



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2024 – 03:15 pm BST

PDB ID : 4C3I
Title : Structure of 14-subunit RNA polymerase I at 3.0 Å resolution, crystal form C2-100
Authors : Fernandez-Tornero, C.; Moreno-Morcillo, M.; Rashid, U.J.; Taylor, N.M.I.; Ruiz, F.M.; Gruene, T.; Legrand, P.; Steuerwald, U.; Muller, C.W.
Deposited on : 2013-08-24
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
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

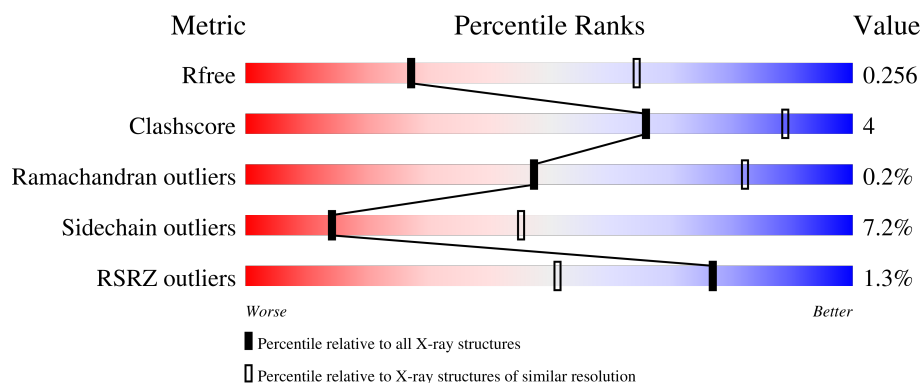
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





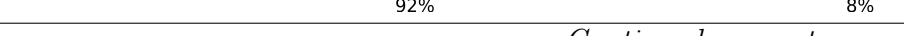
The reported resolution of this entry is 3.00 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1664	
2	B	1203	
3	C	335	
4	D	137	
5	E	215	

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Mol	Chain	Length	Quality of chain
6	F	155	
7	G	326	
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 34252 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 I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1484	Total	C	N	O	S	0	0	0
			11695	7388	2031	2213	63			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1176	Total	C	N	O	S	0	0	0
			9322	5898	1629	1745	50			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	304	Total	C	N	O	S	0	0	0
			2418	1536	414	460	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	59	Total	C	N	O	0	0	0
			466	292	80	94			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	12	SER	THR	conflict	UNP P50106

- 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	215	Total	C	N	O	S	0	0	0
			1759	1116	310	321	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			823	522	144	154	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	259	Total	C	N	O	S	0	0	0
			2052	1301	348	398	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1072	676	181	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	124	Total	C	N	O	S	0	0	0
			942	584	160	189	9			

- 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	69	Total	C	N	O	S	0	0	0
			569	362	101	100	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUB-UNIT RPAC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	103	Total	C	N	O	S	0	0	0
			810	506	132	167	5			

- 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	45	Total	C	N	O	S	0	0	0
			359	221	71	63	4			

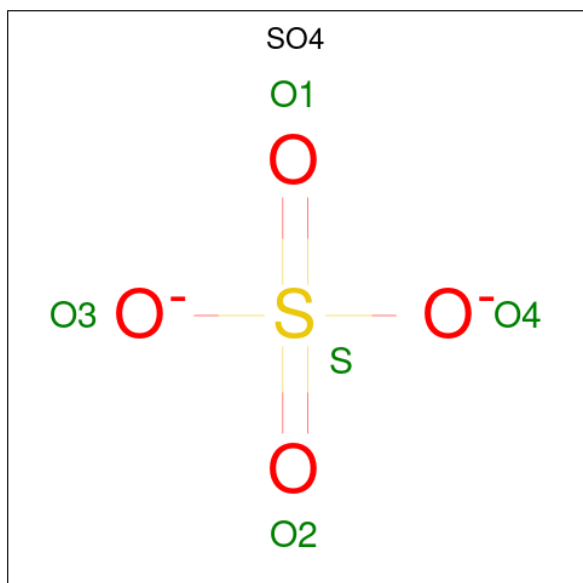
- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	105	Total	C	N	O	0	0	0
			831	528	137	166			

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	139	Total	C	N	O	S	0	0	0
			1103	706	179	214	4			

- Molecule 15 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	O	S	0	0
			5	4	1		
15	A	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		

