



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 03:45 PM BST

PDB ID : 6N60
Title : Escherichia coli RNA polymerase sigma70-holoenzyme bound to upstream fork promoter DNA and Microcin J25 (MccJ25)
Authors : Braffman, N.; Hauver, J.; Campbell, E.A.; Darst, S.A.
Deposited on : 2018-11-23
Resolution : 3.68 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:

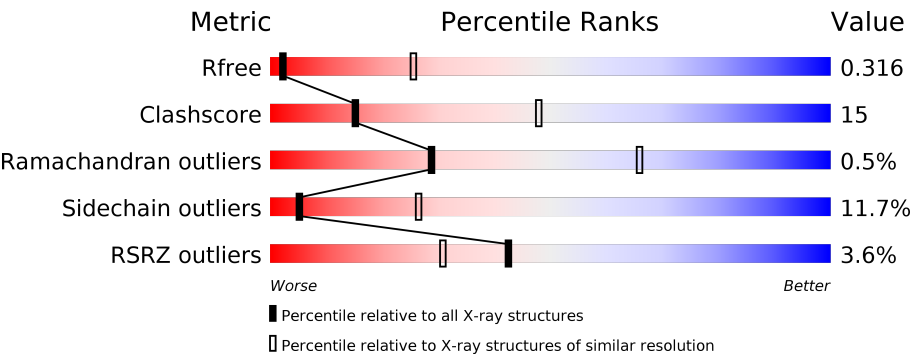
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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}	130704	1013 (3.84-3.52)
Clashscore	141614	1070 (3.84-3.52)
Ramachandran outliers	138981	1036 (3.84-3.52)
Sidechain outliers	138945	1033 (3.84-3.52)
RSRZ outliers	127900	1471 (3.86-3.50)

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 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	239	<div><div>10%</div><div><div></div><div>67%</div><div>28%</div><div>••</div></div></div>
1	B	239	<div><div>2%</div><div><div></div><div>51%</div><div>35%</div><div>5%</div><div>9%</div></div></div>
2	C	1342	<div><div>2%</div><div><div></div><div>61%</div><div>33%</div><div>5%</div><div>•</div></div></div>
3	D	1409	<div><div>3%</div><div><div></div><div>54%</div><div>29%</div><div>5%</div><div>12%</div></div></div>
4	E	91	<div><div>8%</div><div><div></div><div>53%</div><div>29%</div><div>5%</div><div>13%</div></div></div>
5	F	612	<div><div>2%</div><div><div></div><div>35%</div><div>14%</div><div>•</div><div>48%</div></div></div>

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Mol	Chain	Length	Quality of chain
6	M	21	<div><div></div><div>10%</div><div>29%</div><div>57%</div><div>10%</div><div>5%</div></div>
7	N	29	<div><div></div><div>52%</div><div>48%</div></div>
8	T	24	<div><div></div><div>54%</div><div>42%</div><div></div></div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 27705 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1759	1094	312	347	6			
1	B	218	Total	C	N	O	S	0	0	0
			1638	1023	284	325	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP P0A7Z4
A	236	VAL	-	expression tag	UNP P0A7Z4
A	237	LEU	-	expression tag	UNP P0A7Z4
A	238	PHE	-	expression tag	UNP P0A7Z4
A	239	GLN	-	expression tag	UNP P0A7Z4
B	235	GLU	-	expression tag	UNP P0A7Z4
B	236	VAL	-	expression tag	UNP P0A7Z4
B	237	LEU	-	expression tag	UNP P0A7Z4
B	238	PHE	-	expression tag	UNP P0A7Z4
B	239	GLN	-	expression tag	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10470	6569	1822	2036	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1236	Total	C	N	O	S	0	0	0
			9578	6015	1711	1806	46			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	expression tag	UNP P0A8T7
D	1408	LEU	-	expression tag	UNP P0A8T7
D	1409	GLU	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	318	Total	C	N	O	S	0	0	0
			2399	1499	442	446	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	149	ASN	ASP	conflict	UNP Q0P6L9
F	?	-	LEU	deletion	UNP Q0P6L9

- Molecule 6 is a protein called Microcin J25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	21	Total	C	N	O	0	0	0
			144	95	23	26			

- Molecule 7 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	N	29	Total	C	N	O	P	0	0	0
			595	284	106	176	29			

