



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:03 AM UTC

PDB ID : 2JA7 / pdb_00002ja7
Title : CPD lesion containing RNA Polymerase II elongation complex C
Authors : Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.
Deposited on : 2006-11-23
Resolution : 3.80 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

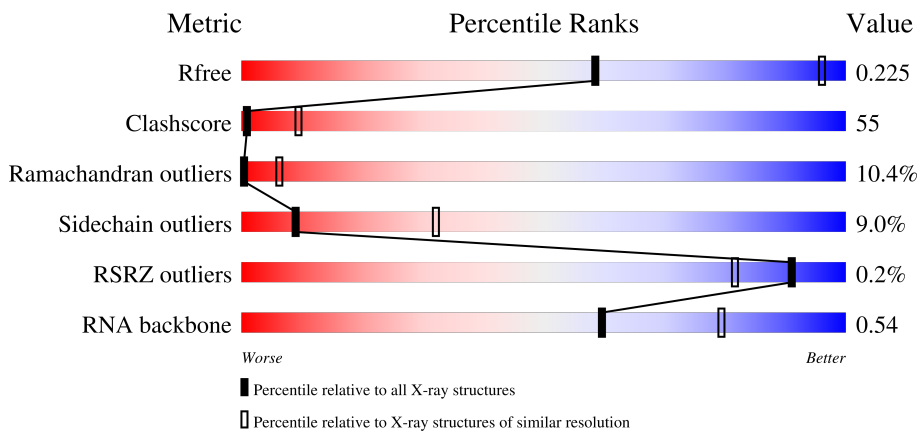
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





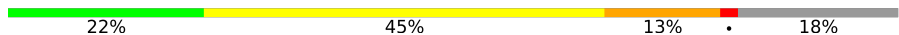

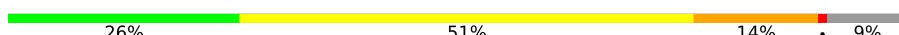
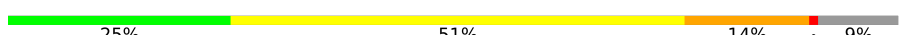
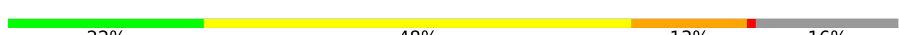
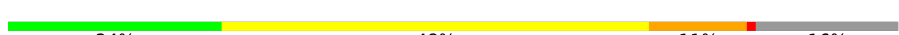



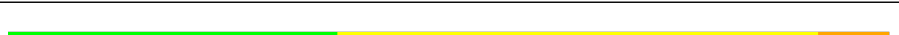

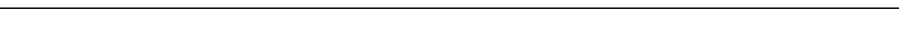
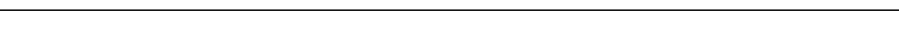
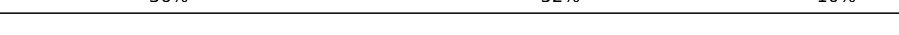

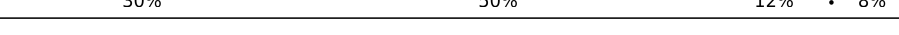
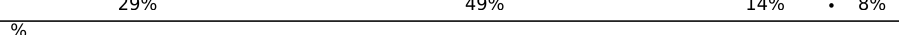

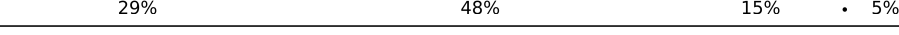


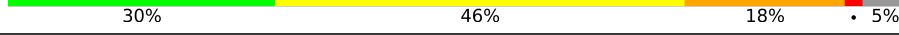

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

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	1	14	
1	4	14	
2	2	25	
2	5	25	


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	3	11	
3	6	11	
4	A	1733	
4	M	1733	
5	B	1224	
5	N	1224	
6	C	318	
6	O	318	
7	D	221	
7	P	221	
8	E	215	
8	Q	215	
9	F	155	
9	R	155	
10	G	171	
10	S	171	
11	H	146	
11	T	146	
12	I	122	
12	U	122	
13	J	70	
13	V	70	
14	K	120	
14	W	120	
15	L	70	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	X	70	 17% 40% 7% 34%

2 Entry composition i

There are 17 unique types of molecules in this entry. The entry contains 63924 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 DNA chain called 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	7	Total	C	N	O	P	0	0	0
			141	69	27	39	6			
1	4	7	Total	C	N	O	P	0	0	0
			141	69	27	39	6			

- Molecule 2 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TTP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	2	18	Total	Br	C	N	O	P	0	0	0
			380	1	186	60	116	17			
2	5	18	Total	Br	C	N	O	P	0	0	0
			380	1	186	60	116	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	10	Total	C	N	O	P	0	0	0
			212	96	41	66	9			
3	6	10	Total	C	N	O	P	0	0	0
			212	96	41	66	9			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1421	Total	C	N	O	S	0	0	0
			11186	7048	1958	2118	62			
4	M	1421	Total	C	N	O	S	0	0	0
			11186	7048	1958	2118	62			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	1115	Total 8866	C 5614	N 1553	O 1644	S 55	0	0	0
5	N	1115	Total 8866	C 5614	N 1553	O 1644	S 55	0	0	0

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	C	267	Total 2101	C 1320	N 349	O 419	S 13	0	0	0
6	O	267	Total 2101	C 1320	N 349	O 419	S 13	0	0	0

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	D	177	Total 1427	C 882	N 256	O 287	S 2	0	0	0
7	P	177	Total 1427	C 882	N 256	O 287	S 2	0	0	0

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	E	214	Total 1752	C 1111	N 309	O 321	S 11	0	0	0
8	Q	214	Total 1752	C 1111	N 309	O 321	S 11	0	0	0

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	F	87	Total 705	C 451	N 119	O 132	S 3	0	0	0
9	R	87	Total 705	C 451	N 119	O 132	S 3	0	0	0

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			
10	S	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			
11	T	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			
12	U	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			
13	V	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			
14	W	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 15 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7

KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			
15	X	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	M	1	Total	Mg	0	0
			1	1		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Zn	0	0
			2	2		
17	B	1	Total	Zn	0	0
			1	1		
17	C	1	Total	Zn	0	0
			1	1		
17	I	2	Total	Zn	0	0
			2	2		
17	J	1	Total	Zn	0	0
			1	1		
17	L	1	Total	Zn	0	0
			1	1		
17	M	2	Total	Zn	0	0
			2	2		
17	N	1	Total	Zn	0	0
			1	1		
17	O	1	Total	Zn	0	0
			1	1		
17	U	2	Total	Zn	0	0
			2	2		
17	V	1	Total	Zn	0	0
			1	1		
17	X	1	Total	Zn	0	0
			1	1		

3 Residue-property plots [i](#)

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: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'

Chain 1: 



- Molecule 1: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'

Chain 4: 



- Molecule 2: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TP*TP*TTP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'

Chain 2: 



- Molecule 2: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TP*TP*TTP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'

Chain 5: 




- Molecule 3: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'

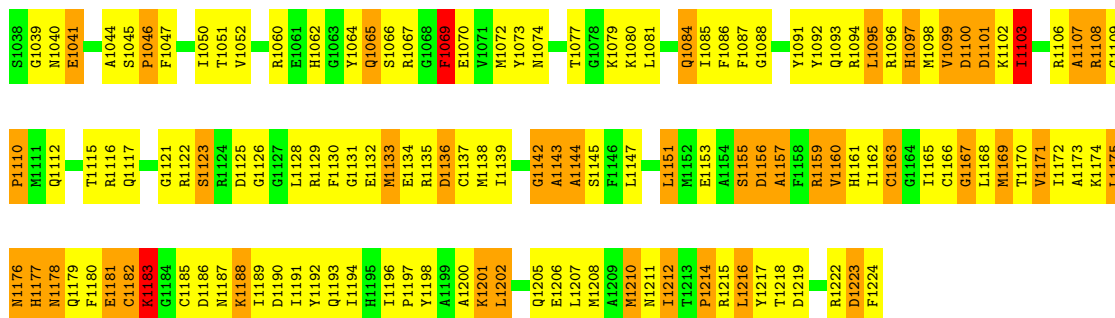
Chain 3: 



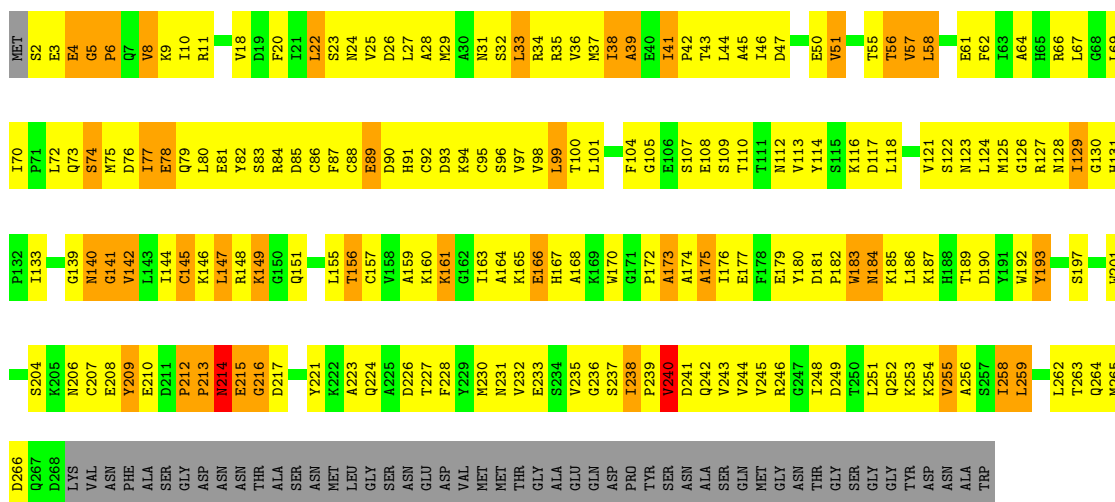
- Molecule 3: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'

Chain 6: 

