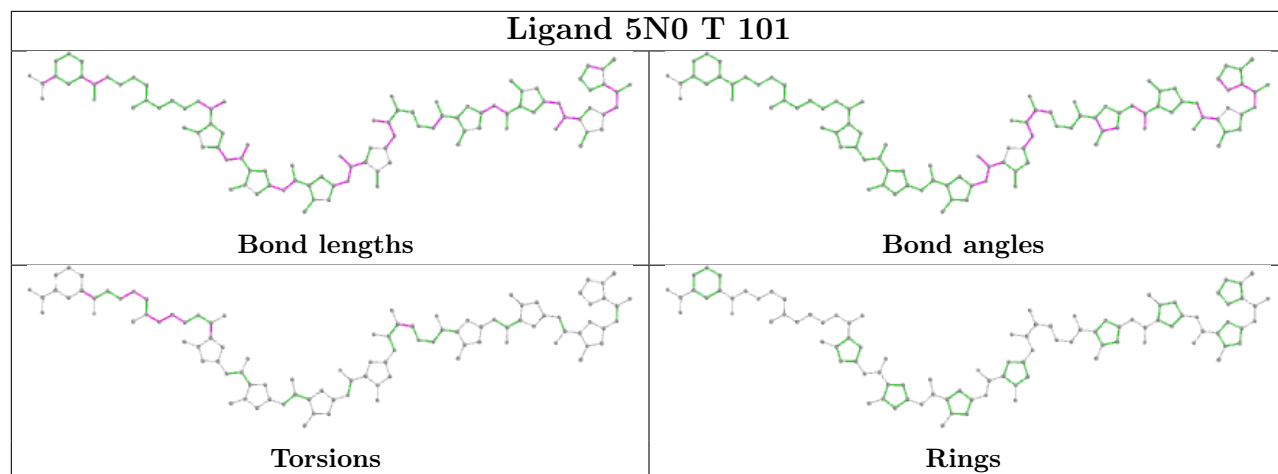
Mol	Chain	Res	Type	Atoms
14	T	101	5N0	C23-C24-C25-N11
14	T	101	5N0	C23-C24-C25-C26
14	T	101	5N0	C47-C44-C49-O9
14	T	101	5N0	C51-C52-N24-C64
14	T	101	5N0	N23-C50-C51-C52

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	101	5N0	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	R	9/9 (100%)	0.55	0 100 100	83, 93, 159, 175	0
2	T	26/30 (86%)	-0.06	0 100 100	109, 168, 239, 254	0
3	N	15/20 (75%)	-0.24	0 100 100	144, 193, 223, 233	0
4	A	1384/1733 (79%)	0.16	45 (3%) 46 41	41, 92, 176, 245	0
5	B	1129/1224 (92%)	0.08	19 (1%) 70 69	33, 76, 148, 223	0
6	C	267/318 (83%)	-0.08	0 100 100	48, 80, 120, 170	0
7	E	212/215 (98%)	0.31	16 (7%) 14 11	66, 122, 185, 231	0
8	F	86/155 (55%)	-0.00	1 (1%) 79 79	61, 93, 145, 204	0
9	H	133/146 (91%)	0.62	11 (8%) 11 8	84, 127, 186, 223	0
10	I	118/122 (96%)	-0.27	0 100 100	58, 93, 138, 203	0
11	J	65/70 (92%)	-0.08	0 100 100	50, 71, 115, 146	0
12	K	114/120 (95%)	0.02	0 100 100	53, 87, 125, 163	0
13	L	43/70 (61%)	0.14	1 (2%) 60 58	67, 113, 175, 206	0
All	All	3601/4232 (85%)	0.11	93 (2%) 56 52	33, 88, 170, 254	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	286	HIS	8.2
5	B	250	PHE	5.6
4	A	141	LEU	5.5
4	A	182	VAL	5.4
4	A	183	GLY	5.2

### 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

There are no monosaccharides in this entry.

## 6.4 Ligands

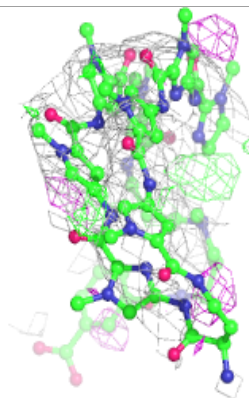
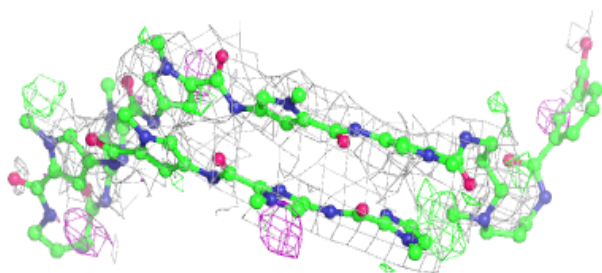
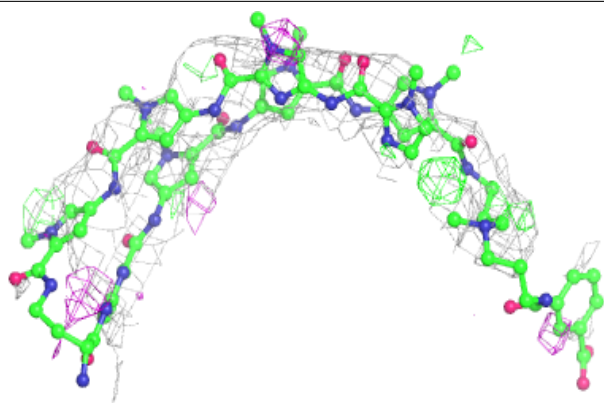
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	5N0	T	101	99/99	0.73	0.33	142,171,236,249	0
15	ZN	A	1801	1/1	0.84	0.05	179,179,179,179	0
15	ZN	B	1301	1/1	0.93	0.14	134,134,134,134	0
15	ZN	I	202	1/1	0.93	0.26	106,106,106,106	0
15	ZN	J	101	1/1	0.93	0.23	86,86,86,86	0
15	ZN	L	101	1/1	0.95	0.09	110,110,110,110	0
15	ZN	A	1802	1/1	0.96	0.15	95,95,95,95	0
16	MG	A	1803	1/1	0.96	0.11	79,79,79,79	0
15	ZN	C	401	1/1	0.99	0.23	81,81,81,81	0
15	ZN	I	201	1/1	0.99	0.16	90,90,90,90	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 5N0 T 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.