



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:19 am GMT

PDB ID : 1H38
Title : STRUCTURE OF A T7 RNA POLYMERASE ELONGATION COMPLEX
AT 2.9Å RESOLUTION
Authors : Tahirov, T.H.; Temyakov, D.; Anikin, M.; Patlan, V.; Mcallister, W.T.; Vasylyev, D.G.; Yokoyama, S.
Deposited on : 2002-08-24
Resolution : 2.90 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

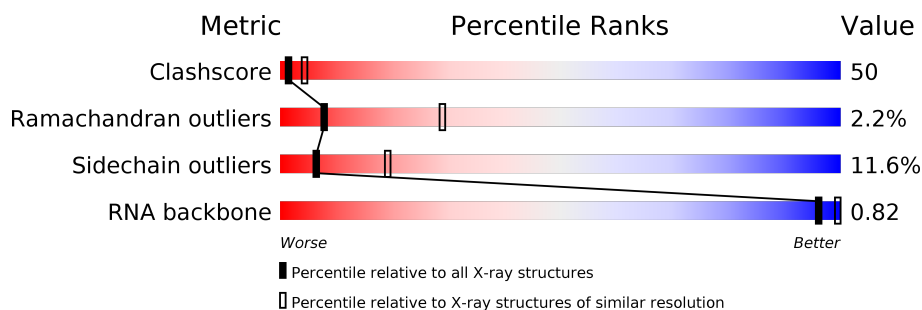
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)

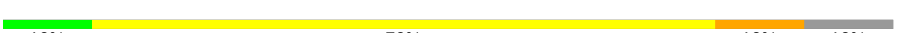


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	883	
1	B	883	
1	C	883	
1	D	883	
2	E	18	
2	H	18	

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Mol	Chain	Length	Quality of chain
2	K	18	
2	N	18	
3	F	12	
3	I	12	
3	L	12	
3	O	12	
4	G	10	
4	J	10	
4	M	10	
4	P	10	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 30948 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	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
1	B	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
1	C	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
1	D	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			

- Molecule 2 is a DNA chain called 5'-D(*GP*GP*GP*AP*AP*TP*CP*GP*AP*CP *AP*TP*CP*GP*CP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	P	0	0	0
			345	164	67	98	16			
2	H	18	Total	C	N	O	P	0	0	0
			367	174	72	104	17			
2	K	17	Total	C	N	O	P	0	0	0
			345	164	67	98	16			
2	N	17	Total	C	N	O	P	0	0	0
			345	164	67	98	16			

- Molecule 3 is a RNA chain called 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
3	I	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
3	L	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			

- Molecule 4 is a DNA chain called 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
4	J	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
4	M	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
4	P	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	310	Total	O	0	0
			310	310		
5	B	352	Total	O	0	0
			352	352		
5	C	185	Total	O	0	0
			185	185		
5	D	177	Total	O	0	0
			177	177		
5	E	13	Total	O	0	0
			13	13		
5	F	16	Total	O	0	0
			16	16		
5	G	12	Total	O	0	0
			12	12		
5	H	20	Total	O	0	0
			20	20		
5	I	11	Total	O	0	0
			11	11		
5	J	9	Total	O	0	0
			9	9		
5	K	17	Total	O	0	0
			17	17		
5	L	5	Total	O	0	0
			5	5		

