



wwPDB X-ray Structure Validation Summary Report

Aug 16, 2023 – 03:54 PM EDT

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

<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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
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) : 2.35

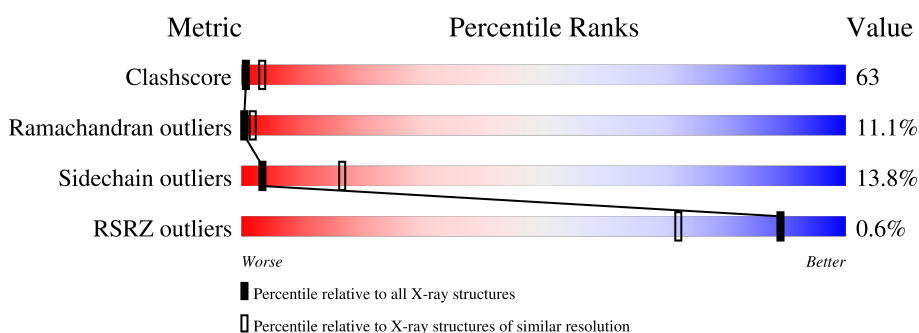
1 Overall quality at a glance

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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	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	<p>%</p> <p>21% 54% 15% 9%</p>
4	E	99	<p>29% 51% 15%</p>
4	O	99	<p>31% 49% 13%</p>
5	F	423	<p>23% 47% 10% 18%</p>
5	P	423	<p>24% 48% 8% 18%</p>

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	B	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	K	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	L	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0

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

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

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

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

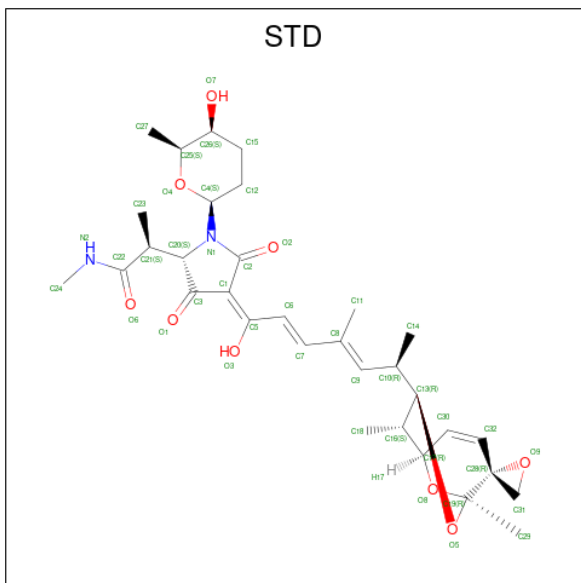
- Molecule 4 is a protein called DNA-directed RNA polymerase omega chain.

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

- Molecule 5 is a protein called DNA-directed RNA polymerase sigma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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: C₃₂H₄₄N₂O₉).



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

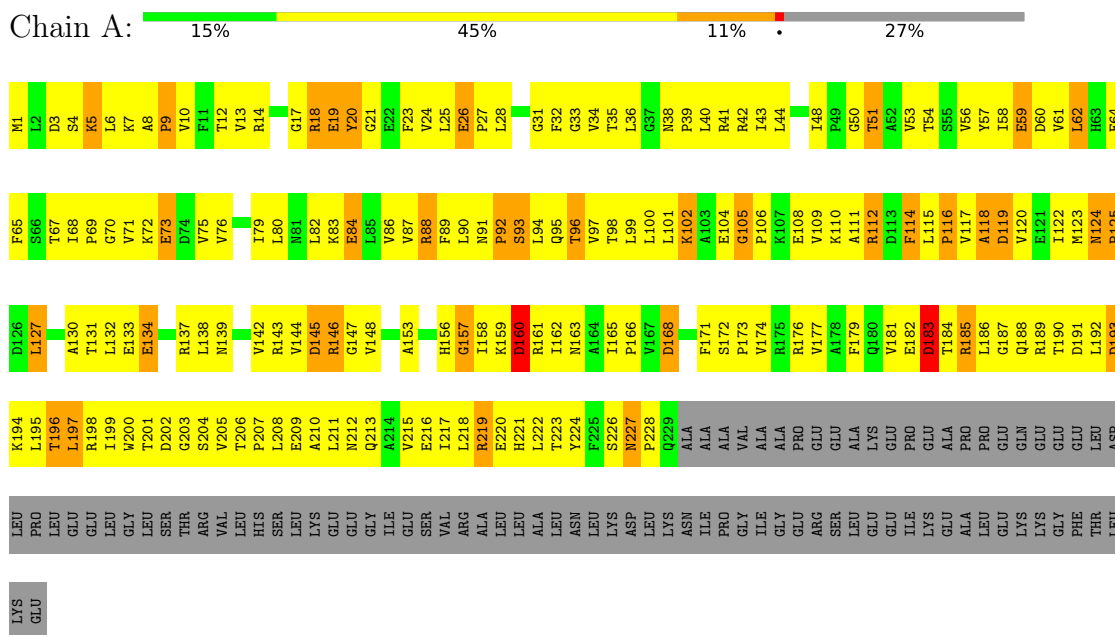
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

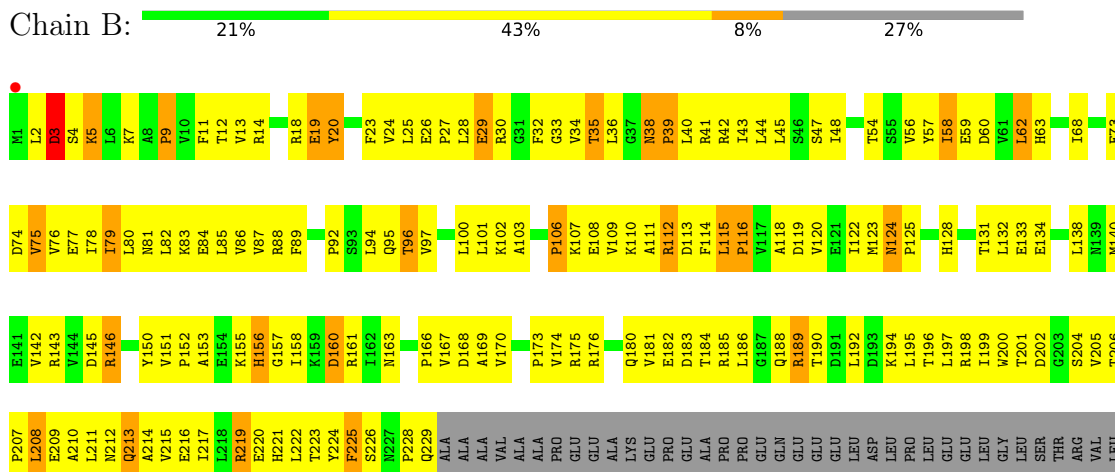
3 Residue-property plots

These plots are drawn for all protein, RNA, 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 alpha chain



