



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:01 PM UTC

PDB ID : 6UU5 / pdb_00006uu5
Title : E. coli sigma-S transcription initiation complex with a 6-nt RNA ("Old" crystal soaked with GTP, UTP, CTP, and dinucleotide GpA for 30 minutes)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 5.40 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
Mogul : 2022.3.0, CSD as543be (2022)
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

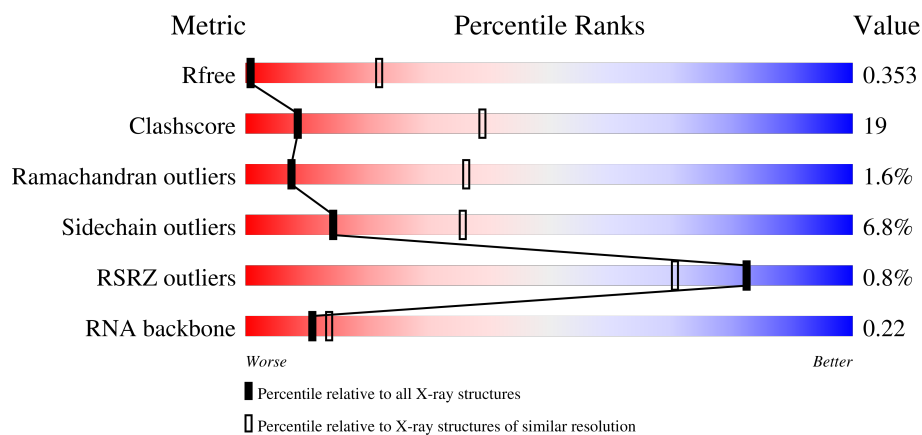
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.40 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.



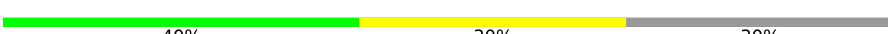
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1060 (6.80-4.00)
Clashscore	190562	1117 (6.80-4.00)
Ramachandran outliers	187476	1020 (6.80-3.96)
Sidechain outliers	187428	1019 (6.86-3.94)
RSRZ outliers	180081	1053 (6.80-4.00)
RNA backbone	3983	1051 (7.50-3.10)

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	AAA	242	2% 62% 30% 5%
1	BBB	242	2% 61% 29% 6%
2	CCC	1342	% 63% 33%
3	DDD	1407	60% 33%

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Mol	Chain	Length	Quality of chain
4	EEE	90	
5	FFF	336	
6	111	50	
7	222	50	
8	333	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	DPO	DDD	1504	-	-	X	-
9	ZN	DDD	1502	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29050 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	AAA	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	BBB	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-6	ALA	-	expression tag	UNP P0A7Z4
AAA	-5	HIS	-	expression tag	UNP P0A7Z4
AAA	-4	HIS	-	expression tag	UNP P0A7Z4
AAA	-3	HIS	-	expression tag	UNP P0A7Z4
AAA	-2	HIS	-	expression tag	UNP P0A7Z4
AAA	-1	HIS	-	expression tag	UNP P0A7Z4
AAA	0	HIS	-	expression tag	UNP P0A7Z4
BBB	-6	ALA	-	expression tag	UNP P0A7Z4
BBB	-5	HIS	-	expression tag	UNP P0A7Z4
BBB	-4	HIS	-	expression tag	UNP P0A7Z4
BBB	-3	HIS	-	expression tag	UNP P0A7Z4
BBB	-2	HIS	-	expression tag	UNP P0A7Z4
BBB	-1	HIS	-	expression tag	UNP P0A7Z4
BBB	0	HIS	-	expression tag	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DDD	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	FFF	277	Total	C	N	O	S	0	0	0
			2253	1411	415	423	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FFF	2	GLY	SER	conflict	UNP P13445
FFF	33	GLU	GLN	conflict	UNP P13445
FFF	329	LEU	-	expression tag	UNP P13445
FFF	330	GLU	-	expression tag	UNP P13445
FFF	331	HIS	-	expression tag	UNP P13445
FFF	332	HIS	-	expression tag	UNP P13445
FFF	333	HIS	-	expression tag	UNP P13445
FFF	334	HIS	-	expression tag	UNP P13445
FFF	335	HIS	-	expression tag	UNP P13445
FFF	336	HIS	-	expression tag	UNP P13445

