



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:43 PM UTC

PDB ID : 6OVR / pdb_00006ovr
Title : X-ray crystal structure of a bacterial reiterative transcription complex of pyrG promoter variant -1G
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2019-05-08
Resolution : 2.84 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

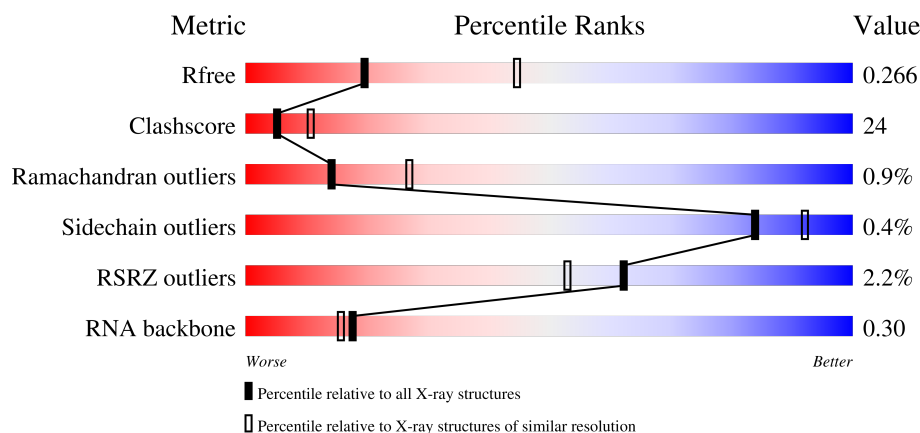
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)
RNA backbone	3983	1035 (3.06-2.62)

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	315	
1	B	315	
2	C	1119	
3	D	1524	

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Mol	Chain	Length	Quality of chain
4	E	99	60%33%5%
5	F	423	9% 47%34%18%
6	G	22	9% 50%36%14%
7	H	27	48%22%30%
8	I	8	25% 38%38%25%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28535 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1107	Total	C	N	O	S	0	0	0
			8726	5523	1551	1628	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1484	Total	C	N	O	S	0	0	0
			11722	7431	2065	2191	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2790	1760	508	518	4			

- Molecule 6 is a DNA chain called DNA (5'-D(P*GP*GP*TP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*GP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	19	Total	C	N	O	P	0	0	0
			387	183	75	110	19			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*CP*TP*GP*AP*TP*GP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	19	Total	C	N	O	P	0	0	0
			394	188	76	112	18			

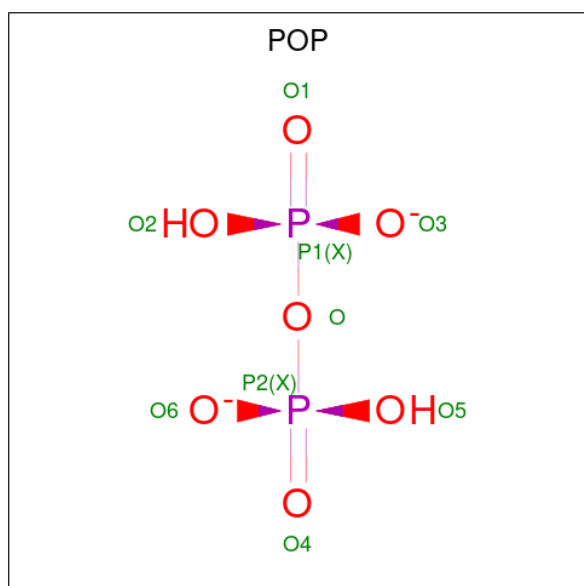
- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*GP*GP*GP*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	8	Total	C	N	O	P	0	0	0
			193	80	40	63	10			

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		

- Molecule 10 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	P	0	0
			9	7	2		