- Molecule 8 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	T	24	Total	C	N	O	P	0	0	0
			492	233	94	141	24			

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		

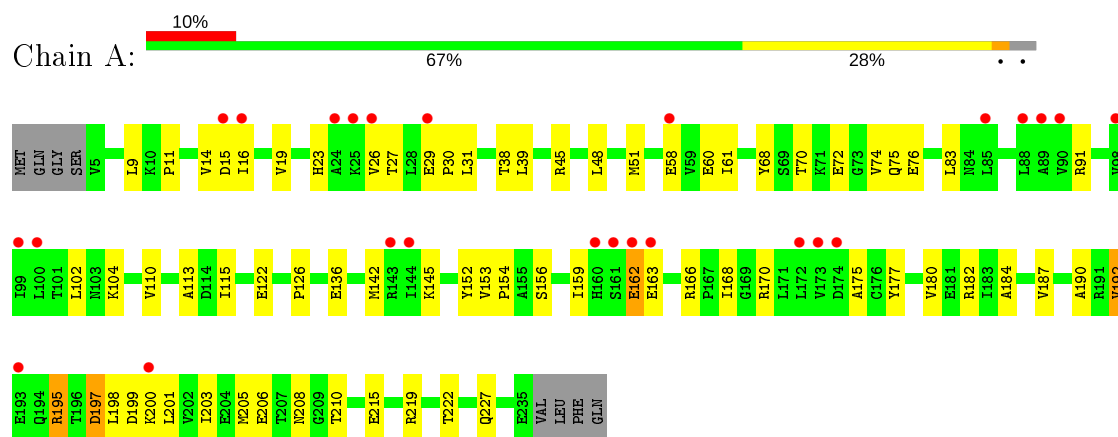
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	Zn	0	0
			2	2		

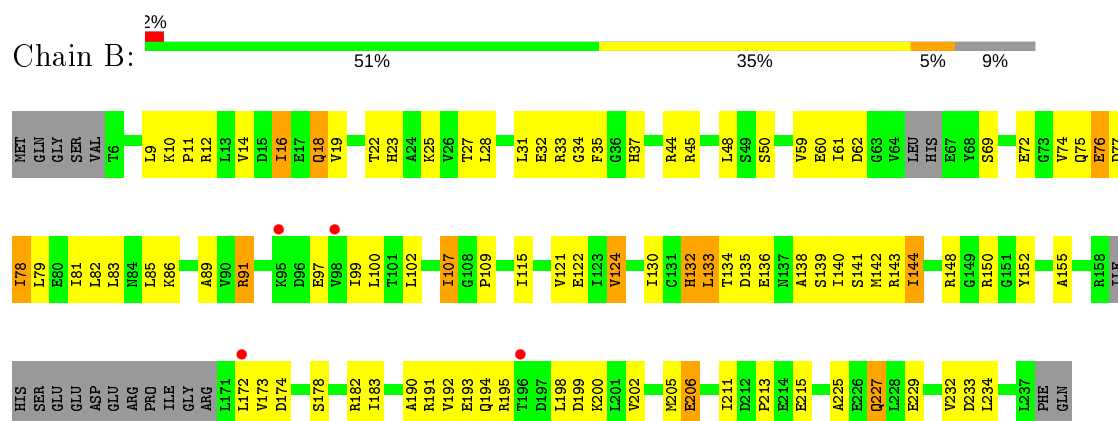
3 Residue-property plots [i](#)

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.

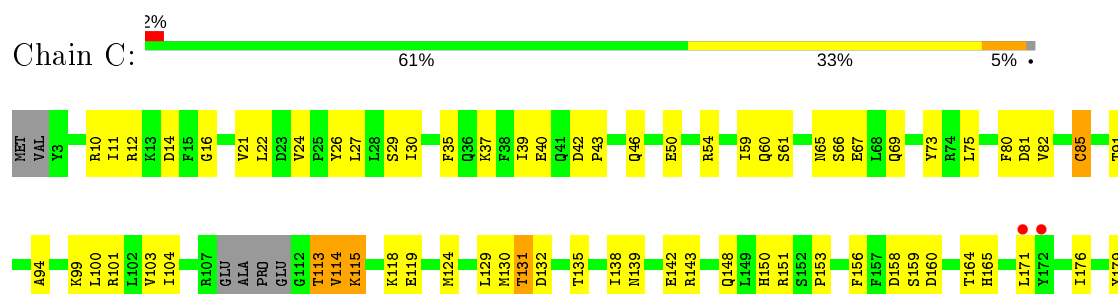
• Molecule 1: DNA-directed RNA polymerase subunit alpha

