



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 05:29 AM EDT

PDB ID : 2PMZ
Title : Archaeal RNA polymerase from Sulfolobus solfataricus
Authors : Murakami, K.S.
Deposited on : 2007-04-23
Resolution : 3.40 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

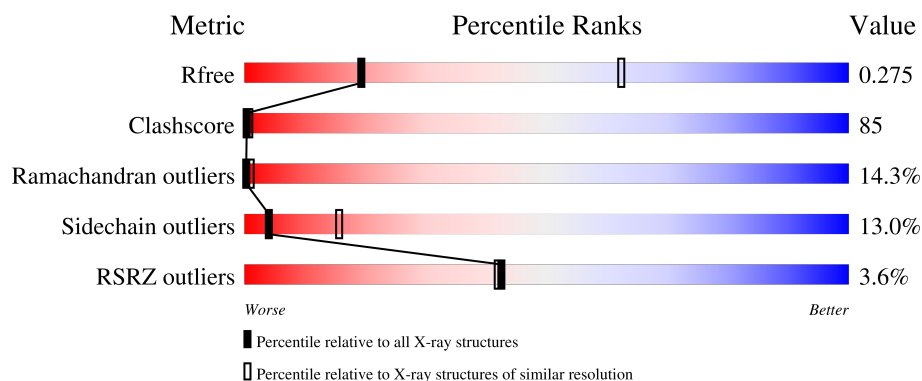
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	880	<div> <div>2%</div> <div>16% 52% 18% 12%</div> </div>
1	Q	880	<div> <div>3%</div> <div>16% 54% 17% 12%</div> </div>
2	C	392	<div> <div>3%</div> <div>11% 42% 15% 29%</div> </div>
2	G	392	<div> <div>3%</div> <div>11% 41% 16% 29%</div> </div>
3	B	1124	<div> <div>2%</div> <div>17% 60% 18% ..</div> </div>

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Mol	Chain	Length	Quality of chain
3	R	1124	
4	D	265	
4	S	265	
5	E	180	
5	T	180	
6	F	113	
6	U	113	
7	H	84	
7	V	84	
8	K	95	
8	W	95	
9	L	92	
9	X	92	
10	N	66	
10	Y	66	
11	P	48	
11	Z	48	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	F3S	D	1001	-	-	X	-
14	F3S	S	1001	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 48122 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	776	Total	C	N	O	S	0	0	0
			6173	3936	1081	1135	21			
1	Q	776	Total	C	N	O	S	0	0	0
			6173	3936	1081	1135	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	279	Total	C	N	O	S	0	0	0
			2169	1376	375	412	6			
2	G	279	Total	C	N	O	S	0	0	0
			2169	1376	375	412	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	1090	Total	C	N	O	S	0	0	0
			8645	5483	1529	1602	31			
3	R	1090	Total	C	N	O	S	0	0	0
			8645	5483	1529	1602	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	264	Total	C	N	O	S	0	0	0
			2114	1355	342	403	14			
4	S	264	Total	C	N	O	S	0	0	0
			2114	1355	342	403	14			

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	176	Total	C	N	O	S	0	0	0
			1402	903	236	259	4			
5	T	176	Total	C	N	O	S	0	0	0
			1402	903	236	259	4			

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	89	Total	C	N	O	S	0	0	0
			694	433	115	142	4			
6	U	89	Total	C	N	O	S	0	0	0
			694	433	115	142	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	74	Total	C	N	O		0	0	0
			611	397	109	105				
7	V	74	Total	C	N	O		0	0	0
			611	397	109	105				

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			
8	W	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L	92	Total	C	N	O	S	0	0	0
			723	459	121	141	2			
9	X	92	Total	C	N	O	S	0	0	0
			723	459	121	141	2			

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	64	Total	C	N	O	S	0	0	0
			514	326	94	88	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	Y	64	Total	C	N	O	S	0	0	0
			514	326	94	88	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			
11	Z	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			

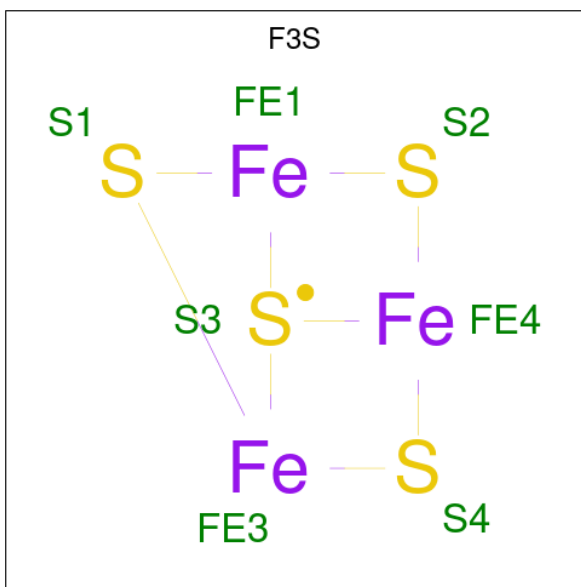
- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Zn	0	0
			1	1		
12	B	1	Total	Zn	0	0
			1	1		
12	N	1	Total	Zn	0	0
			1	1		
12	P	1	Total	Zn	0	0
			1	1		
12	Q	1	Total	Zn	0	0
			1	1		
12	R	1	Total	Zn	0	0
			1	1		
12	Y	1	Total	Zn	0	0
			1	1		
12	Z	1	Total	Zn	0	0
			1	1		

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	Mg	0	0
			1	1		
13	Q	1	Total	Mg	0	0
			1	1		

- Molecule 14 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).

