



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 12:59 PM GMT

PDB ID : 2A6E
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.;
Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.;
RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-02
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

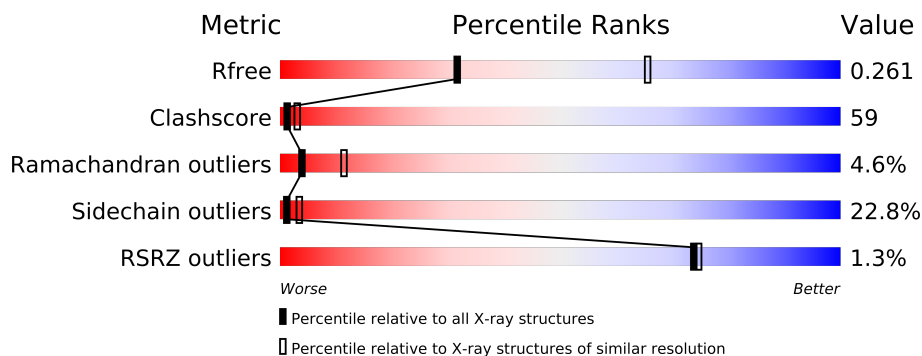
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58679 atoms, of which 0 are hydrogen and 0 are deuterium.

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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	N	1	Total	Mg	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	191	Total	O	0	0
			191	191		
8	B	181	Total	O	0	0
			181	181		
8	C	767	Total	O	0	0
			767	767		
8	D	1100	Total	O	0	0
			1100	1100		
8	E	93	Total	O	0	0
			93	93		
8	F	333	Total	O	0	0
			333	333		
8	K	151	Total	O	0	0
			151	151		
8	L	179	Total	O	0	0
			179	179		
8	M	739	Total	O	0	0
			739	739		

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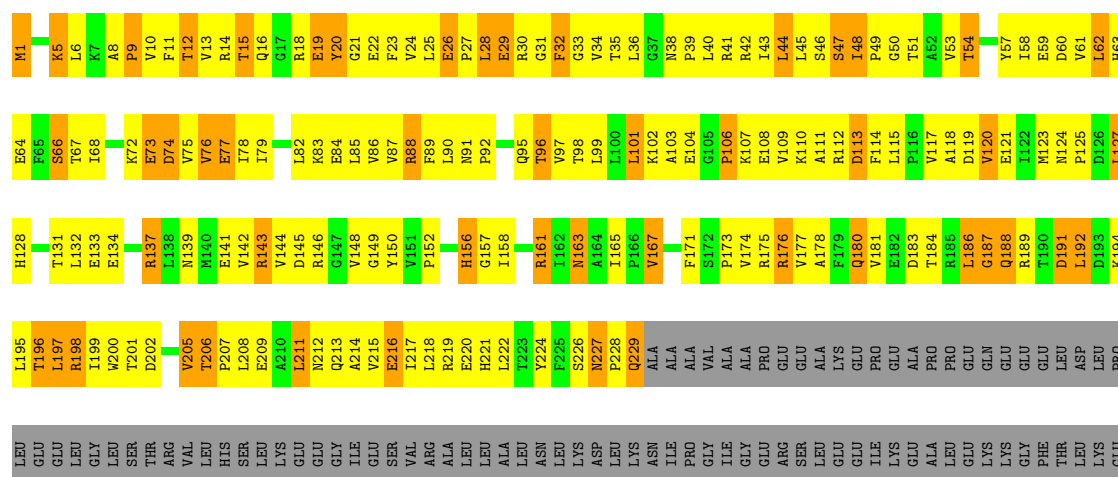
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	1038	Total 1038	O 1038	0	0
8	O	78	Total 78	O 78	0	0
8	P	267	Total 267	O 267	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

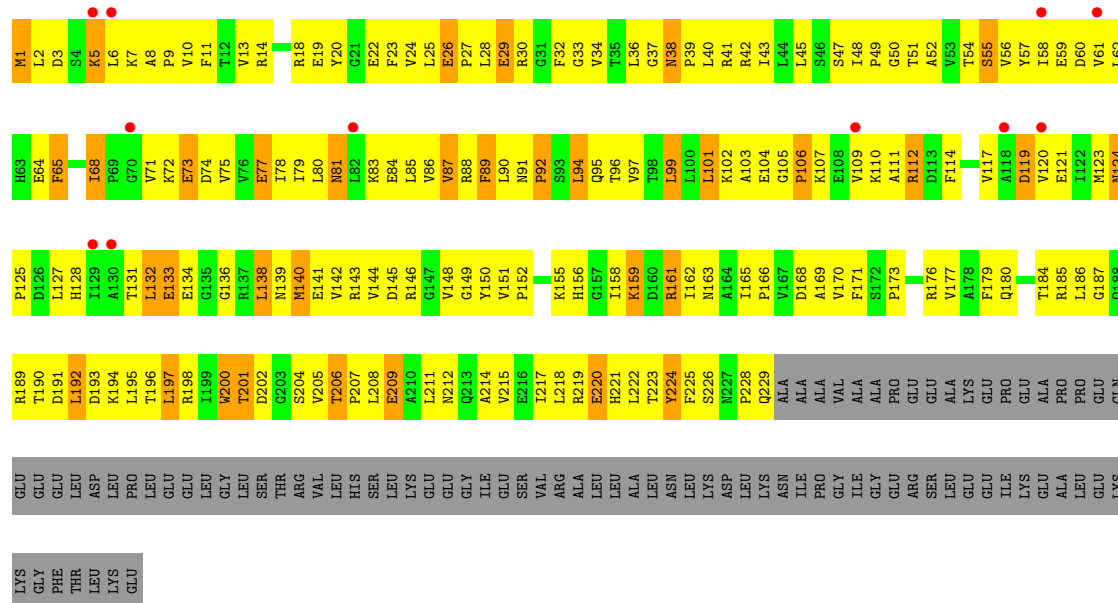
- Molecule 1: DNA-directed RNA polymerase alpha chain