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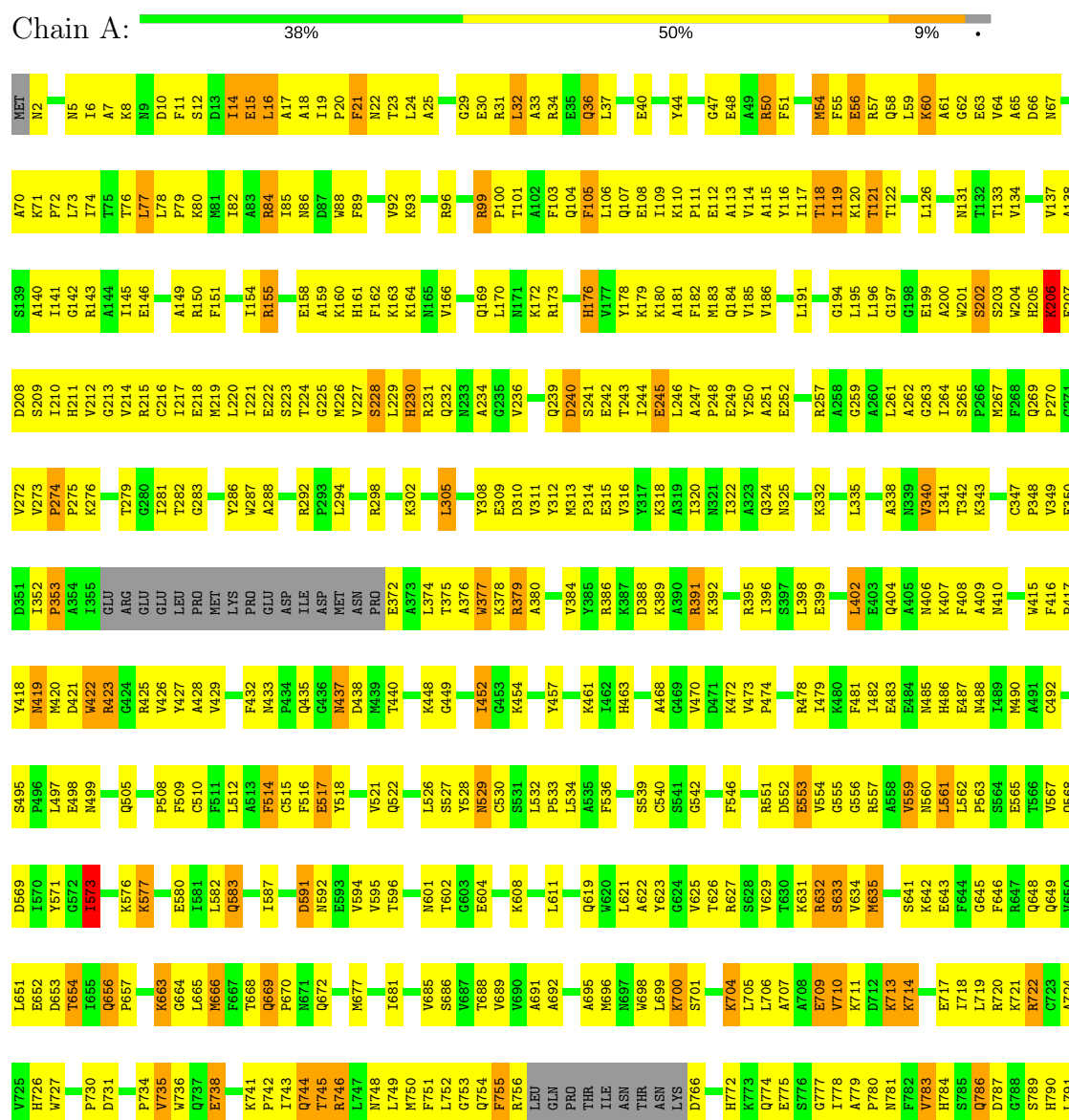
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	8	Total 8	O 8	0	0
5	N	12	Total 12	O 12	0	0
5	O	6	Total 6	O 6	0	0
5	P	9	Total 9	O 9	0	0

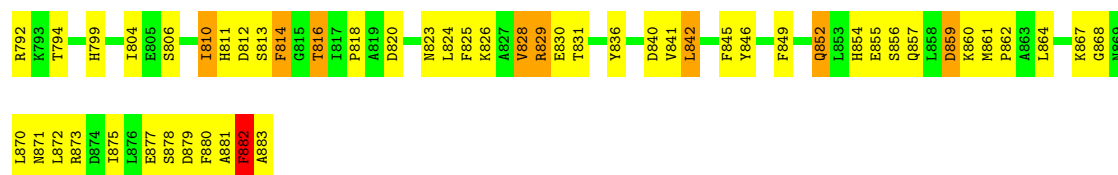
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

