



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:44 AM GMT

PDB ID : 2BE5
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with inhibitor tagetitoxin
Authors : Vassylyev, D.G.; Svetlov, V.; Vassylyeva, M.N.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Artsimovitch, I.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-10-22
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

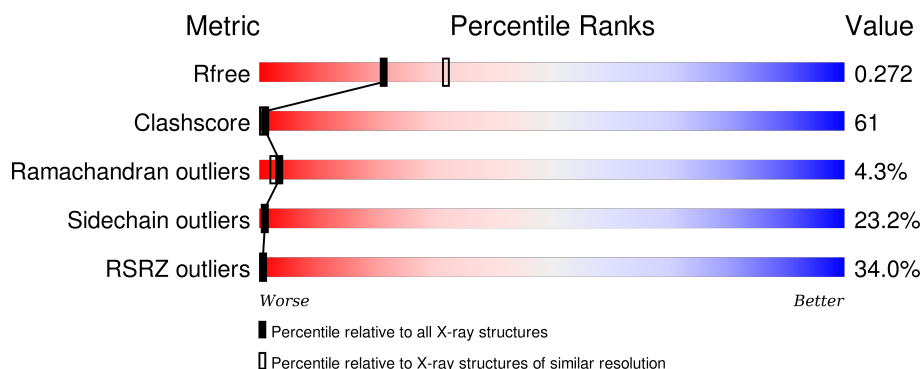
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	

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Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

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
8	TGT	D	9001	-	-	-	X
8	TGT	N	9002	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 61800 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			

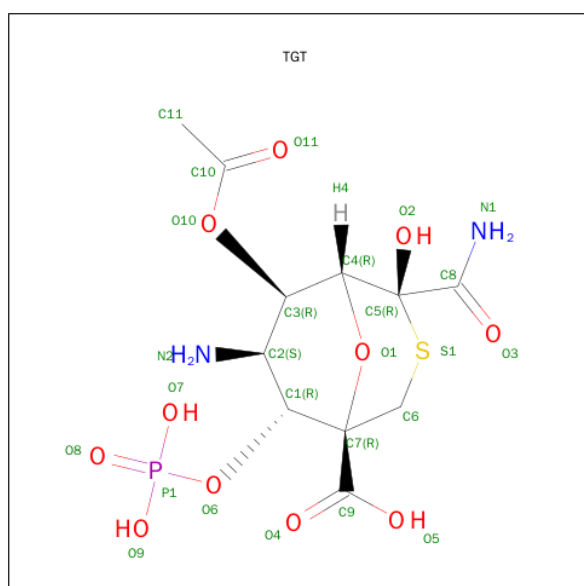
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	N	2	Total	Mg	0	0
			2	2		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is TAGETITOXIN (three-letter code: TGT) (formula: C₁₁H₁₇N₂O₁₁PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	D	1	Total 26	C 11	N 2	O 11	P 1	S 1	0	0
8	N	1	Total 26	C 11	N 2	O 11	P 1	S 1	0	0

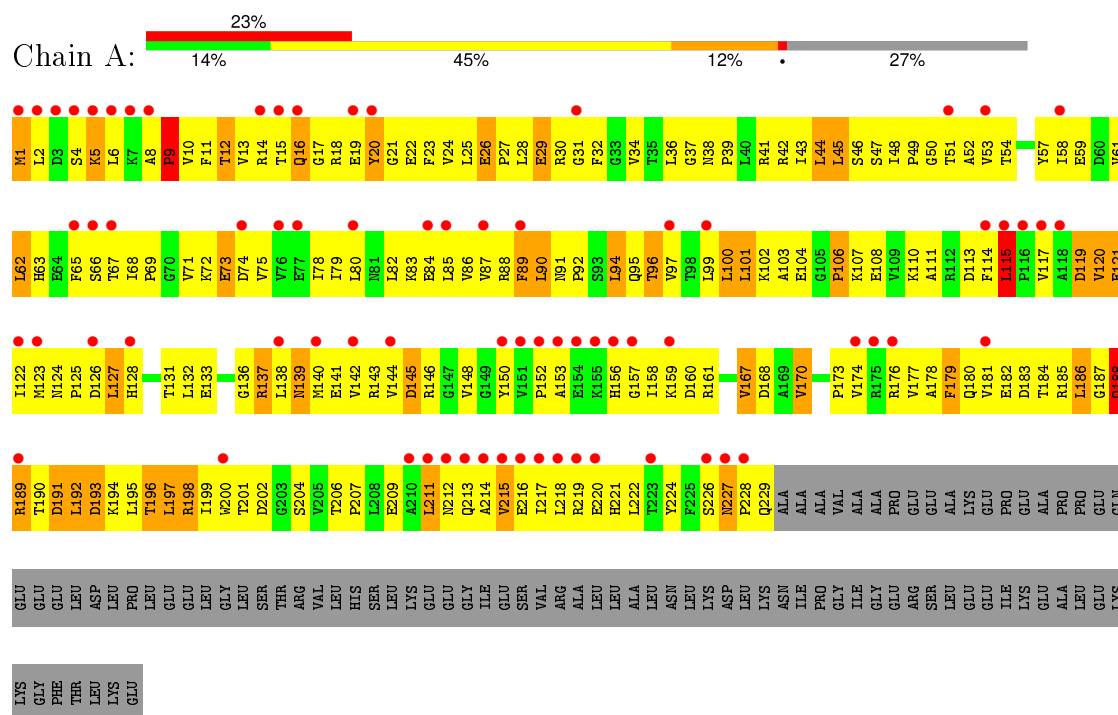
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	250	Total 250	O 250	0	0
9	B	329	Total 329	O 329	0	0
9	C	1321	Total 1321	O 1321	0	0
9	D	1655	Total 1655	O 1655	0	0
9	E	176	Total 176	O 176	0	0
9	F	519	Total 519	O 519	0	0
9	K	278	Total 278	O 278	0	0
9	L	309	Total 309	O 309	0	0
9	M	1236	Total 1236	O 1236	0	0
9	N	1552	Total 1552	O 1552	0	0
9	O	137	Total 137	O 137	0	0
9	P	422	Total 422	O 422	0	0

