



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:10 PM UTC

PDB ID : 2CW0 / pdb_00002cw0
Title : Crystal structure of Thermus thermophilus RNA polymerase holoenzyme at 3.3 angstroms resolution
Authors : Tuske, S.; Sarafianos, S.G.; Wang, X.; Hudson, B.; Sineva, E.; Mukhopadhyay, J.; Birktoft, J.J.; Leroy, O.; Ismail, S.; Clark Jr., A.D.; Dharia, C.; Napoli, A.; Laptenko, O.; Lee, J.; Borukhov, S.; Ebright, R.H.; Arnold, E.
Deposited on : 2005-06-15
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

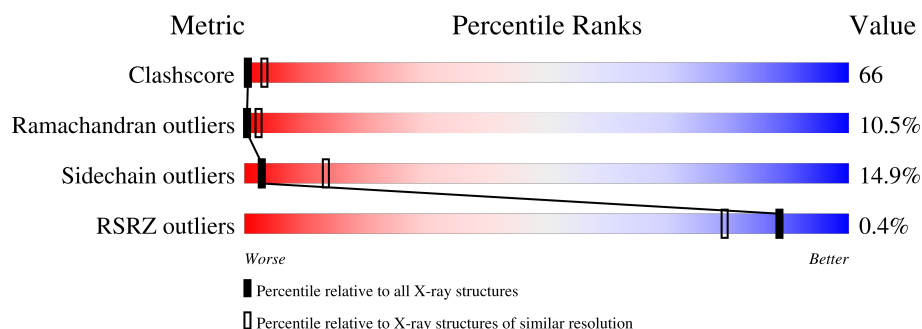
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	17% 42% 13% • 27%
1	B	315	18% 43% 10% • 27%
1	K	315	21% 38% 11% • 27%
1	L	315	17% 44% 11% • 27%
2	C	1119	21% 57% 20% •
2	M	1119	21% 57% 19% •
3	D	1524	18% 49% 22% • 9%

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Mol	Chain	Length	Quality of chain
3	N	1524	%19%48%22%•9%
4	E	99	24%49%18%••
4	O	99	25%49%16%5%•
5	F	423	18%47%14%•18%
5	P	423	22%43%16%•18%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 53962 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 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 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
			2793	1762	504	523	4			
5	P	345	Total	C	N	O	S	0	0	0
			2793	1762	504	523	4			

- Molecule 6 is ZINC ION (CCD ID: 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		

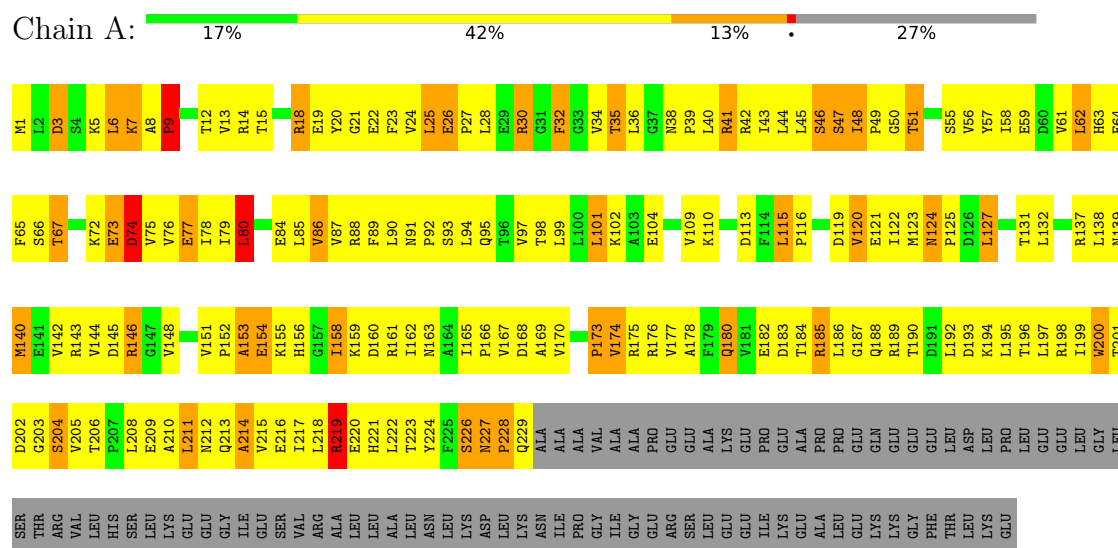
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