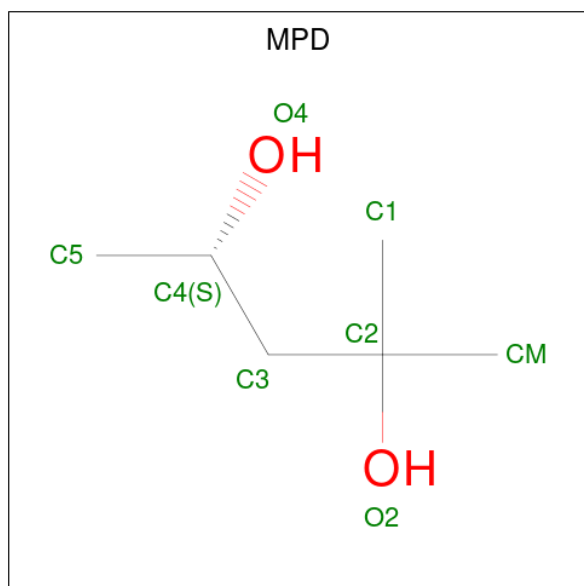
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 18 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).

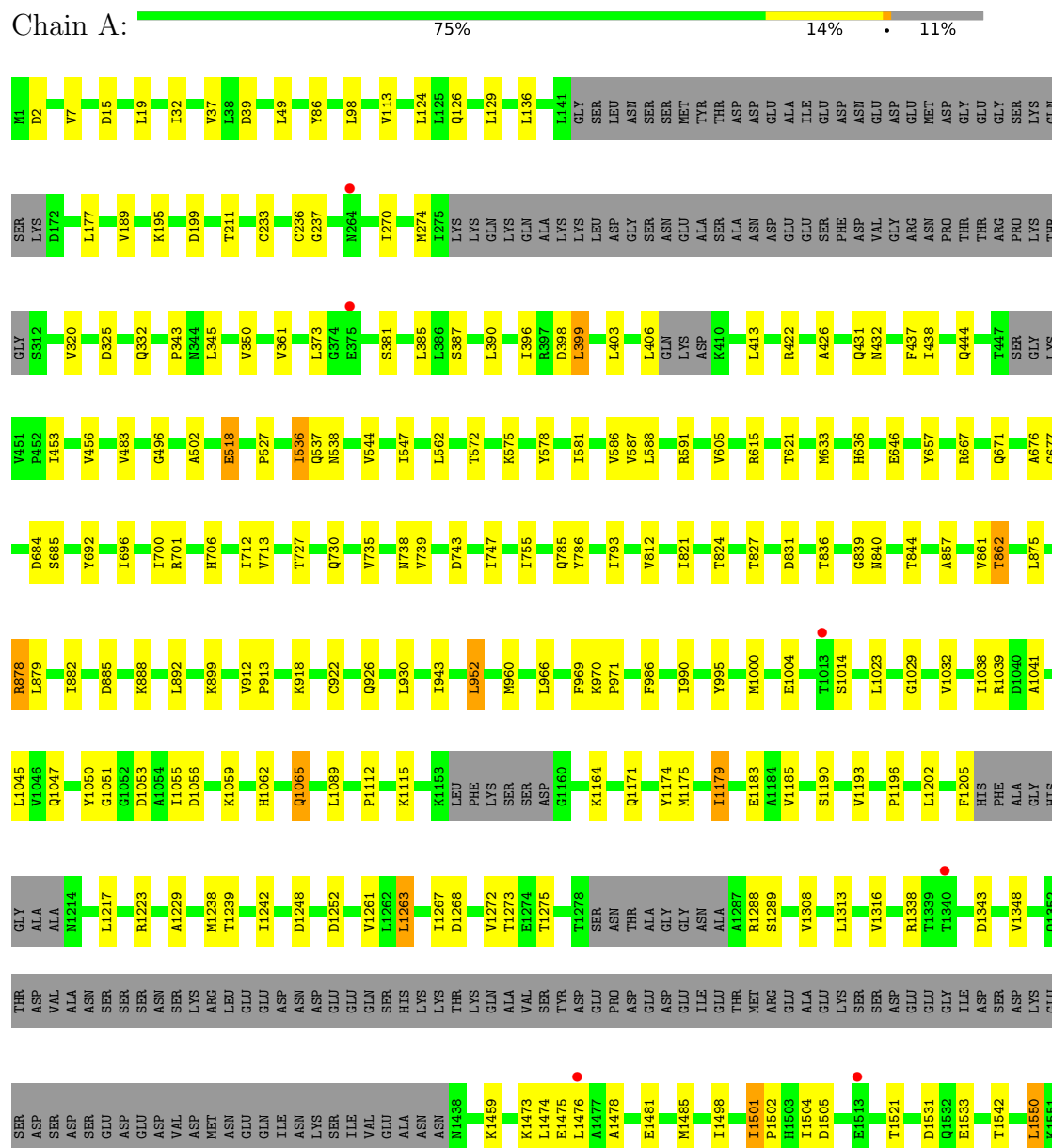