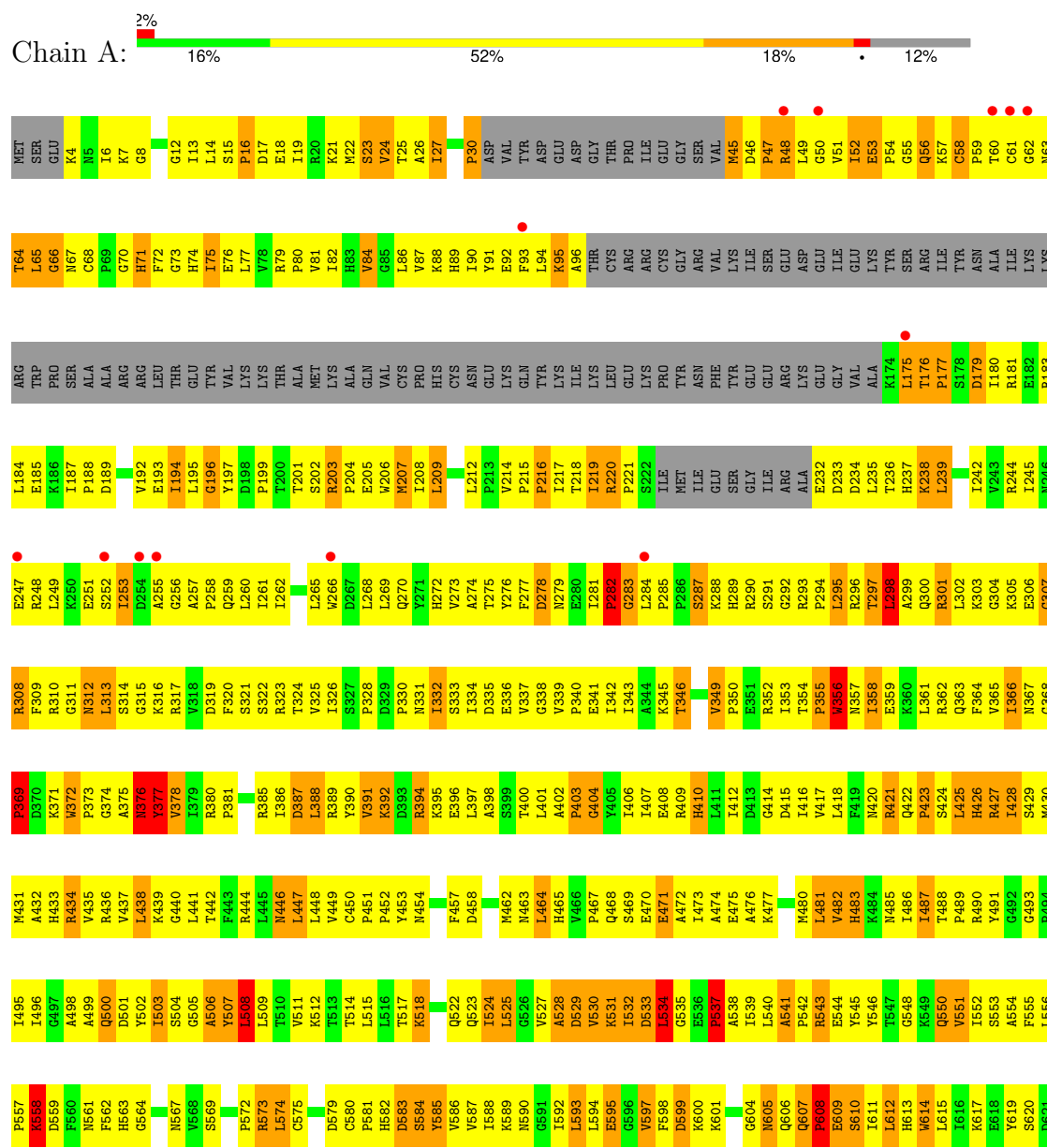


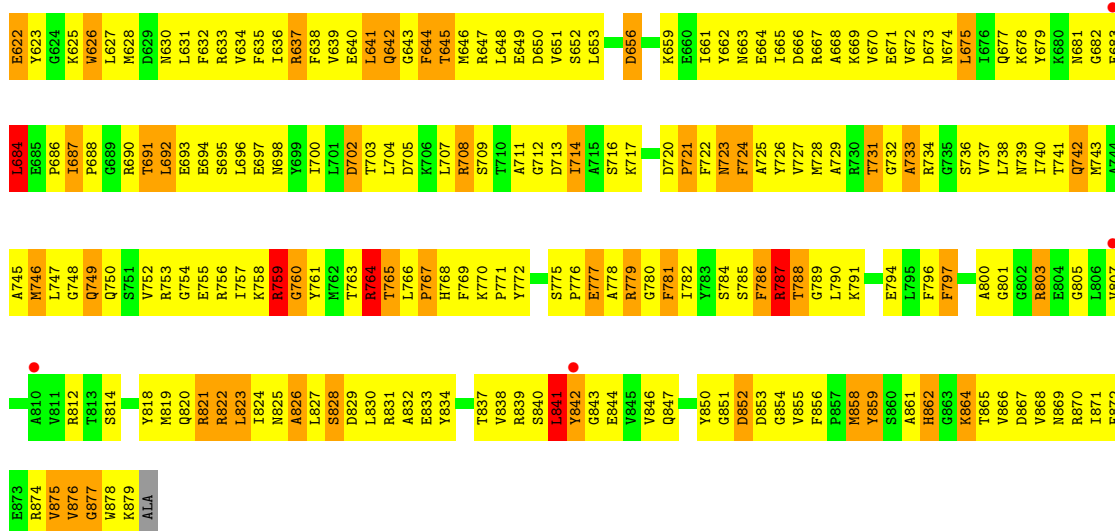
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	Fe	S	0	0
			7	3	4		
14	S	1	Total	Fe	S	0	0
			7	3	4		

3 Residue-property plots

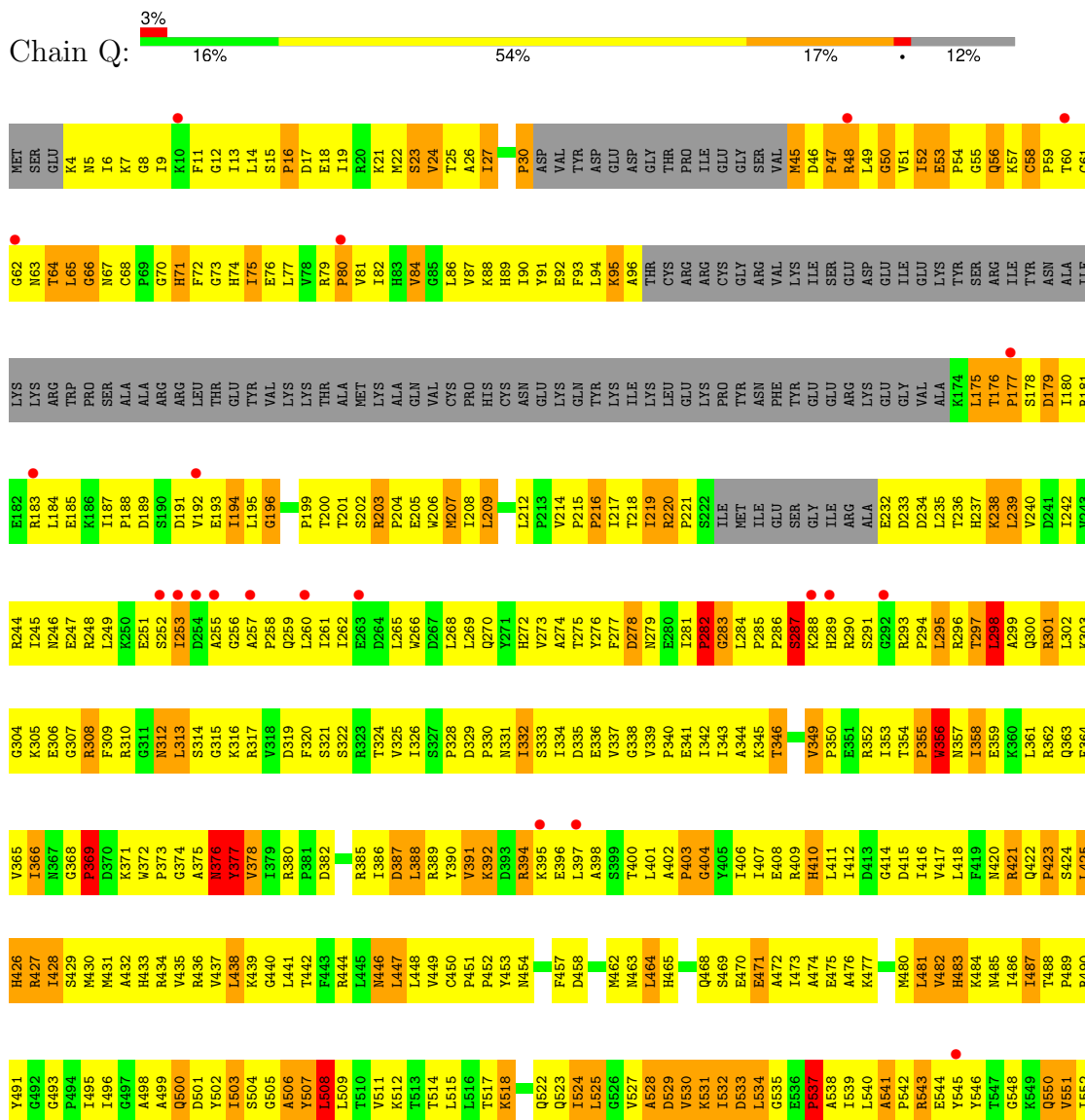
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