- Molecule 6 is a DNA chain called Synthetic DNA 50-MER (promoter non-template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	111	30	Total	C	N	O	P	0	0	0
			618	294	111	183	30			

- Molecule 7 is a DNA chain called Synthetic DNA 50-MER (promoter template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	222	35	Total	C	N	O	P	0	0	0
			716	342	132	208	34			

- Molecule 8 is a RNA chain called RNA 6-mer (dinucleotide GpA primed synthesis).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	333	6	Total	C	N	O	P	0	0	0
			125	57	22	41	5			

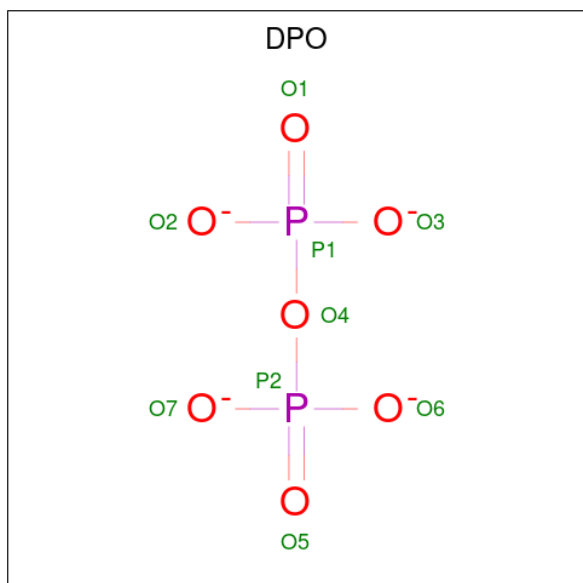
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	DDD	2	Total	Zn	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	DDD	1	Total	Mg	0	0
			1	1		
10	333	1	Total	Mg	0	0
			1	1		

- Molecule 11 is DIPHOSPHATE (CCD ID: DPO) (formula: O₇P₂).

