



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 09:52 am BST

PDB ID : 1I6V  
Title : THERMUS AQUATICUS CORE RNA POLYMERASE-RIFAMPICIN COMPLEX  
Authors : Campbell, E.A.; Korzheva, N.; Mustaev, A.; Murakami, K.; Goldfarb, A.; Darst, S.A.  
Deposited on : 2001-03-05  
Resolution : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

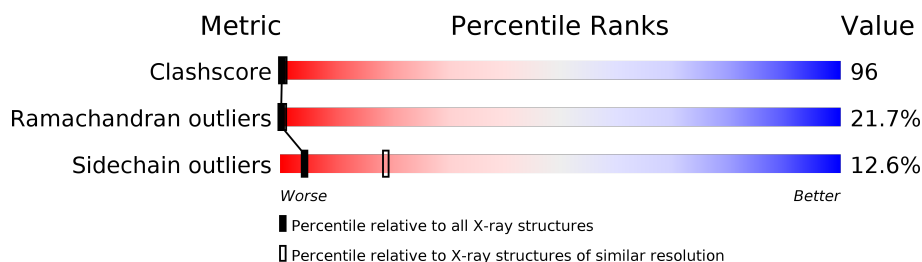
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
2	C	1118	
3	D	1264	
4	E	99	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21292 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1741	1109	299	330	3			
1	B	230	Total	C	N	O	S	0	0	0
			1761	1122	299	337	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	VAL	GLY	CONFLICT	UNP Q9KWU8
A	232	SER	LEU	CONFLICT	UNP Q9KWU8
B	112	VAL	GLY	CONFLICT	UNP Q9KWU8
B	232	SER	LEU	CONFLICT	UNP Q9KWU8

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1113	Total	C	N	O	S	12	0	0
			8508	5386	1514	1585	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LYS	GLU	CONFLICT	UNP Q9KWU7
C	?	-	GLU	DELETION	UNP Q9KWU7
C	1111	VAL	ILE	CONFLICT	UNP Q9KWU7

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1174	Total	C	N	O	S	17	0	0
			8502	5329	1550	1596	27			

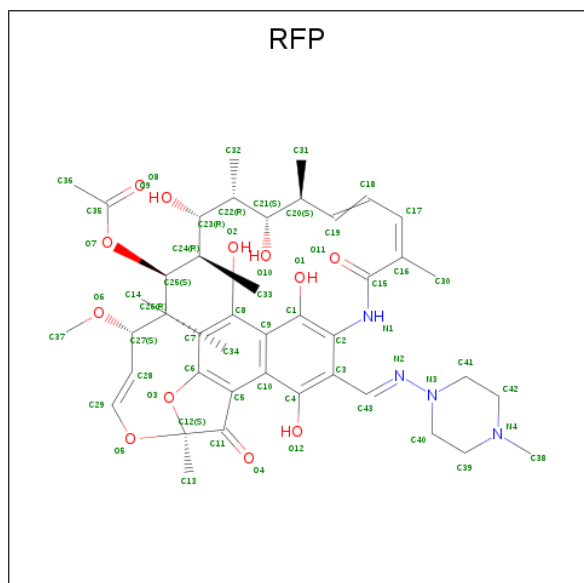
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	ALA	GLY	CONFLICT	UNP Q9KWU6
D	77	ALA	GLY	CONFLICT	UNP Q9KWU6
D	91	ALA	GLY	CONFLICT	UNP Q9KWU6
D	113	ALA	GLY	CONFLICT	UNP Q9KWU6
D	139	ALA	GLY	CONFLICT	UNP Q9KWU6
D	144	ALA	GLY	CONFLICT	UNP Q9KWU6
D	863	THR	VAL	CONFLICT	UNP Q9KWU6
D	866	THR	VAL	CONFLICT	UNP Q9KWU6
D	1009	ASN	LYS	CONFLICT	UNP Q9KWU6

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	98	Total	C	N	O	S	0	0	0
			719	453	132	130	4			

- Molecule 5 is RIFAMPICIN (three-letter code: RFP) (formula:  $C_{43}H_{58}N_4O_{12}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			59	43	4	12		