Chain A:



- Molecule 1: DNA-directed RNA polymerase alpha chain

Chain B:



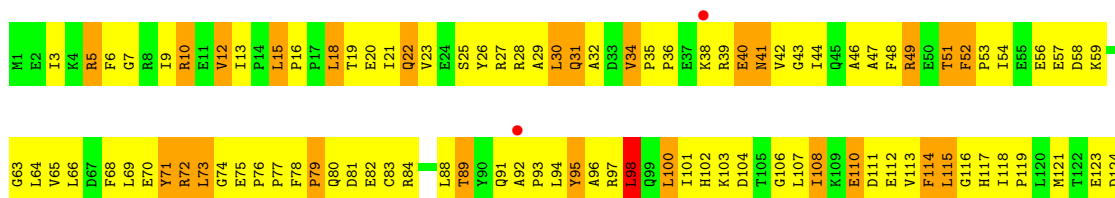
Chain K:



Chain L:



Chain C:



E1083	L1015	L952	V825	L694	G634	A568	G505	P444	A380	V317	R250	M187	G125
S1094	L1016	V953	Y826	L695	T635	V569	N506	E445	A381	V318	D251	K188	S126
F1085	L1017	T954	A828	K696	A636	P570	R507	G446	R382	G319	K252	R189	F127
Q1018	Q1018	P955	A827	L637	L637	L571	I508	A447	R383	G319	V254	K190	I128
V1087	Q1019	G956	R831	D638	D638	R572	A510	R448	F385	R320	V255		I129
P1020	P1020	K957	K832	D698	D698	I573	A509	I449	F386	E321	A255		
L1021	L1021	T958	K833	Y700	R640	A574	E511	G450	F386	E321	Y256	L193	D133
			L833	T701	P641	Q875	R512	L451	S387	T325	Y257	V194	R134
			K834	T702	R642	A576	V513	L452	R388	D326	Y258	L195	R135
			Q835	T703	V643	V514	V514	K327		R327	Y259	L196	R136
			G836	H704	V644	V578	A515	S454		L328	L260	R197	V137
			R837	T705	V645	V579	R516	L455		G329	L261	R198	S138
			K838	T706	V646	M580	B517	A456			A262	V199	Q139
			L839	T707	Q647		K518	A457			D263	L200	I140
			A840	Y708	R648		G519			R332	P264	G291	I141
			R841	T709	V649	L583	R520	A458		T333	R265	Y202	H141
			R842	T710	R650	E584	E584	A459		R334	R266	D203	R142
			H843	T711	K651	R585	P521	A460		T335	R266	Q204	S143
			G844	T712	G652	R586	V522	V461		V336	Y267	Q205	P144
			R845	T713	D653	R588	I523	D462		G337	D268	T206	G145
			K846	T714	L654	R889	S525	E463		E338	L269	L207	V146
			G847	T715	L655	S590	P526	G465		L401	E271	A208	Y147
			V848	K716	A656	S591	E527	F466		K341	A272	E210	F148
			V849	T717	D657	L592	E528	I467		G342	G273	L211	T149
				G718	G658		V529	R468		Q343	R274	G212	D151
				T719	P659	L595	E530	T469		F344	Y275	A213	P152
				T720	A660	T596	F531	P470		R345		Y214	A153
				R721	S661	T597	M532	Y471		V346	E279	E216	R154
				T722	E662	E598	D533	R472		G347	K280	G156	G166
				T723	N663		V534	V474		L348	L281	V218	P163
				R724	G664	G601	S535	V474		A349	G282	G219	R157
				D725	F665	E602	P536	V475		R350			Y158
				T726	L666	E603	K537			L351	L283	G220	I159
				P727	A667	A604	Q538			A352	L284	L221	S161
				H728	L668	K605	V542	V478		P415	L285	M222	G162
				T729	G669	V606	T480	D481		G416	S286	D223	I163
				S730	D670	D607	N543	E482		G417	G287	E224	I163
				E731	N671	G608		V483		L418	R288	S235	P164
				A732	V672	N609	L546	V483		E357	T289	V226	L165
				L733	L673	R610	I547	V484		R358	L290	F227	P166
				R734	V674	I611	F548	M486		K359	A291	A228	R167
				R735	A675	V612	F549	M486		L360	R292	M229	R168
				D736	L676	V613	L550	T487		K361	R293	R230	G169
				L737	M677	R614	E551	A488		G362	F293	P231	P170
				D738	P678	Y615	H52	T489		S363		E232	W171
				E739	F679	Y615	D532	T489		E364	K299	E232	W171
				T740	D680	L620	D554	E490		D365	D300	E233	I172
				G741	G681	V621	A555	E491		S366	E301	A234	D173
				V742	Y682	E622	N556	D492		L367	V302	L235	L174
				T743	N683	Y623	R557	R493		T368	F303	T236	E175
				R744	F684	P624	R557	Y494		P369	L304	R237	V176
				T745	E685	L625	A558	T495		A370	P305	L238	E177
				G746	D686	R626	L559	I496		K371	T306	P239	P178
				A747	A687	R627	M560	A497		L372	L307	F239	P179
				V748	T688	Y628	G561	Q498		V373	G240	L241	G180
				T749	V689	Y629	S562	A499		N374	Y309	L242	V181
				R750	L690	R630	N563	N500		S375	F311	R243	V182
				P751	S691	S632	M564	T501		R376		P244	S183
				V752	G692	N632	Q565	P502		P377	A312	G245	M184
				R624	E693	Q633	T566	E504		L378	R292	D246	K185
							D567			E379	T314		V186