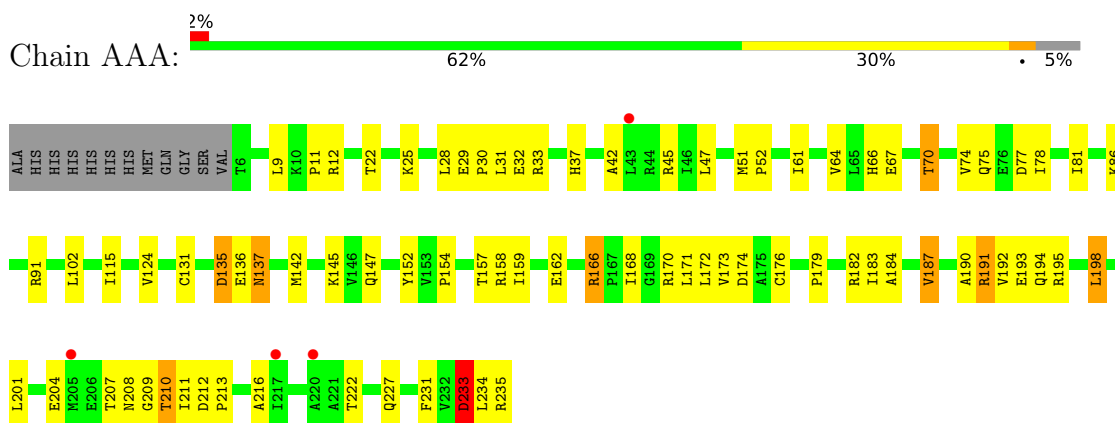


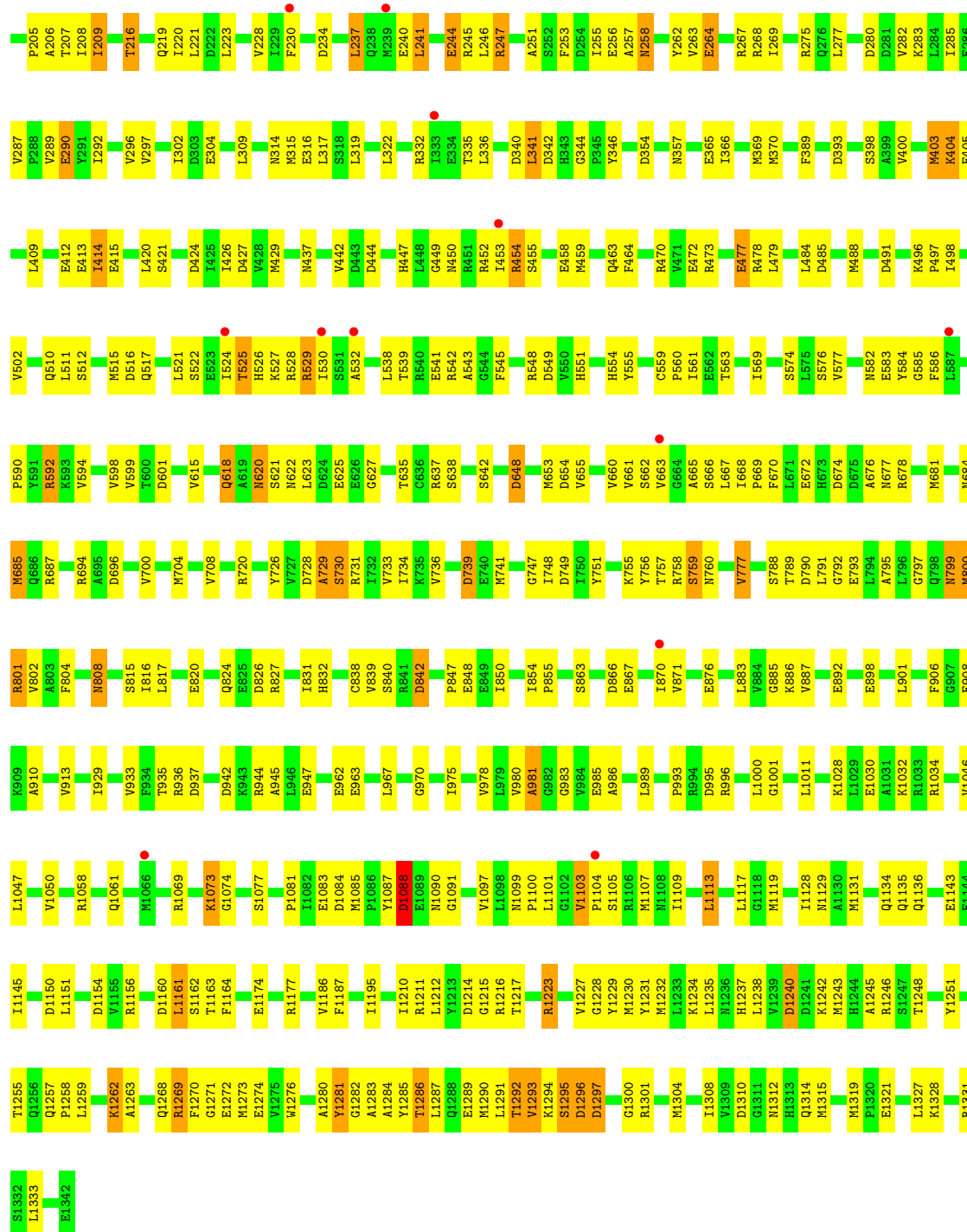
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	DDD	1	Total	O	P	0	0
			9	7	2		

