



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:35 PM UTC

PDB ID : 4WQS / pdb_00004wqs
Title : Thermus thermophilus RNA polymerase backtracked complex
Authors : Murayama, Y.; Sekine, S.; Yokoyama, S.
Deposited on : 2014-10-22
Resolution : 4.31 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

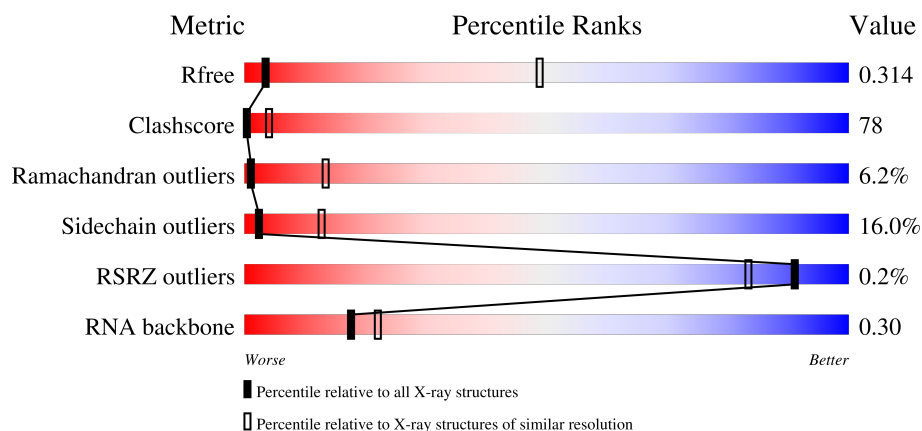
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.31 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.



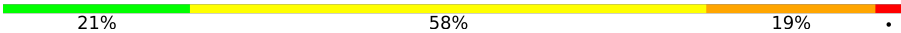
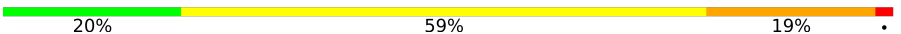
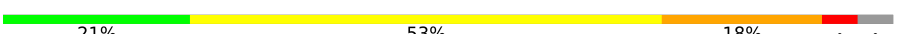
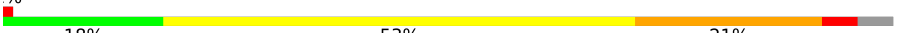
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)
RNA backbone	3983	1036 (5.50-3.10)

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	
1	K	315	
1	L	315	

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	G	28	
5	X	28	
6	H	16	
6	Y	16	
7	I	21	
7	Z	21	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 48166 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	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1151	Total	C	N	O	S	0	0	0
			9097	5753	1629	1682	33			
3	N	1288	Total	C	N	O	S	0	0	0
			10175	6441	1804	1899	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			
4	O	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

- Molecule 5 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	27	Total	C	N	O	P	0	0	0
			548	259	104	158	27			
5	X	27	Total	C	N	O	P	0	0	0
			548	259	104	158	27			

- Molecule 6 is a RNA chain called RNA (5'-R(P*CP*CP*AP*GP*CP*CP*GP*GP*CP*GP*CP*UP*CP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	16	Total	C	N	O	P	0	0	0
			340	151	61	112	16			
6	Y	15	Total	C	N	O	P	0	0	0
			318	141	56	106	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	17	Total	C	N	O	P	0	0	0
			357	169	65	106	17			
7	Z	17	Total	C	N	O	P	0	0	0
			357	169	65	106	17			

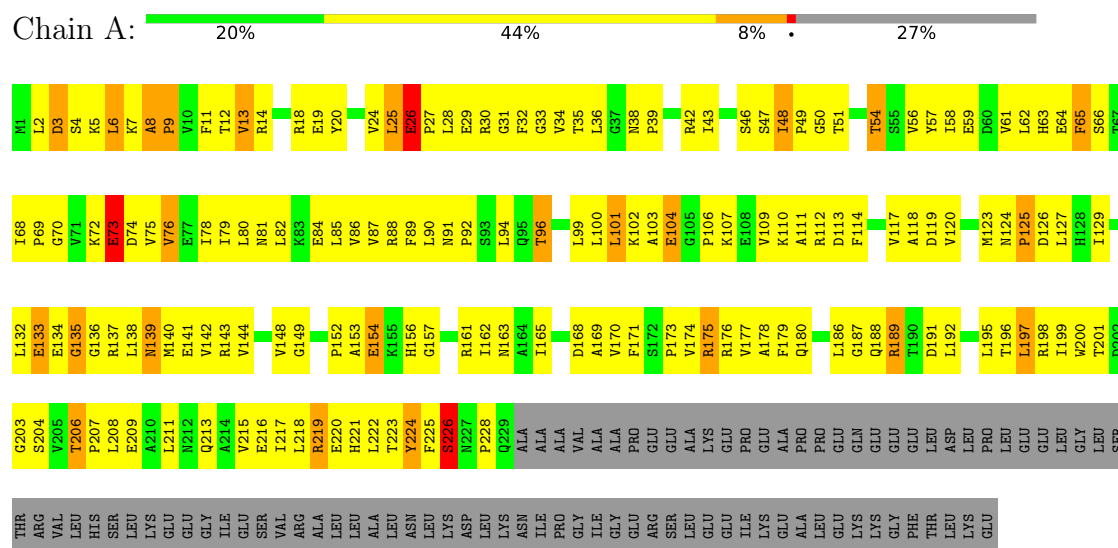
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

