



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:15 AM GMT

PDB ID : 2WAQ
Title : THE COMPLETE STRUCTURE OF THE ARCHAEAL 13-SUBUNIT DNA-DIRECTED RNA POLYMERASE
Authors : Korkhin, Y.; Unligil, U.M.; Littlefield, O.; Nelson, P.J.; Stuart, D.I.; Sigler, P.B.; Bell, S.D.; Abrescia, N.G.A.
Deposited on : 2009-02-11
Resolution : 3.35 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
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

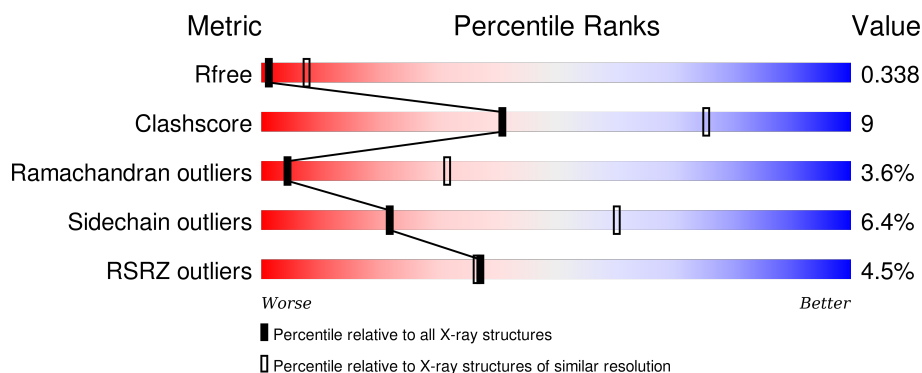
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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 ≥ 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	880	<div> <div>0%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>• •</div> </div> </div>
2	B	1131	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• •</div> </div> </div>
3	C	395	<div> <div>8%</div> <div> <div></div> <div>63%</div> <div>26%</div> <div>• 7%</div> </div> </div>
4	D	265	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>• •</div> </div> </div>
5	E	180	<div> <div>19%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	F	113	
7	G	132	
8	H	84	
9	K	95	
10	L	92	
11	N	66	
12	P	48	
13	Q	104	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 26471 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 RPO1N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6691	4256	1183	1226	26			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE RPO2 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1090	Total	C	N	O	S	0	0	0
			8652	5484	1534	1605	29			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE RPO1C SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	367	Total	C	N	O	S	0	0	0
			2833	1797	481	547	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE RPO3 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	260	Total	C	N	O	S	0	0	0
			2071	1332	334	392	13			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	174	Total	C	N	O	S	0	0	0
			1384	893	232	255	4			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	90	Total	C	N	O	S	0	0	0
			701	439	114	145	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE RPO8 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	113	Total	C	N	O	S	0	0	0
			901	572	152	173	4			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE RPO5 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	74	Total	C	N	O	S	0	0	0
			609	396	108	105				

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE RPO6 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	91	Total	C	N	O	S	0	0	0
			707	454	114	137	2			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	N	64	Total	C	N	O	S	0	0	0
			514	327	93	87	7			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Q	45	Total	C	N	O	S	0	0	0
			387	243	68	75	1			

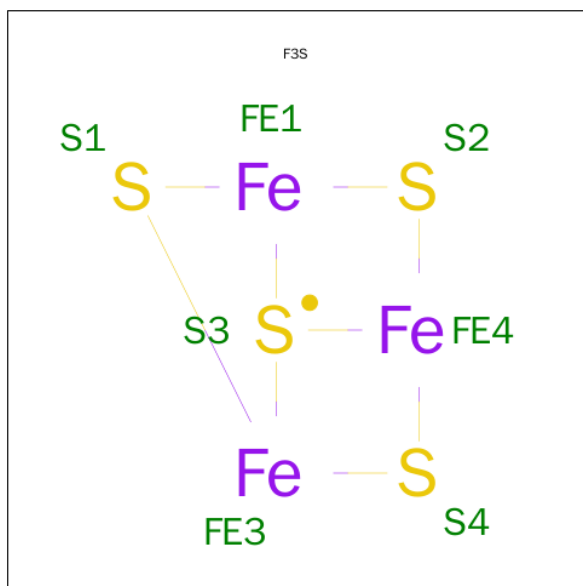
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	P	1	Total 1	Zn 1	0	0
14	B	3	Total 3	Zn 3	0	0
14	A	3	Total 3	Zn 3	0	0
14	C	1	Total 1	Zn 1	0	0
14	N	1	Total 1	Zn 1	0	0

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

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

- Molecule 16 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).

