



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 09:30 pm BST

PDB ID : 2B63  
Title : Complete RNA Polymerase II-RNA inhibitor complex  
Authors : Kettenberger, H.; Eisenfuehr, A.; Brueckner, F.; Theis, M.; Famulok, M.; Cramer, P.  
Deposited on : 2005-09-30  
Resolution : 3.80 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.

---

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 : 2.11  
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) : 2.11

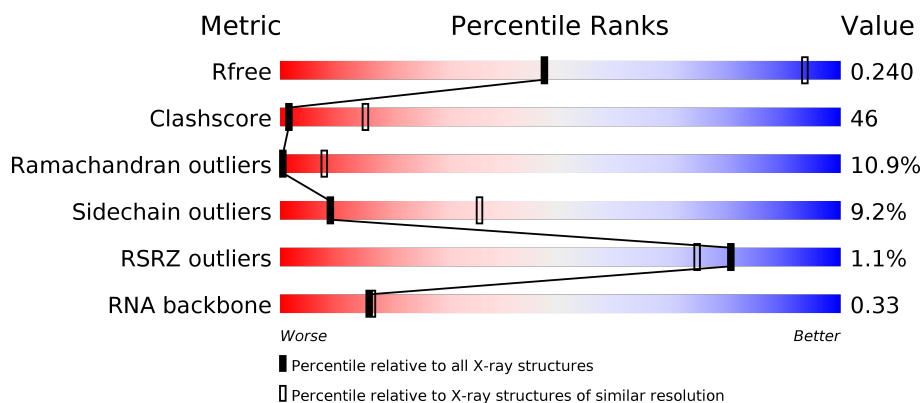
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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 on 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	31	
2	A	1733	
3	B	1224	
4	C	318	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	D	221	
6	E	215	
7	F	155	
8	G	171	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 31731 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 31-MER.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	R	31	Total	Br	C	N	O	P	88	0	0
			666	4	296	119	217	30			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	1112	Total	C	N	O	S	0	0	0
			8836	5594	1548	1639	55			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 5 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	115	Total	C	N	O	S	0	0	0
			924	593	157	172	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

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

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

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

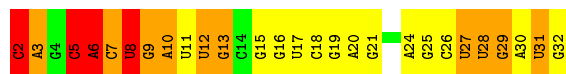
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