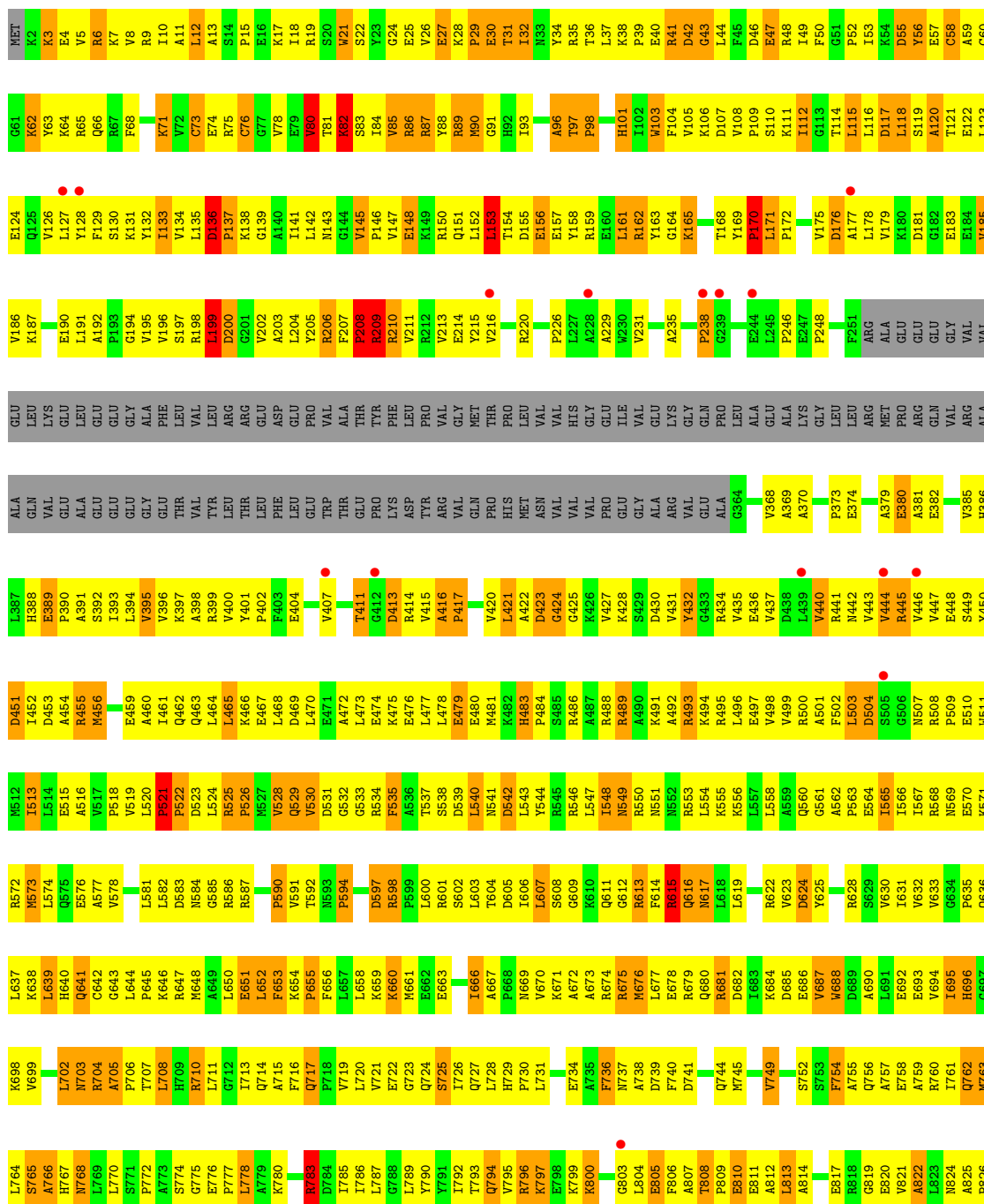
- Molecule 2: DNA-directed RNA polymerase beta chain