- 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		

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

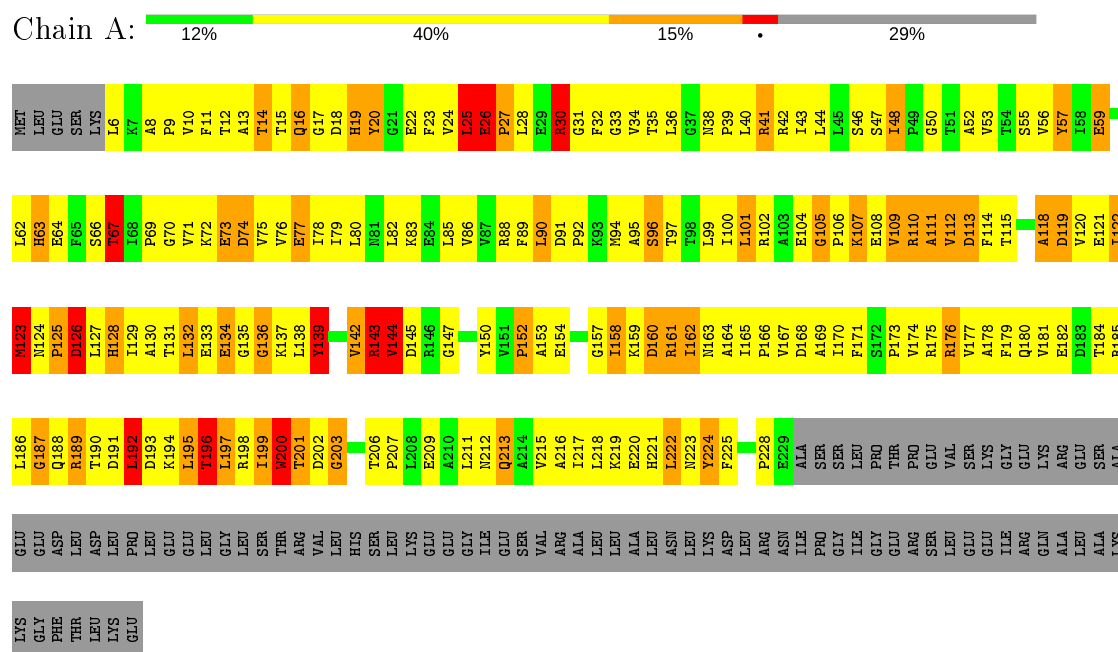
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Zn	0	0
			1	1		

### 3 Residue-property plots

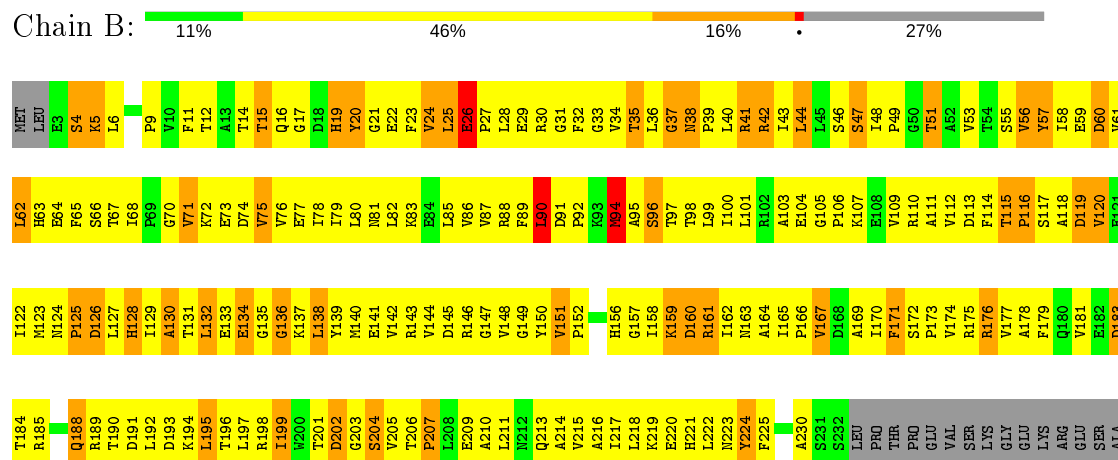
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