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	G	1	Total	C	O	0	0
			8	6	2		

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.

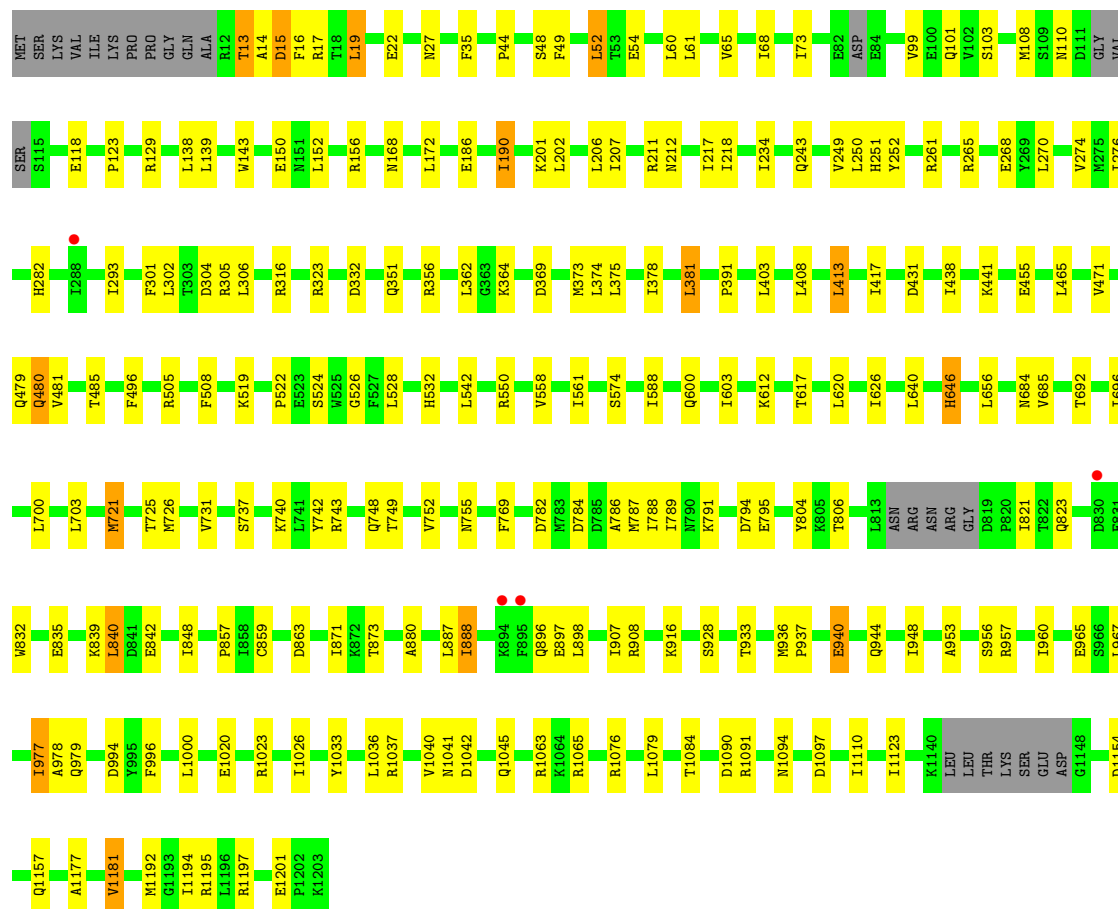
• Molecule 1: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190