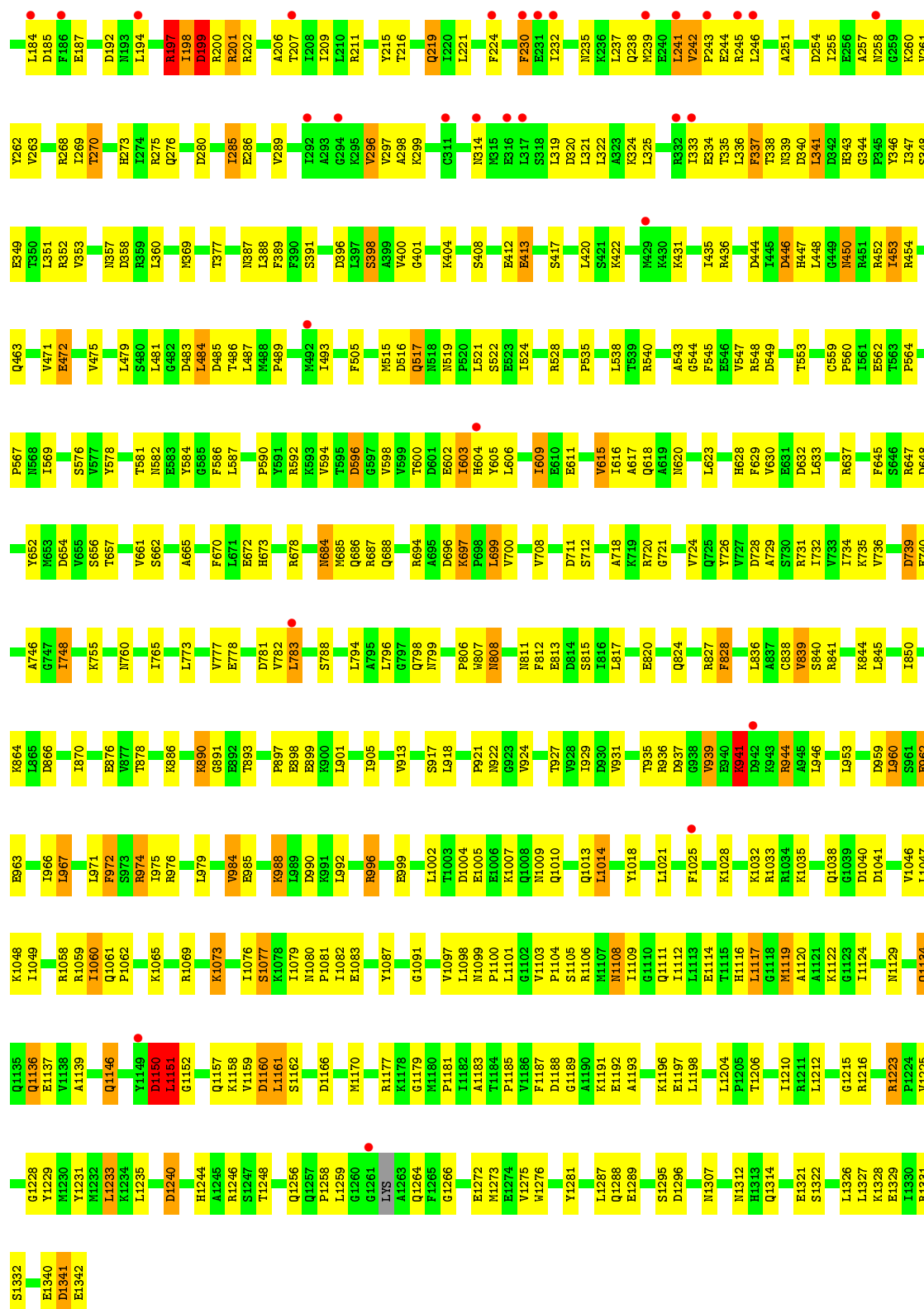


• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

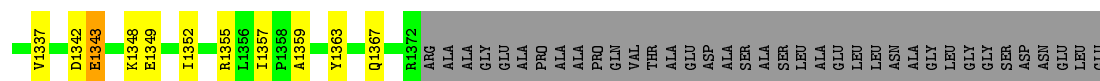




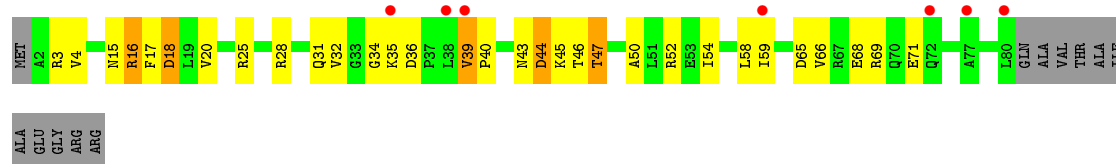
• Molecule 3: DNA-directed RNA polymerase subunit beta'



