



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 10, 2019 – 10:14 PM EST

PDB ID : 4A3F  
Title : RNA Polymerase II initial transcribing complex with a 6nt DNA-RNA hybrid  
and soaked with AMPCPP  
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.  
Deposited on : 2011-09-30  
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](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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

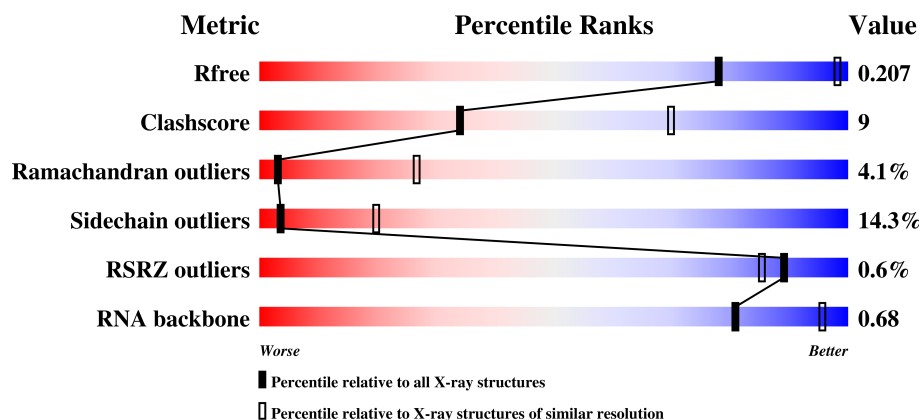
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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.




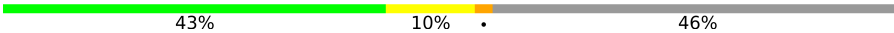









Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1391 (3.60-3.40)
Clashscore	122126	1485 (3.60-3.40)
Ramachandran outliers	120053	1446 (3.60-3.40)
Sidechain outliers	120020	1447 (3.60-3.40)
RSRZ outliers	108989	1303 (3.60-3.40)
RNA backbone	2636	1052 (4.10-2.90)

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. 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	1732	<div> <div></div> <div> <div></div> <div>55%</div> <div>22%</div> <div>5%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	1224	<div> <div></div> <div> <div></div> <div>59%</div> <div>27%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	318	<div> <div></div> <div> <div></div> <div>52%</div> <div>28%</div> <div>•</div> <div>16%</div> </div> </div>
4	D	221	<div> <div></div> <div> <div></div> <div>55%</div> <div>19%</div> <div>5%</div> <div>•</div> <div>19%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	E	215	 69% 29% .
6	F	155	 43% 10% . 46%
7	G	171	 61% 35% . .
8	H	146	 % 66% 21% 5% 9%
9	I	122	 2% 73% 24% . .
10	J	70	 63% 21% 9% 7%
11	K	120	 63% 32% . .
12	L	70	 3% 26% 26% 14% 34%
13	N	14	 79% 21%
14	P	6	 67% 33%
15	T	26	 42% 27% 8% 23%

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32010 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	1425	Total	C	N	O	S	0	0	0
			11197	7051	1958	2126	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	55			

- 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	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called RPB7, 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	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	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	115	Total	C	N	O	S	0	0	1
			920	590	157	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	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called NON TEMPLATE DNA 5'-D(\*TP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*GP\*AP \*GP\*CP\*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	11	Total	C	N	O	P	0	0	0
			226	109	44	63	10			