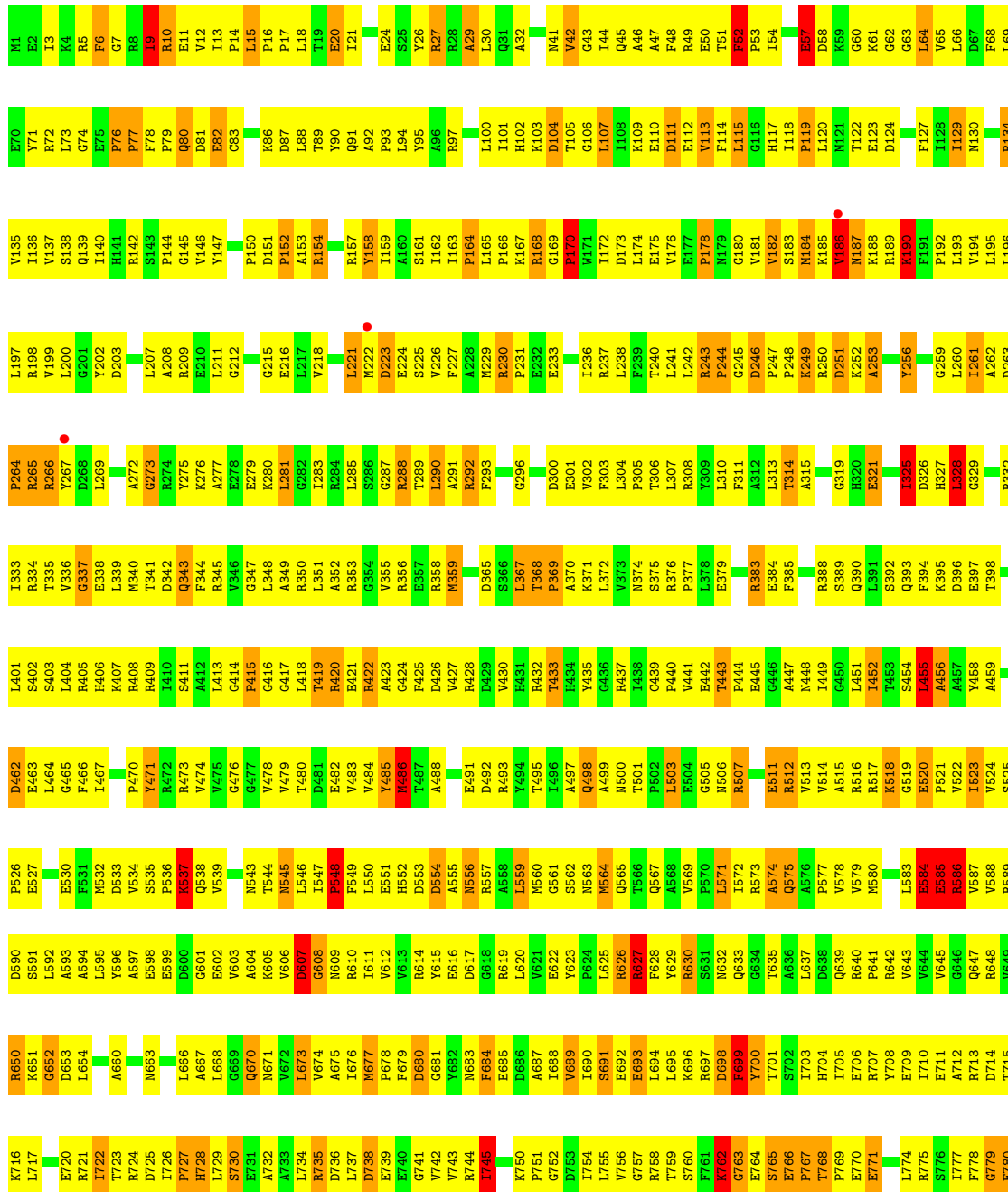
- Molecule 1: DNA-directed RNA polymerase alpha chain

