



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 10:01 PM UTC

PDB ID : 4GZY / pdb_00004gzy
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 : 3.51 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

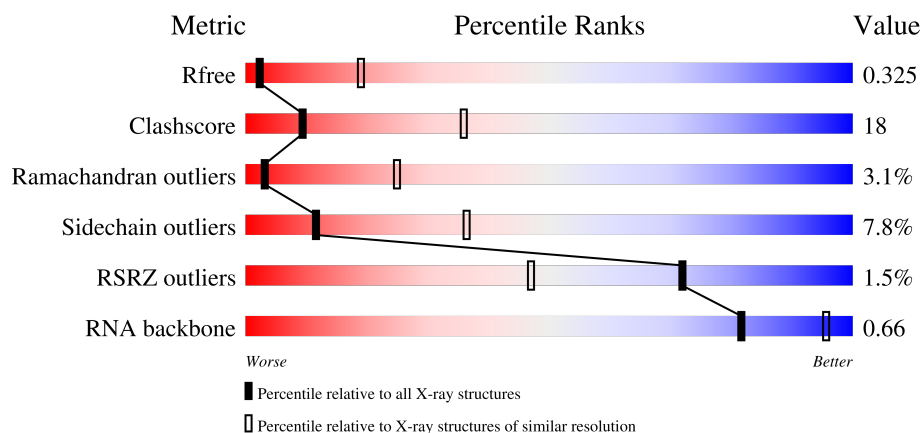
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	42% 25% • 29%
1	B	315	47% 22% • 29%
2	C	1119	2% 53% 38% 5% •
3	D	1534	% 50% 34% 5% 11%

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Mol	Chain	Length	Quality of chain
4	E	99	5% 55% 32% 6% • 6%
5	N	13	69% 15% 15%
6	R	29	10% 17% • 69%
7	T	22	5% 64% 36%

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 (CCD ID: ZN) (formula: Zn).

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

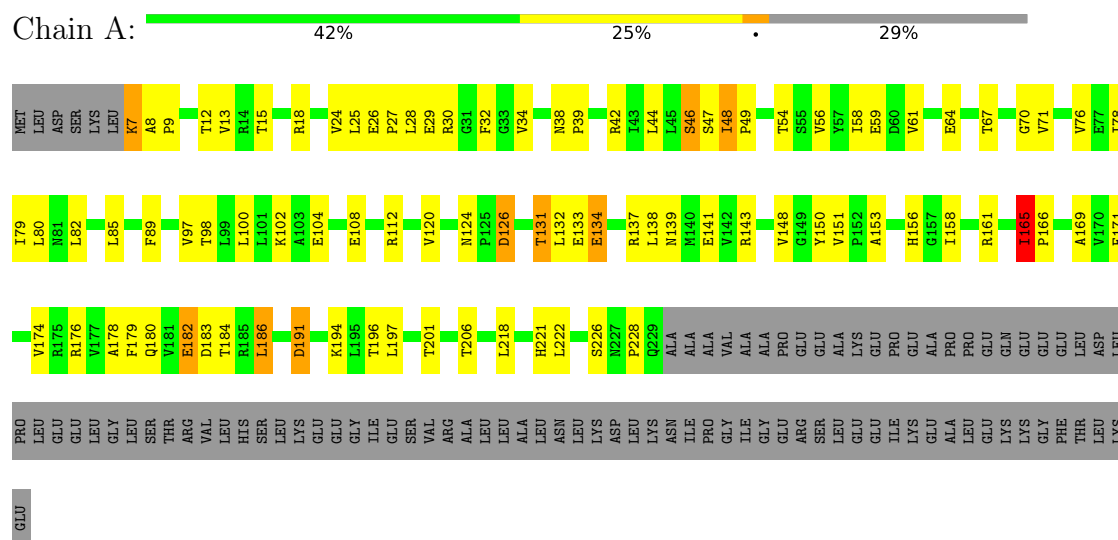
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