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

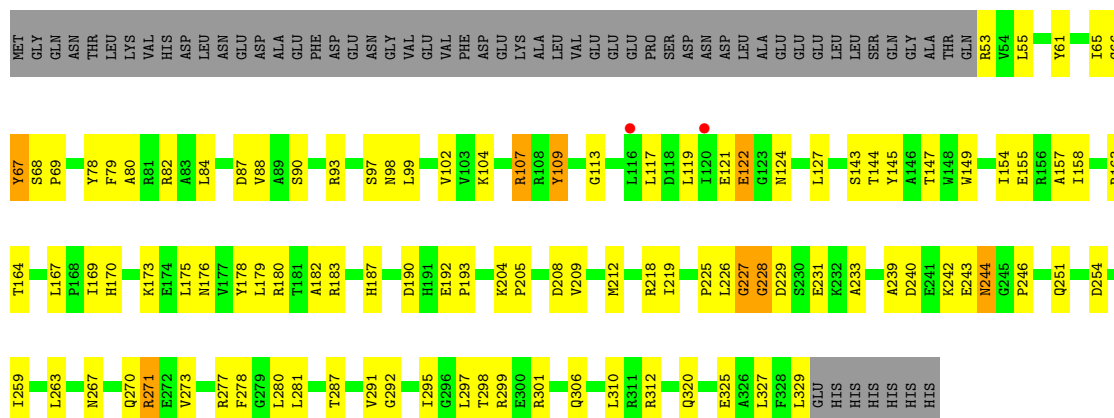




ALA	K1286	R1173	S1068	L980	L872	R799	V717	T611	A520	R425	R339	T212	T111
PRO	L1174	R1175	L1069	S961	E873	L800	S718	L612	E523	A426	Q340	R213	A112
GLN	V1176	L1177	V1060	Y962	V877	V801	F719	T617	G524	T428	P427	R214	H113
VAL	P1179	V1180	V1061	Y963	D878	D802	G731	V618	M525	L429	N341	R220	I114
THR	V1181	D1182	D1062	S965	A879	V803	R732	I619	V526	H430	L342	L223	W115
ALA	D1183	S1183	S1064	S966	V880	Q805	S733	F620	L527	R431	G344	L224	
GLU	E1186	Y1187	D1063	S969	K881	D806	Q736	A621	G529	T434	R346	P234	K118
ASP	E1188	Y1189	S1067	S970	R882	L807	Q739	D622	P530	E443	K347	P247	S119
SER	E1190	Y1191	D1068	S971	R883	V808	G741	I624	E532	E444	D348	M237	L120
ALA	E1192	Y1193	D1073	S972	V884	T810	G742	M625	E533	K445	Y349	L245	P121
LEU	E1194	Y1195	K1079	L982	V886	E811	M743	Y626	R535	Q448	S350	L246	S122
ALA	E1196	Y1197	D1082	D986	D887	D812	M744	T627	L536	Q449	S353	P248	R123
LEU	E1198	Y1199	A1083	D987	D888	T816	G745	F629	Y537	A455	T356	D248	L127
ASN	E1200	Y1201	Q1084	E993	D889	H817	M747	S638	R538	A456	Y360	D256	P131
ALA	E1202	Y1203	A1087	E994	G893	E818	P750	V639	S543	N458	L361	L261	M130
GLY	E1204	Y1205	D1087	S994	V894	G819	D751	M644	L544	A459	R362	R278	I132
LEU	E1206	Y1207	D1090	Y995	C895	T820	G752	V645	H545	D460	L363	L279	R133
GLY	E1208	Y1209	P1091	Y997	C898	M821	S753	A659	V548	D464	H364	L282	I135
SER	E1210	I1210	I1091	G1000	K911	M822	I754	E660	V550	M466	Q365	L283	E136
ASP	E1212	S1211	G1103	G1001	I915	V825	P758	V661	R551	A467	G367	L284	L139
ASN	E1214	I1214	K1104	L1003	G916	I826	I759	A662	L552	V468	K370	L285	S143
GLU	E1216	I1216	A1105	V1011	V917	G829	I760	E663	Y555	L472	K371	L286	M151
LEU	E1218	I1218	E1110	A1018	I918	D830	N762	Q665	K570	E475	M372	L287	T152
GLY	E1220	I1220	D1111	I1019	I923	V831	F763	E666	D571	A476	K378	L288	N163
SER	E1222	I1222	D1112	I1020	G824	L835	R764	Q667	D572	Q477	P379	L289	Q157
ASP	E1224	I1224	D1113	D1021	E925	R836	F769	F668	L572	L478	F380	L290	Q158
ASN	E1226	I1226	D1114	P1022	G926	V839	Q771	Q669	T573	E479	Y382	L291	I159
GLU	E1228	I1228	D1115	T1024	T928	V839	Y772	S670	V574	E487	L385	L292	L160
LEU	E1230	I1230	D1116	M1025	Q929	R842	Y776	V673	L578	T487	L386	L293	T161
GLY	E1232	I1232	D1117	I1026	L930	V843	T777	R678	L579	T490	R388	L294	Q164
SER	E1234	I1234	D1118	M1027	T931	A845	A779	Y679	M581	L491	D304	L295	D174