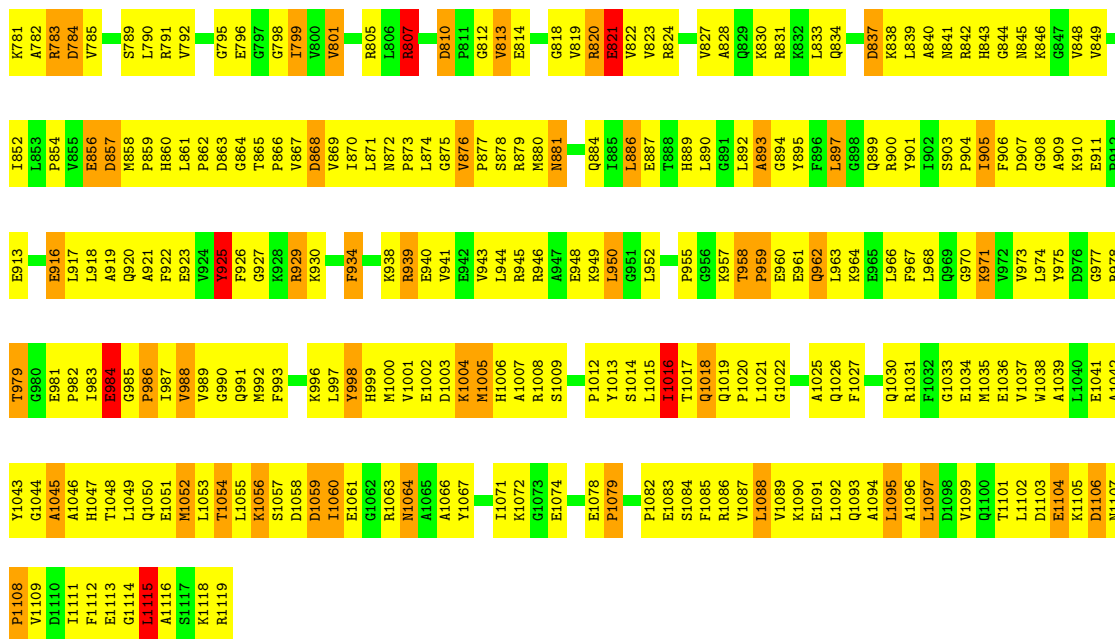


G980	E981	L917	V855	T788	E720	L595	D462	T938	M330	D2683	L196	V186	L69
E982	L918	L918	E856	S789	R721	Y529	E463	S403	R331	P264	L197	I136	E70
Y983	A919	R722	A660	L790	I723	F531	L464	S404	R332	R265	R198	V137	Y71
E984	Q920	T723	E598	S661	T724	E599	G465	L403	I333	R266	V199	S138	R72
G985	A921	P792	H860	E662	R725	S534	F466	R405	R334	Y267	G201	Q139	G74
P986	R922	P793	H861	M663	D726	V535	I467	H406	R335	G202	G201	I140	L73
L987	E923	L726	G664	G601	I726	P536	R468	R407	V336	D268	Y202	H141	G75
V988	Y924	G795	F665	E602	P727	K537	T469	R408	G337	E271	D203	R142	F76
V989	D863	E796	K538	V603	H728	Q538	P470	R409	E338	A272	Q204	S143	P77
G990	G927	I799	F539	F540	S730	V539	Y471	A412	T341	G273	E205	P144	F78
G991	G927	T865	K605	K605	S730	R472	R472	L413	D342	A277	T206	G145	F79
F993	R929	V801	D607	D607	L734	V542	R473	L414	Q343	K276	L207	V146	Q80
K996	K930	R802	G608	G608	R735	M543	V475	G414	F344	E278	R209	F148	D81
L997	G931	G805	M609	M609	R736	T544	T469	G415	R345	E279	E210	F149	E82
M1000	F934	R805	N545	N545	L737	T544	V478	G417	L348	K280	L211	P150	C83
V1001	G935	L806	I611	I611	D738	L546	V479	L418	L349	L281	G220	D151	L88
E1002	V936	R807	P548	P548	G741	I547	T480	L419	A349	G282	G220	P152	T89
D1003	D937	D810	F549	F549	V742	R614	D481	R420	R350	L283	L221	A153	Y90
K1004	K938	P811	L550	L550	V743	R614	E482	E421	L351	R284	H222	R154	Q91
M1005	R939	P812	E551	E551	R744	Y484	V484	A423	A352	G225	D223	P155	A92
H1006	E940	V813	H552	H552	R744	D617	Y485	G424	G354	S225	E224	G156	Q93
A1007	V941	E814	D553	D553	A748	G618	M486	F425	V355	Y158	S225	R157	L94
R1008	E942	L815	D554	D554	E748	R619	T487	D426	R356	T289	F227	Y159	Y95
S1009	V943	K816	A555	A555	V749	L620	A488	V427	E357	A291	A228	A160	A96
G1010	R944	V819	M556	M556	K750	E621	T489	R428	R358	R292	R229	I163	R97
P1011	R945	L822	E685	E685	P751	E622	E490	D429	M359	F293	R230	I163	L100
F1012	R946	G823	L825	L825	I754	M560	E491	V430	S363	G296	R230	P164	L101
D1013	V947	R824	G626	G626	L755	R626	D492	H431	E364	E297	E232	L165	H102
M1014	K949	E825	S622	S622	V756	R627	R493	R432	F298	F298	E233	P166	K103
L1015	L950	Y826	F628	F628	G757	G628	I495	H434	L367	K299	L235	K167	D104
T1016	G951	R827	M664	M664	G757	G628	I496	Y435	L367	K299	L235	R168	I105
F1017	E952	A828	E692	E692	T759	S631	A497	G436	T368	D300	R237	G169	G106
P1020	V953	Q829	S631	S631	S760	E693	R497	R437	I236	E301	L238	P170	G107
L1021	K957	K830	L694	L694	F761	M632	Q498	C439	L372	F303	F239	W171	I108
K1024	P958	R831	L695	L695	K762	Q633	T501	C439	V373	F303	F239	I172	K109
F1027	E960	K832	G696	G696	E766	A636	P502	F440	N374	L304	T240	D173	E110
Q1030	E961	L833	D698	D698	P767	L637	L503	V441	S375	P305	L241	L174	E111
R1031	E962	G834	F699	F699	T768	D638	L503	T443	R376	R308	L242	E175	E112
G1032	E963	G836	Y700	Y700	T768	D638	R507	T444	R376	Y309	L243	E176	V113
E1033	E964	K837	T701	T701	P769	Q639	I508	P444	P377	Y309	P244	E177	F114
M1034	E965	K838	H704	H704	E770	R640	F508	E445	E379	G245	D246	P178	L115
L1035	E966	L839	H705	H705	E771	P641	I508	E445	E379	G245	D246	G116	G116
E1036	E967	A840	I706	I706	L773	R642	V513	G446	A380	L313	P247	H117	H117
E1037	E968	A842	E706	E706	L774	V644	V514	G446	A381	L313	P247	G189	G189
V1037	E969	R843	Y708	Y708	S776	Q644	A515	M448	I382	T314	P248	V181	I118
W1038	G970	G844	E709	E709	I777	Q647	A515	M448	A315	R249	P248	V182	I118
K971	K971	N845	I710	I710	E780	R650	P521	S454	S389	E321	P248	V181	I118
V972	V972	K846	R713	R713	K781	K651	P521	S454	S389	E321	P248	V181	I118
L1040	V973	R849	D714	D714	A782	G652	P521	S454	Q390	Y256	A255	K188	F127
E1041	L974	E850	T715	T715	R783	D653	P521	S454	Q390	Y256	A255	K188	F127
A1042	Y975	K851	K716	K716	D784	L654	P521	S454	L391	Y257	A256	R189	I128
Y1043	D976	L852	L717	L717	D784	L654	P521	S454	S392	Y258	A256	R189	I128
G1044	G977	L853	G718	G718	D784	L654	P521	S454	L391	Y257	A256	R189	I128
A1045	R978	E916	E916	E916	D787	D657	P521	S454	S392	Y258	A256	R189	I128
A1046	T979	E916	E916	E916	D787	D657	P521	S454	L391	Y257	A256	R189	I128