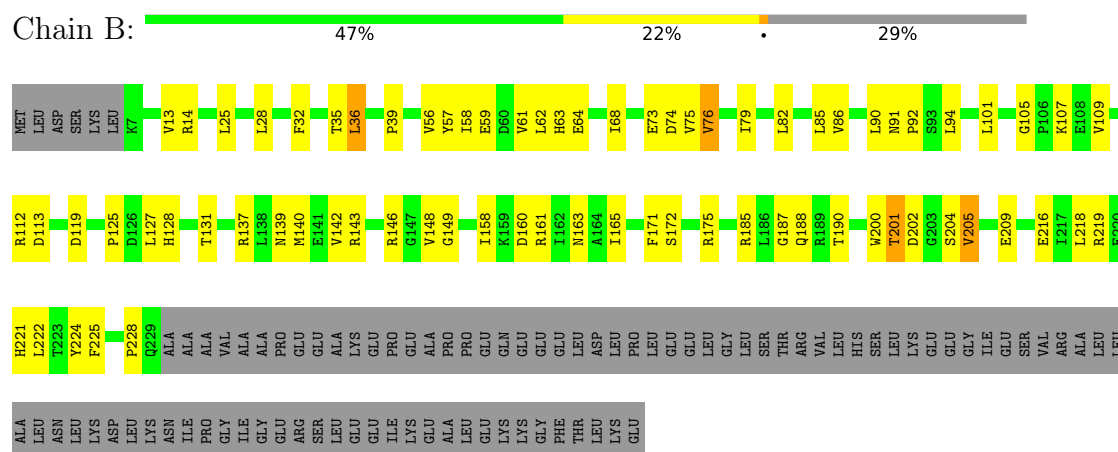
3 Residue-property plots

These plots are drawn for all protein, RNA, 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