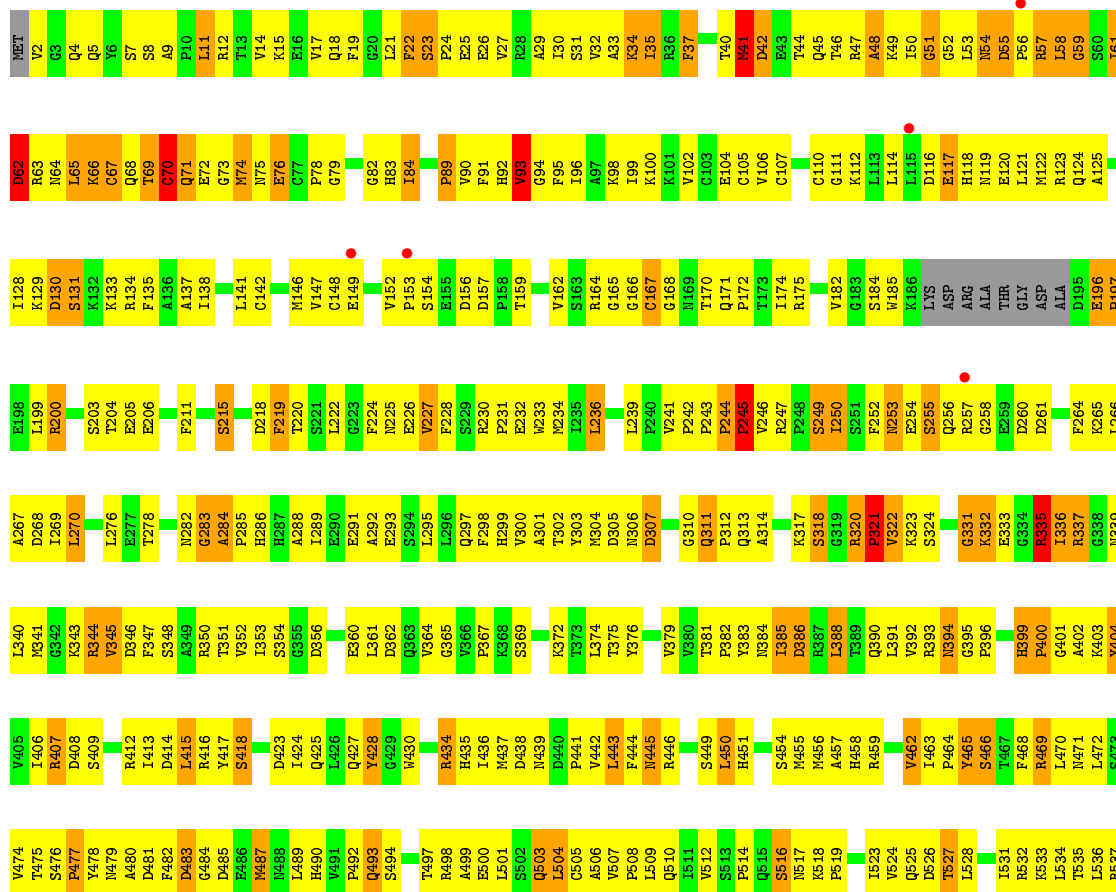
#### • Molecule 1: 31-MER

Chain R: 



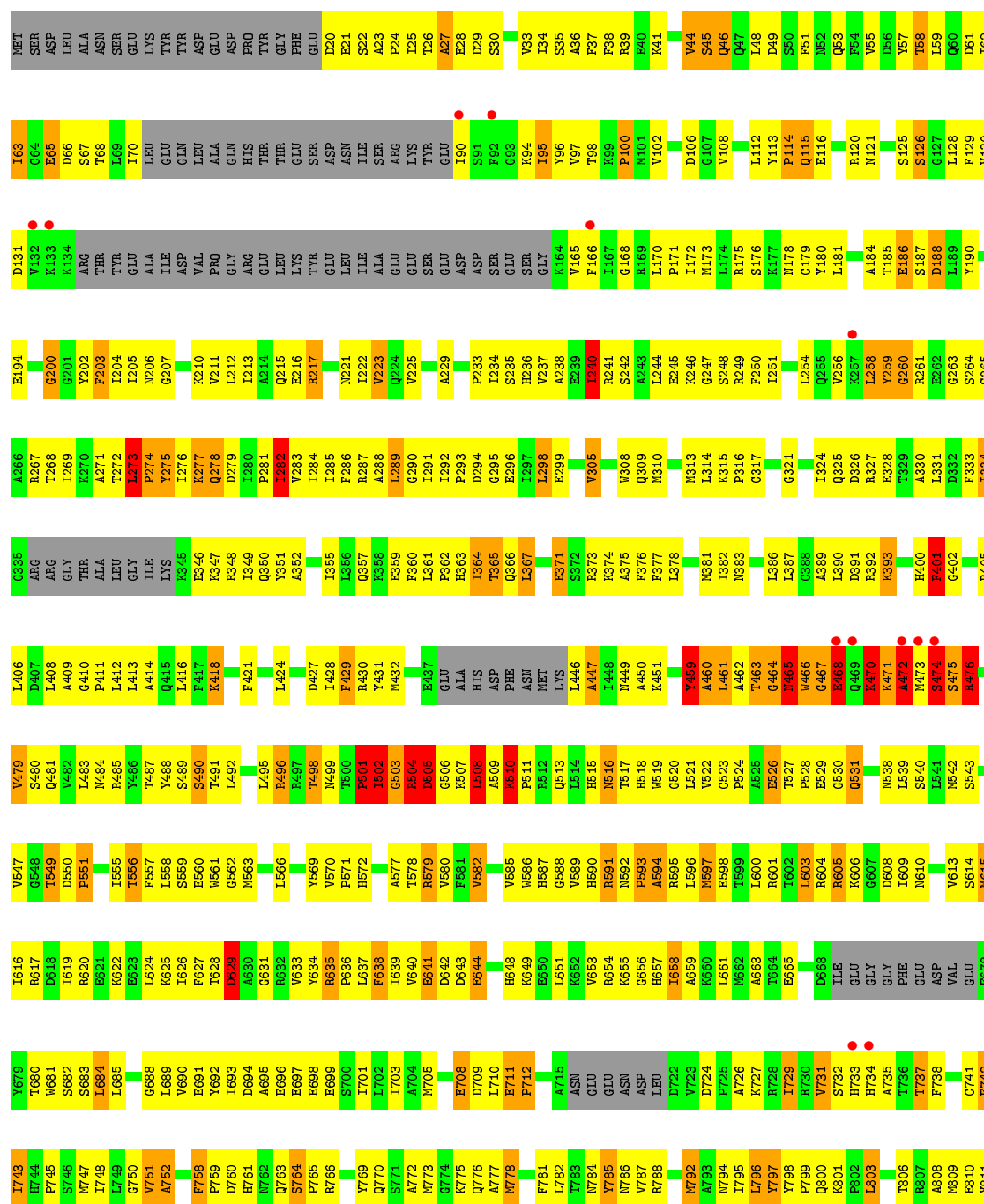
#### • Molecule 2: DNA-directed RNA polymerase II largest subunit