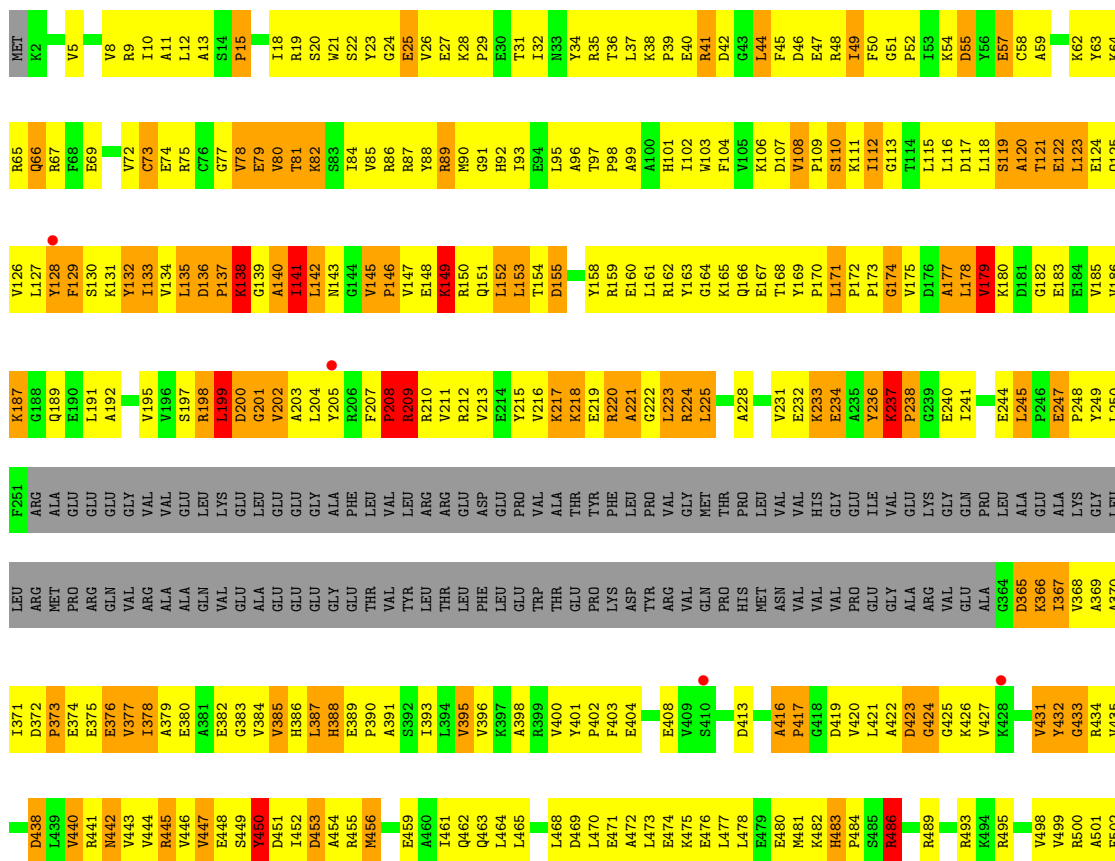
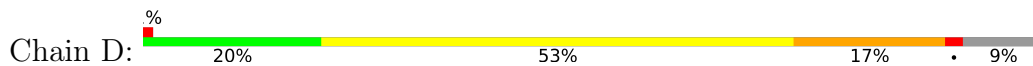


• Molecule 2: DNA-directed RNA polymerase beta chain





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



E1458	E1459	E1460	E1461	E1462	E1463	E1464	E1465	E1466	E1467	E1468	E1469	E1470	E1471	E1472	E1473	E1474	E1475	E1476	E1477	E1478	E1479	E1480	E1481	E1482	E1483	E1484	E1485	E1486	E1487	E1488	E1489	E1490	E1491	E1492	E1493	E1494	E1495	E1496	E1497	E1498	E1499	E1500	E1501	E1502	E1503	E1504	E1505	LVS	GLU	ARG	PRO	ALA	ALA	ALA	ARG	ARG	ARG	GLY	VAL	LYS	ARG
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GLU	GLN	PRO	GLY	LYS	GLN	ALA
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● Molecule 3: DNA-directed RNA polymerase subunit beta' chain