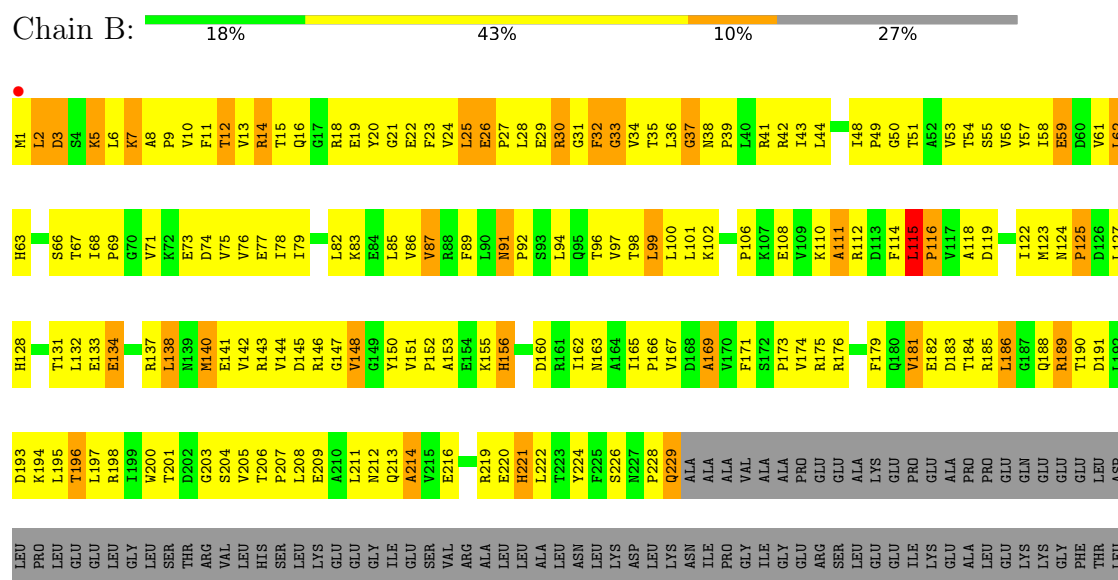
3 Residue-property plots

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

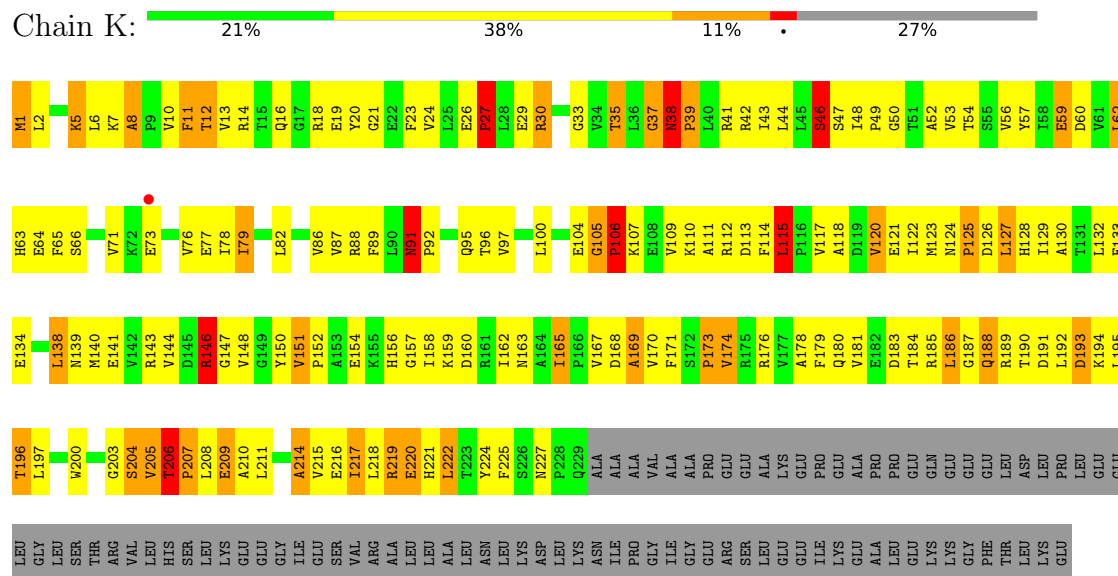


• Molecule 1: DNA-directed RNA polymerase alpha chain



LYS
GLU

• Molecule 1: DNA-directed RNA polymerase alpha chain

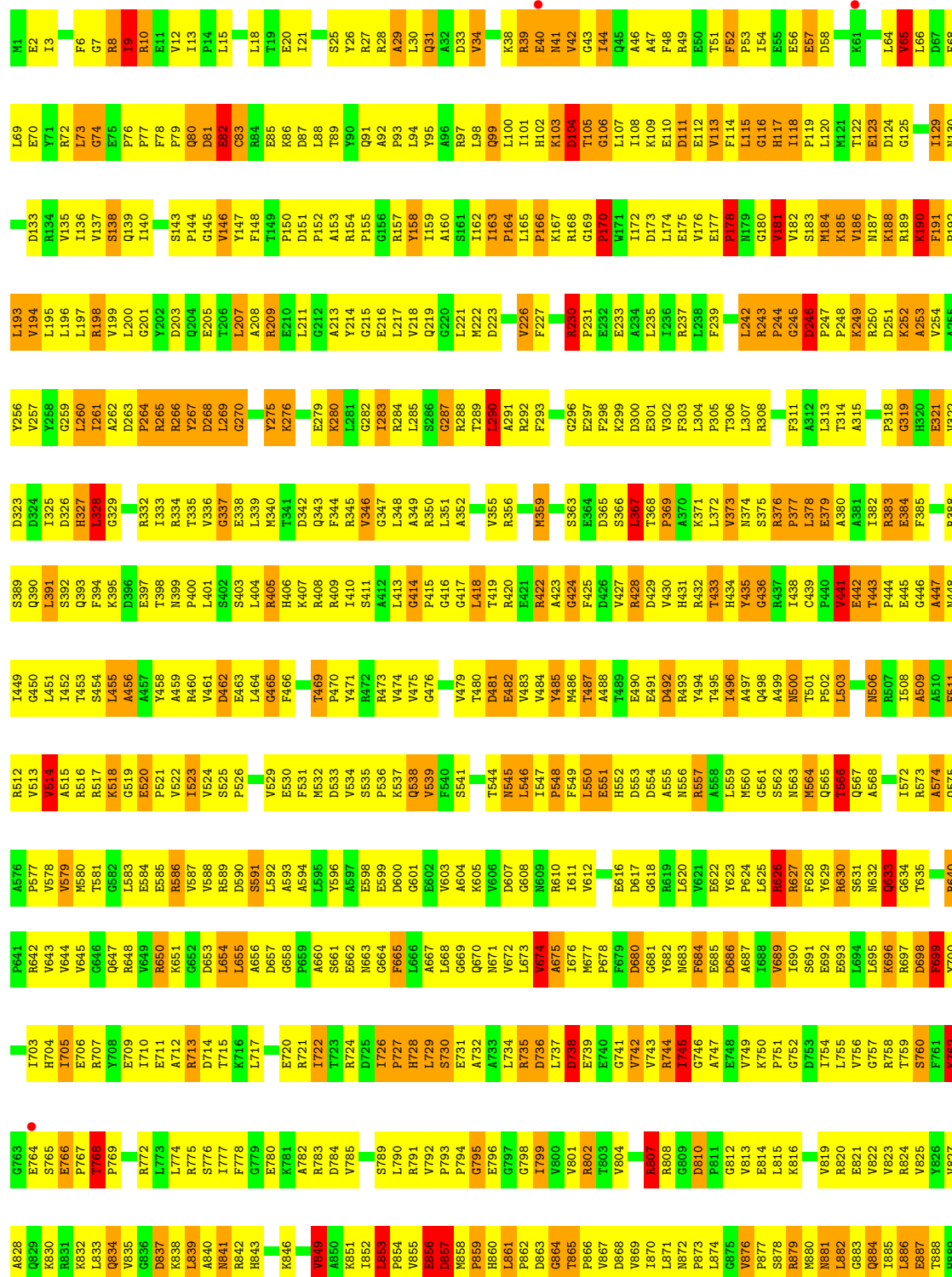


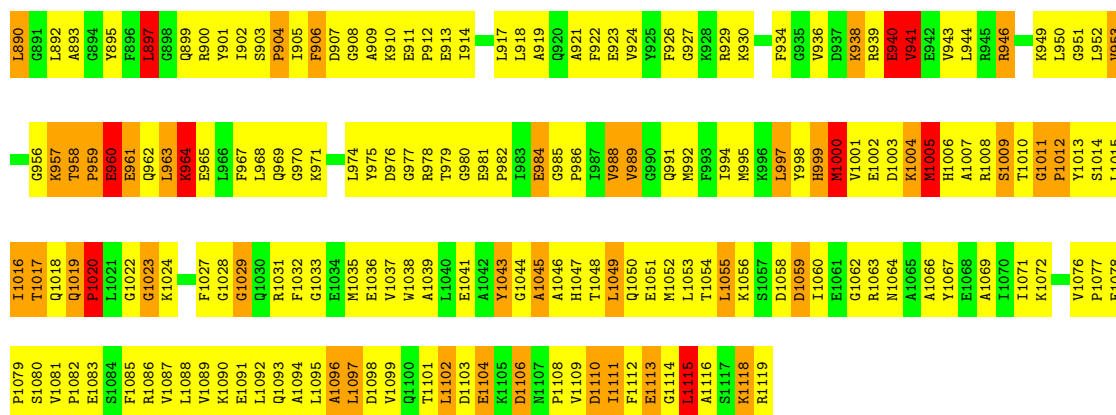
S1014	L944	V819	G758	V689	R626	G565	P502	C439	L372	L310	P244	M184	D124	G62
L1015	R945	R820	R759	I690	R627	T586	L503	G442	V373	F311	G245	K185	G125	G63
T1016	E821	L882	T759	S691	F628	A567	E504	T443	S374	A312	D246	V186	S126	L64
Q1018	R946	V822	S760	E692	Y629	A568	E505	T443	S375	L313	P247	N187	F127	V65
Q1019	R948	R823	S761	N506	S631	V569	N507	P444	P376	T314	K188	K189	I128	L66
P1020	R949	R824	K762	L694	R630	P570	R507	E445	R377	A315	K249	K190	I129	D67
L1021	L950	V825	G763	L695	N632	L571	T508	O446	L378	C316	R250	K191	G131	F68
G1022	G951	Y826	E764	K696	Q633	L572	A509	A447	E379	V317	D251	F191	A132	L89
G1023	L952	Q829	S765	R697	G634	R573	A510	N448	G318	P318	K252	P192	G133	E70
K1024	K957	R830	E766	D698	Y635	A574	E511	I449	R383	G319	A253	L193	D133	Y71
E1027	E960	R831	F767	L699	A636	Q575	R512	G450	E384	H320	V194	L195	R134	R72
G1028	L963	R832	T768	Y700	L637	A576	V513	I452	F385	G321	Y256	L196	V135	L73
Q1030	K964	L833	E770	S702	Q639	V578	A515	T453	S387	V322	T286	L197	V136	G74
R1031	E965	Q834	E771	I703	R640	V579	R516	S454	R388	D323	G259	R198	V137	E75
F1032	L966	V835	R772	H704	P641	M580	R517	I455	S389	D324	G259	R199	S138	P76
G1033	F967	G836	L773	R707	R642	G582	R518	G459	Q390	D326	T281	L200	Q139	F77
E1034	R968	V838	R774	Y708	V644	L583	E520	G459	S392	L328	D283	L201	H141	F78
M1035	Q969	A840	R775	E709	V645	E584	P521	G462	Q393	G329	T284	D203	S143	Q80
E1036	G970	R842	I777	I710	Q646	E585	V522	I463	F394	N330	R265	Q204	P144	E82
V1037	K971	R843	E780	A712	Q647	R586	V523	E463	K395	R331	R266	E205	G145	C83
V1038	V972	H844	K781	R713	R648	V587	V524	L464	D396	R332	Y287	T206	V146	R84
E1041	L974	G844	A782	R713	V649	V588	S525	G465	E397	I333	D288	A208	Y147	E85
A1042	Y975	N845	R783	L717	K651	D590	E526	I467	T398	R334	G273	R209	F148	K86
Y1043	D976	Q846	D784	G718	G652	S591	V529	R468	K399	T385	R274	R209	T149	D87
G1044	G977	V848	K786	R721	D653	L592	E530	T469	S403	G337	Y275	E210	P150	L88
