



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:46 PM UTC

PDB ID : 5W1S / pdb_00005w1s
Title : X-ray crystal structure of Escherichia coli RNA polymerase and TraR complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2017-06-04
Resolution : 3.81 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

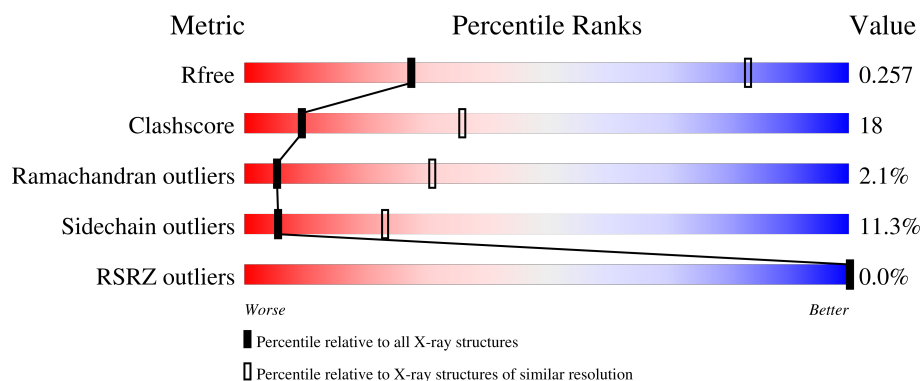
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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.



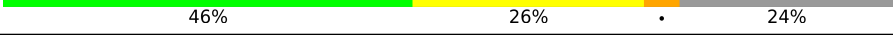
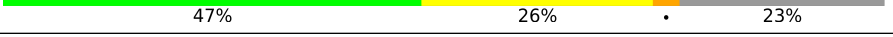
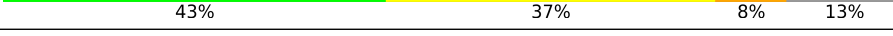
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	329	45% 39% 12% ••
1	B	329	39% 24% • 34%
1	G	329	36% 29% 5% 31%
1	H	329	41% 22% • 34%
2	C	1342	56% 38% 6%

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Mol	Chain	Length	Quality of chain
2	I	1342	 60%35%5%
3	D	1407	 46%32%5%17%
3	J	1407	 46%31%5%18%
4	E	91	 62%27%9%.
4	K	91	 46%31%.21%
5	F	613	 46%26%.24%
5	L	613	 47%26%.23%
6	M	79	 49%33%5%.11%
6	N	79	 43%37%8%13%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56825 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10564	6628	1838	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1173	Total	C	N	O	S	0	0	0
			9095	5718	1628	1703	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	72	Total	C	N	O	S	0	0	0
			573	350	110	112	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is a protein called Protein TraR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	70	Total	C	N	O	S	0	0	0
			557	346	103	103	5			
6	N	69	Total	C	N	O	S	0	0	0
			552	343	102	102	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	74	HIS	-	expression tag	UNP P41065
M	75	HIS	-	expression tag	UNP P41065
M	76	HIS	-	expression tag	UNP P41065
M	77	HIS	-	expression tag	UNP P41065
M	78	HIS	-	expression tag	UNP P41065
M	79	HIS	-	expression tag	UNP P41065
N	74	HIS	-	expression tag	UNP P41065
N	75	HIS	-	expression tag	UNP P41065
N	76	HIS	-	expression tag	UNP P41065
N	77	HIS	-	expression tag	UNP P41065
N	78	HIS	-	expression tag	UNP P41065
N	79	HIS	-	expression tag	UNP P41065

