



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2026 – 10:33 AM UTC

PDB ID : 3HOU / pdb_00003hou
Title : Complete RNA polymerase II elongation complex I with a T-U mismatch
Authors : Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.;
Lehmann, E.; Vassylyev, D.; Cramer, P.
Deposited on : 2009-06-03
Resolution : 3.20 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

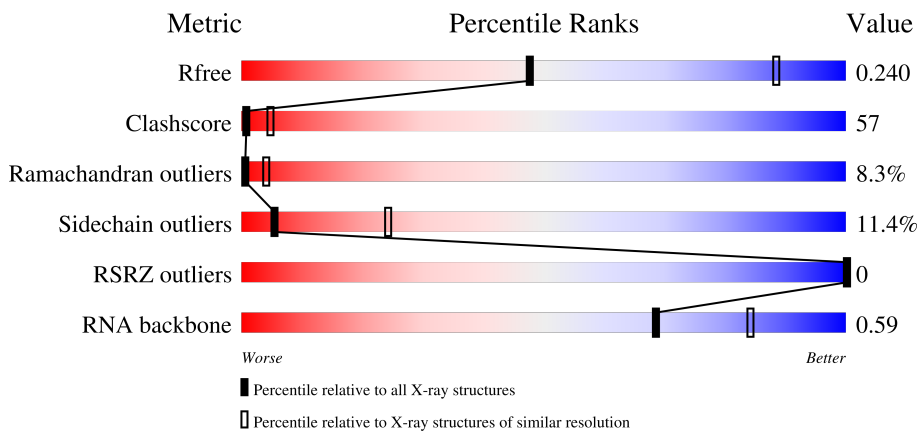
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



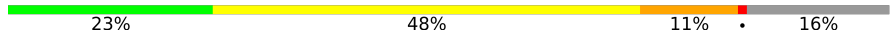
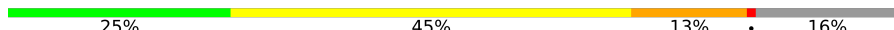

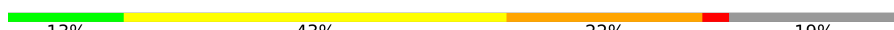
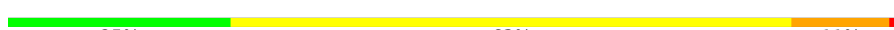




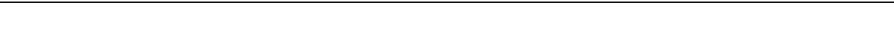

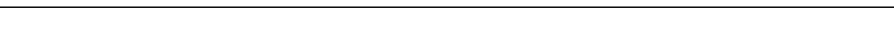
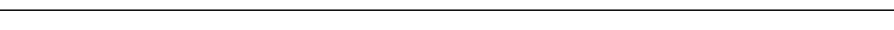










Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	1733	
1	M	1733	
2	B	1224	
2	N	1224	

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Mol	Chain	Length	Quality of chain
3	C	318	
3	O	318	
4	D	221	
4	P	221	
5	E	215	
5	Q	215	
6	F	155	
6	R	155	
7	G	171	
7	S	171	
8	H	146	
8	T	146	
9	I	122	
9	U	122	
10	J	70	
10	V	70	
11	K	120	
11	W	120	
12	L	70	
12	X	70	
13	1	26	
13	4	26	
14	2	13	
14	5	13	
15	3	17	

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Mol	Chain	Length	Quality of chain
15	6	17	 29% 35% 35%

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 63664 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			
1	M	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1104	Total	C	N	O	S	0	0	0
			8779	5560	1537	1627	55			
2	N	1104	Total	C	N	O	S	0	0	0
			8779	5560	1537	1627	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			
3	O	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			
4	P	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			
8	T	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			
9	U	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			
12	X	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*A*AP*GP*TP*AP*GP*TP*TP*AP*TP*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
13	1	18	Total	Br	C	N	O	P	0	0	0
			368	1	176	66	108	17			
13	4	18	Total	Br	C	N	O	P	0	0	0
			368	1	176	66	108	17			

- Molecule 14 is a DNA chain called 5'-D(*A*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	6	Total	C	N	O	P	0	0	0
			117	58	20	34	5			
14	5	6	Total	C	N	O	P	0	0	0
			117	58	20	34	5			

- Molecule 15 is a RNA chain called 5'-R(*UP*GP*CP*AP*UP*U*UP*CP*GP*AP*CP*CP*AP*GP*GP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	11	Total	C	N	O	P	0	0	0
			230	104	41	75	10			
15	6	11	Total	C	N	O	P	0	0	0
			230	104	41	75	10			