Chain M: 

R978	R979	G980	E981	P982	P983	E984	G985	P986	P987	P988	P989	G990	G991	P992	P993	P994	M995	K996	L997	H998	M1000	V1001	E1002	D1003	K1004	M1005	L1006	A1007	R1008	S1009	P1012	Y1013	S1014	L1015	L1016	T1017	Q1018	Q1019	P1020	L1021	K1024	F1027	Q1030	R1031	F1032	G1033	E1034	M1035	L1036	V1037	V1038	A1039	L1040	E1041																																																																																																																																																																																																																																																																																																																																																																																																																										
D907	G908	L909	K910	E911	P912	E913	G914	K915	E916	L917	L918	A919	Q920	A921	E922	E923	V924	Y925	F926	K927	K928	P929	D930	K931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970																																																																																																																																																																																																																																																																																																																																																																																																																	
D937	K938	L939	A940	E941	P942	E943	G944	K945	E946	L947	L948	V949	Q950	A951	E952	E953	V954	Y955	F956	K957	K958	P959	D960	K961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000	E1001	E1002	E1003	E1004	E1005	E1006	E1007	E1008	E1009	E1010	E1011	E1012	E1013	E1014	E1015	E1016	E1017	E1018	E1019	E1020	E1021	E1022	E1023	E1024	E1025	E1026	E1027	E1028	E1029	E1030	E1031	E1032	E1033	E1034	E1035	E1036	E1037	E1038	E1039	E1040	E1041																																																																																																																																																																																																																																																																																																																																																																								
E771	R772	L773	L774	R775	R776	L777	F778	F779	E780	K781	E782	R783	E784	F785	E786	E787	E788	E789	L790	R791	F792	F793	F794	G795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	K814	P815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000	E1001	E1002	E1003	E1004	E1005	E1006	E1007	E1008	E1009	E1010	E1011	E1012	E1013	E1014	E1015	E1016	E1017	E1018	E1019	E1020	E1021	E1022	E1023	E1024	E1025	E1026	E1027	E1028	E1029	E1030	E1031	E1032	E1033	E1034	E1035	E1036	E1037	E1038	E1039	E1040	E1041																																																																																																																																																																																																		
D638	Q639	R640	P641	R642	P643	V644	V645	V646	Q647	R648	V649	R650	K651	G652	D653	L654	D655	E656	E657	A658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	D680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000	E1001	E1002	E1003	E1004	E1005	E1006	E1007	E1008	E1009	E1010	E1011	E1012	E1013	E1014	E1015	E1016	E1017	E1018	E1019	E1020	E1021	E1022	E1023	E1024	E1025	E1026	E1027	E1028	E1029	E1030	E1031	E1032	E1033	E1034	E1035	E1036	E1037	E1038	E1039	E1040	E1041																																																													
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L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	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	L																																																																																																																																																																																																																																																																																																																																																		

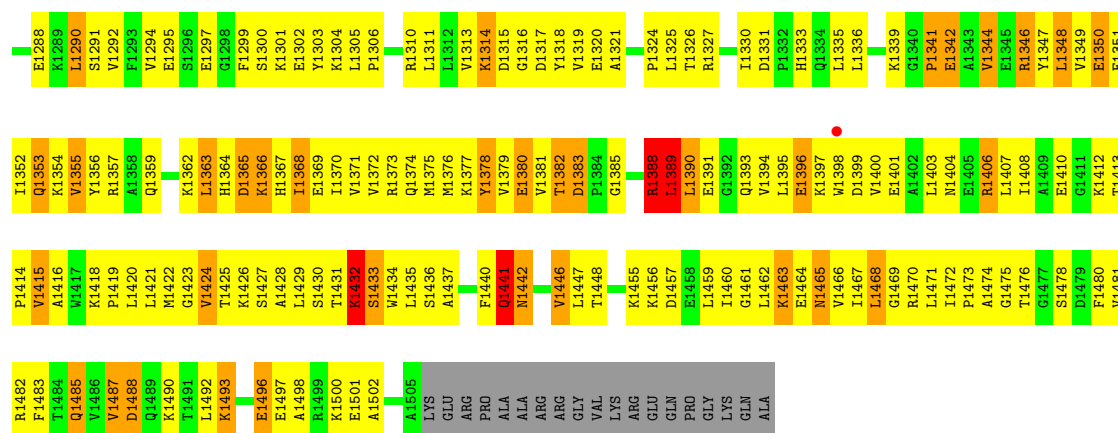


Chain D:



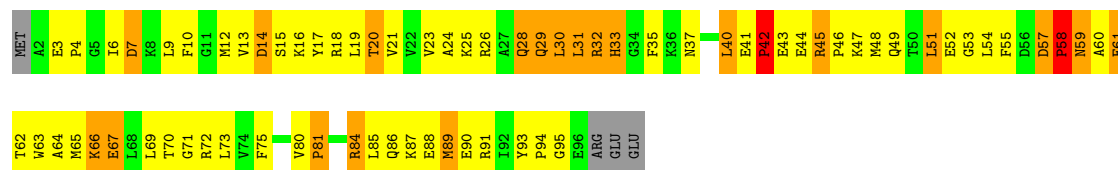


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V1224	A1150	T1088	M1023	I951	R884	A821	A755	A690	S629	I567	G506	R445	GLY	VAL
A1225	R1151	A1089		D952	I885	V822	Q756	L691	V630	R568	N507	V446	ARG	VAL
A1226		D1090	S1026	D953	V886	L823		E692	I631	N569	R508	V447	ALA	VAL
	L1156	G1091	A1028	A954	A887	N824	A759	E693	V632	E570	P509	E448	GLU	ALA
G1230	L1160	X1093	R1029	V955	E888	R824	R760	V694	V633	K571	E510	S449	GLN	GLN
E1231	E1161	T1094	G1036	I956	A889	P826	I761	I695	G634	R572	M511	Y450	VAL	VAL
P1232	E1162	L1094	M1031	P957	V890	L827	Q762	R696	P635	M573	M512	D451	GLU	GLY
G1233	G1163	R1096	E1182	E958	E891	K828	M763	K697	Q636	L574	L513	I452	ALA	ALA
T1234	G1163	K1096	P1032	E959	R892	R829	L764	K698	L637	Q575	L514	D453	GLU	GLU
Q1235	R1164	L1097	Q1033	K960	E893	A830	S765	V699	K638	E576	E515	A454	GLU	GLU
L1236	Y1165	L1098	Q1034	K961	K894	G831	A766	V700	L639	A577	A516	R455	GLY	GLY
T1237	L1166	X1099	I1035	Q962	V895	R832	H767	L701	H640	V578	V517	R456	GLY	ALA
M1238	S1167	D1100	R1036	Y963	A896	E833	L770	L702	Q641	D579	P518	K397	PHE	LEU
R1239	M1168	V1101	Q1037	L964	A897	T834		M703	G642	A580	V519	E459	THR	LEU
T1240	V1102	L1102	L1038	E965	E898	R835		R704	L581	R399	L520	R399	VAL	VAL
F1241	V1171	H1103	C1039	E966	R899	R836	S774	A705	L644	V460	P521	I461	TYR	TYR
H1242	H1172	E1104	G1040	D968	I900	G837	G775	F706	P645	D583	P522	Q462	LEU	ARG
T1243	L1173	L1105	L1041	R969	Q901	R838	E776	T707	R646	N584	D523	Q463	THR	ARG
G1244	L1174	V1106	R1042	K970	L902	L839	F777	L708	R647	G585	L524	L464	LEU	GLU
G1245	L1175	R1107		L971		K840	L778	H709	M648	R586	R525	L465	PHE	ASP
V1246	K1176	V1108	M1045	L972	Q906	Y841	A779	R710	A649	R587	P526	K466	LEU	GLU
A1247		E1109	Q1046	Q973	R908	V842	K780	L711	L650	G588	N527	E467	GLU	PRO
G1248	E1179	A1110	K1047	I974	K908	R843	F781	L712	E851	A589	V528	L468	TRP	VAL
A1249		D1111	P1048	E975	N909	A844	S782			P590	Q529	D469	ALA	ALA
	E1182	C1112	S1049	Q976	S910	N845	R783	A715	K654	V591	V530	L470	THR	THR
I1252	I1183	G1113	G1050	E979	L911	R846	D784	F716	P655	T592	D531	E471	PRO	TYR
T1253	Q1184	E1051	L1051		K912	D847	I785	Q717	F656	N583	G532	A472	LYS	PHE
Q1254	E1185	T1115	T1052		D913	E848	I786	P718	L657	P594	G533	L473	ASP	LEU
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R1258		S1119	P1056	E987	Q917	A852		E723	M662	P599	S538	L478	PRO	THR
V1259	C1194	L1122	V1057	R988	A918	R853	I792	Q723	E663	L600	D539	E479	HIS	PRO
I1260	Q1195	F1123	S1058	Y989	F919	V863	T793	Q724	R663	R601		E480	LEU	LEU
E1261	T1196	Q1124	S1059		L920	I857	Q794	S725	K664	S602	D542	R481	ASN	VAL
L1262	R1197	Q1124	S1060	T992	R921	V858	V795	I726	G665	G609	N549	R488	VAL	VAL
F1263	Y1198	P1125	F1061	L993	P1125	R869	R796	Q727	L666	L603	L543	K482	VAL	VAL
E1264	G1199	D1126	R1062	Q994		L860	K797	L728	A667	T604	V544	H483	HIS	VAL
A1265	V1200	E1127	E1063	L995	K926	Q861	E798	H729	P668	D605	R545	P484	VAL	GLY
R1266	C1201	V1128	G1064	W996	T927	D862	K799	P730	N669	L606	R546	S485	GLU	GLY
Q1202	Q1202	T1129	L1065	T997	A928	R863	K800	L731	V670	L607	L547	R486	PRO	ILE
P1268	K1203	R1130	T1066	E998	R929	V864	G801	C732	K671	S608	L548	R487	GLY	VAL
K1269	C1204	L1130	V1067	T999	R930	T865	A802	C733	A672	G609	N549	R488	ALA	GLU
A1270	Y1205	R1133	L1068	E1001	L931	R866	G803	E734	R673	K610	R550	R489	ARG	LYS
K1271	G1206	L1134	E1069	E1001	D932	R867	L804	A735	A674	Q611	N551	A490	VAL	GLY
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V1273	D1208	K1136	F1071	V1003	L934	Y868	F806	N737	M676	R613	R553	A492	ALA	PRO
L1274	L1209	R1137	I1072	T1004	K935	K871	A807	A738	L677	F614	L554	R493	LEU	LEU
S1275	S1210	A1138	S1073	Q1005	Y936	R872	T808	D739	E678	G616	K556	R495	ALA	GLU
E1276	M1211	D1139	S1074	A1006	Y937	L873	P809		R679	Q616	L557	R496	VAL	ALA
I1277	A1212	I1140	H1075	A1007		E874	E810	D743	K680	N617	L558	V368	GLY	GLY
D1278	R1213	E1141	G1076	F1008	T940	T875	E811	Q744	R681	K621	L559	E497	LYS	LYS
G1279	P1214	A1142	A1077	K1009	T944	R876	A812	M745	D882	R622	Q560	V498	GLY	GLY
V1280	V1215	G1143	G1078	M1010	T944	P877	L813	V749	G684	A622	Q561	R500	LEU	LEU
L1281	L1144	K1079	K1079	S945	T944	R878	A814		R685	L439	P373	V440	ARG	ARG
R1282	Y1145	G1080		C946	S945	R879	E817	P750	D885	D624	P525	F502	NET	ARG
I1283	A1220	G1146	A1085	P1019	C946	R879	E817	L751	R686	G625	R563	A379	NET	ARG
E1284	G1222	V1148	L1086	L1020	T948	L881	R818	S752	L681	S626	E564	N442	PRO	PRO



