wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 11:36 AM EDT

PDB ID	:	4Y52
Title	:	Crystal structure of 5-Carboxycytosine Recognition by RNA Polymerase II during Transcription Elongation.
Authors	:	Wang, L.; Chong, J.; Wang, D.
Deposited on	:	2015-02-11
Resolution	:	3.50 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

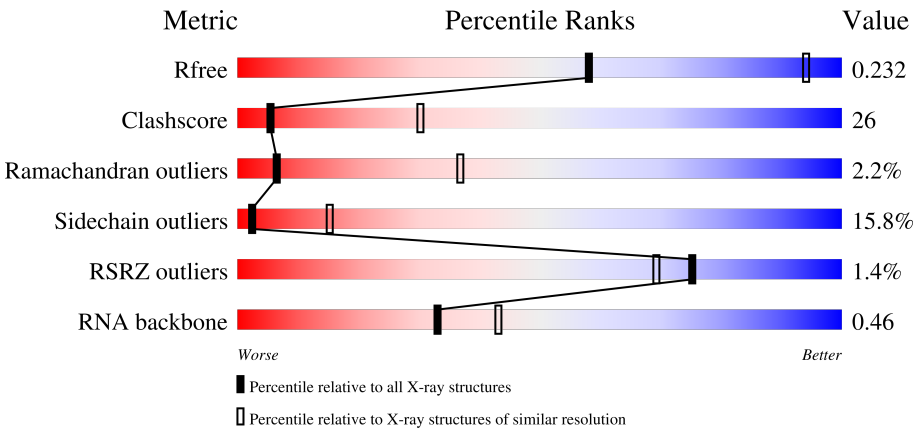
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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	A	1733	2% 42% 31% 7% 20%
2	B	1224	% 49% 35% 6% • 10%
3	C	318	43% 34% 7% 16%
4	E	215	% 58% 36% 5%

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Mol	Chain	Length	Quality of chain
5	F	155	25% 25% • 46%
6	H	146	2% 39% 42% 8% • 9%
7	I	122	43% 40% 14% •
8	J	70	33% 46% 14% 7%
9	K	120	68% 24% • 5%
10	L	70	4% 24% 30% 9% • 36%
11	T	29	24% 14% 72% 14%
12	N	14	14% 14% 79% 7%
13	R	9	56% 22% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	1CC	T	19[A]	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 29189 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 protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1393	10953	6908	1921	2063	61	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1103	8762	5549	1532	1626	55	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	214	1752	1111	309	321	11	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	84	679	434	115	127	3	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	133	1068	673	180	211	4	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	I	119	971	596	179	186	10	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	L	45	358	221	71	62	4	0	0	0

- Molecule 11 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
11	T	29	609	290	111	179	29	0	1	0

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP *GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
12	N	14	284	137	49	85	13	0	0	0

- Molecule 13 is a RNA chain called RNA (5'-D(*AP*UP*GP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	R	9	198	89	42	59	8	0	0	0

