



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 05:02 am BST

PDB ID : 4GZZ  
Title : Crystal structures of bacterial RNA Polymerase paused elongation complexes  
Authors : Weixlbaumer, A.; Leon, K.; Landick, R.; Darst, S.A.  
Deposited on : 2012-09-06  
Resolution : 4.29 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

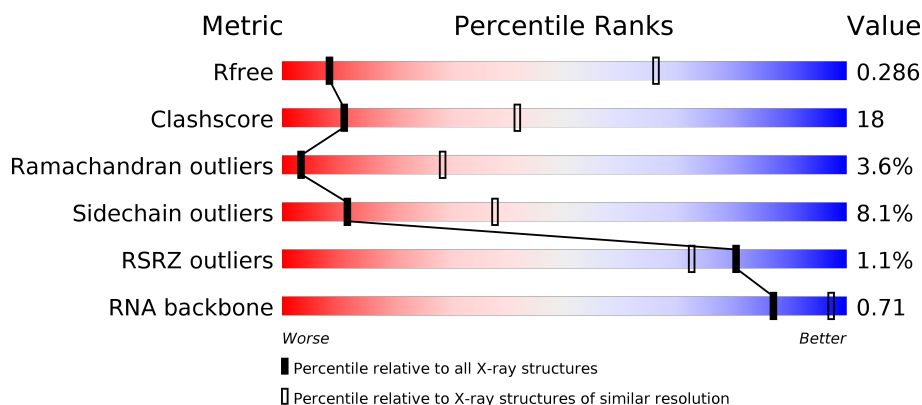
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.29 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)
RNA backbone	3102	1058 (5.60-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>26%</div> <div>•</div> <div>29%</div> </div> </div>
1	B	315	<div> <div>48%</div> <div>22%</div> <div>•</div> <div>29%</div> </div>
2	C	1119	<div> <div>54%</div> <div>38%</div> <div>5%</div> <div>•</div> </div>
3	D	1534	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>34%</div> <div>5%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	99	 40% 45% 7% • 6%
5	N	13	 46% 38% 15%
6	R	16	 6% 44% 6% 44%
7	T	22	 50% 50%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24400 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	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	B	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1083	Total	C	N	O	S	0	0	0
			8548	5412	1524	1588	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1358	Total	C	N	O	S	0	0	0
			10714	6780	1900	2001	33			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1525	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1526	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1527	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1528	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1529	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1530	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1531	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1532	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1533	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1534	HIS	-	EXPRESSION TAG	UNP Q8RQE8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			

- Molecule 5 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	N	11	Total	C	N	O	P	0	0	0
			225	107	43	64	11			

- Molecule 6 is a RNA chain called RNA transcript.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	9	Total	C	N	O	P	0	0	0
			191	85	31	66	9			

- Molecule 7 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	T	22	Total	C	N	O	P	0	0	0
			447	213	81	131	22			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

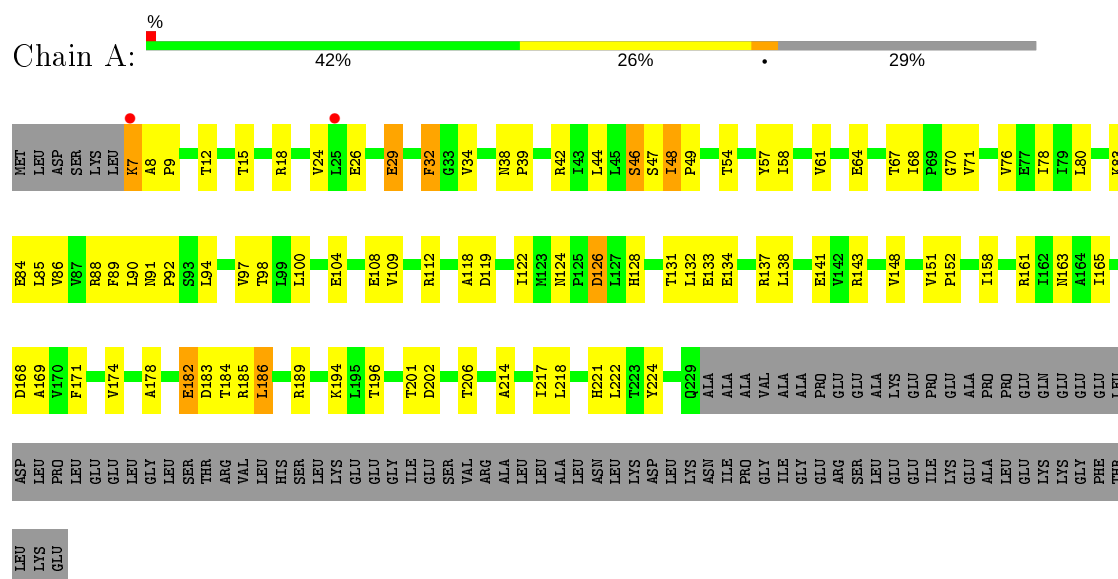
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

