



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:14 AM GMT

PDB ID : 1ZYR
Title : Structure of Thermus thermophilus RNA polymerase holoenzyme in complex with the antibiotic streptolydigin
Authors : Tuske, S.; Sarafianos, S.G.; Wang, X.; Hudson, B.; Sineva, E.; Mukhopadhyay, J.; Birktoft, J.J.; Leroy, O.; Ismail, S.; Clark, A.D.; Dharia, C.; Napoli, A.; Laptenko, O.; Lee, J.; Borukhov, S.; Ebright, R.H.; Arnold, E.
Deposited on : 2005-06-10
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

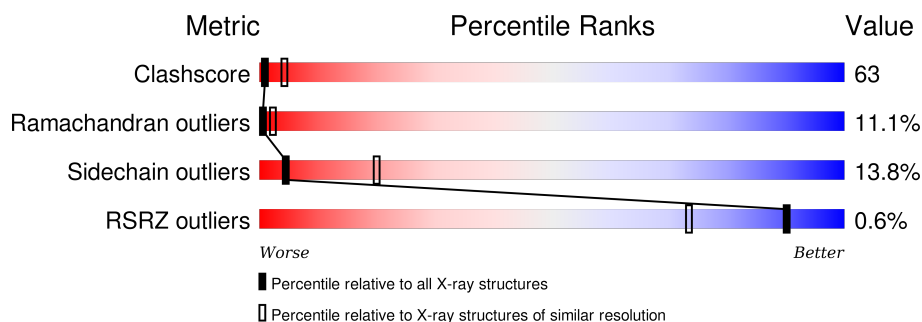
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	
3	D	1524	

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Mol	Chain	Length	Quality of chain
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

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
7	ZN	N	9003	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 54048 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 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 subunit beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10975	6953	1941	2048	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10975	6953	1941	2048	33			

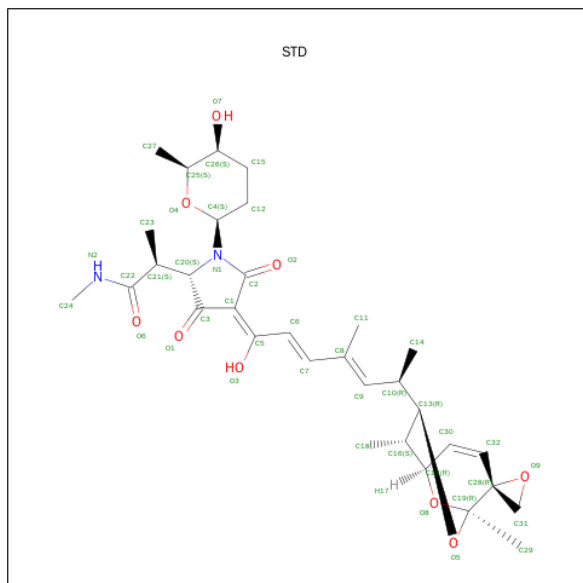
- Molecule 4 is a protein called DNA-directed RNA polymerase omega chain.

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 DNA-directed RNA polymerase sigma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2793	1762	504	523	4			
5	P	345	Total	C	N	O	S	0	0	0
			2793	1762	504	523	4			

- Molecule 6 is STREPTOLYDIGIN (three-letter code: STD) (formula: $C_{32}H_{44}N_2O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			43	32	2	9		
6	M	1	Total	C	N	O	0	0
			43	32	2	9		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

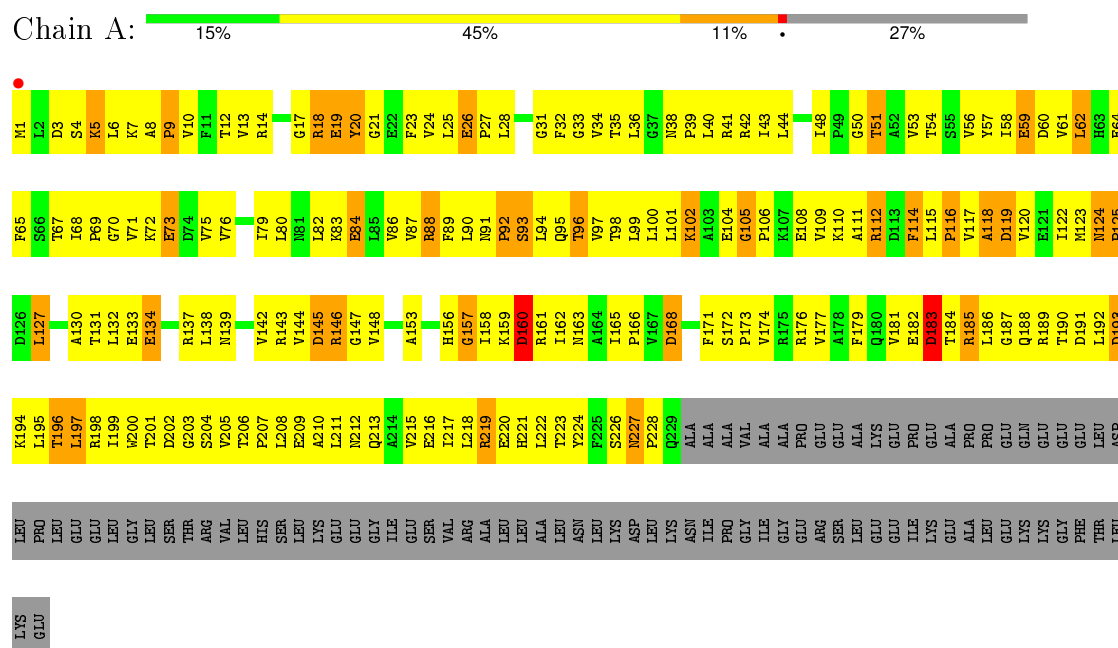
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