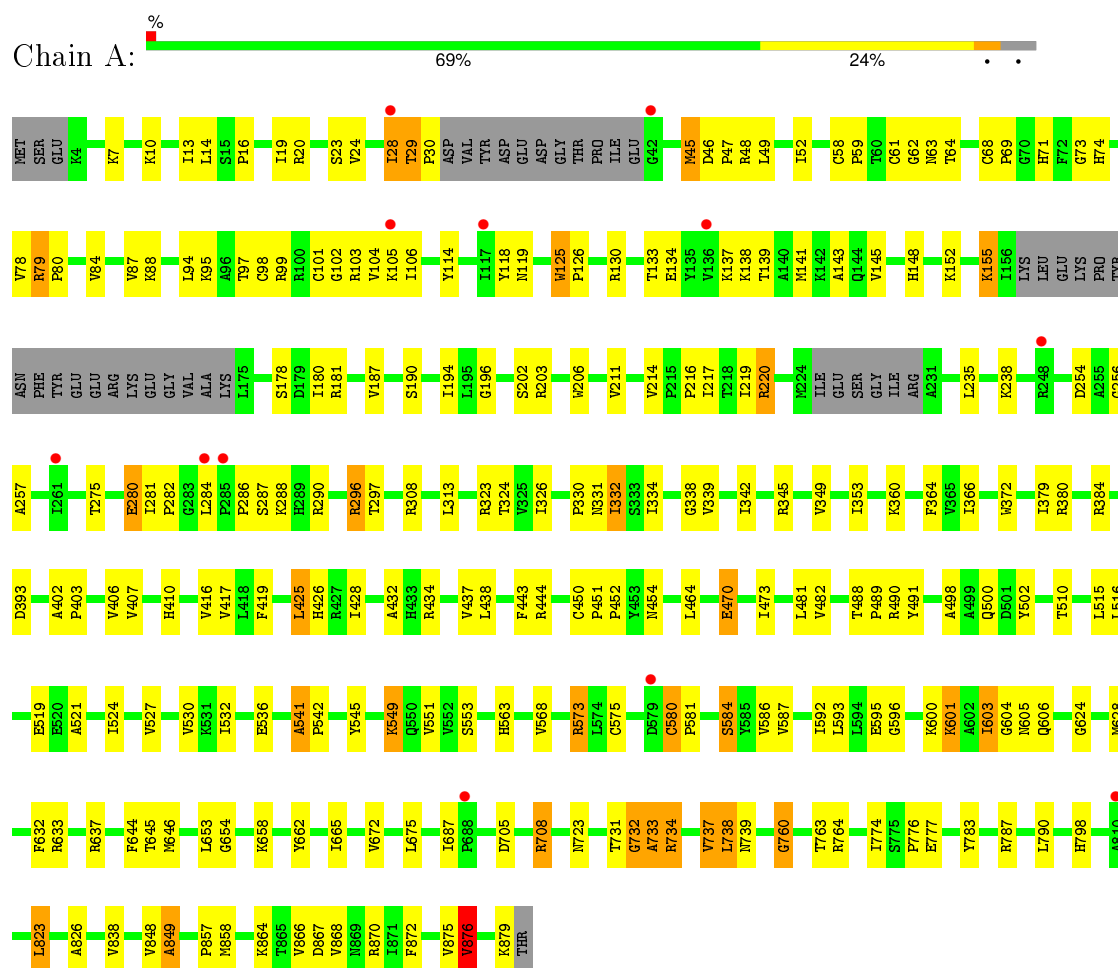


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total 7	Fe 3	S 4	0	0

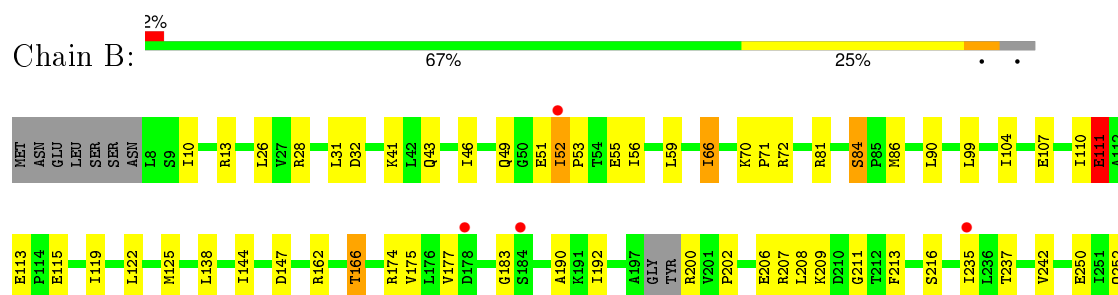