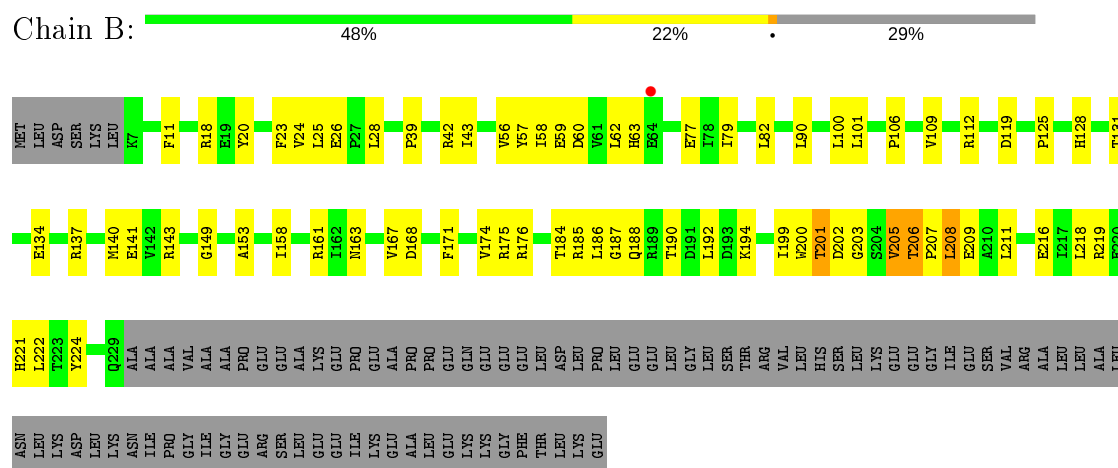
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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



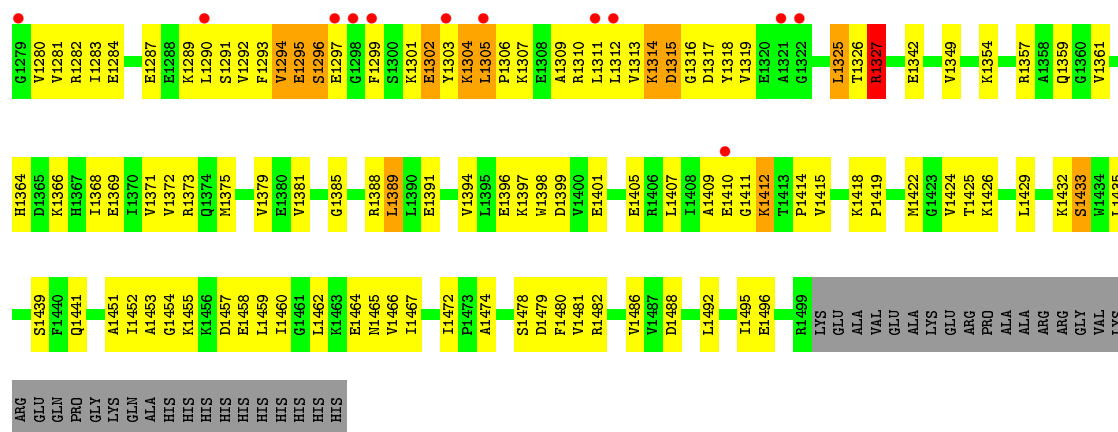
- Molecule 2: DNA-directed RNA polymerase subunit beta