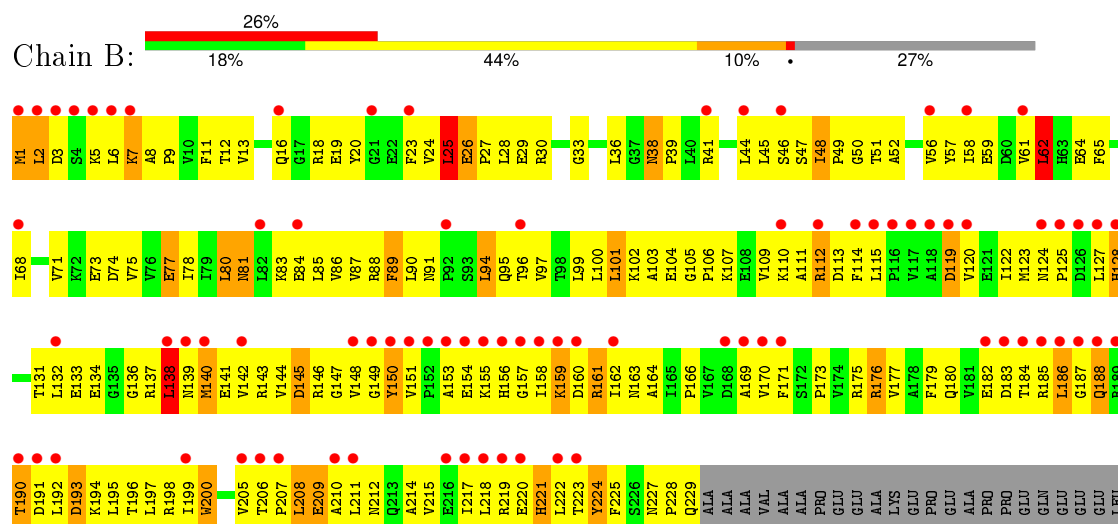
3 Residue-property plots

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



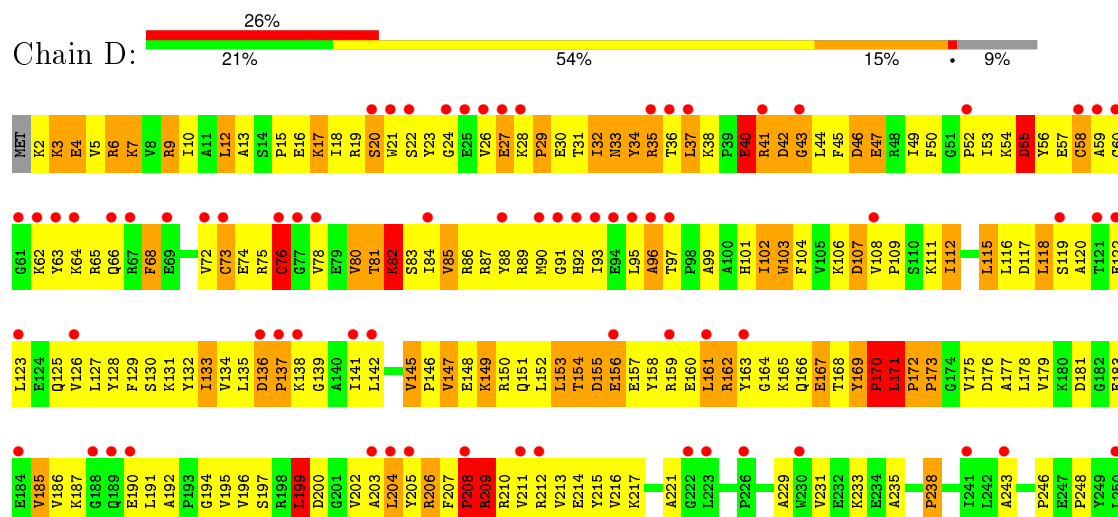
- Molecule 1: DNA-directed RNA polymerase alpha chain

- Molecule 1: DNA-directed RNA polymerase alpha chain

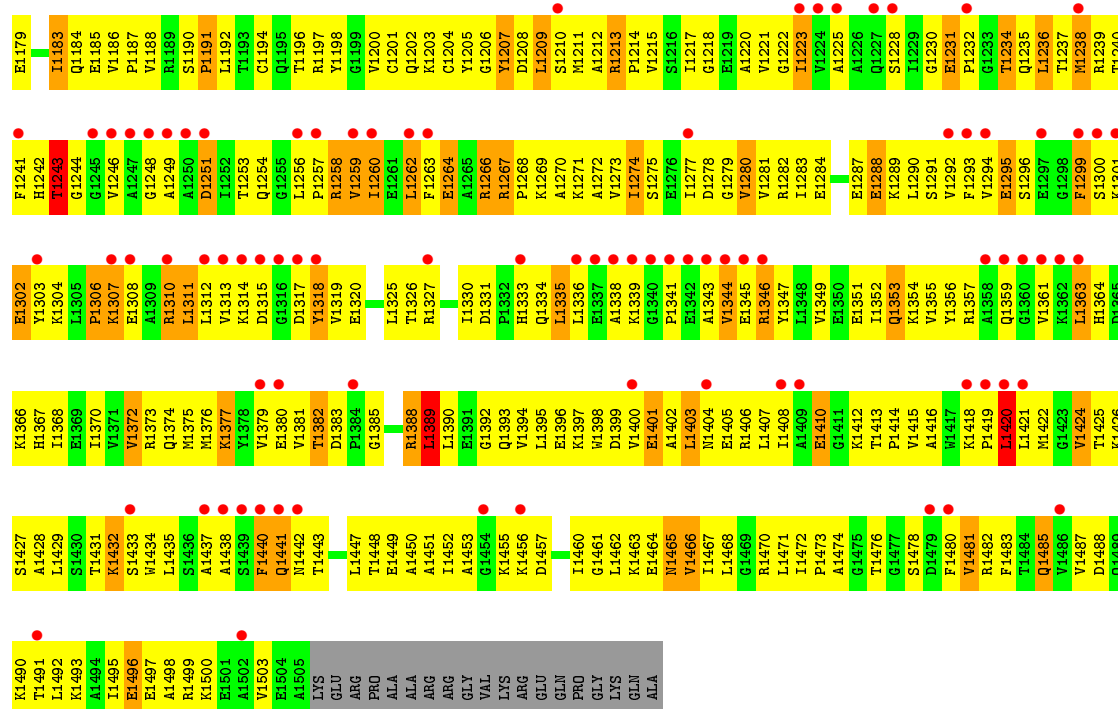


Chain C:

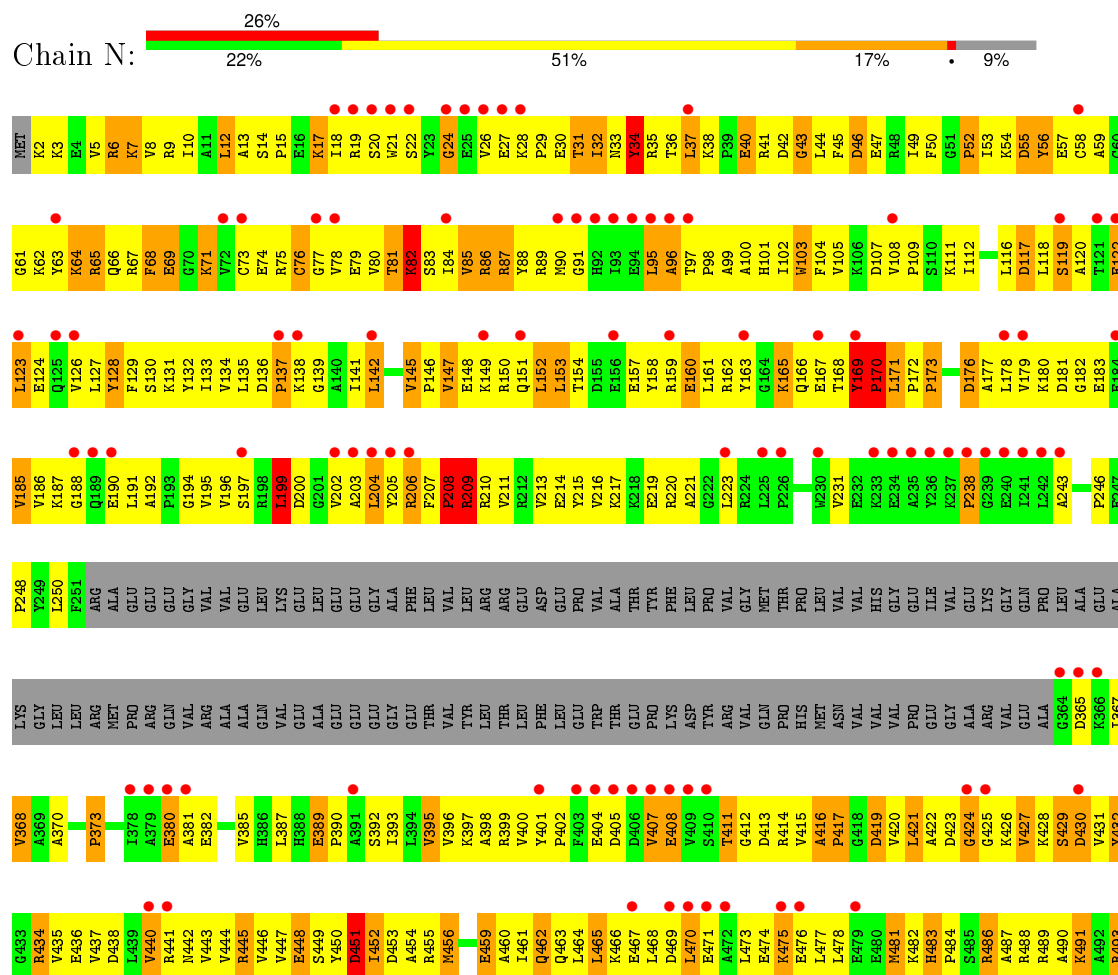




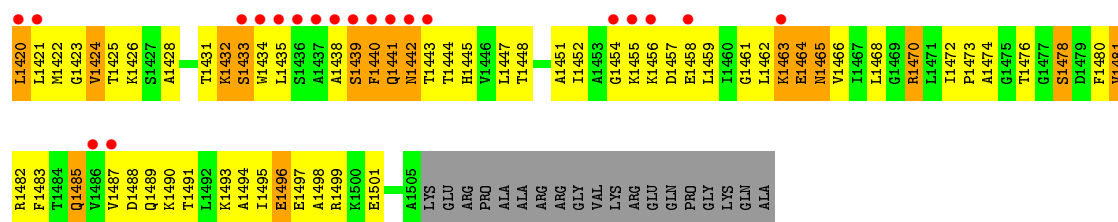
M1116	E1054	K926	V863	G803	D741	R679	M617	L557	I496	V435	P373	F251
Y1117	V1055	T927	V864	L804	G742	Q690	L613	L558	E497	E436	E374	ARG
I1118	P1056	A928	V865	E805	D743	R681	L619	A559	V498	V437		ALA
S1119	V1057	R929	V866	F806	Q744	D682	G620	Q560	V499	D438		GLU
P1120	R1058	L930	R867	A907	M745	L683	K621	R500	G561	V377		GLU
P1121	S1059	L931	V868	T808	A746	K684	R622	A562	R501	L439		GLN
L1122	S1060	D932	R869	P809	V747	D685	V623	P563	A501	V440		GLY
F1123	F1061	A933	G870	E810	H748	E686	D624	P564	P502	R441		VAL
T1124	T1062	L934	R871	E811	V749	V687	G625	L565	D504	M442		ARG
P1125	E1063	R935	R872	A812	P750	V688	G626	I566	S505	V443		VAL
D1126	L1064	V936	L873	L813	S751	D689	G627	S505	S626	R444		ALA
E1127	L1065	V937	E874	A814	S752	D690	R628	R568	S506	V445		GLN
V1128	L1066	G938	R875	A815	S753	L691	S629	R569	R507	V446		LYS
T1129	V1067	P939	S876	H816	F754	E682	V630	E570	R508	V447		GLU
S1130	L1068	T940	R877	E817	F755	E683	L631	K571	P509	E448		ALA
G1131	E1069	F941	G878	R818	Q756	V694	V632	R572	E388	V449		GLU
L1132	F1070	S942	R879	G819	A757	L695	G633	M573	E389	E388		GLU
R1135	F1071	T943	L880	E820	E758	H696	G634	M574	D451	P390		GLY
K1136	L1072	T944	L881	V821	A759	G697	P635	Q575	L574	L452		ALA
I1137	S1073	S945	R882	A822	R760	K698	Q636	E576	D453	L453		PHE
A1138	S1074	G946	E883	L823	L761	V699	L637	A516	A454	R455		LEU
D1139	H1075	T947	R884	N824	Q762	V700	K638	V578	R455	A454		VAL
T1140	G1076	T948	L885	A825	M763	L701	L639	D579	V395	V395		LEU
E1141	A1077	T949	V886	P826	L764	L702	H640	A580	K397	K397		ARG
L1144	K1078	G950	V890	I827	S765	N703	Q641	L581	E459	A397		LEU
Y1145	X1079	D951		K828	A766	R704	C642	L582	L460	R399		ASP
Y1146	A1082	D952	E893	V829	H767	A705	G643	D583	L461	R399		LEU
R1147	A1085	E954	R894	A830	N768	P706	G644	N584	Q463	V400		GLU