3 Residue-property plots

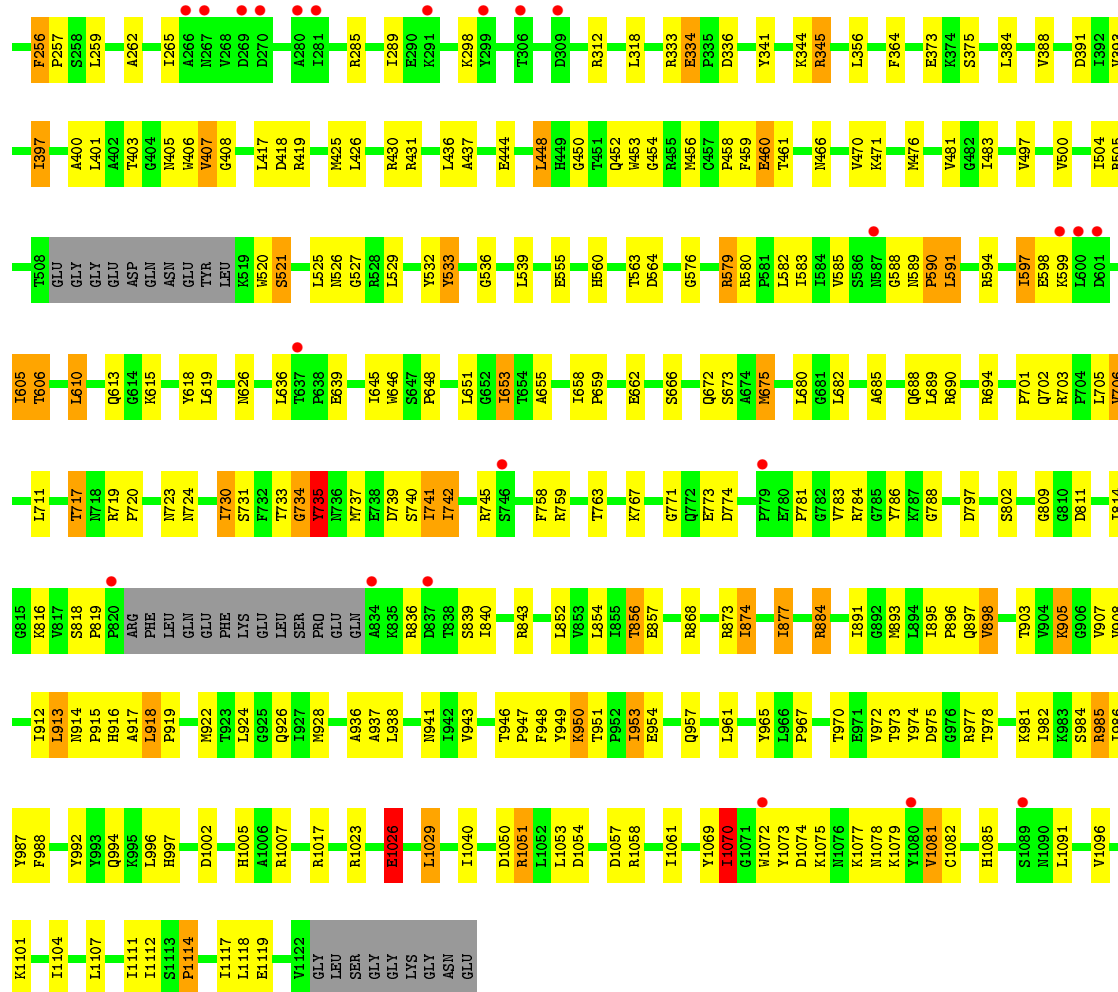
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 RPO1N SUBUNIT

