



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2024 – 09:33 am BST

PDB ID : 4BBS  
Title : Structure of an initially transcribing RNA polymerase II-TFIIB complex  
Authors : Sainsbury, S.; Niesser, J.; Cramer, P.  
Deposited on : 2012-09-27  
Resolution : 3.60 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)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

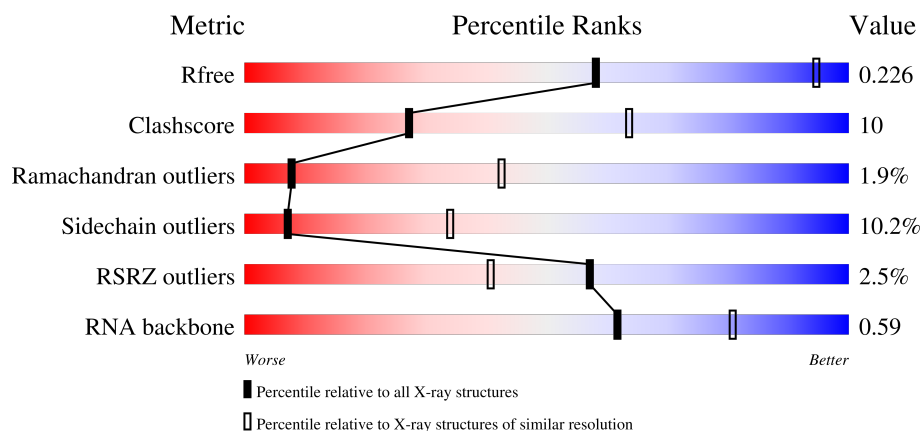
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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  $\geq 3$ , 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	A	1733	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>21%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	1224	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>26%</div> <div>•</div> <div>6%</div> </div> </div>
3	C	318	<div> <div></div> <div> <div>57%</div> <div>24%</div> <div>•</div> <div>16%</div> </div> </div>
4	D	221	<div> <div></div> <div> <div>52%</div> <div>22%</div> <div>6%</div> <div>19%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	14	
15	P	6	
16	T	27	

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
18	MG	A	2459	-	-	-	X

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 33420 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
1	A	1419	Total	C	N	O	S	0	0	0
			11170	7039	1953	2116	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1150	Total	C	N	O	S	0	0	0
			9095	5751	1598	1690	56			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

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

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

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

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	189	Total	C	N	O	S	0	0	0
			1357	838	240	267	12			

- Molecule 14 is a DNA chain called 5'-D(\*GP\*GP\*CP\*AP\*CP\*AP\*AP\*CP\*TP\*GP\*CP\*GP\*CP\*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	7	Total	C	N	O	P	0	0	0
			139	67	29	37	6			

- Molecule 15 is a RNA chain called 5'-R(\*AP\*UP\*AP\*UP\*CP\*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

- Molecule 16 is a DNA chain called 5'-D(\*AP\*GP\*CP\*GP\*CP\*AP\*GP\*TP\*TP\*GP\*TP\*GP\*CP\*TP\*AP\*TP\*GP\*AP\*TP\*AP\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	17	Total	C	N	O	P	0	0	0
			350	169	56	108	17			