MET	K2	K3	E4	V5	R6	K7	R8	V9	I10	A11	L12	A13	S14	P15	E16	K17	I18	S22	Y23	G24	E25	V26	E27	K28	P29	E30	T31	I32	N33	Y34	R35	L36	L37	K38	P39	E40	R41	L44	F45	D46	E47	R48	F50	G51	P52	L53	K54	D55	Y56	E57	C58	A59	C60	G61	L62	Y63
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K64	R65	Q66	R67	E68	E69	G70	K71	V72	C73	E74	R75	C76	G77	V78	R79	K80	T81	V82	S83	I84	V85	R86	R87	Y88	R89	M90	G91	H92	I93	H94	L95	L96	A99	P98	A100	H101	I102	I103	F104	V105	K106	D107	V108	P109	S110	K111	I112	G113	T114	L115	L116	D117	C118	S119	A120	V185	K186	E187	L122	L123
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E124	Q125	V126	E127	R128	G129	S130	K131	V132	C133	V134	L135	D136	P137	K138	G139	A140	I141	L142	N143	P146	V147	E148	K149	R150	Q151	L152	L153	T154	D155	L156	E157	R158	R159	R162	Y163	Q166	E167	T168	Y169	P170	L171	P172	P173	G174	V175	D176	A177	L178	L179	V179	E183	E184	V185	K186	E187	G188
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Q189	E190	L191	A192	P193	G194	V195	V196	S197	L198	L199	V202	A203	L204	Y205	R206	PHE	P208	R209	R210	V211	R212	V213	E214	Y215	V216	K217	K218	E219	R220	A221	G222	R224	L225	P226	L227	W230	V231	E232	K233	E234	K237	P238	G239	E240	I241	L242	A243	E244	L245	P246	E247	P248	Y249	F251
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ARG	ALA	GLU	GLY	GLY	VAL	VAL	ALA	ALA	LEU	LEU	GLY	GLU	GLY	GLY	ALA	GLY	PHE	LEU	VAL	LEU	ARG	ARG	LEU	GLY	PRO	TRP	VAL	THR	ALA	THR	TYR	PHE	LEU	ASP	PRO	VAL	GLN	MET	THR	PRO	LEU	ASN	VAL	VAL	HIS	GLY	GLY	ILE	GLY	GLY	ALA	GLY	VAL	GLY	VAL	GLY	GLN	PRO	LEU	LEU	ALA	D365	K366	G367	V368	A369	A370	I371	LEU
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ARG	MET	ARG	ARG	VAL	GLN	ARG	ALA	ALA	ALA	VAL	GLU	GLU	GLU	GLU	GLU	GLY	GLY	THR	VAL	THR	LEU	THR	THR	LEU	TRP	THR	GLU	GLU	ALA	PRO	TYR	ASP	D406	V409	S410	T411	G412	D413	R414	V415	A416	P417	L421	A422	D423	G424	G425	K426	V427	K428	R429	S429	D430	V431	Y432	G433	K434	I371	LEU
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D372	P373	E374	E375	V376	V377	L378	A381	E382	G383	V384	V385	H386	L387	L388	V389	P390	A391	S392	I393	L394	V395	V396	K397	A398	R399	V400	L401	P402	F403	A404	D405	D406	V409	S410	T411	G412	D413	R414	V415	A416	P417	L421	A422	D423	G424	G425	K426	V427	K428	R429	S429	D430	V431	Y432	G433	K434	I371	LEU
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E436	V437	D438	L439	V440	R441	K442	V443	V444	S445	V446	V447	E448	S449	V450	D451	L452	D453	A454	R455	M456	G457	A458	E459	A460	L461	Q462	Q463	L464	L465	K466	E467	L468	D469	L470	E471	A472	L473	E474	K475	S476	L477	L478	E479	E480	M481	K482	H483	P484	S485	R486	A487	A488	R489	R490	K491	A492	R493	K494	R495
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L496	E497	V498	V499	R500	A501	F502	L503	D504	S505	G506	N507	E510	M511	M512	L513	L514	E515	A516	V517	P518	V519	L520	P521	P522	D523	L524	R525	P526	M527	V528	Q529	V530	G533	R534	F535	A536	T537	S538	S539	L540	L543	Y544	R545	R546	L547	L548	I549	M549	R550	N551	M552	L553	R554	K555	R556	V557	L558
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A559	Q560	G561	A562	P563	E564	L565	S566	L567	V568	G569	P570	K571	R572	M573	L574	H575	E576	A577	V578	D579	L582	D583	R584	G585	R586	R587	L588	F589	M590	S591	M592	L593	D594	K595	D597	R598	P599	L600	R601	S602	I603	L604	T605	D605	V606	L607	G608	S609	G610	R613	N617	L618	E619	R620	G621	R622	D623	L624
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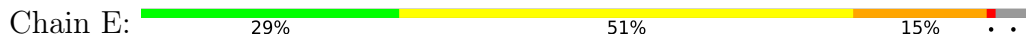
V625	S626	G627	R628	S629	E630	L631	V632	V633	V634	G635	P636	L637	K638	L639	H640	M641	O642	G643	L644	P645	S646	L647	L648	E649	L650	E651	L652	F653	G654	P655	V656	T657	L658	L659	K660	M661	E662	E663	G664	I665	S666	I667	A668	P669	L670	L671	L672	L673	L674	L675	L676	L677	E678	R679	L680	G681	R682	D683	L684	K685
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D685	E686	V687	G688	D689	E690	L691	L692	E693	E694	V695	L696	V699	V700	L701	L702	M703	R704	A705	V706	F707	G708	H709	R710	L711	G712	L713	L714	A715	L716	G717	F718	V719	L720	L721	R722	G723	G724	Q727	L728	H729	I666	A667	P668	M669	V670	K671	A672	S608	G609	R674	R675	L676	L677	E678	R679	L680	G681	R682	D683	L684	K685
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P750	L751	S752	G753	F754	E755	Q756	A757	E758	A759	R760	L761	G762	M763	L764	S765	H766	H767	A768	L769	L770	S771	P772	A773	S774	G775	E776	P777	L778	A779	K780	F781	R782	R783	L784	I785	L786	L787	G788	L789	Y790	Y791	I792	L793	L794	V795	R796	K797	E798	K799	K800	L804	E805	F806	A807	T808	P809	E810	H811	E811
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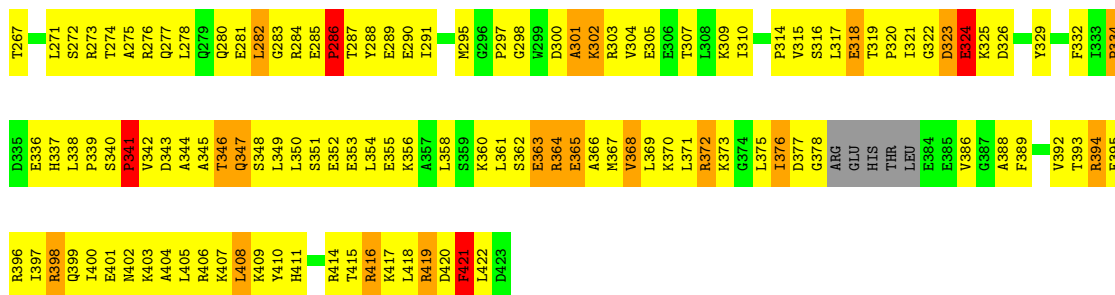
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L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	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	T1000	E1001	T1002	L1003	T1004
E1069	Y1070	F1071	I1072	S1073	S1074	H1075	R1078	K1079	T1084	A1085	L1086	L1087	D1090	S1091	G1092	Y1093	L1094	T1095	R1096	K1097	L1098	V1099	L1100	V1101	H1102	H1103	H1104	H1105	H1106	H1107	R1108	E1109	A1110	D1111	C1112	T1113	T1114	T1115	M1116	Y1117	I1118	S1119	P1120	P1121	L1122	F1123	Q1124	P1125	D1126	E1127	T999	V1128	T1129	R1130	R1133	L1134																																																																											
R1135	K1136	R1137	I1138	D1139	L1144	Y1145	R1146	S1147	V1148	A1149	R1150	E1151	E1152	V1155	G1156	Y1158	L1159	E1160	E1161	E1162	L1163	R1164	Y1165	L1166	S1167	H1168	D1169	D1170	L1171	H1172	L1173	L1174	E1175	K1176	A1177	A1178	E1179	E1182	I1183	V1186	P1187	R1188	R1189	S1190	F1191	L1192	L1193	C1194	T1195	R1197	Y1198	C1201																																																																															
Q1202	K1203	K1204	Y1205	G1206	G1207	D1208	L1209	M1210	A1211	A1212	R1213	A1214	V1215	S1216	I1217	G1218	E1219	A1220	V1221	G1222	I1223	V1224	I1229	G1236	E1231	P1232	G1233	T1234	Q1235	L1236	M1238	R1239	T1240	F1241	H1242	T1243	D1251	I1252	T1253	G1255	L1256	P1257	R1258	V1259	I1260	E1261	F1262	F1263	L1264	A1265	R1266	R1267	P1268	K1269	A1270																																																																												
K1271	A1272	V1273	L1274	S1275	E1276	L1277	D1278	G1279	V1280	V1281	R1282	L1283	E1284	E1285	T1286	E1287	E1288	K1289	L1290	S1291	F1292	F1293	V1294	E1295	S1296	E1297	S1300	G1301	K1304	L1305	P1306	K1307	E1308	A1309	R1310	L1311	K1314	D1315	D1316	G1317	Y1318	V1319	E1320	A1321	G1322	L1323	L1324	P1325	L1326	L1327	I1330	D1331	H1332	H1333	Q1334																																																																												
L1335	L1336	G1340	P1341	E1342	A1343	V1344	E1345	R1346	V1347	L1348	V1349	E1350	E1351	E1352	Q1353	Y1356	V1361	K1362	L1363	H1364	D1365	K1366	H1367	L1368	E1369	S1370	V1371	L1372	R1373	Q1374	M1375	K1376	K1377	Y1378	V1379	E1380	L1381	T1382	D1383	P1384	G1385	R1388	L1389	L1390	E1391	G1392	Q1393	L1394	L1395	E1396	K1397	L1398	D1399	V1400	E1401																																																																												
A1402	L1403	M1404	E1405	L1406	L1407	I1408	A1409	E1410	G1411	A1412	L1413	T1414	V1415	A1416	V1417	L1418	P1419	L1420	L1421	M1422	G1423	V1424	T1425	K1426	S1427	A1428	T1431	K1432	S1433	V1434	L1435	S1436	A1437	A1438	S1439	F1440	Q1441	M1442	T1443	V1446	L1447	T1448	E1449	A1450	A1451	T1452	A1453	G1454	K1455	L1456	D1457	L1458	E1459	I1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467																																																																						
E1464	M1465	V1466	L1467	L1468	G1469	R1470	L1471	L1472	P1473	A1474	Y1475	T1476	G1477	S1478	D1479	F1480	V1481	R1482	F1483	T1484	Q1485	V1486	V1487	L1488	Q1489	L1490	T1491	L1492	K1493	E1496	E1497	K1500	E1501	A1502	V1503	E1504	M1505	LYS	GLU	ARG	PRO	ALA	ALA	ALA	ARG	ARG	GLY	VAL	LYS	ARG	GLU	GLN	PRO	GLY	LYS	GLN	ALA																																																																										