A1045	R978	V849	R787	I722	L654	A593	F531	P470	L404	E338	R276	G212	D151	T89
A1046	T979	A850	T788	I723	L655	A594	M532	Y471	R405	K339	A277	A213	P152	Y90
H1047	K980	R851	S789	R724	G658	V596	D533	R472	H406	N340	E278	Y214	R154	Q91
T1048	E981	L852	R790	D725	P659	A597	S535	R473	R408	T341	G215	G215	P155	L94
L1049	P982	L853	K791	I726	A660	E598	P536	V474	R409	D342	E216	E156	G156	Y95
Q1050	R983	P854	V792	P727	S661	E599	K537	G476	L410	Q343	G282	L217	R157	A96
E1051	E984	V855	P793	H728	E662	D600	Q538	G477	S411	R345	R284	Q219	Y158	R97
M1052	G985	L818	G794	L729	N663	G601	V539	V478	G414	Y346	L285	G220	I159	L98
L1053	P986	D857	G795	S730	G664	E602	F540	V479	G415	G347	S286	L221	S161	Q99
T1054	I987	M858	E796	E731	P665	V603	S541	T480	P415	L348	G287	K222	I162	L100
L1055	V988	P859	G797	E731	L666	A604	V542	D481	G416	A349	R288	D223	I163	I101
K1056	V989	R735	G798	L734	A667	K605	N543	E482	G417	R350	T289	E224	I163	H102
S1057	G990	D736	I799	R736	L668	V606	T544	V483	L418	L351	L290	S225	P164	K103
D1058	Q991	R736	V800	D736	G669	D607	N545	V484	T419	A352	V226	P166	L165	D104
D1059	M992	Q801	V801	L737	Q670	G608	L546	Y485	R420	R353	R292	F227	P166	T105
I1060	F993	K671	R802	D738	G671	N609	I547	M486	G424	G354	F293	A228	K167	G106
E1061	G994	V672	T803	E739	P677	R610	P543	T487	G425	V355	G296	M229	R168	L107
G1062	L997	L673	V804	E740	L673	V612	F549	A488	F425	R356	E297	R230	G169	I108
L1063	Y998	G675	R805	G741	V674	V613	L550	T489	D426	P231	K297	E232	P170	K109
A1066	H999	V743	L806	V742	A675	R614	E551	E490	V427	R358	F298	E232	Y171	E110
Y1067	D1003	R744	R807	V743	L676	R615	H552	E491	R428	K359	K299	E233	D173	D111
A1068	K1004	R745	G809	E616	P678	E616	A555	D492	D429	D300	A234	L174	L174	E112
A1069	M1005	I745	D810	D617	F679	D617	N556	Y494	V430	E363	E301	E175	E175	V113
I1070	I1005	E748	P811	D680	V679	D680	N560	T495	H431	E364	V302	T236	V176	F114
I1071	S1009	V749	G812	G681	V681	V621	L559	I496	R432	D365	F303	R237	E177	L115
E1074	T1010	K750	V813	V682	V621	V621	M560	A497	T433	S366	L304	L238	E177	G116
D1075	G1011	P751	E814	N683	E622	E622	G561	Q498	H434	L367	P305	F239	P178	H117
V1076	P1012	G752	L815	P623	P623	P623	S562	A499	Y435	T388	T240	G150	P179	P119
P1077	Y1013	R879	G818	E685	E685	L625	M564	N500	G436	P369	L307	L241	Y181	T122
														E123