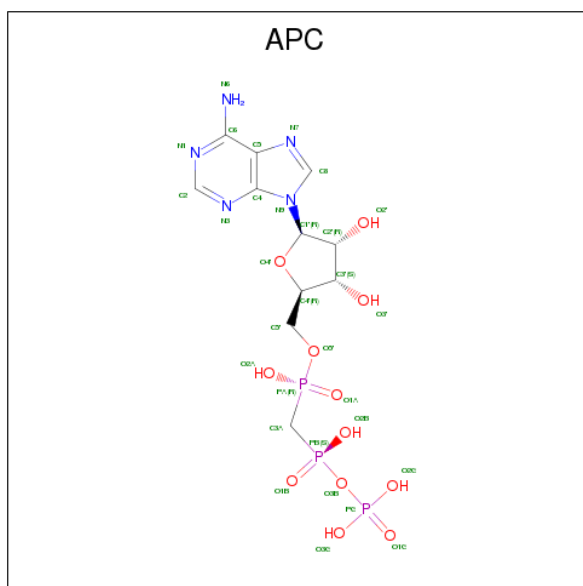
- Molecule 14 is a RNA chain called TRANSCRIPT RNA 5'-R(\*CP\*CP\*AP\*GP\*GP\*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	6	Total	C	N	O	P	0	0	0
			130	58	26	40	6			

- Molecule 15 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*DTP \*TP\*TP\*CP\*C BRU\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	20	Total	Br	C	N	O	P	0	0
			404	1	194	63	126	20		

- Molecule 16 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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

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

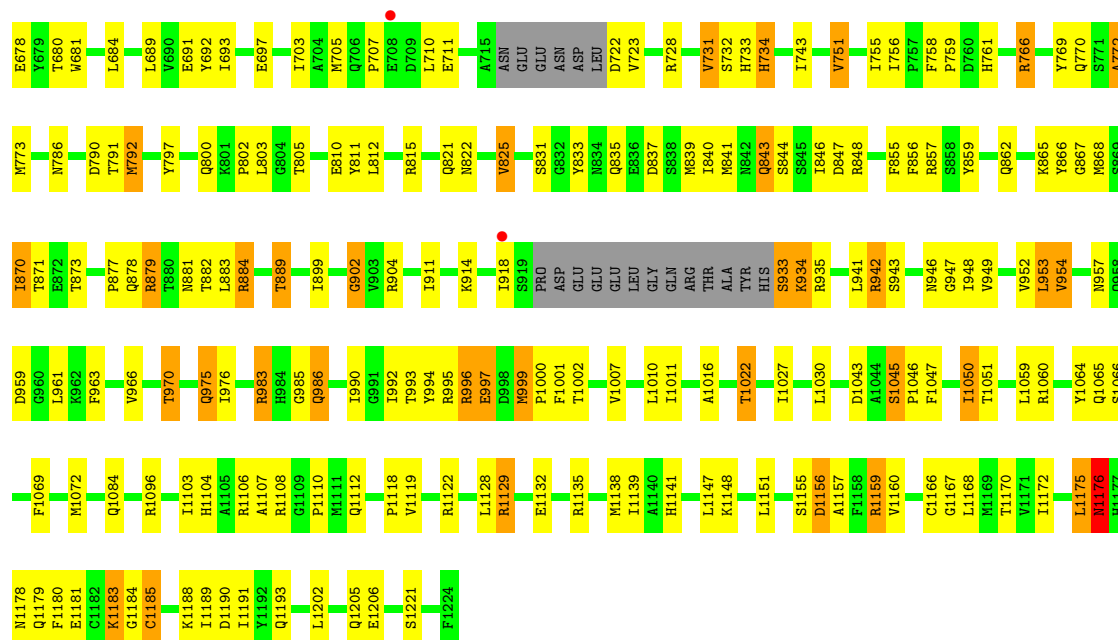
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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