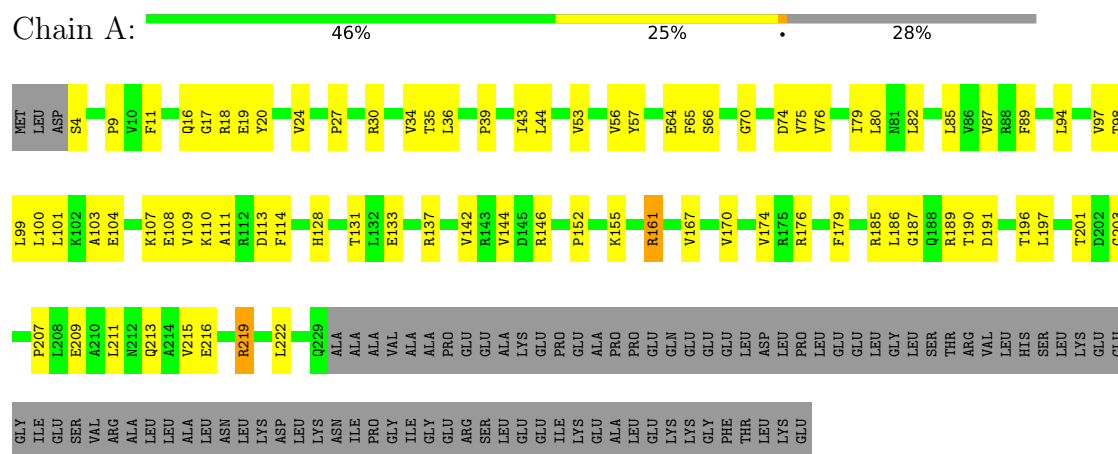
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Zn	0	0
			2	2		