#### • Molecule 1: DNA-DIRECTED RNA POLYMERASE



#### • Molecule 1: DNA-DIRECTED RNA POLYMERASE




- Molecule 2: DNA-DIRECTED RNA POLYMERASE



R805	V867	G927	G990	E1051	F1112
L806	D868	K928	Q991	M1052	E1113
R807	V869	R929	N992	L1053	G1114
	I870	G930	F993	T1054	L1115
D810	L871	G931	I994	K1055	ALA
P811	S872	E932	N995	K1056	SER
G812	P873	G933	K996	S1057	LYS
V813	L874	G934	L997	D1058	ARG
E814	G875	G935	Y998	D1059	
K816	V876	V936	H999	I1060	
P817	P877	D937	E1061	E1061	
G818	S878	K938	V1001	G1062	
V819	R879	R939	E1002	E1063	
R820	M880	E940	D1003		
E821	N881		K1004	A1066	
V822	L882	V943	M1005	Y1067	
R824	Q884	L944	H1006	Q1068	
V825	L885	A945	A1007	A1069	
F826	L886	R946	R1008	I1070	
V827	L887	A947	S1009	I1071	
A828	T888	K949	T1010	K1072	
	H889	L950	G1011	G1073	
	L890	G951	P1012	E1074	
	G891	L952	Y1013	D1075	
	L892	V953	S1014	V1076	
	A893	S954	L1015	F1077	
	Q894		I1016	E1078	
	V895		T1017	P1079	
	F896		Q1018	S1080	
	G897		I019	V1081	
	L897		P1020	P1082	
	G898		L1021	E1083	
	Q899		G1022	S1084	
	R900		K1023	F1085	
	N901		K1024	L1086	
	I902		A1025	V1087	
	S903		Q1026	L1088	
	H843		F1027	V1089	
	G844		G1028	A1090	
	N845		G1029	E1091	
	K846		Q1030	L1092	
	G847		R1031	Q1093	
	V848		F1032	A1094	
	V849		G1033	L1095	
	A850		E1034	A1096	
	K851		M1035	L1097	
	L852		E1036	D1098	
	L853		Y1037	V1099	
	P854		W1038	Q1100	
	V855		A1039	T1101	
	E856		L1040	L1102	
	D857		E1041	D1103	
	L917		A1042	E1104	
	M858		Y1043	K1105	
	P859		G1044	D1106	
	H860		A1045	M1107	
	L861			P1108	
	P862			V1109	
	D863			D1110	
	G864			L1111	
	P866				

• Molecule 3: DNA-DIRECTED RNA POLYMERASE

Chain D: 