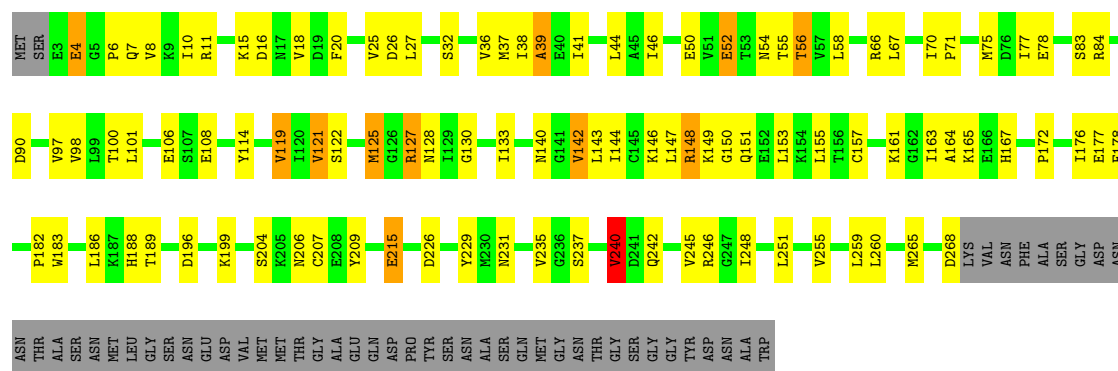






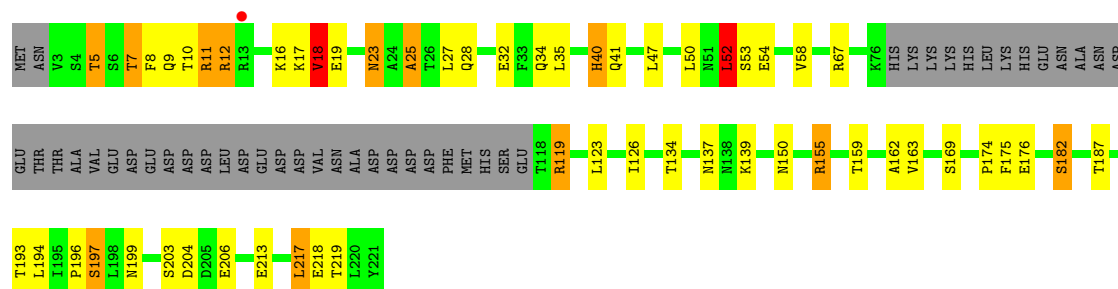
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 52% 28% 16%



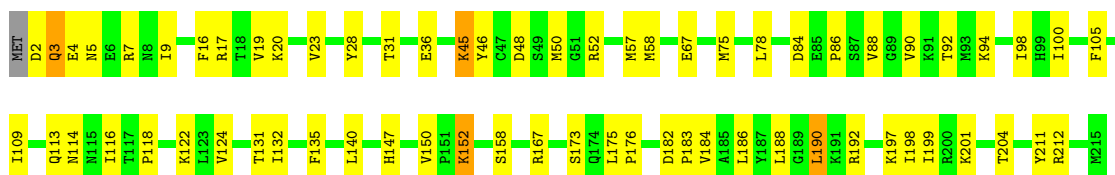
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D: 55% 19% 5% 19%

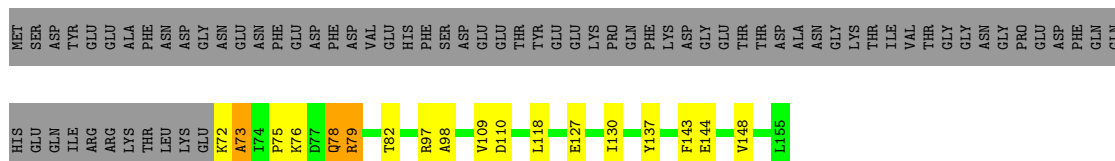


• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

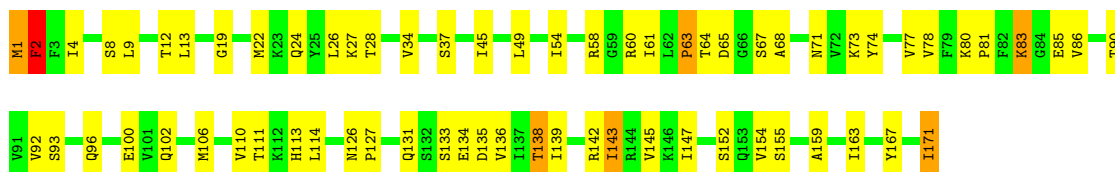
Chain E: 69% 29%



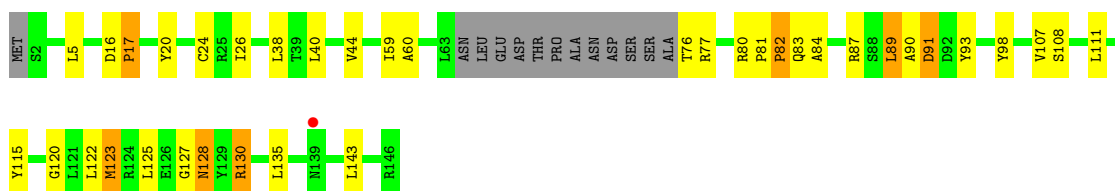
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