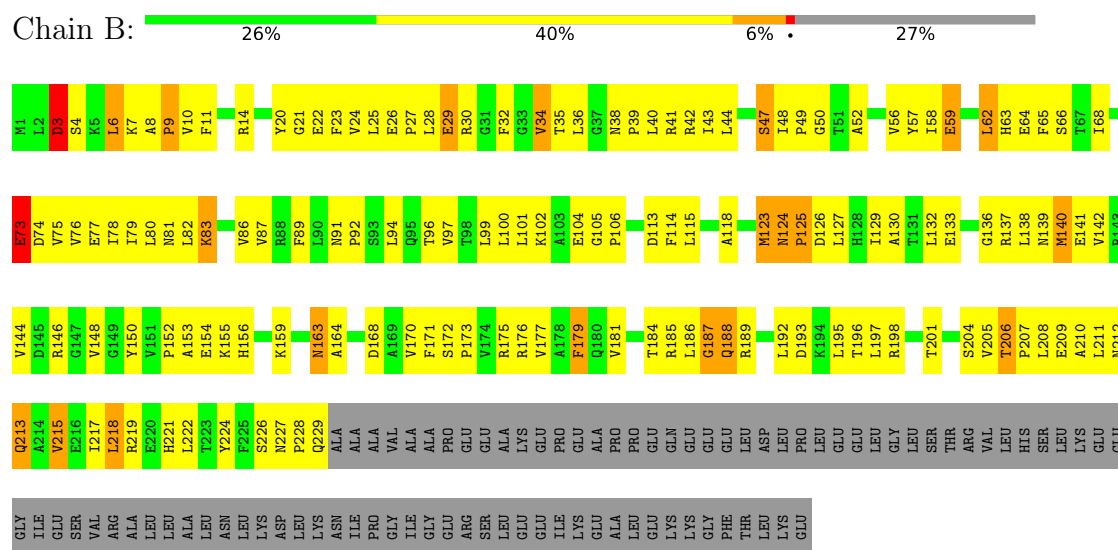
3 Residue-property plots

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

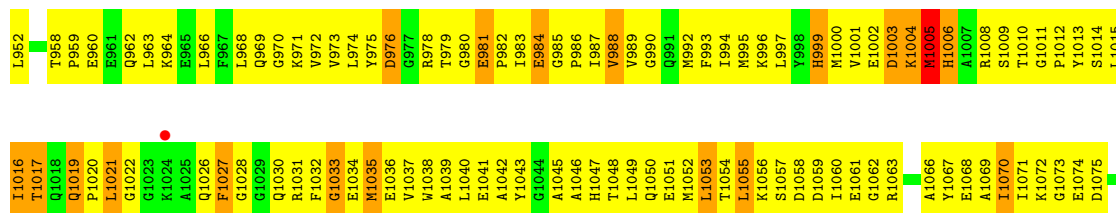


- Molecule 1: DNA-directed RNA polymerase subunit alpha

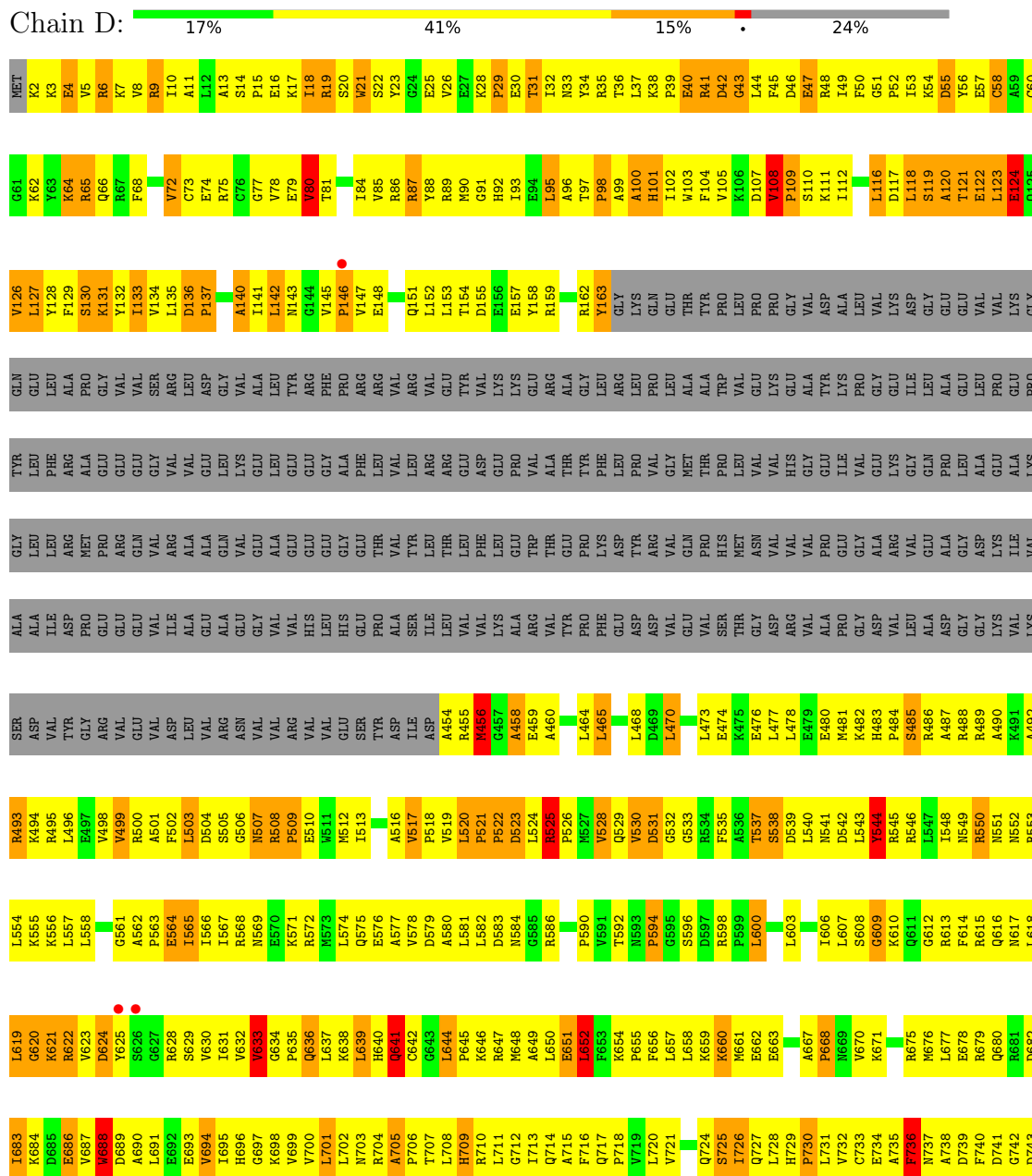
S1084	P1020	E960	A893	R831	S760	D698	L637	P577	E511	E442	T314	K252	K188
F1085	L1021	E961	G894	K832	F761	F699	D638	V678	R512	T443	T317	A253	R189
R1086	G1022	Q962	F896	L833	K762	T700	Q639	V579	V513	P444	V317	Y256	K190
V1087	L963	L963	F896	Q834	G763	T701	Q639	M580	V514			Y256	F191
L1088	L1024	Q964	L897	G835	E764	S702	P641	T581	A515	L451	G319	Y258	F192
V1089	A1025	E965	G898	G836	S765	I703	R642	G582	R516	L452	H320	Y258	L193
K1090	Q1026	L966	Q899	D837	E766	H704	V643	L583	R517	T453	E321	G259	V194
E1091	F1027	L967	R900	K838	P767	I705	V644	E584	K518	S454	V322	L260	L195
L1092	G1028	L968	Y901	L839	T768	E706	V645	E585	G519	L455	D323	L261	L196
Q1093	Q1029	Q969	I902	A840	E769	R707	Q646	R586	E520	A456	D324	A262	L197
A1094	G1030	G970	S903	R841	F770	I708	Q647	V587	P521	A457	I325	D263	L198
L1095	R1031	K971	P904	R842	E771	E709	R648	V588	I522	Y458	D326	P264	V199
A1096	F1032	R905	I905	R843	R772	I710	V649	R589	I523	A459	H327	R265	
L1097	G1033	V973	F906				R650	D590	V524	R460	L328	R266	Y202
D1098	M1034	L974	D907	K946	S776	R713	R651	S525	S525	V461	G329	Y267	D203
V1099	M1035	G947	R714	G947	E780	D714	Q652	L592	P526	E463	G330	D268	Q204