S771	L711	E651	G585	LEU	A460	L127	LYS	MET
S772	G712	L652	R586	PRO	Q462	Y128	ARG	LYS
S773	I713	F653	R587	ARG	K463	F129	GLN	K3
S774	Q714	K654	G588	MET	E463	M130	ARG	E4
S775	I715	P655	S589	VAL	L464	K131	PHE	V6
S776	F716	F656	P590	GLN	L465	Y132	E69	R6
S777	P777	L657	G591	VAL	K466	I133	A70	K7
S778	Q718	L658	R592	ASP	E467	V134	K71	V8
S779	P719	K659	R598	GLY	L468	L135	V72	R9
S780	L720	K660	P599	GLY	D469	D136	LYS	I10
S781	V721	M661	L601	ARG	L470	P137	R75	A11
S782	E722	E662	R601	PHE	A471	C137	C76	L12
S783	G723	E663	S602	ASP	K472	D143	A77	L11
S784	Q724	K664	L603	T537	L473	T144	V78	P15
S785	S725	A665	T604	S538	E474	V145	E79	G15
S786	I726	F666	D605	D539	E475	P146	V80	Y19
S787	Q727	E667	L606	LEU	E480	K149	T81	S20
S788	L728	P668	L607	ASP	K481	R150	R82	M21
S789	H729	M669	S608	D542	L482	Q151	S83	S22
S790	P730	K670	G609	L543	H483	Y152	I84	Y23
S791	L731	K671	Q610	Y544	G484	L152	V85	G24
S792	V732	E672	Q611	R545	S485	L153	R86	E25
S793	Q733	A673	G612	R546	R486	T154	R87	V26
S794	Q734	K674	R613	L547	E487	D155	Y88	E27
S795	E735	R675	F614	R548	L488	X20	R89	K28
S796	F736	M676	Q615	LEU	R489	X30	M90	P29
S797	Q737	L677	R616	ASP	A490	K150	A91	E30
S798	A738	E678	L617	N552	K491	X60	H92	T31
S799	P739	R679	L618	R553	A492	X70	I93	ILE
S800	F740	Q680	L619	L554	R493	X80	E94	ASN
A805	D741	R681	G620	K555	K494	X90	L95	TTR
	Q742	D682	K621	K556	R495	A100	A96	ARG
	D743	L683	R622	L557	L496	X200	T97	THR
	A807	Q744	K684	V623	E497	X210	P98	LEU
S808	M745	D685	R624	L559	V498	Y220	A99	LYS
S809	A746	E686	E625	G560	V499	X230	A100	PRO
S810	V747	R687	S626	P661	R500	X240	W103	GLU
S811	H748	L688	G627	A562	F502	X250	ASP	ARG
A814	V749	D689	R628	P563	E503	X30	F104	GLY
A815	L751	A690	S629	E564	L504	X310	V105	LEU
S816	S752	L691	V630	L565	D504	X320	K106	PHE
S817	E753	E692	I631	L566	S505	X320	D107	LYS
V821	Q754	R693	V632	R567	G506	X330	V108	ASP
	F754	V694	V633	E568	N507	X350	P109	GLU
	A755	L695	G634	N569	R508	X360	S110	ARG
	Q756	H696	P635	E570	P509	X370	K111	ILE
L823	E757	G697	Q636	K571	E510	X390	I112	PHE
S824	S758	K698	L637	R572	M511	X400	A113	GLY
S825	A759	V699	R638	R573	M512	X410	A113	PRO
S826	P760	L700	L639	L574	L513	X420	T114	ILE
L827	I761	L701	H640	Q675	L514	X430	L116	LYS
S828	Q762	L702	Q641	E576	E515	X440	D117	ASP
S829	R763	N703	G642	A577	A516	X450	L118	TTR
S830	L764	R704	G643	V578	V517	D453	S119	GLU
S831	S765	A705	L644	D579	P518	R454	A120	CYS
S832	F766	P706	P645	A580	V519	R455	T121	ALA
S833	H767	T707	R647	V581	L520	G456	G57	CYS
S834	N768	L708	K647	L582	P521	H457	P521	GLY
S835	L769	H709	M648	D583	P522	A458	Q125	LYS
S836	L770	P710	D649	N584	R523	V459	V126	TTR