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

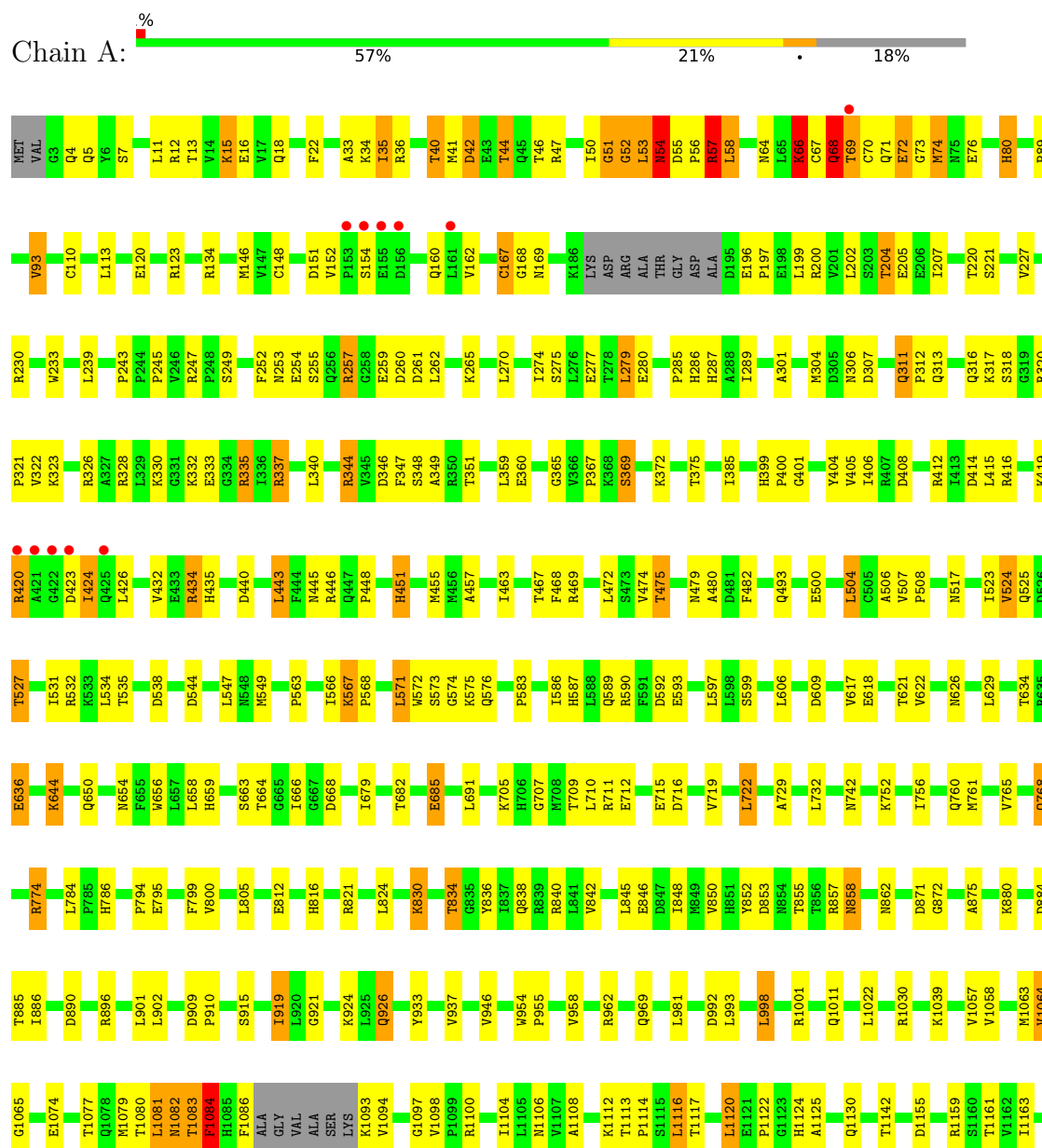
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	2	Total	Mg	0	0
			2	2		