Q1100	I1036						D653	A593		L464	R331	L269	E205
T1101	V1037	G977	L717	A850	R783	L717	L654	A594	F531	L464	R332	G270	T206
L1102	W1038	R978	G718	K851	D784	G718	L655	L595	M532	G465	I333	E271	L207
D1103	A1039	T979	F719	L852	V785	F719	A656	V596	D533	F466	R334	A272	A208
E1104	L980	L918	E720	L853	D787	R721	D657	A597	L401	L467	T335	G273	R209
K1105	E981	A919	R722	P854	D787	I722	Q658	E598	S402	R468	V336	R274	E210
D1106	P982	Q920	I722	V855	T788	T723	A667	E599	S403	T469	G337	Y275	L211
L1107	I983	A921	R723	E856	T788	R723	A667	D600	R405	P470	E338	K276	G212
N1108	F922	D857	R724	D857	S789	R724	L668	G601	V539	Y471	L339	A277	A213
V1109	E923	R858	D725	R858	L790	D725	Q683	R602	F540	R472	K340	E278	Y214
D1110	V924	P859	I726	P859	R792	I726	Q674	V603	S541	R480	R345	L285	Q219
I1111	Y925	H860	F727	H860	V912	F727	Q675	A604	V542	D481	R346	L285	G220
F1112	F926	L861	R728	L861	R793	R728	L666	R605	N543	E482	G347	G287	L221
E1113	G927	P862	L729	P862	F794	L729	A667	V606	T544	V483	L348	G287	M222
G1114	K928	D863	S730	D863	G795	S730	L668	D607	N545	V484	R350	T289	E224
L1115	R929	G864	E796	G864	E796	E732	Q676	G608	L546	Y485	R351	L290	S225
A1116	K930	T865	G797	T865	R797	A732	Q677	R609	L547	M486	A352	A291	V226
R1119	G931	P866	R798	P866	R798	R733	N671	R610	P548	T487	R353	R292	F227
	E932	V867	L799	V867	L799	L734	L672	I611	F549	T489	G354	F293	
	G933	D868	V800	D868	V800	R735	L673	V612	L550	E490	V355	E294	R230
	V936	L870	R802	L870	R802	D736	V674	V613		E491	E357	G296	P231