ASN	E1236	I1236	D1119	S1032	R935	E846	R780	N680	V582	S492	A305	L296	F176
GLU	E1238	I1238	D1120	S1033	H936	L849	K781	K681	V583	I499	R311	L297	M192
LEU	E1240	I1240	D1121	F1037	I937	K850	G782	T685	K585	I500	R312	L298	D193
ASP	E1242	I1242	D1122	T1038	I937	G851	L783	W686	G586	V501	R313	L299	L194
ASN	E1244	I1244	D1123	M1040	A940	T853	A784	M697	Y589	P502	R314	L300	G173
GLY	E1246	I1246	D1124	M1041	A941	V858	D785	M698	S503	Q504	R315	L301	E175
LEU	E1248	I1248	D1125	I1042	R943	L857	T786	M699	S590	Q505	R316	L302	F176
SER	E1250	I1250	D1126	G1043	A944	V858	A787	Q702	I591	V506	R317	L303	M192
ASN	E1252	I1252	D1127	Q1044	A945	L857	L788	T703	V592	V506	R318	L304	D193
GLU	E1254	I1254	D1128	T1047	S948	P859	K789	E704	A595	G509	R319	L305	L194
LEU	E1256	I1256	D1129	T1048	I950	R860	T790	E705	L510	L510	R320	L306	E197
ASP	E1258	I1258	D1130	E1051	I951	L863	N792	V706	K599	E414	R321	L307	C198
SER	E1260	I1260	D1131	E1052	K955	L864	S793	I707	M604	T514	R322	L308	L205
ASN	E1262	I1262	D1132	L1053	G856	L864	G794	N708	M604	T514	R323	L309	G333
GLY	E1264	I1264	D1133	T1054	S957	W868	Y795	R709	C608	C517	R324	L310	N209
LEU	E1266	I1266	D1134	G1055	I958	C869	L796	D710	Y609	V518	R325	L311	S210
GLY	E1268	I1268	D1135	G1056	K959	C869	T797	Q716	R610	N519	R326	L312	G336
SER	E1270	I1270	D1136	G1057	K960	C869	R798				R327	L313	
ASN	E1272	I1272	D1137	G1058	K961	C869					R328	L314	
GLU	E1274	I1274	D1138	G1059	K962	C869					R329	L315	
LEU	E1276	I1276	D1139	G1060	K963	C869					R330	L316	
ASP	E1278	I1278	D1140	G1061	K964	C869					R331	L317	
ASN	E1280	I1280	D1141	G1062	K965	C869					R332	L318	
GLY	E1282	I1282	D1142	G1063	K966	C869					R333	L319	
LEU	E1284	I1284	D1143	G1064	K967	C869					R334	L320	
SER	E1286	I1286	D1144	G1065	K968	C869					R335	L321	
ASN	E1288	I1288	D1145	G1066	K969	C869					R336	L322	
GLU	E1290	I1290	D1146	G1067	K970	C869					R337	L323	
LEU	E1292	I1292	D1147	G1068	K971	C869					R338	L324	
ASP	E1294	I1294	D1148	G1069	K972	C869					R339	L325	
ASN	E1296	I1296	D1149	G1070	K973	C869					R340	L326	
GLY	E1298	I1298	D1150	G1071	K974	C869					R341	L327	
LEU	E1300	I1300	D1151	G1072	K975	C869					R342	L328	
ASP	E1302	I1302	D1152	G1073	K976	C869					R343	L329	
ASN	E1304	I1304	D1153	G1074	K977	C869					R344	L330	
GLY	E1306	I1306	D1154	G1075	K978	C869					R345	L331	
LEU	E1308	I1308	D1155	G1076	K979	C869					R346	L332	