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



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



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

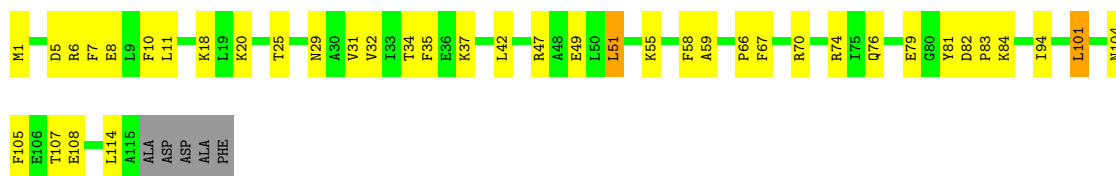


• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5




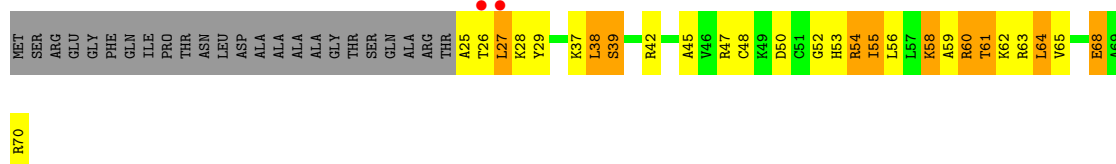
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:  63% 32%




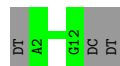
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:  3% 26% 26% 14% 34%



- Molecule 13: NON TEMPLATE DNA 5'-D(\*TP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*TP)-3'

Chain N:  79% 21%



- Molecule 14: TRANSCRIPT RNA 5'-R(\*CP\*CP\*AP\*GP\*GP\*AP)-3'

Chain P:  67% 33%



- Molecule 15: 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*DTP\*TP\*TP\*CP\*CBRU\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'

Chain T:  42% 27% 8% 23%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	221.60Å 391.30Å 283.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.89 – 3.50 52.78 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.89-3.50) 98.2 (52.78-3.40)	Depositor EDS
$R_{merge}$	0.68	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.156 , 0.185 0.180 , 0.207	Depositor DCC
$R_{free}$ test set	3255 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	110.5	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 101.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.036 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32010	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: MG, APC, ZN, BRU

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	0.54	0/11397	0.86	13/15415 (0.1%)
2	B	0.52	0/9029	0.81	3/12171 (0.0%)
3	C	0.49	0/2133	0.78	1/2891 (0.0%)
4	D	0.53	0/1444	0.84	1/1935 (0.1%)
5	E	0.46	0/1788	0.71	0/2406
6	F	0.57	0/691	0.80	0/933
7	G	0.53	0/1368	0.83	0/1844
8	H	0.51	0/1086	0.80	0/1470
9	I	0.46	0/989	0.76	0/1331
10	J	0.55	0/541	0.83	0/727
11	K	0.50	0/938	0.75	0/1267
12	L	0.52	0/365	0.95	0/485
13	N	1.11	0/254	1.01	0/391
14	P	1.13	0/145	0.78	0/224
15	T	1.36	4/426 (0.9%)	1.12	1/652 (0.2%)
All	All	0.55	4/32594 (0.0%)	0.83	19/44142 (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
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	25	DT	N1-C2	7.74	1.44	1.38
15	T	25	DT	C1'-N1	7.62	1.59	1.49
15	T	13	DA	C3'-O3'	5.37	1.50	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	25	DT	N1-C6	5.08	1.41	1.38