	D937	L871	R803	L871	R803	R737	A675	R614	B583	D492	R358	E297	A234
	H999	N872	R804	N872	R804	D738	A676	V615	D554	T496	D365	F298	L235
	M1000	P873	R805	P873	R805	E739	N677	E616	A555	A497	D429	K299	L236
	V1001	L874		L874		E740	F678	D617	N556	A498	V430	D300	R237
	E1002	G875	P811	G875	P811	G741	F679	G618	R557	Q498	V302	E301	L238
	K1003	V876	G812	V876	G812	V742	Q681	R619	A558	A499	T368	F303	F239
	A1004	P877	V613	P877	V613	R743	N681	L620	A568	N500	P369	L304	T240
	H1006	R878	E814	R878	E814	I745	N683	V621	S562	T501	T433	P305	L242
	A1007	R879	L815	R879	L815	G746	F684	E622	G561	P502	H434	T306	R243
	R1008	N880	K816	N880	K816	A747	E685	P624	N563	L503	V435	L372	P244
	E1009	L882	P817	L882	P817	E748	D686	R626	M564	Q498	G436	R308	G245
	T1010	G883	G818	G883	G818	V749	A687	R627	O565	A499	H431	Y309	T246
	G1011	Q884	V619	Q884	V619	K750	L688	R627	T566	N500	T369	L310	P247
	P1012	L885	R820	L885	R820	P751	V689	F628	Q567		A370	P305	F311
	Y1013	L886	R824	L886	R824	G752	N691	V629	P570	L496	K371	T306	R250
	S1014	E887	V826	E887	V826	D753	E692	R630	L571	P503	L372	L307	A312
	I1015	T883	Y826	T883	Y826	I754	E693	R631	I572	E435	G436	G245	
	I1016	H889	V827	H889	V827	V755	L694	Q633	A573	N506	R437	Y309	T246
	Q1017	L890	A828	L890	A828	V756	L695	G634	A574	R507	I438	L310	P247
	Q1018	G891	R829	G891	R829	G757	L696	T635	A575	L508	C439	F311	
	Q1019	L892	K830	L892	K830	T759	R697	A636	A576	A510	P440	L312	R250

