



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:03 AM GMT

PDB ID : 4A3D  
Title : RNA POLYMERASE II INITIAL TRANSCRIBING COMPLEX WITH A  
6NT DNA-RNA HYBRID  
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.  
Deposited on : 2011-09-30  
Resolution : 3.40 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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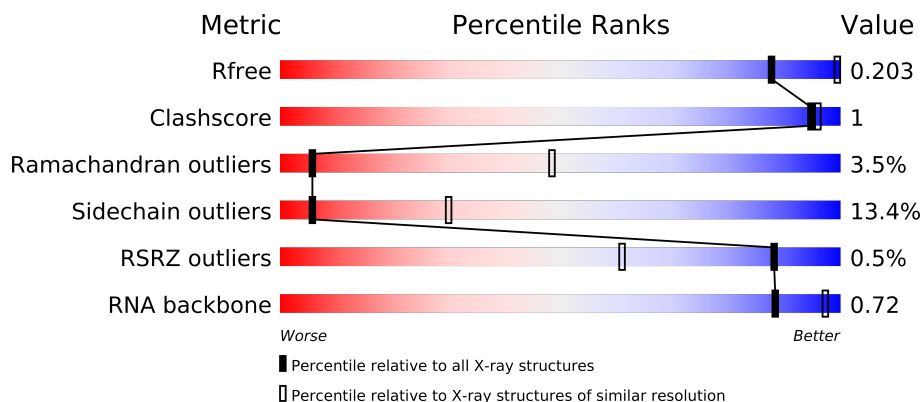
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.40 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))
$R_{free}$	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)
RNA backbone	1838	1002 (4.02-2.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1732	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

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Mol	Chain	Length	Quality of chain
13	N	14	
14	P	6	
15	T	26	

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31937 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1422	Total	C	N	O	S	0	0	0
			11174	7037	1954	2121	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	10	Total	C	N	O	P	0	0	0
			207	99	39	59	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 TEMPLATE DNA 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*BRUP\*GP\*GP\*TP\*CP\*AP\*TP\*TP)-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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

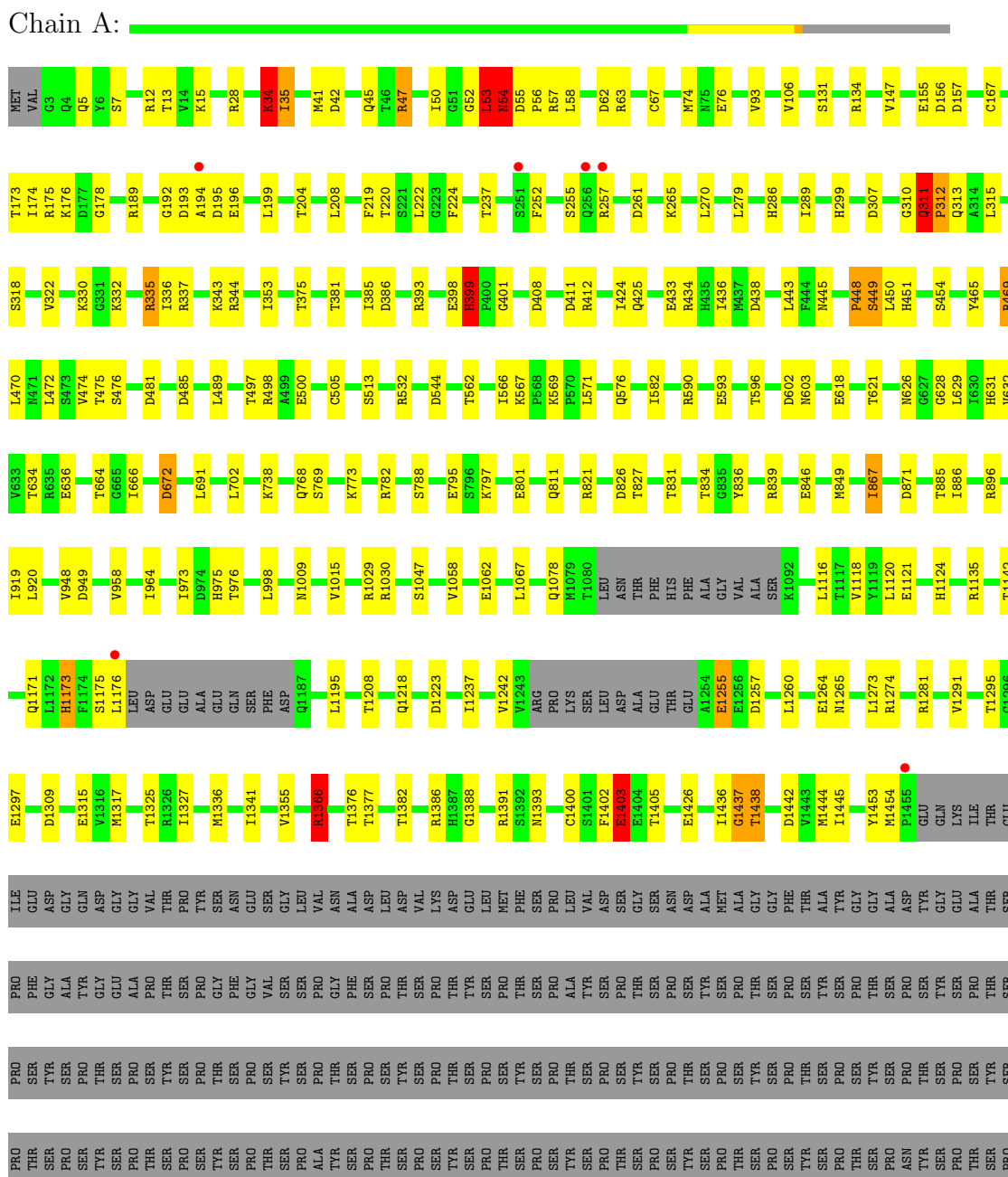
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	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 errors 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.