V1466	V1467	L1468	G1469	R1470	L1471	L1472	P1473	V1474	P1475	G1476	G1477	V1478	D1479	F1480	V1481	R1482	F1483	T1484	Q1485	V1486	V1487	D1488	Q1489	R1490	T1491	L1492	G1496	GLU	ALA	ARG	LYS	GLU	LYS	ARG	ARG	PRQ	ARG	PRQ	VAL	ARG	ARG	GLN	PRQ	GLY	LYS	GLY	LEU													
E1405	R1406	L1407	T1408	V1409	GLU	GLY	LYS	V1413	P1414	V1415	R1416	V1417	K1418	P1419	L1420	M1421	M1422	G1423	V1424	T1425	K1426	V1427	A1428	L1429	S1430	T1431	K1432	S1433	V1434	L1435	S1436	A1437	A1438	F1439	Q1440	Q1441	M1442	T1443	L1444	L1447	T1448	E1449	A1450	A1451	A1452	A1453	G1454	K1455	K1456	D1457	E1458	L1459	F1460	G1461	L1462	K1463	K1464	N1465		
P1341	E1342	V1343	V1344	V1345	R1346	V1347	L1348	V1349	D1350	E1351	I1352	Q1353	K1354	V1355	F1356	R1357	V1361	V1362	L1363	H1364	D1365	K1366	H1367	I1368	E1369	I1370	V1371	V1372	L1373	Q1374	M1375	K1376	K1377	Y1378	V1379	E1380	V1381	T1382	D1383	P1384	R1388	L1389	L1390	E1391	Q1392	Q1393	V1394	L1395	E1396	D1397	K1398	H1399	V1400	E1401	A1402	K1403	N1404			
V1273	L1274	S1275	V1276	I1277	D1278	G1279	E1280	V1281	L1282	I1283	L1290	S1291	V1292	F1293	V1294	F1299	S1300	K1301	E1302	Y1303	K1304	L1305	P1306	K1307	D1308	A1309	R1310	L1311	L1312	V1313	K1314	D1315	G1316	D1317	Y1318	V1319	E1320	G1321	G1322	Q1323	L1324	L1325	T1326	R1327	G1328	A1329	L1330	D1331	P1332	H1333	Q1334	L1335	L1336	E1337	A1338	K1339	G1340			
A1212	R1213	P1214	V1215	S1216	I1217	G1218	E1219	A1220	G1221	V1222	V1223	V1224	A1225	A1226	E1227	S1228	E1231	P1232	G1233	T1234	Q1235	L1236	T1237	M1238	R1239	T1240	PHE	HIS	THR	GLY	GLY	VAL	ALA	VAL	G1249	T1250	D1251	T1252	P1253	Q1254	G1255	L1256	P1257	R1258	V1259	E1261	L1262	F1263	E1264	A1265	R1266	G1267	E1268	K1269	A1270	K1271	A1272			
A1150	R1151	E1152	V1153	E1154	A1155	L1156	R1159	L1160	E1161	E1162	G1163	R1164	Y1165	L1166	S1167	L1168	E1169	D1170	V1171	H1172	F1173	L1174	I1175	K1176	A1177	E1179	E1182	V1183	R1184	E1185	V1186	P1187	V1188	R1189	S1190	P1191	L1192	T1193	G1194	Q1195	T1196	R1197	G1198	V1199	V1200	C1201	Q1202	K1203	C1204	Y1205	G1206	Y1207	D1208	L1209	S1210	M1211				
T1088	A1089	D1090	S1091	G1092	Y1093	L1094	T1095	R1096	L1097	L1098	V1099	D1100	V1101	A1102	H1103	E1104	T1105	V1106	V1107	E1108	E1109	A1110	D1111	C1112	G1113	T1114	Y1117	I1118	S1119	L1122	F1123	Q1124	M1125	D1126	E1127	V1128	T1129	R1130	T1131	L1132	R1133	L1134	R1135	R1137	S1138	D1139	I1140	E1141	S1142	G1143	L1144	Y1145	G1146	R1147	V1148	L1149				
A1028	R1029	G1030	S1031	Q1032	R069	Q1034	L1035	R1036	L1037	Q1038	C1039	G1040	M1041	R1042	G1043	E1044	M1045	Q1046	K1047	P1048	S1049	G1050	E1051	T1052	F1053	E1054	V1055	P1056	V1057	S1058	S1059	S1060	F1061	E1062	E1063	G1064	L1065	T1066	V1067	L1068	E1069	Y1070	F1071	L1072	S1073	E1074	H1075	G1076	A1077	R1078	K1079	G1080	G1081	L1082	D1083	T1084	A1085	L1086	R1087	
L964	E965	D966	A967	D968	P905	R969	K970	R972	Q973	Q974	C975	Q976	A977	Y978	N980	L983	T984	D985	R988	N989	M924	D990	Q991	Y992	R993	Q994	L995	N996	T999	S1000	E1001	K935	Y936	V1002	V1003	T1004	Q1005	A1006	V1007	F1008	N1009	N1010	F1011	E1012	E1013	N1014	D952	D953	A954	V955	P1019	L1020	P957	E958	V1022	M1023	K960	Q961	R962	Y963
R837	R838	L839	K840	N845	P846	D847	E848	A849	L850	L851	L852	V853	A854	R855	G856	L857	L858	D859	L860	Q861	D862	T863	V864	M824	T865	T866	R867	L869	G870	R871	R872	L873	T875	S876	P877	G878	R879	L880	L881	F882	A883	R884	V886	G887	E888	A889	V890	G891	D892	E893	K894	V895	A896	Q897	E898	L899				

• Molecule 4: DNA-DIRECTED RNA POLYMERASE

Chain E: 19% 62% 18%

K1	A2	E3	P4	G5	L6	D7	L8	L9	F10	G11	M12	V13	D14	S15	K16	R17	Y18	F19	T20	L21	G22	GLU	K25	R26	A27	Q28	Q29	L30	L31	R32	R33	R34	F35	K36	R37	T38	V39	L40	E41	P42	E43	E44	K47	M48	R49	T50	L51	E52	E53	L54	Y55	D56	D57	P58	N59	A60	V61	T62
M63	A64	R65	K66	R67	L68	L69	T70	G71	R72	L73	F74	F75	G76	E77	N78	L79	R80	P81	E82	D83	R84	L85	D86	R89	L92	Y93	P94	T95	E98	ALA	ARG	LYS	GLU	LYS	GLU	LYS	ALA	PRQ	ARG	ARG	PRQ	VAL	ARG	ARG	GLN	PRQ	GLY	LYS	GLY	LEU								