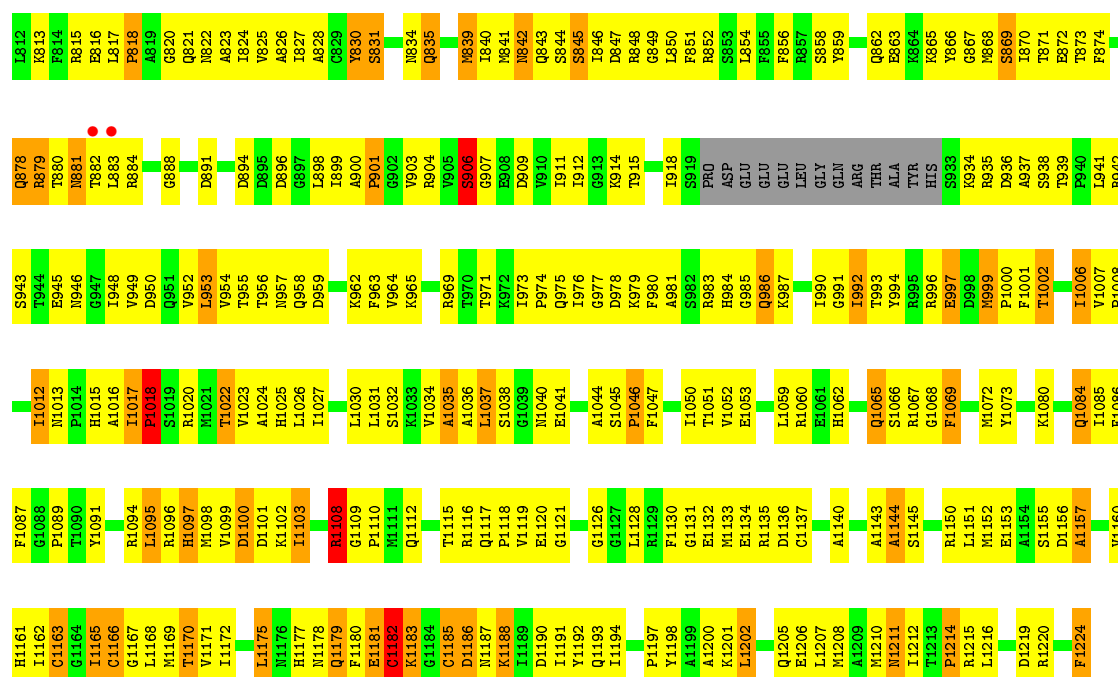
Chain A: 