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	HIS	N-CA-CB	7.22	123.60	110.60
1	A	34	LYS	C-N-CA	6.76	138.61	121.70
1	A	57	ARG	C-N-CA	5.96	136.60	121.70
1	A	54	ASN	C-N-CA	5.95	136.58	121.70
1	A	34	LYS	N-CA-C	-5.92	95.02	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide

## 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	11197	0	11257	222	0
2	B	8859	0	8901	185	0
3	C	2095	0	2051	56	0
4	D	1434	0	1460	25	0
5	E	1752	0	1776	33	0
6	F	679	0	701	10	0
7	G	1340	0	1357	37	0
8	H	1068	0	1040	21	0
9	I	971	0	927	10	0
10	J	532	0	542	14	0
11	K	920	0	929	22	0
12	L	363	0	386	15	0
13	N	226	0	126	0	0
14	P	130	0	66	1	0
15	T	404	0	227	6	0
16	A	31	0	14	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
18	A	1	0	0	0	0
All	All	32010	0	31760	583	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 9.

The worst 5 of 583 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:867:ILE:CD1	1:A:867:ILE:CG1	1.79	1.60
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.43	0.98
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.48	0.95
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.54	0.90
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.55	0.87

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	1417/1732 (82%)	1225 (86%)	135 (10%)	57 (4%)	3	27
2	B	1095/1224 (90%)	951 (87%)	92 (8%)	52 (5%)	2	23
3	C	264/318 (83%)	237 (90%)	20 (8%)	7 (3%)	5	36
4	D	174/221 (79%)	153 (88%)	11 (6%)	10 (6%)	2	19

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	212/215 (99%)	196 (92%)	12 (6%)	4 (2%)	9	43
6	F	82/155 (53%)	77 (94%)	4 (5%)	1 (1%)	14	53
7	G	169/171 (99%)	156 (92%)	9 (5%)	4 (2%)	6	38
8	H	129/146 (88%)	104 (81%)	17 (13%)	8 (6%)	1	17
9	I	117/122 (96%)	93 (80%)	19 (16%)	5 (4%)	3	25
10	J	63/70 (90%)	53 (84%)	7 (11%)	3 (5%)	2	22
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	24 (54%)	12 (27%)	8 (18%)	0	1
All	All	3879/4564 (85%)	3377 (87%)	343 (9%)	159 (4%)	3	27

5 of 159 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	58	LEU
1	A	169	ASN
1	A	189	ARG
1	A	251	SER

### 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	1243/1519 (82%)	1046 (84%)	197 (16%)	3	16
2	B	966/1061 (91%)	833 (86%)	133 (14%)	4	21
3	C	234/274 (85%)	206 (88%)	28 (12%)	5	26
4	D	160/200 (80%)	131 (82%)	29 (18%)	2	10
5	E	196/197 (100%)	176 (90%)	20 (10%)	8	34
6	F	74/137 (54%)	66 (89%)	8 (11%)	7	31
7	G	152/152 (100%)	128 (84%)	24 (16%)	3	16
8	H	117/128 (91%)	108 (92%)	9 (8%)	14	46

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	113/116 (97%)	102 (90%)	11 (10%)	9	35
10	J	60/65 (92%)	50 (83%)	10 (17%)	2	13
11	K	99/102 (97%)	85 (86%)	14 (14%)	4	20
12	L	40/57 (70%)	29 (72%)	11 (28%)	0	3
All	All	3454/4008 (86%)	2960 (86%)	494 (14%)	3	20

5 of 494 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	348	ARG
2	B	837	ASP
9	I	83	ASN
2	B	401	PHE
2	B	570	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	572	HIS
2	B	975	GLN
9	I	108	HIS
2	B	573	GLN
2	B	842	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	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 ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
15	BRU	T	22	15,14	14,21,22	1.70	3 (21%)	17,30,33	3.01	4 (23%)

