



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 03:06 pm GMT

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

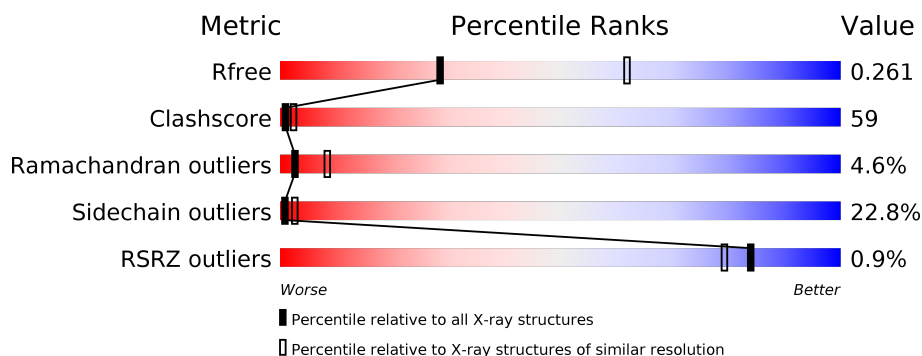
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>23%51%17%•9%</div></div>
3	N	1524	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>24%51%15%•9%</div></div>
4	E	99	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>22%52%20%••</div></div>
4	O	99	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>28%48%19%•</div></div>
5	F	423	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>19%47%14%•18%</div></div>
5	P	423	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>22%49%10%18%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58679 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
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

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

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

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

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

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

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

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

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

- Molecule 8 is water.

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

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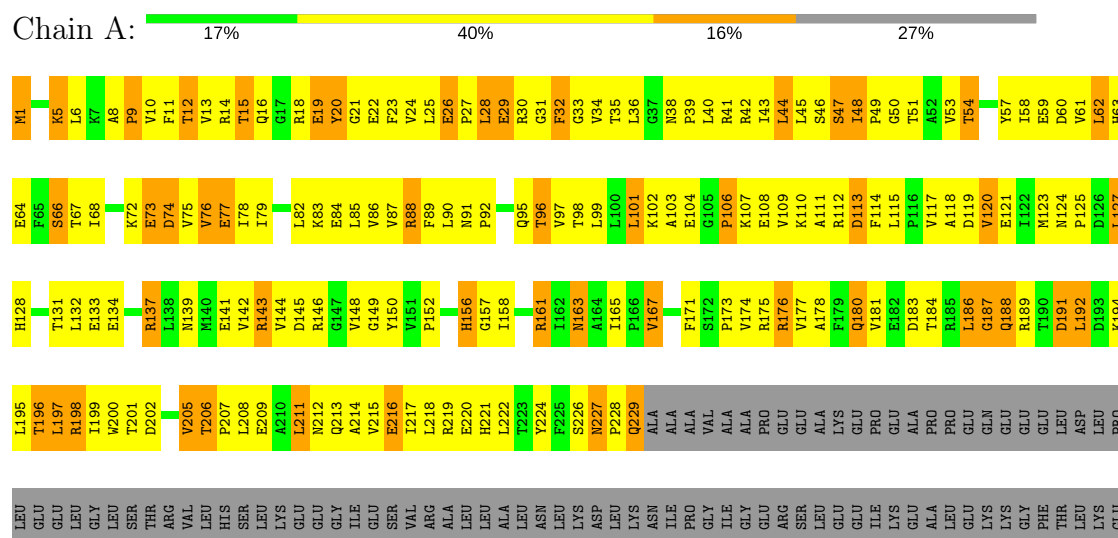
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	1038	Total 1038	O 1038	0	0
8	O	78	Total 78	O 78	0	0
8	P	267	Total 267	O 267	0	0