V1148	L1086	V955	V895	R832	L770	L707	P645	R525	L464	P402		VAL
R1151	L1087	P957	R897	E833	L771	H709	K646	R586	L465	F403		ALA
E1152	T1088	E958	R898	T834	P772	R710	M643	R587	K466	E404		THR
E1153	L1089	E959	S1026	T835	A773	R711	A649	G588	E467	D405		THR
E1154	D1090	R960	S1027	R836	E776	L711	A649	A589	L468	D405		PHE
E1155	S1091	K961	R1029	R838	P777		L650	P590	L468	D405		PHE
L1156	G1092	Q962	L1030	L839	E777		L652	V591	L470	V407		LEU
L1157	V1093	V963	P903	K840	L778		L652	T592	E471	V409		VAL
G1158	L1094	L964	V904	E841		A715	L652	G532	L472	S410		VAL
V1159	T1095	E965	P905	V842		F716	P653	G533	L473	T411		GLY
L1160	R1096	Q966	Q906	F843		Q717	P653	G533	L473	T411		GLY
L1161	K1097	A967	E907	A844		P718	P654	P594	L476	G412		THR
E1162	L1098	E968	N908	N845		V719	P655	G595	L476	D413		THR
G1163	D1100	R969	S910	P846		L720	F656	S596	L477	R414		LEU
T1164	V1101	L970	L911	D847		E721	L657	D597	L477	R414		NET
L1165	T1102	L971	R912	E848		E722	L658	R598	L478	V415		VAL
L1166	H1103	Q973	L850	A849		L728	L659	P599	L478	V415		VAL
S1167	E1104	R1042	L914	L851		H729	K660	L600	E479	R417		VAL
M1168	L1105	E976	V915	A852		P730	K661	L601	E480	V417		HIS
D1169	V1106	Q976	V916	V853		L731	E667	R601	E480	G418		GLY
D1170	V1107		Q917	A854		I732	P668	D542	A487	L421		PRO
R1171	E1108	E979	R918	H855		V732	M669	S602	K482	L421		ILE
H1172	A1109	F919	V919	G856		Q733	V670	L603	P483	A422		VAL
L1173	P1048	L933	L921	I857		E734	K671	R544	R488	D423		GLY
L1174	D1111	T984	R921	V858		R796	A672	Q611	R489	S429		ALA
L1175	G1112	T984	L922	D859		K797	F736	N551	A490	D430		GLU
L1176	G1113	E987	G923	V860		E798	R675	R613	A492	V431		ALA
A1177	T1114	R988	N924	L860		K800	M676	F614	R493	G432		LYS
A1178	T1115	Y989	E925	D862		F740	E678	Q616	K494	G433		GLY
									K495	A370		LEU



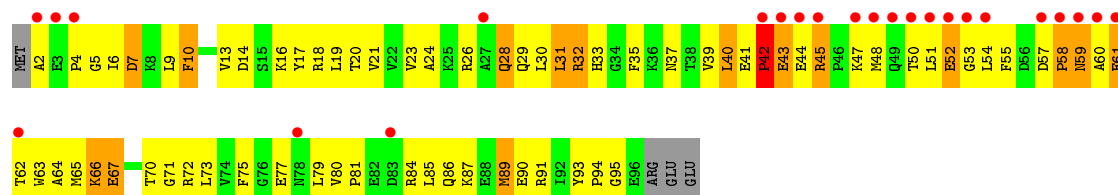
• Molecule 3: DNA-directed RNA polymerase beta' chain