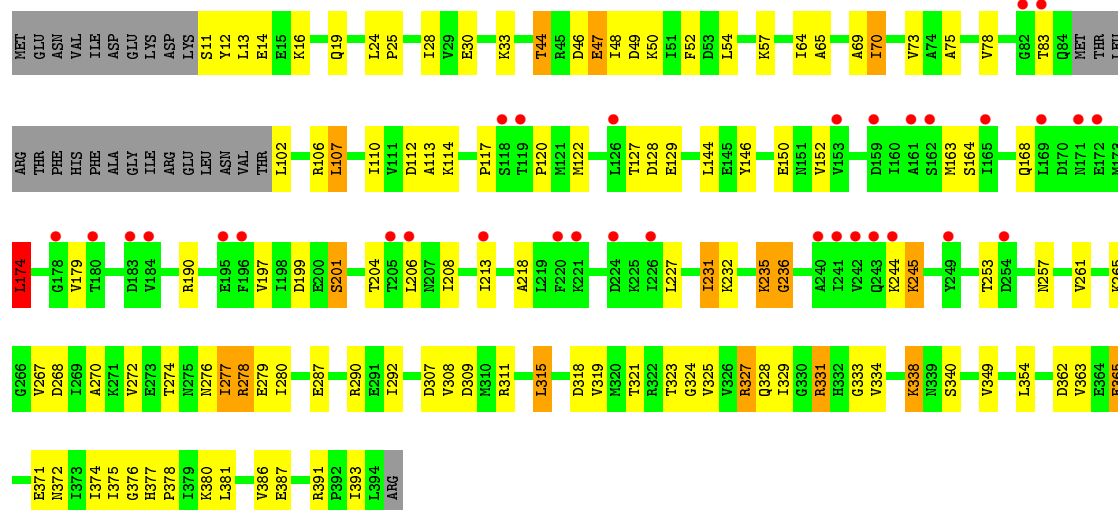


• Molecule 2: DNA-DIRECTED RNA POLYMERASE RPO2 SUBUNIT

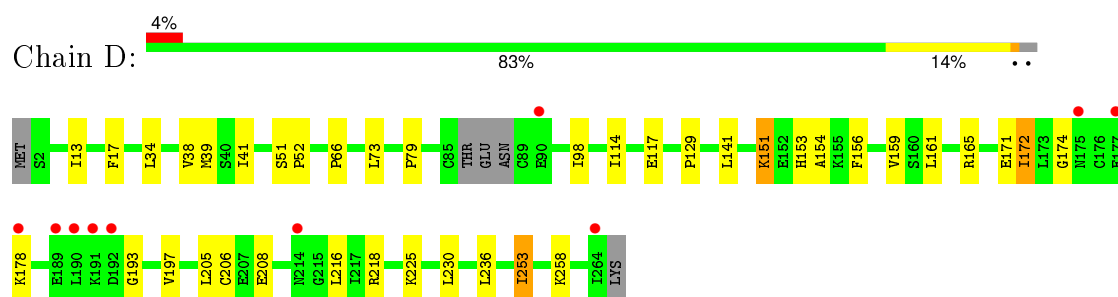




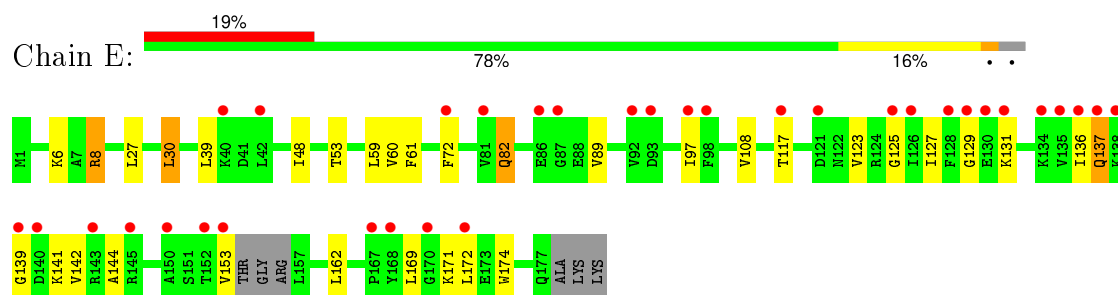
• Molecule 3: DNA-DIRECTED RNA POLYMERASE RPO1C SUBUNIT