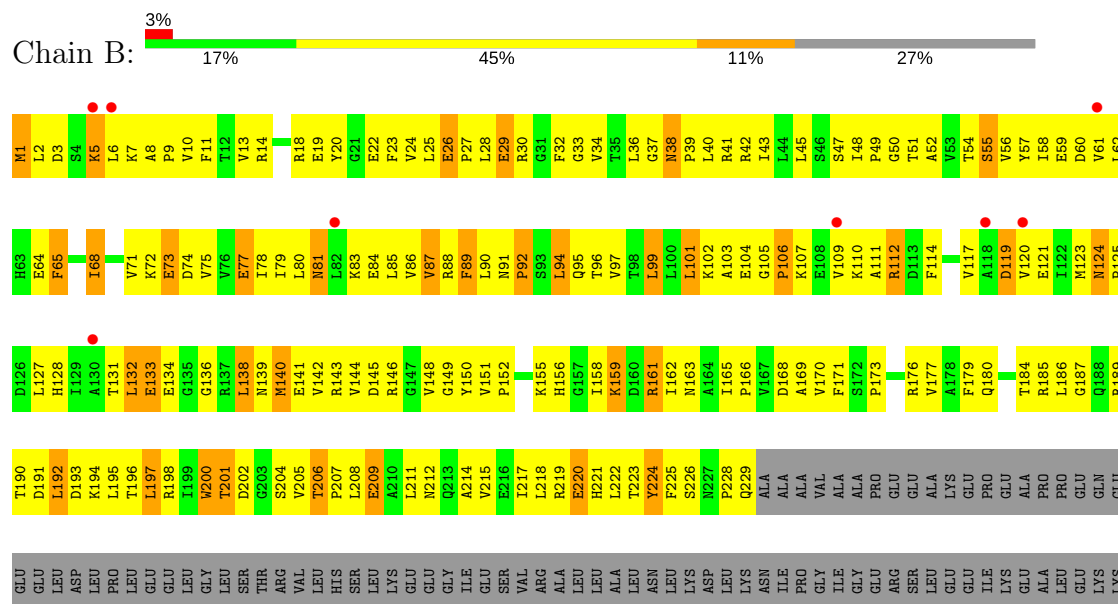
3 Residue-property plots

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

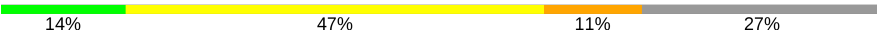


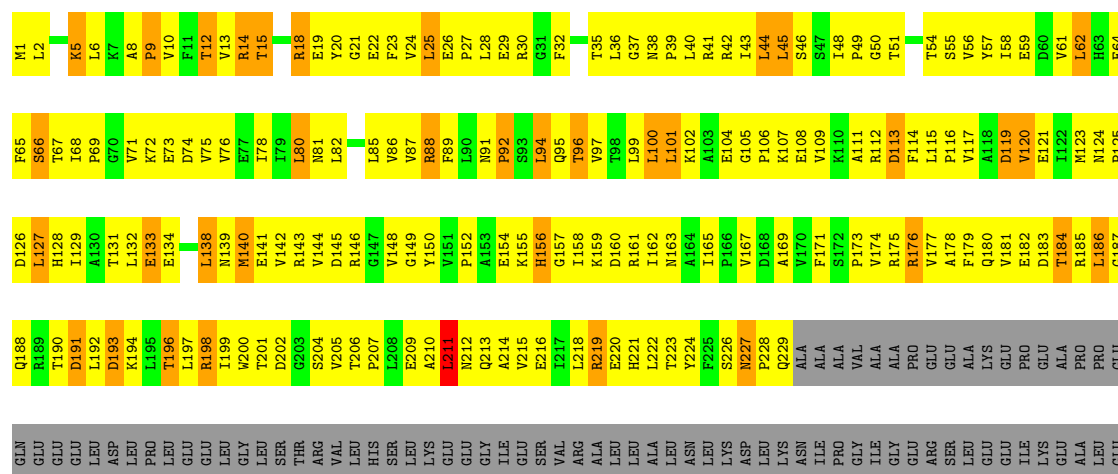
• Molecule 1: DNA-directed RNA polymerase alpha chain



GLY
PHE
THR
LEU
LYS
GLU


• Molecule 1: DNA-directed RNA polymerase alpha chain

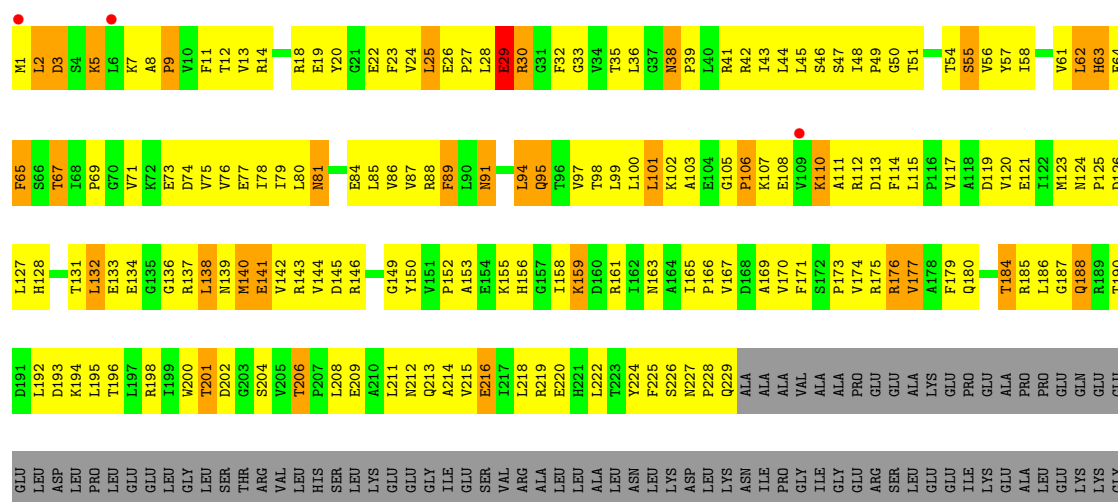
Chain K: 