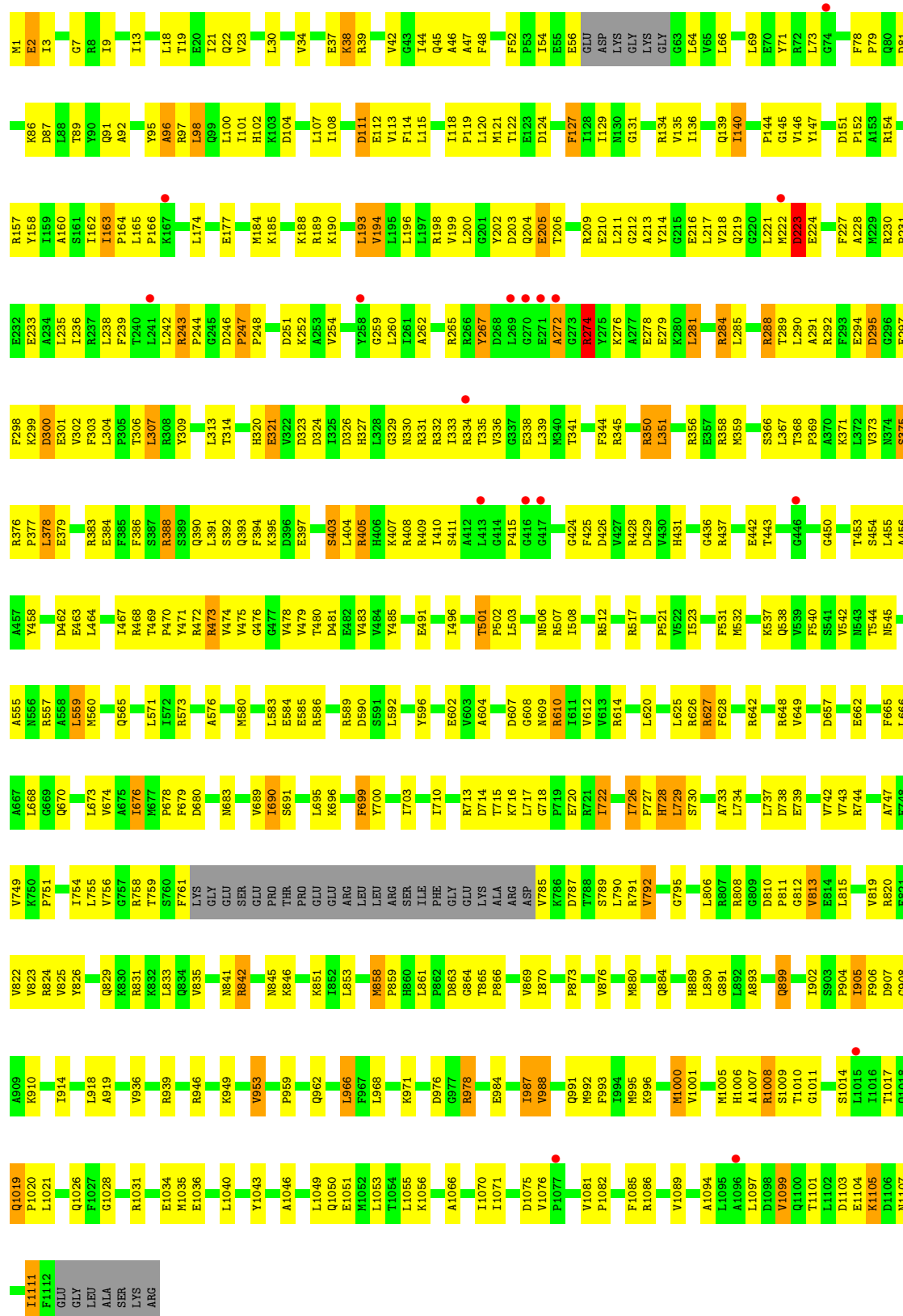


• Molecule 1: DNA-directed RNA polymerase subunit alpha

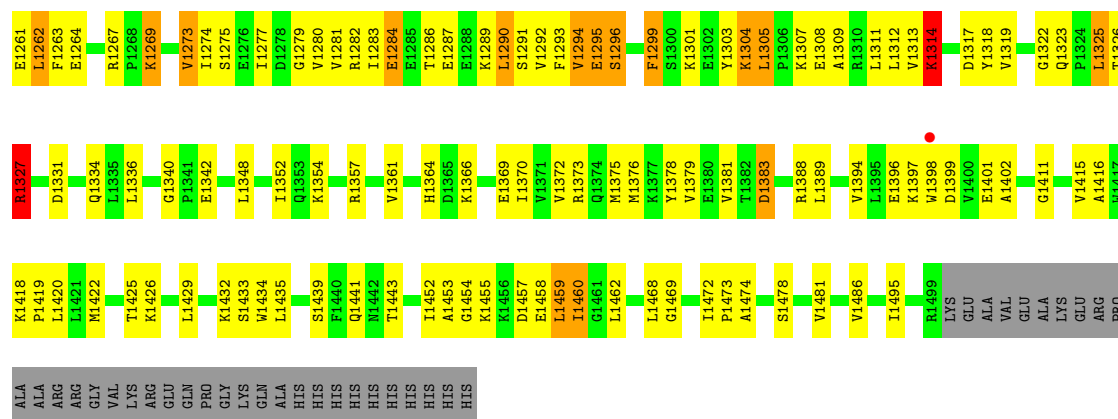


• Molecule 2: DNA-directed RNA polymerase subunit beta

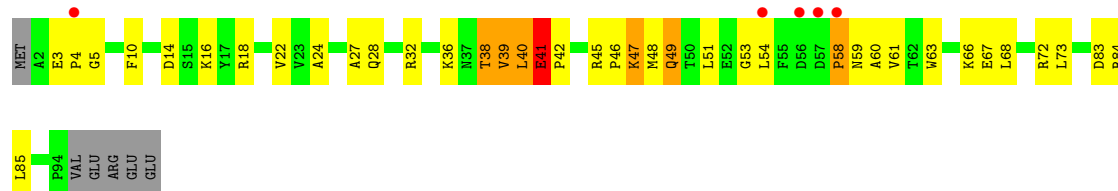




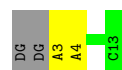
Y1165	S1074	L983	R872	R796	A715	D624	N541	R441	E362	GLU	TYR	T163	A96	MET
L1174	A1077	D985	L873	K797	F716	Y625	D642	V446	A362	ILE	LYS	Y169	A96	K2
I1183	K1078	D985	E874	K799	Q717		L543	V447	G364	VAL	PRO	L171	A100	K7
Q1184	K1079	R988	P877	K800	V719	R628	Y548	Y450	D365	LYS	GLU	P172	H101	K17
E1185	D1083	Q991	I880	A802	L720	S629	R550	D451	K366	GLN	ILE	V175	I102	I18
V1188	L1086	L995	L881	G803	G723	V630	R653	I452	V368	PRO	ALA	D176	W103	
R1189	L1087	W996	L881	E805	G725		K555	I453	A369	LEU	GLU	A177	F104	G24
Q1195	R1096	E1001	D892	F806	S725	H640	K555	A454	A370	ALA	LEU	V179	V108	K28
T1196	S1091	K1002	V895	A807	I726	Q641	K558	A458	I371	ALA	GLU	K180	S110	P29
R1197	R1096	V1003	L902	T808	Q727	C642	L557	T461	E374	LYS	PRO	D181	K111	E30
G1199	V1099	F1008	L908	E810	E734	G643	L558	L473	E376	GLY	TYR	G182	I112	T31
V1200	V1106	F1011	Q917	E811	A735	L644	K560	L473	V377	LEU	PHE	E183	T114	I32
C1204	V1107	F1012	D739	L813	Q737	P645	G561	L477	A379	ARG	ALA	V185	L115	L37
Y1205	V1107	F1012	F740	A814	D741	M648	P563	E480	E382	PRO	GLU	K187	L116	K38
Y1207	R1108	F1012	D741	A815	G742	A649	E564	E480	E382	ARG	GLU	L191	S119	P39
D1208	E1109	E1012	F919	H816	G742	L850	L566	P484	V385	GLN	GLU	A192	L123	E40
L1209	G1112	E1013	R921	E817	Q744	P655	L567	P484	V385	VAL	VAL	E124	E124	D42
S1210	T1115	E1014	L922	E820	M745	F656	N569	S485	H388	ALA	ALA	V195	L127	D46
M1211	T1115	E1015	T927	A822	A746	L657	N569	S485	E389	ALA	GLU	R198	Y128	I49
A1212	T1118	E1016	K935	E822	H748	L658	E570	A487	P390	GLN	LEU	R198	F129	F50
R1213	S1119	E1017	R939	A822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	G51
P1214	S1119	E1018	T940	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	P52
V1215	T1123	E1019	F941	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	I53
G1218	P1125	E1020	S942	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	K54
E1219	D1126	E1021	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	D55
A1220	E1127	E1022	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	Y56
P1232	T1128	E1023	F939	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	C58
Q1235	T1129	E1024	T940	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	A59
L1236	T1130	E1025	F941	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	G60
THR	S1131	E1026	S942	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	G61
MET	L1132	E1027	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	K62
ARG	R1133	E1028	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	Y63
THR	L1134	E1029	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	R65
PHE	R1135	E1030	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	E74
HIS	K1136	E1031	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	R75
THR	L1137	E1032	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	V78
THR	R1138	E1033	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	E79
GLY	L1139	E1034	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	V80
VAL	G1146	E1035	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	T81
ALA	R1147	E1036	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	K82
GLY	R1151	E1037	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	S83
ALA	V1155	E1038	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	I84
ALA	L1156	E1039	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	V85
ASP	E1161	E1040	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	R86
ILE	E1162	E1041	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	R87
THR	G1163	E1042	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	Y88
Q1264	R1164	E1043	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	R89
R1258		E1044	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	I93
		E1045	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1046	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1047	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1048	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1049	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1050	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1051	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1052	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1053	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1054	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1055	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1056	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1057	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1058	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1059	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1060	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1061	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1062	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1063	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1064	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1065	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1066	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1067	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1068	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1069	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1070	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1071	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1072	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1073	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1074	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1075	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1076	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1077	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1078	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1079	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1080	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1081	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1082	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1083	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1084	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1085	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1086	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1087	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1088	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1089	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
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		E1091	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1092	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1093	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1094	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1095	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1096	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1097	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1098	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1099	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1100	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1101	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1102	T943	E822	H748	K659	R572	R488	A391	VAL	LYS	D200	S130	
		E1103	T943											



• Molecule 4: DNA-directed RNA polymerase subunit omega



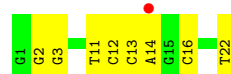
• Molecule 5: non-template DNA



• Molecule 6: RNA transcript



• Molecule 7: template DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.21Å 207.21Å 203.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.77 – 3.51 49.77 – 3.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.77-3.51) 87.9 (49.77-3.51)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8_1069, CNS	Depositor
R, R_{free}	0.263 , 0.322 0.265 , 0.325	Depositor DCC
R_{free} test set	3199 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	95.9	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24400	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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