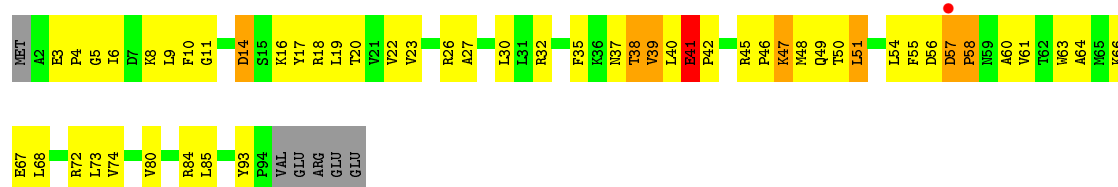


C1204	V1106	Y989	V890	K300	A715	R613	P522	V431	V353	GLY	LEU	L161	K82	MET
Y1205	V1107	D990	E891	G801	V719	F614	D523	V432	V354	MET	ALA	R162	S83	K2
G1206	R1108	Q991	D892	A802	L720	R615	L524	P355	V355	ALA	ALA	Y163	S84	
Y1207	E1109	L993	L902	G803	V721	R616	R525	P356	P356	TRP	TRP	G164	V85	V5
D1208	L1209	L993	L903	E805	E722	R617	P526	R434	E357	VAL	VAL	K165	R86	
S1210	G1112	E1001	V904	P806	G723	L618	M527	V435	G358	VAL	GLU	Q166	R87	A11
M1211	T1115	V1002	P905	A807	Q724	K621	T537	V447	A359	VAL	LYS	E167	Y88	
R1213	S1119	V1003	K908	T808	S725	D624	S538	E448	R360	HIS	GLU	T168	S14	
G1218	E1127	F1008	Q917	L813	Q726	Y625	D539	S449	V361	GLY	ALA	Y169	P15	
E1219	V1128	F1011	R921	H816	S729	Y626	L540		A362	TRR	TRR	H101	H101	
A1220	T1129	E1012	L922	E817	T726	Y627	L541		A363	ILE	LYS	H102	I18	
A1225	R1130	E1013	K925	P809	Q727	S626	D542		G364	VAL	PRO	W103	R19	
A1226	S1131	E1013	K926	P809	L728	G627	D543		D365	GLY	GLY			
Q1227	L1132	V1007	Q917	L813	H729	R628	L543		A366	LYS	GLU	D107	G24	
S1228	R1133	F1008	Q917	L813	H729	R629	L544		V367	GLY	ILE	V108		
T1229	R1136	F1008	Q917	L813	H729	R630	L545		V368	GLN	LEU	P109	K28	
G1230	K1136	F1008	Q917	L813	H729	R631	L546		V369	PRO	ALA	P109	P29	
E1231	D1139	F1008	Q917	L813	H729	R632	L547		V370	LEU	GLU	L178	E30	
P1232	D1142	F1008	Q917	L813	H729	R633	L548		V371	ALA	LEU	K111	T31	
Q1235	G1146	F1008	Q917	L813	H729	R634	L549		V372	GLU	PRO	L115	I32	
L1236	R1147	F1008	Q917	L813	H729	R635	L550		V373	ALA	GLU	L116	N33	
THR	R1148	F1008	Q917	L813	H729	R636	L551		V374	LYS	PRO	D117		
MET	R1149	F1008	Q917	L813	H729	R637	L552		V375	GLY	TRR	L118	L37	
GLY	R1150	F1008	Q917	L813	H729	R638	L553		V376	LEU	PHE	K38		
VAL	R1151	F1008	Q917	L813	H729	R639	L554		V377	LEU	ARG	V185	P39	
ALA	R1152	F1008	Q917	L813	H729	R640	L555		V378	ARG	ARG	V186	E40	
GLY	R1153	F1008	Q917	L813	H729	R641	L556		V379	MET	ALA	E190	R41	
ASP	R1154	F1008	Q917	L813	H729	R642	L557		V380	PRO	GLU	L191	L44	
ILE	R1155	F1008	Q917	L813	H729	R643	L558		V381	ARG	GLU	Q125	F45	
THR	R1156	F1008	Q917	L813	H729	R644	L559		V382	VAL	GLY	L127	D46	
VAL	R1157	F1008	Q917	L813	H729	R645	L560		V383	ALA	VAL	V128	E47	
GLY	R1158	F1008	Q917	L813	H729	R646	L561		V384	ALA	VAL	S130	R48	
ALA	R1159	F1008	Q917	L813	H729	R647	L562		V385	ALA	GLU	K131	F50	