LYS
LYS
GLY
PHE
THR
LEU
LYS
GLU

• Molecule 1: DNA-directed RNA polymerase alpha chain

Chain L: 

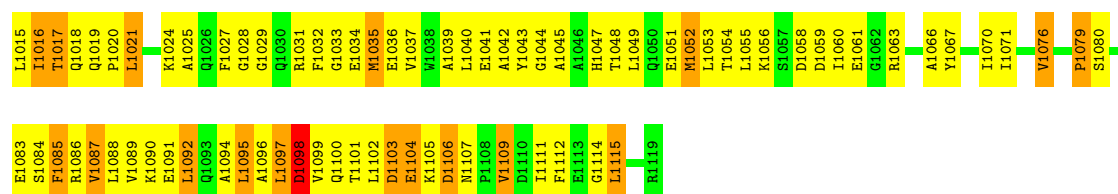


PHE
THR
LEU
LYS
GLU

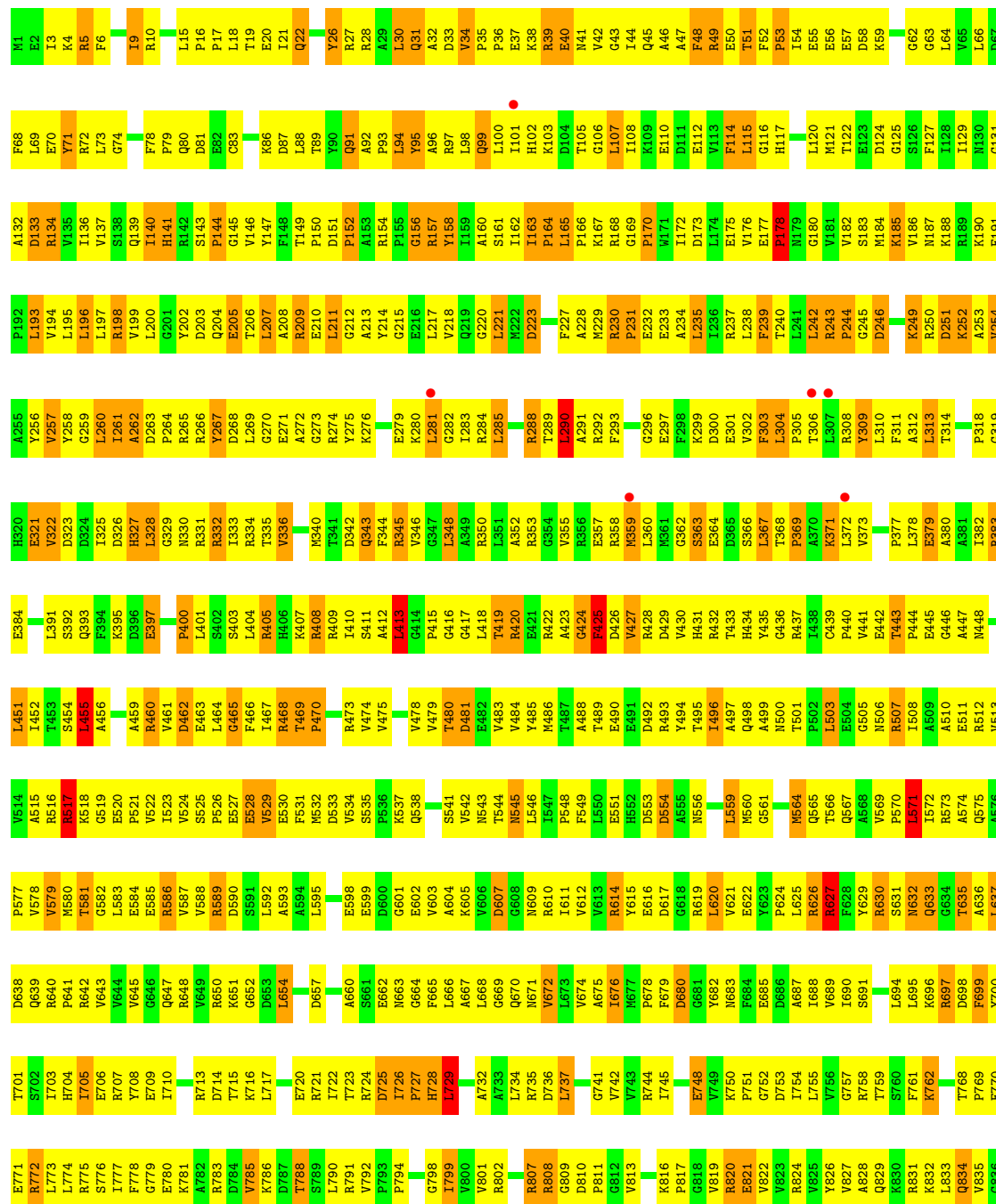
• Molecule 2: DNA-directed RNA polymerase beta chain