5.1 Standard geometry

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	0.40	0/1791	0.83	4/2436 (0.2%)
1	B	0.39	0/1791	0.84	1/2436 (0.0%)
2	C	0.39	0/8711	0.87	19/11784 (0.2%)
3	D	0.40	1/10897 (0.0%)	0.85	21/14726 (0.1%)
4	E	0.40	0/768	0.91	2/1035 (0.2%)
5	N	0.11	0/252	0.57	0/386
6	R	0.11	0/212	0.23	0/328
7	T	0.12	0/500	0.58	0/768
All	All	0.39	1/24922 (0.0%)	0.84	47/33899 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	101	HIS	CG-ND1	5.18	1.44	1.38

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	705	ALA	CA-C-N	-10.81	106.33	119.84
3	D	705	ALA	C-N-CA	-10.81	106.33	119.84
2	C	792	VAL	CA-C-N	8.76	129.40	120.38
2	C	792	VAL	C-N-CA	8.76	129.40	120.38
2	C	247	PRO	N-CA-C	8.16	120.65	110.70

There are no chirality outliers.

There are no planarity outliers.

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	1759	0	1805	59	0
1	B	1759	0	1805	54	0
2	C	8548	0	8650	386	0
3	D	10714	0	10936	415	0
4	E	754	0	769	25	0
5	N	225	0	124	1	0
6	R	191	0	95	7	0
7	T	447	0	248	6	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	24400	0	24432	880	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 880 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:610:ARG:HG3	2:C:610:ARG:HH11	1.16	1.08
3:D:346:ARG:NH1	3:D:347:VAL:O	1.89	1.05
2:C:405:ARG:NH1	2:C:442:GLU:OE2	1.90	1.04
2:C:274:ARG:NH1	2:C:284:ARG:HH12	1.54	1.03
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.25	0.98

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/315 (70%)	193 (87%)	19 (9%)	9 (4%)	2	19
1	B	221/315 (70%)	199 (90%)	21 (10%)	1 (0%)	24	57
2	C	1077/1119 (96%)	901 (84%)	149 (14%)	27 (2%)	4	28
3	D	1352/1534 (88%)	1112 (82%)	189 (14%)	51 (4%)	2	20
4	E	91/99 (92%)	74 (81%)	14 (15%)	3 (3%)	3	23
All	All	2962/3382 (88%)	2479 (84%)	392 (13%)	91 (3%)	3	25

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	THR
2	C	2	GLU
2	C	111	ASP
2	C	164	PRO
2	C	213	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/273 (72%)	187 (95%)	9 (5%)	24	50
1	B	196/273 (72%)	189 (96%)	7 (4%)	31	57
2	C	912/941 (97%)	832 (91%)	80 (9%)	9	32
3	D	1147/1289 (89%)	1055 (92%)	92 (8%)	11	35
4	E	82/88 (93%)	72 (88%)	10 (12%)	5	22
All	All	2533/2864 (88%)	2335 (92%)	198 (8%)	11	36

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	371	ILE

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Mol	Chain	Res	Type
3	D	892	ASP
3	D	400	VAL
3	D	694	VAL
3	D	1001	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1064	ASN
3	D	350	HIS
4	E	28	GLN
3	D	125	GLN
3	D	388	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	8/29 (27%)	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 ⓘ

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 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 [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	223/315 (70%)	-0.15	0 100 100	45, 90, 147, 194	0
1	B	223/315 (70%)	-0.21	0 100 100	40, 86, 139, 173	0
2	C	1083/1119 (96%)	0.03	17 (1%) 70 45	32, 101, 186, 255	0
3	D	1358/1534 (88%)	0.01	23 (1%) 69 43	34, 102, 194, 264	0
4	E	93/99 (93%)	0.15	5 (5%) 31 18	58, 107, 184, 204	0
5	N	11/13 (84%)	0.62	0 100 100	369, 412, 462, 465	0
6	R	9/29 (31%)	0.80	0 100 100	178, 188, 215, 227	0
7	T	22/22 (100%)	0.88	1 (4%) 38 20	202, 334, 453, 466	0
All	All	3022/3446 (87%)	0.00	46 (1%) 72 47	32, 100, 193, 466	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	802	ALA	5.3
4	E	56	ASP	4.5
2	C	417	GLY	4.0
4	E	57	ASP	3.6
3	D	1090	ASP	3.5

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
8	ZN	D	1601	1/1	0.78	0.14	188,188,188,188	0
9	MG	D	1603	1/1	0.97	0.05	46,46,46,46	0
8	ZN	D	1602	1/1	0.99	0.04	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.