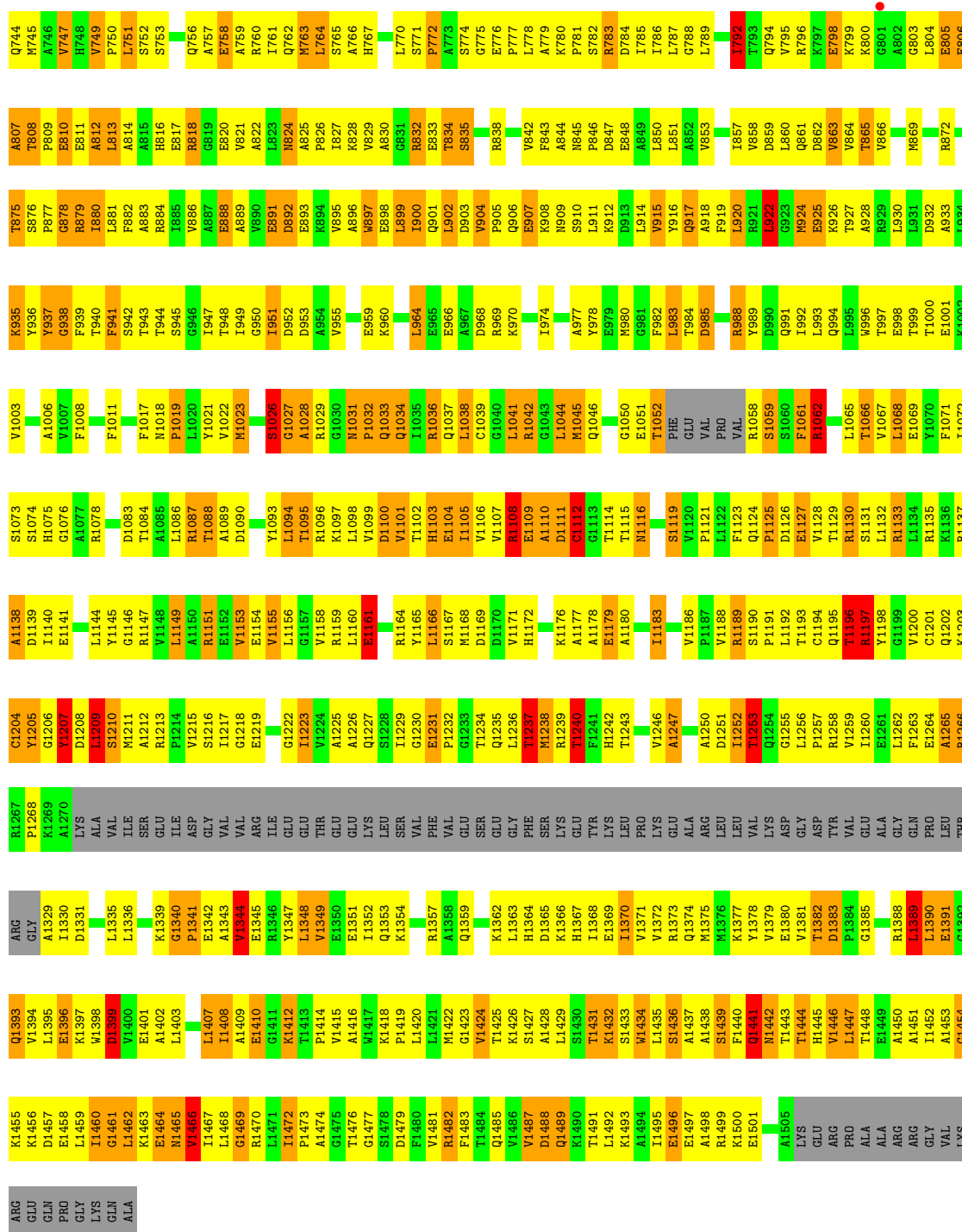
- Molecule 2: DNA-directed RNA polymerase subunit beta