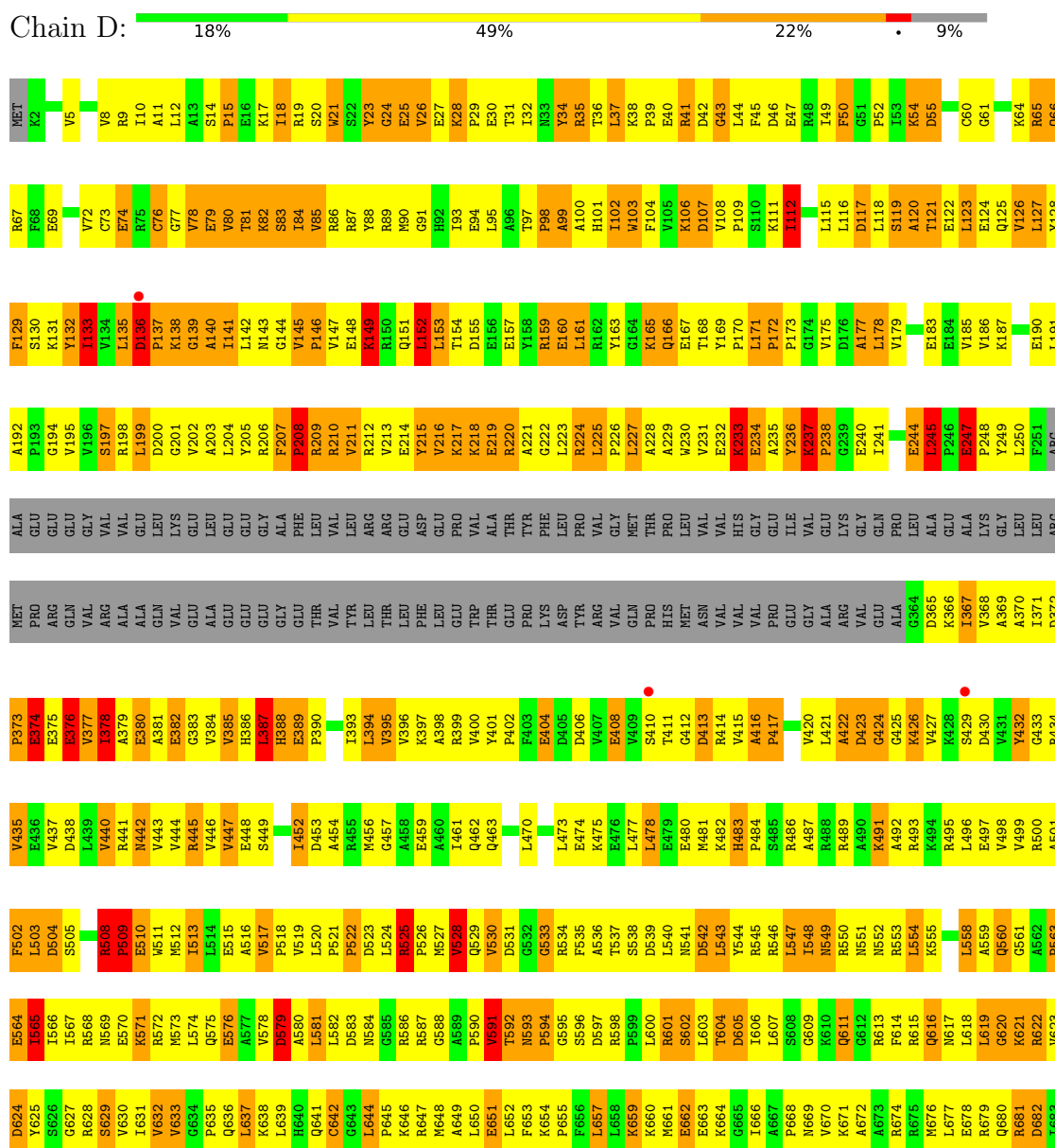
• Molecule 2: DNA-directed RNA polymerase beta chain