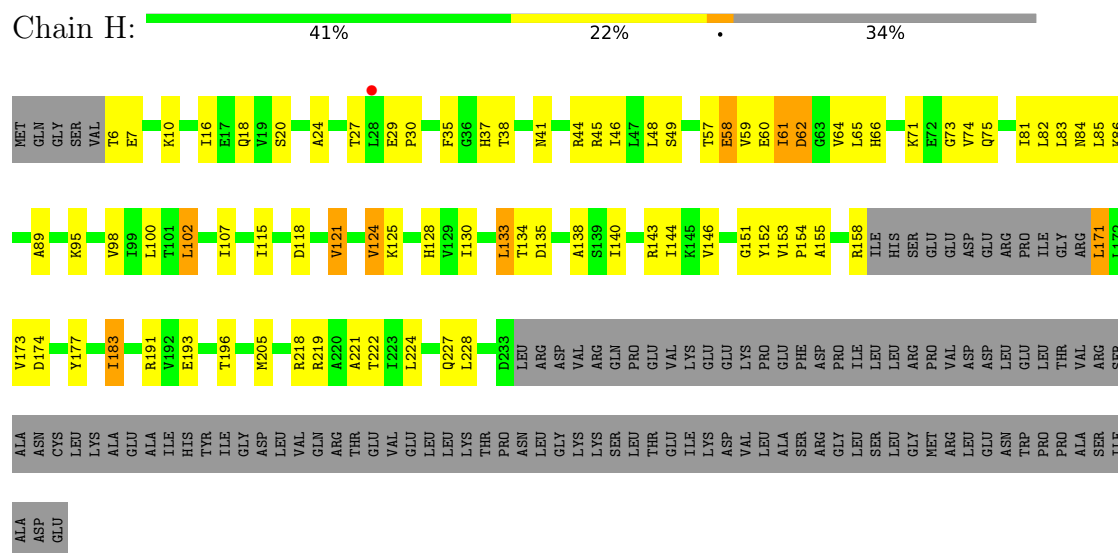
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	J	1	Total	Mg	0	0
			1	1		

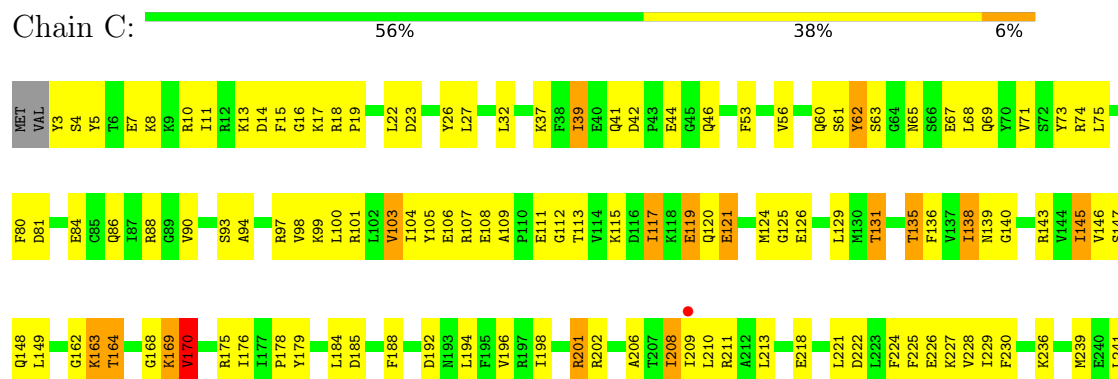
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