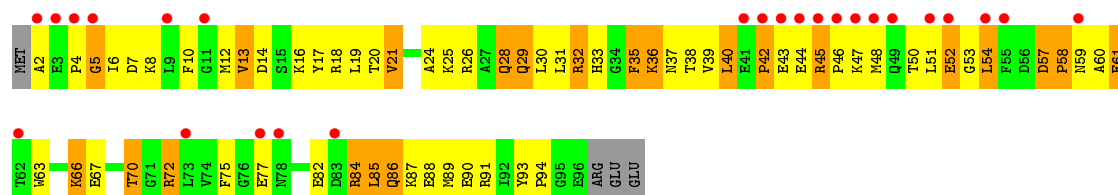
G1360	V1361	F1298	T1237	I1175	T1114	T1052	D990	T927	V866	G803	D743	R879	Q616	K555	K494
K1362	L1363	F1299	M1238	A1176	T1115	F1053	Q991	A928	R867	L804	Q744	Q880	M617	K556	R495
L1364	H1365	S1300	M1239	A1177	T1116	V1054	Y992	R929	Y868	E805	A745	R881	L618	L557	E497
H1366	H1367	K1301	T1240	A1178	Y1117	V1055	L993	L930	M869	R806	A746	M882	L619	L558	
D1368	K1369	L1302	F1241	E1182	L1118	P1056	Q994	L931	G870	A807	V747	I683	G620	G561	R500
K1370	K1371	L1303	H1242	I1183	S1119	V1057	L995	D932	K371	R809	H748	D885	K621	A562	L501
H1372	L1373	K1304	T1243	T1184	F1120	R1058	Q996	A933	R872	E810	V749	D886	R622	A563	F502
L1374	L1375	P1305	G1244	Q1185	L1122	S1059	T997	Y937	L873	E811	W750	E886	V623	E564	D504
L1376	L1377	L1306	E1245	E1186	F1123	F1061	T999	Y937	T875	A812	W751	D688	Y625	I565	S505
L1378	L1379	L1307	P1246	P1187	K1124	R1062	T1000	Y937	T876	S753	S753	D689		I566	
L1380	L1381	L1308	G1247	Q1188	P1125	E1064	E1001	T940	P877	F754	A765	A690	R628	I567	G506
L1382	L1383	L1309	E1248	V1189	P1126	G1063	K1002	F941	G878	E817	A766	L691	R629	R568	N507
L1384	L1385	L1310	L1249	S1190	E1127	L1065	V1003	S942	R879		Q756	E892	V630	N507	R508
L1386	L1387	L1311	A1250	P1191	T1128	T1067	T1004	T943	I880	E820	A757	E893	I631	E570	R509
L1388	L1389	L1312	P1251	P1192	Q1005	V1067	Q1005	T944	L881	W821	E758	V694	V632	K571	E510
L1390	L1391	L1313	T1252	T1193	A1006	L1068	A1006	S945	R882	A822	A759	I695	V633	R572	M511
L1392	L1393	L1314	T1253	T1194	V1007	E1069	A1007	Q946	F883	L823	A883	H696	G634	M573	M512
L1394	L1395	L1315	Q1254	T1195	F1008	Y1070	F1008	T947	R884	N824	W761	G697	P635	L574	L513
L1396	L1397	L1316	Q1255	Q1196	K1009	F1071	K1009	T948	R885	A825	Q762	K698	Q636	Q575	L514
L1398	L1399	L1317	P1256	T1197	M1010	T1072	V886	T949	V886	P826	W763	V699	L637	E576	E515
L1400	L1401	L1318	R1257	R1197	L1011	S1073	A887	Q950	A887	I827	L764	W700	K638	A516	A516
L1402	L1403	L1319	G1198	G1199	F1012	S1074	E888	I951	E888	K828	S765	I701	L639	V577	V577
L1404	L1405	L1320	E1200	D1201	E1013	A1077	A889	D952	A889	W829	A766	L702	H640	P518	P518
L1406	L1407	L1321	V1202	Q1202	M1014		V890	D953	E891	A830	H767	N703	Q641	D580	V519
L1408	L1409	L1322	T1203	G1203	F1017	G1080	D992	A954	E891	G831	W768	R704	C642	L581	L520
L1410	L1411	L1323	R1204	K1204	G1018	G1081	N1018	V955	D992	R832	L769	A705	G643	L582	P521
L1412	L1413	L1324	E1205	E1205	G1082	G1081	L1018	I956	E893	E833	L770	P706	L644	D583	P522
L1414	L1415	L1325	G1206	G1206	A1083	A1082	P1019	P957	K894	T834	S771	T707	P645	N584	L524
L1416	L1417	L1326	L1207	L1207	D1083	D1083	L1020	P958	V895	S835	P772	L708	G646	G585	L524
L1418	L1419	L1327	P1208	P1208	L1084	L1084	V1021	R959	A896	W836	A773	H709	R647	R586	R525
L1420	L1421	L1328	G1209	G1209	A1085	A1085	Y1022	R960	A897	G837	S774	R710	M648	R587	P526
L1422	L1423	L1329	D1209	D1209	L1086	L1086	M1023	R961	E898	R838	G775	L711	A649	G588	M527
L1424	L1425	L1330	S1210	S1210	T1087	T1087	Y1023	Q962	L999	L839	W776	G712	E850	P528	Q529
L1426	L1427	L1331	M1211	M1211	G1088	G1088	S1026	Y963	I900	K840	P777	I713	E851	V591	V530
L1428	L1429	L1332	A1212	A1212	A1089	A1089	G1027	L964	Q901	W842	L778	Q714	K654	D531	D531
L1430	L1431	L1333	R1213	R1213	D1090	D1090	A1028	E965	L902	F843	W780	A715	P855	G532	G532
L1432	L1433	L1334	P1214	P1214	S1091	S1091	R1029	E966	D903	R843	F781	F716	F656	G533	G533
L1434	L1435	L1335	G1215	G1215	G1092	G1092	Y904	A967	P905	A844	S782	Q717	L657	G595	R534
L1436	L1437	L1336	T1216	T1216	L1094	L1094	P1032	P968	Q906	P846	R783	F718	L657	F535	F535
L1438	L1439	L1337	D1217	D1217	T1095	T1095	Q1033	R969	E907	D847	D784	W719	K659	D597	A536
L1440	L1441	L1338	G1218	G1218	K1096	K1096	Q1034	L971	K908	E848	W785	L720	K660	T537	R598
L1442	L1443	L1339	E1219	E1219	G1097	G1097	L1035	R972	N909	A849	L786	S725	M661	P599	S538
L1444	L1445	L1340	R1220	R1220	L1098	L1098	R1036	Q973	S910	L850	L787	I726	E662	L600	D539
L1446	L1447	L1341	G1222	G1222	V1099	V1099	Q1037	Q974	L911	L851	W788	Q727	E663	R601	D539
L1448	L1449	L1342	I1223	I1223	D1100	D1100	L1038	E975	K912	A852	L789	L728		S602	N541
L1450	L1451	L1343	E1224	E1224	V1101	V1101	C1039	Q976	E913	W853	W790	H729	I666	D542	D542
L1452	L1453	L1344	T1225	T1225	G1163	G1163	G1040	A977	L914	A854	V791	P730	A667	L543	L543
L1454	L1455	L1345	A1226	A1226	T1102	T1102	L1041	Q977	V915	H855	W792	L731	P668	T604	T604
L1456	L1457	L1346	E1227	E1227	E1103	E1103	L1042	X978	V916	G856	W793	V732	M669	D605	V544
L1458	L1459	L1347	R1228	R1228	I1104	I1104	Q1043	E979	Q917	R857	Q794	C733	V670	L606	R545
L1460	L1461	L1348	E1289	E1289	V1106	V1106	G1043	R980	L920	I857	W795	W734	K671	L607	R546
L1462	L1463	L1349	L1289	L1289	L1107	L1107	M1045	F982	R921	W858	A796	A735	A672	S608	L547
L1464	L1465	L1350	G1230	G1230	R1108	R1108	Q1046	Q981	L921	D859	W796	A736	K672	G609	L548
L1466	L1467	L1351	E1231	E1231	E1109	E1109	K1047	T985	R922	L860	K797	F736	A673	K610	N549
L1468	L1469	L1352	P1232	P1232	T1109	T1109	P1048	Q986	L923	Q861	W798	N737	R674	Q611	R550
L1470	L1471	L1353	G1233	G1233	A1110	A1110	Q1049	Q987	G923	D862	K799	R800	K675	G612	N551
L1472	L1473	L1354	T1234	T1234	D1111	D1111	S1049	E987	E925	W863	W799	F740	M676	R613	N552
L1474	L1475	L1355	E1235	E1235	C1112	C1112	G1050	R988	E925	W864	R801	D741	L677	F614	R553
L1476	L1477	L1356	L1236	L1236	G1113	G1113	E1051	Y989	K926	T865	A802	G742	E678	R615	L554