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

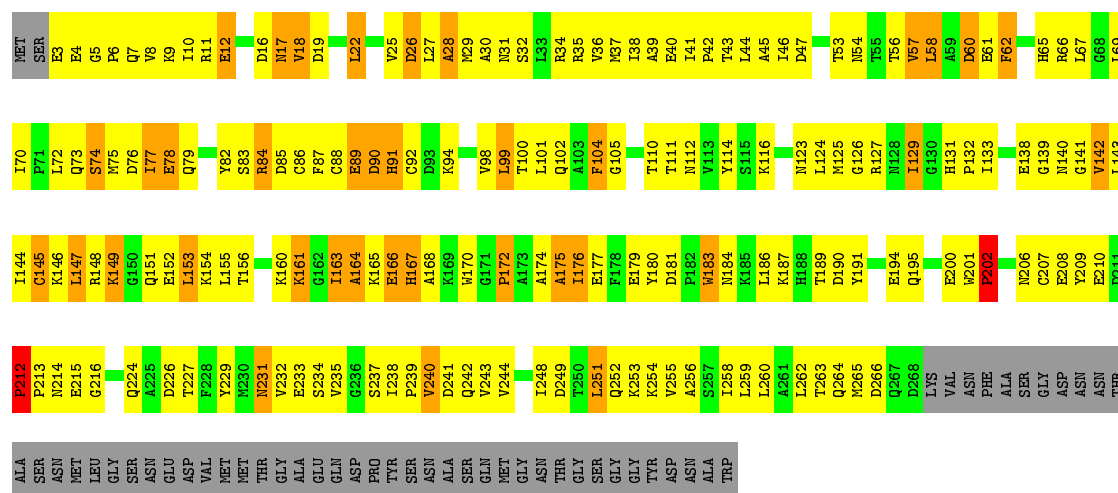






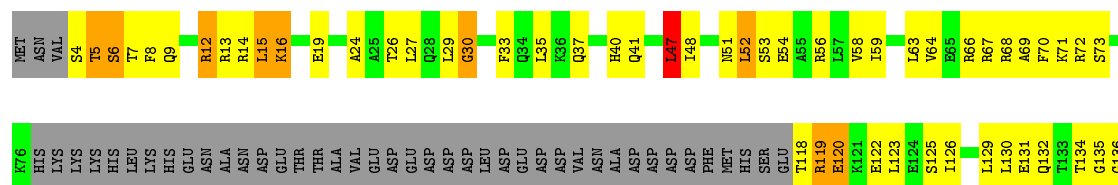
• Molecule 4: DNA-directed RNA polymerase II 45 kDa polypeptide

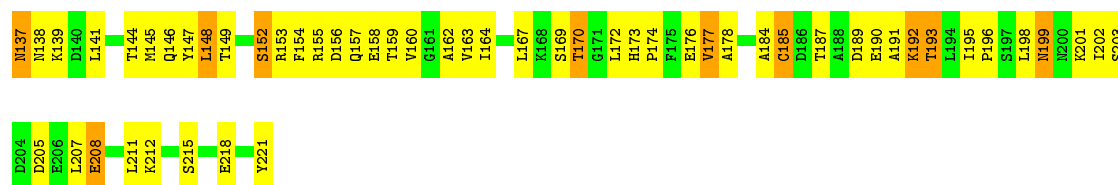
Chain C: 27% 45% 12% 16%



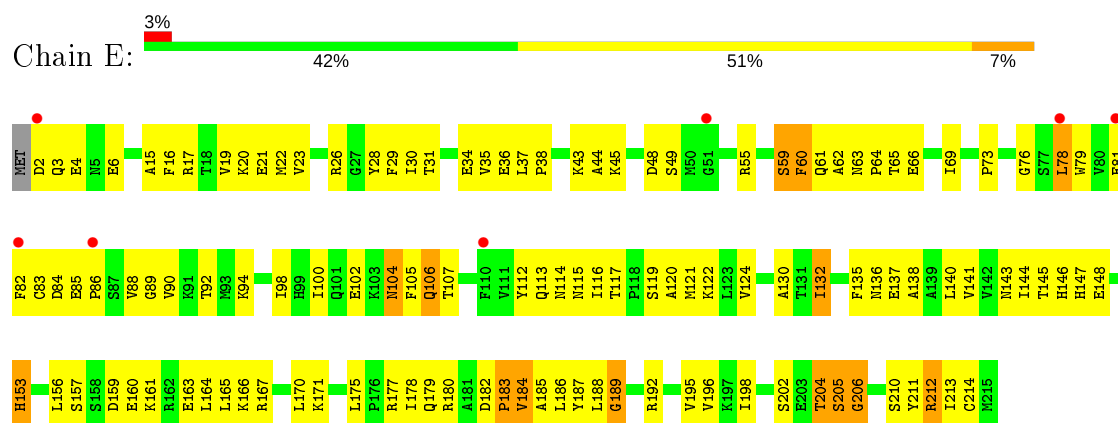
• Molecule 5: DNA-directed RNA polymerase II 32 kDa polypeptide