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

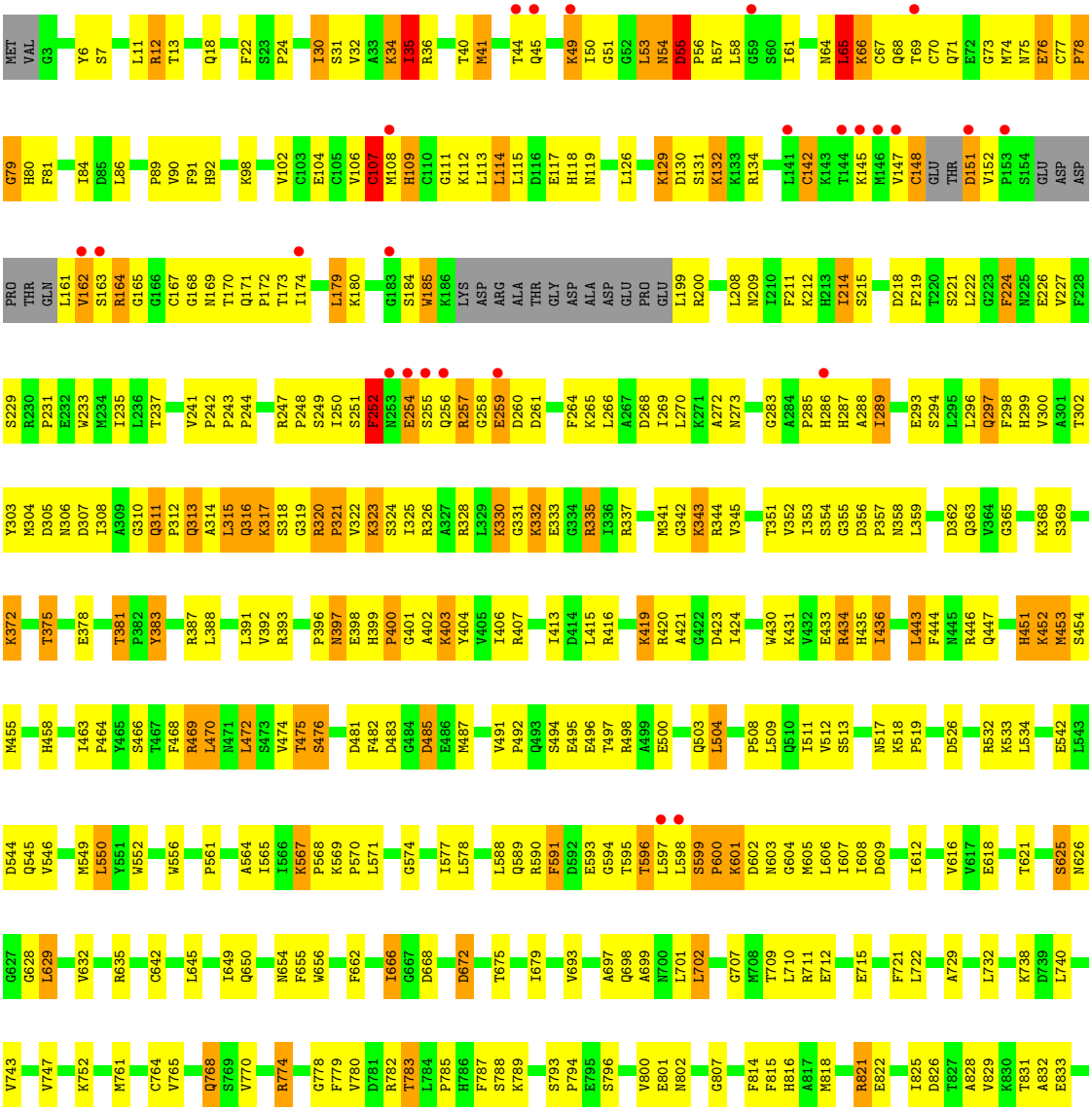
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	A	1	1	1	0	0