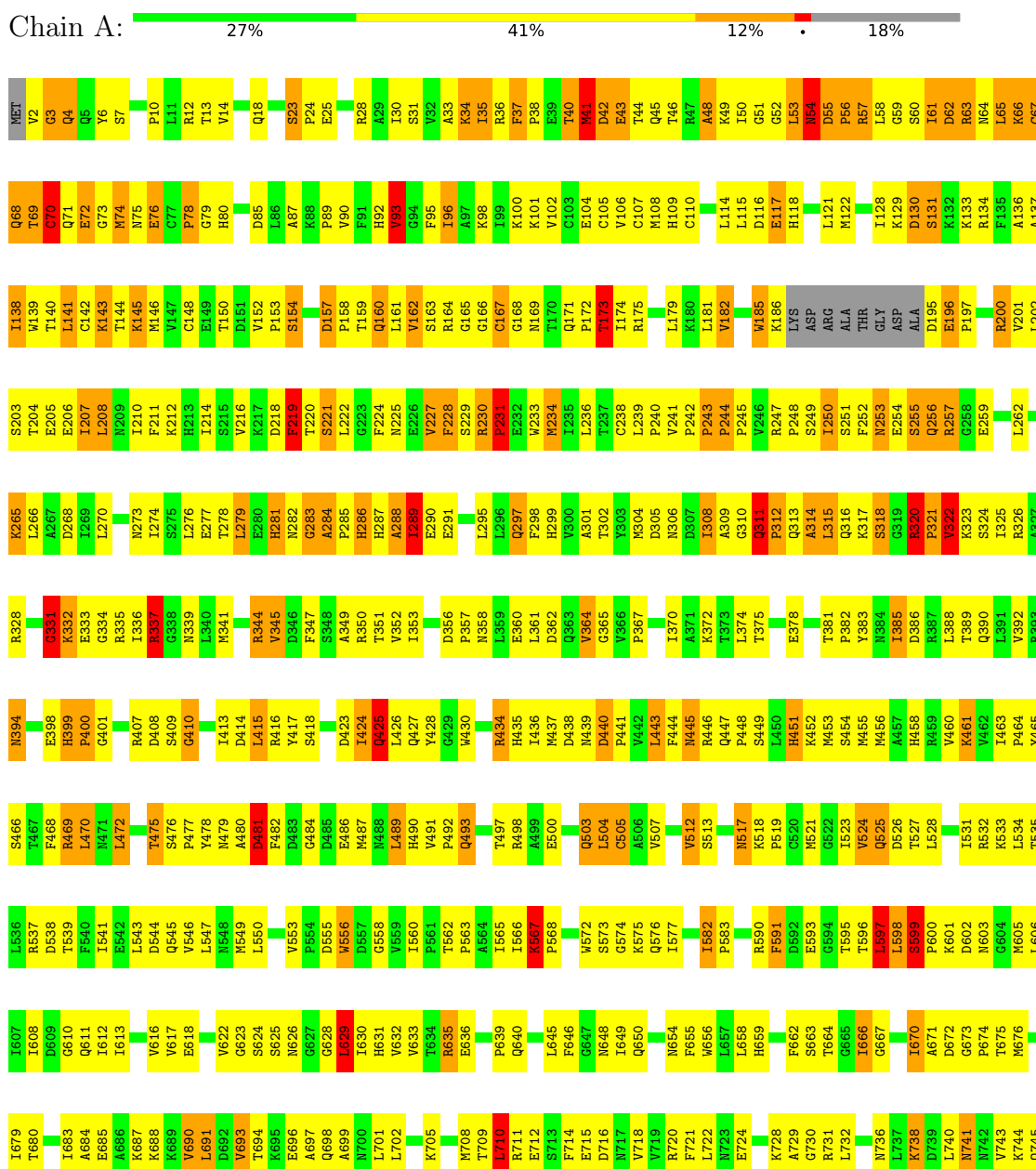
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

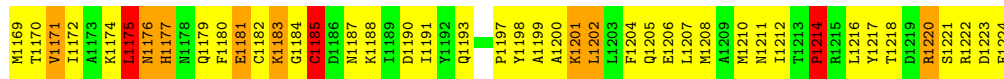
3 Residue-property plots

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 II subunit RPB1

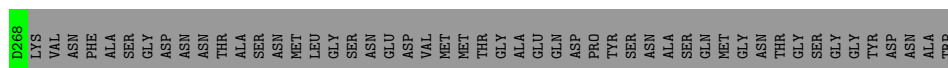
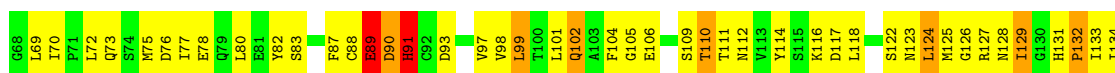
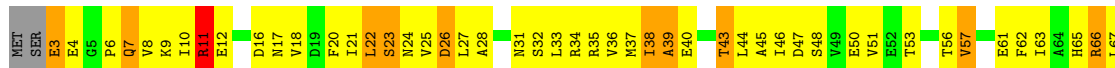