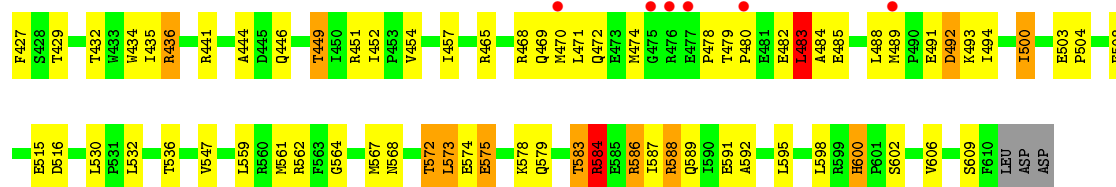
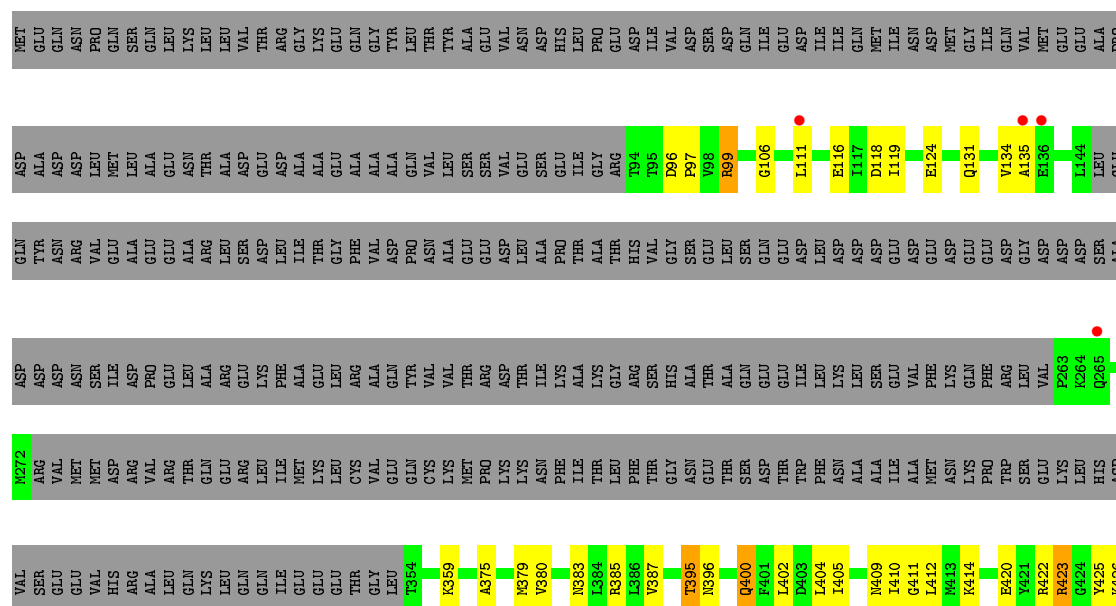
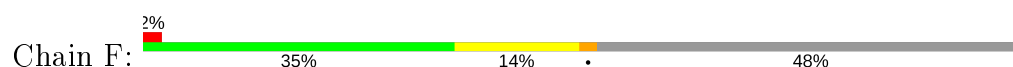
L1261	K1192	SER	SER	I975	C888	F773	V682	A577	A482	Y360	L265	E183	R98	VAL
L1262	W1193	SER	SER	R978	D889	I774	W685	M881	T487	L361	N266	D193	R99	LYS
K1263	R1194	LEU	LEU	R979	G893	R780	W686	M882	M488	R362	D267	L194	E100	ASP
L1264	L1195	VAL	VAL	T980	G894	R781	W687	K585	M489	L363	L268	E197	R101	LEU
T1265	L1196	LEU	LEU	E981	C895	L783	M690	N593	L491	R364	Y269	C198	E106	LEU
M1268	N1197	ALA	ARG	L982	A896	T786	M697	Q594	L492	C367	N274	E199	P110	PHE
A1269	F1198	ILE	SER	K983	Y899	T787	M698	A595	M495	L368	R278	Q200	P111	LEU
E1270	E1200	PRO	ALA	L984	G900	S793	D699	L596	E496	A373	R279	L201	H113	GLN
G1271	G1201	GLU	GLU	E987	R901	T797	N700	G597	E497	R282	R278	R202	I114	ALA
R1203	R1202	THR	ARG	E988	D902	R798	L701	K598	P498	E203	L282	E203	W115	THR
E1205	E1203	ALA	ALA	E993	L903	R799	Q702	K599	L499	R283	L283	E204	F116	LYS
E1274	G1274	GLY	GLY	E994	A904	T703	T703	A600	L500	P379	D284	L205	L117	THR
L1275	E1275	GLY	GLY	R905	G906	E704	E704	I601	Y382	Y382	D289	L206	K118	GLU
E1277	E1277	THR	LYS	R906	H907	D802	I707	S602	D504	L208	D289	T208	S119	E16
E1278	E1278	ASP	ASP	H908	H907	Q805	N708	K603	D505	R209	L290	L120	F17	F17
Q1279	Q1279	LEU	LEU	I908	R909	D806	R709	G608	N706	L121	L291	S210	D18	D18
V1280	V1280	ARG	ARG	I909	I909	L807	Q712	R609	V507	L412	Y292	E211	P121	A19
E1281	E1281	PRO	PRO	M910	M910	R807	Q713	G610	V507	L413	E295	T212	R123	
Y1282	Y1282	ALA	ALA	Q911	G912	R808	Q714	R611	L510	D413	E296	K213	I124	P27
S1283	S1283	LYS	LYS	E913	E913	T810	Q715	L612	T514	E414	K296	R214	R31	R31
V1285	V1217	ILE	ILE	A914	A914	E811	Q716	G613	T514	E415	L299	K215	S32	S32
K1286	K1218	VAL	VAL	W917	W917	D812	F719	L614	C517	V415	L300	L216	W33	W33
	F1145	ASP	ASP			D813	N720	K615	V518	R417	E301	L217	K40	K40
	E1146	GLN	GLN	Q921	Q921	C814	S721	P616	L527	E418	E301	L218	P41	P41
	A1147	ALA	ALA	Q922	Q922	G815	I722	T617	L527	E419	D304	L219	E136	E136
	R1148	ASN	ASN	E925	E925	T816	I723	T617	L527	E420	D304	L220	E42	E42
	I1155	ASP	ASP	P926	P926	H817	R731	F620	P630	L422	R312	L221	Y140	Y140
	E1158	VAL	VAL	T931	T931	E818	Q732	G632	K531	R425	R312	L222	F141	F141
	I1159	ILE	ILE	F935	F935	R842	S733	A633	E532	R426	L316	L223	E142	E142
	G1160	GLU	GLU	H936	H936	A845	A735	I641	E533	P427	T317	L224	S143	S143
	T1161	VAL	VAL	I937	I937	E846	I737	W645	E534	H430	R320	Q228	Y144	Y144