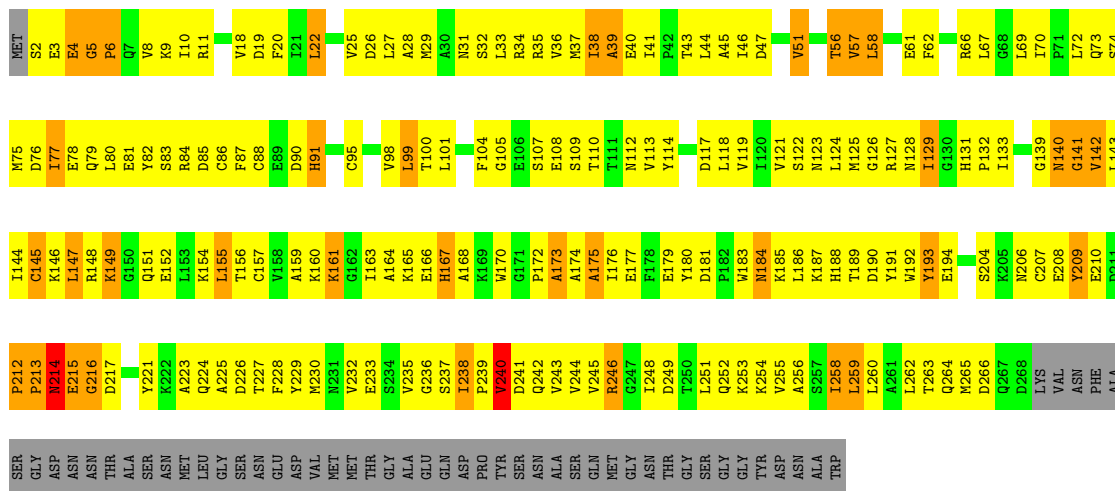
V1066	L1067	Q1070	S1071	L1072	G1073	E1074	P1075	A1076	T1077	M1078	M1079	T1080	L1081	ASN	THR	PHE	HIS	PHE	ALA	GLY	VAL	ALA	SER	K1092	K1093	V1094	T1095	S1096	G1097	V1098	P1099	R1100	L1101	K1102	M1106	V1107	M1110	M1111	K1112	T1113	P1114	S1115	L1116	T1117	V1118	Y1119	L1120	E1121	P1122	H1123	H1124	A1125	A1126	D1127	E1129																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
K834	Q835	L836	F837	V838	K839	E840	K841	F842	L843	F844	G845	V846	W847	P848	P849	P850	P851	P852	P853	P854	P855	P856	P857	P858	P859	P860	P861	P862	P863	P864	P865	P866	P867	P868	P869	P870	P871	P872	P873	P874	P875	P876	P877	P878	P879	P880	P881	P882	P883	P884	P885	P886	P887	P888	P889	P890	P891	P892	P893	P894	P895	P896	P897	P898	P899	P900	P901	P902	P903	P904	P905	P906	P907	P908	P909	P910	P911	P912	P913	P914	P915	P916	P917	P918	P919	P920	P921	P922	P923	P924	P925	P926	P927	P928	P929	P930	P931	P932	P933																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
E801	R802	S803	Y804	R805	K806	G807	L808	T809	R810	Q811	Q812	D813	D814	F815	H816	A817	M818	R819	E820	G821	F822	F823	L824	I825	D826	T827	A828	R829	R830	R831	T832	R833	R834	G835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	D847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
E731	L732	V733	L734	K735	K736	K737	V738	L739	L740	N741	N742	V743	K744	Q745	L746	V747	G748	G749	F750	G751	G752	S753	F754	F755	F756	F757	F758	A759	Q760	M761	R762	A763	G764	V765	E766	A767	Q768	R769	N770	L771	T772	F773	G774	G775	G776	G777	G778	F779	V780	D781	R782	T783	L784	F785	H786	F787	S788	K789	L790	T791	R792	L793	E794	S795	L796	L797	L798	L799	L800	G801	F802	F803	F804	F805	F806	F807	F808	F809	F810	F811	F812	F813	F814	F815	F816	F817	F818	F819	F820	F821	F822	F823	F824	F825	F826	F827	F828	F829	F830	F831	F832	F833	F834	F835	F836	F837	F838	F839	F840	F841	F842	F843	F844	F845	F846	F847	F848	F849	F850	F851	F852	F853	F854	F855	F856	F857	F858	F859	F860	F861	F862	F863	F864	F865	F866	F867	F868	F869	F870	F871	F872	F873	F874	F875	F876	F877	F878	F879	F880	F881	F882	F883	F884	F885	F886	F887	F888	F889	F890	F891	F892	F893	F894	F895	F896	F897	F898	F899	F900	F901	F902	F903	F904	F905	F906	F907	F908	F909	F910	F911	F912	F913	F914	F915	F916	F917	F918	F919	F920	F921	F922	F923	F924	F925	F926	F927	F928	F929	F930	F931	F932	F933																																																																																																																																																																																																																																																																																																																																																																																																											
E656	L657	L658	G659	F660	F661	F662	S663	T664	G665	L666	G667	L668	L669	L670	A671	D672	G673	P674	T675	M676	L677	L678	L679	T680	T681	T682	T683	A684	V685	W686	W687	W688	W689	W690	W691	W692	W693	W694	W695	W696	W697	W698	W699	W700	L701	T702	T703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	R1000	G1002	K1003																																																																																																																																																																																																																																																											
K403	Y404	V405	L406	R407	D408	S409	G410	D411	L412	L413	D414	T415	L416	R417	Y418	S419	S420	S421	S422	S423	S424	S425	S426	S427	S428	S429	S430	S431	S432	S433	S434	S435	S436	S437	S438	S439	S440	S441	S442	S443	S444	S445	S446	S447	S448	S449	S450	S451	S452	S453	S454	S455	S456	S457	S458	S459	S460	S461	S462	S463	S464	S465	S466	S467	S468	S469	S470	S471	S472	S473	S474	S475	S476	S477	S478	S479	S480	S481	S482	S483	S484	S485	S486	S487	S488	S489	S490	S491	S492	S493	S494	S495	S496	S497	S498	S499	S500	S501	S502	S503	S504	S505	S506	S507	S508	S509	S510	S511	S512	S513	S514	S515	S516	S517	S518	S519	S520	S521	S522	S523	S524	S525	S526	S527	S528	S529	S530	S531	S532	S533	S534	S535	S536	S537	S538	S539	S540	S541	S542	S543	S544	S545	S546	S547	S548	S549	S550	S551	S552	S553	S554	S555	S556	S557	S558	S559	S560	S561	S562	S563	S564	S565	S566	S567	S568	S569	S570	S571	S572	S573	S574	S575	S576	S577	S578	S579	S580	S581	S582	S583	S584	S585	S586	S587	S588	S589	S590	S591	S592	S593	S594	S595	S596	S597	S598	S599	S600	S601	S602	S603	S604	S605	S606	S607	S608	S609	S610	S611	S612	S613	S614	S615	S616	S617	S618	S619	S620	S621	S622	S623	S624	S625	S626	S627	S628	S629	S630	S631	S632	S633	S634	S635	S636	S637	S638	S639	S640	S641	S642	S643	S644	S645	S646	S647	S648	S649	S650	S651	S652	S653	S654	S655	S656	S657	S658	S659	S660	S661	S662	S663	S664	S665	S666	S667	S668	S669	S670	S671	S672	S673	S674	S675	S676	S677	S678	S679	S680	S681	S682	S683	S684	S685	S686	S687	S688	S689	S690	S691	S692	S693	S694	S695	S696	S697	S698	S699	S700	S701	S702	S703	S704	S705	S706	S707	S708	S709	S710	S711	S712	S713	S714	S715	S716	S717	S718	S719	S720	S721	S722	S723	S724	S725	S726	S727	S728	S729	S730	S731	S732	S733	S734	S735	S736	S737	S738	S739	S740	S741	S742	S743	S744	S745	S746	S747	S748	S749	S750	S751	S752	S753	S754	S755	S756	S757	S758	S759	S760	S761	S762	S763	S764	S765	S766	S767	S768	S769	S770	S771	S772	S773	S774	S775	S776	S777	S778	S779	S780	S781	S782	S783	S784	S785	S786	S787	S788	S789	S790	S791	S792	S793	S794	S795	S796	S797	S798	S799	S800	S801	S802	S803	S804	S805	S806	S807	S808	S809	S810	S811	S812	S813	S814	S815	S816	S817	S818	S819	S820	S821	S822	S823	S824	S825	S826	S827	S828	S829	S830	S831	S832	S833	S834	S835	S836	S837	S838	S839	S840	S841	S842	S843	S844	S845	S846	S847	S848	S849	S850	S851	S852	S853	S854	S855	S856	S857	S858	S859	S860	S861	S862	S863	S864	S865	S866	S867	S868	S869	S870	S871	S872	S873	S874	S875	S876	S877	S878	S879	S880	S881	S882	S883	S884	S885	S886	S887	S888	S889	S890	S891	S892	S893	S894	S895	S896	S897	S898	S899	S900	S901	S902	S903	S904	S905	S906	S907	S908	S909	S910	S911	S912	S913	S914	S915	S916	S917	S918	S919	S920	S921	S922	S923	S924	S925	S926	S927	S928	S929	S930	S931	S932	S933	S934	S935	S936	S937	S938	S939	S940	S941	S942	S943	S944	S945	S946	S947	S948	S949	S950	S951	S952	S953	S954	S955	S956	S957	S958	S959	S960	S961	S962	S963	S964	S965	S966	S967	S968	S969	S970	S971	S972	S973	S974	S975	S976	S977	S978	S979	S980	S981	S982	S983	S984	S985	S986	S987	S988	S989	S990	S991	S992	S993	S994	S995	S996	S997	S998	S999	S1000
N273	I274	S275	L276	E277	T278	L279	E280	H281	K282	N283	G283	F284	P285	H286	H287	A288	F288	S289	R290	P291	E292	W293	M294	I295	G166	T297	F298	L299	V300	A301	L239	T302	I170	Y303	M304	P242	P243	P244	P245	V246	R247	A309	G310	S249	D250	S251	P252	N253	Q316	E254	S255	ASP	Q256	R257	G258	E259	D260	D261	L262	T263	F264	K265	L266	T204	L267	A268	E206	L207	L208	N209	K271	G334																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
R385	I386	R387	G388	N389	L340	M341																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															