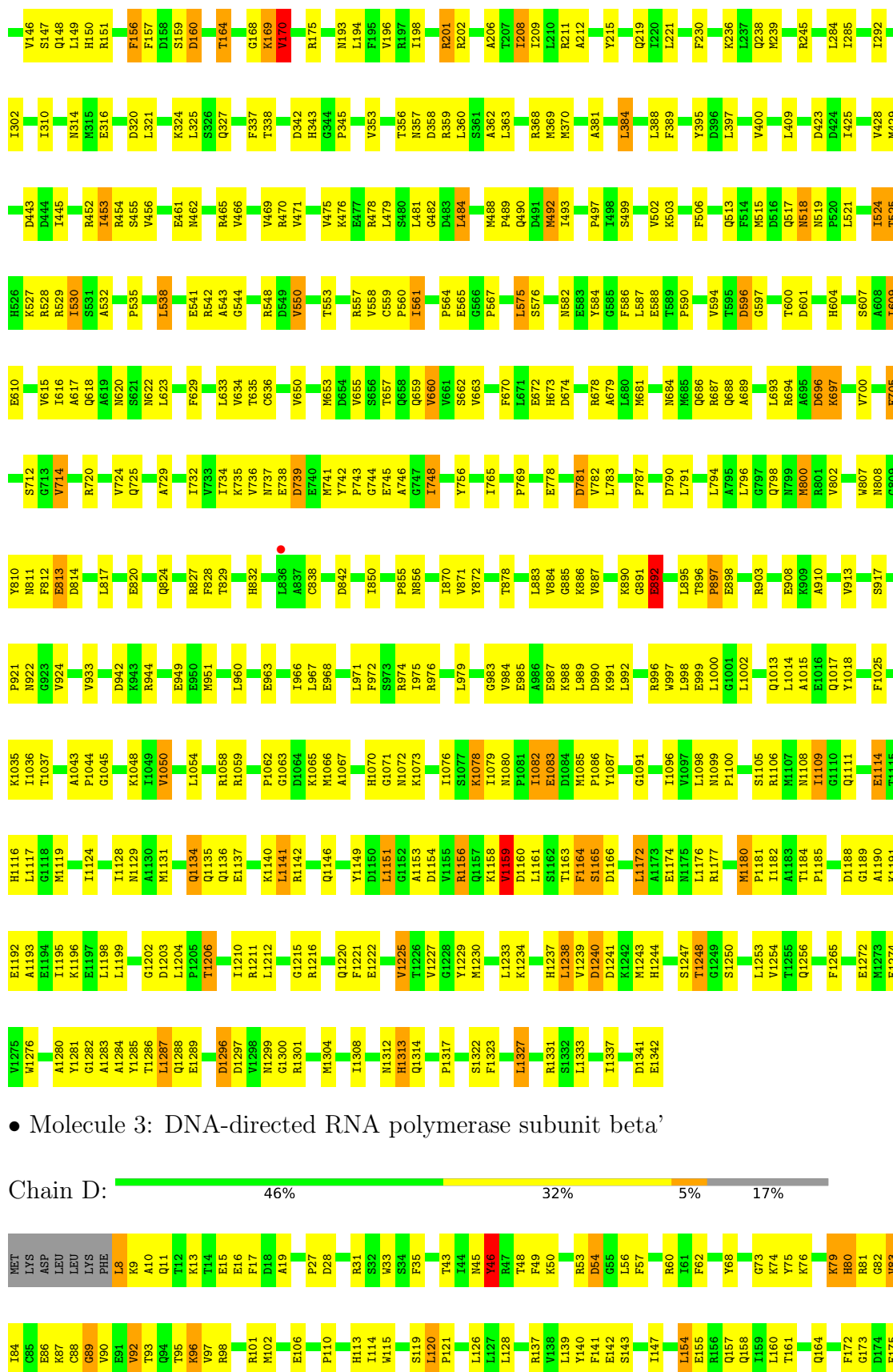
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total 2	Zn 2	0	0
8	J	2	Total 2	Zn 2	0	0
8	M	1	Total 1	Zn 1	0	0
8	N	1	Total 1	Zn 1	0	0

- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta

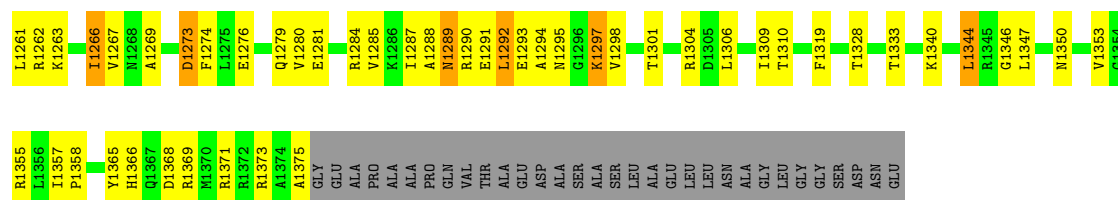




GLY	L1314	I1233	I1155	VAL	ASP	SER	R798	R709	Y609	D505	P427	Y349	T262	F176
LEU	S1318	E1236	I1156	ASP	PRO	ASN	R801	D710	Y506	V506	T428	I355	S263	M180
GLY	F1319	V1237	A1157	ALA	HIS	VAL	Q805	Q711	L614	D264	H430	T356	L265	L188
SER	I1320	Q1238	E1158	GLN	THR	LYS	T810	Q716	P616	L510	R431	V357	N266	L189
ASP	S1324	Y1241	I1159	ASN	PRO	VAL	E811	V717	A621	Y512	L432	P359	L268	K190
ASN	Q1325	R1242	G1161	VAL	ILE	ASN	D812	S718	A633	M513	G433	R362	S191	M192
GLU	F1326	L1243	I1162	VAL	THR	SER	D813	F719	M625	T514	I434	N274	D193	L194
	T1329	V1246	S1164	PRO	GLU	SER	H817	W721	A633	R515	F437	R363	R275	
	L1332	G1247	F1165	GLY	VAL	LYS	T820	S721	M625	D516	E438	H364	L279	
	T1333	I1248	G1166	THR	SER	LYS	H821	W722	A633	C517	P439	Q365	L282	E197
	R1341	K1251	K1167	ASP	PHE	VAL	R822	W724	S638	V518	I442	G367	C198	
	D1342	V1255	T1169	MET	VAL	ILE	R823	W725	S639	V526	K445	M372	L282	
	E1343	I1256	G1170	PRO	ARG	THR	H824	R731	V639	L527	A446	A373	P288	L201
	L1344	V1257	G1171	ALA	PHE	SER	R825	Q732	G640	T528	I447	L374	I291	R202
	R1345	M1260	R1173	TYR	THR	ARG	R826	S733	I641	G529	Q448	E375	V292	E203
	G1346	L1261	R1174	PHE	ASP	ASN	R827	A734	P647	E532	L449	L376	L205	L206
	L1347	L1261	G1175	LEU	THR	THR	G828	Q736	E658	A534	H450	F377	E295	E207
	V1353	A1264	I1177	LEU	GLY	LEU	R831	W737	A659	R535	P451	P379	K296	
	G1354	T1265	T1178	GLY	GLN	LYS	R832	Q738	E660	L536	V453	M298	K297	S210
	R1355	I1266	D1181	ALA	THR	ILE	R833	Q739	V661	A542	G454	Y382	D304	K213
	L1356	G1270	G1182	ILE	THR	ASP	R834	L740	I664	H545	D460	G385	A305	K214
	P1358	S1271	D1184	VAL	ARG	GLU	L835	A741	F668	R548	D462	L386	L306	K215
	T1361	P1272	P1185	LEU	GLN	PHE	R839	W743	F668	V548	G463	E386	L307	I221
	H1366	D1273	Y1186	GLU	THR	ARG	R842	G745	L672	K549	D464	L387	G310	K222
	R1373	L1275	M1189	ASP	ASP	THR	R843	L746	R678	V550	Q465	T392	R311	L223
	G1376	E1276	K1192	LEU	GLU	LYS	T844	W750	V679	R551	M466	T393	R312	L224
GLU	ALA	Q1279	R1194	GLN	THR	LYS	D847	F754	N680	E556	L472	K395	G313	E225
ALA	PRO	E1281	F1199	THR	GLY	TYR	R848	T754	K681	D558	T473	K398	I394	A226
ALA	ALA	S1283	G1201	SER	LEU	VAL	R850	P758	V686	A559	L474	K399	A315	F227
ALA	PRO	R1284	E1202	ALA	SER	VAL	T853	R764	I685	E562	A476	M400	I316	S230
PRO	PRO	V1285	R1203	ALA	LEU	PRO	R857	L770	A688	L569	Q477	E405	N320	P234
GLN	VAL	K1286	R1206	ALA	SER	ALA	P859	Q771	A689	K570	L478	A406	R322	E235
THR	THR	M1289	R1206	ALA	ALA	LYS	R860	Y772	N690	D571	M484	V407	P323	L238
THR	THR	A1294	S1211	GLN	GLU	GLY	L863	T776	V693	T573	T487	V408	L324	L239
ASP	ASP	A1294	E1215	GLU	ARG	ASP	L864	R780	K694	R576	N488	M330	K325	V241
ALA	ALA	K1297	I1220	GLY	THR	GLY	R865	K781	K695	R576	N489	I331	P246	P247
SER	SER	V1298	L1221	GLY	ALA	GLN	E866	G782	A696	L579	I490	Q335	D248	
ALA	ALA	G1299	R1222	VAL	VAL	VAL	E866	G782	M697	M580	L491	Q336	P251	L252
SER	SER	A1300	L1223	GLY	GLY	GLY	L872	T786	M698	M581	E418	R337	P254	P255
LEU	LEU	T1301	L1223	ASP	ASP	ASP	L872	T786	L701	Q594	A494	E418	L342	L252
ALA	ALA	R1304	H1227	PRO	ARG	THR	N875	K789	Q702	G496	N495	E418	L343	P254
GLU	GLU	R1304	H1228	THR	THR	THR	N876	T790	G497	K598	E497	E418	L343	L255
LEU	LEU	I1309	T1229	ALA	VAL	VAL	N877	T790	T705	I601	I500	E418	K345	K346
LEU	LEU	T1310	T1230	ALA	ALA	ALA	N882	S793	V705	I601	I500	E418	R346	V347
ASN	ASN			LEU	LEU	LEU	R883	T797	T705	I601	I500	E418	R346	R259
ALA	ALA			TRP	TRP	TRP								D348

