wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2023 – 07:48 PM EDT

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)

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

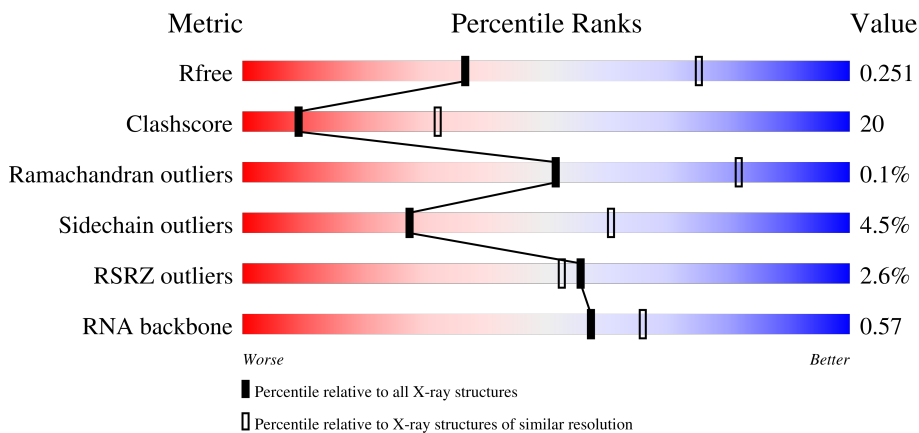|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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	Percentile Ranks	Value
Rfree		0.251
Clashscore		20
Ramachandran outliers		0.1%
Sidechain outliers		4.5%
RSRZ outliers		2.6%
RNA backbone		0.57

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 >=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 <=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	89% 11%
2	T	30	20% 63% • 13%
3	N	20	10% 65% 25%
4	A	1733	3% 50% 28% • 20%

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

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 199	C 88	N 40	O 62	P 9	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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 1731	C 1100	N 305	O 315	S 11	0	0	0

- 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 684	C 437	N 115	O 129	S 3	0	0	0

- 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 1064	C 670	N 179	O 211	S 4	0	0	0

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

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

- 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 532	C 339	N 93	O 94	S 6	0	0	0

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

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

- 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 337	C 208	N 66	O 59	S 4	0	0	0

- 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-pyr role-2-carbonyl]amino}-1H-pyrrole-2-carbonyl)amino]butanoyl}amino)-1-methyl-1H-imida zole-2-carbonyl]amino}-1-methyl-1H-pyrrole-2-carbonyl)amino]-1-methyl-1H-pyrrole-2-car bonyl}amino)-1-methyl-1H-pyrrole-2-carbonyl]amino}propyl)(methyl)amino]propyl}carba moyl)benzoic acid (three-letter code: 5N0) (formula: $C_{64}H_{75}N_{23}O_{12}$) (labeled as "Ligand of Interest" by depositor).

5N0
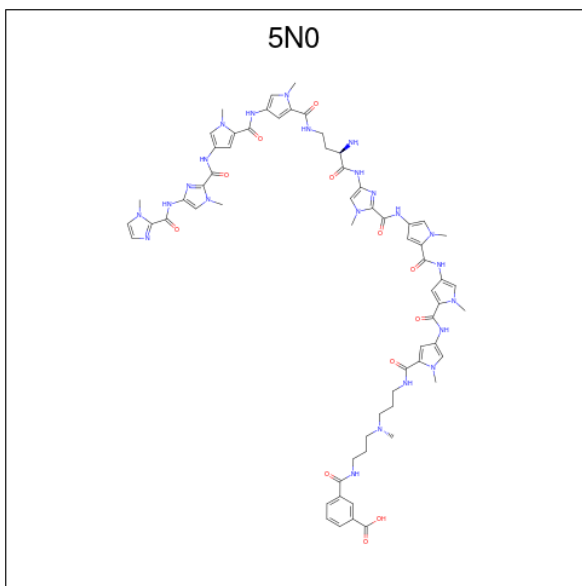
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
14	T	1	99	64	23	12	0	0

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

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

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

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
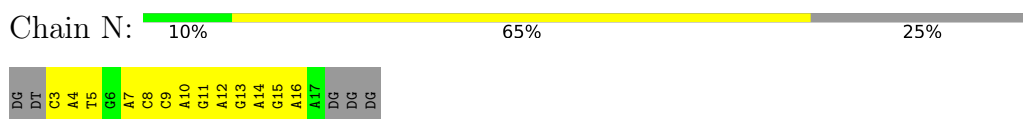
- Molecule 1: RNA