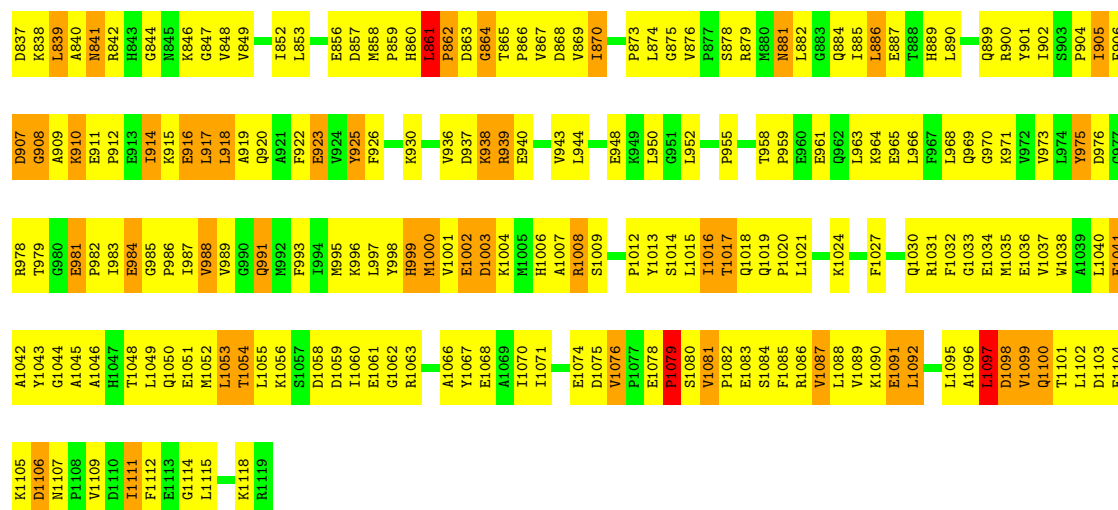
Chain C: 