Chain D: 31% 40% 9% 20%

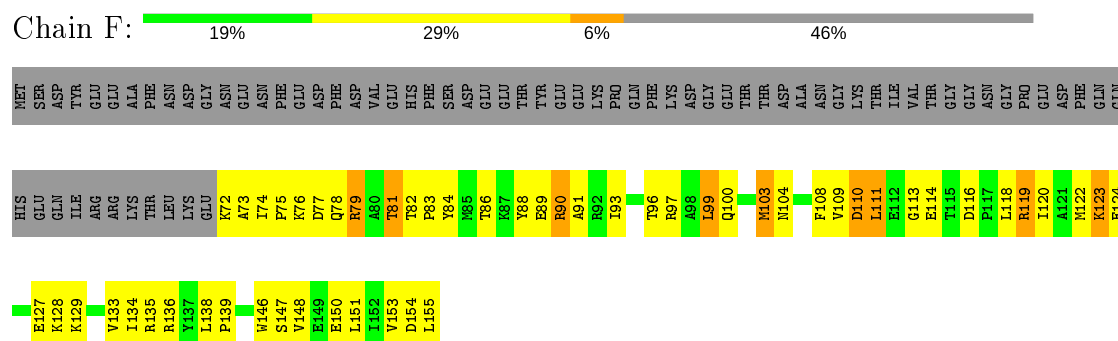




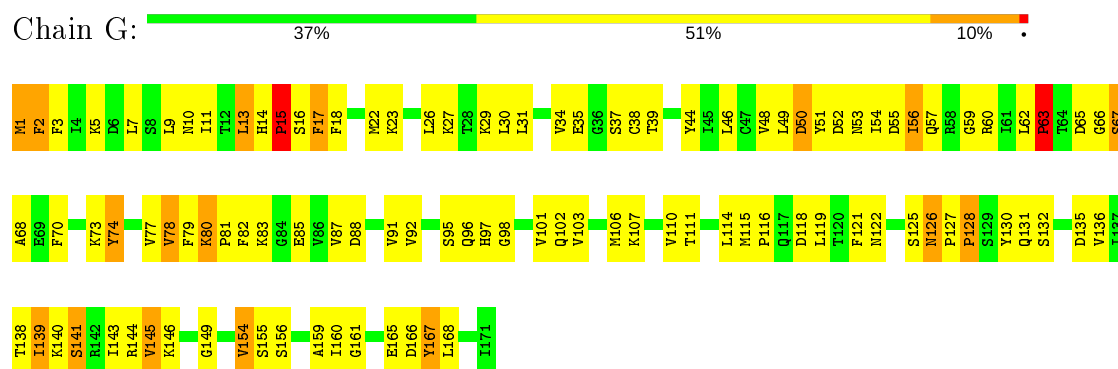
- Molecule 6: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