● Molecule 4: DNA-directed RNA polymerase omega chain



WET	A2	E3	P4	L9	F10	V13	K16	Y17	R18	L19	T20	D21	V22	V23	A24	K25	R26	A27	Q28	Q29	L30	L31	R32	F35	T38	V39	L40	E41	P42	E43	E44	R45	P46	K47	M48	Q49	T50	L51	E52	G53	L54	F55	D56	D57	F58	N59	A60	E61	T62	H63	A64	H65	K66	E67
L68	L69	T70	G71	R72	L73	E77	M78	L79	V80	P81	E82	D83	Q86	R87	E88	H89	Y93	P94	Q95	E96	ARG	GLU	GLU	F35	T38	V39	L40	E41	P42	E43	E44	R45	P46	K47	M48	Q49	T50	L51	E52	G53	L54	F55	D56	D57	F58	N59	A60	E61	T62	H63	A64	H65	K66	E67

● Molecule 4: DNA-directed RNA polymerase omega chain



4 Data and refinement statistics i

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	1.12 (at 3.00Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.281 0.258 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtrriage
Anisotropy	0.354	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , -24.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.499 for -h,-k,l 0.499 for h,-h-k,-l 0.044 for -k,-h,-l	Xtrriage
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

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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:D:141:ILE:H	3:D:141:ILE:HD12	1.11	1.16
3:N:172:PRO:HB3	3:N:178:LEU:HD22	1.22	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	6
1	B	227/315 (72%)	167 (74%)	46 (20%)	14 (6%)	1	8
1	K	227/315 (72%)	154 (68%)	45 (20%)	28 (12%)	0	1
1	L	227/315 (72%)	169 (74%)	41 (18%)	17 (8%)	1	5
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	1
3	D	1388/1524 (91%)	940 (68%)	286 (21%)	162 (12%)	0	1
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	171 (85%)	31 (15%)	2	13
1	B	202/273 (74%)	178 (88%)	24 (12%)	5	22
1	K	202/273 (74%)	172 (85%)	30 (15%)	3	14
1	L	202/273 (74%)	175 (87%)	27 (13%)	4	17
2	C	941/941 (100%)	829 (88%)	112 (12%)	5	22
2	M	941/941 (100%)	816 (87%)	125 (13%)	4	17
3	D	1170/1279 (92%)	972 (83%)	198 (17%)	2	11
3	N	1170/1279 (92%)	1000 (86%)	170 (14%)	3	15
4	E	83/87 (95%)	71 (86%)	12 (14%)	3	15
4	O	83/87 (95%)	72 (87%)	11 (13%)	4	17
5	F	300/370 (81%)	261 (87%)	39 (13%)	4	19
5	P	300/370 (81%)	281 (94%)	19 (6%)	18	51
All	All	5796/6446 (90%)	4998 (86%)	798 (14%)	3	17

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

Mol	Chain	Res	Type
1	L	140	MET
2	M	881	ASN
2	M	24	GLU
1	L	126	ASP

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Mol	Chain	Res	Type
2	M	420	ARG

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

Mol	Chain	Res	Type
2	M	704	HIS
3	N	768	ASN
2	M	845	ASN
3	N	125	GLN
3	N	1184	GLN

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 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	-	42,47,47	2.12	13 (30%)	47,73,73	1.74	9 (19%)
6	STD	M	1120	-	42,47,47	1.93	12 (28%)	47,73,73	2.01	12 (25%)

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	-	-	7/31/101/101	0/6/5/5
6	STD	M	1120	-	-	12/31/101/101	0/6/5/5

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1525	STD	C22-N2	4.98	1.40	1.33
6	D	1525	STD	C26-C25	4.63	1.60	1.52
6	D	1525	STD	O5-C19	4.46	1.47	1.43
6	D	1525	STD	O8-C19	4.16	1.46	1.43
6	M	1120	STD	C26-C25	4.12	1.59	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1120	STD	O4-C4-N1	6.75	113.28	105.92
6	D	1525	STD	C29-C19-C28	-5.62	108.73	113.30
6	M	1120	STD	C29-C19-C28	-5.16	109.10	113.30
6	M	1120	STD	O8-C19-C29	5.00	109.86	105.64
6	D	1525	STD	C19-O5-C13	4.56	117.72	112.80