Chain R:
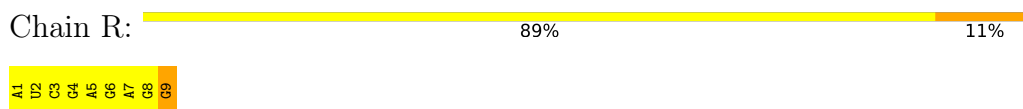
- Molecule 2: Template strand DNA
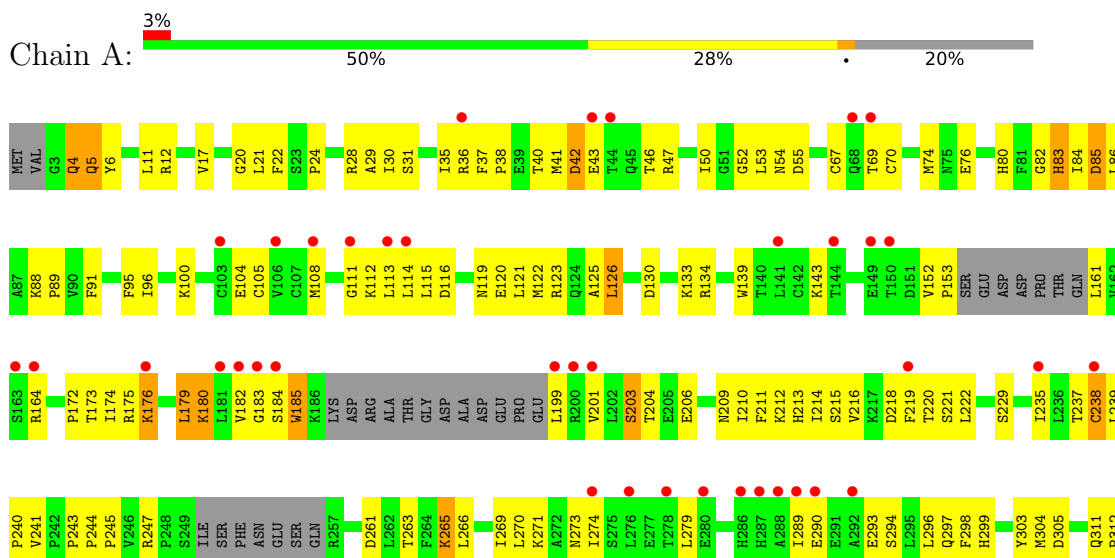
Chain T:
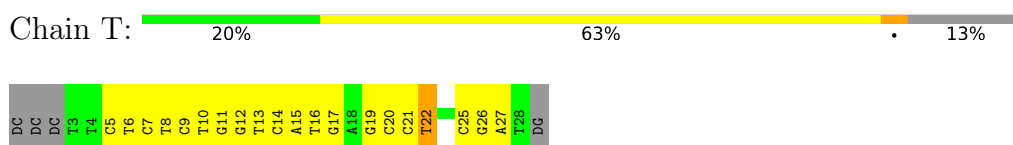
- Molecule 3: Non-template DNA

Chain N:

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

Chain A:

PRO LYS GLN ASP GLU GLN LYS HIS ASN GLU ASN GLU ASN SER ARG

● Molecule 5: DNA-directed RNA polymerase II subunit RPB2
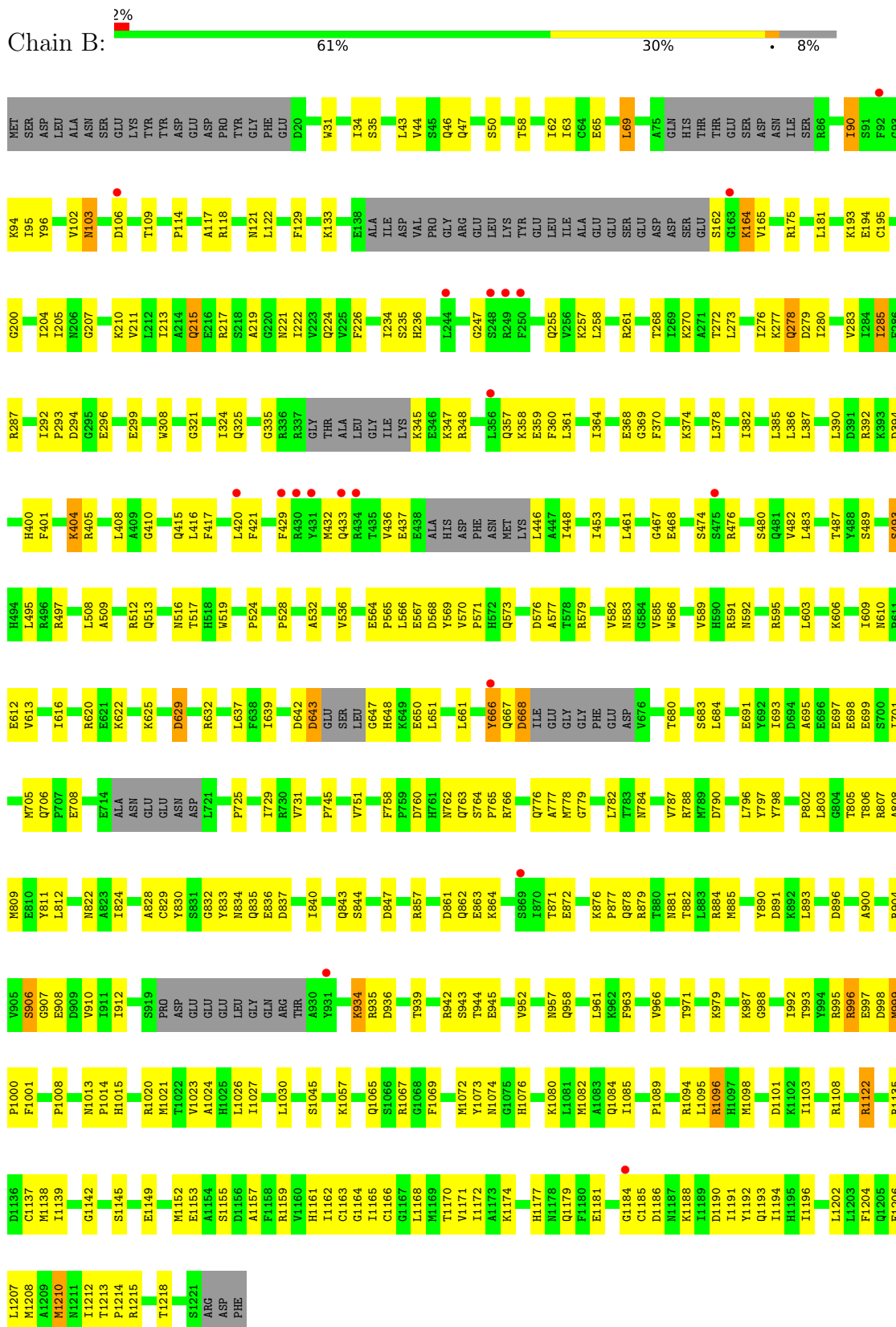
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

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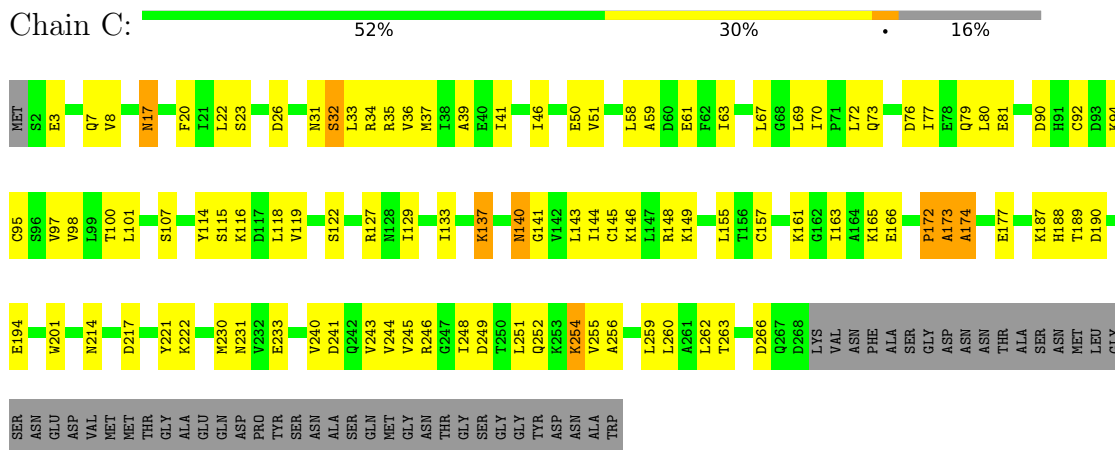
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1
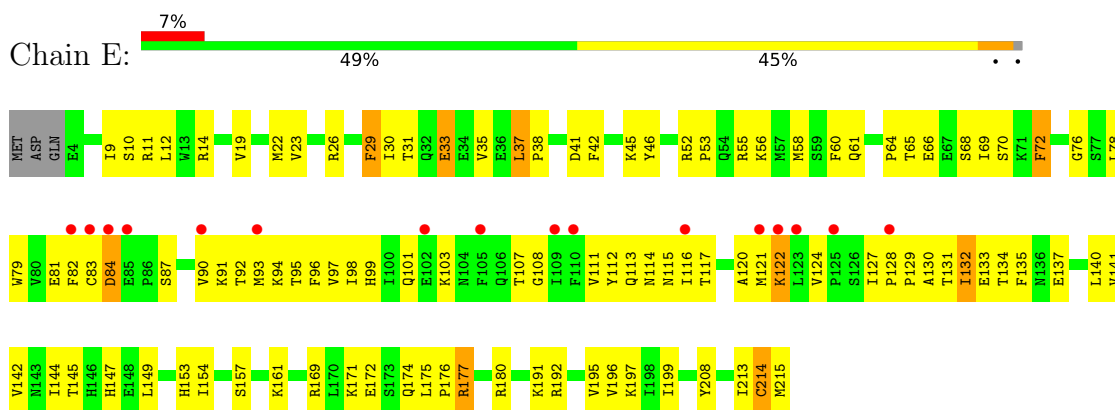
Chain E:

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

Chain F:

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

Chain H:

T76 W79 Q83 A84 G85 D86 L89 A90 D91 D92 Y93 D94 Y95 V96 M97 Y98 G99 T100 A101 Y102 K103 F104 V107 S108 K109 D110 L111 I112 A113 V114 Y115 Y116 S117 F118 L122 M123 R124 L125 E126 G127 N128 Y129 R130 N131 L132 N133 N134 L135 K136 Q137 E138 N139 L142 L143
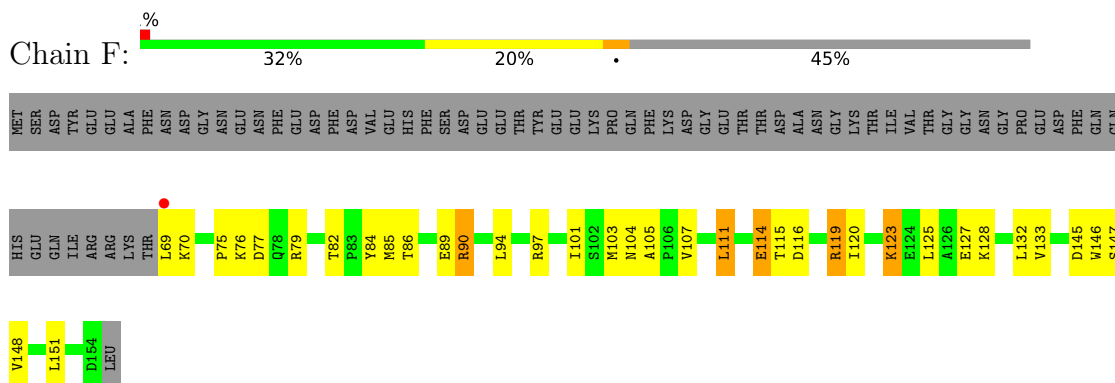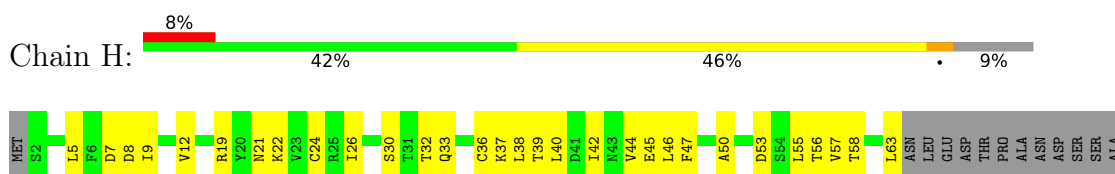
I144 R145 R146
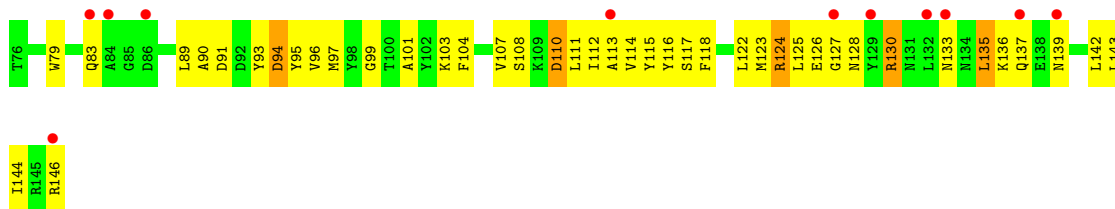
• Molecule 10: DNA-directed RNA polymerase II subunit RPB9