	I1162	THR	THR	R937	R937	D847	R738	I646	E535	R431	R321	Q229	V145	V145
	V1163	ASP	ASP	GLY	GLY	V848	Q739	P647	L536	L432	R322	Q230	F49	F49
	S1164	MET	MET	ALA	ALA	L849	L740	E648	E439	E439	P323	R234	E155	E155
	F1165	PRO	PRO	ALA	ALA	K850	A741	K649	H545	L442	L324	E235	L56	L56
	K1166	ALA	ALA	ALA	ALA	R854	G742	K650	E546	Q448	R330	W236	F57	F57
	K1167	GLN	GLN	SER	SER	A854	N743	H651	V550	Q449	R334	W241	F62	F62
	E1168	THR	THR	ARG	ARG	L857	R744	E657	R551	A459	E338	Y244	Y68	Y68
	T1169	PHE	PHE	ALA	ALA	V858	L745	E658	E554	D462	R339	L245	L71	L71
	K1170	LEU	LEU	ALA	ALA	M747	L746	V661	E555	G463	L343	P246	K74	K74
	G1171	PRO	PRO	ALA	ALA	I754	I754	A662	A559	D464	L343	L249	L165	L165
	K1172	GLY	GLY	S948	S948	H865	P758	E663	N560	Q465	R346	R250	D167	D167
	R1173	LYS	LYS	I950	I950	Q867	I759	I664	E563	Q466	V347	R251	L166	L166
	E1174	ALA	ALA	Q951	Q951	T862	T760	E666	L563	V468	D348	L252	T161	T161
	T1178	VAL	VAL	I958	I958	N875	A761	E667	E564	D469	R347	L253	E162	E162
	P1179	GLN	GLN	K959	K959	N767	N767	A675	E565	L474	Y349	L254	E163	E163
	V1180	LEU	LEU	L960	L960	K881	F763	G676	L474	D475	R352	L255	Q164	Q164
	D1181	THR	THR	L961	L961	V882	R764	E677	L569	E476	R352	D256	Y165	Y165
	D1184	ASP	ASP	L962	L962	V883	R765	E678	E570	L477	R353	D257	L166	L166
	F1185	GLY	GLY	V963	V963	V884	L770	E679	E571	L478	R354	D258	D167	D167
	Y1186	VAL	VAL	K972	K972	V885	Q771	N680	E572	L479	R355	D259	L167	L167
	P1191	ILE	ILE	K973	K973	V886	Q772	N681	E573	L480	R356	D260	L168	L168
		SER	SER	K974	K974	V887	Q773	N682	E574	L481	R357	D261	L169	L169
				K975	K975	V888	Q774	N683	E575	L482	R358	D262	L170	L170
				K976	K976	V889	Q775	N684	E576	L483	R359	D263	L171	L171
				K977	K977	V890	Q776	N685	E577	L484	R360	D264	L172	L172
				K978	K978	V891	Q777	N686	E578	L485	R361	D265	L173	L173
				K979	K979	V892	Q778	N687	E579	L486	R362	D266	L174	L174
				K980	K980	V893	Q779	N688	E580	L487	R363	D267	L175	L175
				K981	K981	V894	Q780	N689	E581	L488	R364	D268	L176	L176
				K982	K982	V895	Q781	N690	E582	L489	R365	D269	L177	L177
				K983	K983	V896	Q782	N691	E583	L490	R366	D270	L178	L178
				K984	K984	V897	Q783	N692	E584	L491	R367	D271	L179	L179
				K985	K985	V898	Q784	N693	E585	L492	R368	D272	L180	L180
				K986	K986	V899	Q785	N694	E586	L493	R369	D273	L181	L181
				K987	K987	V900	Q786	N695	E587	L494	R370	D274	L182	L182
				K988	K988	V901	Q787	N696	E588	L495	R371	D275	L183	L183