ASP	R1160	F1008	Q917	L813	H729	R648	L563		V386	GLN	LEU	Y132	I49	
THR	R1161	F1008	Q917	L813	H729	R649	L564		V387	VAL	LYS	G133	G51	
ILE	R1162	F1008	Q917	L813	H729	R650	L565		V388	GLU	GLY	P52	P52	
THR	R1163	F1008	Q917	L813	H729	R651	L566		V389	ALA	LEU	L134	I53	
Q1254	R1164	F1008	Q917	L813	H729	R652	L567		V390	GLU	GLU	D136	R54	
R1258	R1165	F1008	Q917	L813	H729	R653	L568		V391	GLU	GLU	P137	D55	
E1261	R1166	F1008	Q917	L813	H729	R654	L569		V392	GLY	ALA	K138	Y56	
L1262	R1167	F1008	Q917	L813	H729	R655	L570		V393	GLY	PHE	G139	E57	
F1263	R1168	F1008	Q917	L813	H729	R656	L571		V394	GLY	LEU	R209	G58	
K1269	R1169	F1008	Q917	L813	H729	R657	L572		V395	THR	LEU	R210	A59	
A1272	R1170	F1008	Q917	L813	H729	R658	L573		V396	VAL	VAL	L142	O60	
T1273	R1171	F1008	Q917	L813	H729	R659	L574		V397	THR	LEU	P146	Y63	
I1274	R1172	F1008	Q917	L813	H729	R660	L575		V398	LEU	ARG	V147	K64	
S1275	R1173	F1008	Q917	L813	H729	R661	L576		V399	LEU	GLU	E148	R65	
E1276	R1174	F1008	Q917	L813	H729	R662	L577		V400	PHE	ASP	Q151	F68	
I1277	R1175	F1008	Q917	L813	H729	R663	L578		V401	LEU	GLU	L152		
D1278	R1176	F1008	Q917	L813	H729	R664	L579		V402	GLU	PRO	L153	C73	
	R1177	F1008	Q917	L813	H729	R665	L580		V403	TRP	VAL	T154	E74	
	R1178	F1008	Q917	L813	H729	R666	L581		V404	ALA	ALA	T155	R75	
	R1179	F1008	Q917	L813	H729	R667	L582		V405	THR	THR	E156		
	R1180	F1008	Q917	L813	H729	R668	L583		V406	PHE	PHE	E157	V78	
	R1181	F1008	Q917	L813	H729	R669	L584		V407	LEU	LEU	E158	E79	
	R1182	F1008	Q917	L813	H729	R670	L585		V408	VAL	PRO	Y159	V80	
	R1183	F1008	Q917	L813	H729	R671	L586		V409	THR	VAL	E160	T81	
	R1184	F1008	Q917	L813	H729	R672	L587		V410	LEU	VAL			
	R1185	F1008	Q917	L813	H729	R673	L588		V411	THR	ARG			
	R1186	F1008	Q917	L813	H729	R674	L589		V412	LEU	GLU			
	R1187	F1008	Q917	L813	H729	R675	L590		V413	PHE	ASP			
	R1188	F1008	Q917	L813	H729	R676	L591		V414	LEU	GLU			
	R1189	F1008	Q917	L813	H729	R677	L592		V415	LEU	ASP			
	R1190	F1008	Q917	L813	H729	R678	L593		V416	LEU	GLU			
	R1191	F1008	Q917	L813	H729	R679	L594		V417	GLU	PRO			
	R1192	F1008	Q917	L813	H729	R680	L595		V418	GLU	VAL			
	R1193	F1008	Q917	L813	H729	R681	L596		V419	TRP	VAL			
	R1194	F1008	Q917	L813	H729	R682	L597		V420	ALA	ALA			
	R1195	F1008	Q917	L813	H729	R683	L598		V421	THR	THR			