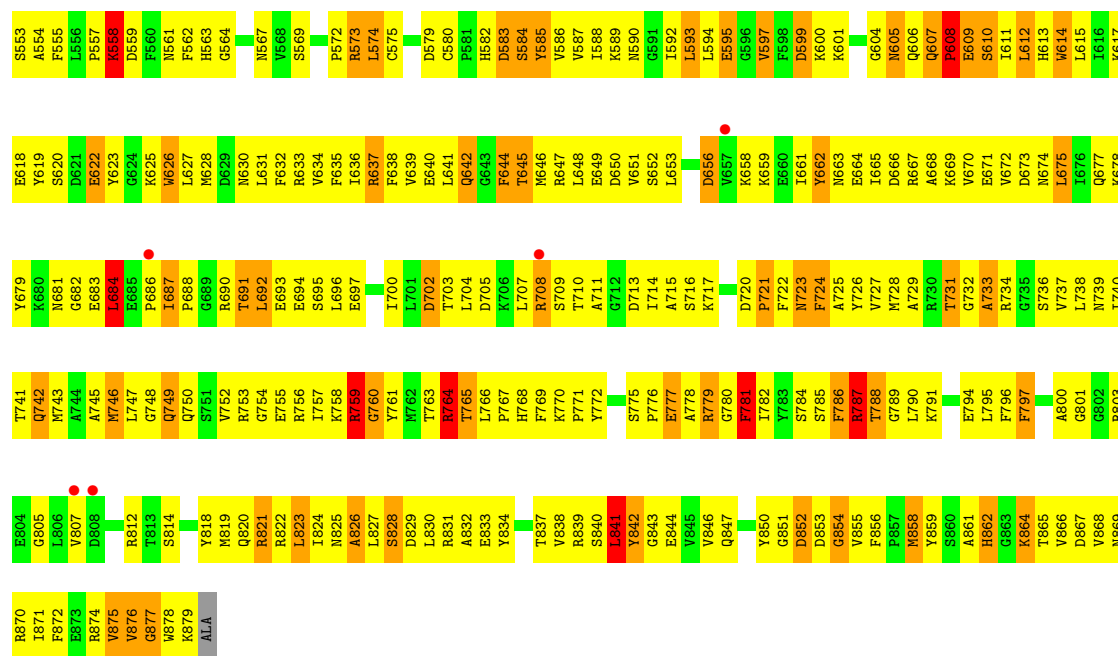
• Molecule 1: DNA-directed RNA polymerase subunit A



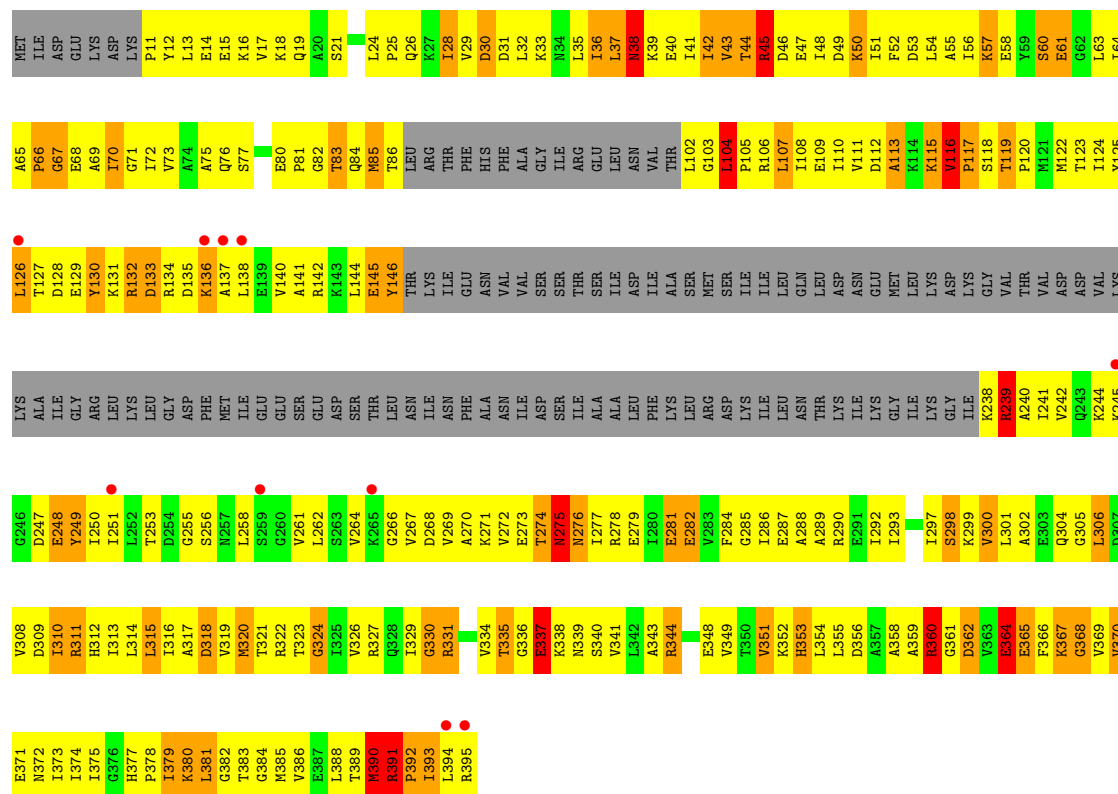


• Molecule 1: DNA-directed RNA polymerase subunit A



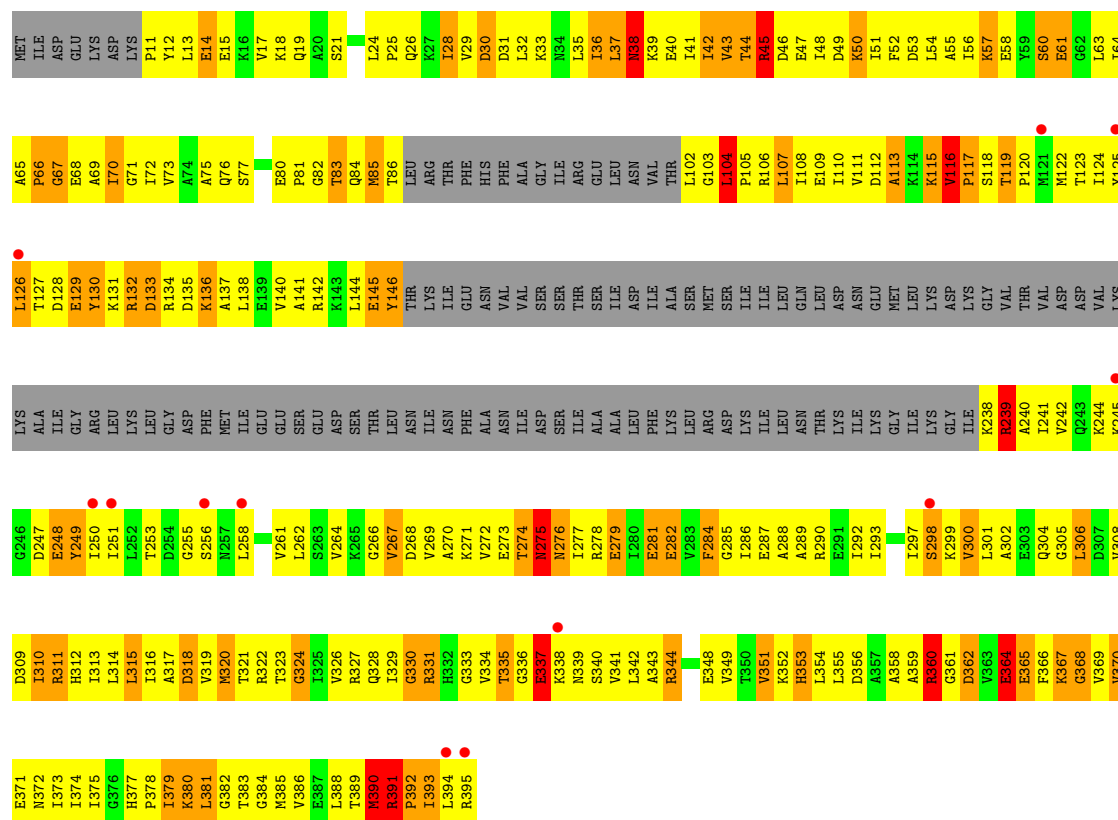


• Molecule 2: DNA-directed RNA polymerase subunit A''