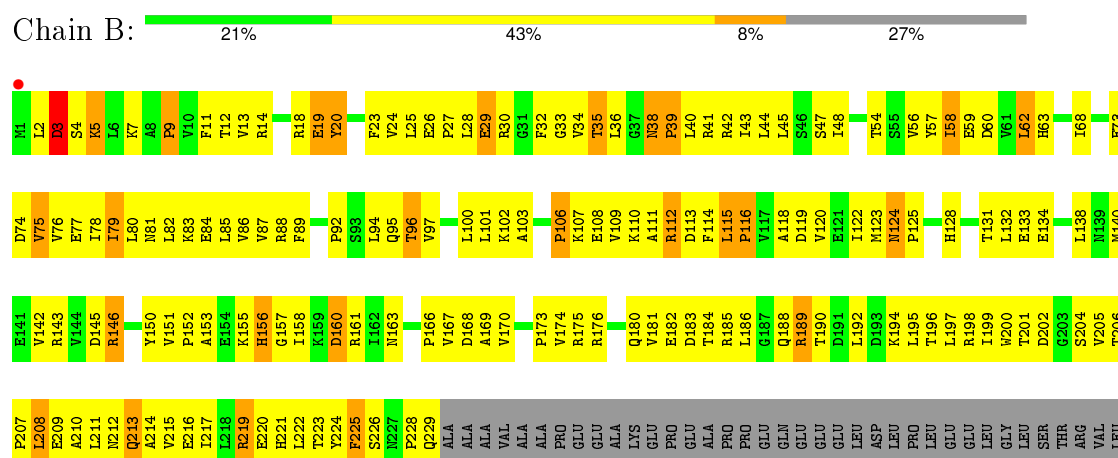
3 Residue-property plots

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

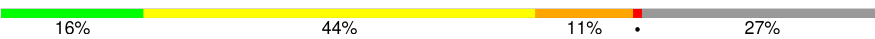


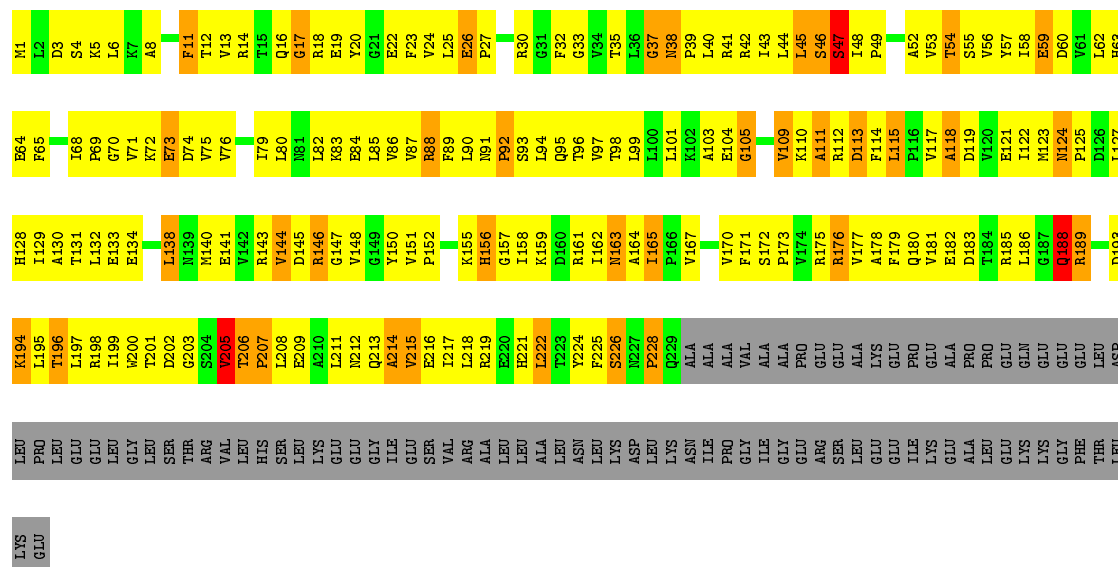
• Molecule 1: DNA-directed RNA polymerase alpha chain



HIS
SER
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GLY
GLY
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ALA
LEU
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LYS
GLY
PHE
THR
LEU
LYS
GLU

• Molecule 1: DNA-directed RNA polymerase alpha chain

Chain K: 