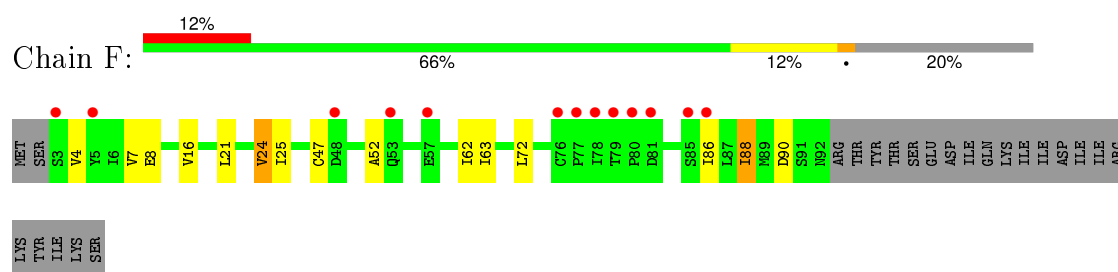
• Molecule 4: DNA-DIRECTED RNA POLYMERASE RPO3 SUBUNIT



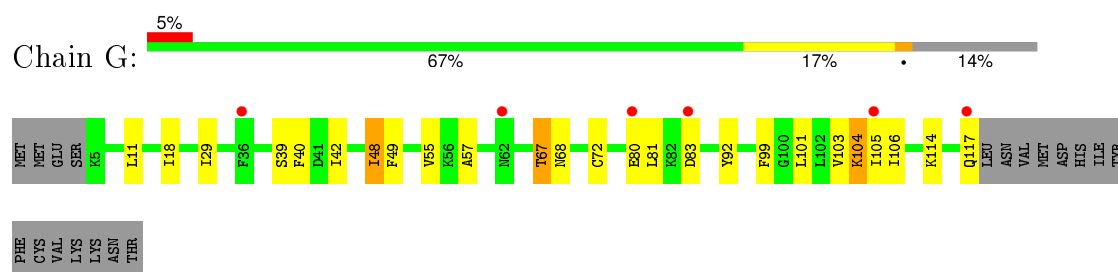
• Molecule 5: DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT



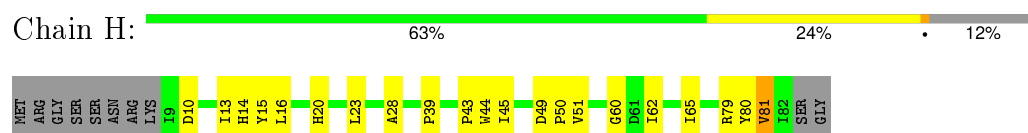
• Molecule 6: DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT



• Molecule 7: DNA-DIRECTED RNA POLYMERASE RPO8 SUBUNIT

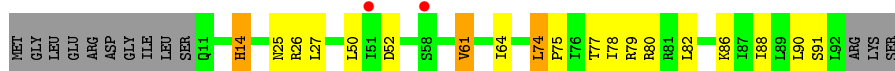


• Molecule 8: DNA-DIRECTED RNA POLYMERASE RPO5 SUBUNIT

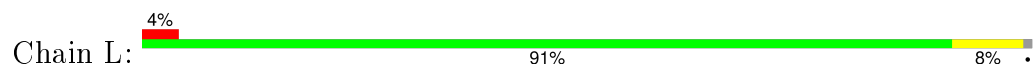


• Molecule 9: DNA-DIRECTED RNA POLYMERASE RPO6 SUBUNIT

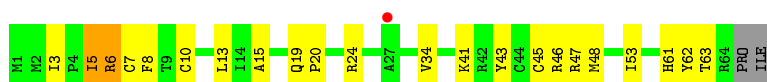




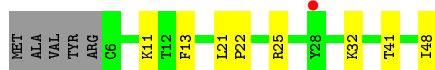
• Molecule 10: DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT



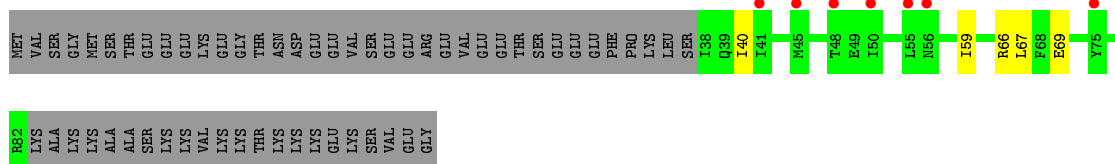
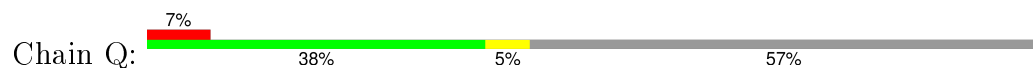
• Molecule 11: DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT



• Molecule 12: DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT



• Molecule 13: DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	193.50Å 212.62Å 129.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.78 – 3.35 42.78 – 3.20	Depositor EDS
% Data completeness (in resolution range)	77.0 (42.78-3.35) 72.5 (42.78-3.20)	Depositor EDS
R_{merge}	0.00	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.271 , 0.341 0.270 , 0.338	Depositor DCC
R_{free} test set	3012 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 31.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63954 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	26471	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, F3S, 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	0.33	0/6834	0.52	0/9247
2	B	0.32	0/8816	0.52	0/11926
3	C	0.34	0/2857	0.53	1/3847 (0.0%)
4	D	0.31	0/2106	0.50	0/2845
5	E	0.34	0/1405	0.47	0/1899
6	F	0.33	0/709	0.44	0/961
7	G	0.34	0/913	0.48	0/1224
8	H	0.34	0/623	0.52	0/845
9	K	0.33	0/667	0.51	0/903
10	L	0.29	0/717	0.47	0/968
11	N	0.33	0/524	0.45	0/706
12	P	0.37	0/354	0.51	0/475
13	Q	0.37	0/391	0.50	0/522
All	All	0.33	0/26916	0.51	1/36368 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	174	LEU	CA-CB-CG	5.09	127.01	115.30

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	6691	0	6758	138	0
2	B	8652	0	8795	191	0
3	C	2833	0	2992	76	0
4	D	2071	0	2116	24	0
5	E	1384	0	1444	15	0
6	F	701	0	708	7	0
7	G	901	0	912	13	0
8	H	609	0	640	12	0
9	K	658	0	692	10	0
10	L	707	0	739	3	0
11	N	514	0	528	15	0
12	P	346	0	375	4	0
13	Q	387	0	388	2	0
14	A	3	0	0	0	0
14	B	3	0	0	0	0
14	C	1	0	0	0	0
14	N	1	0	0	0	0
14	P	1	0	0	0	0
15	A	1	0	0	0	0
16	D	7	0	0	0	0
All	All	26471	0	27087	460	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 460 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:ASP:HA	1:A:870:ARG:HH22	1.14	1.12
2:B:110:ILE:HA	2:B:111:GLU:HB2	1.10	1.07
2:B:110:ILE:HA	2:B:111:GLU:CB	1.86	1.03
2:B:110:ILE:CA	2:B:111:GLU:HB2	1.96	0.95
2:B:953:ILE:HD13	2:B:953:ILE:H	1.35	0.92

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	833/880 (95%)	692 (83%)	112 (13%)	29 (4%)	4	32
2	B	1082/1131 (96%)	908 (84%)	127 (12%)	47 (4%)	3	26
3	C	363/395 (92%)	288 (79%)	61 (17%)	14 (4%)	4	29
4	D	256/265 (97%)	227 (89%)	25 (10%)	4 (2%)	12	49
5	E	170/180 (94%)	152 (89%)	16 (9%)	2 (1%)	16	56
6	F	88/113 (78%)	74 (84%)	11 (12%)	3 (3%)	5	33
7	G	111/132 (84%)	96 (86%)	13 (12%)	2 (2%)	11	47
8	H	72/84 (86%)	59 (82%)	8 (11%)	5 (7%)	1	12
9	K	80/95 (84%)	69 (86%)	7 (9%)	4 (5%)	3	21
10	L	89/92 (97%)	79 (89%)	8 (9%)	2 (2%)	8	43
11	N	62/66 (94%)	50 (81%)	10 (16%)	2 (3%)	5	34
12	P	41/48 (85%)	32 (78%)	7 (17%)	2 (5%)	3	22
13	Q	43/104 (41%)	36 (84%)	6 (14%)	1 (2%)	8	42
All	All	3290/3585 (92%)	2762 (84%)	411 (12%)	117 (4%)	4	31