- Molecule 3: DNA-directed RNA polymerase subunit beta'





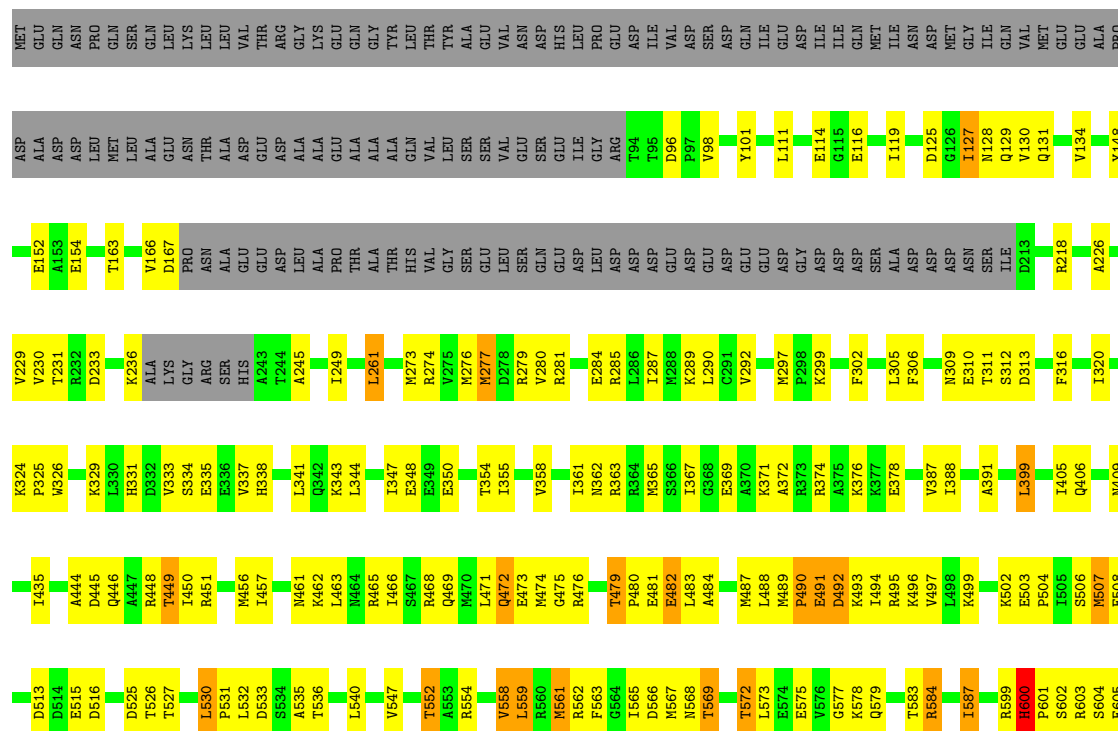
• Molecule 4: DNA-directed RNA polymerase subunit omega