	R1196	F1008	Q917	L813	H729	R684	L599		V422	PHE	PHE			
	R1197	F1008	Q917	L813	H729	R685	L600		V423	LEU	LEU			
	R1198	F1008	Q917	L813	H729	R686	L601		V424	LEU	LEU			
	R1199	F1008	Q917	L813	H729	R687	L602		V425	VAL	PRO			
	R1200	F1008	Q917	L813	H729	R688	L603		V426	THR	THR			
	R1201	F1008	Q917	L813	H729	R689	L604		V427	ALA	ALA			
	R1202	F1008	Q917	L813	H729	R690	L605		V428	THR	THR			
	R1203	F1008	Q917	L813	H729	R691	L606		V429	PHE	PHE			
	R1204	F1008	Q917	L813	H729	R692	L607		V430	LEU	LEU			
	R1205	F1008	Q917	L813	H729	R693	L608		V431	VAL	VAL			
	R1206	F1008	Q917	L813	H729	R694	L609		V432	THR	THR			
	R1207	F1008	Q917	L813	H729	R695	L610		V433	LEU	LEU			
	R1208	F1008	Q917	L813	H729	R696	L611		V434	VAL	VAL			
	R1209	F1008	Q917	L813	H729	R697	L612		V435	THR	THR			
	R1210	F1008	Q917	L813	H729	R698	L613		V436	ALA	ALA			
	R1211	F1008	Q917	L813	H729	R699	L614		V437	LEU	LEU			
	R1212	F1008	Q917	L813	H729	R700	L615		V438	VAL	VAL			
	R1213	F1008	Q917	L813	H729	R701	L616		V439	THR	THR			
	R1214	F1008	Q917	L813	H729	R702	L617		V440	LEU	LEU			
	R1215	F1008	Q917	L813	H729	R703	L618		V441	VAL	VAL			
	R1216	F1008	Q917	L813	H729	R704	L619		V442	THR	THR			
	R1217	F1008	Q917	L813	H729	R705	L620		V443	ALA	ALA			
	R1218	F1008	Q917	L813	H729	R706	L621		V444	LEU	LEU			
	R1219	F1008	Q917	L813	H729	R707	L622		V445	VAL	VAL			
	R1220	F1008	Q917	L813	H729	R708	L623		V446	THR	THR			
	R1221	F1008	Q917	L813	H729	R709	L624		V447	LEU	LEU			
	R1222	F1008	Q917	L813	H729	R710	L625		V448	VAL	VAL			
	R1223	F1008	Q917	L813	H729	R711	L626		V449	THR	THR			
	R1224	F1008	Q917	L813	H729	R712	L627		V450	ALA	ALA			
	R1225	F1008	Q917	L813	H729	R713	L628		V451	LEU	LEU			
	R1226	F1008	Q917	L813	H729	R714	L629		V452	VAL	VAL			
	R1227	F1008	Q917	L813	H729	R715	L630		V453	THR	THR			
	R1228	F1008	Q917	L813	H729	R716	L631		V454	ALA	ALA			
	R1229	F1008	Q917	L813	H729	R717	L632		V455	LEU	LEU			
	R1230	F1008	Q917	L813	H729	R718	L633		V456	VAL	VAL			
	R1231	F1008	Q917	L813	H729	R719	L634		V457	THR	THR			
	R1232	F1008	Q917	L813	H729	R720	L635		V458	ALA	ALA			
	R1233	F1008	Q917	L813	H729	R721	L636		V459	LEU	LEU			
	R1234	F1008	Q917	L813	H729	R722	L637		V460	VAL	VAL			
	R1235	F1008	Q917	L813	H729	R723	L638		V461	THR	THR			
	R1236	F1008	Q917	L813	H729	R724	L639		V462	ALA				