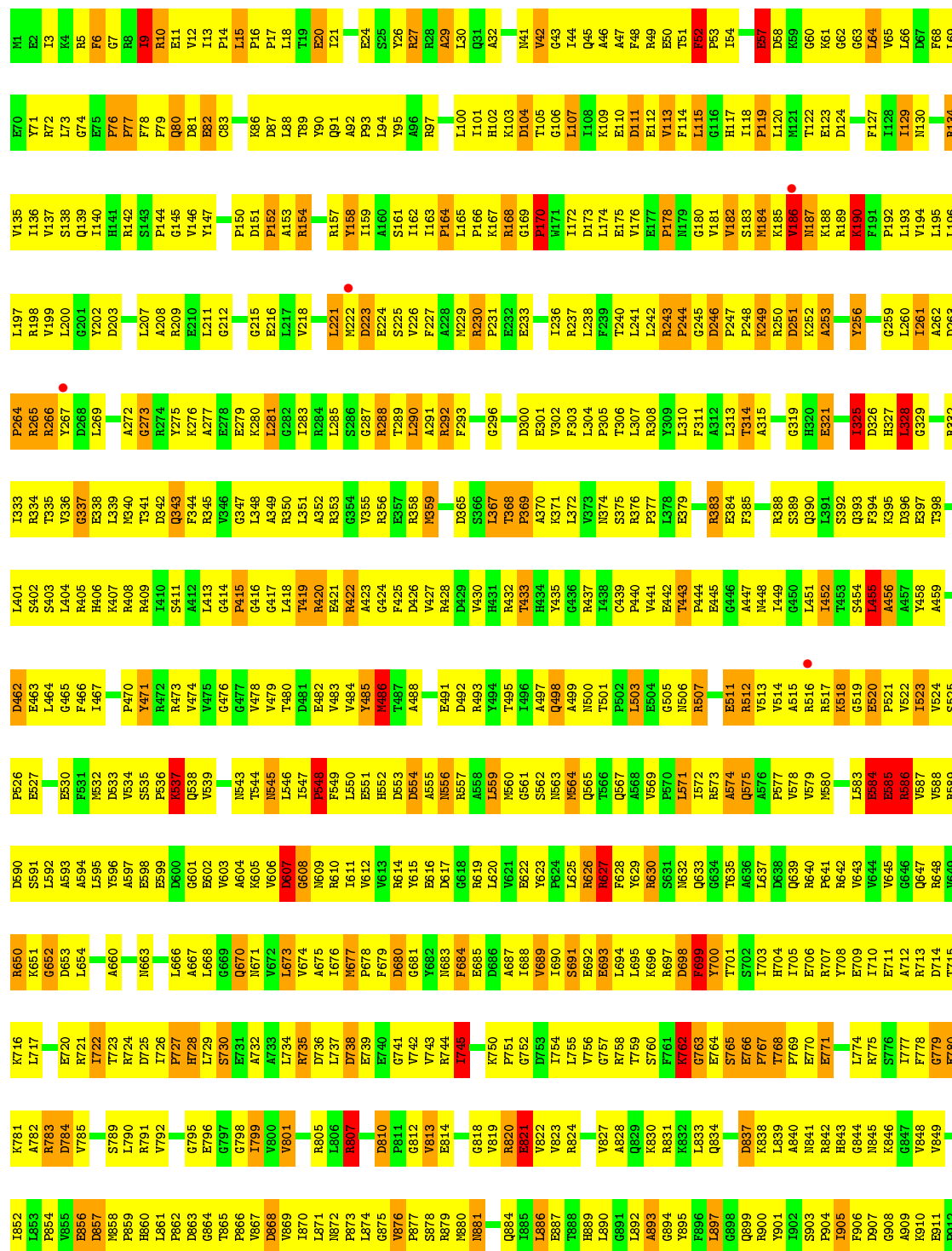


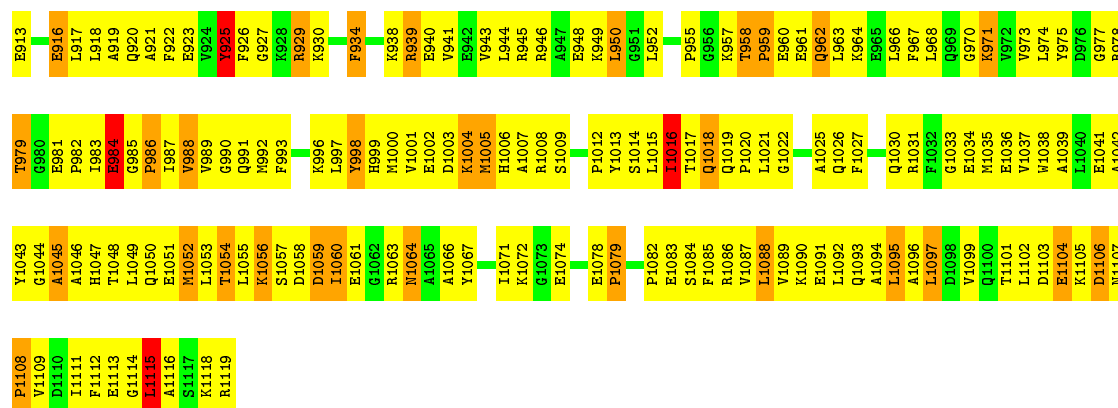
H1047	G980	L917	V855	E720	G658	L595	V529	D462	T398	R330	D263	L196	V135	L69
T1048	E981	L918	E856	R721	P659	L596	E530	E463	S403	R331	P264	L197	I136	E70
L1049	P982	A919	D857	I722	A660	A937	F531	L464	S403	R332	R265	L198	V137	Y71
Q1050	L983	Q920	H858	T723	S661	E598	V534	G465	L404	R333	R266	V199	S138	R72
M1051	E984	A921	P859	R724	E662	E599	V535	F466	R405	R334	Y267	G201	Q139	L73
E1052	K985	F922	H860	R725	N663	D600	S334	L467	H406	R335	D268	G202	I140	G74
L1053	L986	E923	L861	I726	G664	G601	P536	R468	K407	V336	Y270	Y202	E75	E75
T1054	P987	V924	P862	P727	P665	E602	K537	T469	R408	R337	E271	D203	R142	P76
L1055	V988	Y925	D863	R728	L666	V603	Q538	P470	R409	E338	A272	Q204	S143	P77
K1056	P989	F926	G864	L729	A667	A604	V539	Y471	A412	T341	G273	Q205	S143	P77
S1057	G990	G927	T865	S730	L668	K605	F540	R472	G413	Q342	K276	T206	G145	F78
D1058	F983	K928	P866	L734	G669	V606	S541	R473	G414	Q343	K277	L207	Y147	Q80
L1059		R929	V867	R735	N670	D607	V542	Y474	G415	Q344	E278	Q208	D81	D81
G1062	K996	K930	D868	R736	N672	G608	N543	Y475	P415	R345	E279	R209	F148	E82
R1063	L997	G931	L870	D736	L673	N609	T544		G416		E280	E210	T149	C83
A1064	M1000	F934	L871	D738	V674	N545	N546	Y478	L418	L348	G281	L211	P150	
A1065	V1001	G935	N872	G741	A675	L611	L546	T480	T419	A349	L282	G220	D151	L88
A1066	P1002	V936	P873	V742	L676	V613	P548	T481	R420	R350	I283	L221	P152	T89
Y1067	D1003	D937	L874	V743	N677	L614	F549	E482	E421	L351	R284	M222	A154	Y90
I1070	K1004	R939	G875	R744	P678	L615	E551	Y484	R422	R352	L285	D223	A92	Q91
L1071	M1005	E940	P877	R744	F679	E616	H552	Y485	G423	R353	E224	G156	P155	A92
K1072	H1006	V941	S878		D680	D617	H553	Y486	G424	G354	E225	S225	G157	P93
G1073	A1007	E942	S879	A747	G681	G618	D553	T487	F425	V355	R288	V226	Y158	L94
E1074	R1008	V943	H880	E748	Y682	D554	D554	Y488	D426	R356	L290	F227	I159	A96
D1075	S1009	L944	N881	V749	N683	L620	A555	A488	Y427	E357	A291	A228	A160	R97
V1076	T1010	R945	L882	R750	F684	V621	N556	T489	R428	R358	R292	M229		
P1077	G1011	R946	D883	P751	E685	E622		E490	D429	M359	F293	R230	I163	L100
P1078	P1012	A947	G884	T754	A687	L625	M560	E491	H430	S363	G296	R231	P164	I101
P1079	Y1013	E948	L885	L755	L688	R626	G561	D492	R431	E364	E297	E232	L165	H102
S1080	S1014	K949	L886	V756	V689	R627	S562	Y494	T433		F298	E233	P166	K103
V1081	L1015	L950	E897	G757	L690	F628	S563	T495	H434	L367	K299	L235	K167	D104
E1082	T1016	G951	T888	T759	S691	V629	M564	Y496	Y435	T368	D300	R236	G169	T105
S1084		V953	H889	T759	E692	R630		A497	G436	P369	V302	R307	P170	L107
F1085	P1020	K957	L891	F761	E693	S631	Q567	Q498	R437		F303	L238	W171	K108
R1086	L1021	T958	L892	K762	L694	N632	A568	T501	L438	L372	L304	T240	L172	K109
V1087	K1024	P959	A893	E766	R696		P570	P502	C439	V373	P305	L241	D173	E110
V1089	F1027	E960	Y895	P767	R697	A636	L571	L503	P440	N374		L242	L174	D111
K1090		E961	F896	T768	D698	L637	I572		E442	S375	R308	R243	E175	E112
E1091		Q962	L897	P769	F699	D638		R507	T443	P377	Y309	P244	E177	F113
L1092	Q1030	L963		E770	Y700	Q639	Q575	I508	E445	L378	G245	R245	P178	L115
Q1093	R1031	K964	R900	E771	T701	R640	A576		G446	E379	D246	D246	M179	G116
A1094	F1032	E965	T901	R772	H704	P641	P577	V513	A447	A380	P247	P247	G180	H117
L1095	G1033	L966	I902	L773	I705	R642	V578	V514	N448	A381	K248	P248	V182	I118
A1096	E1034	F967	S903	L774	E706	V644	M580	A515	I449	R383	K249	K249	V182	
L1097	M1035	L968	P304	R775	R707	V645		R516	G450	E384	R250	R250	S183	M121
D1098	E1036	Q969	I905	S776	Y708	G646	L583	R517	L451	F385	D251	D251	M184	T122
V1099	V1037	G970	P906	I777	E709	Q647	E584	K518	L452	F386	K252	K252	K185	E123
Q1100	W1038	K971	D907		I710		E585	G519	I452		A253	A253	V186	D124
T1101	A1039	V972	K910	E780	R713	R650	E586	E520	T453	S389	G320	V254	M187	F127
L1102	L1040	V973	E912	R781	D714	K651	R587	P521	S454	Q390	K188	A255	K188	I128
D1103	E1041	L974	P912	A782	L715	G652	V588	V522	L455	L391	V322	Y257	K189	I129
E1104	A1042	Y975	P912	R783	T715	D653	R589	V524	A457	S392	I325	Y258	F191	N130
K1105	Y1043	D976	E915	D784	K716	L654	D590	S525	Y458		D326	G259	P192	G131
D1106	G1044	G977	I914	S785	L717	L655	S591	S526	A459	R395	H327	L260	L193	A132
N1107	A1045	R978	K915	K786	P718	A656	L592	E527	R460	D396	L328	L261	L194	D133
P1108		T979	E916	D787	P719	D657		E528	V461	E397	G329	A262	L195	R134