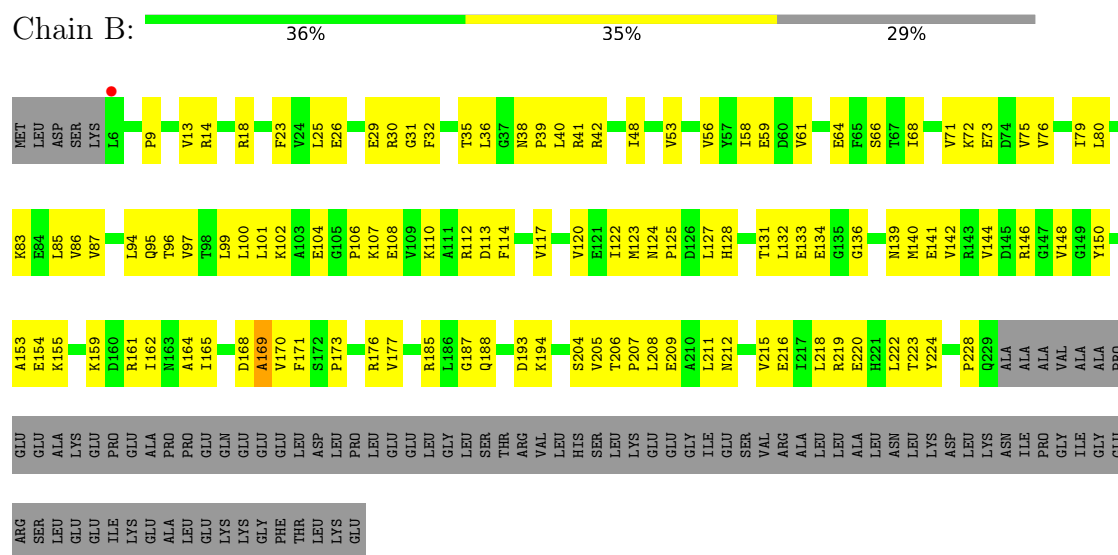
3 Residue-property plots

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 subunit alpha

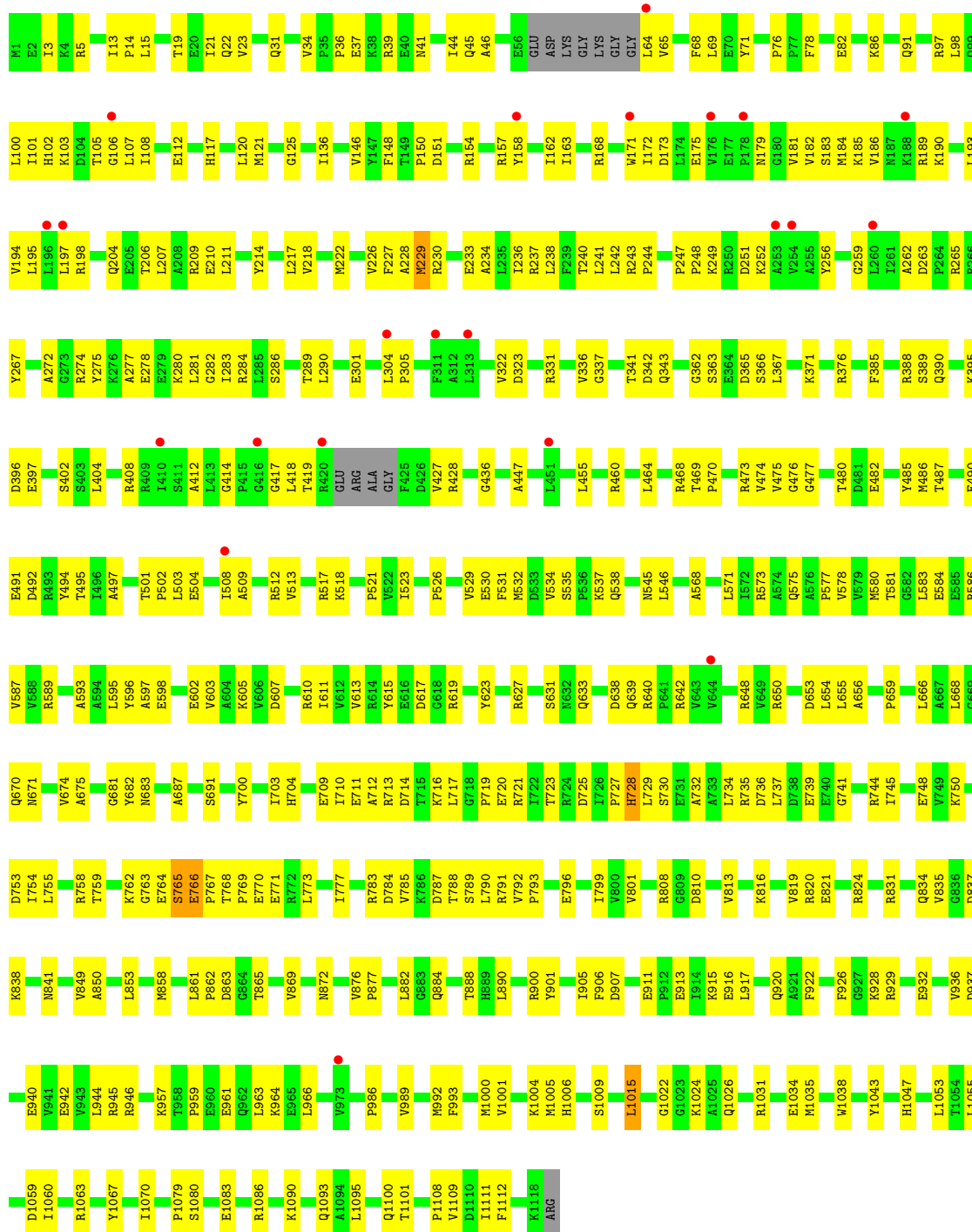


• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta





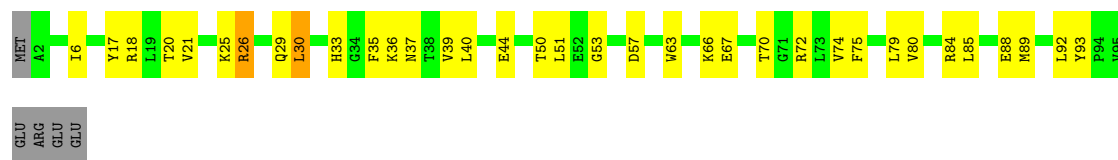
• Molecule 3: DNA-directed RNA polymerase subunit beta'