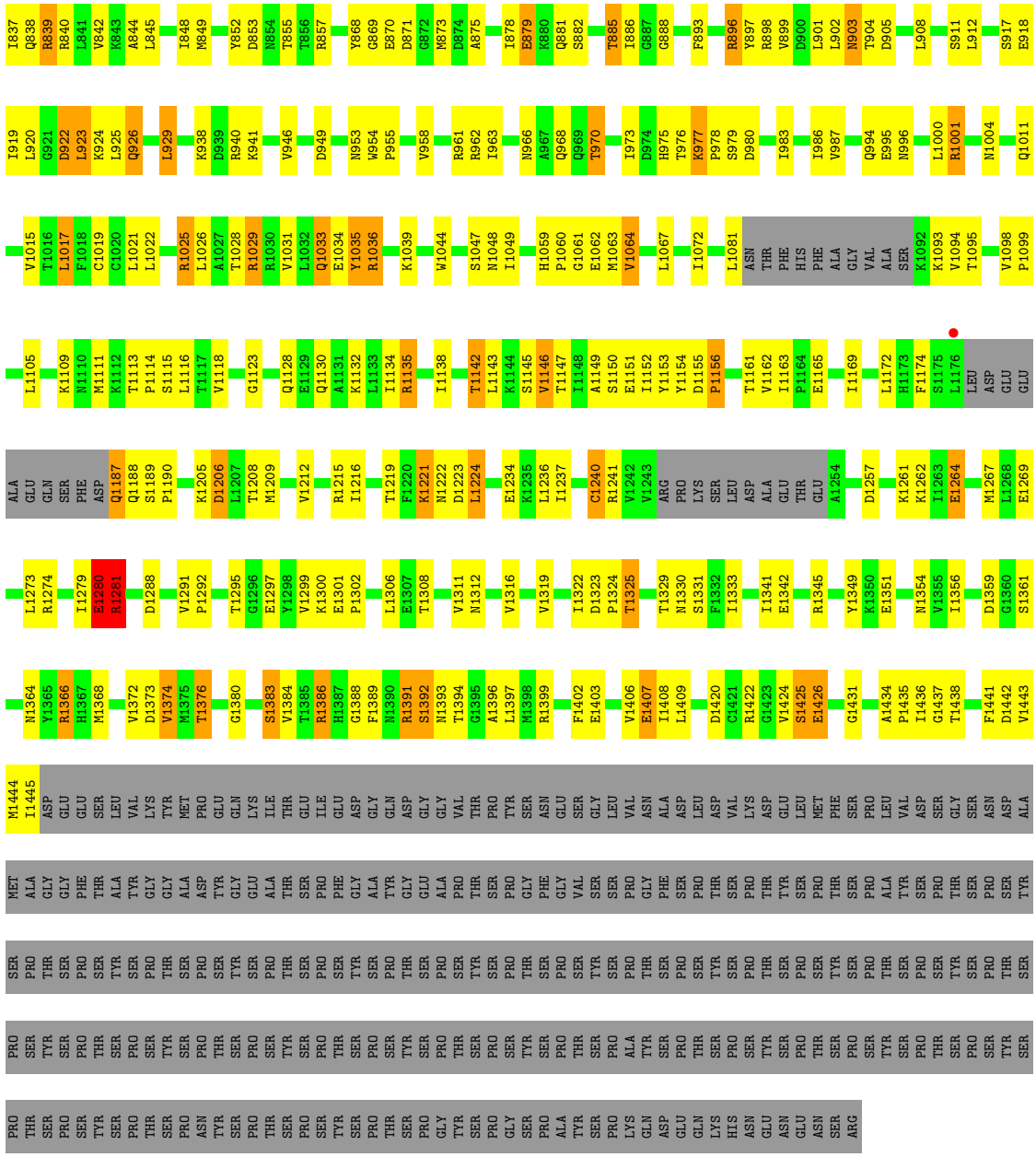
3 Residue-property plots (i)

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: DNA-directed RNA polymerase II subunit RPB1