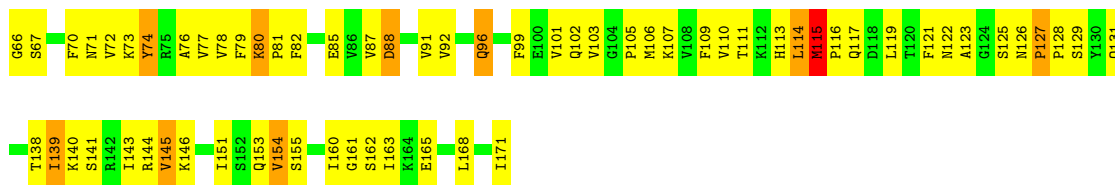
• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE



• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE

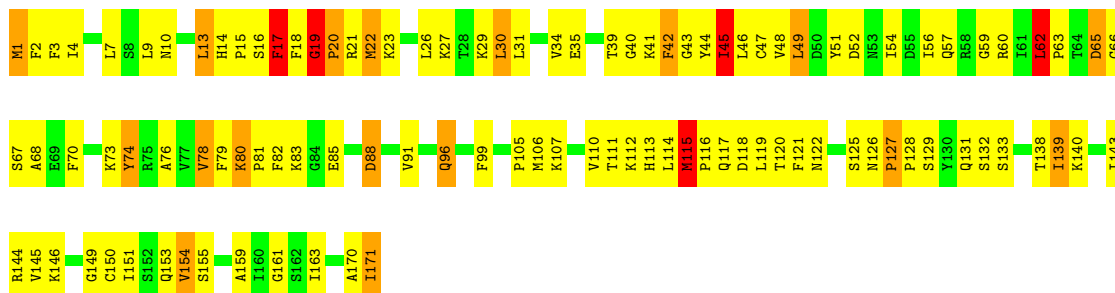


• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE



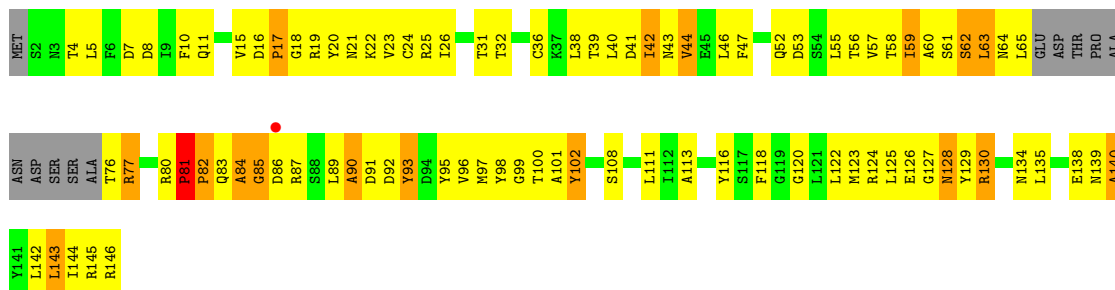
- Molecule 10: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE

Chain S: 38% 49% 10%



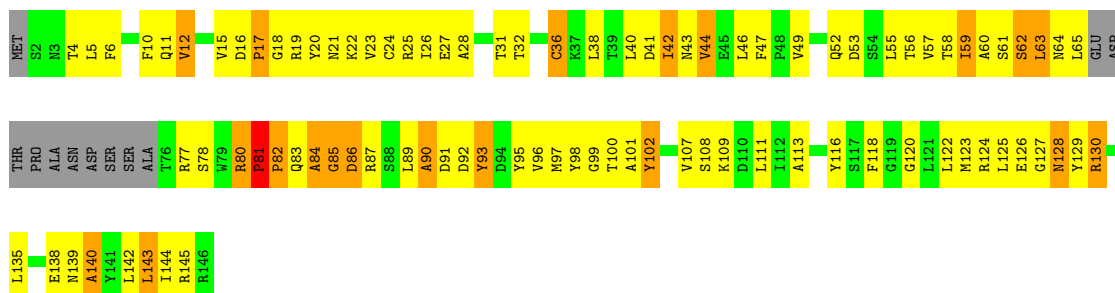
- Molecule 11: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