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

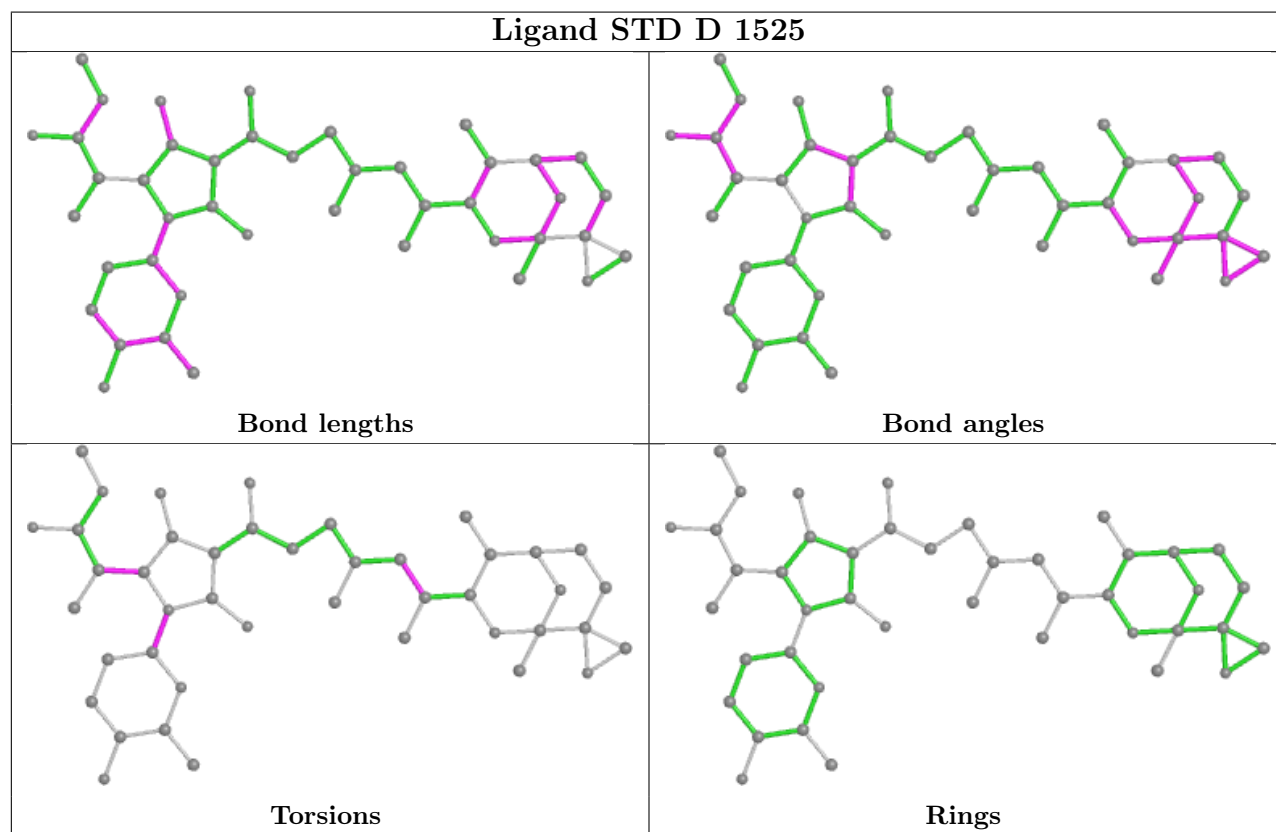
Mol	Chain	Res	Type	Atoms
6	D	1525	STD	N1-C20-C21-C22
6	D	1525	STD	N1-C20-C21-C23
6	D	1525	STD	C3-C20-C21-C23
6	M	1120	STD	O4-C4-N1-C20
6	M	1120	STD	C9-C10-C13-C16

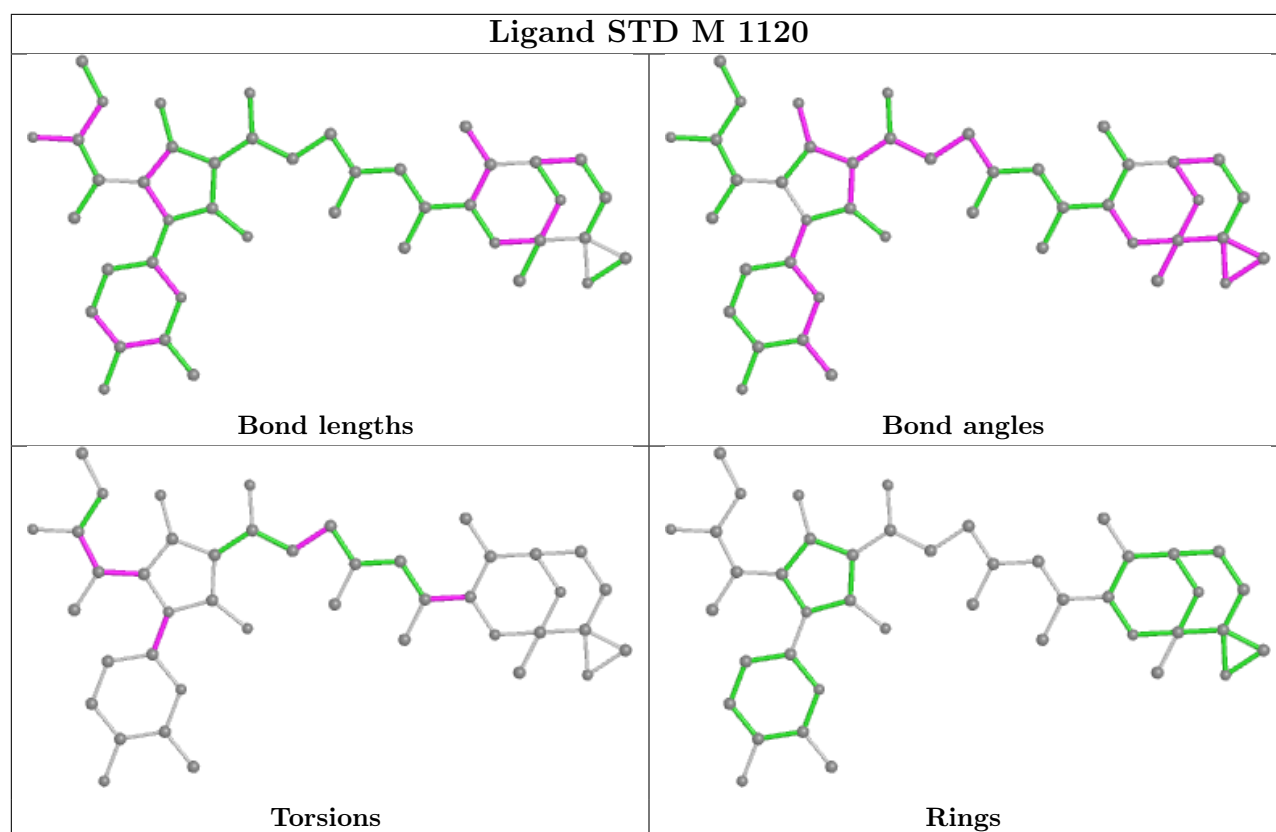
There are no ring outliers.