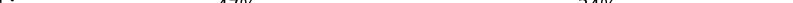
G1461	P1332	ASP	A1142	A1028	E898	Q794	A690	L496	S410	K343	V259	K180	P98
L1462	H1333	ILE	G1143	R1029	L899	V795	L691	R500	T411	D344	E266	D181	A99
N1465	L1336	THR	Y1145	Q1033	E901	E798	E692	E693	G412	G182	G182	E183	H101
V1466	L1336		G1146	Q1034	L902	K799	E694	L503	D413	E184	E267	E184	I102
L1471	P1341		R1147	L1038	D903	K800	I695	R508	V420	Q347	F269	E185	Q103
E1342	E1342		V1148	Q1039	V904	L804	V689	P509	G425	M351	L270	V186	F104
V1344	A1345		R1151	G1040	Q905	T808	V700	E510	G425	N352	V271	K187	V105
E1351	V1344		V1155	R1042	E907	L701	L702	M511	V431	V353	L272	G188	S110
F1480	E1351		R1159	M1045	S910	E810	R703	M512	V432	V354	R273	E189	K111
T1484	L1363		R1164	Q1046	Y916	E812	R704	I513	G435	P356	D276	L191	I112
Q1485	H1364		Y1165	Q1047	Q917	L813	L711	V517	E436	E357	E277	A192	L116
V1486	D1366		L1166	R1048	Q917	G712	G712	L520	E437	G958	P278	V195	D117
V1487	K1366		L1167	P1048	R921	L713	L713	P521	V437	A359	V279	V196	L118
L1492	V1371		S1168	G1050	L922	G819	Q714	P522	D438	R360	A280	S197	L122
K1493	V1372		M1168	T1052	G923	E820	Q717	R525	R441	V361	T281	K198	E122
A1494	R1373		V1171	T1053	M924	N824	P718	P526	N442	E362	Y282	L199	L123
I1495	Q1374		A1177	P1054	Y936	I827	V719	M527	V443	G364	F283	E124	E124
E1496	M1375		A1177	E1054	Y937	K828	L720	V528	V444	D365	P285	Q125	V126
E1497	M1376		A1177	T1057	G938	L644	L720	Q529	V445	K366	V286	L204	L127
A1498	K1377		V1188	V1057	G938	P645	Q724	V530	V446	I367	G287	Y205	Y128
R1499	V1378		R1189	V1067	F939	V829	Q724	D531	V447	V368	K288	R206	
A1502	V1379		R1189	L1068	F941	E833	Q727	S449	E448	I371	E296	F207	I133
VAL	D1386		R1197	E1069	F941	T834	F736	R534	Y449	D372	L297	P208	V194
GLU	L1390		Y1198	T1072	I947	R838	F736	Y544	D451	P373	E299	L209	L135
ALA	E1391		G1199	H1075	T948	V842	F740	I548	E454	E374	K300	R210	D136
LYS	V1398		K1203	G1076	I949	N845	G742	L548	R455	E374	G301	V211	P137
GLU	D1399		C1204	T1084	D952	M845	D743	R553	M456	E380	Q302	E214	V147
ARG	E1405		P1214	T1088	I956	E848	M745	K555	G457	E380	E306	V216	E148
ARG	A1409		I1217	G1092	E975	L860	V747	L557	A460	A381	K217	K218	K149
GLY	G1410		A1225	L1098	T984	Q861	H748	L558	L465	E382	G309	L217	L152
VAL	T1413		I1229	V1099	D985	T865	P750	I565	L465	V385	L310	G222	D155
ARG	L1420		T1234	V1107	R986	T874	Q756	I566	L468	H385	R312	L223	D156
GLN	L1421		Q1235	R1108	E987	T875	Q756	I567	D469	H388	R313	R224	E157
PHO	M1422		L1236	E1109	R988	S876	I761	E570	L470	E389	R315	V231	Y158
GLY	K1432		T1237	A1110	Y989	T876	Q762	K571	E474	P390	Q316	Y236	R159
LYS	K1433		ARG	D1111	I992	R879	M763	R572	M481	S392	A319	K237	E160
GLN	W1434		THR	C1112	T999	L881	H767	M573	K482	I393	A320	E240	L151
ALA			THR	G1113	V1003	A773	A773	L574	H483	L394	Q321	T241	K165
	A1438		PHE	T1114	V1007	I885	Q880	D579	S485	A398	V322	L242	E167
			HIS	D1126	V1007	V886	R691	A580	R486	E398	E326	L245	T168
	N1442		THR	D1126	V1007	V886	R691	A580	R487	E398	E327	L245	Y169
			GLY	T1129	N1014	E888	L683	L581	A487	Y401	E327	L245	P170
	V1446		GLY	R1130	N1014	E888	L683	L581	A487	Y401	E327	L245	L171
			VAL	R1130	N1014	E888	L683	L581	A487	Y401	E327	L245	P172
			ALA	R1137	P1019	V895	L767	R587	K491	D405	E327	L245	Q166
	A1450		GLY	R1137	P1019	V895	L767	R587	K491	D405	E327	L245	E167
	K1455		ALA	E1141	M1023	V895	L767	R587	K491	D405	E327	L245	T168