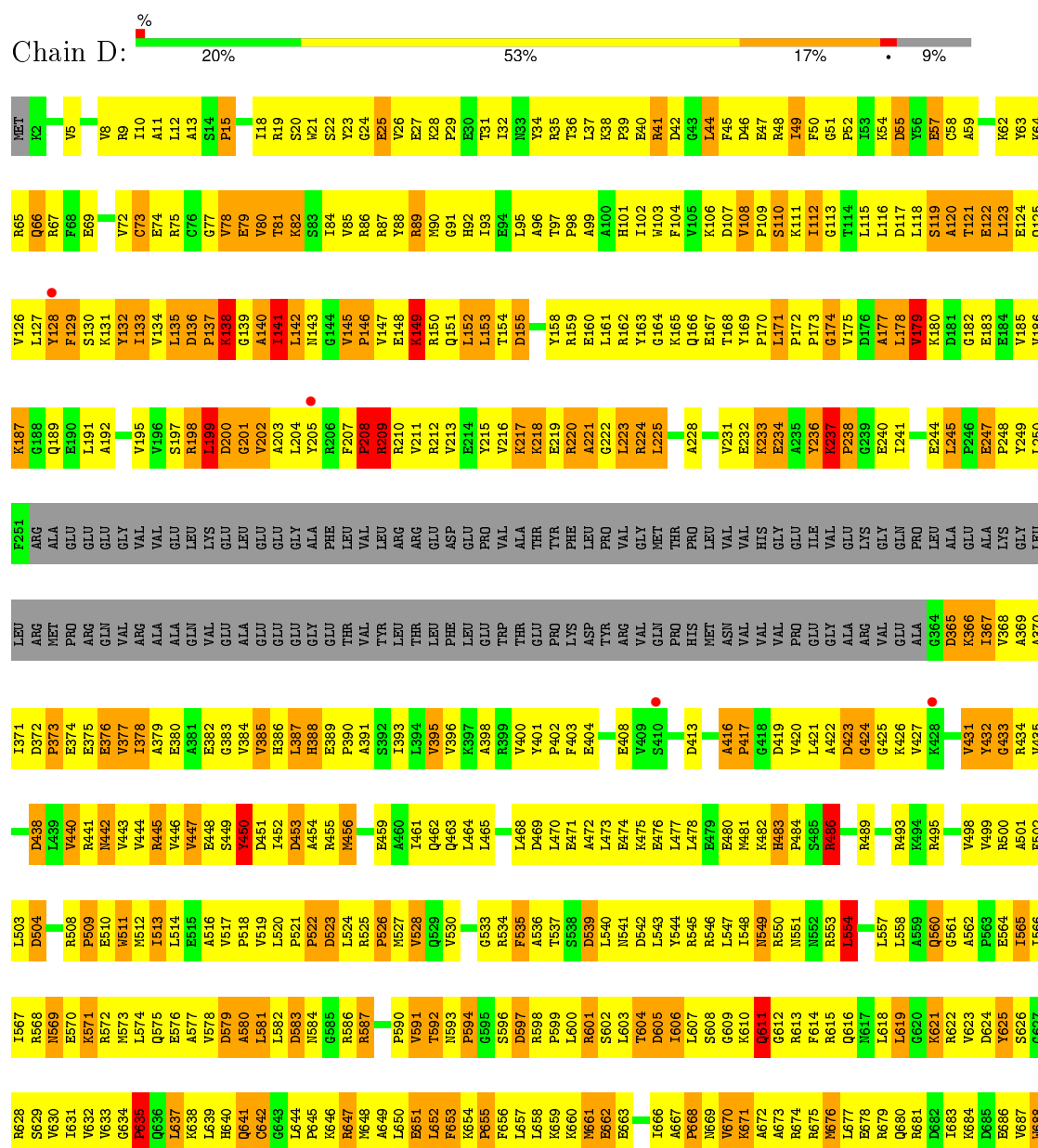
• Molecule 2: DNA-directed RNA polymerase beta chain