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
15	BRU	T	22	15,14	-	0/3/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	O5'-C5'	-3.32	1.40	1.44
15	T	22	BRU	C2-N3	-2.53	1.33	1.38
15	T	22	BRU	C4-C5	4.16	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C5-C4-N3	-4.19	118.62	123.64
15	T	22	BRU	C2'-C1'-N1	-2.45	108.57	114.27
15	T	22	BRU	O4'-C1'-N1	5.21	116.57	107.78
15	T	22	BRU	C4-N3-C2	9.88	123.56	115.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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
16	APC	A	2455	-	28,33,33	3.39	13 (46%)	27,52,52	2.44	7 (25%)

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
16	APC	A	2455	-	-	0/15/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	2455	APC	C8-N9	-3.10	1.33	1.36
16	A	2455	APC	C8-N7	-2.72	1.29	1.34
16	A	2455	APC	C5-N7	-2.43	1.31	1.39
16	A	2455	APC	C6-N1	-2.18	1.27	1.37
16	A	2455	APC	C4-N3	-2.06	1.32	1.35

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	2455	APC	N3-C2-N1	-8.86	121.28	128.86
16	A	2455	APC	C4-C5-N7	-4.56	105.00	109.41
16	A	2455	APC	PG-O3B-PB	-3.15	121.35	132.40
16	A	2455	APC	C5'-C4'-C3'	-2.24	106.86	115.29
16	A	2455	APC	C5-C6-N6	2.07	124.69	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2455	APC	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.45
1	B	351:TYR	C	352:ALA	N	3.24

## 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	1425/1732 (82%)	-0.26	11 (0%) 86 80	58, 110, 173, 226	0
2	B	1115/1224 (91%)	-0.19	6 (0%) 90 87	69, 123, 181, 210	0
3	C	266/318 (83%)	-0.34	0 100 100	81, 110, 148, 178	0
4	D	178/221 (80%)	-0.20	1 (0%) 89 85	85, 121, 175, 193	0
5	E	214/215 (99%)	-0.21	0 100 100	91, 148, 190, 200	0
6	F	84/155 (54%)	-0.51	0 100 100	68, 92, 125, 138	0
7	G	171/171 (100%)	-0.20	0 100 100	82, 109, 145, 167	0
8	H	133/146 (91%)	0.17	1 (0%) 86 80	121, 153, 184, 218	0
9	I	119/122 (97%)	-0.13	3 (2%) 57 50	120, 158, 195, 213	0
10	J	65/70 (92%)	-0.31	0 100 100	90, 106, 145, 161	0
11	K	115/120 (95%)	-0.42	0 100 100	79, 110, 141, 156	0
12	L	46/70 (65%)	-0.02	2 (4%) 35 30	100, 180, 195, 199	0
13	N	11/14 (78%)	-0.39	0 100 100	181, 210, 266, 271	0
14	P	6/6 (100%)	-0.20	0 100 100	91, 95, 119, 147	0
15	T	19/26 (73%)	-0.34	0 100 100	84, 141, 264, 267	0
All	All	3967/4610 (86%)	-0.23	24 (0%) 89 85	58, 117, 182, 271	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	ARG	3.8
1	A	1176	LEU	3.7
2	B	340	ALA	3.6
8	H	139	ASN	3.6
2	B	509	ALA	3.2

## 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
15	BRU	T	22	20/21	0.95	0.16	86,97,107,113	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
16	APC	A	2455	31/31	0.88	0.24	112,115,143,144	0
17	ZN	L	1071	1/1	0.95	0.06	211,211,211,211	0
17	ZN	I	1122	1/1	0.97	0.05	201,201,201,201	0
18	MG	A	2458	1/1	0.98	0.16	86,86,86,86	0
17	ZN	A	2456	1/1	0.99	0.07	138,138,138,138	0
17	ZN	C	1269	1/1	0.99	0.12	93,93,93,93	0
17	ZN	I	1121	1/1	0.99	0.13	134,134,134,134	0
17	ZN	B	2225	1/1	0.99	0.21	81,81,81,81	0
17	ZN	J	1066	1/1	1.00	0.23	95,95,95,95	0
17	ZN	A	2457	1/1	1.00	0.15	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.