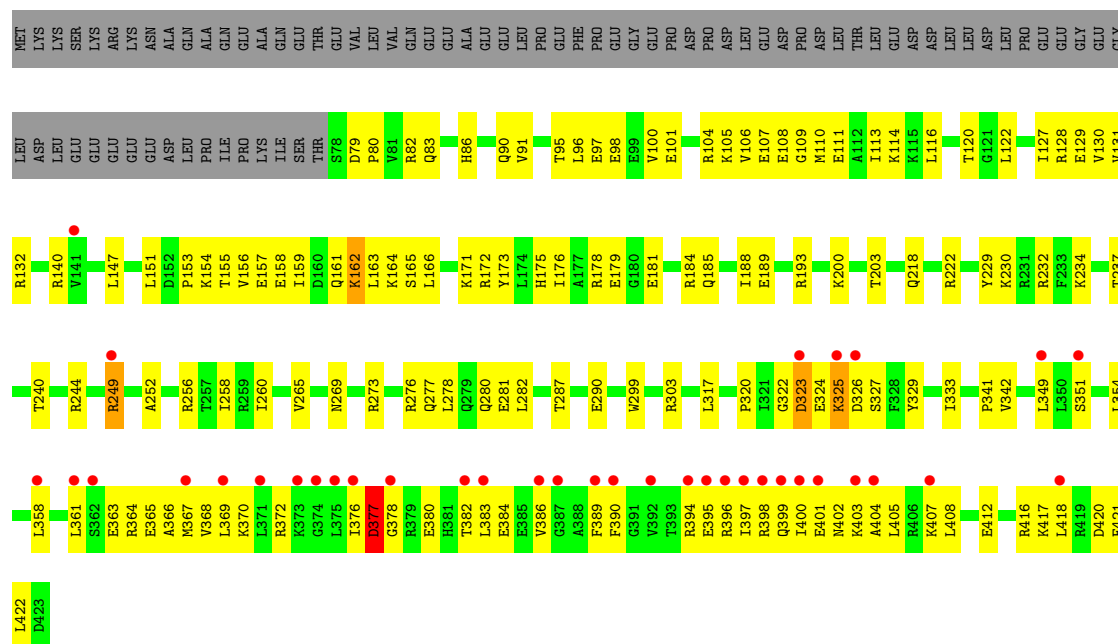
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 60% 33% • 5%