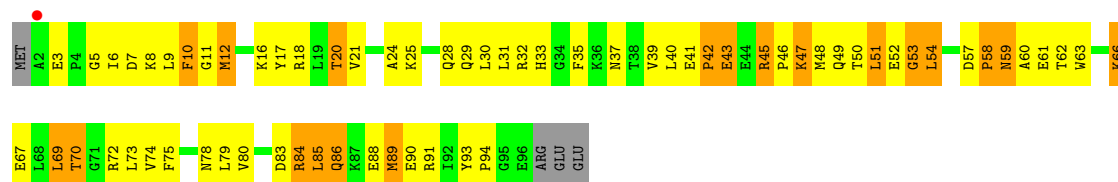
• Molecule 4: RNA polymerase omega chain

Chain E:



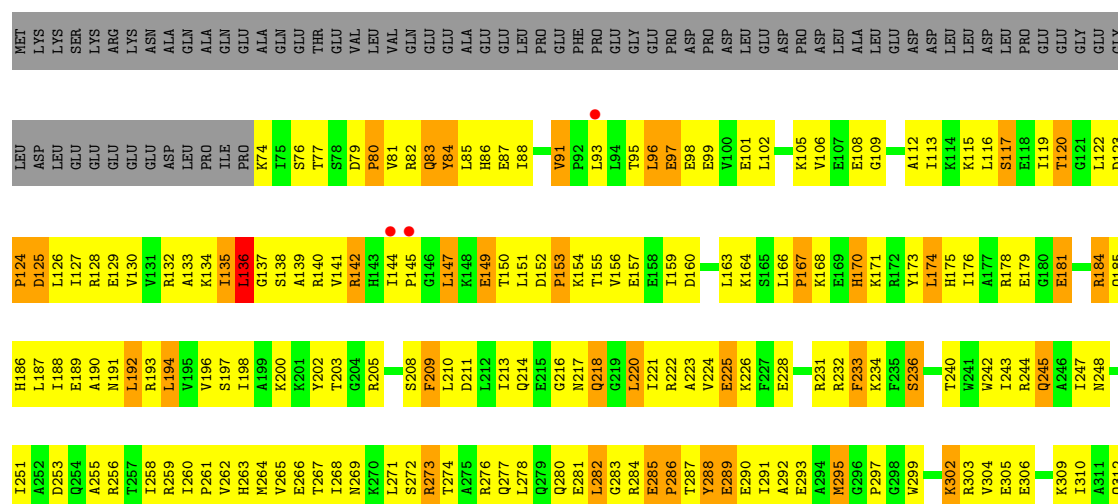
• Molecule 4: RNA polymerase omega chain