- Molecule 7: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

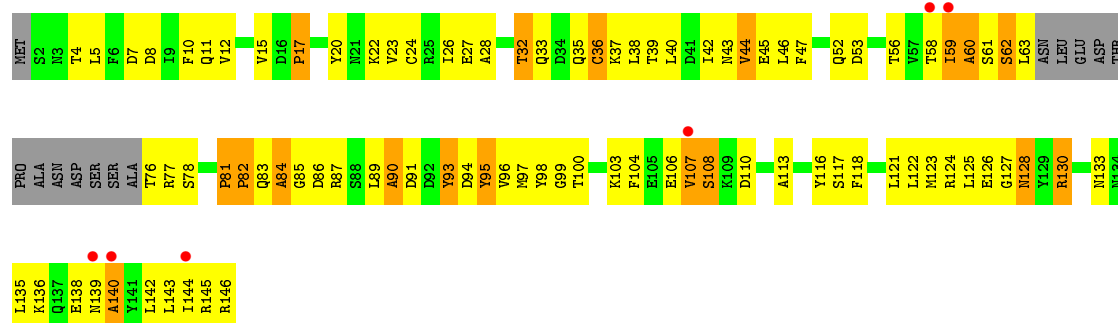


- Molecule 8: DNA-directed RNA polymerase II 19 kDa polypeptide

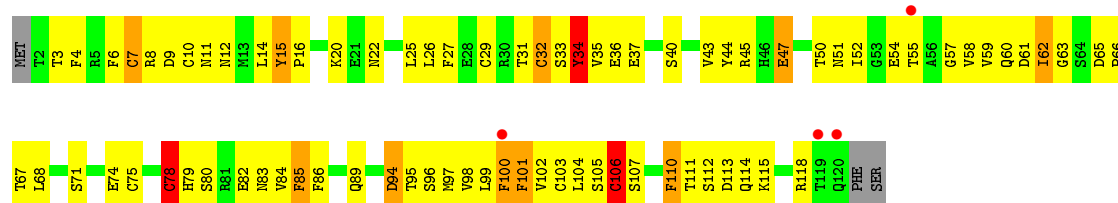


- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

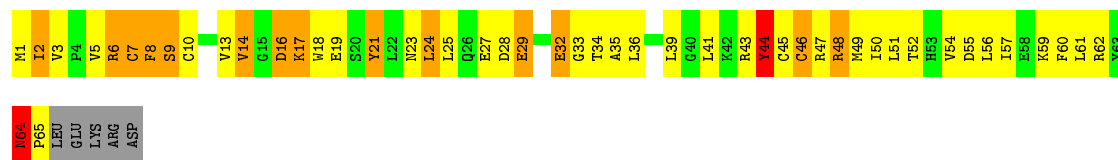




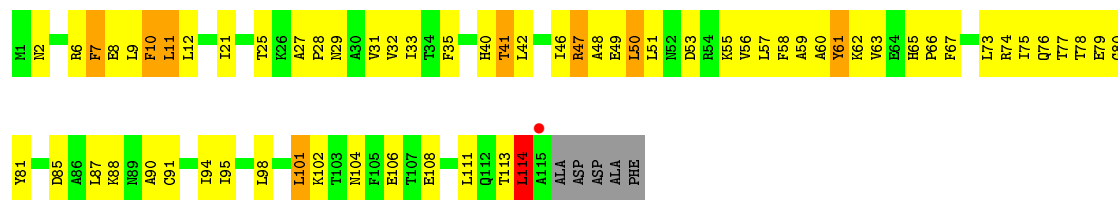
- Molecule 10: DNA-directed RNA polymerase II subunit 9



- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10



- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



T61	
V65	
Q66	
F67	
E68	
A69	
R70	

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.59Å 399.81Å 286.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 49.15 – 3.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.80) 99.1 (49.15-3.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.252 , 0.273 0.214 , 0.240	Depositor DCC
$R_{free}$ test set	8121 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	121.4	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 64.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	31731	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 1.87% 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: 5BU, ZN, 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	0.93	1/652 (0.2%)	1.19	4/1017 (0.4%)
2	A	0.48	0/11339	0.74	5/15334 (0.0%)
3	B	0.47	0/9008	0.78	19/12146 (0.2%)
4	C	0.47	0/2133	0.75	1/2891 (0.0%)
5	D	0.45	0/1365	0.68	0/1837
6	E	0.44	0/1788	0.67	0/2406
7	F	0.56	0/691	0.76	0/933
8	G	0.51	0/1368	0.75	0/1844
9	H	0.39	0/1086	0.64	0/1470
10	I	0.39	0/989	0.70	0/1331
11	J	0.51	0/541	0.82	0/727
12	K	0.46	0/942	0.68	0/1272
13	L	0.53	0/365	0.75	0/485
All	All	0.48	1/32267 (0.0%)	0.76	29/43693 (0.1%)

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
1	R	0	2
11	J	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	2	C	C3'-C2'	5.33	1.58	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	GLY	N-CA-C	-10.94	85.76	113.10
3	B	273	LEU	C-N-CD	-9.80	99.03	120.60
1	R	2	C	O4'-C1'-N1	9.55	115.84	108.20
3	B	508	LEU	N-CA-C	-8.97	86.78	111.00
1	R	5	C	C2'-C3'-O3'	7.04	124.98	109.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	J	44	TYR	Sidechain
1	R	2	C	Sidechain
1	R	5	C	Sidechain

## 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	R	666	0	331	42	0
2	A	11140	0	11217	1087	0
3	B	8836	0	8871	910	0
4	C	2095	0	2051	242	0
5	D	1356	0	1319	118	0
6	E	1752	0	1776	129	0
7	F	679	0	701	56	0
8	G	1340	0	1357	132	0
9	H	1068	0	1040	123	0
10	I	971	0	928	83	0
11	J	532	0	542	84	0
12	K	924	0	934	78	0
13	L	363	0	386	41	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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31731	0	31453	2875	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 46.