Chain H: 30% 50% 12% 8%

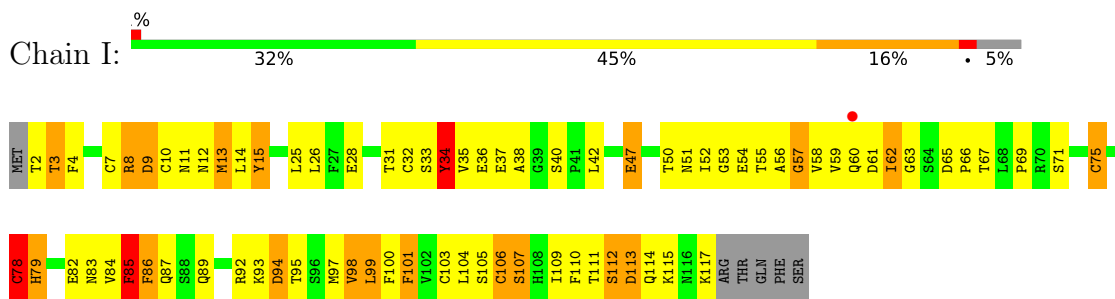


- Molecule 11: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

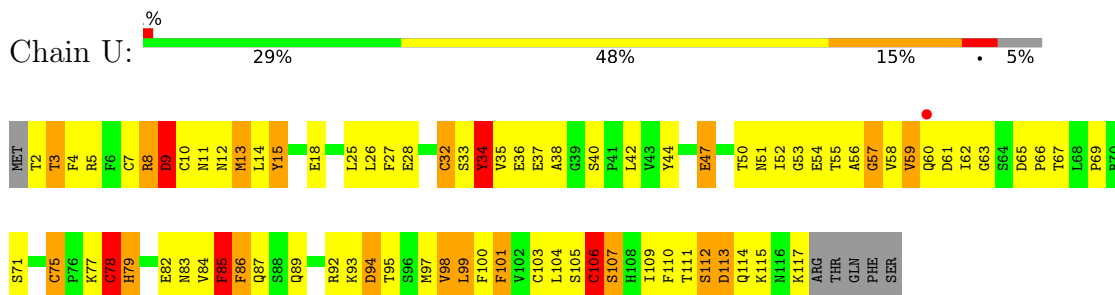
Chain T: 29% 49% 14% 8%



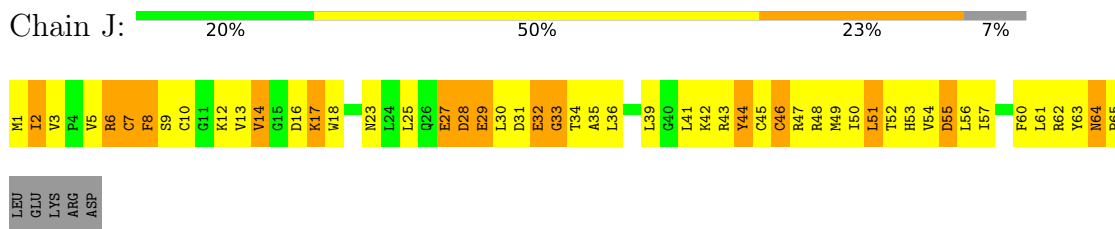
- Molecule 12: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9



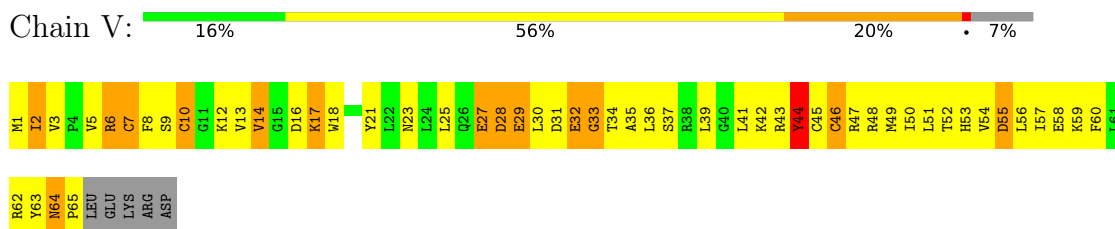
- Molecule 12: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9



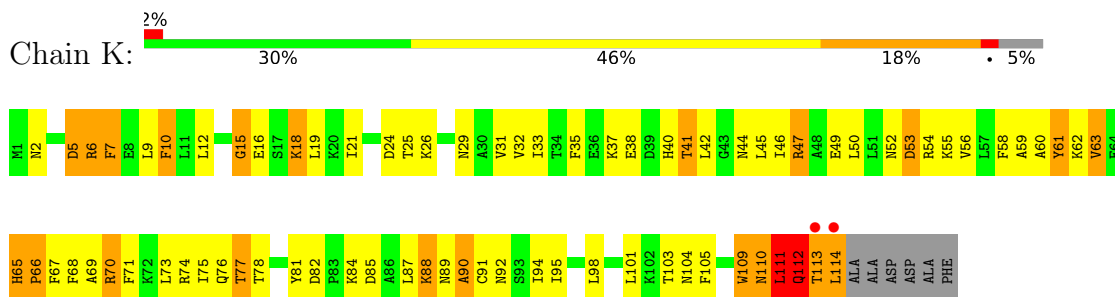
- Molecule 13: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10



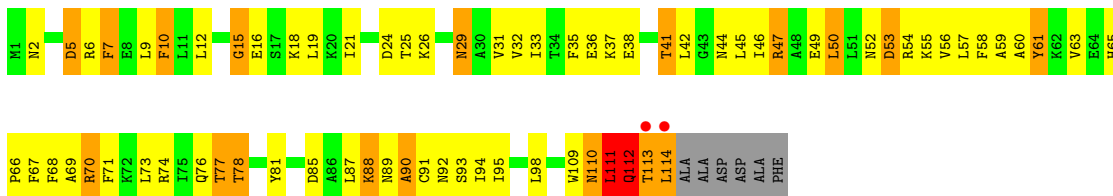
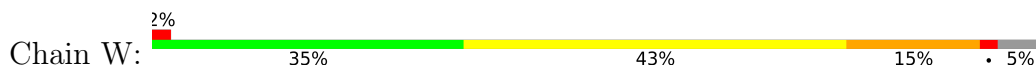
- Molecule 13: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10