Chain O:



• Molecule 5: RNA polymerase sigma factor rpoD

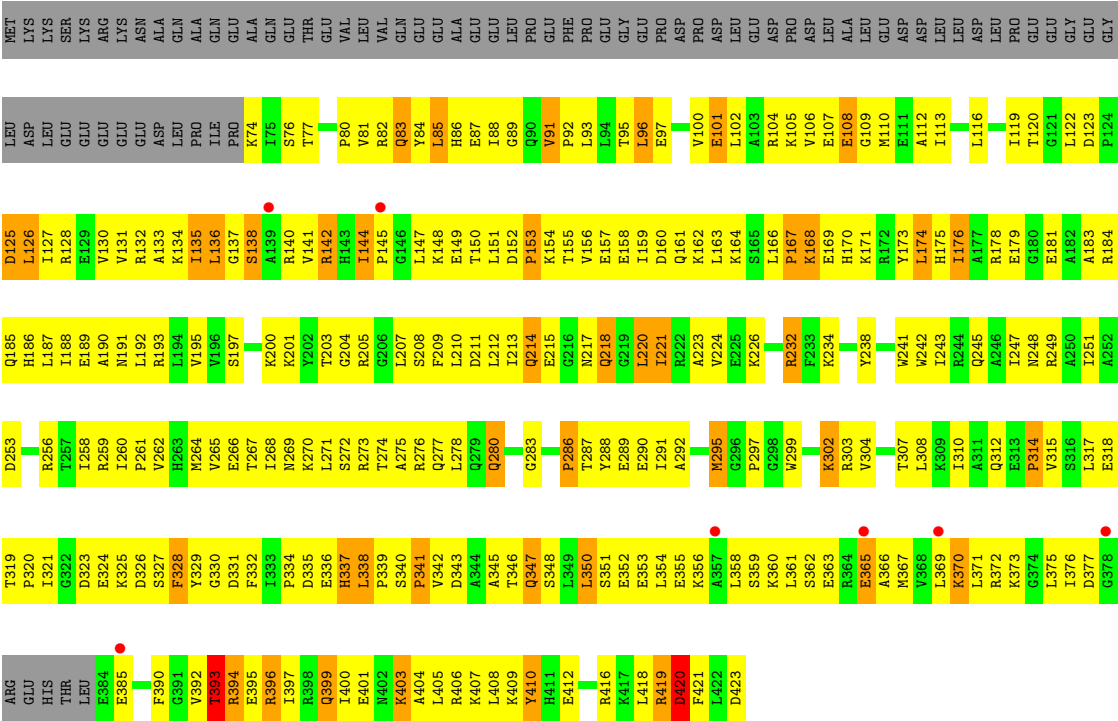
Chain F:





● Molecule 5: RNA polymerase sigma factor rpoD

Chain P:



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.80) 92.0 (24.96-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.268 0.227 , 0.261	Depositor DCC
R_{free} test set	21166 reflections (6.13%)	DCC
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 80.1	EDS
Estimated twinning fraction	0.499 for -h,-k,l 0.068 for h,-h-k,-l 0.068 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 366401 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	58679	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.80	1/1838 (0.1%)	0.88	1/2498 (0.0%)
1	B	0.75	0/1838	0.82	2/2498 (0.1%)
1	K	0.75	0/1838	0.86	2/2498 (0.1%)
1	L	0.72	0/1838	0.78	1/2498 (0.0%)
2	C	0.84	0/8997	0.90	8/12164 (0.1%)
2	M	0.82	0/8997	0.89	7/12164 (0.1%)
3	D	0.84	0/10975	0.94	20/14836 (0.1%)
3	N	0.83	0/10975	0.93	18/14836 (0.1%)
4	E	0.84	0/783	0.97	0/1054
4	O	0.88	0/783	1.00	1/1054 (0.1%)
5	F	0.75	0/2812	0.82	3/3781 (0.1%)
5	P	0.75	0/2812	0.80	1/3781 (0.0%)
All	All	0.82	1/54486 (0.0%)	0.90	64/73662 (0.1%)

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	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	5.57	1.44	1.34

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	199	LEU	CA-CB-CG	-8.69	95.30	115.30
1	B	138	LEU	CA-CB-CG	8.01	133.72	115.30
3	N	1389	LEU	CA-CB-CG	7.77	133.18	115.30
5	P	136	LEU	CA-CB-CG	7.49	132.51	115.30
3	N	76	CYS	CA-CB-SG	6.73	126.11	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	132	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	216	0
1	B	1806	0	1861	199	0
1	K	1806	0	1861	208	0
1	L	1806	0	1861	206	0
2	C	8829	0	8933	1184	0
2	M	8829	0	8933	1106	0
3	D	10797	0	10873	1450	0
3	N	10797	0	10873	1345	0
4	E	769	0	775	97	0
4	O	769	0	775	108	0
5	F	2771	0	2844	336	0
5	P	2771	0	2844	342	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	1	0	0	0	0
7	N	1	0	0	0	0
8	A	191	0	0	37	0
8	B	181	0	0	34	0
8	C	767	0	0	174	0
8	D	1100	0	0	234	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	93	0	0	14	0
8	F	333	0	0	58	0
8	K	151	0	0	30	0
8	L	179	0	0	49	0
8	M	739	0	0	195	0
8	N	1038	0	0	225	0
8	O	78	0	0	24	0
8	P	267	0	0	61	0
All	All	58679	0	54294	6401	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 59.