The worst 5 of 2875 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)
5:D:40:HIS:HB3	8:G:73:LYS:NZ	1.60	1.16
2:A:1329:THR:HG22	2:A:1331:SER:H	1.01	1.12
3:B:827:ILE:HG12	3:B:1012:ILE:HD11	1.18	1.11
3:B:463:THR:HB	3:B:465:ASN:HB2	1.32	1.10
1:R:3:A:OP2	3:B:531:GLN:HB3	1.50	1.10

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	
2	A	1406/1733 (81%)	973 (69%)	278 (20%)	155 (11%)	0	8
3	B	1096/1224 (90%)	754 (69%)	214 (20%)	128 (12%)	0	6
4	C	264/318 (83%)	172 (65%)	62 (24%)	30 (11%)	0	7
5	D	173/221 (78%)	116 (67%)	36 (21%)	21 (12%)	0	6
6	E	212/215 (99%)	155 (73%)	42 (20%)	15 (7%)	1	17
7	F	82/155 (53%)	72 (88%)	9 (11%)	1 (1%)	13	50
8	G	169/171 (99%)	133 (79%)	19 (11%)	17 (10%)	0	9
9	H	129/146 (88%)	89 (69%)	23 (18%)	17 (13%)	0	5
10	I	117/122 (96%)	83 (71%)	23 (20%)	11 (9%)	0	11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0	1
12	K	113/120 (94%)	83 (74%)	25 (22%)	5 (4%)	2	25
13	L	44/70 (63%)	19 (43%)	16 (36%)	9 (20%)	0	2
All	All	3868/4565 (85%)	2684 (69%)	761 (20%)	423 (11%)	0	8

5 of 423 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	31	SER
2	A	48	ALA
2	A	55	ASP
2	A	57	ARG
2	A	58	LEU

### 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	
2	A	1239/1520 (82%)	1146 (92%)	93 (8%)	13	44
3	B	964/1061 (91%)	854 (89%)	110 (11%)	5	28
4	C	234/274 (85%)	211 (90%)	23 (10%)	8	33
5	D	140/200 (70%)	128 (91%)	12 (9%)	10	40
6	E	196/197 (100%)	186 (95%)	10 (5%)	24	54
7	F	74/137 (54%)	63 (85%)	11 (15%)	3	18
8	G	152/152 (100%)	137 (90%)	15 (10%)	8	32
9	H	117/128 (91%)	113 (97%)	4 (3%)	37	64
10	I	113/116 (97%)	97 (86%)	16 (14%)	3	21
11	J	60/65 (92%)	51 (85%)	9 (15%)	3	18
12	K	99/102 (97%)	90 (91%)	9 (9%)	9	36
13	L	40/57 (70%)	37 (92%)	3 (8%)	13	44
All	All	3428/4009 (86%)	3113 (91%)	315 (9%)	9	35

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	531	GLN
3	B	953	LEU
10	I	101	PHE
3	B	603	LEU
3	B	778	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	449	ASN
3	B	686	ASN
10	I	12	ASN
3	B	469	GLN
3	B	518	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	31/31 (100%)	16 (51%)	3 (9%)

5 of 16 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	3	A
1	R	6	A
1	R	7	C
1	R	8	U
1	R	9	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	2	C
1	R	5	C
1	R	6	A

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

4 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
1	5BU	R	17	1	15,22,23	1.65	3 (20%)	17,32,35	4.04	3 (17%)
1	5BU	R	12	1	15,22,23	1.96	3 (20%)	17,32,35	4.39	7 (41%)
1	5BU	R	28	1	15,22,23	2.43	3 (20%)	17,32,35	4.43	5 (29%)
1	5BU	R	27	1	15,22,23	1.98	3 (20%)	17,32,35	4.09	3 (17%)