5 of 117 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	734	ARG
1	A	737	VAL
2	B	28	ARG
2	B	111	GLU

5.3.2 Protein sidechains [i](#)

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	729/766 (95%)	680 (93%)	49 (7%)	20	59
2	B	941/975 (96%)	866 (92%)	75 (8%)	15	50
3	C	315/341 (92%)	289 (92%)	26 (8%)	14	48
4	D	233/238 (98%)	226 (97%)	7 (3%)	48	80
5	E	154/158 (98%)	145 (94%)	9 (6%)	25	64
6	F	84/107 (78%)	79 (94%)	5 (6%)	24	62
7	G	106/125 (85%)	102 (96%)	4 (4%)	40	75
8	H	67/75 (89%)	66 (98%)	1 (2%)	72	89
9	K	72/83 (87%)	70 (97%)	2 (3%)	51	82
10	L	79/80 (99%)	78 (99%)	1 (1%)	76	90
11	N	58/60 (97%)	53 (91%)	5 (9%)	13	46
12	P	39/43 (91%)	38 (97%)	1 (3%)	54	83
13	Q	43/96 (45%)	41 (95%)	2 (5%)	32	71
All	All	2920/3147 (93%)	2733 (94%)	187 (6%)	22	60

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	591	LEU
2	B	854	LEU
7	G	67	THR
2	B	613	GLN
2	B	717	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	565	GLN
2	B	442	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 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	F3S	D	1001	4	0,9,9	0.00	-	0,15,15	0.00	-

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	F3S	D	1001	4	-	0/0/24/24	0/0/3/3

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, 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	841/880 (95%)	-0.05	12 (1%) 78 79	40, 69, 119, 184	0
2	B	1090/1131 (96%)	0.08	27 (2%) 61 60	43, 71, 136, 201	0
3	C	367/395 (92%)	0.46	33 (8%) 12 12	48, 81, 151, 202	0
4	D	260/265 (98%)	0.26	10 (3%) 44 44	66, 93, 131, 200	0
5	E	174/180 (96%)	0.96	34 (19%) 1 2	58, 144, 188, 210	0
6	F	90/113 (79%)	0.83	13 (14%) 3 3	95, 175, 222, 230	0
7	G	113/132 (85%)	0.37	6 (5%) 30 30	66, 105, 147, 156	0
8	H	74/84 (88%)	0.02	0 100 100	60, 84, 103, 108	0
9	K	82/95 (86%)	0.01	2 (2%) 62 62	50, 67, 90, 99	0
10	L	91/92 (98%)	0.17	4 (4%) 38 37	51, 90, 121, 140	0
11	N	64/66 (96%)	0.00	1 (1%) 74 75	60, 71, 113, 140	0
12	P	43/48 (89%)	0.17	1 (2%) 64 64	72, 93, 135, 146	0
13	Q	45/104 (43%)	1.00	7 (15%) 3 3	83, 121, 150, 169	0
All	All	3334/3585 (92%)	0.19	150 (4%) 37 36	40, 81, 156, 230	0

The worst 5 of 150 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	153	VAL	5.8
5	E	135	VAL	5.7
2	B	267	ASN	5.3
5	E	87	GLY	5.0
6	F	81	ASP	4.9

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

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

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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
14	ZN	B	1400	1/1	0.98	0.21	-0.39	62,62,62,62	0
16	F3S	D	1001	7/7	0.98	0.16	-1.01	67,67,67,67	0
14	ZN	P	50	1/1	0.97	0.08	-1.16	71,71,71,71	0
14	ZN	B	1300	1/1	0.99	0.06	-1.70	62,62,62,62	0
14	ZN	A	1300	1/1	1.00	0.04	-1.86	58,58,58,58	0
14	ZN	N	100	1/1	0.97	0.14	-2.03	63,63,63,63	0
14	ZN	A	1350	1/1	0.97	0.07	-2.44	58,58,58,58	0
14	ZN	C	1000	1/1	0.98	0.05	-	58,58,58,58	0
14	ZN	B	1500	1/1	0.99	0.08	-	62,62,62,62	0
15	MG	A	1400	1/1	0.92	0.36	-	58,58,58,58	0
14	ZN	A	1360	1/1	0.98	0.20	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.