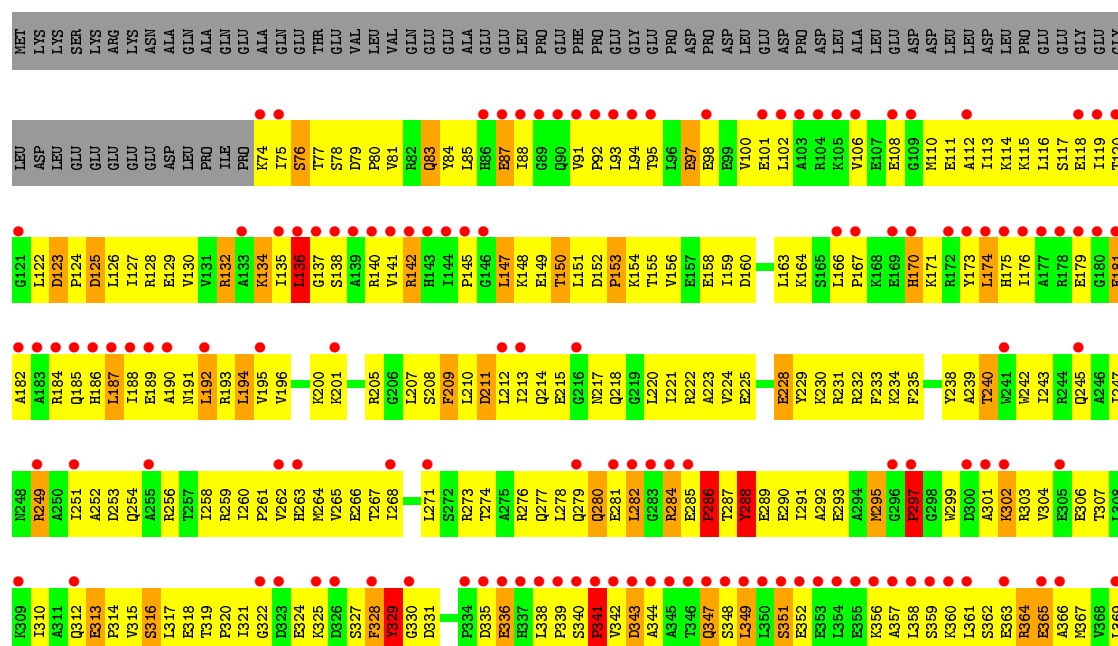
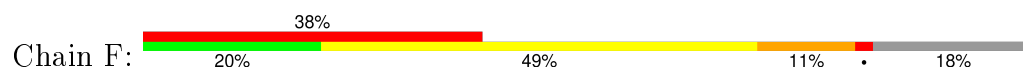
• Molecule 4: RNA polymerase omega chain