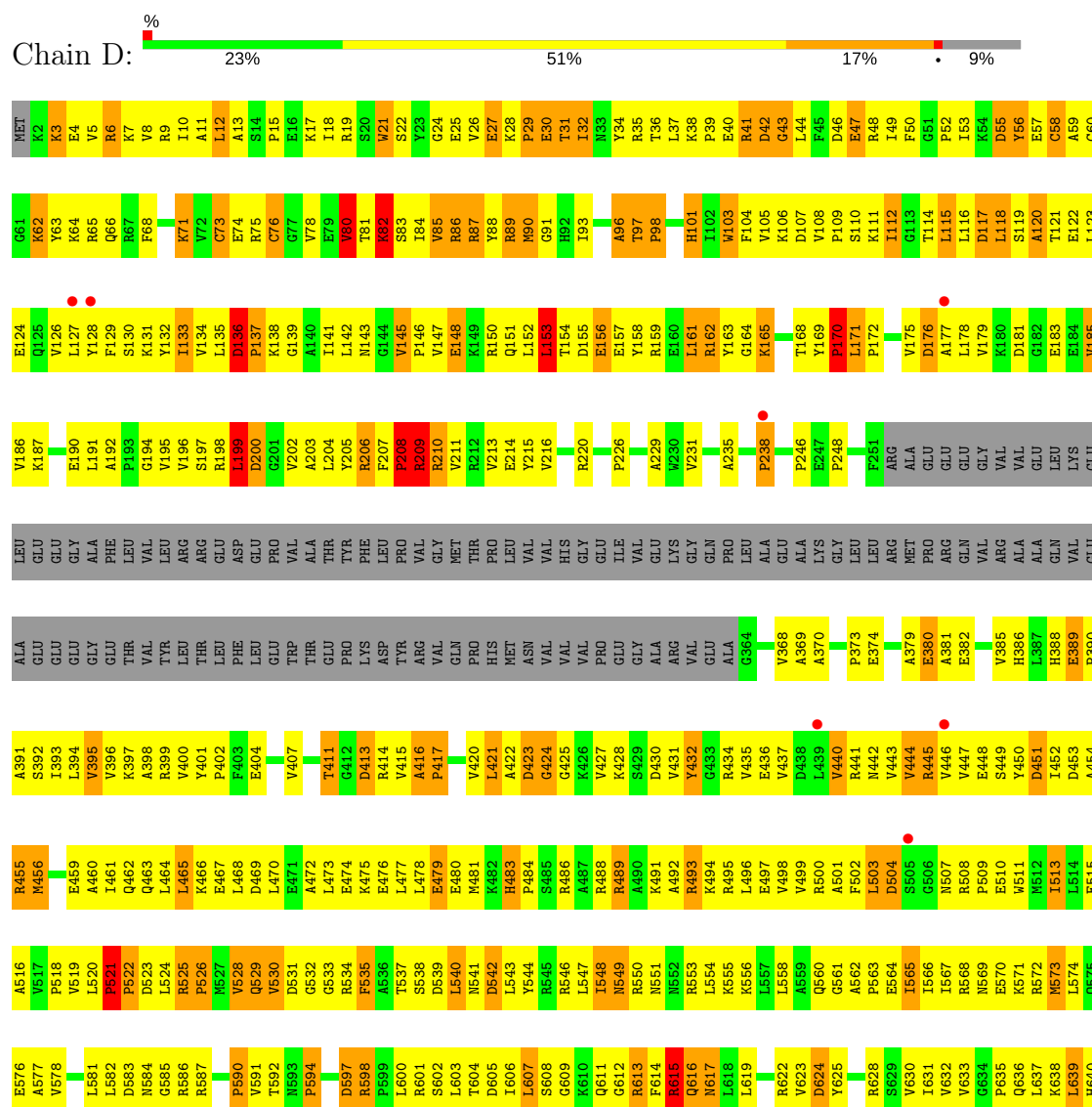


• Molecule 2: DNA-directed RNA polymerase beta chain





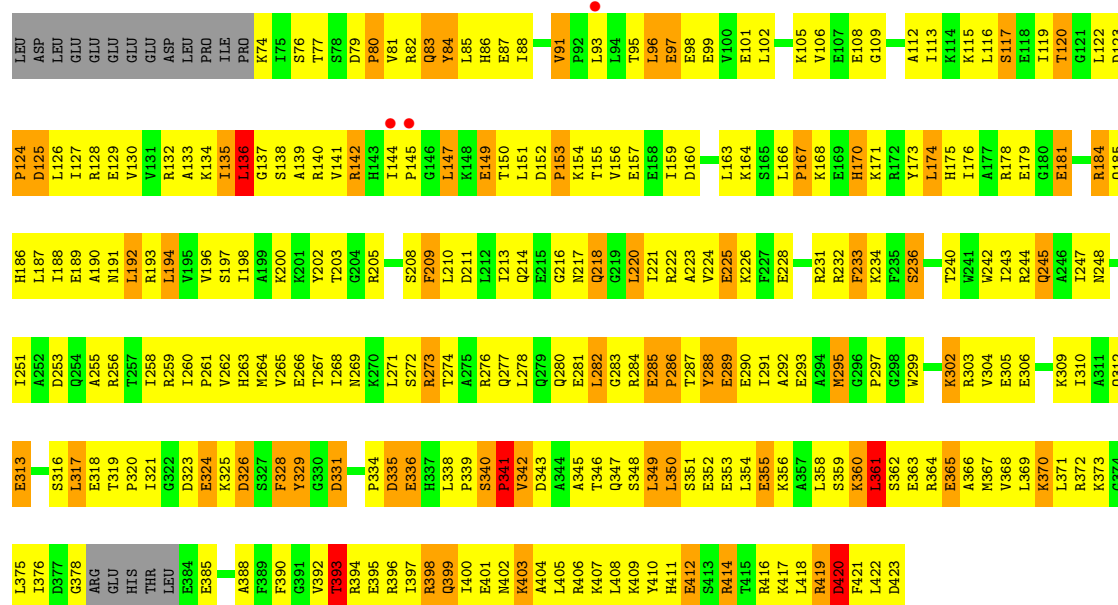
• Molecule 3: DNA-directed RNA polymerase beta' chain