H1025	H1026	I1027	I1028	L0901	L0902	L1030	L1031	L1032	L1033	L1034	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1049	L1050	L1051	L1052	L1053	L1056	L1060	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1091	L1094	L1095	L1097	L1098																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
M957	Q958	Q959	G960	L961	Q962	F963	Q964	K965	Q966	Q967	Q968	Q969	Q970	Q971	Q974	Q975	Q976	Q977	D978	K979	F980	R983	H984	G985	T989	I990	G991	I992	I993	Y994	R995	R996	R997	D998	M999	P1000	F1001	G1004	L1005	V1007	P1008	D1009	L1010	L1011	L1012	L1013	A1016	I1017	P1018	L1019	L1095	L1020	M1021	T1022																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
D896	G897	L898	L899	L900	L901	G902	L903	L904	L905	L906	L907	L908	L909	L910	L911	K914	T915	T916	F917	L918	L919	PRD	ASP	GLU	GLU	GLU	LEU	GLY	GLN	ARG	THR	ALA	THR	HIS	K934	D936	A937	S938	T939	L940	L941	R942	S943	T944	E945	L946	G947	L948	Y949	D950	L951	L952	L953	L954	L955	L956	L957																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
E836	D837	S838	M839	L840	M841	M842	Q843	S844	S845	L846	D847	R848	G849	L850	L851	R852	R853	L854	F855	F856	R857	S858	Y859	M860	D861	Q862	E863	K864	K865	Y866	M867	M868	S869	L870	T871	E872	T873	F874	E875	K876	P877	R878	T880	ASN	THR	LEU	R884	M885	K886	H887	G888	T889	Y890	L952	L953	L954	L955	L956	L957																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
H773	G774	L775	Q776	A777	M778	G779	L780	F781	L782	L783	M784	L785	M786	L787	L788	M789	D790	L791	M792	L793	R794	L795	L796	L797	L798	L799	Q800	K801	F802	L803	L804	L805	L806	L807	L808	L809	E810	L811	L812	L813	L814	L815	L816	L817	L818	Q821	M822	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	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
E708	D709	L710	E711	E714	L715	ASN	GLU	GLU	ASN	ASN	LEU	LEU	D722	L723	D724	L725	K727	L603	L604	T605	E606	D607	D608	L609	M610	P611	E612	M613	S614	M615	L616	R617	D618	L619	R620	E621	K622	E623	L624	K625	L626	E627	L628	L629	A630	G631	R632	L633	Y634	Y635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	S702	L703	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	S732	L733	H734	L735	L736	T737	F738	L739	L740	L741	L742	L743	H744	L745	L746	S747	M747	L748	L749	G750	L751	A752	L753	L754	L755	L756	L757	L758	L759	D760	H761	N762	Q763	S764	E699	E698	E697	E696	Y695	L694	E693	E692	L691	L690	L689	L688	L687	L686	L685	L684	L683	L682	L681	L680	L679	L678	L677	L676	L675	L674	L673	L672	L671	L670	L669	L668	L667	L666	L665	L664	L663	L662	L661	L660	L659	L658	L657	L656	L655	L654	L653	L652	L651	L650	L649	L648	L647	L646	L645	L644	L643	L642	L641	L640	L639	L638	L637	L636	L635	L634	L633	L632	L631	L630	L629	L628	L627	L626	L625	L624	L623	L622	L621	L620	L619	L618	L617	L616	L615	L614	L613	L612	L611	L610	L609	L608	L607	L606	L605	L604	L603	L602	L601	Q531	D532	E533	E534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	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	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022
R384	L385	L386	L387	C388	L389	D391	R392	K393	D394	Q395	D396	D397	R398	R399	E400	H401	G402	R405	L406	D407	D408	L409	L410	L411	L412	L413	L414	L415	L416	F417	K418	R419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	R430	Y431	M432	Q433	R434	T435	V436	E437	GLU	ARG	ALA	HIS	ASP	GLY	LYS	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										



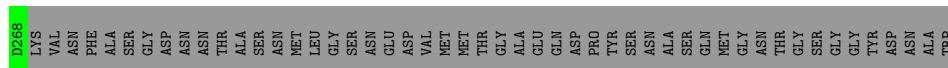
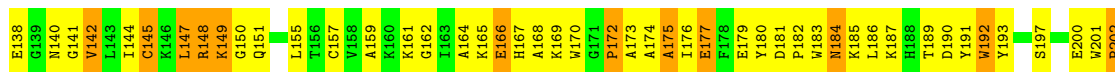
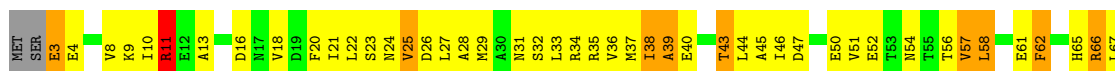
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 23% 48% 11% 16%



• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain O: 25% 45% 13% 16%



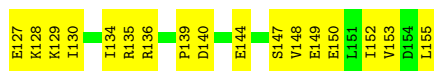
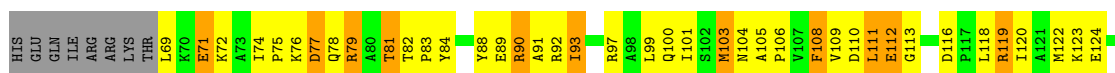
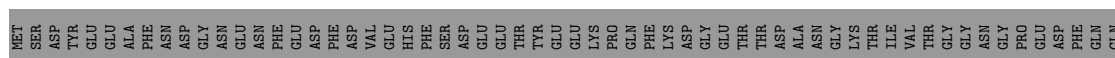
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 20% 44% 13% 19%