Chain M: 25% 59% 14%





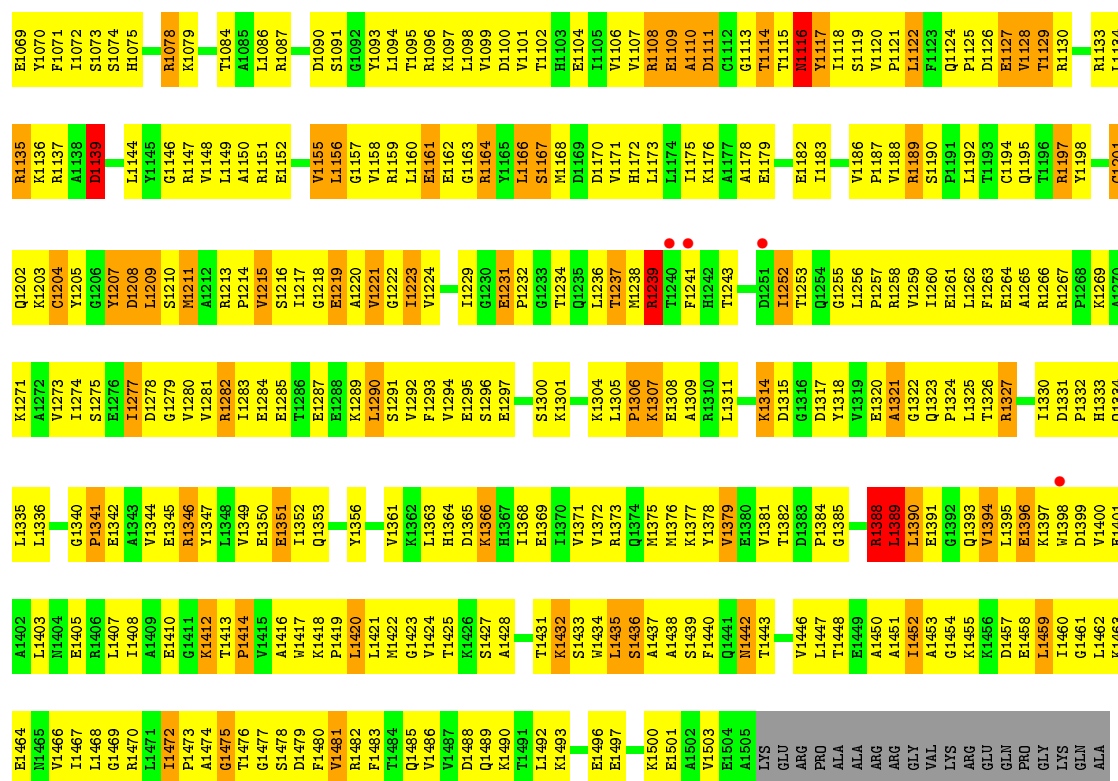
● Molecule 3: DNA-directed RNA polymerase subunit beta' chain



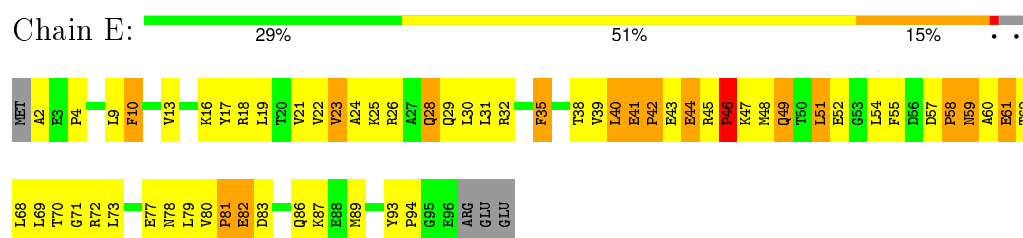
- Molecule 3: DNA-directed RNA polymerase subunit beta' chain