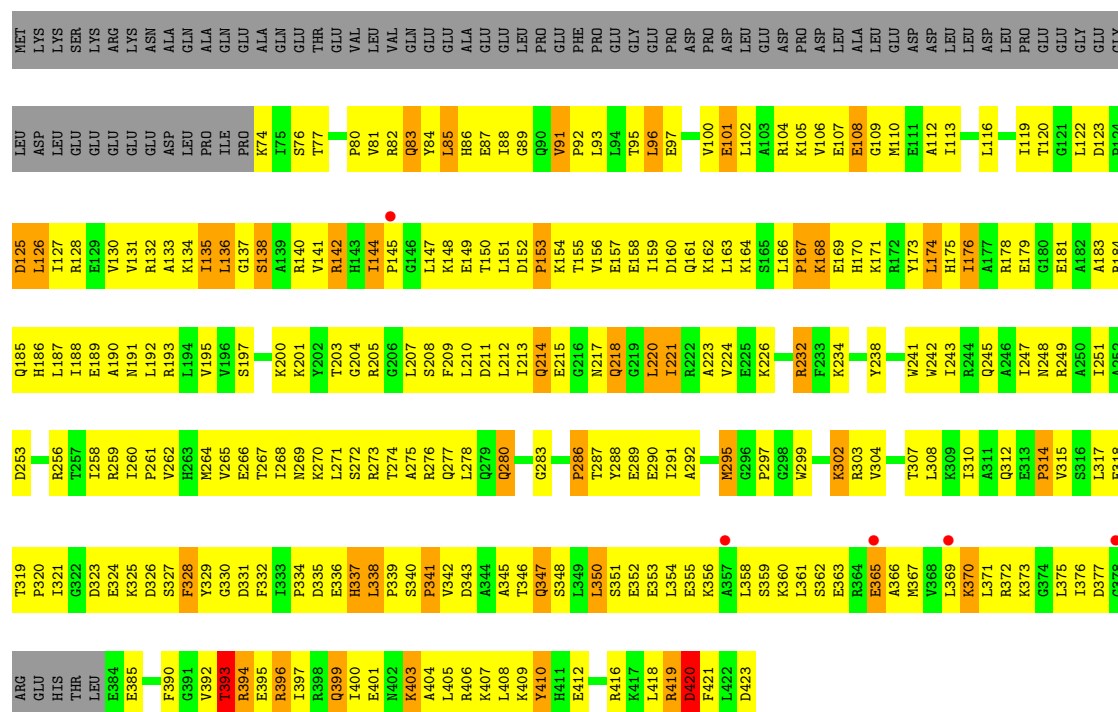
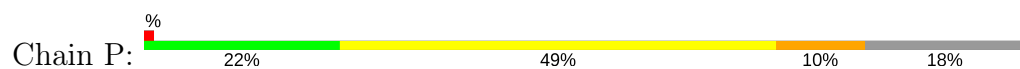
- Molecule 3: DNA-directed RNA polymerase beta' chain