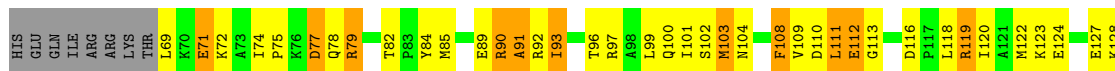
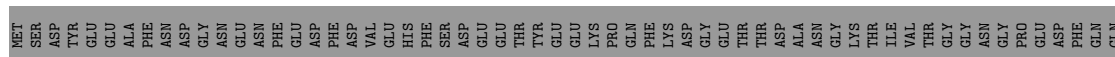
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 19% 30% 7% 44%



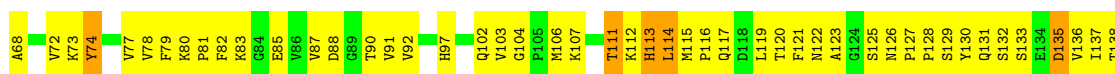
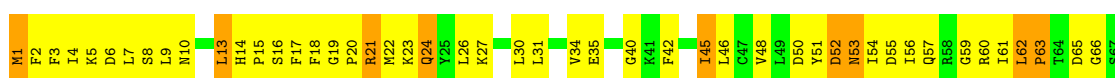
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain R: 21% 28% 8% 44%




- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 34% 57% 9%




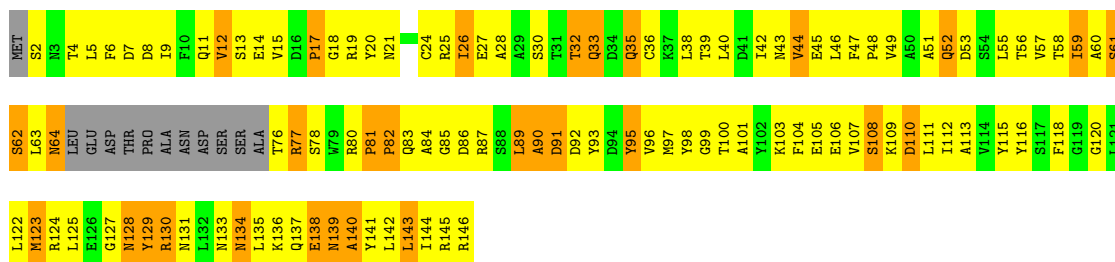
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain S: 




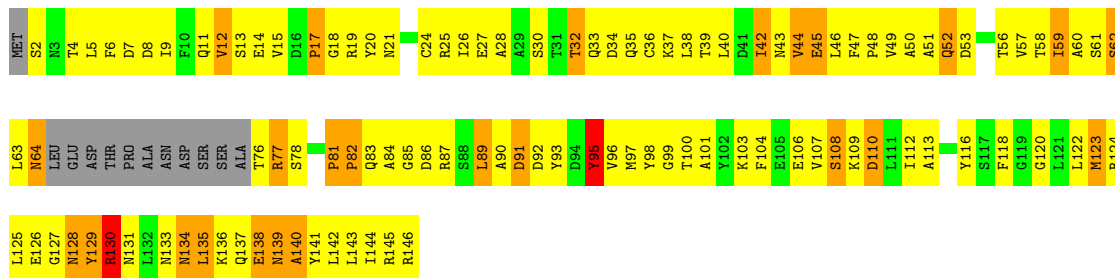
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 

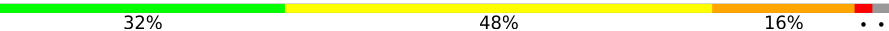


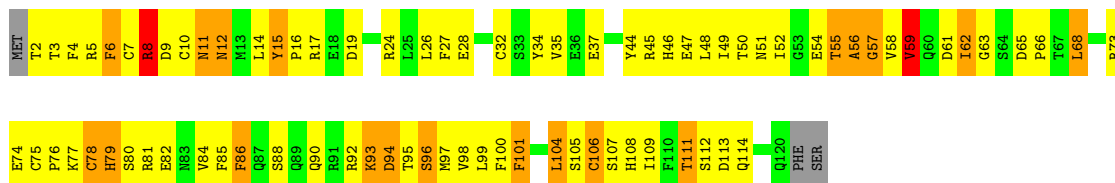
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain T: 



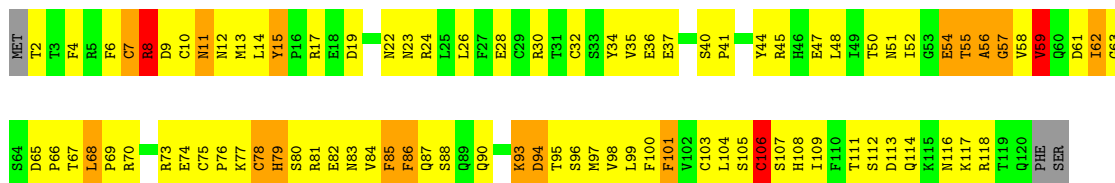
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 