Chain M: 21% 57% 19%



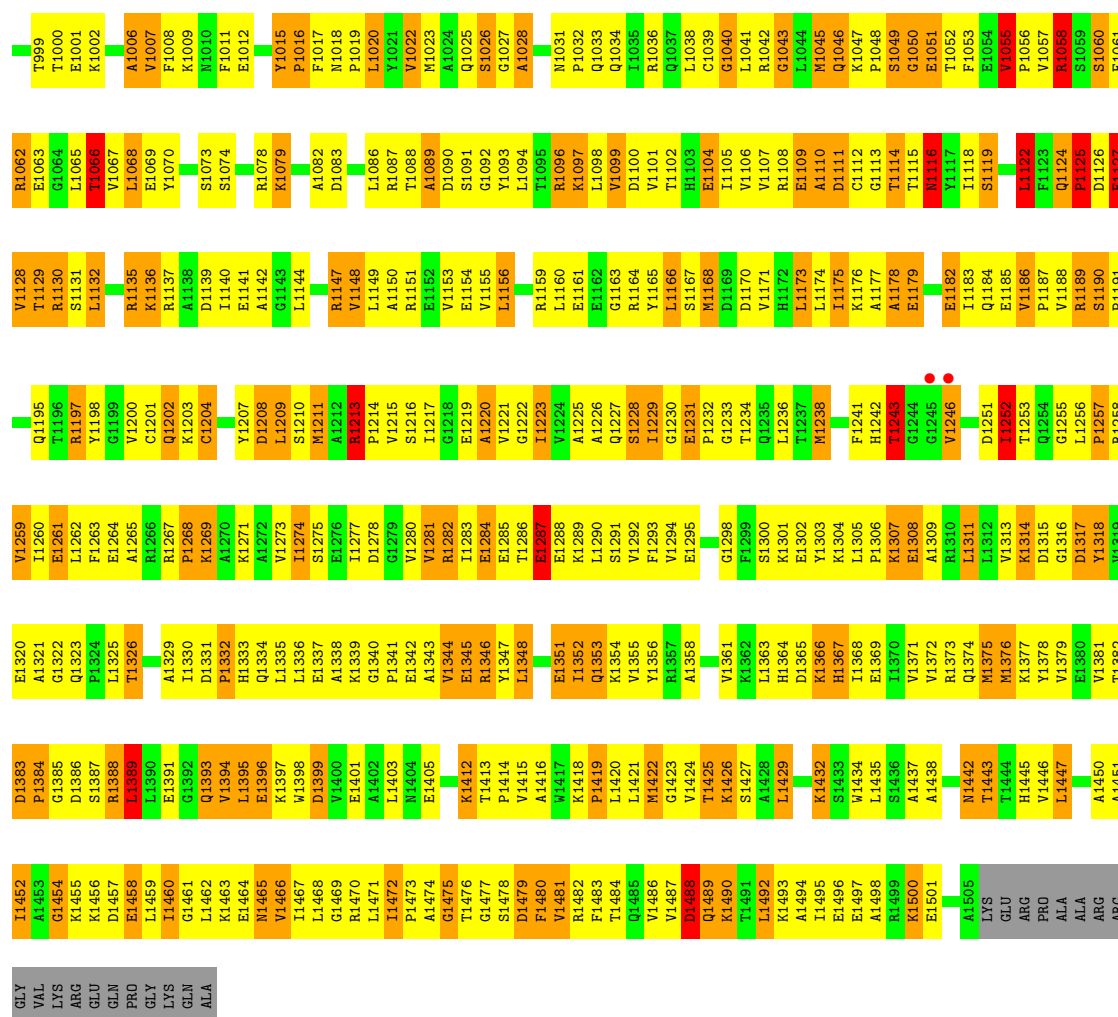


• Molecule 3: DNA-directed RNA polymerase beta' chain



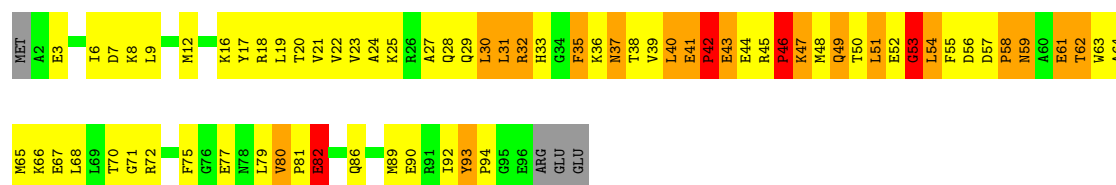


A933	B872	E811	A746	D682	R622	A559	V499	V435	P373	MET	ALA	E190	L127	R65	MET
L934	L873	A812	V747	I683	V623	Q660	R500	E436	E374	PRO	GLU	L191	Y128	Q66	K2
K936		A813		K684	D524	G561	A501	A437	E376	ARG	GLU	A192	F129	Q67	K3
Y937	S876	A814	P750	D685	G625	A562	F502	D438	E375	GLN	GLU	P193	S130	F68	E4
G938	B877	A815	L751	G686	S626	P563	L503	L439	V377	VAL	GLY	G194	K131	E69	V5
F939	G878	H816	S752	G687	G627	E564	D504	V440	I378	ARG	VAL	V195	Y132	G70	R6
T940	R879	E817	S753		R628	I565	S505	R441	A379	ALA	VAL	V196	I183	K71	K7
	I880	R318	F754	A890	S629	I566	G506	I442	E380	ALA	GLU	S197	V134	V72	V8
F941	L881	G819	A755	L691	V630	I567	N507	V443	A381	ALA	GLN	R198	L135	C73	R9
S942	F882	E820	Q756	G692	I631	R568	R508	V444	E382	VAL	LYS	L199	D136	E74	A11
T943	F883	G693	A757	G693	V632	N569	P509	R445	G383	GLU	GLU	D200	P137	R75	A12
S944	R884	A822	E758	V694	V633	E570	E510	V446	V384	ALA	LEU	G201	K138	C76	L13
G945	L885	L823	A759	G695	G634	G671	V511	V447	V385	GLU	GLU	V202	G139	G77	A13
	R886	N824	R760		P635	R572	N512	E448	H386	GLU	GLU	A203	A140	V78	S14
I947	A887	A825	I761	K698	Q636	M573	L513	S449	L387	GLY	GLY	L204	I141	E79	P15
T948	E888	P826	Q762	V699	L637	L574	L514	V450	H388	GLY	ALA	L205	L142	V80	E16
I949	A889	I927	M763	V700	K638	Q575	E515	D451	E389	GLU	PHE	R206	N143	T81	K17
G950	V890	K828	L764	L701	L439	E576	A516	I452	P390	THR	LEU	F207	G144	K82	I18
I951	E891	V829	S765	L702	H640	A577	V517	D453	A391	VAL	VAL	P208	V145	S83	R19
D952	B892	A830	A766	N703	Q641	V678	P518	A454		TYR	LEU	R209	P146	I84	S22
	E893	G831	R767	R704	C642	D579	P519	R455	L394	LEU	ARG	R210	V147	R85	Y23
A954	K894	R832	N768	A705	G643		L520	A456	V395	THR	ARG	V211	E148	R86	G24
V955	V895	E833	L769	P706	L644	R587	P521		V396	LEU	GLU	R212	K149	R87	
I956	A896	T834	L770	L707	K645	D583	P522	I461	K397	PHE	ASP	V213	R150	Y88	E27
P957	V897	S771	S771	L708	R646	N584	D523	Q462	A398	LEU	GLU	E214	Q151	M90	K28
E958	E898	V836	P772	H709	R647	G585	L524	Q463	R399	GLU	PRO	Y215	L152	G91	P29
	L899	G837		R710	M648	R586	R525	L464	V400	TRP	VAL	V216	L153	H92	E30
K960	R900	R838	E776	L711	G649	N593	P526	L465	Y401	THR	ALA	K217	T154	I93	T31
G961	Q901	L839	P777	G712	L850	G588	N527	K466	P402	GLU	THR	R218	D155		