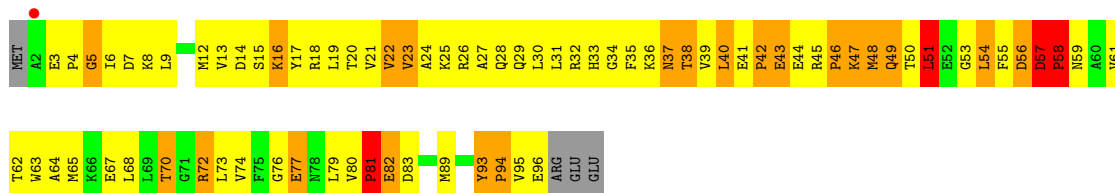


• Molecule 3: DNA-directed RNA polymerase subunit beta'





E1001	L934	G870	P809	V749	E686	V623	G561	A501	R441	PRO	MET	ALA	G194	V126	K64
G871	K935	K871	E810	P750	V687	D624	A562	F502	R442	GLU	PRO	GLU	G194	L127	K65
L872	E936	L872	E811	P751	V688	Y625	P563	L503	V443	GLU	ARG	GLU	V196	F128	K66
L873	Y937	L873	A812	S752	D689	S626	E564	D504	V444	GLN	GLN	GLU	G196	F129	K67
E874	L813	E874	L813	S753	A690	G627	I565	S505	V444	VAL	VAL	GLY	S197	F130	F68
L875	L814	L875	A814	S754	L691	R628	I566	G506	R445	ILE	ARG	VAL	R198	K131	E69
S876	A815	S876	A815	A755	E692	G629	I567	N507	V446	ALA	ALA	VAL	L199	Y132	
P877	H816	P877	H816	Q756	E693	V630	R568	R508	V447	GLU	ALA	GLU	D200	I133	V72
E878	E817	E878	E817	A757	E694	L631	R569	P509	E448	LEU	GLN	LEU	G201	V134	C73
R879	R818	R879	R818	E758	L695	V632	E570	E510	S449	VAL	VAL	GLY	V202	E74	E74
G819	G819	G819	G819	A759	R696	V633	K571	W511		GLY	GLU	GLU	A203	D136	R75
E820	E820	E820	E820	A760	G697	G634	B572	R512	1452	VAL	ALA	LEU	L204	P137	C76
R821	R821	R821	R821	R761	K698		B573	I513	D453	VAL	GLU	GLU	Y205	G138	G77
L761	L761	L761	L761	R761	K698		L574	L514	A454	HIS	GLU	GLU	R206	G139	V78
Q762	Q762	Q762	A822	Q762	V699	L637	L574	L514	A454	LEU	GLU	GLY	F207	A140	E79
M763	M763	M763	L823	M763	V700	K638	Q575	E515	R455	LEU	GLU	GLY	PRO	I141	R80
L764	L764	L764	L701	L764	V700	L639	E576	A516	R456	HIS	GLY	ALA	ARG	N142	T81
S765	S765	S765	L701	S765	L702	R640	A577	G517	R456	GLU	GLU	PHE	ARG	L142	T81
A766	A766	A766	H640	A766	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
H767	H767	H767	H640	H767	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
R768	R768	R768	H640	R768	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L769	L769	L769	H640	L769	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L770	L770	L770	H640	L770	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
S771	S771	S771	H640	S771	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
P772	P772	P772	H640	P772	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
A773	A773	A773	H640	A773	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
S774	S774	S774	H640	S774	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
G775	G775	G775	H640	G775	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
E776	E776	E776	H640	E776	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L777	L777	L777	H640	L777	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
A778	A778	A778	H640	A778	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
R779	R779	R779	H640	R779	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
K780	K780	K780	H640	K780	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
P781	P781	P781	H640	P781	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
S782	S782	S782	H640	S782	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
R783	R783	R783	H640	R783	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
D784	D784	D784	H640	D784	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L785	L785	L785	H640	L785	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
R786	R786	R786	H640	R786	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
G787	G787	G787	H640	G787	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L788	L788	L788	H640	L788	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L789	L789	L789	H640	L789	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
Y790	Y790	Y790	H640	Y790	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L791	L791	L791	H640	L791	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L852	L852	L852	H640	L852	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
V853	V853	V853	H640	V853	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
A854	A854	A854	H640	A854	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
H855	H855	H855	H640	H855	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L856	L856	L856	H640	L856	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L857	L857	L857	H640	L857	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L858	L858	L858	H640	L858	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L859	L859	L859	H640	L859	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L860	L860	L860	H640	L860	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L861	L861	L861	H640	L861	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L862	L862	L862	H640	L862	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L863	L863	L863	H640	L863	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L864	L864	L864	H640	L864	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L865	L865	L865	H640	L865	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L866	L866	L866	H640	L866	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L867	L867	L867	H640	L867	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L868	L868	L868	H640	L868	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L869	L869	L869	H640	L869	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L870	L870	L870	H640	L870	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L871	L871	L871	H640	L871	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L872	L872	L872	H640	L872	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L873	L873	L873	H640	L873	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L874	L874	L874	H640	L874	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L875	L875	L875	H640	L875	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L876	L876	L876	H640	L876	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L877	L877	L877	H640	L877	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L878	L878	L878	H640	L878	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L879	L879	L879	H640	L879	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L880	L880	L880	H640	L880	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L881	L881	L881	H640	L881	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L882	L882	L882	H640	L882	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L883	L883	L883	H640	L883	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L884	L884	L884	H640	L884	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L885	L885	L885	H640	L885	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L886	L886	L886	H640	L886	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L887	L887	L887	H640	L887	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L888	L888	L888	H640	L888	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L889	L889	L889	H640	L889	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L890	L890	L890	H640	L890	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L891	L891	L891	H640	L891	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L892	L892	L892	H640	L892	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L893	L893	L893	H640	L893	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L894	L894	L894	H640	L894	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L895	L895	L895	H640	L895	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L896	L896	L896	H640	L896	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L897	L897	L897	H640	L897	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L898	L898	L898	H640	L898	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L899	L899	L899	H640	L899	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L900	L900	L900	H640	L900	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L901	L901	L901	H640	L901	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L902	L902	L902	H640	L902	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L903	L903	L903	H640	L903	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L904	L904	L904	H640	L904	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG	N142	T81
L905	L905	L905	H640	L905	L702	H640	A577	G517	R456	GLU	GLU	PHE	ARG		