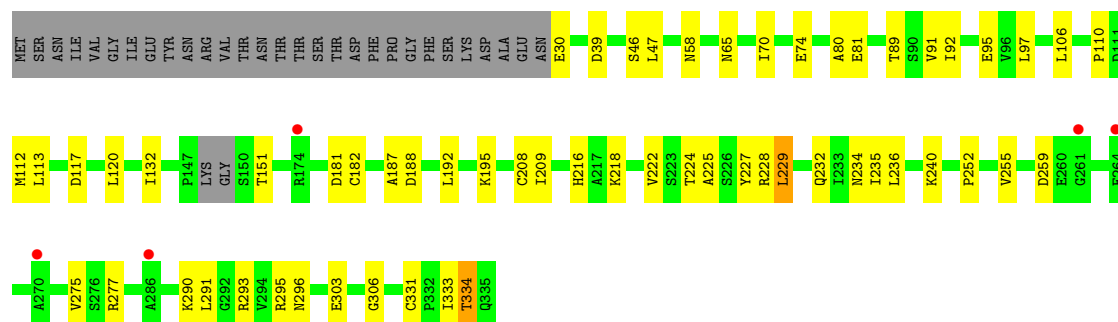
• Molecule 2: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135

Chain B: 80% 17% ..



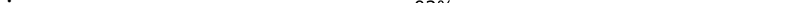
• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPA1

Chain C: 73% 17% 9%



• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

T80	L89	P100	PRO ALA GLN ASP PHE SER SER ALA ALA ALA PRO ILE ILE GLN VAL SER THR THR GLU LYS LYS GLU THR SER ILE ILE GLY VAL SER ALA THR GLY GLY LYS LYS THR THR PHE ASP ASP GLU	MET MET GLY SER ARG ARG THR GLY ASN ASN ASN S12 A13 T14 T15 L16 P19 V20 V21 I22 H23 A24 T25 Q26 L27 H30 M49 ILE ILE ASP SER SER THR THR MET MET ASN THR THR ILE SER SER GLY ASN ALA ALA ASP ALA ASP ALA ALA ALA VAL VAL ALA ASN THR THR SER SER LEU ASN TLE ASP
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- Chain E:  92% 8%


Category	Value	Color
M1	1	Green
E4	2	Green
N5	3	Green
E6	4	Green
N7	5	Green
M8	6	Green
N9	7	Green
K56	8	Green
D84	9	Orange
M93	10	Red
Q106	11	Green
F110	12	Red
A120	13	Green
L123	14	Green
T131	15	Yellow
V141	16	Green
V142	17	Green
H147	18	Green
E148	19	Green
L149	20	Yellow
E163	21	Green
R167	22	Red
L175	23	Yellow
K191	24	Green
M215	25	Green

- Chain F: 56% 8% 35%

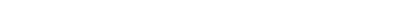
R92	SER
M103	ASP
V107	TYR
F108	GLU
V109	ALA
D110	PHE
L111	ASN
T115	GLY
K128	ASN
R135	ASN
S147	GLU
V148	PHE
E149	ASP
E150	VAL
L151	GLU
D154	HIS
LEU	PHE

- Chain G: 67% 12% . 21%

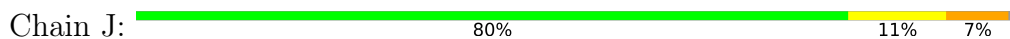
L249	V120
L250	V124
ASP	P127
ALA	E134
ASP	H144
GLU	E174
GLU	GLU
GLY	ASP
ASN	ALA
GLY	ASP
Y260	VAL
R264	TLE
A267	ASN
D303	THR
E316	ASP
SER	GLU
ASN	ASN
ASP	ASN
GLY	GLY
GLU	ASN
SER	ASN
SER	ASN
ASP	ASN
SER	LYS
ASP	ASP
	SER
	ASN
	GLY
	GLY
	SER
	ASN
	SER
	LEU
	GLY
	LYS
	PHE
	SER
	PHE
	GLY
	ASN
	ARG
	SER
	L214
	W217
	E223
	K228
	T246
	MET
	SER
	GLN
	VAL
	LYS
	ARG
	ALA
	N8
	A14
	I17
	K18
	K21
	K22
	N26
	E30
	K31
	N32
	C37
	I38
	V39
	I43
	A44
	L45
	V46
	V47
	A50
	P51
	L54
	P57
	V61
	Q64
	N75
	V81
	D93
	P94
	L96
	SER
	LYS
	GLU
	D99
	L104
	I107
	T109

- Chain H: 