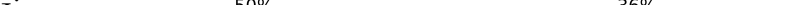


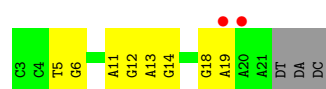
- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 

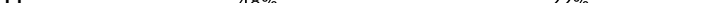


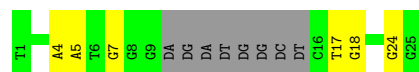
- Molecule 6: DNA (5'-D(P*GP*GP*TP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*GP*AP*AP*A)-3')

Chain G: 



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*CP*TP*GP*AP*TP*GP*CP*AP*GP*G)-3')

Chain H:  48% 22% 30%



- Molecule 8: RNA (5'-D^{*}(GTP))-R(P^{*}GP^{*}GP^{*}GP^{*}GP^{*}GP^{*}GP^{*}G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.90Å 101.42Å 295.19Å 90.00° 98.64° 90.00°	Depositor
Resolution (Å)	41.69 – 2.84 41.69 – 2.84	Depositor EDS
% Data completeness (in resolution range)	96.5 (41.69-2.84) 96.4 (41.69-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.222 , 0.268 0.222 , 0.266	Depositor DCC
R_{free} test set	1997 reflections (1.56%)	wwPDB-VP
Wilson B-factor (Å ²)	79.0	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28535	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: GTP, MG, POP, ZN

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	0.45	0/1814	0.72	0/2466
1	B	0.48	0/1799	0.75	2/2447 (0.1%)
2	C	0.47	2/8892 (0.0%)	0.72	2/12028 (0.0%)
3	D	0.55	2/11928 (0.0%)	0.78	6/16127 (0.0%)
4	E	0.51	1/775 (0.1%)	0.77	1/1045 (0.1%)
5	F	0.55	4/2835 (0.1%)	0.76	3/3816 (0.1%)
6	G	0.54	0/434	0.60	0/666
7	H	0.38	0/442	0.54	0/680
8	I	0.44	0/181	0.59	0/283
All	All	0.51	9/29100 (0.0%)	0.75	14/39558 (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	1
3	D	0	2
5	F	0	1
All	All	0	4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	642	CYS	C-N	15.00	1.41	1.33
5	F	249	ARG	NE-CZ	10.08	1.44	1.33
5	F	249	ARG	CB-CG	9.74	1.81	1.52
5	F	249	ARG	CZ-NH2	-8.90	1.21	1.33
3	D	521	PRO	CA-C	6.74	1.58	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	249	ARG	NE-CZ-NH2	8.46	126.81	119.20
3	D	1151	ARG	CA-CB-CG	7.58	129.26	114.10
3	D	302	GLN	N-CA-C	-6.92	99.88	110.32
3	D	302	GLN	CA-C-N	-6.81	112.75	119.90
3	D	302	GLN	C-N-CA	-6.81	112.75	119.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Peptide
3	D	1129	THR	Peptide
3	D	65	ARG	Peptide
5	F	389	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	88	0
1	B	1767	0	1816	120	0
2	C	8726	0	8814	444	0
3	D	11722	0	11950	618	13
4	E	761	0	778	44	0
5	F	2790	0	2853	186	11
6	G	387	0	212	9	0
7	H	394	0	217	9	0
8	I	193	0	88	3	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	C	9	0	0	0	0
11	D	2	0	0	0	0
All	All	28535	0	28562	1397	13

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 24.