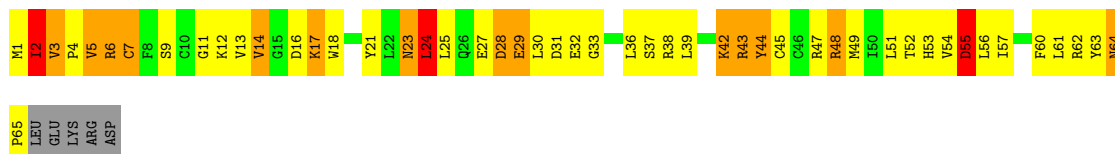
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain U: 



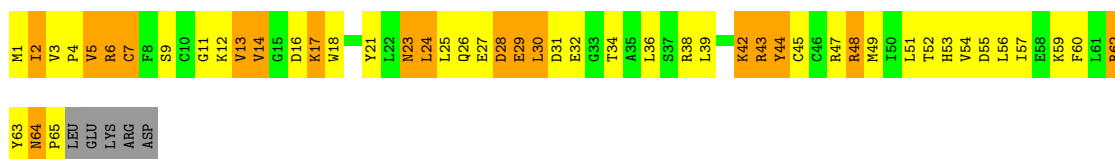
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 21% 47% 20% 7%



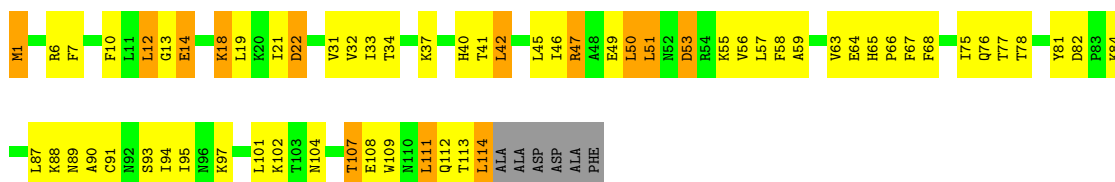
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain V: 21% 46% 26% 7%



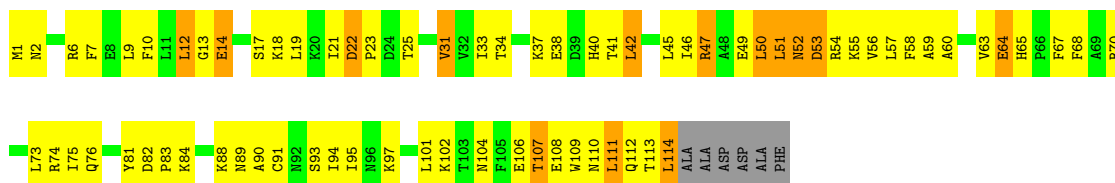
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K: 42% 42% 11% 5%



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain W: 34% 49% 12% 5%

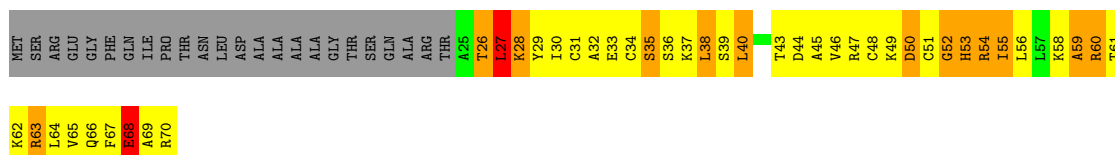
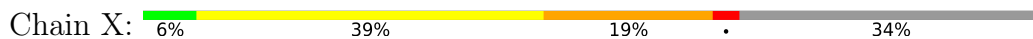


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

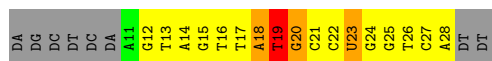
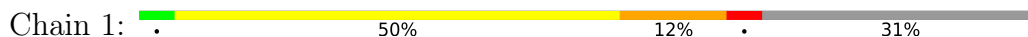
Chain L: 6% 39% 17% 34%



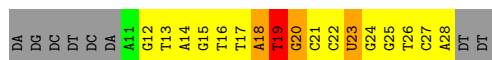
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



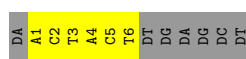
- Molecule 13: 5'-D(*AP*GP*CP*TP*CP*A*AP*GP*TP*AP*GP*TP*TP*AP*TP*GP*CP*C P*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'



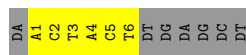
- Molecule 13: 5'-D(*AP*GP*CP*TP*CP*A*AP*GP*TP*AP*GP*TP*TP*AP*TP*GP*CP*C P*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'



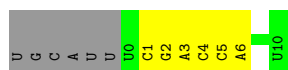
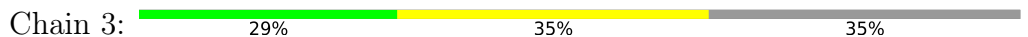
- Molecule 14: 5'-D(*A*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'



- Molecule 14: 5'-D(*A*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'