Y962	L902	L778	L713	G713	E651	V528	V528	E467	F403	PRO	TYR	E219		E94	I32
Y963	D903	Y841	A779	Q714	L652	P590	Q529	L468	E404	LYS	PHE	R220	Y158	L95	N33
L964	I904	V842	K780	A715	F653	V591	V530	D469	P405	LEU	LEU	A221		A96	Y34
E965	P905	F843	F781	F716	K654	T592	D531	L470	D406	TYR	PRO	G222	L161	T97	R35
E966	Q906	A844	S782	Q717	P655	N593	G532	E472	V407	ARG	VAL	L223	R162	P98	T36
A967	E907	N845	R783	P718	F656	P594	G533	A471	E408	VAL	GLY	R224		A99	L37
D968	K908	P846	D784	L719	L657	G595	R534	L473	V409	GLN	MET	L225	K165	A100	K38
R969	N909	D847	I785	L720	L658	S596	F535	E474	S410	PRO	THR	P226	Q166	H101	P39
K970	S910	E848	I786	V721	K659	D597	A536	K475	T411	HIS	PRO	L227	E167	I102	E40
L971	L911	A849	L787	E722	K660	R598	T537	E476	G412	MET	LEU	A228	T168	W103	R41
L972	K912	P599			M661	P599	S538	L477	D413	ASN	VAL	A229	Y169	F104	D42
	D913	L851			E662	L600	D539	L478	R414	VAL	VAL	W230	P170	K106	G43
E975	L914	A852	I726	Q727	E663	R601	L540		V415	VAL	HIS	V231	L171	D107	L44
Q976	V915	V853	L728	L728	K664	S602	N541	M481	A416	VAL	GLY	E232	P172	V108	F45
A977	Y916	L854	T793	H729	G665	L603	D542	K482	P417	VAL	ILE	K233	P173	P109	D46
Y978	Q917	H855	Q794	P730	I666	D605	L543	H483	G416	PRO	GLU	E234	G174		E47
E979	A918	G856	V795	L731	A667	R546	T544	P484		GLY	VAL		V175		R48
	F919	I857	R796	V732	P668	L606	R546	S485	L421	ALA	GLU	P238	D176	I112	I49
	V858	G797	K798	C733	N669		L547	A487	D423	ARG	LYS	G239	L178	L115	G51
	E798	K799	K799	E734	V670	G609	T548	R488	G426	VAL	GLN	E240	V179	L116	P52
L983	R921	L860	G800	A735	K671	Q610	N549	R489	G426	ALA	PRO	I241	K180	D117	I53
D985	G923	Q861	F736	N737	A672	Q612	R550	A490	K426	LEU			D181	L118	K54
R986	M924	R862	G801	G737	R674	R613	N551	K491	V427	ALA	ALA	L245	E183	S119	D55
E987	E925	V863	A738	A738	G675		N552	A492	K428	GLU	GLU	P246	G182	A120	
R988	K926	V864	V864	D739	R676	Q616	R553	R493	S429	ALA	ALA	E247	E184	T121	
D990	T927	T865	L804	F740	M676	Q617	R554	K494	D430	LYS	LYS	P248	V185	E122	C58
Q991	A928	F806	N617	D741	L677	N617	L554	K494	P430	GLY	GLY	P249	V186	L123	A59
I992	R929	A807	G742	G742	E578	L613	R555	R495	V431	THR	THR	Y249	K187	L124	
	L930	M869	L743	L743	R679	L619	K556	L496	G432	LEU	LEU	L250	G188	E124	K62
	L931	G870	Q744	Q744	Q680	G620	L557	E497	R433	LEU	LEU	F251	Q125	Q125	Y63
L995	W996	K871	E810	M745	R681	K621	L558	V498	R434	ARG	ARG		Q189	V126	K64