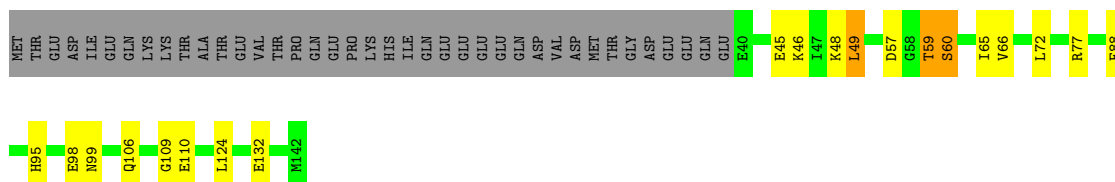
Category	Item	Value
MET	MET	0.00
	S3	0.00
	N3	0.00
S30	S30	0.00
	Q33	0.00
	D34	0.00
Q35	Q35	0.00
	C36	0.00
	L40	0.00
D53	D53	0.00
	N64	0.00
	LEU	0.00
GLU	GLU	0.00
	ASP	0.00
	THR	0.00
P80	P80	0.00
	ALA	0.00
	ASN	0.00
ASP	ASP	0.00
	SER	0.00
	SER	0.00
A75	A75	0.00
	T76	0.00
	R77	0.00
A84	A84	0.00
	L89	0.00
	Y93	0.00
K103	K103	0.00
	V107	0.00
	S108	0.00
K109	K109	0.00
	D110	0.00
	L111	0.00
Y115	Y115	0.00
	G119	0.00
	M123	0.00
K136	K136	0.00
	N139	0.00
	R145	0.00

- Chain I:  16% 80% 4%

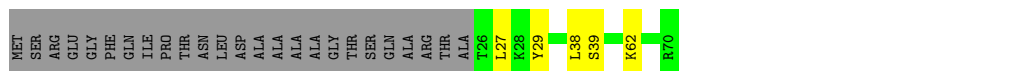
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



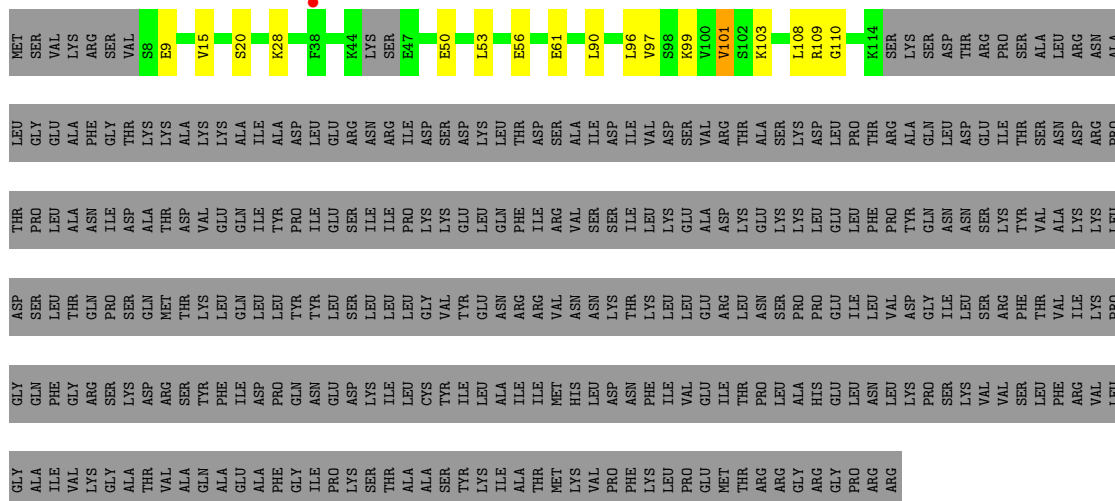
- Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2



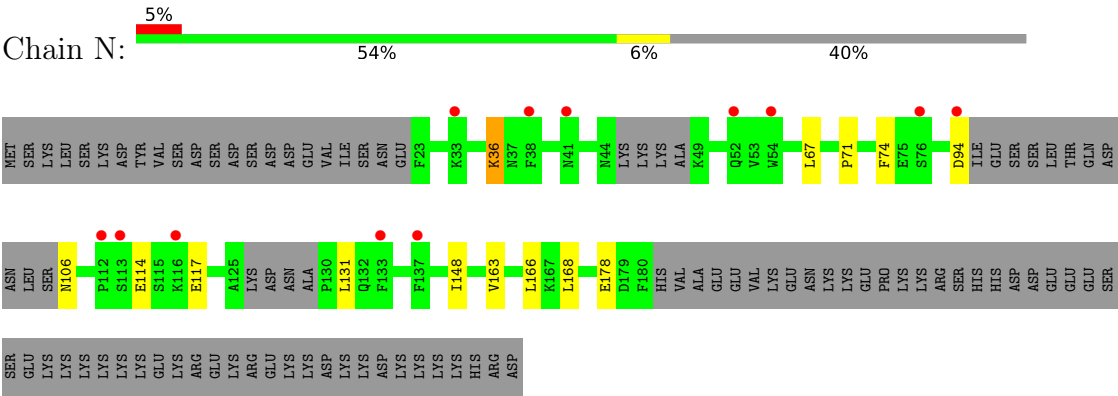
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



- Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49



● Molecule 14: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	400.53Å 140.22Å 122.89Å 90.00° 100.14° 90.00°	Depositor
Resolution (Å)	84.00 – 3.00 84.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (84.00-3.00) 99.1 (84.00-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.199 , 0.231 0.219 , 0.256	Depositor DCC
R_{free} test set	6617 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	93.9	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34252	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, MPD, SO4

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	0.39	0/11907	0.58	0/16088
2	B	0.39	0/9527	0.59	0/12879
3	C	0.39	0/2469	0.61	0/3347
4	D	0.39	0/472	0.53	0/639
5	E	0.40	0/1795	0.55	0/2416
6	F	0.39	0/838	0.54	0/1129
7	G	0.39	0/2094	0.58	0/2843
8	H	0.39	0/1090	0.57	0/1476
9	I	0.40	0/955	0.55	0/1288
10	J	0.40	0/578	0.62	0/775
11	K	0.39	0/821	0.60	0/1108
12	L	0.38	0/361	0.60	0/478
13	M	0.38	0/846	0.52	0/1136
14	N	0.37	0/1124	0.52	0/1512
All	All	0.39	0/34877	0.58	0/47114

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11695	0	11764	116	0
2	B	9322	0	9187	93	0
3	C	2418	0	2401	24	0
4	D	466	0	466	3	0
5	E	1759	0	1788	7	0
6	F	823	0	841	7	0
7	G	2052	0	2016	17	0
8	H	1072	0	1042	7	0
9	I	942	0	935	7	0
10	J	569	0	585	12	0
11	K	810	0	801	11	0
12	L	359	0	381	1	0
13	M	831	0	820	10	0
14	N	1103	0	1106	6	0
15	A	10	0	0	0	0
15	K	5	0	0	0	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	B	1	0	0	0	0
18	G	8	0	14	2	0
All	All	34252	0	34147	270	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 4.

The worst 5 of 270 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:712:ILE:H	11:K:106:GLN:HE22	1.22	0.88
2:B:99:VAL:HG21	2:B:417:ILE:HD11	1.55	0.87
2:B:16:PHE:HD2	2:B:978:ALA:HB2	1.51	0.75
1:A:86:TYR:H	1:A:431:GLN:HE22	1.36	0.72
1:A:824:THR:HG23	2:B:1023:ARG:HB2	1.71	0.71

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	1466/1664 (88%)	1393 (95%)	71 (5%)	2 (0%)	51	85
2	B	1166/1203 (97%)	1094 (94%)	70 (6%)	2 (0%)	47	82
3	C	300/335 (90%)	284 (95%)	16 (5%)	0	100	100
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
7	G	251/326 (77%)	234 (93%)	16 (6%)	1 (0%)	34	72
8	H	130/146 (89%)	119 (92%)	10 (8%)	1 (1%)	19	57
9	I	122/125 (98%)	109 (89%)	11 (9%)	2 (2%)	9	40
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	101/142 (71%)	96 (95%)	5 (5%)	0	100	100
12	L	43/70 (61%)	39 (91%)	4 (9%)	0	100	100
13	M	101/415 (24%)	93 (92%)	8 (8%)	0	100	100
14	N	131/233 (56%)	123 (94%)	8 (6%)	0	100	100
All	All	4244/5236 (81%)	3996 (94%)	240 (6%)	8 (0%)	47	82

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	GLY
2	B	532	HIS
2	B	1154	ASP
1	A	1338	ARG
8	H	84	ALA