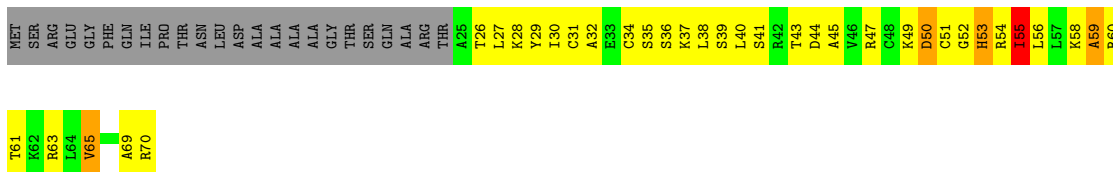
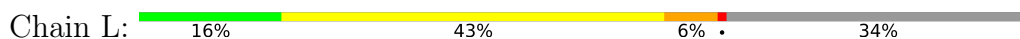
- Molecule 14: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE



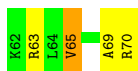
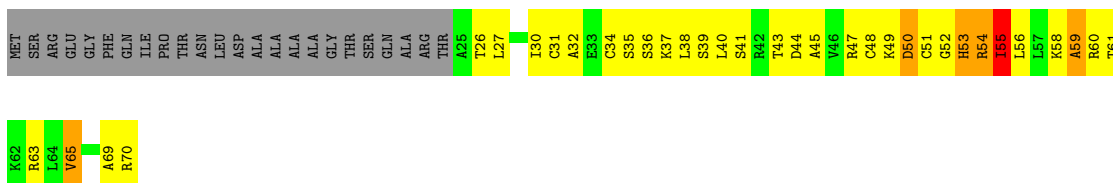
- Molecule 14: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE



- Molecule 15: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE



- Molecule 15: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	394.36Å 221.86Å 283.11Å 90.00° 90.56° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-3.80) 96.7 (50.00-3.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.275 0.215 , 0.225	Depositor DCC
R_{free} test set	9042 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	116.2	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 169.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.024 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.024 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.024 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.020 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.308 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	63924	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: MG, ZN, BRU, TT

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	1	0.80	0/158	1.68	9/242 (3.7%)
1	4	0.80	0/158	1.68	9/242 (3.7%)
2	2	0.78	0/357	1.55	12/544 (2.2%)
2	5	0.78	0/357	1.55	12/544 (2.2%)
3	3	1.10	1/237 (0.4%)	1.80	9/368 (2.4%)
3	6	1.09	0/237	1.74	8/368 (2.2%)
4	A	0.60	0/11385	1.12	95/15393 (0.6%)
4	M	0.60	0/11385	1.12	102/15393 (0.7%)
5	B	0.57	0/9037	1.06	68/12181 (0.6%)
5	N	0.56	0/9037	1.06	60/12181 (0.5%)
6	C	0.59	0/2138	1.08	14/2896 (0.5%)
6	O	0.60	0/2138	1.07	14/2896 (0.5%)
7	D	0.50	0/1437	1.08	16/1925 (0.8%)
7	P	0.51	0/1437	1.10	19/1925 (1.0%)
8	E	0.51	0/1788	1.00	13/2406 (0.5%)
8	Q	0.52	0/1788	0.99	11/2406 (0.5%)
9	F	0.70	0/716	1.15	4/964 (0.4%)
9	R	0.69	0/716	1.15	6/964 (0.6%)
10	G	0.59	0/1368	1.14	15/1844 (0.8%)
10	S	0.58	0/1368	1.16	14/1844 (0.8%)
11	H	0.48	0/1102	1.02	7/1492 (0.5%)
11	T	0.48	0/1102	1.04	10/1492 (0.7%)
12	I	0.48	0/962	1.03	4/1295 (0.3%)
12	U	0.48	0/962	1.06	5/1295 (0.4%)
13	J	0.58	0/541	0.99	1/727 (0.1%)
13	V	0.61	0/541	1.04	2/727 (0.3%)
14	K	1.32	9/937 (1.0%)	1.44	17/1265 (1.3%)
14	W	1.33	9/937 (1.0%)	1.42	11/1265 (0.9%)
15	L	0.54	0/366	0.93	0/485
15	X	0.56	0/366	0.97	0/485
All	All	0.62	19/65058 (0.0%)	1.11	567/88054 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	2
2	5	0	1
5	B	0	1
5	N	0	1
All	All	0	5

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	W	112	GLN	CA-C	19.96	1.79	1.52
14	K	112	GLN	CA-C	19.65	1.79	1.52
14	W	112	GLN	N-CA	13.63	1.63	1.46
14	K	113	THR	CA-C	13.61	1.70	1.53
14	W	113	THR	CA-C	13.60	1.70	1.53

The worst 5 of 567 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	W	113	THR	N-CA-C	22.31	137.68	108.24
14	K	113	THR	N-CA-C	21.20	137.48	108.23
3	3	2	C	OP2-P-O3'	-17.44	55.69	108.00
4	A	242	PRO	CA-C-N	16.50	131.54	119.66
4	A	242	PRO	C-N-CA	16.50	131.54	119.66

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	20	DC	Sidechain
2	2	26	DC	Sidechain
2	5	20	DC	Sidechain
5	B	486	TYR	Sidechain
5	N	486	TYR	Sidechain

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	1	141	0	81	11	0
1	4	141	0	81	12	0
2	2	380	0	218	37	0
2	5	380	0	218	34	0
3	3	212	0	110	15	0
3	6	212	0	110	10	0
4	A	11186	0	11266	1373	0
4	M	11186	0	11266	1359	0
5	B	8866	0	8898	1041	0
5	N	8866	0	8898	1070	0
6	C	2101	0	2055	272	0
6	O	2101	0	2055	258	0
7	D	1427	0	1451	152	0
7	P	1427	0	1451	153	0
8	E	1752	0	1776	144	0
8	Q	1752	0	1776	138	0
9	F	705	0	730	88	0
9	R	705	0	730	84	0
10	G	1340	0	1357	162	0
10	S	1340	0	1357	169	0
11	H	1084	0	1057	124	0
11	T	1084	0	1057	128	0
12	I	944	0	899	117	0
12	U	944	0	899	120	0
13	J	532	0	542	104	0
13	V	532	0	542	115	0
14	K	919	0	929	117	0
14	W	919	0	929	107	0
15	L	364	0	386	42	0
15	X	364	0	386	44	0
16	A	1	0	0	0	0
16	M	1	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	1	0	0	0	0
17	M	2	0	0	0	0
17	N	1	0	0	0	0
17	O	1	0	0	0	0
17	U	2	0	0	0	0
17	V	1	0	0	0	0
17	X	1	0	0	0	0
All	All	63924	0	63510	6988	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 55.