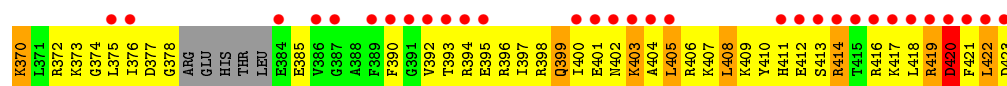


• Molecule 4: RNA polymerase omega chain

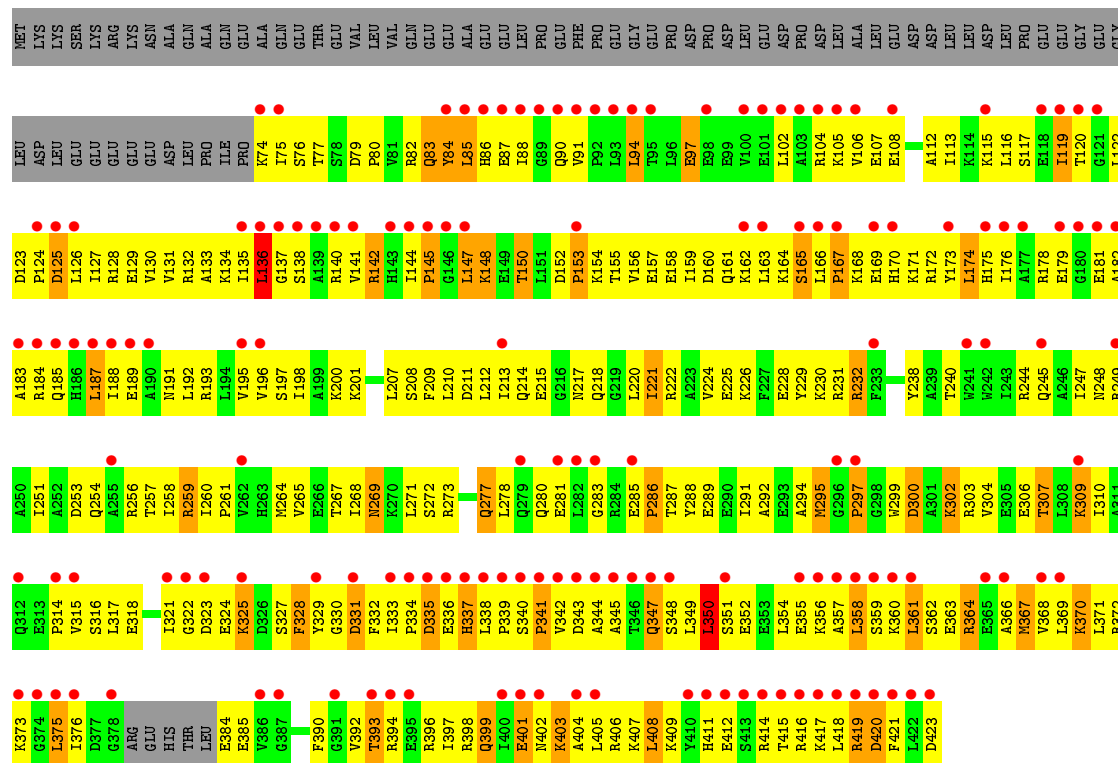
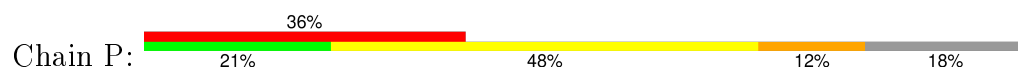


• Molecule 5: RNA polymerase sigma factor rpoD





● 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 – 2.40 36.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.40) 95.2 (36.81-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.274 0.235 , 0.272	Depositor DCC
R_{free} test set	34795 reflections (6.11%)	DCC
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , -79.6	EDS
Estimated twinning fraction	0.500 for H, K, L 0.500 for -H, -K, L 0.499 for -h,-k,-l 0.065 for h,-h-k,-l 0.065 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for -H, -K, L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 604645 reflections	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	61800	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

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	0.77	0/1838	0.86	3/2498 (0.1%)
1	B	0.70	0/1838	0.83	4/2498 (0.2%)
1	K	0.76	0/1838	0.85	4/2498 (0.2%)
1	L	0.73	0/1838	0.76	0/2498
2	C	0.81	0/8997	0.89	8/12164 (0.1%)
2	M	0.80	2/8997 (0.0%)	0.89	12/12164 (0.1%)
3	D	0.82	0/10975	0.92	21/14836 (0.1%)
3	N	0.80	1/10975 (0.0%)	0.92	17/14836 (0.1%)
4	E	0.80	0/783	0.94	0/1054
4	O	0.81	0/783	0.92	0/1054
5	F	0.71	0/2812	0.81	1/3781 (0.0%)
5	P	0.72	0/2812	0.78	2/3781 (0.1%)
All	All	0.79	3/54486 (0.0%)	0.89	72/73662 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	733	CYS	CB-SG	-5.54	1.72	1.81
2	M	202	TYR	CD2-CE2	5.05	1.47	1.39
2	M	682	TYR	CD2-CE2	5.02	1.46	1.39

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LEU	CA-CB-CG	10.11	138.56	115.30
3	N	199	LEU	CA-CB-CG	-8.78	95.11	115.30
2	M	557	ARG	NE-CZ-NH2	7.73	124.17	120.30
3	D	199	LEU	CA-CB-CG	-7.64	97.72	115.30
3	N	1389	LEU	CA-CB-CG	7.54	132.65	115.30

There are no chirality outliers.

There are no planarity outliers.

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	232	0
1	B	1806	0	1861	217	0
1	K	1806	0	1861	195	0
1	L	1806	0	1861	216	0
2	C	8829	0	8933	1248	0
2	M	8829	0	8933	1139	0
3	D	10797	0	10873	1481	0
3	N	10797	0	10873	1398	0
4	E	769	0	775	101	0
4	O	769	0	775	98	0
5	F	2771	0	2844	350	0
5	P	2771	0	2844	345	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	N	2	0	0	0	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	D	26	0	15	3	0
8	N	26	0	14	1	0
9	A	250	0	0	46	0
9	B	329	0	0	67	0
9	C	1321	0	0	266	0
9	D	1655	0	0	324	0
9	E	176	0	0	32	0
9	F	519	0	0	103	0
9	K	278	0	0	43	0
9	L	309	0	0	68	0
9	M	1236	0	0	259	0
9	N	1552	0	0	306	0
9	O	137	0	0	23	0
9	P	422	0	0	84	0
All	All	61800	0	54323	6611	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 61.