- Molecule 15: 5'-R(*UP*GP*CP*AP*UP*U*UP*CP*GP*AP*CP*CP*AP*GP*GP*CP*U)-3'



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	394.26Å 221.61Å 283.45Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (40.00-3.20) 90.8 (40.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.233 , 0.252 0.234 , 0.240	Depositor DCC
R_{free} test set	20910 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.018 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.017 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.017 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.257 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	63664	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, BRU

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	0.63	3/11342 (0.0%)	1.15	99/15337 (0.6%)
1	M	0.62	1/11342 (0.0%)	1.15	96/15337 (0.6%)
2	B	0.59	0/8948	1.08	55/12062 (0.5%)
2	N	0.58	0/8948	1.09	53/12062 (0.4%)
3	C	0.59	0/2133	1.11	15/2891 (0.5%)
3	O	0.59	0/2133	1.10	13/2891 (0.4%)
4	D	0.51	0/1444	1.15	19/1935 (1.0%)
4	P	0.64	0/1444	1.24	18/1935 (0.9%)
5	E	0.53	0/1788	1.12	12/2406 (0.5%)
5	Q	0.54	0/1788	1.13	11/2406 (0.5%)
6	F	0.70	0/717	1.26	4/967 (0.4%)
6	R	0.68	0/717	1.25	5/967 (0.5%)
7	G	0.54	0/1368	1.15	12/1844 (0.7%)
7	S	0.69	0/1368	1.27	11/1844 (0.6%)
8	H	0.47	0/1094	1.04	4/1481 (0.3%)
8	T	0.47	0/1094	1.04	7/1481 (0.5%)
9	I	0.50	0/989	1.10	6/1331 (0.5%)
9	U	0.50	0/989	1.06	5/1331 (0.4%)
10	J	0.60	0/541	1.09	2/727 (0.3%)
10	V	0.58	0/541	1.04	1/727 (0.1%)
11	K	0.55	0/937	1.00	4/1265 (0.3%)
11	W	0.56	0/937	0.99	5/1265 (0.4%)
12	L	0.64	0/365	1.16	2/485 (0.4%)
12	X	0.63	0/365	1.16	2/485 (0.4%)
13	1	0.40	0/389	1.01	1/597 (0.2%)
13	4	0.39	0/389	1.01	1/597 (0.2%)
14	2	0.36	0/130	0.75	0/198
14	5	0.35	0/130	0.73	0/198
15	3	0.45	0/256	0.79	0/397
15	6	0.45	0/256	0.78	0/397
All	All	0.59	4/64882 (0.0%)	1.12	463/87846 (0.5%)

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	B	0	1
2	N	0	2
13	1	0	4
13	4	0	4
All	All	0	11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	MET	SD-CE	6.51	1.95	1.79
1	M	437	MET	SD-CE	5.76	1.94	1.79
1	A	1398	MET	SD-CE	5.56	1.93	1.79
1	A	55	ASP	CA-C	-5.38	1.46	1.52

The worst 5 of 463 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	71	GLU	N-CA-C	-13.70	95.91	113.17
6	R	71	GLU	N-CA-C	-13.55	96.10	113.17
5	E	5	ASN	N-CA-C	-12.47	97.50	113.72
5	Q	5	ASN	N-CA-C	-12.36	97.65	113.72
1	M	3	GLY	N-CA-C	-11.12	98.93	115.72

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	1	18	DA	Sidechain
13	1	19	DT	Sidechain
13	1	20	DG	Sidechain
13	1	21	DC	Sidechain
2	B	833	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	A	11143	0	11217	1232	0
1	M	11143	0	11217	1236	0
2	B	8779	0	8808	1124	0
2	N	8779	0	8808	1136	0
3	C	2095	0	2051	244	0
3	O	2095	0	2051	246	0
4	D	1434	0	1460	165	0
4	P	1434	0	1460	288	0
5	E	1752	0	1776	198	0
5	Q	1752	0	1776	217	0
6	F	705	0	731	88	0
6	R	705	0	731	79	0
7	G	1340	0	1357	154	0
7	S	1340	0	1357	212	0
8	H	1076	0	1046	178	0
8	T	1076	0	1046	163	0
9	I	971	0	929	128	0
9	U	971	0	929	137	0
10	J	532	0	542	98	0
10	V	532	0	542	98	0
11	K	919	0	929	84	0
11	W	919	0	929	88	0
12	L	363	0	387	89	0
12	X	363	0	387	89	0
13	1	368	0	203	25	0
13	4	368	0	203	23	0
14	2	117	0	70	13	0
14	5	117	0	70	11	0
15	3	230	0	121	8	0
15	6	230	0	121	8	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
16	M	2	0	0	0	0
16	N	1	0	0	0	0
16	O	1	0	0	0	0
16	U	2	0	0	0	0
16	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	X	1	0	0	0	0
All	All	63664	0	63254	7250	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 57.