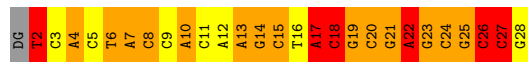


- Molecule 5: DNA (28-MER)

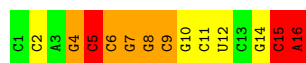




- Molecule 5: DNA (28-MER)



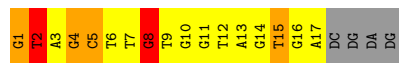
- Molecule 6: RNA (5'-R(P*CP*CP*AP*GP*CP*CP*GP*GP*CP*GP*CP*UP*CP*GP*CP*A)-3')



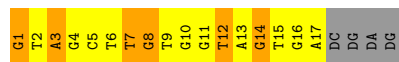
- Molecule 6: RNA (5'-R(P*CP*CP*AP*GP*CP*CP*GP*GP*CP*GP*CP*UP*CP*GP*CP*A)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	155.98Å 155.98Å 495.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.15 – 4.31 44.15 – 4.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.15-4.31) 99.4 (44.15-4.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 4.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.281 , 0.311 0.284 , 0.314	Depositor DCC
R_{free} test set	3821 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	106.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 156.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.499 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	48166	wwPDB-VP
Average B, all atoms (Å ²)	250.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% 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

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	0.51	0/1838	1.09	14/2498 (0.6%)
1	B	0.53	0/1838	1.07	7/2498 (0.3%)
1	K	0.57	1/1838 (0.1%)	1.09	10/2498 (0.4%)
1	L	0.53	0/1838	1.10	15/2498 (0.6%)
2	C	0.63	1/8997 (0.0%)	1.25	110/12164 (0.9%)
2	M	0.61	0/8997	1.23	93/12164 (0.8%)
3	D	0.65	2/9249 (0.0%)	1.30	126/12482 (1.0%)
3	N	0.66	0/10344	1.27	118/13968 (0.8%)
4	E	0.63	0/784	1.45	11/1057 (1.0%)
4	O	0.57	0/784	1.30	9/1057 (0.9%)
5	G	0.56	0/614	1.46	14/943 (1.5%)
5	X	0.53	0/614	1.52	17/943 (1.8%)
6	H	0.75	0/378	1.34	5/585 (0.9%)
6	Y	0.75	0/353	1.17	4/546 (0.7%)
7	I	0.49	0/400	1.21	3/616 (0.5%)
7	Z	0.46	0/400	1.04	2/616 (0.3%)
All	All	0.62	4/49266 (0.0%)	1.25	558/67133 (0.8%)

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
5	G	0	10
5	X	0	11
6	H	0	4
6	Y	0	5
7	I	0	6
7	Z	0	4
All	All	0	40

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1246	VAL	CA-CB	5.50	1.61	1.54
3	D	726	ILE	CA-CB	-5.21	1.48	1.54
1	K	76	VAL	CA-CB	-5.04	1.48	1.54
2	C	702	SER	CA-C	-5.01	1.46	1.52

The worst 5 of 558 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	93	TYR	CA-C-N	17.64	137.32	118.97
4	E	93	TYR	C-N-CA	17.64	137.32	118.97
3	D	1247	ALA	N-CA-C	-16.96	92.82	111.14
3	N	1209	LEU	N-CA-C	-15.19	85.96	109.96
3	D	1209	LEU	N-CA-C	-15.05	86.17	109.96

There are no chirality outliers.

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	G	10	DA	Sidechain
5	G	2	DT	Sidechain
5	G	3	DC	Sidechain
5	G	4	DA	Sidechain
5	G	9	DC	Sidechain

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	1806	0	1861	267	0
1	B	1806	0	1861	189	0
1	K	1806	0	1861	205	0
1	L	1806	0	1861	213	0
2	C	8829	0	8933	1477	0
2	M	8829	0	8933	1485	0
3	D	9097	0	9316	1681	0
3	N	10175	0	10401	1839	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	770	0	784	130	0
4	O	770	0	784	159	0
5	G	548	0	301	114	0
5	X	548	0	301	93	0
6	H	340	0	176	78	0
6	Y	318	0	165	58	0
7	I	357	0	194	68	0
7	Z	357	0	194	71	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
All	All	48166	0	47926	7443	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 78.