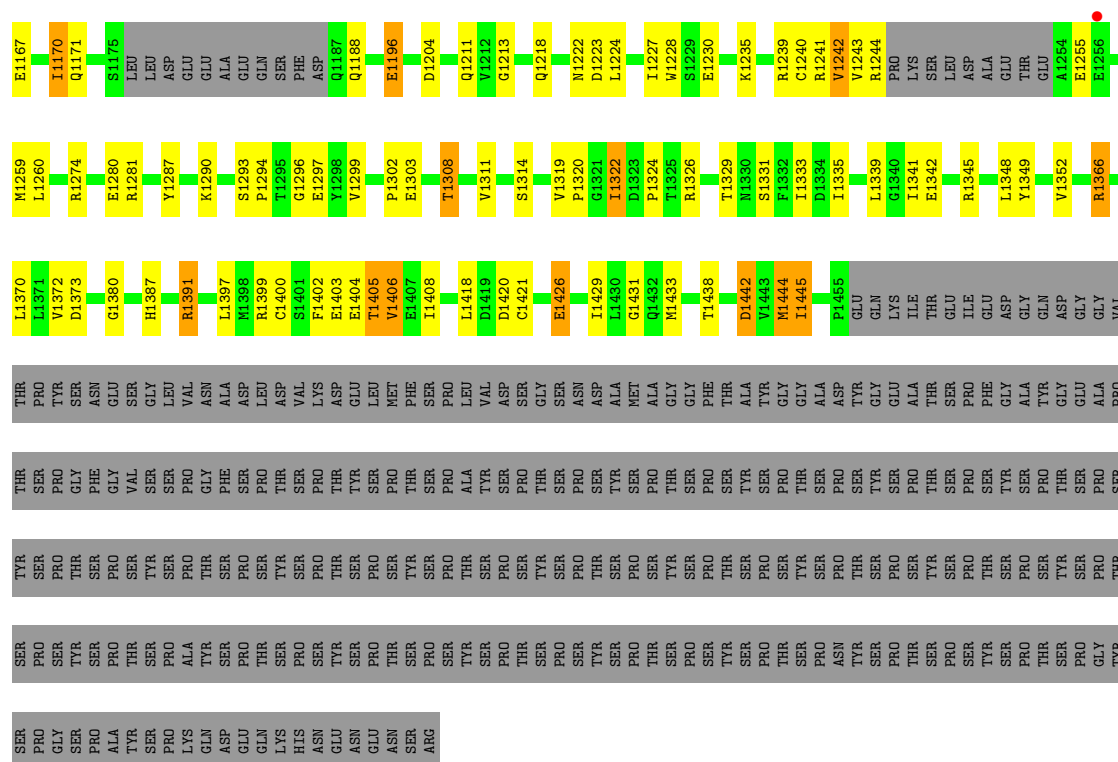
### 3 Residue-property plots

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.

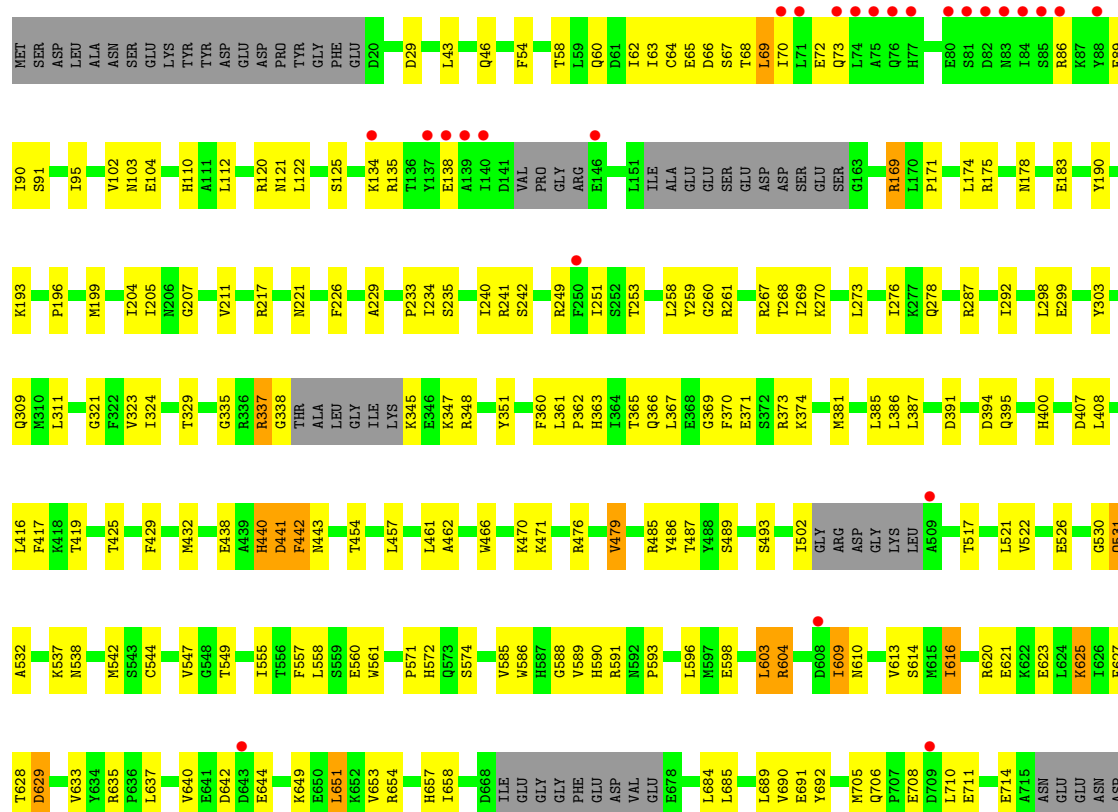
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