The worst 5 of 7250 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:N:510:LYS:HG3	2:N:511:PRO:HD3	1.21	1.17
1:A:855:THR:HG21	1:A:857:ARG:HE	1.08	1.16
9:U:111:THR:HG22	9:U:113:ASP:H	1.05	1.15
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.23	1.15
5:Q:124:VAL:HG13	5:Q:132:ILE:HB	1.28	1.15

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	1406/1733 (81%)	1075 (76%)	225 (16%)	106 (8%)	1 5
1	M	1406/1733 (81%)	1073 (76%)	228 (16%)	105 (8%)	1 5
2	B	1082/1224 (88%)	800 (74%)	186 (17%)	96 (9%)	0 3
2	N	1082/1224 (88%)	798 (74%)	186 (17%)	98 (9%)	0 3
3	C	264/318 (83%)	202 (76%)	41 (16%)	21 (8%)	1 4
3	O	264/318 (83%)	203 (77%)	42 (16%)	19 (7%)	1 6
4	D	174/221 (79%)	120 (69%)	37 (21%)	17 (10%)	0 2
4	P	174/221 (79%)	122 (70%)	34 (20%)	18 (10%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	212/215 (99%)	155 (73%)	41 (19%)	16 (8%)	1	5
5	Q	212/215 (99%)	159 (75%)	37 (18%)	16 (8%)	1	5
6	F	85/155 (55%)	72 (85%)	11 (13%)	2 (2%)	4	28
6	R	85/155 (55%)	72 (85%)	11 (13%)	2 (2%)	4	28
7	G	169/171 (99%)	141 (83%)	23 (14%)	5 (3%)	3	23
7	S	169/171 (99%)	139 (82%)	23 (14%)	7 (4%)	2	17
8	H	130/146 (89%)	85 (65%)	25 (19%)	20 (15%)	0	0
8	T	130/146 (89%)	85 (65%)	25 (19%)	20 (15%)	0	0
9	I	117/122 (96%)	77 (66%)	28 (24%)	12 (10%)	0	2
9	U	117/122 (96%)	78 (67%)	28 (24%)	11 (9%)	0	3
10	J	63/70 (90%)	43 (68%)	9 (14%)	11 (18%)	0	0
10	V	63/70 (90%)	42 (67%)	10 (16%)	11 (18%)	0	0
11	K	112/120 (93%)	89 (80%)	20 (18%)	3 (3%)	4	25
11	W	112/120 (93%)	89 (80%)	19 (17%)	4 (4%)	2	19
12	L	44/70 (63%)	19 (43%)	15 (34%)	10 (23%)	0	0
12	X	44/70 (63%)	19 (43%)	15 (34%)	10 (23%)	0	0
All	All	7716/9130 (84%)	5757 (75%)	1319 (17%)	640 (8%)	0	4

5 of 640 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	43	GLU
1	A	57	ARG
1	A	62	ASP
1	A	63	ARG

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	
1	A	1239/1520 (82%)	1102 (89%)	137 (11%)	6	25
1	M	1239/1520 (82%)	1105 (89%)	134 (11%)	6	27
2	B	958/1061 (90%)	847 (88%)	111 (12%)	5	24
2	N	958/1061 (90%)	840 (88%)	118 (12%)	4	22
3	C	234/274 (85%)	206 (88%)	28 (12%)	5	23
3	O	234/274 (85%)	204 (87%)	30 (13%)	4	20
4	D	160/200 (80%)	135 (84%)	25 (16%)	2	13
4	P	160/200 (80%)	122 (76%)	38 (24%)	1	4
5	E	196/197 (100%)	185 (94%)	11 (6%)	19	52
5	Q	196/197 (100%)	185 (94%)	11 (6%)	19	52
6	F	77/137 (56%)	70 (91%)	7 (9%)	9	34
6	R	77/137 (56%)	70 (91%)	7 (9%)	9	34
7	G	152/152 (100%)	140 (92%)	12 (8%)	11	40
7	S	152/152 (100%)	127 (84%)	25 (16%)	2	12
8	H	118/128 (92%)	107 (91%)	11 (9%)	8	33
8	T	118/128 (92%)	108 (92%)	10 (8%)	10	37
9	I	113/116 (97%)	101 (89%)	12 (11%)	6	27
9	U	113/116 (97%)	104 (92%)	9 (8%)	11	40
10	J	60/65 (92%)	51 (85%)	9 (15%)	3	15
10	V	60/65 (92%)	51 (85%)	9 (15%)	3	15
11	K	99/102 (97%)	90 (91%)	9 (9%)	9	34
11	W	99/102 (97%)	88 (89%)	11 (11%)	6	25
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	15
12	X	40/57 (70%)	34 (85%)	6 (15%)	3	15
All	All	6892/8018 (86%)	6106 (89%)	786 (11%)	5	24

5 of 786 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	907	THR
2	N	645	SER
1	M	1033	GLN
1	M	874	ASP
2	N	167	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 265 such sidechains are listed below:

Mol	Chain	Res	Type
5	Q	3	GLN
5	Q	114	ASN
9	U	120	GLN
5	E	99	HIS
5	E	3	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	3	10/17 (58%)	0	0
15	6	10/17 (58%)	0	0
All	All	20/34 (58%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