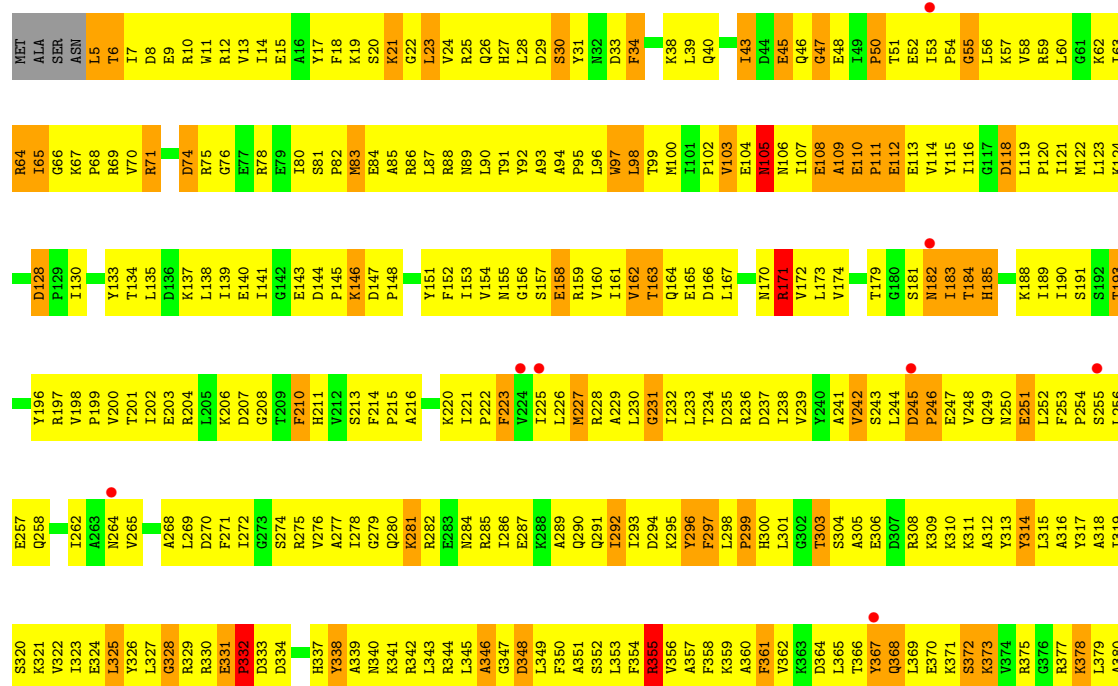


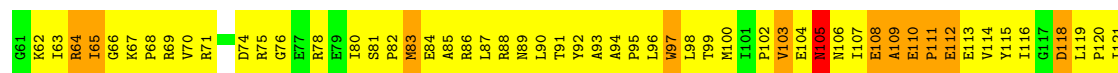
• Molecule 2: DNA-directed RNA polymerase subunit A''