SER	E1310	I1310	D1156	G1077	K980	C869					R347	L333	
ASN	E1312	I1312	D1157	G1078	K981	C869					R348	L334	
GLY	E1314	I1314	D1158	G1079	K982	C869					R349	L335	
LEU	E1316	I1316	D1159	G1080	K983	C869					R350	L336	
SER	E1318	I1318	D1160	G1081	K984	C869					R351	L337	
ASN	E1320	I1320	D1161	G1082	K985	C869					R352	L338	
GLY	E1322	I1322	D1162	G1083	K986	C869					R353	L339	
LEU	E1324	I1324	D1163	G1084	K987	C869					R354	L340	
SER	E1326	I1326	D1164	G1085	K988	C869					R355	L341	
ASN	E1328	I1328	D1165	G1086	K989	C869					R356	L342	
GLY	E1330	I1330	D1166	G1087	K990	C869					R357	L343	
LEU	E1332	I1332	D1167	G1088	K991	C869					R358	L344	
SER	E1334	I1334	D1168	G1089	K992	C869					R359	L345	
ASN	E1336	I1336	D1169	G1090	K993	C869					R360	L346	
GLY	E1338	I1338	D1170	G1091	K994	C869					R361	L347	
LEU	E1340	I1340	D1171	G1092	K995	C869					R362	L348	
SER	E1342	I1342	D1172	G1093	K996	C869					R363	L349	
ASN	E1344	I1344	D1173	G1094	K997	C869					R364	L350	
GLY	E1346	I1346	D1174	G1095	K998	C869					R365	L351	
LEU	E1348	I1348	D1175	G1096	K999	C869					R366	L352	
SER	E1350	I1350	D1176	G1097	K1000	C869					R367	L353	
ASN	E1352	I1352	D1177	G1098	K1001	C869					R368	L354	
GLY	E1354	I1354	D1178	G1099	K1002	C869					R369	L355	
LEU	E1356	I1356	D1179	G1100	K1003	C869					R370	L356	
SER	E1358	I1358	D1180	G1101	K1004	C869					R371	L357	
ASN	E1360	I1360	D1181	G1102	K1005	C869					R372	L358	
GLY	E1362	I1362	D1182	G1103	K1006	C869					R373	L359	
LEU	E1364	I1364	D1183	G1104	K1007	C869					R374	L360	
SER	E1366	I1366	D1184	G1105	K1008	C869					R375	L361	
ASN	E1368	I1368	D1185	G1106	K1009	C869					R376	L362	
GLY	E1370	I1370	D1186	G1107	K1010	C869					R377	L363	
LEU	E1372	I1372	D1187	G1108	K1011	C869					R378	L364	
SER	E1374	I1374	D1188	G1109	K1012	C869					R379	L365	
ASN	E1376	I1376	D1189	G1110	K1013	C869					R380	L366	
GLY	E1378	I1378	D1190	G1111	K1014	C869					R381	L367	
LEU	E1380	I1380	D1191	G1112	K1015	C869					R382	L368	
SER	E1382	I1382	D1192	G1113	K1016	C869					R383	L369	
ASN	E1384	I1384	D1193	G1114	K1017	C869					R384	L370	
GLY	E1386	I1386	D1194	G1115	K1018	C869					R385	L371	
LEU	E1388	I1388	D1195	G1116	K1019	C869					R386	L372	
SER	E1390	I1390	D1196	G1117	K1020	C869					R387	L373	
ASN	E1392	I1392	D1197	G1118	K1021	C869					R388	L374	
GLY	E1394	I1394	D1198	G1119	K1022	C869					R389	L375	
LEU	E1396	I1396	D1199	G1120	K1023	C869					R		