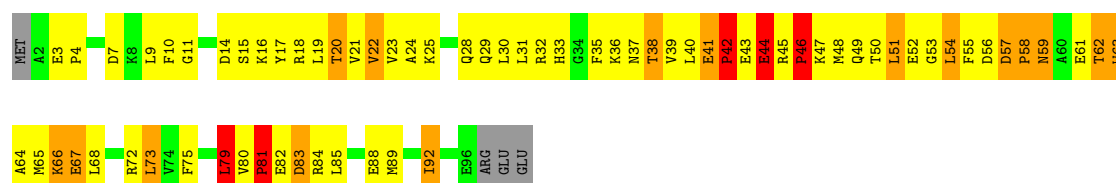
• Molecule 4: RNA polymerase omega chain

Chain E: 24% 49% 18% . .

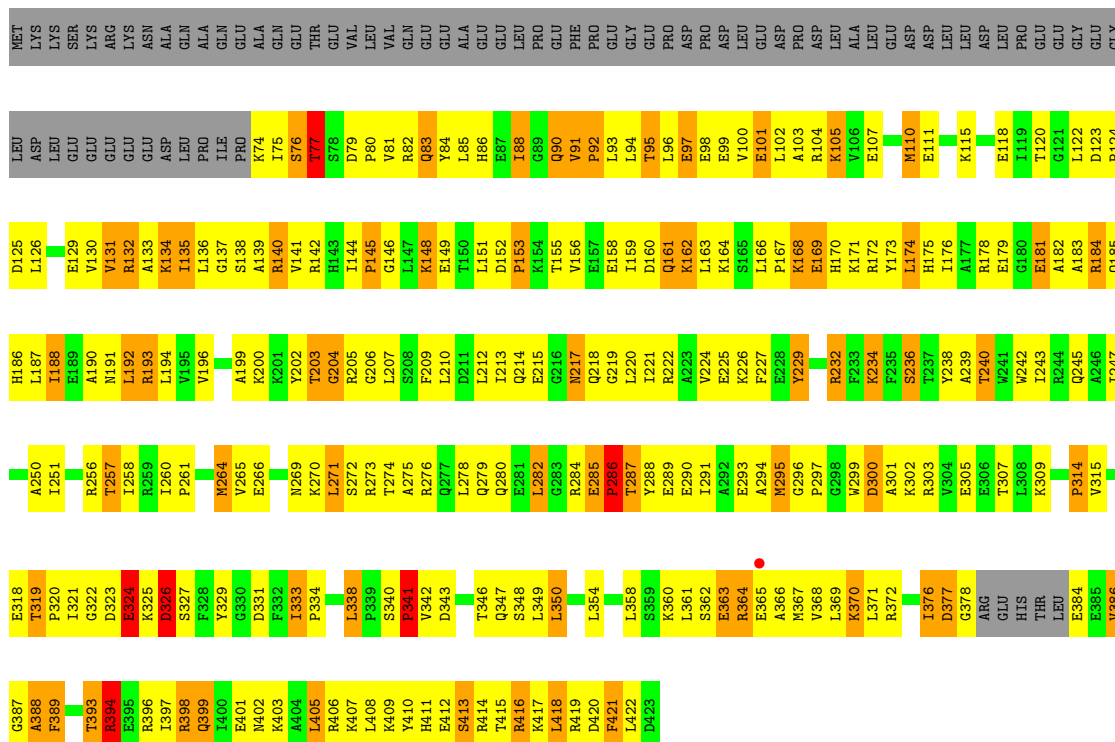
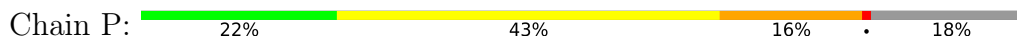


• Molecule 4: RNA polymerase omega chain

Chain O: 25% 49% 16% 5% .



Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	236.15Å 236.15Å 249.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	84.1 (30.00-3.30) 47.3 (30.00-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.320 0.277 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	97.4	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.499 for h,-h-k,-l 0.064 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	53962	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 6.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.58	0/1838	1.19	20/2498 (0.8%)
1	B	0.42	0/1838	1.02	8/2498 (0.3%)
1	K	0.61	0/1838	1.17	18/2498 (0.7%)
1	L	0.49	0/1838	1.08	18/2498 (0.7%)
2	C	0.57	0/8997	1.27	130/12164 (1.1%)
2	M	0.58	0/8997	1.25	123/12164 (1.0%)
3	D	0.60	2/11165 (0.0%)	1.29	156/15088 (1.0%)
3	N	0.58	0/11165	1.29	170/15088 (1.1%)
4	E	0.52	0/783	1.31	14/1054 (1.3%)
4	O	0.51	0/783	1.35	13/1054 (1.2%)
5	F	0.49	1/2836 (0.0%)	1.16	39/3812 (1.0%)
5	P	0.51	0/2836	1.17	35/3812 (0.9%)
All	All	0.57	3/54914 (0.0%)	1.25	744/74228 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
3	N	0	3
5	F	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1186	VAL	CA-CB	-5.92	1.50	1.54
5	F	313	GLU	C-N	5.66	1.41	1.33
3	D	1255	GLY	C-N	-5.35	1.26	1.33