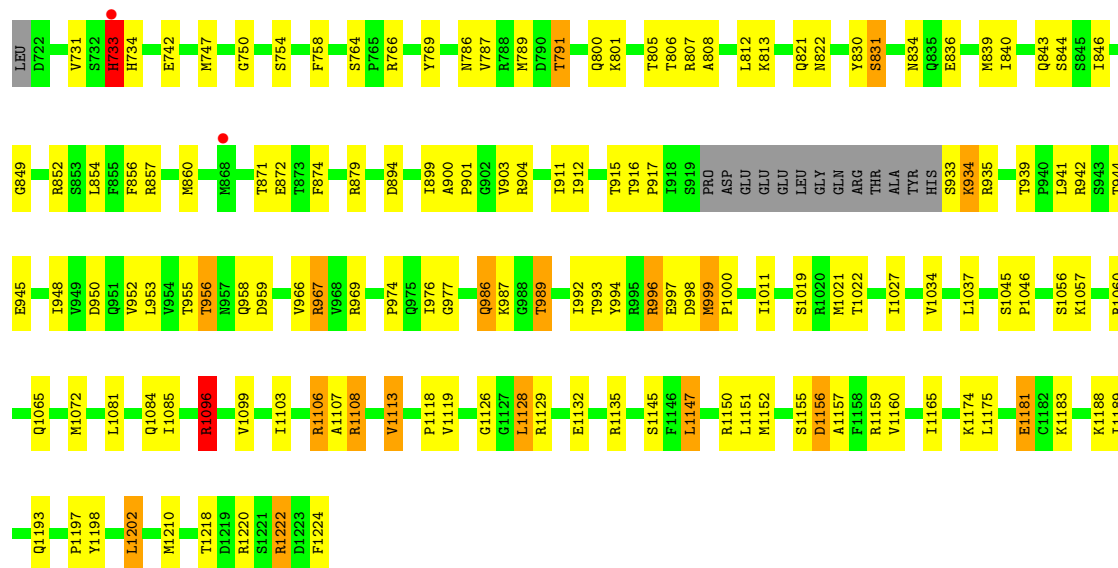






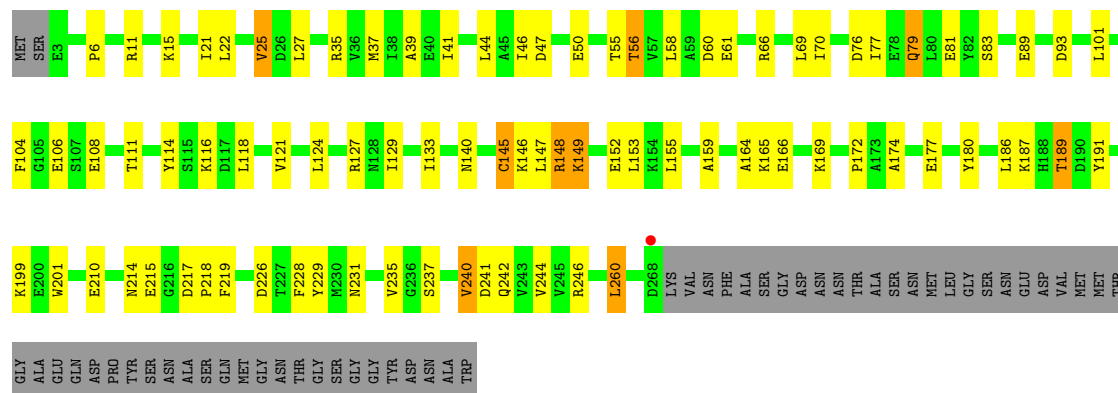
● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2