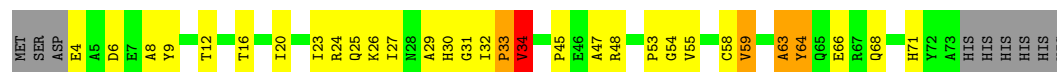
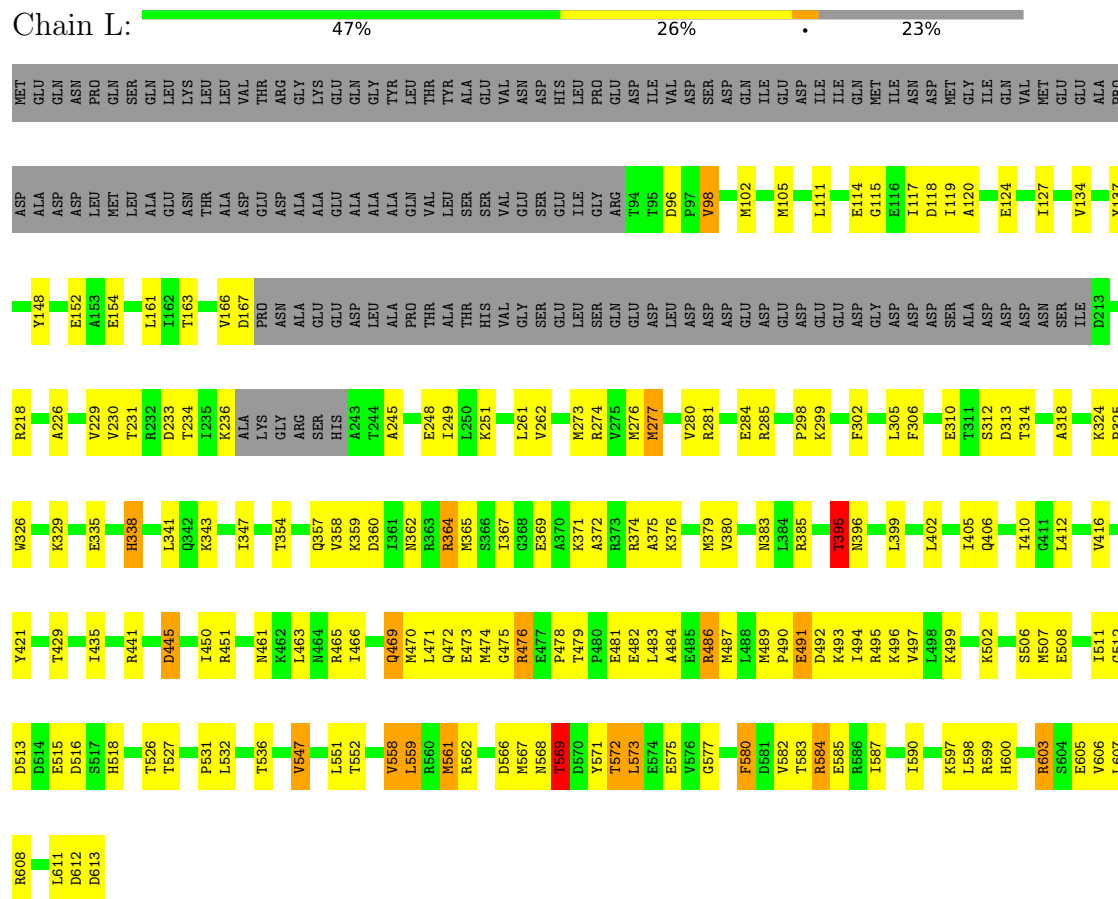


• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.48Å 206.04Å 310.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.81 49.84 – 3.81	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.84-3.81) 86.4 (49.84-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.60 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.208 , 0.262 0.212 , 0.257	Depositor DCC
R_{free} test set	2000 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	156.4	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 217.7	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	0.95	EDS
Total number of atoms	56825	wwPDB-VP
Average B, all atoms (Å ²)	239.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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

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	0.24	0/2524	0.74	2/3421 (0.1%)
1	B	0.22	0/1697	0.69	0/2300
1	G	0.22	0/1777	0.63	0/2408
1	H	0.25	0/1681	0.71	3/2278 (0.1%)
2	C	0.24	0/10733	0.67	0/14482
2	I	0.22	0/10735	0.63	3/14484 (0.0%)
3	D	0.24	0/9235	0.69	4/12472 (0.0%)
3	J	0.22	0/9140	0.65	0/12341
4	E	0.21	0/693	0.61	0/935
4	K	0.19	0/575	0.38	0/774
5	F	0.21	0/3864	0.63	0/5194
5	L	0.20	0/3872	0.61	0/5205
6	M	0.29	0/567	0.76	1/766 (0.1%)
6	N	0.30	0/562	0.75	0/759
All	All	0.23	0/57655	0.66	13/77819 (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
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	2
5	F	0	1
All	All	0	9

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	PRO	CA-C-N	6.17	132.81	121.70
1	A	323	PRO	C-N-CA	6.17	132.81	121.70
1	H	29	GLU	C-N-CD	-5.98	107.44	120.60
3	D	746	LEU	CA-C-N	-5.71	112.79	122.67
3	D	746	LEU	C-N-CA	-5.71	112.79	122.67

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
5	F	600	HIS	Peptide

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	2490	0	2542	121	0
1	B	1677	0	1703	61	0
1	G	1755	0	1773	80	0
1	H	1662	0	1687	61	0
2	C	10564	0	10571	441	0
2	I	10566	0	10576	365	0
3	D	9095	0	9222	397	0
3	J	9001	0	9167	385	0
4	E	691	0	695	26	0
4	K	573	0	587	20	0
5	F	3813	0	3880	129	0
5	L	3821	0	3884	116	0
6	M	557	0	547	31	0
6	N	552	0	542	44	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	2	0	0	0	0
8	J	2	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
All	All	56825	0	57376	2038	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 18.

The worst 5 of 2038 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:45:ARG:HG2	1:B:38:THR:HB	1.42	1.02
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.42	1.01
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.38	1.00
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.44	0.99
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.46	0.96

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	317/329 (96%)	247 (78%)	52 (16%)	18 (6%)	1	15
1	B	213/329 (65%)	194 (91%)	15 (7%)	4 (2%)	6	32
1	G	225/329 (68%)	199 (88%)	20 (9%)	6 (3%)	4	27
1	H	212/329 (64%)	196 (92%)	12 (6%)	4 (2%)	6	32
2	C	1338/1342 (100%)	1201 (90%)	118 (9%)	19 (1%)	9	37
2	I	1338/1342 (100%)	1197 (90%)	120 (9%)	21 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1169/1407 (83%)	1038 (89%)	104 (9%)	27 (2%)	5	30
3	J	1151/1407 (82%)	1026 (89%)	99 (9%)	26 (2%)	5	30
4	E	87/91 (96%)	80 (92%)	5 (6%)	2 (2%)	5	30
4	K	70/91 (77%)	61 (87%)	8 (11%)	1 (1%)	9	37
5	F	462/613 (75%)	426 (92%)	28 (6%)	8 (2%)	7	34
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	7	34
6	M	68/79 (86%)	56 (82%)	7 (10%)	5 (7%)	1	11
6	N	67/79 (85%)	56 (84%)	6 (9%)	5 (8%)	1	11
All	All	7180/8380 (86%)	6402 (89%)	624 (9%)	154 (2%)	5	31