M1023	I951	R884	W821	A755	A690	S629	I567	G506	R445	E382	GLN	GLY	G182	E122	G61
S1026	D952	I885	A822	Q756	L691	V630	R568	N507	V446	E382	VAL	GLY	E183	E122	K62
G1027	D953	R886	L823	Q756	E692	I631	N569	R508	V447	V385	ARG	VAL	E184	E124	Y63
R1029	A955	A887	N824	A759	E693	V632	E570	P509	E448	H388	ALA	VAL	V185	Q125	K64
G1030	I956	A889	A825	R760	V694	V633	K571	E510	S449	H388	ALA	GLU	V186	V126	R65
M1031	P957	V890	P826	I761	I695	G634	R572	N511	Y450	E389	GLN	LEU	K187	L127	Q66
E958	K828	E891	L827	Q762	H696	P635	M573	M512	D451	P390	VAL	LYS	G188	Y128	R67
E959	R828	E892	K828	M763	G697	Q636	L574	E513	D452	A391	GLU	GLU	L191	F129	F68
K960	W829	D892	W829	L764	G698	L637	Q575	E515	D453	S392	ALA	LEU	E192	S130	E69
K961	A830	E893	A830	Q765	E699	K638	E576	E515	A454	I393	GLU	GLU	I393	K131	G70
Q1034	K961	K894	C831	A766	V700	L639	A577	A516	R455	L394	GLU	GLY	F193	Y132	K71
I1035	Q962	V895	R832	H767	L701	H640	V578	W517	M456	V395	GLU	GLY	G194	Y133	V72
R1036	Q963	A896	E833	Q641	L702	Q641	D579	F518	M456	V396	GLY	ALA	V195	I133	K72
Q1037	L864	R897	T834	L770	W703	C642	A580	V519	E459	K397	GLY	ALA	V196	C73	C73
E965	E965	E898	W836	Q774	R704	G643	L581	L520	A460	A398	GLU	PHE	G196	E74	E74
C1038	E968	R899	S835	S774	L705	L644	L582	E520	I461	R299	VAL	VAL	R198	D136	R75
G1040	Q968	I900	C837	G775	P706	P645	D583	P522	Q462	V400	TYR	LEU	G199	K138	C76
L1041	R969	Q901	R838	E776	L707	K646	N584	D523	Q463	Y401	LEU	ARG	D200	G139	E79
R1042	K970	L902	L839	P777	L708	R647	G585	L524	L464	P402	THR	ARG	G201	E140	E79
M1045	L971	Q906	K840	L778	W709	R648	R586	R525	L465	F403	LEU	GLU	V202	I141	I141
Q1046	L972	K906	Y841	A779	R710	A649	R587	P526	K466	E404	PHE	ASP	A203	L142	T81
K1047	Q973	K907	W842	K780	L711	L650	G588	M527	K467	D405	LEU	LEU	L204	N143	K82
T974	E974	K908	F843	P781	G712	E651	A589	V528	L468	D406	GLU	PRO	Y205	G144	S83
E975	Q975	K909	A844	S782	W712	E651	P590	Q529	D469	V407	THR	VAL	R206	Y145	I84
Q976	S910	R845	R845	R783	A715	K654	V591	W530	L470	E408	THR	ALA	F207	P146	V85
E1050	L911	P846	P846	D784	F716	P655	T592	D531	E471	T411	PRO	THR	P208	Y147	R86
G1051	E912	K912	D847	I785	Q717	F656	N593	G532	A472	T411	GLU	TYR	R209	E148	R87
F1052	D913	E848	E848	I786	P718	L657	P594	G533	L473	G412	LYS	PHE	R210	K149	Y88
T1053	L914	A849	A849	L787	W719	L658	G595	R534	E474	D413	ASP	LEU	V211	R150	R89
Y915	L850	L850	L850	G788	L720	K659	S596	F535	K475	R414	TYR	PRO	R212	Q151	M90
P1056	Q917	L851	L851	L789	W721	K660	D597	A536	E476	V415	ARG	VAL	V213	L152	
E957	Q917	A852	A852	I792	E722	K661	R598	S538	L477	P417	GLN	GLY	E214	L153	
R988	G918	W853	W853	T793	G723	E662	P599	W537	L478	G418	PRO	MET	V215	T154	E94
Y989	F919	R919	R919	K794	Q724	E663	L600	D539	E479	G418	PRO	THR	V216	D155	L95
L920	R920	S725	S725	Q794	Q724	E663	L600	D539	E479	G418	PRO	THR	V216	D155	L95
S1059	R920	S725	S725	Q794	Q724	E663	L600	D539	E479	G418	PRO	THR	V216	D155	L95
E1060	I992	R921	W858	R795	T726	G665	S602	D542	E480	D419	HIS	PRO	K217	E156	A96
F1061	L993	R859	R859	R796	Q727	L666	S602	D542	E480	D419	HIS	PRO	K217	E156	A96
R1062	Q994	L860	L860	K797	L728	A667	T604	L543	K482	V420	ASN	VAL	R220	E157	T97
L995	K926	Q861	Q861	E798	H729	P668	D605	Y544	H483	L421	VAL	VAL	A221	Y158	P98
W996	T927	D862	W863	K799	P730	N669	L606	R546	P484	A422	VAL	HIS	A221	R159	A99
G1064	Q966	T927	D862	K799	P730	N669	L606	R546	P484	A422	VAL	HIS	A221	R159	A99
L1065	T997	A928	W863	K800	L731	V670	L607	L547	R486	G424	VAL	GLY	L223	A100	H101
T1066	E998	R929	W864	G801	W732	K671	S608	L548	A487	C426	PRO	GLU	V231	I102	
V1067	T999	L930	T865	A802	C733	A672	G609	N549	R488	K426	GLU	ILE	V231	Y163	F103
L1068	T1000	L931	W866	G803	W734	A673	K610	R550	R488	V427	GLY	VAL	P238	G164	F104
E1069	E1001	D932	R867	L804	A735	R674	Q611	R550	R489	K428	ALA	GLU	P238	K165	V105
Y1070	K1002	A933	W868	E805	F736	R675	G612	N552	A490	S429	ARG	LYS	G239	Q166	K106
F1071	V1003	L934	K871	F806	N737	M676	R613	R553	K491	D430	VAL	GLY	E240	E167	D107
I1072	Q1004	K935	L871	A807	A738	L677	F614	L554	A492	V431	GLU	GLN	L241	T168	V108
S1073	Q1005	Y936	R872	T808	W739	E678	R615	K555	R493	C432	ALA	PRO	L242	Y169	P109
W1074	A1006	Y937	L873	P809	D739	R679	Q616	K556	R495	C433	ALA	ALA	A243	P170	S110
H1075	V1007	T940	E874	E810	D743	Q680	M617	K556	L496	R434	ALA	ALA	E244	L171	K111
G1076	F1008	T940	T875	E811	Q744	R681	K621	L558	E497	V435	ARG	GLY	L245	P172	I112
A1077	K1009	T944	S876	A812	W745	D682	R622	A559	V498	E436	LYS	LYS	P246	P173	G113
R1078	N1010	T944	P877	L813	L683	L683	R622	Q560	V499	D438	ALA	GLY	E247	G174	T114
K1079	G945	S945	K878	A814	W749	G684	W623	G560	R500	L439	GLY	GLY	P248	V175	L115
G1080	N1018	G946	R879	A814	W749	G684	W623	G561	R500	L439	LEU	LEU	F251	D176	L116
P1019	I947	G946	R879	A814	W749	G684	W623	G561	R500	L439	LEU	LEU	F251	D176	L116
A1085	L1020	T948	L880	E817	L751	E686	W625	A562	F502	V440	ARG	ARG	ALA	L178	L118
R1086	V1022	G950	F882	R818	S752	W687	W626	E564	L503	N442	MET	MET	ALA	V179	S119
			A883	E820	F754	D689	R628	I566	S505	V444	PRO	PRO	GLU	K180	A120
															T121