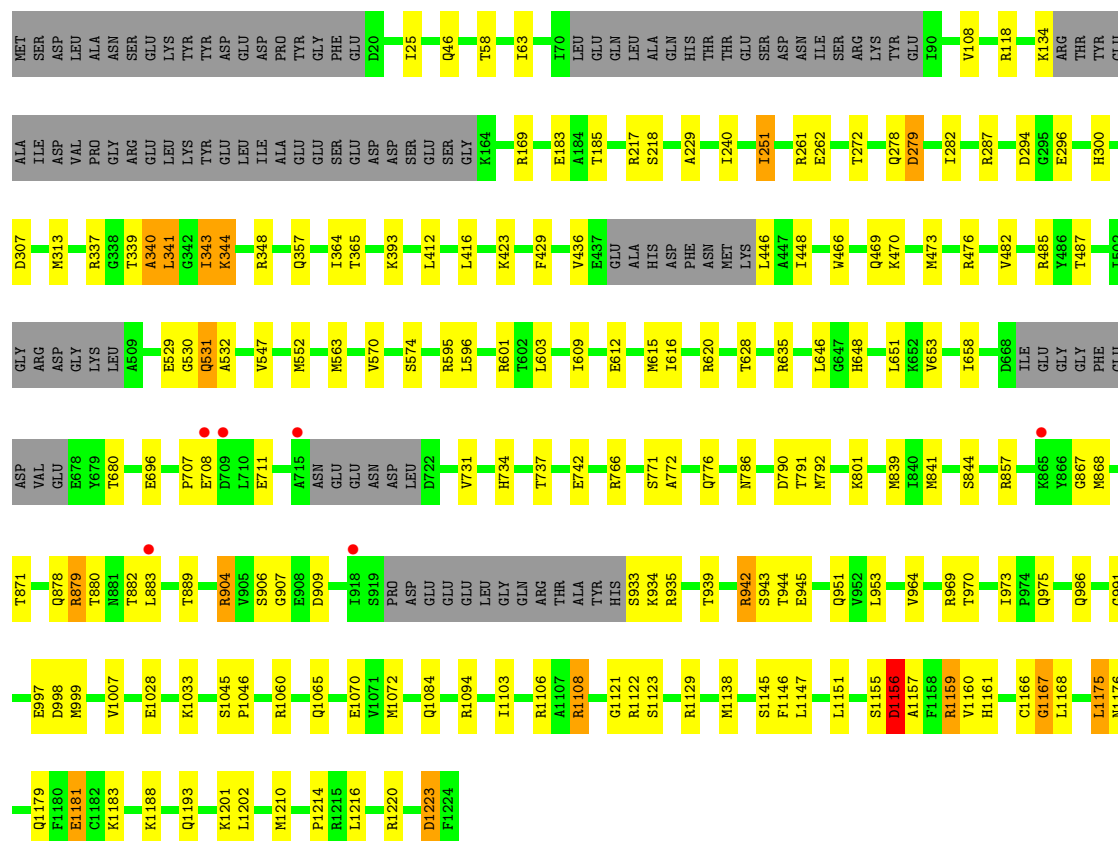
#### • Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