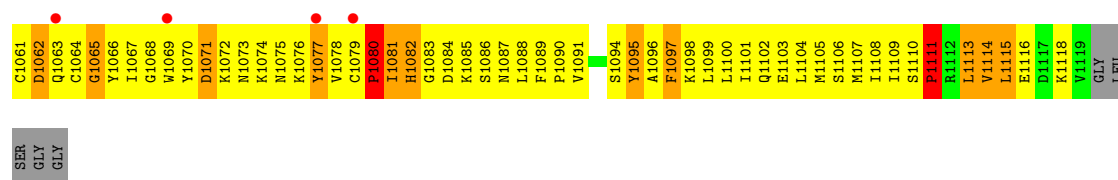


● Molecule 3: DNA-directed RNA polymerase subunit B

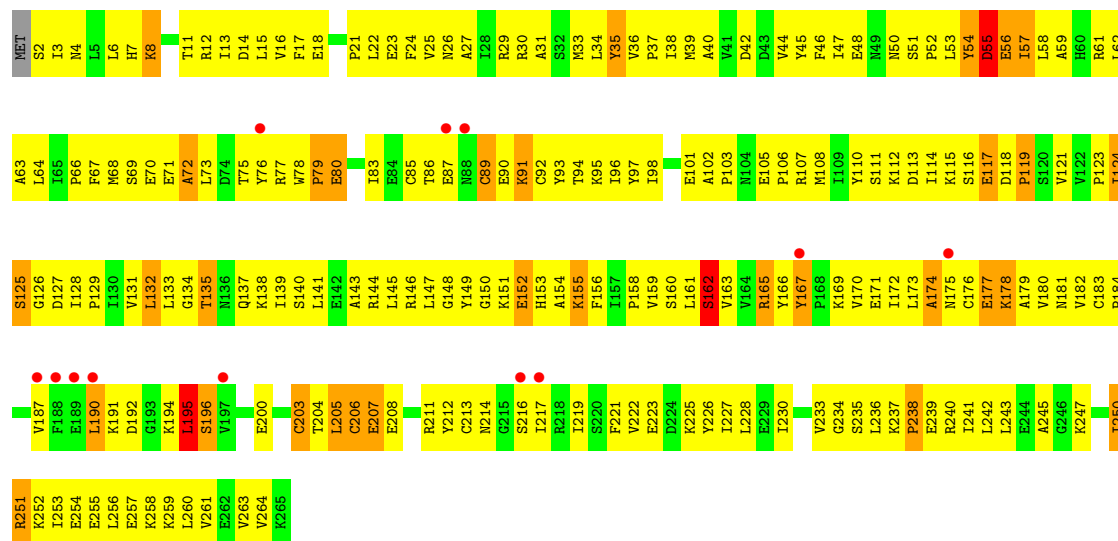




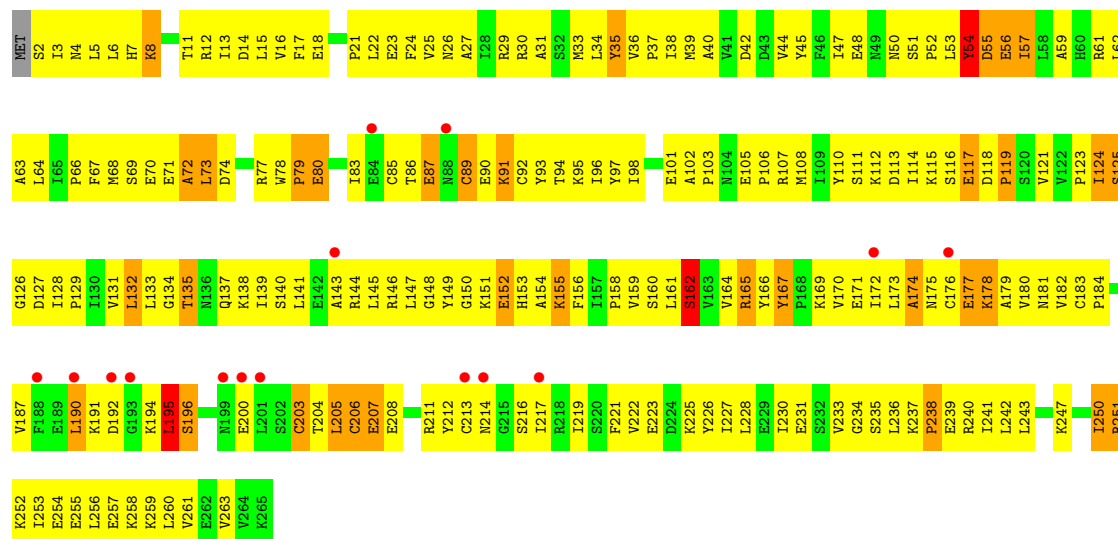
L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060																																																																																																																																
S936	G875	D876	K877	F878	A879	S880	P881	H882	Q883	Q884	K885	G886	V887	L888	E889	Q890	L891	T892	P893	Q894	V895	E896	I897	L952	L963	P964	D965	A966	T967	E968	V969	P970	I971	D972	G973	R974	T975	G976	K977	K978	I979		R882	I983	P984	F985	G986	V987	G988	P989	Y990	S991	K992	L993	H994	T995	M996		K1000																																																																																																																																
K813	V814	S815	P816	P817	R818	PHE	LEU	GLN	GLU	PHE	LYS	GLU	LEU	SER	GLN	GLU	GLN	GLN	A831	K832	K833	D834	T835	S836	T837	V838	T839	R840		E843	R844	G845	R846	D847	D848	L849	V850	L851	R852	T853	E854	T855	A856	E857	G858	N859	T860	L861	V862	K863	V864	R865	R866	R867	L868	L869	R870	P871	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
V626	A627	L628	V629	P630	L631	L632	P633	P634	T635	T636	H637	V638	L639	E640	E641	L642	P643	P644	P645	P646	P647	L648	G649	G650	T651	A652	S653	L654	L655	P656	P657	P658	L659	L660	L661	Q662	S663	P664	R665		Y666	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																																																														
I663	N664	E665	V666	H667	V668	N669	C670	D671	G672	G673	R674	V675	R676	S677	P678	L679	S680	I681	V682		N683	P684	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																																																																																																			
E441	A442	R443	D444	L445	H446	G447	T448	Q449	W450	A451	R452	V453	M454	C455	F456	E457	T458	P459	E460	G461	M462	N463	S464	G465	L466	V467	P468	Q469	R470	L471	L472	M473	A474	Q475	I476	A477	V478	G479	L480	M481	E482	R483	M484	V485	E486	K487	T488	L489	Y490	E491	N492	G493	V494	H495	E496	V497	L498	E499	V500																																																																																																																																
I501	ARG	ARG	VAL	THR	GLU	GLY	GLY	GLY	ASP	GLN	ASN	GLU	TYR	L515	K516	W517	S518	K519	V520	L521		R525	L526	I527	G528	Y529	E530	Q531	L532	D533	G534	E535	L536	A537	N538	K539	L540	R541	D542	R543	R544	R545		E548	I549	S550	D551	E552	V553	N554	V555	G556	H557	E558	V559	T560	D561	F562																																																																																																																																	
L379	A380	K381	K382	L383	L384	V385	R386	P387	D388	L389	G390	V391	E392	R393	I394	R395	H396	A397	L398	G399	T400	G401	N402	V403	Y404	G405	K406	R407		V410	S411	Q412	L413	L414	D415	R416	T417	M418	V419	L420	S421	M422		H425	L426	R427	R428	V429	L430	S431	M432	L433	A434	R435	E436	Q437	P438	N439	F440																																																																																																																																
L379	A380	K381	K382	L383	L384	V385	R386	P387	D388	L389	G390	V391	E392	R393	I394	R395	H396	A397	L398	G399	T400	G401	N402	V403	Y404	G405	K406	R407		V410	S411	Q412	L413	L414	D415	R416	T417	M418	V419	L420	S421	M422		H425	L426	R427	R428	V429	L430	S431	M432	L433	A434	R435	E436	Q437	P438	N439	F440																																																																																																																																
E441	A442	R443	D444	L445	H446	G447	T448	Q449	W450	A451	R452	V453	M454	C455	F456	E457	T458	P459	E460	G461	M462	N463	S464	G465	L466	V467	P468	Q469	R470	L471	L472	M473	A474	Q475	I476	A477	V478	G479	L480	M481	E482	R483	M484	V485	E486	K487	T488	L489	Y490	E491	N492	G493	V494	H495	E496	V497	L498	E499	V500																																																																																																																																
I501	ARG	ARG	VAL	THR	GLU	GLY	GLY	GLY	ASP	GLN	ASN	GLU	TYR	L515	K516	W517	S518	K519	V520	L521		R525	L526	I527	G528	Y529	E530	Q531	L532	D533	G534	E535	L536	A537	N538	K539	L540	R541	D542	R543	R544	R545		E548	I549	S550	D551	E552	V553	N554	V555	G556	H557	E558	V559	T560	D561	F562																																																																																																																																	
I563	N564	E565	V566	H567	V568	N569	C570	D571	G572	G573	R574	V575	R576	S577	P578	L579	S580	I581	V582		N586	P587	L588	V589	T590	L591	E592	D593	I594	E595	K596	L597	H598	L599	M600	L601	I602	F603	D604	D605	D606	L607	V608	R609		K612	I613	E614	V615	L616	D617	A618	V619	G620	H621	E622	N623	A624	F625																																																																																																																																
V626	A627	L628	V629	P630	L631	L632	P633	P634	T635	T636	H637	V638	L639	E640	E641	L642	P643	P644	P645	P646	P647	L648	G649	G650	T651	A652	S653	L654	L655	P656	P657	P658	L659	L660	L661	Q662	S663	P664	R665		Y666	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																																																														
R691	A692	H693	L694	P695	H696	Y697	P698	Q699	R700	P701	L702	V703	L704	E641	L642	P643	P644	P645	P646	P647	L648	G649	G650	T651	A652	S653	L654	L655	P656	P657	P658	L659	L660	L661	Q662	S663	P664	R665		Y666	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																																																															
R691	A692	H693	L694	P695	H696	Y697	P698	Q699	R700	P701	L702	V703	L704	E641	L642	P643	P644	P645	P646	P647	L648	G649	G650	T651	A652	S653	L654	L655	P656	P657	P658	L659	L660	L661	Q662	S663	P664	R665		Y666	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																																																															
R691	A692	H693	L694	P695	H696	Y697	P698	Q699	R700	P701	L702	V703	L704	E641	L642	P643	P644	P645	P646	P647	L648	G649	G650	T651	A652	S653	L654	L655	P656	P657	P658	L659	L660	L661	Q662	S663	P664	R665		Y666	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																																																															
R691	A692	H693	L694	P695	H696	Y697	P698	Q699	R700	P701	L702	V703	L704	E641	L642	P643	P644	P645	P646	P647	L648	G649	G650	T651	A652	S653	L654	L655	P656	P657	P658	L659	L660	L661	Q662	S663	P664	R665		Y666	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	L																																																																																																											