• Molecule 5: RNA polymerase sigma factor rpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.80) 92.0 (24.96-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.268 0.227 , 0.261	Depositor DCC
R_{free} test set	21166 reflections (5.78%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.068 for h,-h-k,-l 0.068 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	58679	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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: ZN, MG

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	N	0	1

All (1) bond length outliers are listed below:

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

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

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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	132	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	216	0
1	B	1806	0	1861	199	0
1	K	1806	0	1861	208	0
1	L	1806	0	1861	206	0
2	C	8829	0	8933	1184	0
2	M	8829	0	8933	1106	0
3	D	10797	0	10873	1450	0
3	N	10797	0	10873	1345	0
4	E	769	0	775	97	0
4	O	769	0	775	108	0
5	F	2771	0	2844	336	0
5	P	2771	0	2844	342	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	1	0	0	0	0
7	N	1	0	0	0	0
8	A	191	0	0	37	0
8	B	181	0	0	34	0
8	C	767	0	0	174	0
8	D	1100	0	0	234	0
8	E	93	0	0	14	0
8	F	333	0	0	58	0

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

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 59.

The worst 5 of 6401 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:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.28	1.11
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.12	1.08
2:C:135:VAL:HG11	2:C:407:LYS:HA	1.36	1.04
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.14	1.04
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.20	1.04

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%)	202 (89%)	21 (9%)	4 (2%)	9	30
1	B	227/315 (72%)	202 (89%)	21 (9%)	4 (2%)	9	30
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	9	30
1	L	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	9	30
2	C	1117/1119 (100%)	917 (82%)	150 (13%)	50 (4%)	3	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	1117/1119 (100%)	907 (81%)	159 (14%)	51 (5%)	2	8
3	D	1388/1524 (91%)	1123 (81%)	191 (14%)	74 (5%)	2	6
3	N	1388/1524 (91%)	1110 (80%)	195 (14%)	83 (6%)	2	4
4	E	93/99 (94%)	74 (80%)	16 (17%)	3 (3%)	4	15
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	4	15
5	F	341/423 (81%)	283 (83%)	42 (12%)	16 (5%)	2	8
5	P	341/423 (81%)	285 (84%)	40 (12%)	16 (5%)	2	8
All	All	6786/7590 (89%)	5582 (82%)	892 (13%)	312 (5%)	2	8

5 of 312 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	83/87 (95%)	64 (77%)	19 (23%)	1	2
5	F	295/370 (80%)	228 (77%)	67 (23%)	1	3
5	P	295/370 (80%)	249 (84%)	46 (16%)	3	9
All	All	5692/6446 (88%)	4395 (77%)	1297 (23%)	1	2

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

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

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

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

5.3.3 RNA ⓘ

There are no RNA 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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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%)	-0.38	0 100 100	38, 65, 92, 117	0
1	B	229/315 (72%)	-0.27	8 (3%) 44 33	53, 95, 115, 121	0
1	K	229/315 (72%)	-0.37	0 100 100	41, 66, 93, 122	0
1	L	229/315 (72%)	-0.39	3 (1%) 77 71	52, 94, 114, 127	0
2	C	1119/1119 (100%)	-0.35	8 (0%) 87 83	23, 81, 110, 119	0
2	M	1119/1119 (100%)	-0.39	6 (0%) 90 88	27, 79, 109, 122	0
3	D	1392/1524 (91%)	-0.33	12 (0%) 84 79	17, 68, 113, 130	0
3	N	1392/1524 (91%)	-0.35	16 (1%) 80 75	27, 69, 110, 138	0
4	E	95/99 (95%)	-0.35	0 100 100	47, 85, 115, 133	0
4	O	95/99 (95%)	-0.49	1 (1%) 80 75	40, 76, 97, 111	0
5	F	345/423 (81%)	-0.40	3 (0%) 84 79	46, 84, 112, 131	0
5	P	345/423 (81%)	-0.39	5 (1%) 75 69	54, 87, 112, 125	0
All	All	6818/7590 (89%)	-0.36	62 (0%) 84 79	17, 77, 111, 138	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	ALA	5.1
3	D	1240	THR	4.7
3	N	1243	THR	4.7
3	D	1243	THR	4.5
5	F	145	PRO	4.4

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 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. 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
7	MG	N	9002	1/1	0.94	0.13	64,64,64,64	0
7	MG	D	9001	1/1	0.97	0.15	67,67,67,67	0
6	ZN	N	7113	1/1	0.98	0.10	87,87,87,87	0
6	ZN	D	7058	1/1	0.98	0.07	109,109,109,109	0
6	ZN	D	7112	1/1	0.99	0.14	75,75,75,75	0
6	ZN	N	7059	1/1	0.99	0.11	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.