The worst 5 of 6988 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)
14:W:112:GLN:CB	14:W:112:GLN:CG	1.76	1.59
14:K:112:GLN:CB	14:K:112:GLN:CG	1.75	1.56
14:K:112:GLN:C	14:K:112:GLN:CA	1.79	1.55
14:W:112:GLN:CA	14:W:112:GLN:C	1.79	1.54
4:A:855:THR:HG21	4:A:857:ARG:HE	1.09	1.18

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
4	A	1410/1733 (81%)	968 (69%)	288 (20%)	154 (11%)	0 5
4	M	1410/1733 (81%)	964 (68%)	291 (21%)	155 (11%)	0 5
5	B	1096/1224 (90%)	762 (70%)	222 (20%)	112 (10%)	0 7
5	N	1096/1224 (90%)	765 (70%)	217 (20%)	114 (10%)	0 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	264/318 (83%)	172 (65%)	64 (24%)	28 (11%)	0	6
6	O	264/318 (83%)	171 (65%)	63 (24%)	30 (11%)	0	5
7	D	173/221 (78%)	125 (72%)	27 (16%)	21 (12%)	0	4
7	P	173/221 (78%)	124 (72%)	32 (18%)	17 (10%)	0	7
8	E	212/215 (99%)	155 (73%)	42 (20%)	15 (7%)	1	12
8	Q	212/215 (99%)	156 (74%)	42 (20%)	14 (7%)	1	13
9	F	84/155 (54%)	67 (80%)	11 (13%)	6 (7%)	1	12
9	R	84/155 (54%)	67 (80%)	12 (14%)	5 (6%)	1	14
10	G	169/171 (99%)	125 (74%)	37 (22%)	7 (4%)	2	20
10	S	169/171 (99%)	132 (78%)	28 (17%)	9 (5%)	1	16
11	H	131/146 (90%)	87 (66%)	27 (21%)	17 (13%)	0	3
11	T	131/146 (90%)	83 (63%)	30 (23%)	18 (14%)	0	3
12	I	114/122 (93%)	83 (73%)	19 (17%)	12 (10%)	0	6
12	U	114/122 (93%)	81 (71%)	22 (19%)	11 (10%)	0	7
13	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0	1
13	V	63/70 (90%)	36 (57%)	15 (24%)	12 (19%)	0	1
14	K	112/120 (93%)	86 (77%)	14 (12%)	12 (11%)	0	6
14	W	112/120 (93%)	86 (77%)	17 (15%)	9 (8%)	1	10
15	L	44/70 (63%)	16 (36%)	21 (48%)	7 (16%)	0	2
15	X	44/70 (63%)	17 (39%)	19 (43%)	8 (18%)	0	2
All	All	7744/9130 (85%)	5363 (69%)	1574 (20%)	807 (10%)	0	6

5 of 807 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	44	THR
4	A	48	ALA
4	A	57	ARG
4	A	62	ASP
4	A	65	LEU

5.3.2 Protein sidechains [i](#)

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	
4	A	1244/1520 (82%)	1123 (90%)	121 (10%)	8	29
4	M	1244/1520 (82%)	1127 (91%)	117 (9%)	8	30
5	B	967/1061 (91%)	889 (92%)	78 (8%)	11	35
5	N	967/1061 (91%)	888 (92%)	79 (8%)	10	35
6	C	235/274 (86%)	211 (90%)	24 (10%)	7	27
6	O	235/274 (86%)	215 (92%)	20 (8%)	10	33
7	D	159/200 (80%)	135 (85%)	24 (15%)	3	16
7	P	159/200 (80%)	132 (83%)	27 (17%)	2	13
8	E	196/197 (100%)	190 (97%)	6 (3%)	35	57
8	Q	196/197 (100%)	190 (97%)	6 (3%)	35	57
9	F	77/137 (56%)	69 (90%)	8 (10%)	7	26
9	R	77/137 (56%)	68 (88%)	9 (12%)	5	22
10	G	152/152 (100%)	140 (92%)	12 (8%)	11	36
10	S	152/152 (100%)	139 (91%)	13 (9%)	10	33
11	H	119/128 (93%)	113 (95%)	6 (5%)	22	47
11	T	119/128 (93%)	113 (95%)	6 (5%)	22	47
12	I	110/116 (95%)	96 (87%)	14 (13%)	4	21
12	U	110/116 (95%)	94 (86%)	16 (14%)	3	17
13	J	60/65 (92%)	55 (92%)	5 (8%)	10	34
13	V	60/65 (92%)	55 (92%)	5 (8%)	10	34
14	K	99/102 (97%)	88 (89%)	11 (11%)	6	24
14	W	99/102 (97%)	87 (88%)	12 (12%)	5	21
15	L	40/57 (70%)	37 (92%)	3 (8%)	12	38
15	X	40/57 (70%)	37 (92%)	3 (8%)	12	38
All	All	6916/8018 (86%)	6291 (91%)	625 (9%)	9	32

5 of 625 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	N	615	MET
10	S	45	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	N	839	MET
5	N	603	LEU
6	O	172	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 204 such sidechains are listed below:

Mol	Chain	Res	Type
4	M	427	GLN
5	N	236	HIS
13	V	53	HIS
4	M	631	HIS
4	M	926	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	3	9/11 (81%)	1 (11%)	0
3	6	9/11 (81%)	1 (11%)	0
All	All	18/22 (81%)	2 (11%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	3	3	G
3	6	3	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	TT	2	18	2	40,43,44	4.85	8 (20%)	58,69,72	2.20	14 (24%)
2	BRU	5	22	3,2	18,21,22	0.41	0	25,30,33	1.24	3 (12%)
2	BRU	2	22	3,2	18,21,22	0.42	0	25,30,33	1.16	2 (8%)
2	TT	5	18	2	40,43,44	4.84	7 (17%)	58,69,72	2.21	13 (22%)

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
2	TT	2	18	2	-	10/18/105/106	0/5/6/6
2	BRU	5	22	3,2	-	2/7/21/22	0/2/2/2
2	BRU	2	22	3,2	-	2/7/21/22	0/2/2/2
2	TT	5	18	2	-	10/18/105/106	0/5/6/6

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	18	TT	C5-C6	-21.70	1.31	1.55
2	2	18	TT	C5-C6	-21.55	1.31	1.55
2	2	18	TT	C5T-C6T	-20.03	1.33	1.55
2	5	18	TT	C5T-C6T	-19.68	1.33	1.55
2	2	18	TT	C6-N1	-4.30	1.39	1.46