SER TYR  
SER PRO  
SER PRO  
THR THR  
SER PRO  
GLY TYR  
SER PRO  
SER PRO  
GLY GLY  
SER PRO  
ALA TYR  
SER SER  
PRO PRO  
LYS LYS  
GLN ASP  
ASP GLU  
GLN GLN  
LYS HIS  
ASN ASN  
GLU ASN  
ASN ASN  
SER SER

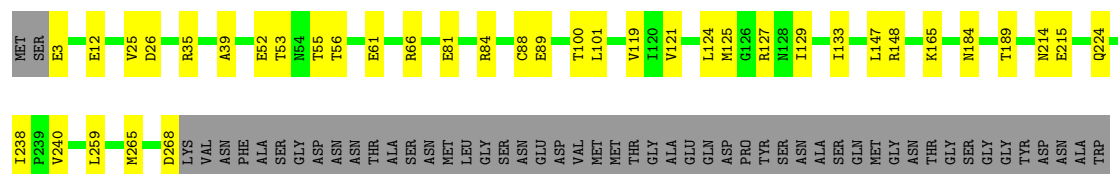
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

Chain B:



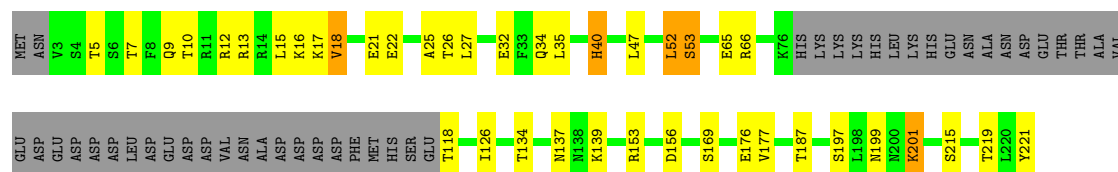
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:



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

Chain D:



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

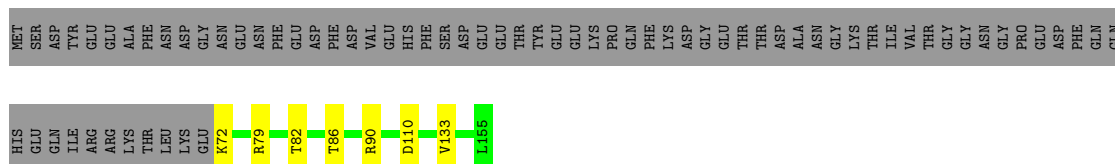


Chain E: 



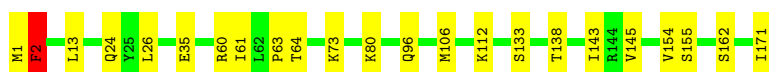
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 



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

Chain G: 



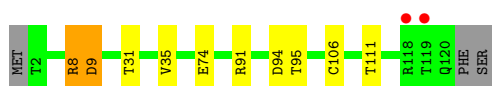
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H: 



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

Chain I: 



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

Chain J: 



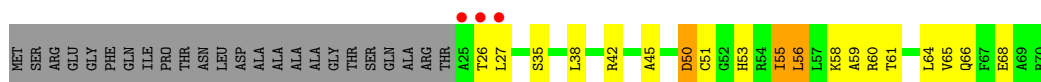
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K: 