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	162	GLU
1	A	167	PRO

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	278/286 (97%)	222 (80%)	56 (20%)	1	8
1	B	186/286 (65%)	163 (88%)	23 (12%)	4	21
1	G	193/286 (68%)	162 (84%)	31 (16%)	2	14
1	H	183/286 (64%)	167 (91%)	16 (9%)	9	33
2	C	1154/1157 (100%)	1022 (89%)	132 (11%)	5	23
2	I	1154/1157 (100%)	1034 (90%)	120 (10%)	7	26
3	D	962/1168 (82%)	857 (89%)	105 (11%)	6	25
3	J	960/1168 (82%)	857 (89%)	103 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	21
4	K	62/75 (83%)	56 (90%)	6 (10%)	8	29
5	F	417/540 (77%)	374 (90%)	43 (10%)	7	27
5	L	418/540 (77%)	373 (89%)	45 (11%)	6	25
6	M	59/68 (87%)	55 (93%)	4 (7%)	14	40
6	N	59/68 (87%)	55 (93%)	4 (7%)	14	40
All	All	6157/7160 (86%)	5460 (89%)	697 (11%)	5	23

5 of 697 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	542	ARG
3	J	505	ASP
2	I	635	THR
2	I	538	LEU
2	I	1225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	139	ASN
2	I	1146	GLN
5	L	446	GLN
2	I	343	HIS
2	I	766	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9
1	A	319/329 (96%)	-0.93	0	100	100	152, 220, 344, 468	0
1	B	217/329 (65%)	-0.94	0	100	100	140, 238, 332, 383	0
1	G	227/329 (68%)	-0.98	0	100	100	204, 264, 358, 416	0
1	H	216/329 (65%)	-0.86	1 (0%)	87	71	204, 298, 387, 432	0
2	C	1340/1342 (99%)	-0.90	1 (0%)	92	87	104, 197, 403, 528	0
2	I	1340/1342 (99%)	-0.95	1 (0%)	92	87	127, 264, 377, 485	0
3	D	1173/1407 (83%)	-0.87	0	100	100	101, 174, 294, 419	0
3	J	1155/1407 (82%)	-0.95	0	100	100	125, 213, 329, 431	0
4	E	89/91 (97%)	-1.06	0	100	100	160, 216, 269, 393	0
4	K	72/91 (79%)	-1.03	0	100	100	227, 323, 429, 470	0
5	F	468/613 (76%)	-0.93	0	100	100	137, 239, 365, 477	0
5	L	469/613 (76%)	-1.01	0	100	100	162, 251, 379, 489	0
6	M	70/79 (88%)	-0.91	0	100	100	226, 315, 399, 479	0
6	N	69/79 (87%)	-0.99	0	100	100	325, 403, 501, 568	0
All	All	7224/8380 (86%)	-0.93	3 (0%)	100	100	101, 230, 372, 568	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	209	ILE	2.4
1	H	28	LEU	2.2
2	I	836	LEU	2.1

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
7	MG	D	2001	1/1	0.88	0.05	251,251,251,251	0
7	MG	J	2001	1/1	0.93	0.06	170,170,170,170	0
8	ZN	N	101	1/1	0.93	0.06	465,465,465,465	0
8	ZN	M	101	1/1	0.97	0.03	468,468,468,468	0
8	ZN	J	2002	1/1	0.97	0.05	229,229,229,229	0
8	ZN	D	2003	1/1	0.98	0.14	334,334,334,334	0
8	ZN	D	2002	1/1	0.98	0.03	182,182,182,182	0
8	ZN	J	2003	1/1	1.00	0.01	126,126,126,126	0

6.5 Other polymers [i](#)

There are no such residues in this entry.