• Molecule 5: RNA polymerase sigma factor RpoS



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.36Å 153.77Å 231.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 5.40 49.00 – 5.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.00-5.40) 98.2 (49.00-5.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 5.39Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.295 , 0.362 0.283 , 0.353	Depositor DCC
R_{free} test set	770 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	225.3	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 358.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	29050	wwPDB-VP
Average B, all atoms (Å ²)	345.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: DPO, 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	AAA	0.96	0/1809	1.24	0/2450
1	BBB	0.97	0/1789	1.24	3/2425 (0.1%)
2	CCC	0.93	0/10745	1.30	12/14499 (0.1%)
3	DDD	0.96	0/10729	1.29	10/14487 (0.1%)
4	EEE	0.89	0/629	1.36	0/847
5	FFF	0.99	0/2282	1.32	2/3076 (0.1%)
6	111	0.30	0/691	0.56	0/1063
7	222	0.31	0/802	0.56	0/1234
8	333	0.38	0/139	0.72	0/215
All	All	0.92	0/29615	1.26	27/40296 (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	CCC	0	1

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	563	THR	CB-CA-C	9.30	123.30	109.63
2	CCC	1084	ASP	CA-CB-CG	7.64	120.24	112.60
3	DDD	460	ASP	CA-CB-CG	6.56	119.16	112.60
2	CCC	454	ARG	CB-CA-C	-6.52	100.01	111.22
2	CCC	1310	ASP	N-CA-C	-6.25	105.65	113.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	CCC	1282	GLY	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	AAA	1787	0	1813	76	1
1	BBB	1767	0	1789	77	0
2	CCC	10576	0	10591	429	0
3	DDD	10568	0	10781	493	5
4	EEE	627	0	634	14	0
5	FFF	2253	0	2298	118	7
6	111	618	0	341	30	3
7	222	716	0	397	29	1
8	333	125	0	66	9	0
9	DDD	2	0	0	2	0
10	333	1	0	0	0	0
10	DDD	1	0	0	0	0
11	DDD	9	0	0	3	0
All	All	29050	0	28710	1089	12

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 19.

The worst 5 of 1089 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:DDD:843:VAL:HG11	3:DDD:883:ARG:CB	1.46	1.46
3:DDD:843:VAL:CG1	3:DDD:883:ARG:CB	1.99	1.40
3:DDD:843:VAL:CG1	3:DDD:883:ARG:HB2	1.49	1.40
6:111:54:DA:H2''	6:111:55:DC:C5	1.64	1.30
3:DDD:392:THR:HG21	5:FFF:320:GLN:O	1.27	1.27

The worst 5 of 12 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:67:TYR:CE1	5:FFF:299:ARG:NH2[3_644]	0.94	1.26
5:FFF:67:TYR:CZ	5:FFF:299:ARG:NH2[3_644]	1.07	1.13
5:FFF:67:TYR:CD1	5:FFF:299:ARG:NH2[3_644]	1.75	0.45
5:FFF:67:TYR:CE2	5:FFF:299:ARG:NH2[3_644]	1.89	0.31
5:FFF:67:TYR:CZ	5:FFF:299:ARG:CZ[3_644]	1.98	0.22