The worst 5 of 744 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1209	LEU	N-CA-C	-18.83	83.67	108.34
2	C	728	HIS	N-CA-C	18.52	131.58	111.03
3	N	207	PHE	CA-C-N	16.12	139.98	119.84
3	N	207	PHE	C-N-CA	16.12	139.98	119.84
2	M	728	HIS	N-CA-C	14.48	131.69	113.88

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	132	TYR	Sidechain
5	F	84	TYR	Sidechain
3	N	1015	TYR	Sidechain
3	N	1318	TYR	Sidechain
3	N	132	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	261	0
1	B	1806	0	1861	197	0
1	K	1806	0	1861	202	0
1	L	1806	0	1861	215	0
2	C	8829	0	8933	1212	0
2	M	8829	0	8933	1265	0
3	D	10975	0	11211	1833	0
3	N	10975	0	11210	1775	0
4	E	769	0	775	96	0
4	O	769	0	775	92	0
5	F	2793	0	2873	316	0
5	P	2793	0	2873	380	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	53962	0	55027	7240	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 66.

The worst 5 of 7240 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)
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.21	1.20
2:C:1016:ILE:HD13	2:C:1016:ILE:H	1.06	1.16
3:D:907:GLU:HG2	3:D:1027:GLY:H	1.02	1.16
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.22	1.15
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.27	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%)	167 (74%)	39 (17%)	21 (9%)	0	3
1	B	227/315 (72%)	177 (78%)	37 (16%)	13 (6%)	1	9
1	K	227/315 (72%)	161 (71%)	39 (17%)	27 (12%)	0	1
1	L	227/315 (72%)	166 (73%)	44 (19%)	17 (8%)	1	6
2	C	1117/1119 (100%)	781 (70%)	226 (20%)	110 (10%)	0	3
2	M	1117/1119 (100%)	769 (69%)	215 (19%)	133 (12%)	0	1
3	D	1388/1524 (91%)	941 (68%)	293 (21%)	154 (11%)	0	2
3	N	1388/1524 (91%)	907 (65%)	332 (24%)	149 (11%)	0	2
4	E	93/99 (94%)	67 (72%)	17 (18%)	9 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	93/99 (94%)	59 (63%)	20 (22%)	14 (15%)	0	1
5	F	341/423 (81%)	241 (71%)	67 (20%)	33 (10%)	0	3
5	P	341/423 (81%)	249 (73%)	57 (17%)	35 (10%)	0	2
All	All	6786/7590 (89%)	4685 (69%)	1386 (20%)	715 (10%)	0	2

5 of 715 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	B	3	ASP
1	B	118	ALA
1	B	160	ASP
2	C	7	GLY

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%)	176 (87%)	26 (13%)	4	17
1	B	202/273 (74%)	180 (89%)	22 (11%)	6	23
1	K	202/273 (74%)	170 (84%)	32 (16%)	2	12
1	L	202/273 (74%)	186 (92%)	16 (8%)	11	36
2	C	941/941 (100%)	802 (85%)	139 (15%)	3	13
2	M	941/941 (100%)	802 (85%)	139 (15%)	3	13
3	D	1170/1279 (92%)	972 (83%)	198 (17%)	2	10
3	N	1170/1279 (92%)	974 (83%)	196 (17%)	2	11
4	E	83/87 (95%)	71 (86%)	12 (14%)	3	14
4	O	83/87 (95%)	72 (87%)	11 (13%)	4	17
5	F	300/370 (81%)	257 (86%)	43 (14%)	3	14
5	P	300/370 (81%)	269 (90%)	31 (10%)	7	25
All	All	5796/6446 (90%)	4931 (85%)	865 (15%)	3	13

5 of 865 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	186	LEU
2	M	686	ASP
3	N	1348	LEU
1	L	26	GLU
1	K	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	431	HIS
3	N	549	ASN
2	M	639	GLN
2	M	1018	GLN
3	N	748	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	229/315 (72%)	-1.29	0 100 100	41, 64, 87, 113	0
1	B	229/315 (72%)	-1.07	1 (0%) 88 79	47, 121, 143, 143	0
1	K	229/315 (72%)	-1.25	1 (0%) 88 79	28, 63, 88, 111	0
1	L	229/315 (72%)	-1.27	0 100 100	41, 79, 99, 116	0
2	C	1119/1119 (100%)	-1.22	2 (0%) 91 86	12, 67, 133, 143	0
2	M	1119/1119 (100%)	-1.19	3 (0%) 90 82	6, 71, 122, 133	0
3	D	1392/1524 (91%)	-1.21	7 (0%) 87 76	7, 60, 125, 143	0
3	N	1392/1524 (91%)	-1.17	9 (0%) 85 73	5, 65, 134, 143	0
4	E	95/99 (95%)	-1.21	0 100 100	54, 84, 100, 106	0
4	O	95/99 (95%)	-1.25	0 100 100	46, 86, 117, 121	0
5	F	345/423 (81%)	-1.21	0 100 100	48, 81, 113, 121	0
5	P	345/423 (81%)	-1.26	1 (0%) 90 82	47, 73, 110, 123	0
All	All	6818/7590 (89%)	-1.20	24 (0%) 88 79	5, 70, 129, 143	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1247	ALA	6.9
3	N	224	ARG	4.4
3	N	412	GLY	3.8
3	N	1245	GLY	3.3
2	C	180	GLY	3.3

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	D	1527	1/1	0.99	0.02	19,19,19,19	0
6	ZN	D	1526	1/1	1.00	0.01	78,78,78,78	0
6	ZN	N	1525	1/1	1.00	0.02	108,108,108,108	0
6	ZN	N	1526	1/1	1.00	0.01	72,72,72,72	0
6	ZN	D	1525	1/1	1.00	0.01	107,107,107,107	0
7	MG	N	1527	1/1	1.00	0.02	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.