				K989	K989	V902	Q788	N697	E589	L496	R372	D276	L184	L184
				K990	K990	V903	Q789	N698	E590	L497	R373	D277	L185	L185
				K991	K991	V904	Q790	N699	E591	L498	R374	D278	L186	L186
				K992	K992	V905	Q791	N700	E592	L499	R375	D279	L187	L187
				K993	K993	V906	Q792	N701	E593	L500	R376	D280	L188	L188
				K994	K994	V907	Q793	N702	E594	L501	R377	D281	L189	L189
				K995	K995	V908	Q794	N703	E595	L502	R378	D282	L190	L190
				K996	K996	V909	Q795	N704	E596	L503	R379	D283	L191	L191
				K997	K997	V910	Q796	N705	E597	L504	R380	D284	L192	L192
				K998	K998	V911	Q797	N706	E598	L505	R381	D285	L193	L193
				K999	K999	V912	Q798	N707	E599	L506	R382	D286	L194	L194
				K1000	K1000	V913	Q799	N708	E600	L507	R383	D287	L195	L195
				K1001	K1001	V914	Q800	N709	E601	L508	R384	D288	L196	L196
				K1002	K1002	V915	Q801	N710	E602	L509	R385	D289	L197	L197
				K1003	K1003	V916	Q802	N711	E603	L510	R386	D290	L198	L198
				K1004	K1004	V917	Q803	N712	E604	L511	R387	D291	L199	L199
				K1005	K1005	V918	Q804	N713	E605	L512	R388	D292	L200	L200
				K1006	K1006	V919	Q805	N714	E606	L513	R389	D293	L201	L201
				K1007	K1007	V920	Q806	N715	E607	L514	R390	D294	L202	L202
				K1008	K1008	V921	Q807	N716	E608	L515	R391	D295	L203	L203
				K1009	K1009	V922	Q808	N717	E609	L516	R392	D296	L204	L204
				K1010	K1010	V923	Q809	N718	E610	L517	R393	D297	L205	L205
				K1011	K1011	V924	Q810	N719	E611	L518	R394	D298	L206	L206
				K1012	K1012	V925	Q811	N720	E612	L519	R395	D299	L207	L207
				K1013	K1013	V926	Q812	N721	E613	L520	R396	D300	L208	L208
				K1014	K1014	V927	Q813	N722	E614	L521	R397	D301	L209	L209
				K1015	K1015	V928	Q814	N723	E615	L522	R398	D302	L210	L210
				K1016	K1016	V929	Q815	N724	E616	L523	R399	D303	L211	L211
				K1017	K1017	V930	Q816	N725	E617	L524	R400	D304	L212	L212
				K1018	K1018	V931	Q817	N726	E618	L525	R401	D305	L213	L213
				K1019	K1019	V932	Q818	N727	E619	L526	R402	D306	L214	L214
				K1020	K1020	V933	Q819	N728	E620	L527	R403	D307	L215	L215
				K1021	K1021	V934	Q820	N729	E621	L528	R404	D308	L216	L216
				K1022	K1022	V935	Q821	N730	E622	L529	R405	D309	L217	L217
				K1023	K1023	V936	Q822	N731	E623	L530	R406	D310	L218	L218
				K1024	K1024	V937	Q823	N732	E624	L531	R407	D311	L219	L219
				K1025	K1025	V938	Q824	N733	E625	L532	R408	D312	L220	L220
				K1026	K1026	V939	Q825	N734	E626	L533	R409	D313	L221	L221
			</											