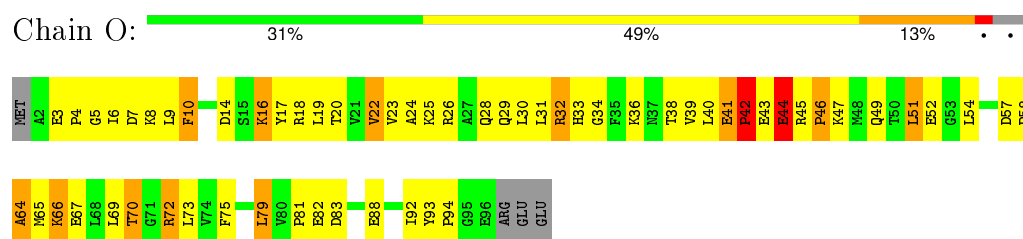
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F1008	K935	E874	L813	L751	E686	S625	Q560	E497	V437	F373	ALA	E190	Q125	R65
K1009	Y936	T975	A814	S752	V687	G627	A561	V498	D439	E375	GLU	A192	V126	Q66
N1010	Y937	S876	A815	S753	W688	G628	A562	V499	L438	E376	ARG	F129	L127	R67
F1011	G938	P877	H816	F754	D689	S629	E563	R500	V440	E376	GLN	P193	F128	F68
F1012	F939	G878	E817	A755	E690	V630	E564	A501	R441	V377	GLY	F129	F129	E69
E1012	T940	R879	R818	A756	L691	L631	I565	F502	W442	I378	VAL	V195	S130	G70
Y1015	S942	L880	E820	A757	E692	V632	I566	L503	V443		VAL	V196	K131	K71
P1016	T943	L881	E821	E758	E693	V633	I567	L504	V444		ALA	S197	Y132	V72
F1017	T944	A883	A822	A759	E694	G634	R568	S505	R445	C382	GLN	C73	I133	C73
N1018	S945	R884	A823	R760	I695	P635	R569	G506	V446	C383	VAL	L139	V134	E74
P1019	G946	I885	L824	I761	Q636	Q637	E570	N507	W447	V384	GLY	L135	L135	R75
L1020	T947	R886	A825	Q762	L637	L638	K571		E448	V385	ALA	L136	D136	C76
Y1021	T948	A887	P826	M763	K638	K639	R572	E510	S449	H386	GLU	A203	P137	G77
Y1022	T949	E888	P827	L764	L701	L639	M573	M511	Y450	L387	GLU	L204	K138	V78
M1023	G950	R889	L828	A766	L702	H640	L574	M512	Y451	L387	GLY	Y205	K139	E79
	I951	V890	K828	Q772	R703	Q641	Q575	L513	I452	E389	ALA	R206	A140	V80
		V891	W829	H767	R704	Q642	E576	L514	D453	P390	PHE	F207	I141	T81
		E891	A830	W768	A705	G643	A577	E515	A454	A391	LEU	P208	L142	K82
		D892	G831	L769	P706	L644	V578	A516	S449	S392	VAL	R209	N143	S83
		E893	R832	L770	L707	P645	D579	M517	Y456	L393	LEU	R210		I84
		K894	E833	S771	L708	H646	P518	P519	Y457	L394	ARG	V211	P146	V85
		V895	T834	P772	H709	R647	E458	V519	A458	V395	THR	R212	V147	R86
		A896	S835	A773	R710	N648	D583	L520	E459	V396	GLU	V213	GLY	R87
		R897	V836	S774	L711	N649	N584	P521	A460	K397	ASP	E214	E149	Y88
		E898	G837	G775	G712	L650	G585	P522	I461	A398	GLY	Y215	R150	R89
		L899	R838	E776	L713	E651	R586	D523	Q463	R399	PRO	V216	Q151	M90
		I900	L839	P777	Q714	L652	R587	L524	Q463	V400	VAL	R217	L152	G91
		Q901	K840	L778	A715	F653	P590	R525	L464	Y401	ALA	K218	L153	H92
		L902	H841	A779	F716	K654	P526	P527	L465	P402	THR	E219	T154	I93
		D903	R842	K780	Q717	P655	V591	N527	K466	F403	TYR	R220	D155	E94
		V904	F843	F781	P656	P656	T592	V528	E467	E404	PHE	A221	E156	L95
		F905	A844	S782	L719	L657	N593	Q529	L468	D405	LEU	G222	E157	A96
		R906	N845	R783	L720	L658	R594	V530	L470	D406	PRO	R224	Y158	T97
		E907	P846	D784	E721	K659	S596		L471		ARG	R225	R159	P98
		K908	E847	I785	E722	K660	S597	E533	E472	V409	VAL	L226		A99
			E848	I786	G723	N661	R598	R534	A471	S410	GLN	P226	R162	A100
			A849	L787	Q724	E662	P599	F535	L473	T411	PRO	L227	Y183	H101
			E850	G788		E663	L600	A536	E474	G412	HIS			I102
			L851	L789	Q727	K664	R601	T537	K475	D413	LEU	W230	Q166	W103
			A852	Y790	L728	G665	S602	S538	E476	R414	ASN	V231	E167	F104
			V853	Y791	H729	P666	S602	D539	L477	V415	VAL	E232	T168	V105
			A854	I792	P730	A667	L603	L540	L478	A416	VAL	K233	Y169	K106
			H855	I793	L731	P668	T604		E479	P417	VAL	E234	P170	D107
			G856	Q794	V732	N669	D605	L543	E480	L421	GLY		L171	V108
			L857	V795		V670	L606	Y544	M481	L421	ILE	K237	P172	P109
			V858	R796	F736	K671	L607	R545	K482	A422	GLY	P238	P173	S110
			D859	K797	N737	A672	S608	R546	H483	D423	ALA	G239	P173	S110
			L860	E798	A738	A673	G609	L547	P484	G424	ARG	E240	G174	K111
			Q861	K799	D739	R674		T548	S485	G425	VAL	I241	D176	I112
			D862	K800	F740	R675	R613	N549	A486	K426	GLY	L242	A177	G113
			V863		D741	R676		R550	A487	V427	GLU	A243	L178	T114
			E864	L804	G742	L677	N617	N551	R488	K428	ALA	E244	V179	L115
			R867	E805	G743	E678	L618	N552	R488	S429	LEU	L245		L116
			V868	F806	Q744	R679	L619	R553	A490	D430	GLU	P246	E183	D117
			N869	A807	N745	Q680	G620	L554	K491	V431	ALA	E247	E184	L118
			R870	T808	A746	R681	K621	K555	A492	Y432	LYS	P248	V185	S119
			K871	P609	V747	D682	R622	K556	K493	G433	GLY	Y249	V186	A120
			E872	E910	H748	L683	V623	L557	K494	R434	LEU	K250	K187	E121
			R872	E911	V749	K684	D624	L558	R495	V435	LEU	F251	G188	L123



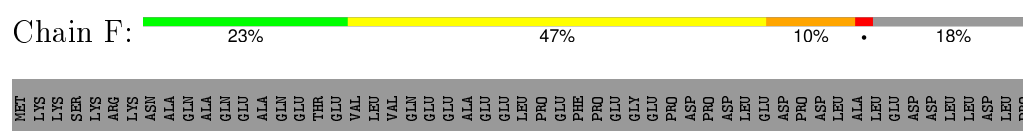
• Molecule 4: DNA-directed RNA polymerase omega chain