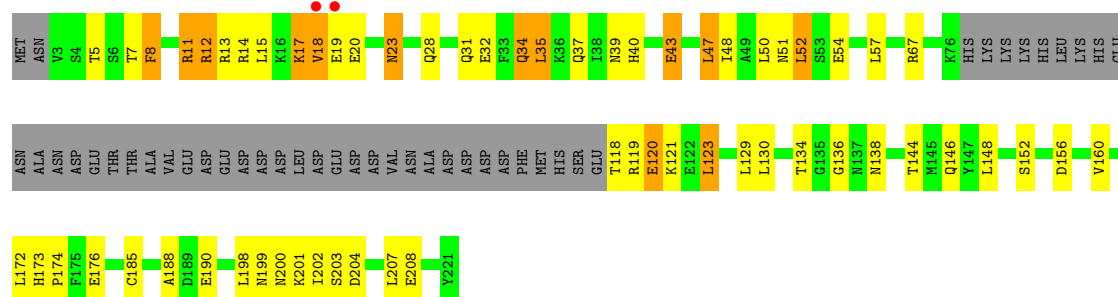
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 57% 24% 16%



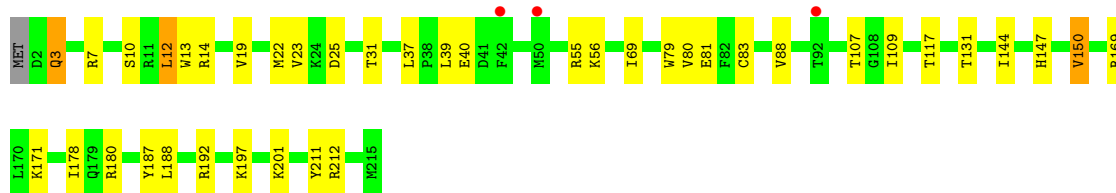
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D: 52% 22% 6% 19%



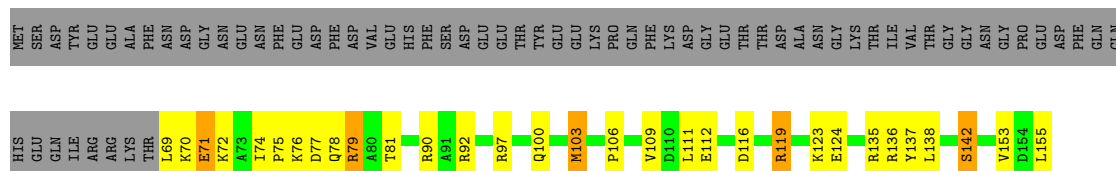
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E: 81% 17%



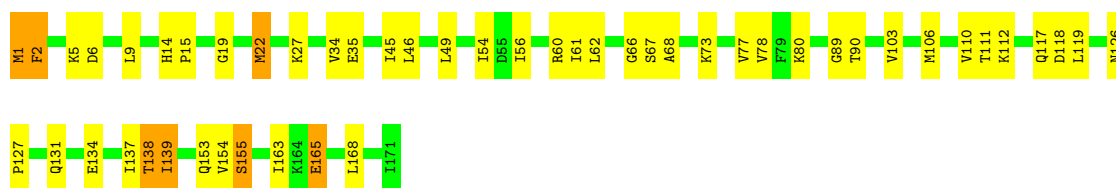
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 36% 17% 44%



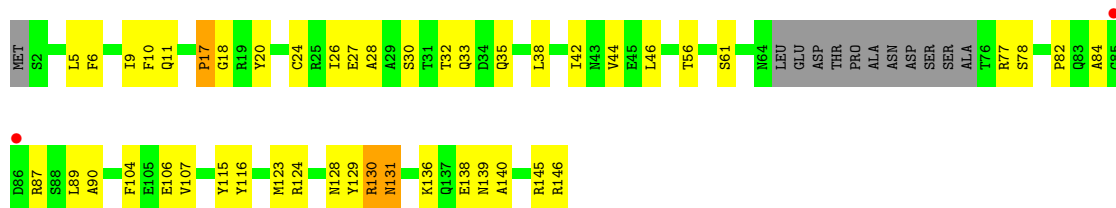
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G: 71% 25%