• Molecule 4: DNA-directed RNA polymerase subunit omega



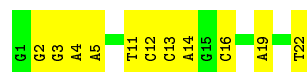
• Molecule 5: non-template DNA



• Molecule 6: RNA transcript



• Molecule 7: template DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	286.55Å 286.55Å 199.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.78 – 4.29 38.79 – 4.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.78-4.29) 87.8 (38.79-4.29)	Depositor EDS
$R_{merge}$	0.44	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 4.28Å)	Xtriage
Refinement program	PHENIX 1.8_1069, CNS	Depositor
R, $R_{free}$	0.234 , 0.285 0.236 , 0.286	Depositor DCC
$R_{free}$ test set	2074 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	164.3	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	24400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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	0.26	0/1791	0.47	0/2436
1	B	0.28	0/1791	0.47	0/2436
2	C	0.28	0/8711	0.51	0/11784
3	D	0.28	0/10897	0.50	1/14726 (0.0%)
4	E	0.29	0/768	0.55	0/1035
5	N	0.44	0/252	1.08	0/386
6	R	0.21	0/212	0.77	0/328
7	T	0.44	0/500	1.08	0/768
All	All	0.29	0/24922	0.53	1/33899 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	705	ALA	C-N-CD	5.17	139.25	128.40

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	1759	0	1805	65	0
1	B	1759	0	1805	50	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8548	0	8650	371	0
3	D	10714	0	10936	408	1
4	E	754	0	769	40	0
5	N	225	0	124	3	0
6	R	191	0	95	10	0
7	T	447	0	248	10	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	24400	0	24432	882	1

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 882 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)
2:C:428:ARG:HH12	3:D:1086:LEU:HD21	1.24	0.98
2:C:610:ARG:HH11	2:C:610:ARG:HG3	1.27	0.96
2:C:846:LYS:NZ	6:R:29:U:OP1	1.99	0.96
1:B:188:GLN:O	3:D:646:LYS:NZ	2.00	0.94
1:A:80:LEU:HD21	2:C:573:ARG:HH11	1.34	0.92

All (1) 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)
1:B:143:ARG:NH1	3:D:1297:GLU:OE2[3_455]	2.18	0.02

## 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	221/315 (70%)	186 (84%)	29 (13%)	6 (3%)	5	34
1	B	221/315 (70%)	193 (87%)	25 (11%)	3 (1%)	11	47
2	C	1077/1119 (96%)	897 (83%)	144 (13%)	36 (3%)	4	30
3	D	1352/1534 (88%)	1097 (81%)	198 (15%)	57 (4%)	3	25
4	E	91/99 (92%)	73 (80%)	13 (14%)	5 (6%)	2	21
All	All	2962/3382 (88%)	2446 (83%)	409 (14%)	107 (4%)	3	28

5 of 107 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	184	THR
2	C	2	GLU
2	C	111	ASP
2	C	164	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	196/273 (72%)	188 (96%)	8 (4%)	30	56
1	B	196/273 (72%)	189 (96%)	7 (4%)	35	60
2	C	912/941 (97%)	837 (92%)	75 (8%)	11	37
3	D	1147/1289 (89%)	1044 (91%)	103 (9%)	9	33
4	E	82/88 (93%)	70 (85%)	12 (15%)	3	18
All	All	2533/2864 (88%)	2328 (92%)	205 (8%)	11	38

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	58	CYS
3	D	178	LEU
3	D	1433	SER

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Mol	Chain	Res	Type
3	D	68	PHE
3	D	124	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	434	HIS
2	C	609	ASN
3	D	1031	ASN
2	C	431	HIS
3	D	462	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	8/16 (50%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	22	U

There are no RNA pucker outliers to report.

## 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 3 ligands modelled in this entry, 3 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	223/315 (70%)	-0.18	2 (0%) 84 77	52, 116, 169, 205	0
1	B	223/315 (70%)	-0.20	1 (0%) 92 87	53, 107, 163, 198	0
2	C	1083/1119 (96%)	-0.20	5 (0%) 91 86	34, 108, 177, 264	0
3	D	1358/1534 (88%)	-0.12	25 (1%) 68 60	31, 110, 196, 250	0
4	E	93/99 (93%)	-0.05	1 (1%) 80 72	65, 121, 179, 228	0
5	N	11/13 (84%)	-0.21	0 100 100	340, 362, 386, 405	0
6	R	9/16 (56%)	-0.21	0 100 100	201, 206, 235, 243	0
7	T	22/22 (100%)	-0.46	0 100 100	219, 336, 388, 406	0
All	All	3022/3433 (88%)	-0.16	34 (1%) 80 72	31, 111, 192, 406	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	368	VAL	4.5
3	D	1299	PHE	4.0
2	C	372	LEU	3.5
3	D	1276	GLU	3.4
1	A	7	LYS	3.2

### 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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	ZN	D	1601	1/1	0.92	0.14	70,70,70,70	0
9	MG	D	1603	1/1	0.95	0.26	70,70,70,70	0
8	ZN	D	1602	1/1	0.99	0.28	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.