• Molecule 4: DNA-directed RNA polymerase subunit D

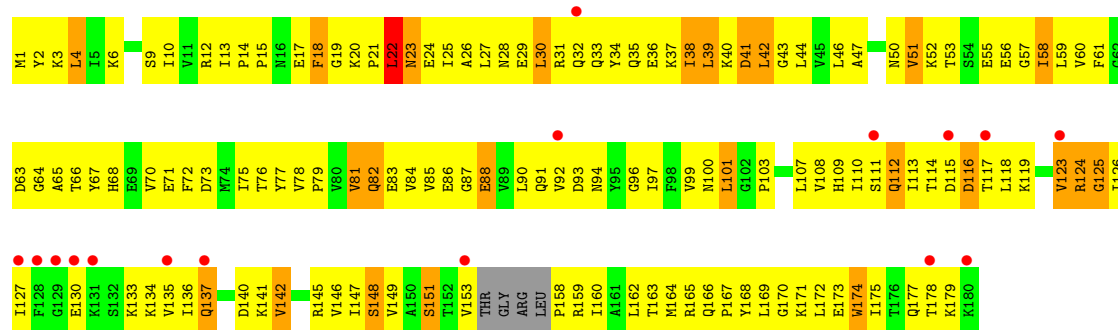


• Molecule 4: DNA-directed RNA polymerase subunit D

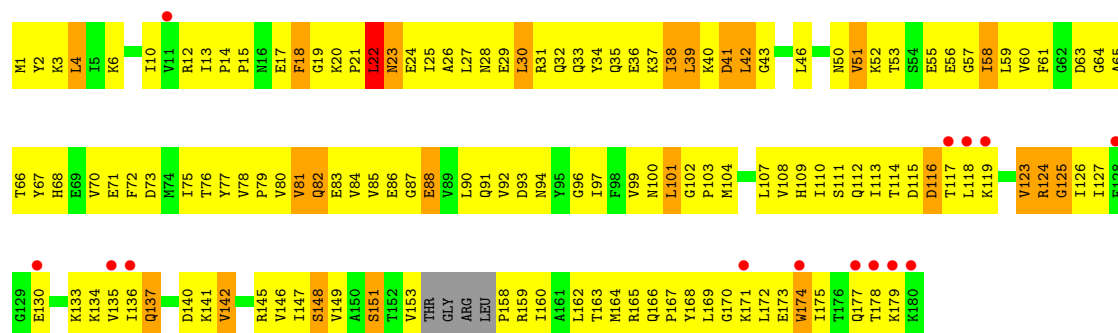


• Molecule 5: DNA-directed RNA polymerase subunit E

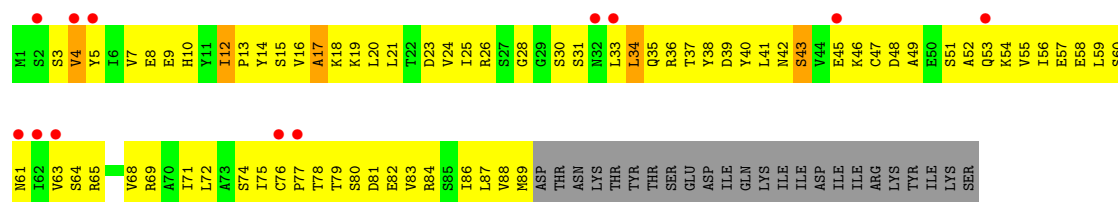
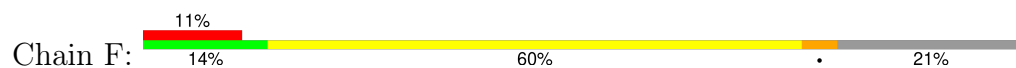




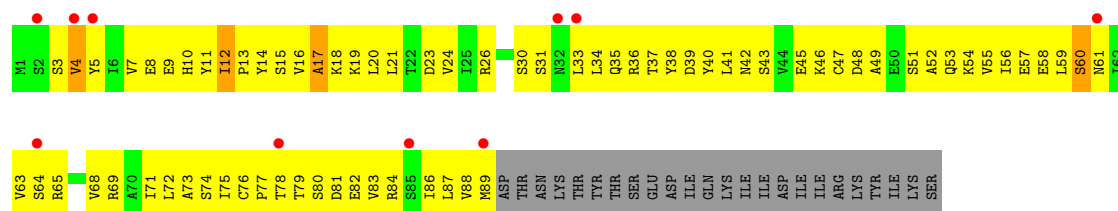
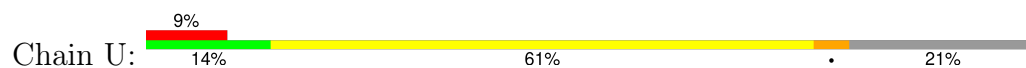
• Molecule 5: DNA-directed RNA polymerase subunit E



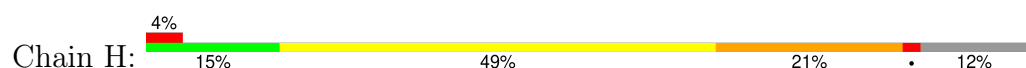
• Molecule 6: DNA-directed RNA polymerase subunit F

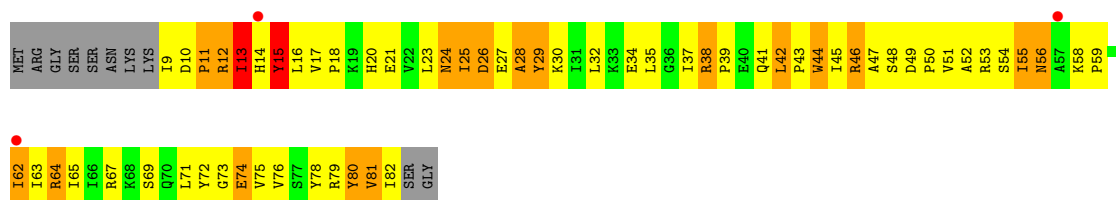


• Molecule 6: DNA-directed RNA polymerase subunit F

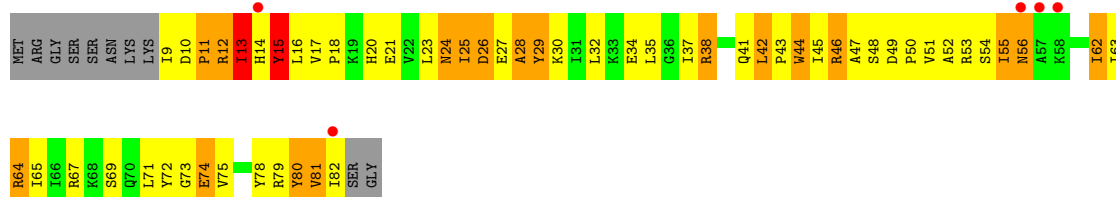
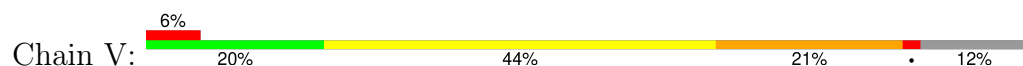


• Molecule 7: DNA-directed RNA polymerase subunit H

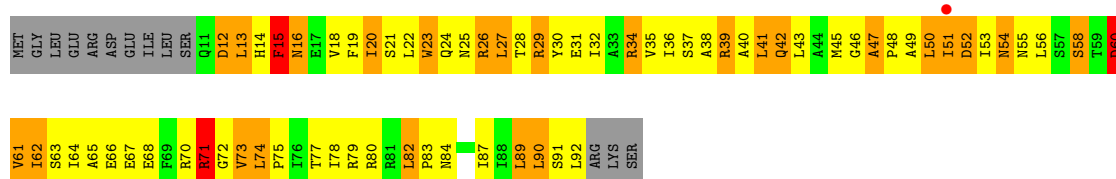




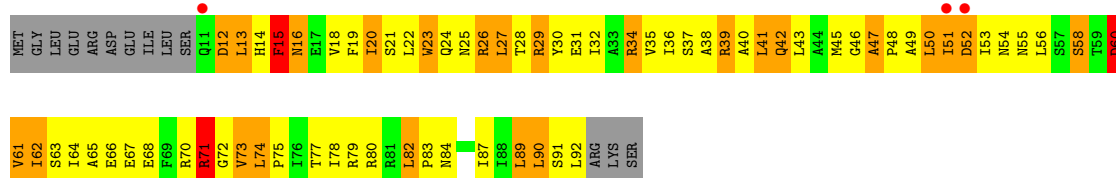
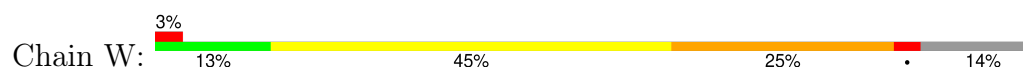
• Molecule 7: DNA-directed RNA polymerase subunit H



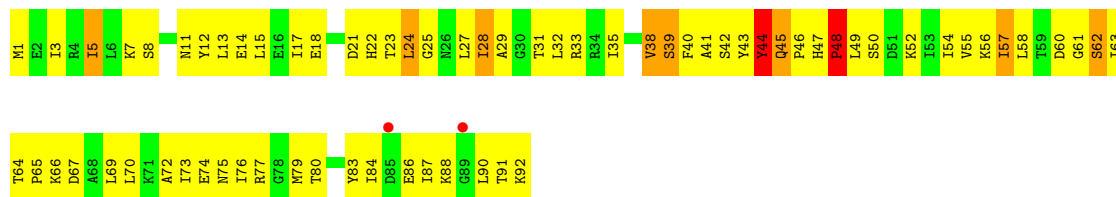
• Molecule 8: DNA-directed RNA polymerase subunit K