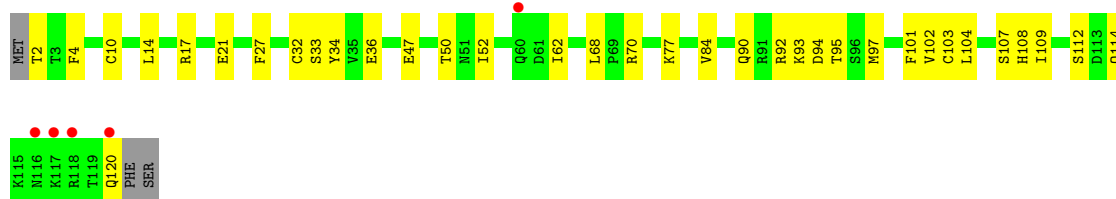
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H: 60% 29% 8%



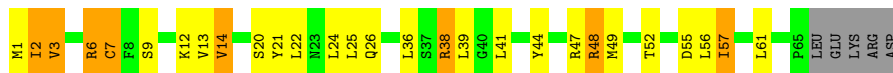
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I: 4% 69% 29%



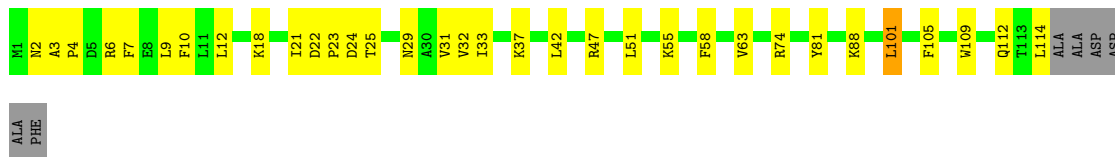
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:  53% 29% 11% 7%

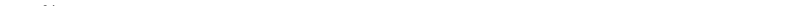


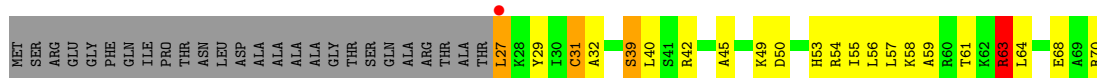
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:  68% 27% 5%



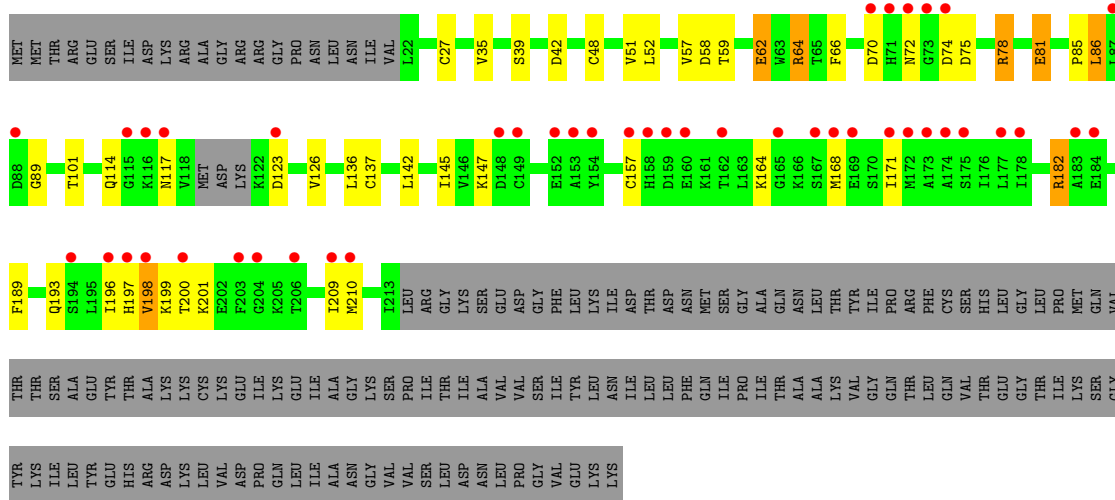
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L: 




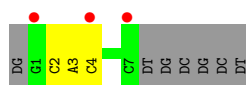
- Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB

Chain M: 



- Molecule 14: 5'-D(\*GP\*GP\*CP\*AP\*CP\*AP\*AP\*CP\*TP\*GP\*CP\*GP\*CP\*TP)-3'

Chain N: 




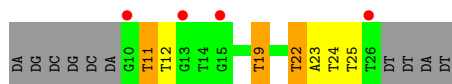
- Molecule 15: 5'-R(\*AP\*UP\*AP\*UP\*CP\*AP)-3'