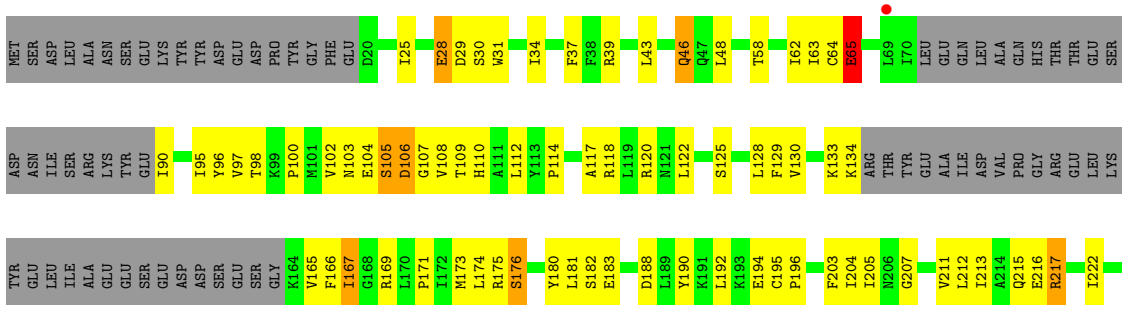
Chain A: 2% 42% 31% 7% 20%

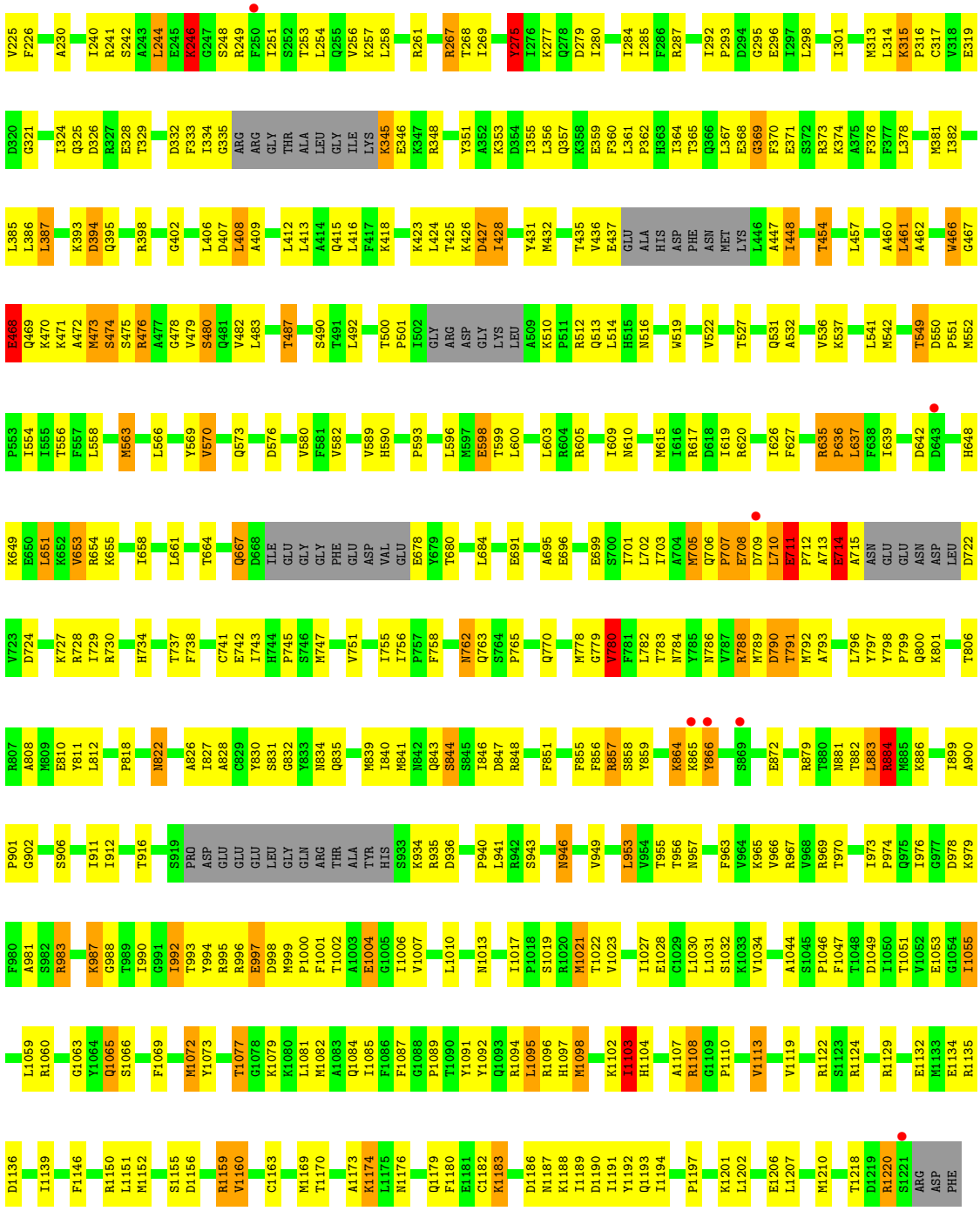




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

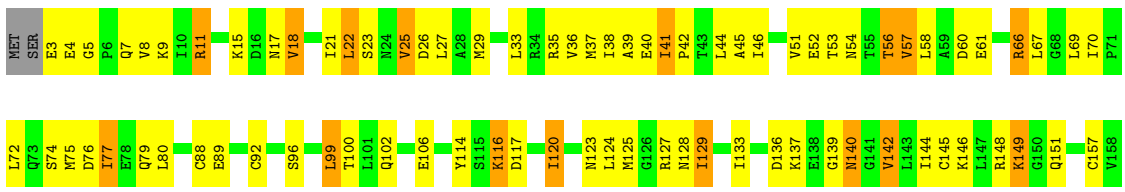
Chain B:

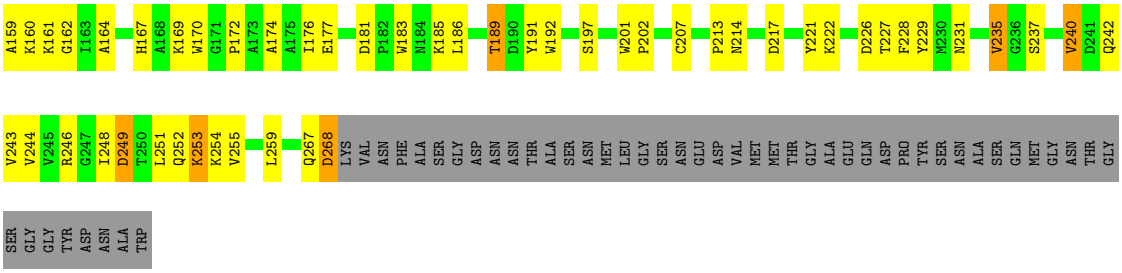




- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

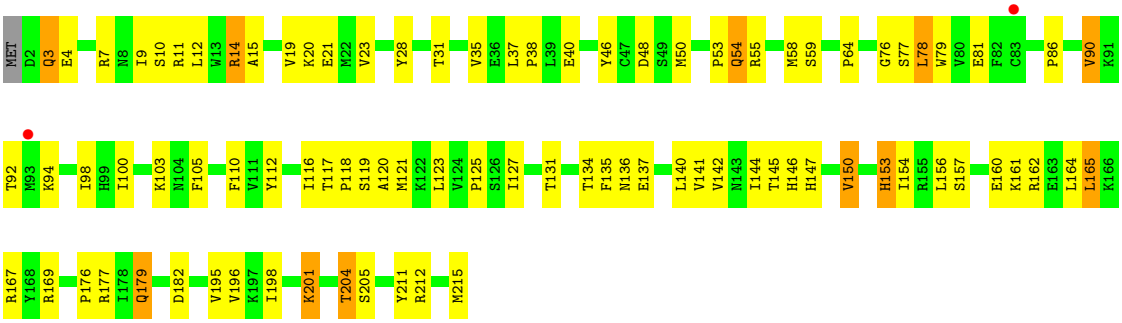
Chain C:





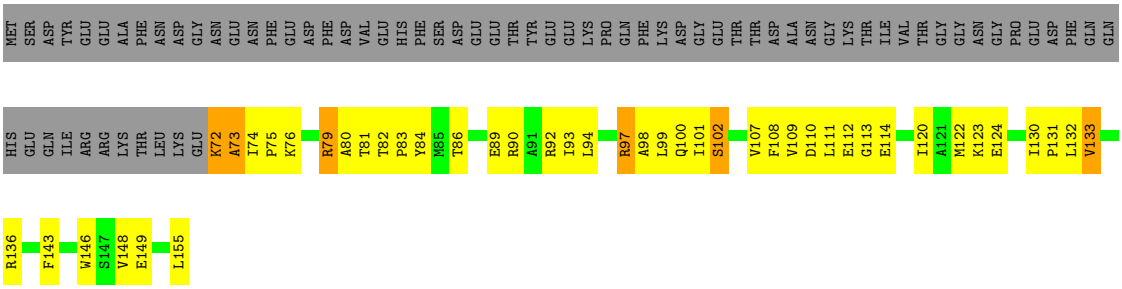
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



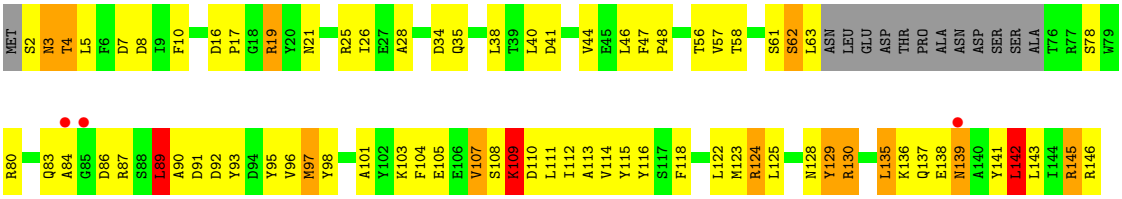
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



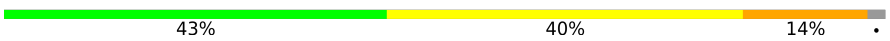
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