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.45Å 199.45Å 289.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.30)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.276 , 0.359	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

## 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, RFP, 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	0.43	0/1775	0.77	1/2417 (0.0%)
1	B	0.42	1/1795 (0.1%)	0.77	1/2447 (0.0%)
2	C	0.41	0/8672	0.80	7/11752 (0.1%)
3	D	0.44	1/8439 (0.0%)	0.84	19/11447 (0.2%)
4	E	0.37	0/730	0.71	0/991
All	All	0.42	2/21411 (0.0%)	0.81	28/29054 (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
1	A	0	1
2	C	0	1
3	D	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1270	ALA	C-N	-12.09	1.06	1.34
1	B	94	MET	SD-CE	5.75	2.10	1.77

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270	ALA	O-C-N	-19.05	92.23	122.70
3	D	1270	ALA	C-N-CA	13.67	155.87	121.70
3	D	1270	ALA	CA-C-N	12.08	143.77	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	580	MET	N-CA-C	6.98	129.85	111.00
3	D	1166	LEU	CA-CB-CG	6.22	129.61	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
2	C	1013	TYR	Sidechain
3	D	1165	TYR	Sidechain
3	D	1268	PRO	Mainchain
3	D	1270	ALA	Mainchain

## 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	1741	0	1747	348	0
1	B	1761	0	1754	316	0
2	C	8508	0	8421	1817	0
3	D	8502	0	8002	1671	0
4	E	719	0	685	138	0
5	C	59	0	56	6	0
6	D	1	0	0	0	0
7	D	1	0	0	0	0
All	All	21292	0	20665	4041	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 96.

The worst 5 of 4041 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)
1:B:94:MET:SD	1:B:94:MET:CE	2.10	1.39
2:C:690:ILE:HB	2:C:852:ILE:HG22	1.19	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1280:VAL:HG12	3:D:1281:VAL:HG23	1.25	1.16
2:C:491:GLU:HA	2:C:531:PHE:HA	1.29	1.15
3:D:772:PRO:HG3	3:D:778:LEU:HB2	1.28	1.14

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	222/314 (71%)	111 (50%)	61 (28%)	50 (22%)	0	0
1	B	228/314 (73%)	123 (54%)	62 (27%)	43 (19%)	0	1
2	C	1111/1118 (99%)	591 (53%)	277 (25%)	243 (22%)	0	0
3	D	1126/1264 (89%)	588 (52%)	291 (26%)	247 (22%)	0	0
4	E	96/99 (97%)	50 (52%)	24 (25%)	22 (23%)	0	0
All	All	2783/3109 (90%)	1463 (53%)	715 (26%)	605 (22%)	0	0

5 of 605 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	19	HIS
1	A	26	GLU
1	A	59	GLU
1	A	73	GLU

### 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	A	189/271 (70%)	161 (85%)	28 (15%)	3	13
1	B	190/271 (70%)	169 (89%)	21 (11%)	6	23
2	C	870/935 (93%)	770 (88%)	100 (12%)	5	22
3	D	782/1035 (76%)	671 (86%)	111 (14%)	3	15
4	E	67/88 (76%)	62 (92%)	5 (8%)	13	39
All	All	2098/2600 (81%)	1833 (87%)	265 (13%)	4	19

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	710	ILE
2	C	1115	LEU
3	D	1299	PHE
2	C	743	VAL
2	C	859	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	872	ASN
2	C	1030	GLN
3	D	1374	GLN
2	C	881	ASN
2	C	962	GLN

### 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 3 ligands modelled in this entry, 2 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
5	RFP	C	1640	-	63,63,63	1.26	9 (14%)	94,94,94	0.95	4 (4%)