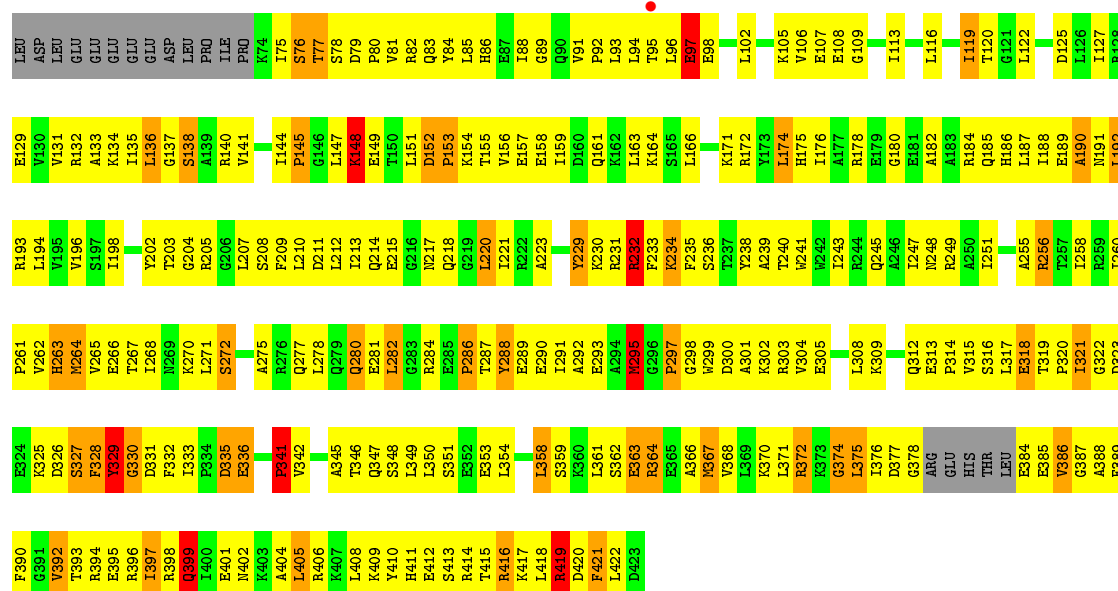


• Molecule 4: DNA-directed RNA polymerase omega chain

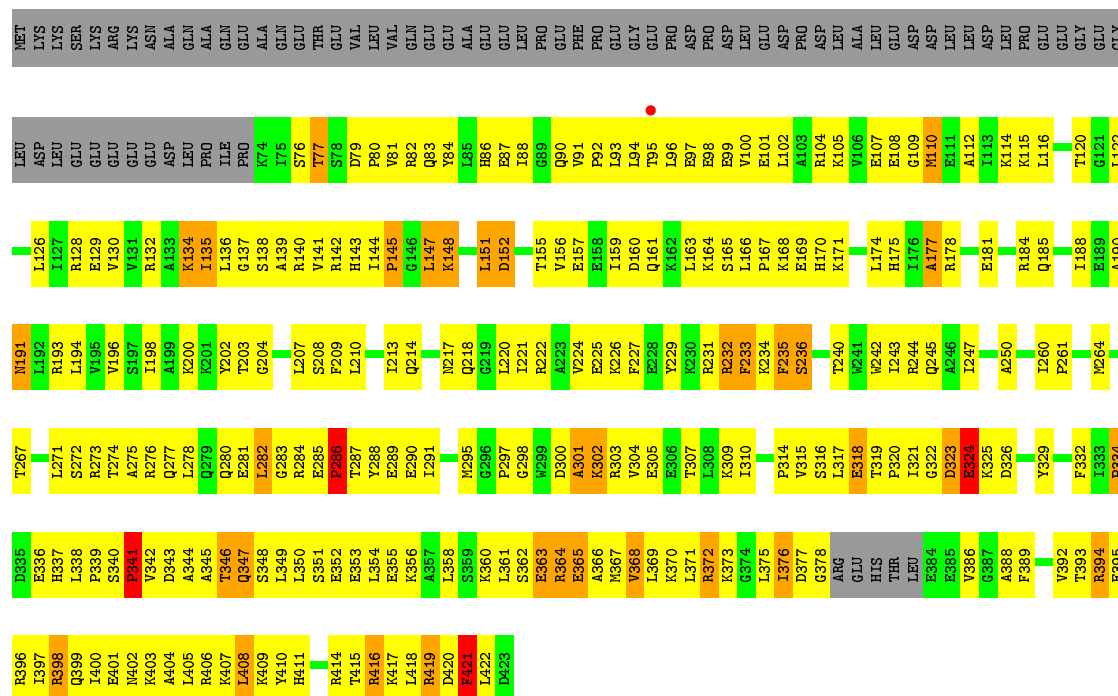


• Molecule 5: DNA-directed RNA polymerase sigma chain





• Molecule 5: DNA-directed RNA polymerase sigma chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	237.00Å 237.00Å 250.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.89 – 3.00	Depositor EDS
% Data completeness (in resolution range)	77.9 (30.00-3.00) 42.8 (29.89-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.261 , 0.281 0.258 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.499 for -h,-k,l 0.499 for h,-h-k,-l 0.049 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 139357 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	54048	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: STD, 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	0.43	0/1838	0.76	0/2498
1	B	0.38	0/1838	0.64	0/2498
1	K	0.46	0/1838	0.75	0/2498
1	L	0.39	0/1838	0.66	0/2498
2	C	0.45	0/8997	0.76	5/12164 (0.0%)
2	M	0.44	0/8997	0.76	5/12164 (0.0%)
3	D	0.46	0/11165	0.78	13/15088 (0.1%)
3	N	0.45	0/11165	0.78	14/15088 (0.1%)
4	E	0.40	0/783	0.77	2/1054 (0.2%)
4	O	0.44	0/783	0.82	1/1054 (0.1%)
5	F	0.41	0/2836	0.70	1/3812 (0.0%)
5	P	0.41	0/2836	0.69	0/3812
All	All	0.44	0/54914	0.76	41/74228 (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
2	C	0	1
3	D	0	1
3	N	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	81	THR	N-CA-C	-7.96	89.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	728	HIS	N-CA-C	7.59	131.49	111.00
4	O	49	GLN	N-CA-C	7.23	130.53	111.00
3	N	1209	LEU	N-CA-C	-7.22	91.50	111.00
3	D	1209	LEU	N-CA-C	-7.04	92.00	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	258	TYR	Sidechain
3	D	132	TYR	Sidechain
3	N	625	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	1806	0	1861	279	0
1	B	1806	0	1861	211	0
1	K	1806	0	1861	232	0
1	L	1806	0	1861	210	0
2	C	8829	0	8933	1148	0
2	M	8829	0	8933	1178	0
3	D	10975	0	11213	1653	0
3	N	10975	0	11212	1616	0
4	E	769	0	775	99	0
4	O	769	0	775	87	0
5	F	2793	0	2873	320	0
5	P	2793	0	2873	362	0
6	D	43	0	44	10	0
6	M	43	0	44	8	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	D	1	0	0	0	0
8	N	1	0	0	0	0
All	All	54048	0	55119	6892	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 63.