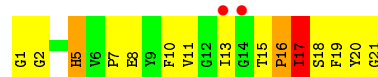
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoD



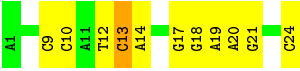
- Molecule 6: Microcin J25



- Molecule 7: non-template strand DNA



● Molecule 8: template strand DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	172.91Å 172.91Å 387.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 3.68 49.55 – 3.68	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.55-3.68) 98.3 (49.55-3.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.263 , 0.306 0.274 , 0.316	Depositor DCC
R_{free} test set	1945 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å ²)	175.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 119.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27705	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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	0.25	0/1780	0.47	0/2415
1	B	0.25	0/1655	0.50	0/2247
2	C	0.26	0/10634	0.47	1/14353 (0.0%)
3	D	0.25	0/9724	0.47	1/13134 (0.0%)
4	E	0.23	0/629	0.40	0/847
5	F	0.25	0/2428	0.50	2/3280 (0.1%)
6	M	0.36	0/149	0.76	0/202
7	N	0.65	1/666 (0.2%)	0.96	1/1026 (0.1%)
8	T	0.64	1/552 (0.2%)	0.86	0/849
All	All	0.28	2/28217 (0.0%)	0.51	5/38353 (0.0%)

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
1	B	0	1
2	C	0	5
3	D	0	3
5	F	0	1
6	M	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	12	DG	C1'-N9	-6.56	1.38	1.47
8	T	13	DC	C1'-N1	5.59	1.56	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	483	LEU	CA-CB-CG	6.04	129.20	115.30
5	F	583	THR	C-N-CA	5.44	135.30	121.70
3	D	224	LEU	CA-CB-CG	5.40	127.72	115.30
2	C	517	GLN	N-CA-C	5.20	125.04	111.00
7	N	11	DT	N3-C4-O4	5.11	122.96	119.90

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	14	VAL	Peptide
2	C	197	ARG	Peptide
2	C	198	ILE	Peptide
2	C	939	VAL	Peptide
2	C	941	LYS	Peptide

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	1759	0	1759	46	0
1	B	1638	0	1629	71	0
2	C	10470	0	10445	333	0
3	D	9578	0	9710	335	0
4	E	627	0	634	21	0
5	F	2399	0	2324	69	0
6	M	144	0	131	15	0
7	N	595	0	329	14	0
8	T	492	0	269	9	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	27705	0	27230	822	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 15.