2 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
13	BRU	4	23	15,13	18,21,22	3.92	1 (5%)	25,30,33	0.99	1 (4%)
13	BRU	1	23	15,13	18,21,22	3.90	1 (5%)	25,30,33	0.99	1 (4%)

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
13	BRU	4	23	15,13	-	1/7/21/22	0/2/2/2
13	BRU	1	23	15,13	-	1/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	23	BRU	BR-C5	-16.55	1.50	1.88
13	1	23	BRU	BR-C5	-16.45	1.50	1.88

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	4	23	BRU	C6-C5-C4	-2.99	117.64	120.67
13	1	23	BRU	C6-C5-C4	-2.99	117.64	120.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	1	23	BRU	O4'-C4'-C5'-O5'
13	4	23	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	4	23	BRU	6	0
13	1	23	BRU	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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	1416/1733 (81%)	-1.70	0 100 100	12, 52, 93, 119	0
1	M	1416/1733 (81%)	-1.68	0 100 100	10, 53, 94, 123	0
2	B	1104/1224 (90%)	-1.61	0 100 100	12, 62, 103, 120	0
2	N	1104/1224 (90%)	-1.59	0 100 100	16, 65, 104, 121	0
3	C	266/318 (83%)	-1.72	0 100 100	24, 52, 83, 100	0
3	O	266/318 (83%)	-1.70	0 100 100	25, 54, 85, 106	0
4	D	178/221 (80%)	-1.57	0 100 100	36, 68, 100, 108	0
4	P	178/221 (80%)	-1.43	0 100 100	55, 85, 105, 113	0
5	E	214/215 (99%)	-1.53	0 100 100	35, 80, 106, 114	0
5	Q	214/215 (99%)	-1.49	0 100 100	35, 82, 107, 119	0
6	F	87/155 (56%)	-1.81	0 100 100	13, 34, 62, 78	0
6	R	87/155 (56%)	-1.83	0 100 100	15, 34, 63, 76	0
7	G	171/171 (100%)	-1.70	0 100 100	37, 55, 85, 99	0
7	S	171/171 (100%)	-1.55	0 100 100	37, 69, 110, 116	0
8	H	134/146 (91%)	-1.39	0 100 100	60, 88, 105, 114	0
8	T	134/146 (91%)	-1.38	0 100 100	66, 89, 104, 116	0
9	I	119/122 (97%)	-1.46	0 100 100	47, 81, 102, 117	0
9	U	119/122 (97%)	-1.45	0 100 100	45, 84, 102, 119	0
10	J	65/70 (92%)	-1.75	0 100 100	23, 52, 74, 91	0
10	V	65/70 (92%)	-1.73	0 100 100	28, 53, 78, 91	0
11	K	114/120 (95%)	-1.74	0 100 100	23, 54, 72, 83	0
11	W	114/120 (95%)	-1.75	0 100 100	21, 54, 74, 84	0
12	L	46/70 (65%)	-1.30	0 100 100	37, 89, 107, 107	0
12	X	46/70 (65%)	-1.31	0 100 100	42, 93, 107, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9	
13	1	17/26 (65%)	-1.34	0	100 100	47, 101, 140, 144	0
13	4	17/26 (65%)	-1.32	0	100 100	50, 102, 139, 142	0
14	2	6/13 (46%)	-0.87	0	100 100	114, 121, 127, 133	0
14	5	6/13 (46%)	-0.84	0	100 100	114, 121, 129, 136	0
15	3	11/17 (64%)	-1.70	0	100 100	88, 93, 131, 133	0
15	6	11/17 (64%)	-1.67	0	100 100	88, 96, 130, 133	0
All	All	7896/9242 (85%)	-1.63	0	100 100	10, 61, 102, 144	0

There are no RSRZ outliers to report.

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
13	BRU	1	23	20/21	0.99	0.04	85,89,94,97	0
13	BRU	4	23	20/21	0.99	0.04	83,89,95,98	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
16	ZN	A	9984	1/1	1.00	0.01	70,70,70,70	0
16	ZN	A	9985	1/1	1.00	0.00	40,40,40,40	0
16	ZN	B	9986	1/1	1.00	0.01	33,33,33,33	0
16	ZN	C	9987	1/1	1.00	0.00	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	ZN	I	9988	1/1	1.00	0.00	65,65,65,65	0
16	ZN	I	9989	1/1	1.00	0.02	117,117,117,117	0
16	ZN	J	9990	1/1	1.00	0.01	52,52,52,52	0
16	ZN	L	9991	1/1	1.00	0.01	90,90,90,90	0
16	ZN	M	9992	1/1	1.00	0.01	74,74,74,74	0
16	ZN	M	9993	1/1	1.00	0.00	37,37,37,37	0
16	ZN	N	9994	1/1	1.00	0.00	38,38,38,38	0
16	ZN	O	9995	1/1	1.00	0.00	43,43,43,43	0
16	ZN	U	9996	1/1	1.00	0.00	71,71,71,71	0
16	ZN	U	9997	1/1	1.00	0.02	119,119,119,119	0
16	ZN	V	9998	1/1	1.00	0.01	52,52,52,52	0
16	ZN	X	9999	1/1	1.00	0.01	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.