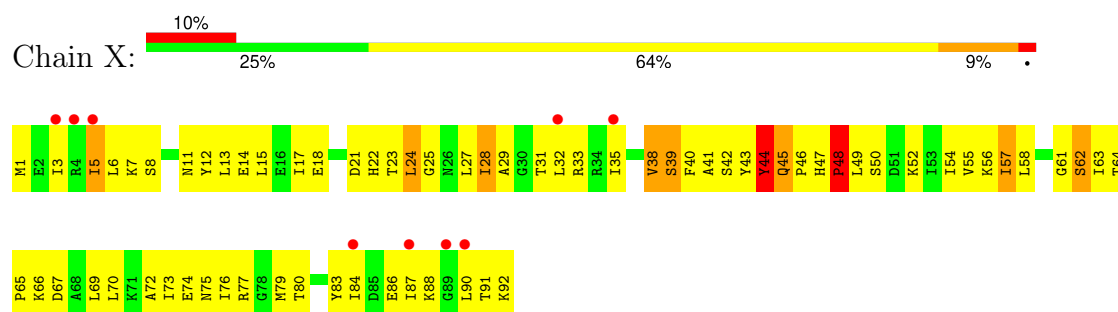
• Molecule 8: DNA-directed RNA polymerase subunit K



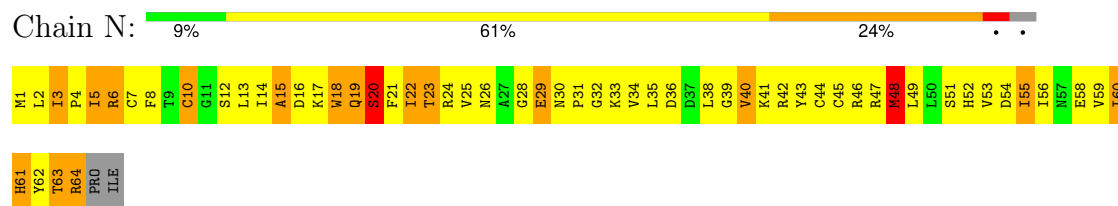
• Molecule 9: DNA-directed RNA polymerase subunit L



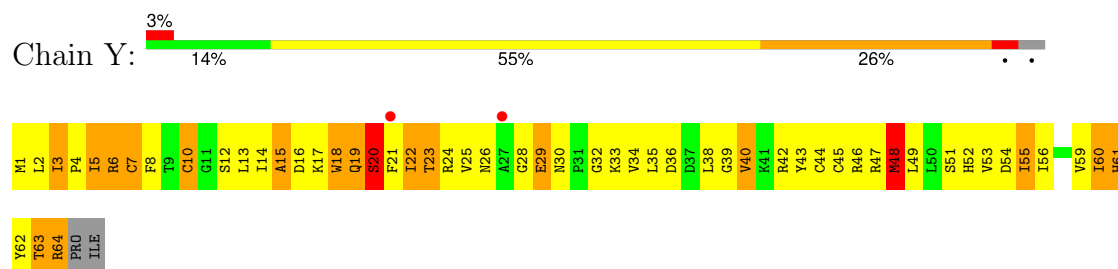
• Molecule 9: DNA-directed RNA polymerase subunit L



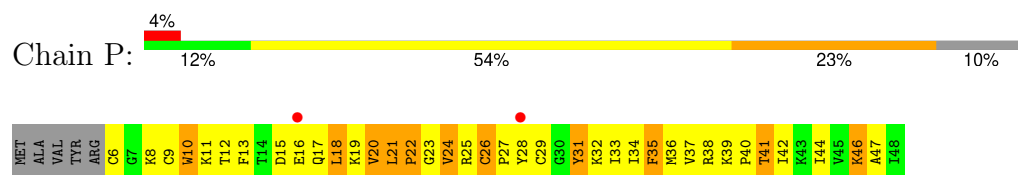
- Molecule 10: DNA-directed RNA polymerase subunit N



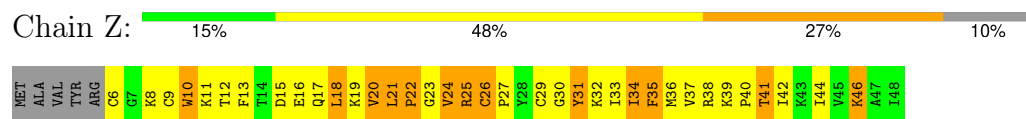
- Molecule 10: DNA-directed RNA polymerase subunit N



- Molecule 11: DNA-directed RNA polymerase subunit P



- Molecule 11: DNA-directed RNA polymerase subunit P



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.82Å 201.24Å 196.05Å 90.00° 100.92° 90.00°	Depositor
Resolution (Å)	39.79 – 3.40 39.79 – 3.40	Depositor EDS
% Data completeness (in resolution range)	80.4 (39.79-3.40) 80.3 (39.79-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.274 , 0.343 0.271 , 0.275	Depositor DCC
R_{free} test set	5323 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	48122	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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: MG, ZN, F3S

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	0.48	0/6306	0.80	4/8539 (0.0%)
1	Q	0.46	0/6306	0.79	4/8539 (0.0%)
2	C	0.46	0/2189	0.81	0/2947
2	G	0.43	0/2189	0.80	0/2947
3	B	0.46	0/8810	0.79	5/11921 (0.0%)
3	R	0.45	0/8810	0.79	3/11921 (0.0%)
4	D	0.40	0/2152	0.68	0/2911
4	S	0.37	0/2152	0.67	0/2911
5	E	0.38	0/1423	0.69	0/1919
5	T	0.37	0/1423	0.69	0/1919
6	F	0.35	0/701	0.63	0/949
6	U	0.35	0/701	0.62	0/949
7	H	0.44	0/625	0.76	0/848
7	V	0.41	0/625	0.76	0/848
8	K	0.50	0/667	0.82	0/903
8	W	0.49	0/667	0.81	0/903
9	L	0.39	0/733	0.72	0/986
9	X	0.38	0/733	0.72	0/986
10	N	0.38	0/523	0.75	0/705
10	Y	0.37	0/523	0.74	0/705
11	P	0.45	0/354	0.68	0/475
11	Z	0.46	0/354	0.67	0/475
All	All	0.44	0/48966	0.77	16/66206 (0.0%)

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
3	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	R	0	1
4	D	0	1
4	S	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	841	LEU	CA-CB-CG	7.67	132.93	115.30
1	Q	841	LEU	CA-CB-CG	7.56	132.69	115.30
3	B	436	GLY	N-CA-C	-6.16	97.70	113.10
3	R	436	GLY	N-CA-C	-5.97	98.17	113.10
1	A	508	LEU	N-CA-C	-5.89	95.11	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	314	TYR	Sidechain
4	D	54	TYR	Sidechain
3	R	314	TYR	Sidechain
4	S	54	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	6173	0	6243	1147	0
1	Q	6173	0	6243	1128	0
2	C	2169	0	2288	501	0
2	G	2169	0	2288	526	0
3	B	8645	0	8782	1656	0
3	R	8645	0	8780	1698	0
4	D	2114	0	2145	357	0
4	S	2114	0	2145	348	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1402	0	1467	222	0
5	T	1402	0	1467	246	0
6	F	694	0	705	129	0
6	U	694	0	705	139	0
7	H	611	0	641	117	0
7	V	611	0	641	125	0
8	K	658	0	692	161	0
8	W	658	0	692	174	0
9	L	723	0	749	94	0
9	X	723	0	749	91	0
10	N	514	0	528	159	0
10	Y	514	0	529	151	0
11	P	346	0	376	63	0
11	Z	346	0	375	58	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	N	1	0	0	0	0
12	P	1	0	0	0	0
12	Q	1	0	0	0	0
12	R	1	0	0	0	0
12	Y	1	0	0	0	0
12	Z	1	0	0	0	0
13	A	1	0	0	0	0
13	Q	1	0	0	0	0
14	D	7	0	0	4	0
14	S	7	0	0	3	0
All	All	48122	0	49230	8272	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 85.