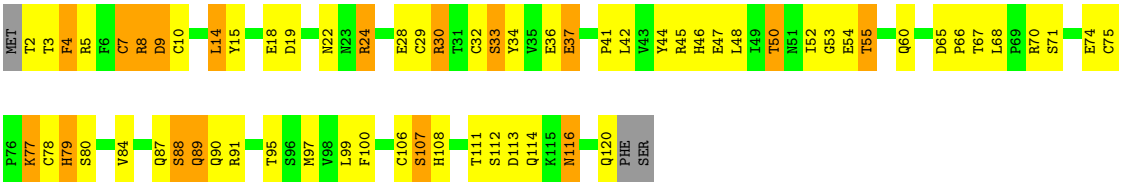
Chain H:



• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

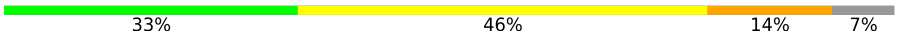
Chain I:

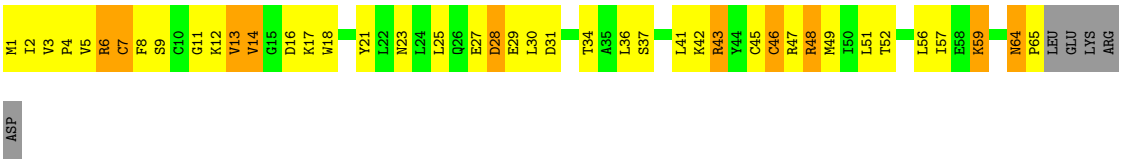




• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



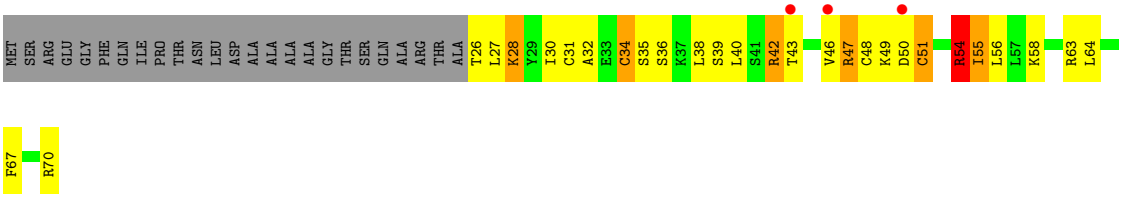


• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:

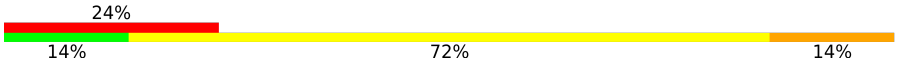
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

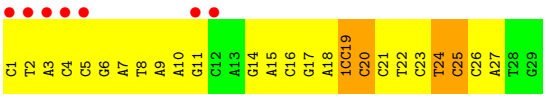
Chain L:



• Molecule 11: DNA (29-MER)

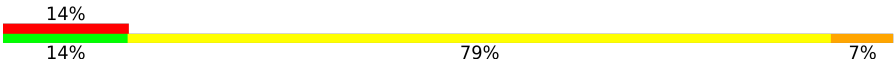
Chain T:

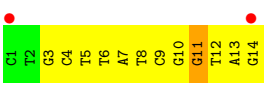




• Molecule 12: DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3')

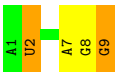
Chain N:





• Molecule 13: RNA (5'-D(*AP*UP*GP*GP*AP*GP*AP*GP*G)-3')

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.70Å 221.64Å 192.41Å 90.00° 100.35° 90.00°	Depositor
Resolution (Å)	49.27 – 3.50 49.27 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.1 (49.27-3.50) 94.2 (49.27-3.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.48Å)	Xtriage
Refinement program	PHENIX, REFMAC	Depositor
R, R_{free}	0.201 , 0.232 0.201 , 0.232	Depositor DCC
R_{free} test set	4090 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	75.7	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 70.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	29189	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1CC, 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	A	0.44	2/11146 (0.0%)	0.67	5/15066 (0.0%)
2	B	0.46	0/8932	0.68	5/12045 (0.0%)
3	C	0.48	0/2133	0.70	0/2891
4	E	0.41	1/1788 (0.1%)	0.56	0/2406
5	F	0.41	0/691	0.64	0/933
6	H	0.37	0/1086	0.65	4/1470 (0.3%)
7	I	0.41	0/989	0.58	0/1331
8	J	0.48	0/541	0.73	0/727
9	K	0.47	0/937	0.64	0/1265
10	L	0.37	0/360	0.63	0/478
11	T	0.59	0/632	1.09	6/969 (0.6%)
12	N	0.39	0/317	0.99	1/488 (0.2%)
13	R	0.57	0/223	1.00	0/348
All	All	0.45	3/29775 (0.0%)	0.68	21/40417 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	38	PRO	N-CD	5.30	1.55	1.47
1	A	400	PRO	N-CD	5.14	1.55	1.47
1	A	321	PRO	N-CD	5.08	1.54	1.47