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
1	5BU	R	17	1	-	0/5/25/26	0/2/2/2
1	5BU	R	12	1	-	0/5/25/26	0/2/2/2
1	5BU	R	28	1	-	4/5/25/26	0/2/2/2
1	5BU	R	27	1	-	2/5/25/26	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	28	5BU	C4-C5	6.75	1.47	1.38
1	R	27	5BU	C4-C5	6.12	1.46	1.38
1	R	12	5BU	C4-C5	5.93	1.46	1.38
1	R	28	5BU	BR-C5	5.46	2.06	1.90
1	R	17	5BU	C4-C5	4.47	1.44	1.38

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	28	5BU	C4-N3-C2	15.47	128.20	115.14
1	R	12	5BU	C4-N3-C2	15.12	127.91	115.14
1	R	27	5BU	C4-N3-C2	14.48	127.37	115.14
1	R	17	5BU	C4-N3-C2	14.20	127.13	115.14
1	R	17	5BU	C5-C4-N3	-7.72	114.40	123.64

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	R	28	5BU	C3'-C4'-C5'-O5'
1	R	28	5BU	C2'-C1'-N1-C6
1	R	28	5BU	O4'-C4'-C5'-O5'
1	R	27	5BU	O4'-C4'-C5'-O5'
1	R	27	5BU	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R	17	5BU	3	0
1	R	12	5BU	4	0
1	R	28	5BU	4	0
1	R	27	5BU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

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, 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	23/31 (74%)	0.19	0 100 100	86, 105, 133, 157	0
2	A	1416/1733 (81%)	-0.37	11 (0%) 86 81	22, 86, 159, 180	0
3	B	1112/1224 (90%)	-0.28	15 (1%) 77 70	26, 95, 168, 180	0
4	C	266/318 (83%)	-0.45	0 100 100	47, 82, 139, 156	0
5	D	177/221 (80%)	-0.35	0 100 100	56, 108, 156, 177	0
6	E	214/215 (99%)	-0.12	7 (3%) 46 38	56, 141, 179, 180	0
7	F	84/155 (54%)	-0.55	0 100 100	28, 59, 98, 122	0
8	G	171/171 (100%)	-0.34	0 100 100	54, 82, 124, 133	0
9	H	133/146 (91%)	0.25	6 (4%) 33 28	105, 144, 178, 180	0
10	I	119/122 (97%)	0.00	4 (3%) 45 37	82, 135, 166, 180	0
11	J	65/70 (92%)	-0.56	0 100 100	48, 78, 125, 133	0
12	K	115/120 (95%)	-0.43	1 (0%) 84 79	45, 83, 113, 143	0
13	L	46/70 (65%)	-0.09	1 (2%) 62 54	73, 139, 174, 179	0
All	All	3941/4596 (85%)	-0.31	45 (1%) 80 74	22, 92, 168, 180	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1176	LEU	5.1
3	B	882	THR	4.5
2	A	149	GLU	3.7
3	B	883	LEU	3.7
6	E	51	GLY	3.6

## 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, 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(Å <sup>2</sup> )	Q<0.9
1	5BU	R	27	21/22	0.77	0.24	140,148,161,171	0
1	5BU	R	28	21/22	0.78	0.25	130,138,155,167	0
1	5BU	R	12	21/22	0.88	0.18	96,112,134,153	0
1	5BU	R	17	21/22	0.91	0.18	88,105,129,149	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 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(Å <sup>2</sup> )	Q<0.9
14	ZN	A	2456	1/1	0.97	0.11	73,73,73,73	0
14	ZN	L	1071	1/1	0.97	0.05	114,114,114,114	0
15	MG	A	2458	1/1	0.98	0.34	20,20,20,20	0
14	ZN	C	1269	1/1	0.98	0.07	48,48,48,48	0
14	ZN	A	2457	1/1	0.99	0.10	46,46,46,46	0
14	ZN	B	2225	1/1	0.99	0.13	66,66,66,66	0
14	ZN	I	1122	1/1	0.99	0.08	176,176,176,176	0
14	ZN	J	1066	1/1	0.99	0.13	65,65,65,65	0
14	ZN	I	1121	1/1	0.99	0.14	85,85,85,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.