Chain I: 65% 29% • •

MET T2 T3 F4 R5 F6 C7 R8 D9 C10 M13 L14 Y15 P16 R17 E18 L26 F27 E28 C29 R30 T31 E36 E37 R45 H46 E47 L48 I49 T50 N51 I52 V59 I62 T67 L68 P69 R70 C75 H79 S80 R81 E82 N83 V84 Q87 V98 L99 F100

F101 V102 C103 I109 F110 T111 S112 D113 Q114 K115 T119 GLN PHE SER
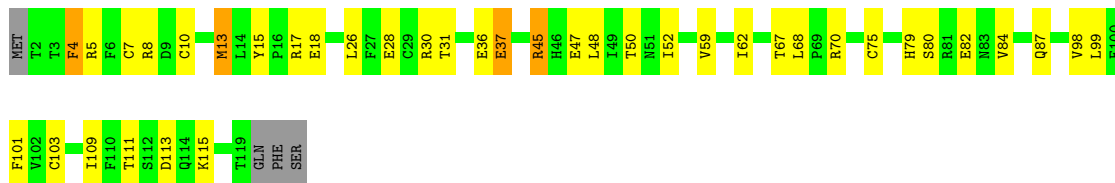
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 60% 30% • 7%

M1 V5 R6 C7 V13 K17 W18 Y21 L36 S37 R38 Y44 C45 C46 R47 R48 M49 I50 L51 D55 L56 I57 E58 K59 F60 L61 N64 P65 LEU GLU LYS ARG ASP

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

Chain K: 63% 32% 5%

M1 N2 F10 L11 L12 K18 I21 D24 T25 K26 I33 E36 K37 E38 T41 L50 L51 N52 D53 V56 L57 F58 A59 A60 Y61 K62 V63 R70 F71 K72 L73 R74 I75 Q76 Y81 K84 L87 K88 N89 A90 C91 I95 K102 T103 N104

F105 E106 T107 E108 L111 L114 ALA ALA ASP ASP ALA PHE

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

Chain L: % 40% 20% • 39%

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA GLY THR SER GLN ALA ARG THR ALA THR LEU K28 C31 S36 K37 L38 T43 D44 A45 C48 K49 L56 L57 K58 A59 R60 T61 K62 R63 L64 V65 Q66 R70

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	64.3	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 71.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	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^2)	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, 5N0

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(^{o})	Ideal(^{o})
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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	93,107,107	2.43	28 (30%)	94,153,153	1.56	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	-	-	17/51/92/92	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	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
14	T	101	5N0	C26-N14	5.74	1.48	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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

There are no chirality outliers.

5 of 17 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 then 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.

Ligand 5N0 T 101	
Bond lengths	Bond angles
Torsions	Rings
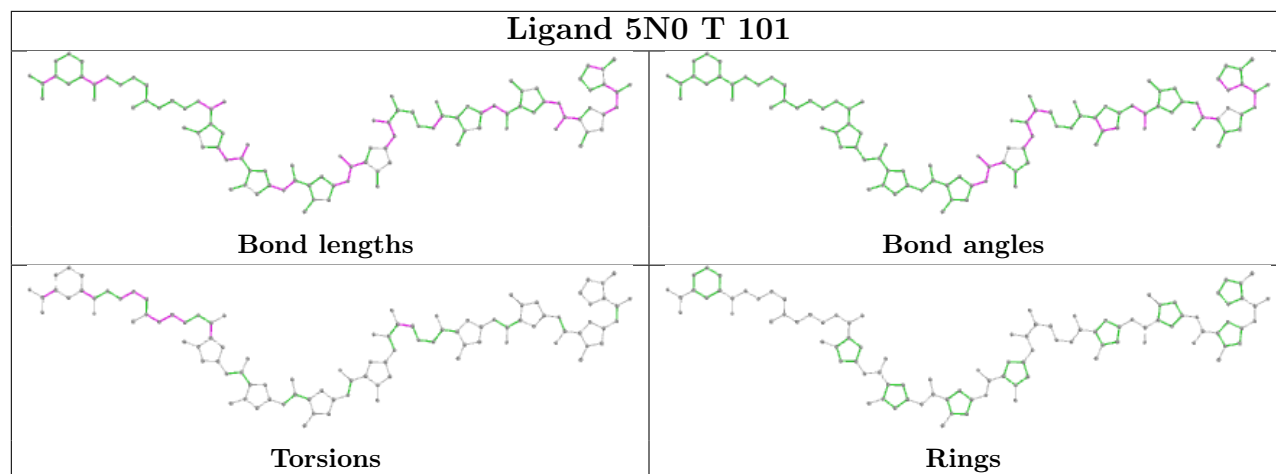
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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, 95th 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^2)	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 ⓘ