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
5	RFP	C	1640	-	-	13/60/85/85	0/5/5/5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1640	RFP	O5-C29	3.47	1.48	1.39
5	C	1640	RFP	O4-C11	3.12	1.27	1.21
5	C	1640	RFP	C5-C10	2.99	1.49	1.43
5	C	1640	RFP	C39-N4	2.98	1.52	1.46
5	C	1640	RFP	C8-C9	2.77	1.51	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1640	RFP	C34-C26-C25	-2.37	107.15	111.40
5	C	1640	RFP	C5-C10-C9	-2.33	115.41	119.66
5	C	1640	RFP	O12-C4-C10	2.16	124.19	119.00
5	C	1640	RFP	C24-C23-C22	2.12	118.97	115.43

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

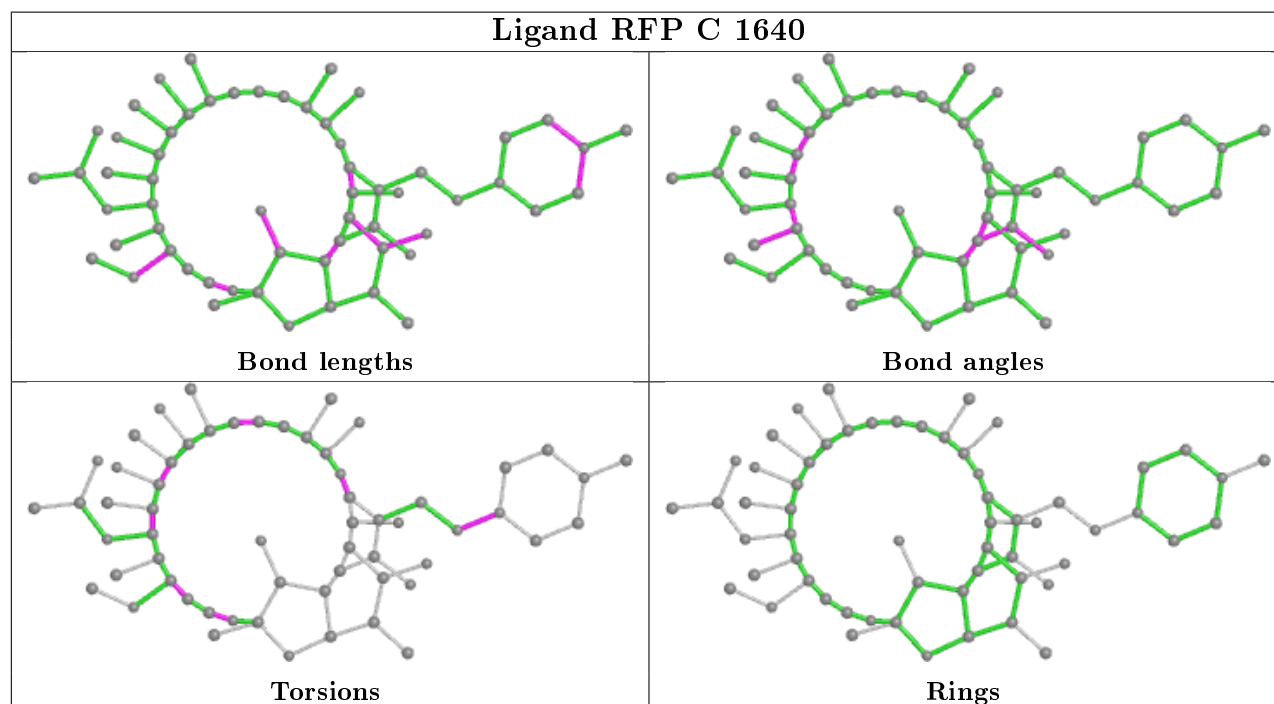
Mol	Chain	Res	Type	Atoms
5	C	1640	RFP	C17-C18-C19-C20
5	C	1640	RFP	C26-C27-C28-C29
5	C	1640	RFP	O6-C27-C28-C29
5	C	1640	RFP	C32-C22-C23-C24
5	C	1640	RFP	C21-C22-C23-C24

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1640	RFP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	155:ASP	C	2(U):UNK	N	54.72
1	D	46(U):UNK	C	452:ILE	N	47.08
1	D	10(U):UNK	C	20(U):UNK	N	15.58
1	D	1270:ALA	C	1271:LYS	N	1.06

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.