The worst 5 of 6892 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:673:LEU:HD23	2:C:867:VAL:HA	1.22	1.20
3:N:172:PRO:HB3	3:N:178:LEU:HD22	1.22	1.16
3:D:141:ILE:H	3:D:141:ILE:HD12	1.11	1.16
2:C:857:ASP:HB2	2:C:978:ARG:HG2	1.29	1.15
3:D:1304:LYS:H	3:D:1304:LYS:HD3	1.03	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	227/315 (72%)	163 (72%)	48 (21%)	16 (7%)	1	7
1	B	227/315 (72%)	167 (74%)	46 (20%)	14 (6%)	2	10
1	K	227/315 (72%)	154 (68%)	45 (20%)	28 (12%)	0	2
1	L	227/315 (72%)	169 (74%)	41 (18%)	17 (8%)	1	6
2	C	1117/1119 (100%)	768 (69%)	229 (20%)	120 (11%)	0	2
2	M	1117/1119 (100%)	758 (68%)	222 (20%)	137 (12%)	0	2
3	D	1388/1524 (91%)	940 (68%)	286 (21%)	162 (12%)	0	2
3	N	1388/1524 (91%)	916 (66%)	317 (23%)	155 (11%)	0	2
4	E	93/99 (94%)	66 (71%)	17 (18%)	10 (11%)	0	2
4	O	93/99 (94%)	56 (60%)	25 (27%)	12 (13%)	0	1
5	F	341/423 (81%)	239 (70%)	57 (17%)	45 (13%)	0	1
5	P	341/423 (81%)	250 (73%)	54 (16%)	37 (11%)	0	2
All	All	6786/7590 (89%)	4646 (68%)	1387 (20%)	753 (11%)	0	2

5 of 753 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	160	ASP
1	A	188	GLN
1	B	3	ASP
1	B	96	THR

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%)	171 (85%)	31 (15%)	3	16
1	B	202/273 (74%)	178 (88%)	24 (12%)	6	26
1	K	202/273 (74%)	172 (85%)	30 (15%)	4	17
1	L	202/273 (74%)	175 (87%)	27 (13%)	5	21
2	C	941/941 (100%)	829 (88%)	112 (12%)	6	26
2	M	941/941 (100%)	816 (87%)	125 (13%)	5	21
3	D	1170/1279 (92%)	972 (83%)	198 (17%)	2	13
3	N	1170/1279 (92%)	1000 (86%)	170 (14%)	4	18
4	E	83/87 (95%)	71 (86%)	12 (14%)	4	18
4	O	83/87 (95%)	72 (87%)	11 (13%)	5	21
5	F	300/370 (81%)	261 (87%)	39 (13%)	5	22
5	P	300/370 (81%)	281 (94%)	19 (6%)	22	60
All	All	5796/6446 (90%)	4998 (86%)	798 (14%)	4	20

5 of 798 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1442	ASN
1	L	1	MET
3	N	1190	SER
4	E	46	PRO

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Mol	Chain	Res	Type
5	F	341	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1489	GLN
1	L	212	ASN
3	N	1334	GLN
5	F	90	GLN
1	K	124	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 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
6	STD	D	1525	-	43,47,47	2.30	15 (34%)	41,73,73	1.65	6 (14%)
6	STD	M	1120	-	43,47,47	2.05	13 (30%)	41,73,73	2.08	9 (21%)

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
6	STD	D	1525	-	-	0/31/101/101	0/2/5/5
6	STD	M	1120	-	-	0/31/101/101	0/2/5/5

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1120	STD	O9-C28	-4.34	1.37	1.43
6	D	1525	STD	O9-C28	-3.35	1.38	1.43
6	D	1525	STD	C4-N1	-2.39	1.42	1.45
6	M	1120	STD	C20-N1	2.08	1.50	1.47
6	D	1525	STD	C28-C32	2.09	1.53	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1525	STD	C29-C19-C28	-5.33	108.73	113.33
6	M	1120	STD	C29-C19-C28	-4.90	109.10	113.33
6	M	1120	STD	O8-C17-C30	-2.62	109.04	111.69
6	D	1525	STD	O8-C17-C30	-2.34	109.33	111.69
6	M	1120	STD	C6-C7-C8	-2.32	122.68	126.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1525	STD	10	0
6	M	1120	STD	8	0

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%)	-0.57	1 (0%) 93 80	32, 58, 89, 110	0
1	B	229/315 (72%)	-0.50	1 (0%) 93 80	45, 96, 120, 124	0
1	K	229/315 (72%)	-0.54	0 100 100	24, 57, 82, 111	0
1	L	229/315 (72%)	-0.61	0 100 100	43, 78, 96, 117	0
2	C	1119/1119 (100%)	-0.54	6 (0%) 91 76	21, 67, 123, 137	0
2	M	1119/1119 (100%)	-0.53	4 (0%) 93 80	21, 69, 120, 130	0
3	D	1392/1524 (91%)	-0.51	10 (0%) 89 70	20, 64, 107, 125	0
3	N	1392/1524 (91%)	-0.46	20 (1%) 78 51	20, 64, 125, 140	0
4	E	95/99 (95%)	-0.55	0 100 100	52, 82, 99, 102	0
4	O	95/99 (95%)	-0.51	0 100 100	46, 86, 114, 119	0
5	F	345/423 (81%)	-0.56	1 (0%) 94 84	53, 77, 97, 104	0
5	P	345/423 (81%)	-0.56	1 (0%) 94 84	47, 81, 97, 108	0
All	All	6818/7590 (89%)	-0.52	44 (0%) 90 73	20, 69, 118, 140	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	406	ASP	5.9
3	D	205	TYR	5.7
3	D	802	ALA	5.6
3	D	801	GLY	5.1
3	N	224	ARG	4.4

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 [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	ZN	N	9003	1/1	0.99	0.24	4.33	55,55,55,55	0
7	ZN	N	9004	1/1	0.99	0.23	1.07	56,56,56,56	0
7	ZN	D	9001	1/1	0.99	0.20	0.52	56,56,56,56	0
7	ZN	D	9002	1/1	0.98	0.22	0.46	47,47,47,47	0
6	STD	M	1120	43/43	0.92	0.20	0.05	39,51,53,56	0
6	STD	D	1525	43/43	0.95	0.17	-0.32	39,59,62,63	0
8	MG	D	9901	1/1	0.97	0.13	-	20,20,20,20	0
8	MG	N	9902	1/1	0.96	0.22	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.