The worst 5 of 822 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:1006:GLY:N	3:D:1009:GLU:OE2	1.92	1.01
5:F:414:LYS:HB2	5:F:434:TRP:HE1	1.30	0.94
3:D:208:THR:O	3:D:214:ARG:NH1	2.01	0.92
5:F:600:HIS:HE2	5:F:602:SER:HG	1.04	0.92
1:B:76:GLU:OE2	1:B:132:HIS:ND1	2.05	0.88

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	229/239 (96%)	204 (89%)	23 (10%)	2 (1%)	17	54
1	B	212/239 (89%)	189 (89%)	23 (11%)	0	100	100
2	C	1329/1342 (99%)	1243 (94%)	77 (6%)	9 (1%)	22	59
3	D	1230/1409 (87%)	1166 (95%)	62 (5%)	2 (0%)	47	78
4	E	77/91 (85%)	73 (95%)	3 (4%)	1 (1%)	12	47
5	F	312/612 (51%)	293 (94%)	18 (6%)	1 (0%)	41	74
6	M	19/21 (90%)	13 (68%)	4 (21%)	2 (10%)	0	7
All	All	3408/3953 (86%)	3181 (93%)	210 (6%)	17 (0%)	29	66

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	199	ASP
2	C	200	ARG
2	C	1151	LEU
1	A	177	TYR
2	C	340	ASP

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	190/206 (92%)	178 (94%)	12 (6%)	18	49
1	B	176/206 (85%)	154 (88%)	22 (12%)	4	23
2	C	1138/1157 (98%)	1001 (88%)	137 (12%)	5	25
3	D	1022/1170 (87%)	901 (88%)	121 (12%)	5	26
4	E	67/75 (89%)	59 (88%)	8 (12%)	5	25
5	F	232/539 (43%)	205 (88%)	27 (12%)	5	27
6	M	13/14 (93%)	9 (69%)	4 (31%)	0	2
All	All	2838/3367 (84%)	2507 (88%)	331 (12%)	5	26

5 of 331 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1083	GLU
3	D	193	ASP
5	F	425	TYR
2	C	1117	LEU
2	C	1326	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1116	HIS
2	C	1314	GLN
3	D	1244	GLN
2	C	1237	HIS
3	D	200	GLN

5.3.3 RNA ⓘ

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 3 ligands modelled in this entry, 3 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/239 (96%)	0.35	25 (10%) 5 4	138, 193, 227, 277	0
1	B	218/239 (91%)	-0.13	4 (1%) 68 56	133, 191, 230, 261	0
2	C	1335/1342 (99%)	-0.11	32 (2%) 59 45	93, 170, 229, 271	0
3	D	1236/1409 (87%)	0.02	46 (3%) 41 29	99, 176, 247, 304	0
4	E	79/91 (86%)	0.27	7 (8%) 9 6	144, 183, 238, 268	0
5	F	318/612 (51%)	0.00	10 (3%) 49 35	128, 190, 250, 265	0
6	M	21/21 (100%)	0.18	2 (9%) 8 5	151, 194, 226, 257	0
7	N	29/29 (100%)	-0.82	0 100 100	139, 222, 253, 255	0
8	T	24/24 (100%)	-0.81	0 100 100	125, 223, 249, 259	0
All	All	3491/4006 (87%)	-0.02	126 (3%) 42 31	93, 179, 240, 304	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	476	ARG	10.1
2	C	243	PRO	9.6
1	A	89	ALA	9.3
1	A	90	VAL	7.5
2	C	230	PHE	6.5

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

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

6.3 Carbohydrates ⓘ

There are no 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
9	MG	D	1501	1/1	0.95	0.25	83,83,83,83	0
10	ZN	D	1503	1/1	0.96	0.21	185,185,185,185	0
10	ZN	D	1502	1/1	0.98	0.12	162,162,162,162	0

6.5 Other polymers [i](#)

There are no such residues in this entry.