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	CYS	C-N-CD	-15.50	86.50	120.60
2	B	474	SER	N-CA-CB	-7.60	99.10	110.50
11	T	24	DT	N3-C4-O4	7.25	124.25	119.90
11	T	24	DT	P-O5'-C5'	-6.69	110.20	120.90
11	T	25	DC	O4'-C4'-C3'	-6.24	102.01	104.50

There are no chirality outliers.

There are no planarity outliers.

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	A	10953	0	11053	638	0
2	B	8762	0	8797	428	0
3	C	2095	0	2051	101	0
4	E	1752	0	1776	67	0
5	F	679	0	701	30	0
6	H	1068	0	1040	102	0
7	I	971	0	927	82	0
8	J	532	0	542	54	0
9	K	919	0	929	24	0
10	L	358	0	381	35	0
11	T	609	0	337	96	0
12	N	284	0	161	30	0
13	R	198	0	100	4	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	29189	0	28795	1511	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 26.

The worst 5 of 1511 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:A:315:LEU:HD23	1:A:316:GLN:CG	1.22	1.56
1:A:315:LEU:CD2	1:A:316:GLN:HG3	1.43	1.44
1:A:315:LEU:HB3	1:A:316:GLN:CB	1.54	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:CD2	1:A:316:GLN:CG	1.96	1.36
11:T:1:DC:H2"	11:T:2:DT:C5'	1.63	1.27

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 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	
1	A	1379/1733 (80%)	1166 (85%)	182 (13%)	31 (2%)	6	37
2	B	1085/1224 (89%)	932 (86%)	125 (12%)	28 (3%)	5	33
3	C	264/318 (83%)	228 (86%)	35 (13%)	1 (0%)	34	72
4	E	212/215 (99%)	184 (87%)	25 (12%)	3 (1%)	11	46
5	F	82/155 (53%)	74 (90%)	7 (8%)	1 (1%)	13	50
6	H	129/146 (88%)	98 (76%)	27 (21%)	4 (3%)	4	30
7	I	117/122 (96%)	97 (83%)	17 (14%)	3 (3%)	5	33
8	J	63/70 (90%)	56 (89%)	6 (10%)	1 (2%)	9	43
9	K	112/120 (93%)	106 (95%)	6 (5%)	0	100	100
10	L	43/70 (61%)	25 (58%)	14 (33%)	4 (9%)	0	8
All	All	3486/4173 (84%)	2966 (85%)	444 (13%)	76 (2%)	6	37

5 of 76 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	286	HIS
1	A	315	LEU
1	A	600	PRO
1	A	1174	PHE

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 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	
1	A	1216/1520 (80%)	1014 (83%)	202 (17%)	2	13
2	B	957/1061 (90%)	820 (86%)	137 (14%)	3	19
3	C	234/274 (85%)	195 (83%)	39 (17%)	2	12
4	E	196/197 (100%)	169 (86%)	27 (14%)	3	20
5	F	74/137 (54%)	61 (82%)	13 (18%)	2	10
6	H	117/128 (91%)	99 (85%)	18 (15%)	2	16
7	I	113/116 (97%)	88 (78%)	25 (22%)	1	5
8	J	60/65 (92%)	47 (78%)	13 (22%)	1	5
9	K	99/102 (97%)	89 (90%)	10 (10%)	7	32
10	L	40/57 (70%)	33 (82%)	7 (18%)	2	10
All	All	3106/3657 (85%)	2615 (84%)	491 (16%)	2	15