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	18	TT	C5T-C5-C6	8.03	97.75	88.36
2	2	18	TT	C5T-C5-C6	7.52	97.15	88.36
2	2	18	TT	C5-C6-N1	6.59	124.39	115.65
2	5	18	TT	C5-C6-C6T	-6.53	79.23	89.26
2	2	18	TT	C5-C6-C6T	-6.33	79.54	89.26

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	18	TT	C3R-C4R-C5R-O5R
2	5	18	TT	C3R-C4R-C5R-O5R

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	2	18	TT	O4R-C4R-C5R-O5R
2	5	18	TT	O4R-C4R-C5R-O5R
2	2	18	TT	C2'-C1'-N1-C6

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	18	TT	4	0
2	5	22	BRU	3	0
2	2	22	BRU	4	0
2	5	18	TT	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	B	2
5	N	2
6	O	1
6	C	1
9	F	1
9	R	1
4	M	1
4	A	1

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	2:SER	C	3:GLU	N	4.13
1	C	2:SER	C	3:GLU	N	4.09
1	B	18:PHE	C	19:GLU	N	3.79
1	N	18:PHE	C	19:GLU	N	3.71
1	F	69:LEU	C	70:LYS	N	3.56

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	1	7/14 (50%)	-0.29	0 100 100	123, 130, 149, 149	0
1	4	7/14 (50%)	-0.06	0 100 100	120, 128, 147, 148	0
2	2	16/25 (64%)	0.03	0 100 100	84, 130, 151, 155	0
2	5	16/25 (64%)	-0.06	0 100 100	87, 132, 150, 153	0
3	3	10/11 (90%)	-0.39	0 100 100	95, 100, 152, 155	0
3	6	10/11 (90%)	-0.21	1 (10%) 12 15	95, 102, 153, 156	0
4	A	1421/1733 (81%)	-0.78	3 (0%) 91 81	22, 88, 163, 200	0
4	M	1421/1733 (81%)	-0.79	4 (0%) 90 78	20, 88, 163, 200	0
5	B	1115/1224 (91%)	-0.67	1 (0%) 92 87	24, 101, 175, 200	0
5	N	1115/1224 (91%)	-0.70	3 (0%) 90 78	23, 101, 174, 200	0
6	C	267/318 (83%)	-0.84	0 100 100	49, 88, 147, 173	0
6	O	267/318 (83%)	-0.83	0 100 100	52, 87, 148, 170	0
7	D	177/221 (80%)	-0.62	0 100 100	72, 121, 166, 183	0
7	P	177/221 (80%)	-0.55	0 100 100	71, 124, 166, 182	0
8	E	214/215 (99%)	-0.56	0 100 100	60, 145, 193, 197	0
8	Q	214/215 (99%)	-0.58	0 100 100	58, 145, 194, 197	0
9	F	87/155 (56%)	-0.89	0 100 100	31, 62, 108, 140	0
9	R	87/155 (56%)	-0.94	0 100 100	31, 63, 109, 138	0
10	G	171/171 (100%)	-0.88	0 100 100	64, 91, 136, 146	0
10	S	171/171 (100%)	-0.84	0 100 100	65, 92, 136, 143	0
11	H	135/146 (92%)	-0.44	1 (0%) 84 65	101, 145, 182, 192	0
11	T	135/146 (92%)	-0.43	0 100 100	99, 146, 181, 191	0
12	I	116/122 (95%)	-0.46	1 (0%) 81 60	82, 139, 170, 195	0
12	U	116/122 (95%)	-0.40	1 (0%) 81 60	81, 138, 170, 194	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	J	65/70 (92%)	-0.93	0 100 100	52, 83, 128, 133	0
13	V	65/70 (92%)	-0.91	0 100 100	46, 81, 130, 136	0
14	K	114/120 (95%)	-0.82	2 (1%) 67 46	48, 92, 120, 170	0
14	W	114/120 (95%)	-0.79	2 (1%) 67 46	47, 92, 118, 167	0
15	L	46/70 (65%)	-0.44	0 100 100	86, 155, 179, 186	0
15	X	46/70 (65%)	-0.40	0 100 100	84, 156, 179, 185	0
All	All	7922/9230 (85%)	-0.72	19 (0%) 91 81	20, 99, 173, 200	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1081	LEU	5.6
4	M	1092	LYS	4.7
12	U	60	GLN	4.5
12	I	60	GLN	3.9
14	W	113	THR	3.5

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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(Å ²)	Q<0.9
2	BRU	2	22	20/21	0.98	0.06	69,76,80,84	0
2	TT	2	18	38/39	0.98	0.08	93,106,123,125	0
2	TT	5	18	38/39	0.98	0.08	95,108,126,127	0
2	BRU	5	22	20/21	0.99	0.05	77,84,87,89	0

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(Å ²)	Q<0.9
17	ZN	I	2457	1/1	0.99	0.02	199,199,199,199	0
16	MG	M	2459	1/1	1.00	0.02	34,34,34,34	0
17	ZN	A	2471	1/1	1.00	0.01	90,90,90,90	0
17	ZN	A	2472	1/1	1.00	0.01	52,52,52,52	0
17	ZN	B	2457	1/1	1.00	0.02	53,53,53,53	0
17	ZN	C	2457	1/1	1.00	0.02	48,48,48,48	0
16	MG	A	2457	1/1	1.00	0.02	50,50,50,50	0
17	ZN	I	2458	1/1	1.00	0.01	94,94,94,94	0
17	ZN	J	2457	1/1	1.00	0.02	70,70,70,70	0
17	ZN	L	2457	1/1	1.00	0.02	116,116,116,116	0
17	ZN	M	2457	1/1	1.00	0.01	87,87,87,87	0
17	ZN	M	2458	1/1	1.00	0.01	51,51,51,51	0
17	ZN	N	2457	1/1	1.00	0.02	54,54,54,54	0
17	ZN	O	2457	1/1	1.00	0.01	39,39,39,39	0
17	ZN	U	2457	1/1	1.00	0.02	91,91,91,91	0
17	ZN	U	2458	1/1	1.00	0.02	178,178,178,178	0
17	ZN	V	2457	1/1	1.00	0.02	67,67,67,67	0
17	ZN	X	2457	1/1	1.00	0.02	120,120,120,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.