The worst 5 of 7443 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:52:PHE:CZ	2:C:68:PHE:HB2	1.22	1.67
3:D:897:TRP:HA	3:D:900:ILE:CG1	1.33	1.56
3:D:1041:LEU:HD11	3:D:1045:MET:SD	1.55	1.44
3:D:705:ALA:HB1	6:H:14:G:N2	1.24	1.40
3:D:744:GLN:CD	5:G:21:DG:H21	1.34	1.34

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	227/315 (72%)	194 (86%)	24 (11%)	9 (4%)	2	18
1	B	227/315 (72%)	195 (86%)	23 (10%)	9 (4%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	227/315 (72%)	193 (85%)	26 (12%)	8 (4%)	3	20
1	L	227/315 (72%)	201 (88%)	17 (8%)	9 (4%)	2	18
2	C	1117/1119 (100%)	893 (80%)	151 (14%)	73 (6%)	1	13
2	M	1117/1119 (100%)	889 (80%)	153 (14%)	75 (7%)	1	12
3	D	1143/1524 (75%)	903 (79%)	167 (15%)	73 (6%)	1	13
3	N	1280/1524 (84%)	1011 (79%)	190 (15%)	79 (6%)	1	13
4	E	93/99 (94%)	67 (72%)	15 (16%)	11 (12%)	0	4
4	O	93/99 (94%)	69 (74%)	13 (14%)	11 (12%)	0	4
All	All	5751/6744 (85%)	4615 (80%)	779 (14%)	357 (6%)	1	13

5 of 357 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	29	GLU
1	A	118	ALA
1	A	133	GLU
1	A	187	GLY

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	202/273 (74%)	181 (90%)	21 (10%)	7	23
1	B	202/273 (74%)	180 (89%)	22 (11%)	6	22
1	K	202/273 (74%)	183 (91%)	19 (9%)	8	27
1	L	202/273 (74%)	177 (88%)	25 (12%)	4	18
2	C	941/941 (100%)	775 (82%)	166 (18%)	2	11
2	M	941/941 (100%)	783 (83%)	158 (17%)	2	12
3	D	968/1279 (76%)	803 (83%)	165 (17%)	2	12
3	N	1088/1279 (85%)	913 (84%)	175 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	84/88 (96%)	66 (79%)	18 (21%)	1	6
4	O	84/88 (96%)	69 (82%)	15 (18%)	2	11
All	All	4914/5708 (86%)	4130 (84%)	784 (16%)	2	13

5 of 784 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	186	VAL
2	M	960	GLU
2	M	261	ILE
2	M	178	PRO
2	M	584	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	669	ASN
3	N	1034	GLN
3	N	744	GLN
3	N	1010	ASN
4	O	29	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	H	15/16 (93%)	5 (33%)	1 (6%)
6	Y	14/16 (87%)	3 (21%)	1 (7%)
All	All	29/32 (90%)	8 (27%)	2 (6%)

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	H	4	G
6	H	5	C
6	H	6	C
6	H	15	C
6	H	16	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	H	5	C
6	Y	5	C

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 4 ligands modelled in this entry, 4 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	229/315 (72%)	-0.94	0 100 100	154, 243, 347, 432	0
1	B	229/315 (72%)	-0.81	0 100 100	202, 343, 460, 525	0
1	K	229/315 (72%)	-0.86	1 (0%) 88 77	157, 255, 375, 500	0
1	L	229/315 (72%)	-0.79	0 100 100	193, 363, 452, 538	0
2	C	1119/1119 (100%)	-0.90	2 (0%) 91 83	12, 213, 336, 454	0
2	M	1119/1119 (100%)	-0.90	3 (0%) 90 80	60, 238, 426, 549	0
3	D	1151/1524 (75%)	-0.93	4 (0%) 90 80	8, 205, 382, 548	0
3	N	1288/1524 (84%)	-0.94	2 (0%) 91 83	81, 249, 452, 545	0
4	E	95/99 (95%)	-0.97	0 100 100	156, 217, 337, 395	0
4	O	95/99 (95%)	-0.87	1 (1%) 78 62	205, 297, 426, 451	0
5	G	27/28 (96%)	-0.72	0 100 100	152, 210, 372, 381	0
5	X	27/28 (96%)	-0.63	0 100 100	238, 279, 353, 374	0
6	H	16/16 (100%)	-0.82	0 100 100	97, 189, 363, 385	0
6	Y	15/16 (93%)	-0.90	0 100 100	208, 249, 351, 378	0
7	I	17/21 (80%)	-0.64	0 100 100	215, 276, 418, 428	0
7	Z	17/21 (80%)	-0.72	0 100 100	264, 305, 348, 352	0
All	All	5902/6874 (85%)	-0.90	13 (0%) 91 83	8, 240, 416, 549	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	626	SER	4.6
2	M	416	GLY	4.1
3	D	146	PRO	4.0
3	N	801	GLY	3.2
2	C	1024	LYS	2.8

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	1.00	0.06	72,72,72,72	0
8	ZN	D	1602	1/1	1.00	0.01	72,72,72,72	0
8	ZN	N	1601	1/1	1.00	0.01	72,72,72,72	0
8	ZN	N	1602	1/1	1.00	0.00	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.