5 of 491 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	319	GLU
7	I	14	LEU
2	B	786	ASN
7	I	4	PHE
8	J	64	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	843	GLN
7	I	108	HIS
2	B	1093	GLN
6	H	3	ASN
2	B	1084	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	2	U
13	R	9	G

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
11	1CC	T	19[A]	11	20,23,24	1.10	2 (10%)	26,33,36	1.24	2 (7%)
11	1CC	T	19[B]	11	20,23,24	1.53	4 (20%)	26,33,36	1.77	8 (30%)

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
11	1CC	T	19[A]	11	-	3/11/25/26	0/2/2/2
11	1CC	T	19[B]	11	-	4/11/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	19[B]	1CC	C2'-C1'	-3.61	1.42	1.52
11	T	19[B]	1CC	O4'-C1'	2.45	1.47	1.42
11	T	19[A]	1CC	C2-N1	-2.22	1.35	1.40
11	T	19[B]	1CC	C2-N1	-2.22	1.35	1.40
11	T	19[B]	1CC	C5-C4	2.22	1.47	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	19[B]	1CC	O4'-C1'-C2'	-3.81	99.05	106.25
11	T	19[A]	1CC	C5-C6-N1	-2.89	119.25	123.10
11	T	19[B]	1CC	C5-C6-N1	-2.89	119.26	123.10
11	T	19[B]	1CC	C3'-C2'-C1'	2.72	109.34	102.54
11	T	19[B]	1CC	O2-C2-N3	-2.60	118.11	122.33

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	19[B]	1CC	C3'-C4'-C5'-O5'
11	T	19[A]	1CC	C3'-C4'-C5'-O5'
11	T	19[A]	1CC	O4'-C4'-C5'-O5'
11	T	19[B]	1CC	O4'-C4'-C5'-O5'
11	T	19[B]	1CC	C2'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	T	19[A]	1CC	7	0
11	T	19[B]	1CC	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 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.

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, 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	A	1393/1733 (80%)	-0.22	26 (1%) 66 61	24, 80, 185, 300	0
2	B	1103/1224 (90%)	-0.35	8 (0%) 87 83	28, 70, 149, 285	0
3	C	266/318 (83%)	-0.59	0 100 100	33, 70, 111, 170	0
4	E	214/215 (99%)	-0.18	2 (0%) 84 79	43, 108, 202, 264	0
5	F	84/155 (54%)	-0.58	0 100 100	54, 83, 139, 196	0
6	H	133/146 (91%)	0.08	3 (2%) 60 54	52, 105, 179, 286	0
7	I	119/122 (97%)	-0.49	0 100 100	43, 85, 133, 169	0
8	J	65/70 (92%)	-0.55	0 100 100	34, 64, 108, 142	0
9	K	114/120 (95%)	-0.39	0 100 100	36, 73, 110, 158	0
10	L	45/70 (64%)	0.21	3 (6%) 17 16	61, 137, 242, 287	0
11	T	28/29 (96%)	0.68	7 (25%) 0 0	54, 278, 349, 351	0
12	N	14/14 (100%)	1.09	2 (14%) 2 3	244, 289, 323, 331	0
13	R	9/9 (100%)	-0.49	0 100 100	56, 68, 129, 140	0
All	All	3587/4225 (84%)	-0.29	51 (1%) 75 69	24, 78, 183, 351	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	GLU	7.3
1	A	1176	LEU	6.8
1	A	153	PRO	4.6
6	H	84	ALA	4.5
2	B	1221	SER	4.3

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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
11	1CC	T	19[A]	22/23	0.87	0.22	37,75,128,168	22
11	1CC	T	19[B]	22/23	0.87	0.22	63,101,153,155	22

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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
15	MG	A	1803	1/1	0.75	0.19	78,78,78,78	0
14	ZN	A	1802	1/1	0.77	0.10	117,117,117,117	0
14	ZN	B	1301	1/1	0.84	0.20	197,197,197,197	0
14	ZN	I	202	1/1	0.87	0.16	96,96,96,96	0
14	ZN	L	101	1/1	0.91	0.12	211,211,211,211	0
14	ZN	A	1801	1/1	0.93	0.13	247,247,247,247	0
14	ZN	C	401	1/1	0.97	0.10	96,96,96,96	0
14	ZN	I	201	1/1	0.98	0.09	100,100,100,100	0
14	ZN	J	101	1/1	0.99	0.20	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.