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	229/315 (72%)	-0.58	0 100 100	32, 58, 89, 110	0
1	B	229/315 (72%)	-0.52	1 (0%) 92 79	45, 96, 120, 124	0
1	K	229/315 (72%)	-0.56	0 100 100	24, 57, 82, 111	0
1	L	229/315 (72%)	-0.62	0 100 100	43, 78, 96, 117	0
2	C	1119/1119 (100%)	-0.55	5 (0%) 92 79	21, 67, 123, 137	0
2	M	1119/1119 (100%)	-0.54	3 (0%) 94 84	21, 69, 120, 130	0
3	D	1392/1524 (91%)	-0.53	10 (0%) 87 69	20, 64, 107, 125	0
3	N	1392/1524 (91%)	-0.48	19 (1%) 75 49	20, 64, 125, 140	0
4	E	95/99 (95%)	-0.56	0 100 100	52, 82, 99, 102	0
4	O	95/99 (95%)	-0.52	0 100 100	46, 86, 114, 119	0
5	F	345/423 (81%)	-0.57	1 (0%) 94 84	53, 77, 97, 104	0
5	P	345/423 (81%)	-0.57	0 100 100	47, 81, 97, 108	0
All	All	6818/7590 (89%)	-0.53	39 (0%) 89 72	20, 69, 118, 140	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	406	ASP	5.8
3	D	802	ALA	5.5
3	D	205	TYR	5.4
3	D	801	GLY	4.9
3	N	224	ARG	4.3

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](#)

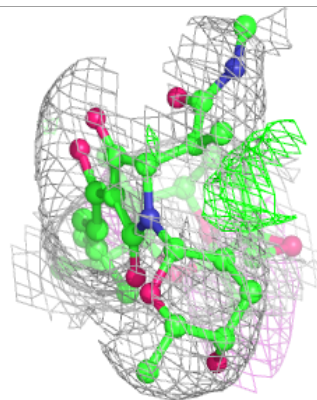
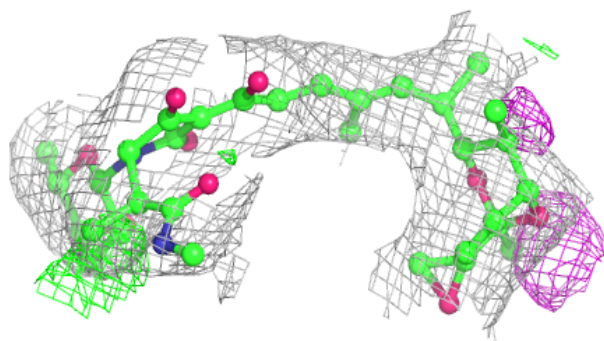
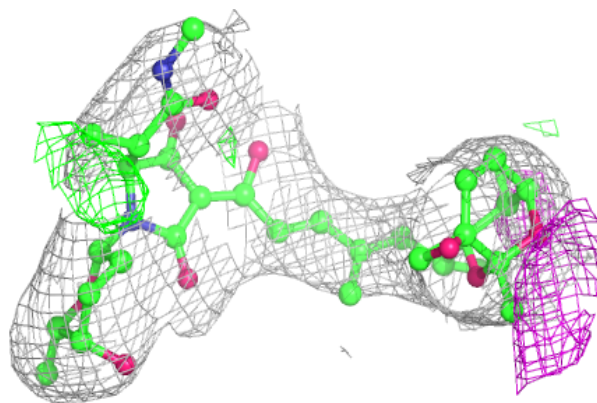
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	STD	M	1120	43/43	0.92	0.20	39,51,53,56	0
6	STD	D	1525	43/43	0.95	0.17	39,59,62,63	0
8	MG	N	9902	1/1	0.96	0.22	30,30,30,30	0
8	MG	D	9901	1/1	0.97	0.13	20,20,20,20	0
7	ZN	D	9002	1/1	0.98	0.22	47,47,47,47	0
7	ZN	N	9004	1/1	0.99	0.23	56,56,56,56	0
7	ZN	D	9001	1/1	0.99	0.20	56,56,56,56	0
7	ZN	N	9003	1/1	0.99	0.24	55,55,55,55	0

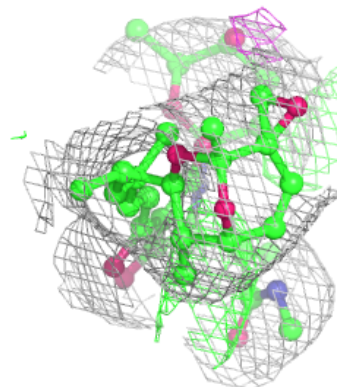
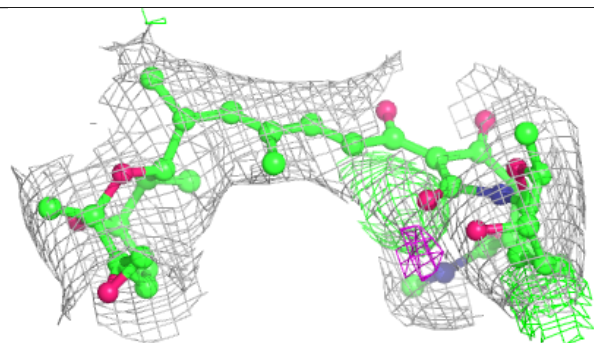
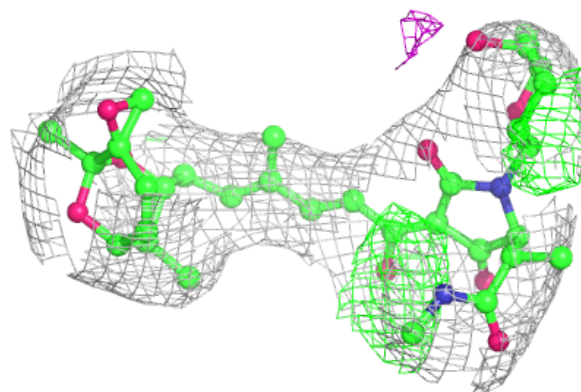
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around STD M 1120:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around STD D 1525:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.