The worst 5 of 1397 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)
5:F:249:ARG:CG	5:F:249:ARG:CB	1.81	1.58
3:D:371:ILE:CD1	3:D:372:ASP:H	1.36	1.38
2:C:605:LYS:HB3	2:C:610:ARG:NH2	1.35	1.36
3:D:411:THR:O	5:F:178:ARG:NH2	1.58	1.36
3:D:411:THR:C	5:F:178:ARG:NH2	1.90	1.27

The worst 5 of 13 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:301:GLY:N	5:F:249:ARG:NH1[4_1349]	1.44	0.76
3:D:300:LYS:O	5:F:249:ARG:NE[4_1349]	1.58	0.62
3:D:302:GLN:N	5:F:249:ARG:NH2[4_1349]	1.66	0.54
3:D:302:GLN:N	5:F:249:ARG:CZ[4_1349]	1.77	0.43
3:D:300:LYS:C	5:F:249:ARG:NE[4_1349]	1.80	0.40

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	224/315 (71%)	211 (94%)	13 (6%)	0	100	100
1	B	222/315 (70%)	202 (91%)	18 (8%)	2 (1%)	14	27
2	C	1101/1119 (98%)	1036 (94%)	53 (5%)	12 (1%)	11	23
3	D	1480/1524 (97%)	1398 (94%)	71 (5%)	11 (1%)	18	35
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/423 (81%)	316 (92%)	23 (7%)	5 (2%)	8	17
All	All	3463/3795 (91%)	3252 (94%)	181 (5%)	30 (1%)	14	27

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	GLU
2	C	363	SER
2	C	418	LEU
2	C	419	THR
3	D	486	ARG

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	199/273 (73%)	198 (100%)	1 (0%)	81	90
1	B	197/273 (72%)	197 (100%)	0	100	100
2	C	931/941 (99%)	929 (100%)	2 (0%)	87	95
3	D	1250/1279 (98%)	1243 (99%)	7 (1%)	78	89
4	E	83/88 (94%)	83 (100%)	0	100	100
5	F	296/371 (80%)	294 (99%)	2 (1%)	76	88
All	All	2956/3225 (92%)	2944 (100%)	12 (0%)	84	92

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1188	VAL
3	D	1234	THR
5	F	377	ASP
3	D	1236	LEU
3	D	302	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	816	HIS
5	F	90	GLN

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Mol	Chain	Res	Type
3	D	861	GLN
3	D	1116	ASN
5	F	269	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	7/8 (87%)	3 (42%)	2 (28%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	3	G
8	I	4	G
8	I	5	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	I	1	GTP
8	I	4	G

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 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	$\# Z > 2$
10	POP	C	1201	-	6,8,8	0.53	0	12,13,13	1.09	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
10	POP	C	1201	-	-	0/6/6/6	-

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 [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(Å ²)	Q<0.9
1	A	226/315 (71%)	0.11	0 100 100	71, 95, 118, 132	0
1	B	224/315 (71%)	0.09	1 (0%) 88 87	68, 96, 126, 146	0
2	C	1107/1119 (98%)	0.14	22 (1%) 65 57	54, 94, 165, 203	0
3	D	1484/1524 (97%)	0.01	14 (0%) 81 76	49, 87, 149, 204	0
4	E	94/99 (94%)	0.29	0 100 100	64, 102, 152, 157	0
5	F	346/423 (81%)	0.50	37 (10%) 11 8	62, 107, 206, 228	0
6	G	19/22 (86%)	0.03	2 (10%) 11 9	66, 123, 229, 241	0
7	H	19/27 (70%)	-0.10	0 100 100	92, 125, 233, 239	0
8	I	7/8 (87%)	0.71	2 (28%) 1 1	68, 83, 172, 195	0
All	All	3526/3852 (91%)	0.12	78 (2%) 62 53	49, 94, 165, 241	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	369	LEU	6.0
5	F	397	ILE	5.4
5	F	375	LEU	5.2
5	F	418	LEU	3.7
5	F	323	ASP	3.6

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
10	POP	C	1201	9/9	0.75	0.09	78,95,107,114	0
9	MG	B	1001	1/1	0.88	0.24	78,78,78,78	0
9	MG	D	2001	1/1	0.93	0.12	48,48,48,48	0
11	ZN	D	2002	1/1	1.00	0.03	113,113,113,113	0
11	ZN	D	2003	1/1	1.00	0.11	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.