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

Chain L: 



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

Chain N:



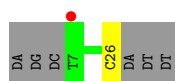
- Molecule 14: TRANSCRIPT RNA 5'-R(\*CP\*CP\*AP\*GP\*GP\*AP)-3'

Chain P:



- Molecule 15: TEMPLATE DNA 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*BRUP\*GP\*GP\*TP\*CP\*AP\*TP\*TP)-3'

Chain T:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	221.91Å 391.36Å 283.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 3.40 49.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.96-3.40) 100.0 (49.96-3.40)	Depositor EDS
$R_{merge}$	0.93	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.161 , 0.186 0.180 , 0.203	Depositor DCC
$R_{free}$ test set	3337 reflections (1.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	95.8	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 78.7	EDS
Estimated twinning fraction	0.034 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
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 168581 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	31937	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0/11374	0.85	10/15383 (0.1%)
2	B	0.51	0/9029	0.79	4/12171 (0.0%)
3	C	0.49	0/2133	0.78	2/2891 (0.1%)
4	D	0.51	0/1444	0.83	2/1935 (0.1%)
5	E	0.48	0/1788	0.71	0/2406
6	F	0.62	0/691	0.81	0/933
7	G	0.52	0/1368	0.81	0/1844
8	H	0.50	0/1086	0.80	0/1470
9	I	0.47	0/989	0.78	0/1331
10	J	0.54	0/541	0.88	1/727 (0.1%)
11	K	0.47	0/938	0.71	0/1267
12	L	0.54	0/365	0.95	0/485
13	N	1.07	0/232	1.06	0/356
14	P	1.21	0/145	0.79	0/224
15	T	1.26	1/426 (0.2%)	1.08	0/652
All	All	0.55	1/32549 (0.0%)	0.82	19/44075 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	26	DC	C1'-N1	5.63	1.56	1.49

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	7.25	123.66	110.60
1	A	34	LYS	C-N-CA	7.21	139.73	121.70
4	D	25	ALA	C-N-CA	6.11	136.98	121.70
1	A	56	PRO	C-N-CA	6.01	136.73	121.70
1	A	35	ILE	N-CA-CB	5.95	124.49	110.80

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11174	0	0	21	0
2	B	8859	0	0	18	0
3	C	2095	0	0	5	0
4	D	1434	0	0	3	0
5	E	1752	0	0	0	0
6	F	679	0	0	0	0
7	G	1340	0	0	5	0
8	H	1068	0	0	1	0
9	I	971	0	0	1	0
10	J	532	0	0	1	0
11	K	920	0	0	1	0
12	L	363	0	0	1	0
13	N	207	0	0	0	0
14	P	130	0	0	0	0
15	T	404	0	0	0	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31937	0	0	45	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

The worst 5 of 45 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:867:ILE:CD1	1:A:867:ILE:CG1	1.83	1.53
3:C:66:ARG:NH2	10:J:3:VAL:O	2.23	0.72
7:G:1:MET:SD	7:G:2:PHE:N	2.63	0.70
7:G:1:MET:CE	7:G:80:LYS:O	2.45	0.65
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.34	0.60

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1414/1732 (82%)	1236 (87%)	126 (9%)	52 (4%)	5	46
2	B	1095/1224 (90%)	968 (88%)	85 (8%)	42 (4%)	5	45
3	C	264/318 (83%)	242 (92%)	20 (8%)	2 (1%)	27	81
4	D	174/221 (79%)	148 (85%)	17 (10%)	9 (5%)	3	32
5	E	212/215 (99%)	195 (92%)	13 (6%)	4 (2%)	12	64
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100	100
7	G	169/171 (99%)	158 (94%)	8 (5%)	3 (2%)	13	65
8	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	2	23
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	8	56
10	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	4	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0	3
All	All	3876/4564 (85%)	3413 (88%)	328 (8%)	135 (4%)	6	48

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	76	GLU
1	A	189	ARG
1	A	195	ASP