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	AAA	228/242 (94%)	214 (94%)	8 (4%)	6 (3%)	4	24
1	BBB	226/242 (93%)	206 (91%)	14 (6%)	6 (3%)	4	24
2	CCC	1339/1342 (100%)	1237 (92%)	77 (6%)	25 (2%)	6	31
3	DDD	1360/1407 (97%)	1253 (92%)	91 (7%)	16 (1%)	10	43
4	EEE	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
5	FFF	275/336 (82%)	256 (93%)	15 (6%)	4 (2%)	8	38
All	All	3505/3659 (96%)	3239 (92%)	209 (6%)	57 (2%)	7	36

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	117	HIS
1	BBB	193	GLU
1	BBB	194	GLN
2	CCC	46	GLN
2	CCC	247	ARG

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	AAA	198/208 (95%)	181 (91%)	17 (9%)	10	29
1	BBB	196/208 (94%)	182 (93%)	14 (7%)	13	35
2	CCC	1156/1157 (100%)	1070 (93%)	86 (7%)	13	33
3	DDD	1135/1168 (97%)	1062 (94%)	73 (6%)	16	37
4	EEE	67/74 (90%)	64 (96%)	3 (4%)	24	45
5	FFF	240/292 (82%)	230 (96%)	10 (4%)	26	47
All	All	2992/3107 (96%)	2789 (93%)	203 (7%)	14	36

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CCC	1293	VAL
3	DDD	591	ILE
5	FFF	244	ASN
3	DDD	60	ARG
3	DDD	256	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	333	5/6 (83%)	2 (40%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	333	18	C
8	333	19	U

There are no RNA pucker outliers to report.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
11	DPO	DDD	1504	10	6,8,8	0.75	0	12,13,13	0.80	0

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
11	DPO	DDD	1504	10	-	0/6/6/6	-

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	DDD	1504	DPO	3	0

5.7 Other polymers [i](#)

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	AAA	230/242 (95%)	-0.49	4 (1%) 69 57	259, 372, 468, 533	0
1	BBB	228/242 (94%)	-0.41	4 (1%) 67 56	220, 350, 469, 536	0
2	CCC	1341/1342 (99%)	-0.57	14 (1%) 79 66	149, 303, 471, 650	0
3	DDD	1362/1407 (96%)	-0.55	6 (0%) 88 78	154, 328, 517, 647	0
4	EEE	79/90 (87%)	-0.75	0 100 100	269, 375, 517, 678	0
5	FFF	277/336 (82%)	-0.51	2 (0%) 84 72	237, 384, 529, 633	0
6	111	30/50 (60%)	-0.40	0 100 100	310, 412, 536, 678	0
7	222	35/50 (70%)	-0.15	0 100 100	271, 388, 687, 743	0
8	333	6/6 (100%)	-0.52	0 100 100	331, 366, 398, 405	0
All	All	3588/3765 (95%)	-0.54	30 (0%) 82 71	149, 332, 504, 743	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	CCC	127	ILE	4.4
1	AAA	43	LEU	3.7
1	BBB	43	LEU	3.6
2	CCC	530	ILE	3.6
5	FFF	116	LEU	3.4

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 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
10	MG	DDD	1503	1/1	0.56	0.19	477,477,477,477	0
11	DPO	DDD	1504	9/9	0.60	0.20	265,283,350,352	0
10	MG	333	101	1/1	0.95	0.09	316,316,316,316	0
9	ZN	DDD	1501	1/1	0.98	0.04	509,509,509,509	0
9	ZN	DDD	1502	1/1	0.99	0.05	376,376,376,376	0

6.5 Other polymers [i](#)

There are no such residues in this entry.