The worst 5 of 6401 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.28	1.11
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.12	1.08
2:C:135:VAL:HG11	2:C:407:LYS:HA	1.36	1.04
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.20	1.04
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.14	1.04

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	227/315 (72%)	202 (89%)	21 (9%)	4 (2%)	13	39
1	B	227/315 (72%)	202 (89%)	21 (9%)	4 (2%)	13	39
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	13	39
1	L	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	13	39
2	C	1117/1119 (100%)	917 (82%)	150 (13%)	50 (4%)	4	12
2	M	1117/1119 (100%)	907 (81%)	159 (14%)	51 (5%)	4	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1388/1524 (91%)	1123 (81%)	191 (14%)	74 (5%)	3	9
3	N	1388/1524 (91%)	1110 (80%)	195 (14%)	83 (6%)	2	6
4	E	93/99 (94%)	74 (80%)	16 (17%)	3 (3%)	6	20
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	6	20
5	F	341/423 (81%)	283 (83%)	42 (12%)	16 (5%)	4	11
5	P	341/423 (81%)	285 (84%)	40 (12%)	16 (5%)	4	11
All	All	6786/7590 (89%)	5582 (82%)	892 (13%)	312 (5%)	4	11

5 of 312 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	147 (73%)	55 (27%)	0	2
1	B	202/273 (74%)	163 (81%)	39 (19%)	2	6
1	K	202/273 (74%)	152 (75%)	50 (25%)	1	2
1	L	202/273 (74%)	158 (78%)	44 (22%)	1	4
2	C	941/941 (100%)	734 (78%)	207 (22%)	1	4
2	M	941/941 (100%)	730 (78%)	211 (22%)	1	4
3	D	1123/1279 (88%)	846 (75%)	277 (25%)	1	2
3	N	1123/1279 (88%)	866 (77%)	257 (23%)	1	3
4	E	83/87 (95%)	58 (70%)	25 (30%)	0	1
4	O	83/87 (95%)	64 (77%)	19 (23%)	1	3
5	F	295/370 (80%)	228 (77%)	67 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	P	295/370 (80%)	249 (84%)	46 (16%)	4 11
All	All	5692/6446 (88%)	4395 (77%)	1297 (23%)	1 3

5 of 1297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	30	LEU
1	L	25	LEU
3	N	1353	GLN
5	F	80	PRO
5	F	361	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	86	GLN
1	L	212	ASN
3	N	1374	GLN
5	F	337	HIS
1	K	156	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	229/315 (72%)	-0.30	0 100 100	38, 65, 92, 117	0
1	B	229/315 (72%)	-0.18	11 (4%) 29 30	53, 95, 115, 121	0
1	K	229/315 (72%)	-0.29	0 100 100	41, 66, 93, 122	0
1	L	229/315 (72%)	-0.31	7 (3%) 47 47	52, 94, 114, 127	0
2	C	1119/1119 (100%)	-0.27	12 (1%) 77 78	23, 81, 110, 119	0
2	M	1119/1119 (100%)	-0.31	7 (0%) 86 88	27, 79, 109, 122	0
3	D	1392/1524 (91%)	-0.24	22 (1%) 68 69	17, 68, 113, 130	0
3	N	1392/1524 (91%)	-0.27	18 (1%) 74 75	27, 69, 110, 138	0
4	E	95/99 (95%)	-0.27	0 100 100	47, 85, 115, 133	0
4	O	95/99 (95%)	-0.42	1 (1%) 77 78	40, 76, 97, 111	0
5	F	345/423 (81%)	-0.33	4 (1%) 75 76	46, 84, 112, 131	0
5	P	345/423 (81%)	-0.32	7 (2%) 62 63	54, 87, 112, 125	0
All	All	6818/7590 (89%)	-0.28	89 (1%) 74 75	17, 77, 111, 138	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	ALA	5.6
3	N	1243	THR	5.1
2	C	307	LEU	5.0
3	D	1240	THR	4.9
3	N	1248	GLY	4.8

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	ZN	D	7112	1/1	0.15	0.64	75,75,75,75	0
6	ZN	N	7059	1/1	0.11	-0.81	100,100,100,100	0
7	MG	N	9002	1/1	0.14	-0.81	64,64,64,64	0
7	MG	D	9001	1/1	0.15	-0.85	67,67,67,67	0
6	ZN	N	7113	1/1	0.10	-1.10	87,87,87,87	0
6	ZN	D	7058	1/1	0.07	-1.76	109,109,109,109	0

6.5 Other polymers

There are no such residues in this entry.