Chain P:  67% 33%



• Molecule 16: 5'-D(\*AP\*GP\*CP\*GP\*CP\*AP\*GP\*TP\*TP\*GP\*TP\*GP\*CP\*TP \*AP\*TP\*GP\*AP\*TP\*AP\*TP\*TP\*TP\*TP\*TP\*AP\*TP)-3'

Chain T:  15% 37% 15% 11% 37%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.17Å 386.01Å 254.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 3.60 49.33 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-3.60) 100.0 (49.33-3.60)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.185 , 0.225 0.182 , 0.226	Depositor DCC
$R_{free}$ test set	2520 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 99.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	33420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.38	0/11372	0.59	1/15380 (0.0%)
2	B	0.36	0/9271	0.56	0/12505
3	C	0.42	0/2133	0.58	0/2891
4	D	0.38	0/1444	0.59	0/1935
5	E	0.32	0/1788	0.51	0/2406
6	F	0.41	0/717	0.63	0/967
7	G	0.43	0/1368	0.61	0/1844
8	H	0.35	0/1094	0.55	0/1481
9	I	0.32	0/989	0.50	0/1331
10	J	0.45	0/541	0.70	1/727 (0.1%)
11	K	0.40	0/937	0.53	0/1265
12	L	0.41	0/353	0.58	0/468
13	M	0.29	0/1373	0.47	0/1863
14	N	0.63	0/156	1.06	0/238
15	P	0.32	0/137	0.81	0/211
16	T	0.62	0/390	1.37	3/601 (0.5%)
All	All	0.38	0/34063	0.59	5/46113 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	19	DT	O4'-C4'-C3'	-7.33	101.57	104.50
1	A	58	LEU	CA-CB-CG	5.74	128.51	115.30
16	T	22	DT	O4'-C1'-N1	5.73	112.01	108.00
10	J	3	VAL	CB-CA-C	-5.61	100.74	111.40
16	T	11	DT	N3-C4-O4	5.18	123.01	119.90

There are no chirality outliers.

There are no planarity outliers.

## 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	A	11170	0	11222	271	0
2	B	9095	0	9055	196	0
3	C	2095	0	2051	54	0
4	D	1434	0	1460	38	0
5	E	1752	0	1776	21	0
6	F	705	0	731	20	0
7	G	1340	0	1357	35	0
8	H	1076	0	1046	25	0
9	I	971	0	927	15	0
10	J	532	0	542	23	0
11	K	919	0	929	19	0
12	L	351	0	374	17	0
13	M	1357	0	1263	27	0
14	N	139	0	79	2	0
15	P	123	0	66	1	0
16	T	350	0	197	6	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
17	M	1	0	0	0	0
18	A	2	0	0	0	0
All	All	33420	0	33075	674	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 10.

The worst 5 of 674 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)
7:G:1:MET:HE3	7:G:80:LYS:H	1.15	1.04
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.30	0.95
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG21	1:A:857:ARG:HE	1.36	0.90
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.59	0.84

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	1409/1733 (81%)	1273 (90%)	104 (7%)	32 (2%)	6	38
2	B	1134/1224 (93%)	1016 (90%)	97 (9%)	21 (2%)	8	42
3	C	264/318 (83%)	245 (93%)	17 (6%)	2 (1%)	19	59
4	D	174/221 (79%)	157 (90%)	12 (7%)	5 (3%)	4	33
5	E	212/215 (99%)	200 (94%)	11 (5%)	1 (0%)	29	68
6	F	85/155 (55%)	81 (95%)	4 (5%)	0	100	100
7	G	169/171 (99%)	152 (90%)	15 (9%)	2 (1%)	13	51
8	H	130/146 (89%)	111 (85%)	15 (12%)	4 (3%)	4	32
9	I	117/122 (96%)	99 (85%)	16 (14%)	2 (2%)	9	45
10	J	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4	31
11	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
12	L	42/70 (60%)	29 (69%)	8 (19%)	5 (12%)	0	5
13	M	185/345 (54%)	164 (89%)	19 (10%)	2 (1%)	14	53
All	All	4096/4910 (83%)	3691 (90%)	327 (8%)	78 (2%)	8	42

5 of 78 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	MET

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	286	HIS
1	A	317	LYS
1	A	593	GLU
1	A	885	THR