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	1306/1465 (89%)	1234 (94%)	72 (6%)	21	57
2	B	1024/1053 (97%)	926 (90%)	98 (10%)	8	32
3	C	269/296 (91%)	244 (91%)	25 (9%)	9	33
4	D	56/116 (48%)	50 (89%)	6 (11%)	6	26
5	E	197/197 (100%)	192 (98%)	5 (2%)	47	79
6	F	90/137 (66%)	86 (96%)	4 (4%)	28	65
7	G	234/291 (80%)	219 (94%)	15 (6%)	17	51
8	H	116/128 (91%)	111 (96%)	5 (4%)	29	66
9	I	109/110 (99%)	98 (90%)	11 (10%)	7	29
10	J	64/65 (98%)	57 (89%)	7 (11%)	6	25
11	K	93/130 (72%)	84 (90%)	9 (10%)	8	31
12	L	40/57 (70%)	37 (92%)	3 (8%)	13	43
13	M	94/371 (25%)	89 (95%)	5 (5%)	22	58
14	N	128/220 (58%)	118 (92%)	10 (8%)	12	42
All	All	3820/4636 (82%)	3545 (93%)	275 (7%)	14	45

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	17	LEU
9	I	99	LEU
13	M	50	GLU
2	B	265	ARG
2	B	217	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	361	HIS

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Mol	Chain	Res	Type
9	I	21	ASN
2	B	755	ASN
8	H	35	GLN
13	M	16	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
15	SO4	A	2664	-	4,4,4	0.15	0	6,6,6	0.04	0
15	SO4	K	1143	-	4,4,4	0.13	0	6,6,6	0.08	0
18	MPD	G	1317	-	7,7,7	0.57	0	9,10,10	0.61	0
15	SO4	A	2665	-	4,4,4	0.14	0	6,6,6	0.08	0

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
18	MPD	G	1317	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	G	1317	MPD	O2-C2-C3-C4
18	G	1317	MPD	C2-C3-C4-C5
18	G	1317	MPD	C2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	1317	MPD	2	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1484/1664 (89%)	-0.26	6 (0%) 92 79	62, 98, 156, 225	0
2	B	1176/1203 (97%)	-0.26	4 (0%) 94 84	60, 107, 142, 176	0
3	C	304/335 (90%)	-0.26	5 (1%) 72 44	93, 122, 160, 197	0
4	D	59/137 (43%)	-0.38	0 100 100	82, 124, 147, 158	0
5	E	215/215 (100%)	-0.26	3 (1%) 75 49	78, 136, 183, 202	0
6	F	100/155 (64%)	-0.48	0 100 100	69, 86, 125, 142	0
7	G	259/326 (79%)	-0.22	1 (0%) 92 79	71, 121, 196, 231	0
8	H	134/146 (91%)	-0.18	3 (2%) 62 33	94, 123, 152, 165	0
9	I	124/125 (99%)	0.78	20 (16%) 1 0	116, 187, 215, 228	0
10	J	69/70 (98%)	-0.12	0 100 100	94, 112, 141, 161	0
11	K	103/142 (72%)	-0.53	0 100 100	82, 106, 136, 171	0
12	L	45/70 (64%)	-0.46	0 100 100	107, 128, 149, 153	0
13	M	105/415 (25%)	-0.01	1 (0%) 82 59	137, 229, 262, 267	0
14	N	139/233 (59%)	0.16	12 (8%) 10 3	111, 249, 267, 276	0
All	All	4316/5236 (82%)	-0.22	55 (1%) 77 51	60, 111, 202, 276	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	98	THR	8.2
9	I	99	LEU	7.0
9	I	118	GLY	6.9
9	I	105	ASP	5.9
9	I	87	PRO	5.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	SO4	A	2665	5/5	0.86	0.20	166,167,168,168	0
18	MPD	G	1317	8/8	0.86	0.37	99,101,103,104	0
15	SO4	A	2664	5/5	0.87	0.12	177,177,178,180	0
16	ZN	I	1127	1/1	0.88	0.11	153,153,153,153	0
17	MG	B	2204	1/1	0.92	0.90	89,89,89,89	0
15	SO4	K	1143	5/5	0.96	0.13	147,147,149,149	0
16	ZN	A	2666	1/1	0.99	0.14	108,108,108,108	0
16	ZN	L	1071	1/1	0.99	0.11	125,125,125,125	0
16	ZN	A	2667	1/1	0.99	0.14	95,95,95,95	0
16	ZN	I	1126	1/1	0.99	0.12	138,138,138,138	0
16	ZN	J	1070	1/1	1.00	0.23	104,104,104,104	0
16	ZN	B	2205	1/1	1.00	0.17	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.