The worst 5 of 8272 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)
1:A:238:LYS:NZ	1:A:297:THR:HB	1.42	1.31
1:Q:238:LYS:NZ	1:Q:297:THR:HB	1.43	1.31
1:A:803:ARG:HG2	3:B:444:ASP:HA	1.20	1.17
1:A:308:ARG:HH21	3:B:1099:LEU:HD13	1.10	1.16
3:R:88:ARG:HD3	3:R:853:THR:HG21	1.25	1.15

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	768/880 (87%)	513 (67%)	136 (18%)	119 (16%)	0	0
1	Q	768/880 (87%)	509 (66%)	141 (18%)	118 (15%)	0	0
2	C	273/392 (70%)	158 (58%)	66 (24%)	49 (18%)	0	0
2	G	273/392 (70%)	161 (59%)	61 (22%)	51 (19%)	0	0
3	B	1084/1124 (96%)	698 (64%)	238 (22%)	148 (14%)	0	1
3	R	1084/1124 (96%)	698 (64%)	237 (22%)	149 (14%)	0	1
4	D	262/265 (99%)	166 (63%)	69 (26%)	27 (10%)	0	3
4	S	262/265 (99%)	167 (64%)	66 (25%)	29 (11%)	0	3
5	E	172/180 (96%)	123 (72%)	31 (18%)	18 (10%)	0	3
5	T	172/180 (96%)	122 (71%)	32 (19%)	18 (10%)	0	3
6	F	87/113 (77%)	56 (64%)	22 (25%)	9 (10%)	0	3
6	U	87/113 (77%)	56 (64%)	23 (26%)	8 (9%)	1	4
7	H	72/84 (86%)	46 (64%)	13 (18%)	13 (18%)	0	0
7	V	72/84 (86%)	44 (61%)	15 (21%)	13 (18%)	0	0
8	K	80/95 (84%)	44 (55%)	19 (24%)	17 (21%)	0	0
8	W	80/95 (84%)	44 (55%)	20 (25%)	16 (20%)	0	0
9	L	90/92 (98%)	64 (71%)	19 (21%)	7 (8%)	1	6
9	X	90/92 (98%)	66 (73%)	17 (19%)	7 (8%)	1	6
10	N	62/66 (94%)	30 (48%)	18 (29%)	14 (23%)	0	0
10	Y	62/66 (94%)	31 (50%)	18 (29%)	13 (21%)	0	0
11	P	41/48 (85%)	24 (58%)	10 (24%)	7 (17%)	0	0
11	Z	41/48 (85%)	23 (56%)	11 (27%)	7 (17%)	0	0
All	All	5982/6678 (90%)	3843 (64%)	1282 (21%)	857 (14%)	0	1

5 of 857 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	58	CYS
1	A	64	THR
1	A	65	LEU
1	A	194	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	675/766 (88%)	580 (86%)	95 (14%)	3	13
1	Q	675/766 (88%)	583 (86%)	92 (14%)	3	14
2	C	237/338 (70%)	201 (85%)	36 (15%)	3	11
2	G	237/338 (70%)	199 (84%)	38 (16%)	2	10
3	B	937/965 (97%)	807 (86%)	130 (14%)	3	13
3	R	937/965 (97%)	810 (86%)	127 (14%)	3	14
4	D	241/242 (100%)	224 (93%)	17 (7%)	14	44
4	S	241/242 (100%)	223 (92%)	18 (8%)	13	41
5	E	156/159 (98%)	142 (91%)	14 (9%)	9	32
5	T	156/159 (98%)	142 (91%)	14 (9%)	9	32
6	F	82/106 (77%)	79 (96%)	3 (4%)	34	62
6	U	82/106 (77%)	79 (96%)	3 (4%)	34	62
7	H	67/75 (89%)	54 (81%)	13 (19%)	1	4
7	V	67/75 (89%)	55 (82%)	12 (18%)	2	6
8	K	72/84 (86%)	57 (79%)	15 (21%)	1	3
8	W	72/84 (86%)	57 (79%)	15 (21%)	1	3
9	L	81/81 (100%)	75 (93%)	6 (7%)	13	42
9	X	81/81 (100%)	75 (93%)	6 (7%)	13	42
10	N	58/60 (97%)	50 (86%)	8 (14%)	3	14
10	Y	58/60 (97%)	49 (84%)	9 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	P	39/43 (91%)	31 (80%)	8 (20%)	1	3
11	Z	39/43 (91%)	31 (80%)	8 (20%)	1	3
All	All	5290/5838 (91%)	4603 (87%)	687 (13%)	4	16

5 of 687 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	335	THR
3	R	959	ARG
3	R	6	THR
2	G	331	ARG
3	R	551	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	275	ASN
3	R	721	ASN
3	R	89	ASN
3	R	439	ASN
3	R	994	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
14	F3S	S	1001	4	0,9,9	-	-	-		
14	F3S	D	1001	4	0,9,9	-	-	-		

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
14	F3S	S	1001	4	-	-	0/3/3/3
14	F3S	D	1001	4	-	-	0/3/3/3

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.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	S	1001	F3S	3	0
14	D	1001	F3S	4	0

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	776/880 (88%)	-0.18	17 (2%) 62 60	23, 75, 132, 186	0
1	Q	776/880 (88%)	-0.03	26 (3%) 45 44	29, 87, 145, 202	0
2	C	279/392 (71%)	-0.06	10 (3%) 42 42	29, 81, 153, 190	0
2	G	279/392 (71%)	0.00	12 (4%) 35 35	42, 97, 153, 181	0
3	B	1090/1124 (96%)	-0.19	17 (1%) 72 70	24, 78, 145, 196	0
3	R	1090/1124 (96%)	-0.10	33 (3%) 50 49	36, 84, 149, 196	0
4	D	264/265 (99%)	0.09	12 (4%) 33 33	44, 94, 144, 179	0
4	S	264/265 (99%)	0.22	15 (5%) 23 24	61, 111, 157, 192	0
5	E	176/180 (97%)	0.38	16 (9%) 9 10	39, 112, 189, 202	0
5	T	176/180 (97%)	0.35	14 (7%) 12 13	57, 113, 176, 202	0
6	F	89/113 (78%)	0.35	12 (13%) 3 4	73, 142, 182, 196	0
6	U	89/113 (78%)	0.59	10 (11%) 5 6	93, 141, 184, 201	0
7	H	74/84 (88%)	0.21	3 (4%) 37 36	46, 90, 137, 165	0
7	V	74/84 (88%)	0.20	5 (6%) 17 19	70, 101, 159, 198	0
8	K	82/95 (86%)	-0.25	1 (1%) 79 77	30, 72, 118, 154	0
8	W	82/95 (86%)	0.03	3 (3%) 41 40	47, 82, 139, 189	0
9	L	92/92 (100%)	0.01	2 (2%) 62 60	42, 81, 125, 200	0
9	X	92/92 (100%)	0.31	9 (9%) 7 9	52, 102, 140, 159	0
10	N	64/66 (96%)	-0.23	0 100 100	60, 90, 124, 174	0
10	Y	64/66 (96%)	-0.02	2 (3%) 49 48	61, 98, 145, 185	0
11	P	43/48 (89%)	-0.03	2 (4%) 31 31	48, 101, 137, 154	0
11	Z	43/48 (89%)	-0.13	0 100 100	64, 100, 144, 180	0
All	All	6058/6678 (90%)	-0.03	221 (3%) 42 42	23, 88, 153, 202	0

The worst 5 of 221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	434	ALA	8.3
5	T	135	VAL	6.6
6	U	33	LEU	6.1
4	D	217	ILE	5.8
6	U	2	SER	5.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
13	MG	A	1003	1/1	0.92	0.18	57,57,57,57	0
12	ZN	R	2001	1/1	0.97	0.06	101,101,101,101	0
12	ZN	B	2001	1/1	0.97	0.11	91,91,91,91	0
13	MG	Q	1003	1/1	0.97	0.25	60,60,60,60	0
14	F3S	D	1001	7/7	0.97	0.12	79,80,80,80	0
14	F3S	S	1001	7/7	0.98	0.11	111,111,112,113	0
12	ZN	Y	1001	1/1	0.99	0.17	93,93,93,93	0
12	ZN	Z	1001	1/1	0.99	0.12	106,106,106,106	0
12	ZN	N	1001	1/1	0.99	0.17	93,93,93,93	0
12	ZN	P	1001	1/1	0.99	0.10	103,103,103,103	0
12	ZN	Q	1002	1/1	0.99	0.05	89,89,89,89	0
12	ZN	A	1002	1/1	0.99	0.06	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.