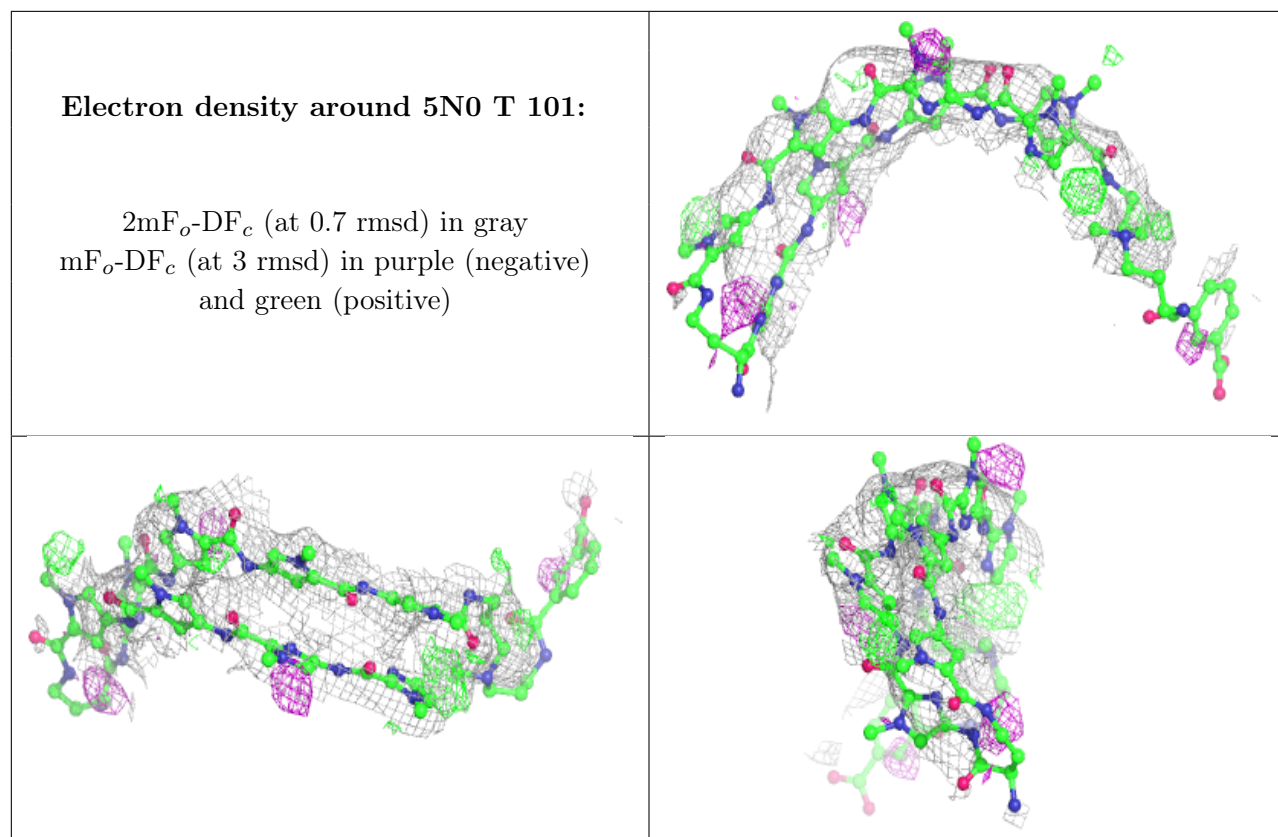There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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($Å^2$)	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:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.