The worst 5 of 6611 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:409:ARG:HA	2:M:454:SER:HA	1.20	1.15
3:D:1045:MET:HG2	3:D:1073:SER:HA	1.33	1.10
3:D:119:SER:HB2	3:D:123:LEU:H	1.23	1.04
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.41	1.02
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.43	1.01

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%)	200 (88%)	22 (10%)	5 (2%)	8	9
1	B	227/315 (72%)	200 (88%)	22 (10%)	5 (2%)	8	9
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	11	13
1	L	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	11	13
2	C	1117/1119 (100%)	927 (83%)	138 (12%)	52 (5%)	3	2
2	M	1117/1119 (100%)	926 (83%)	142 (13%)	49 (4%)	3	2
3	D	1388/1524 (91%)	1155 (83%)	168 (12%)	65 (5%)	3	2
3	N	1388/1524 (91%)	1133 (82%)	187 (14%)	68 (5%)	3	1
4	E	93/99 (94%)	76 (82%)	13 (14%)	4 (4%)	3	2
4	O	93/99 (94%)	76 (82%)	13 (14%)	4 (4%)	3	2
5	F	341/423 (81%)	290 (85%)	35 (10%)	16 (5%)	3	2
5	P	341/423 (81%)	288 (84%)	38 (11%)	15 (4%)	3	2
All	All	6786/7590 (89%)	5671 (84%)	824 (12%)	291 (4%)	3	2

5 of 291 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	231	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%)	149 (74%)	53 (26%)	0	0
1	B	202/273 (74%)	167 (83%)	35 (17%)	2	2
1	K	202/273 (74%)	154 (76%)	48 (24%)	1	1
1	L	202/273 (74%)	152 (75%)	50 (25%)	1	1
2	C	941/941 (100%)	722 (77%)	219 (23%)	1	1
2	M	941/941 (100%)	731 (78%)	210 (22%)	1	1
3	D	1123/1279 (88%)	861 (77%)	262 (23%)	1	1
3	N	1123/1279 (88%)	832 (74%)	291 (26%)	0	0
4	E	83/87 (95%)	65 (78%)	18 (22%)	1	1
4	O	83/87 (95%)	61 (74%)	22 (26%)	0	0
5	F	295/370 (80%)	234 (79%)	61 (21%)	1	1
5	P	295/370 (80%)	242 (82%)	53 (18%)	2	2
All	All	5692/6446 (88%)	4370 (77%)	1322 (23%)	1	1

5 of 1322 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	136	LEU
1	L	197	LEU
3	N	1401	GLU
5	F	249	ARG

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Mol	Chain	Res	Type
1	K	112	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1441	GLN
1	K	229	GLN
3	N	1465	ASN
4	E	28	GLN
5	F	218	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	TGT	D	9001	6	16,27,27	4.14	12 (75%)	19,44,44	2.60	7 (36%)
8	TGT	N	9002	6	16,27,27	4.51	11 (68%)	19,44,44	2.71	5 (26%)

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
8	TGT	D	9001	6	-	0/8/57/57	0/0/2/2
8	TGT	N	9002	6	-	0/8/57/57	0/0/2/2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	9001	TGT	C6-C7	2.25	1.58	1.53
8	N	9002	TGT	C6-C7	2.37	1.58	1.53
8	N	9002	TGT	C2-N2	2.53	1.51	1.47
8	D	9001	TGT	O10-C3	2.88	1.49	1.44
8	D	9001	TGT	P1-O7	3.67	1.67	1.54

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	9002	TGT	O10-C10-O11	-2.54	117.85	122.92
8	D	9001	TGT	O3-C8-N1	-2.32	118.16	123.21
8	D	9001	TGT	O11-C10-C11	-2.28	116.39	124.85
8	D	9001	TGT	O6-C1-C2	2.05	110.68	107.81
8	D	9001	TGT	C6-C7-C1	2.17	118.65	112.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	9001	TGT	3	0
8	N	9002	TGT	1	0

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(Å²)	Q<0.9	
1	A	229/315 (72%)	2.14	73 (31%)	1 1	18, 47, 72, 88	0
1	B	229/315 (72%)	2.89	82 (35%)	0 0	34, 66, 82, 88	0
1	K	229/315 (72%)	1.50	71 (31%)	1 1	21, 43, 70, 92	0
1	L	229/315 (72%)	2.20	72 (31%)	1 1	34, 62, 82, 95	0
2	C	1119/1119 (100%)	3.18	424 (37%)	0 0	15, 58, 81, 94	0
2	M	1119/1119 (100%)	3.29	434 (38%)	0 0	15, 55, 81, 97	0
3	D	1392/1524 (91%)	2.06	399 (28%)	1 1	15, 49, 82, 97	0
3	N	1392/1524 (91%)	2.10	402 (28%)	1 1	16, 48, 83, 105	0
4	E	95/99 (95%)	1.45	24 (25%)	1 1	30, 59, 82, 103	0
4	O	95/99 (95%)	1.80	25 (26%)	1 1	22, 59, 77, 87	0
5	F	345/423 (81%)	4.05	160 (46%)	0 0	38, 63, 83, 97	0
5	P	345/423 (81%)	4.08	152 (44%)	0 0	41, 64, 85, 92	0
All	All	6818/7590 (89%)	2.66	2318 (33%)	0 0	15, 54, 82, 105	0

The worst 5 of 2318 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	854	ALA	69.5
3	N	1246	VAL	62.9
3	N	532	GLY	61.9
3	N	533	GLY	59.1
3	N	1248	GLY	59.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
8	TGT	N	9002	26/26	0.81	0.61	0.79	41,47,51,52	0
8	TGT	D	9001	26/26	0.81	0.44	0.32	44,47,50,52	0
6	MG	N	9006	1/1	0.99	0.04	-0.93	4,4,4,4	0
6	MG	C	9004	1/1	0.97	0.06	-1.11	17,17,17,17	0
7	ZN	N	9059	1/1	0.99	0.06	-1.71	42,42,42,42	0
7	ZN	D	9112	1/1	0.99	0.05	-2.12	50,50,50,50	0
7	ZN	N	9113	1/1	0.99	0.10	-2.36	41,41,41,41	0
7	ZN	D	9058	1/1	1.00	0.17	-4.47	56,56,56,56	0
6	MG	D	9003	1/1	0.98	0.06	-	17,17,17,17	0
6	MG	N	9005	1/1	0.98	0.03	-	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.