### 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	
1	A	1241/1520 (82%)	1112 (90%)	129 (10%)	7	33
2	B	980/1061 (92%)	886 (90%)	94 (10%)	8	37
3	C	234/274 (85%)	211 (90%)	23 (10%)	8	36
4	D	160/200 (80%)	140 (88%)	20 (12%)	4	25
5	E	196/197 (100%)	186 (95%)	10 (5%)	24	58
6	F	77/137 (56%)	67 (87%)	10 (13%)	4	24
7	G	152/152 (100%)	136 (90%)	16 (10%)	7	33
8	H	118/128 (92%)	109 (92%)	9 (8%)	13	45
9	I	113/116 (97%)	101 (89%)	12 (11%)	6	32
10	J	60/65 (92%)	49 (82%)	11 (18%)	1	10
11	K	99/102 (97%)	89 (90%)	10 (10%)	7	34
12	L	39/57 (68%)	35 (90%)	4 (10%)	7	34
13	M	136/299 (46%)	118 (87%)	18 (13%)	4	23
All	All	3605/4308 (84%)	3239 (90%)	366 (10%)	7	34

5 of 366 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	111	THR
7	G	1	MET
3	C	186	LEU
4	D	120	GLU
7	G	139	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	325	GLN
2	B	975	GLN
12	L	53	HIS
5	E	153	HIS
11	K	2	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

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 11 ligands modelled in this entry, 11 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

### 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	A	1419/1733 (81%)	-0.26	12 (0%) 86 75	47, 92, 160, 278	0
2	B	1150/1224 (93%)	-0.27	28 (2%) 59 42	49, 99, 176, 251	0
3	C	266/318 (83%)	-0.28	1 (0%) 92 86	49, 77, 123, 208	0
4	D	178/221 (80%)	-0.17	2 (1%) 80 68	63, 102, 166, 211	0
5	E	214/215 (99%)	0.07	3 (1%) 75 61	73, 130, 188, 213	0
6	F	87/155 (56%)	-0.42	0 100 100	58, 80, 123, 140	0
7	G	171/171 (100%)	-0.34	0 100 100	58, 81, 123, 136	0
8	H	134/146 (91%)	-0.03	2 (1%) 73 60	76, 120, 176, 222	0
9	I	119/122 (97%)	0.03	5 (4%) 36 23	90, 126, 199, 218	0
10	J	65/70 (92%)	-0.48	0 100 100	58, 79, 119, 152	0
11	K	114/120 (95%)	-0.25	0 100 100	57, 80, 129, 153	0
12	L	44/70 (62%)	-0.24	1 (2%) 60 44	80, 128, 181, 210	0
13	M	189/345 (54%)	1.03	44 (23%) 0 0	81, 170, 229, 272	0
14	N	7/14 (50%)	2.04	3 (42%) 0 0	200, 213, 233, 239	0
15	P	6/6 (100%)	1.01	0 100 100	169, 184, 220, 237	0
16	T	17/27 (62%)	1.28	4 (23%) 0 0	163, 197, 261, 274	0
All	All	4180/4957 (84%)	-0.17	105 (2%) 57 41	47, 97, 183, 278	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	73	GLY	5.6
13	M	72	ASN	5.5
1	A	422	GLY	5.2
1	A	69	THR	5.0
2	B	81	SER	4.7

## 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 [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, 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
18	MG	A	2458	1/1	0.78	0.25	109,109,109,109	0
18	MG	A	2459	1/1	0.80	0.74	104,104,104,104	0
17	ZN	L	1071	1/1	0.98	0.07	162,162,162,162	0
17	ZN	M	1216	1/1	0.98	0.06	111,111,111,111	0
17	ZN	I	1122	1/1	0.99	0.04	145,145,145,145	0
17	ZN	J	1066	1/1	0.99	0.17	69,69,69,69	0
17	ZN	A	2457	1/1	0.99	0.12	94,94,94,94	0
17	ZN	C	1269	1/1	1.00	0.07	86,86,86,86	0
17	ZN	I	1121	1/1	1.00	0.09	109,109,109,109	0
17	ZN	A	2456	1/1	1.00	0.05	118,118,118,118	0
17	ZN	B	2225	1/1	1.00	0.16	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.