### 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	1240/1519 (82%)	1062 (86%)	178 (14%)	5	26
2	B	966/1061 (91%)	842 (87%)	124 (13%)	6	32
3	C	234/274 (85%)	206 (88%)	28 (12%)	7	35
4	D	160/200 (80%)	129 (81%)	31 (19%)	2	11
5	E	196/197 (100%)	175 (89%)	21 (11%)	10	43
6	F	74/137 (54%)	67 (90%)	7 (10%)	12	50
7	G	152/152 (100%)	135 (89%)	17 (11%)	9	39
8	H	117/128 (91%)	103 (88%)	14 (12%)	7	35
9	I	113/116 (97%)	106 (94%)	7 (6%)	26	72
10	J	60/65 (92%)	49 (82%)	11 (18%)	2	13
11	K	99/102 (97%)	87 (88%)	12 (12%)	7	35
12	L	40/57 (70%)	27 (68%)	13 (32%)	0	2
All	All	3451/4008 (86%)	2988 (87%)	463 (13%)	6	30

5 of 463 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	436	VAL
2	B	906	SER
10	J	1	MET
2	B	485	ARG
2	B	653	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	5/6 (83%)	1 (20%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	G

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	19,21,22	0.99	1 (5%)	22,30,33	2.42	4 (18%)

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	-	0/5/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	P-OP1	2.31	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C6-N1-C2	-9.58	119.69	122.41
15	T	22	BRU	O4'-C1'-N1	4.08	115.35	107.68
15	T	22	BRU	N3-C2-N1	3.00	118.48	115.97
15	T	22	BRU	C2'-C1'-N1	-2.25	108.25	114.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1422/1732 (82%)	-0.07	6 (0%) 90 68	52, 96, 155, 215	0
2	B	1115/1224 (91%)	-0.01	6 (0%) 88 61	56, 111, 174, 201	0
3	C	266/318 (83%)	-0.14	0 100 100	68, 97, 135, 165	0
4	D	178/221 (80%)	-0.04	0 100 100	77, 110, 162, 182	0
5	E	214/215 (99%)	-0.02	0 100 100	72, 129, 170, 191	0
6	F	84/155 (54%)	-0.18	0 100 100	55, 76, 106, 122	0
7	G	171/171 (100%)	-0.03	0 100 100	65, 96, 135, 153	0
8	H	133/146 (91%)	0.40	0 100 100	110, 136, 175, 195	0
9	I	119/122 (97%)	-0.04	2 (1%) 67 31	107, 137, 173, 189	0
10	J	65/70 (92%)	-0.24	0 100 100	73, 94, 129, 142	0
11	K	115/120 (95%)	-0.14	1 (0%) 81 47	63, 95, 135, 151	0
12	L	46/70 (65%)	0.37	3 (6%) 18 7	92, 161, 182, 184	0
13	N	10/14 (71%)	0.09	0 100 100	158, 184, 239, 246	0
14	P	6/6 (100%)	-0.34	0 100 100	75, 90, 111, 138	0
15	T	20/26 (76%)	-0.04	1 (5%) 28 10	105, 152, 246, 248	0
All	All	3964/4610 (85%)	-0.04	19 (0%) 88 61	52, 105, 168, 248	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	4.3
12	L	25	ALA	3.3
1	A	257	ARG	3.3
12	L	26	THR	3.2
1	A	251	SER	3.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	BRU	T	22	20/21	0.13	-1.26	107,109,114,121	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
16	ZN	I	1121	1/1	0.13	0.28	121,121,121,121	0
16	ZN	B	2225	1/1	0.19	0.02	77,77,77,77	0
16	ZN	J	1066	1/1	0.22	-0.09	91,91,91,91	0
16	ZN	A	2457	1/1	0.14	-0.80	67,67,67,67	0
17	MG	A	2458	1/1	0.16	-0.86	64,64,64,64	0
16	ZN	C	1269	1/1	0.10	-1.07	88,88,88,88	0
16	ZN	A	2456	1/1	0.08	-1.96	133,133,133,133	0
16	ZN	I	1122	1/1	0.04	-2.08	182,182,182,182	0
16	ZN	L	1071	1/1	0.05	-2.86	163,163,163,163	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.