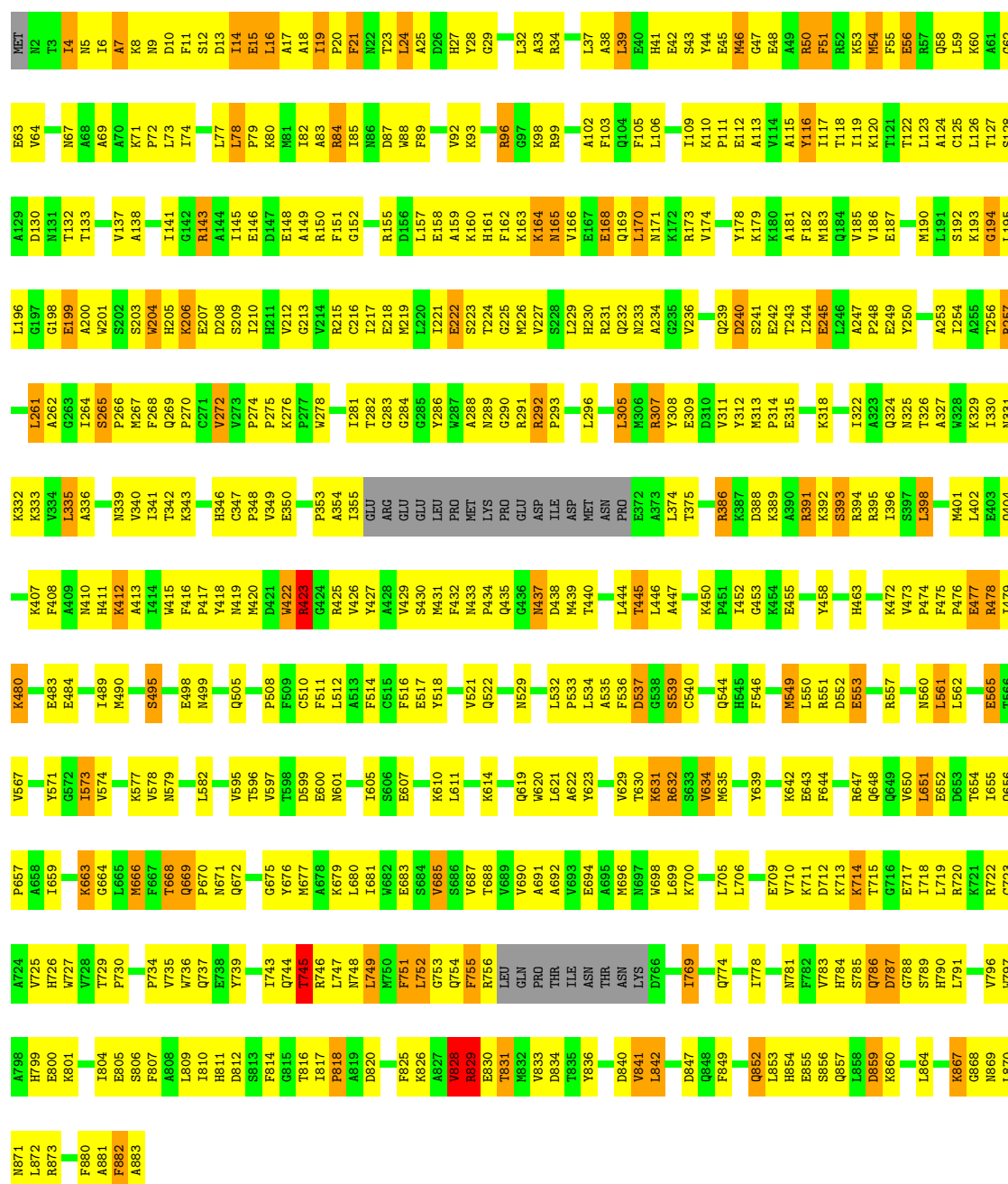
• Molecule 1: DNA-DIRECTED RNA POLYMERASE





• Molecule 1: DNA-DIRECTED RNA POLYMERASE

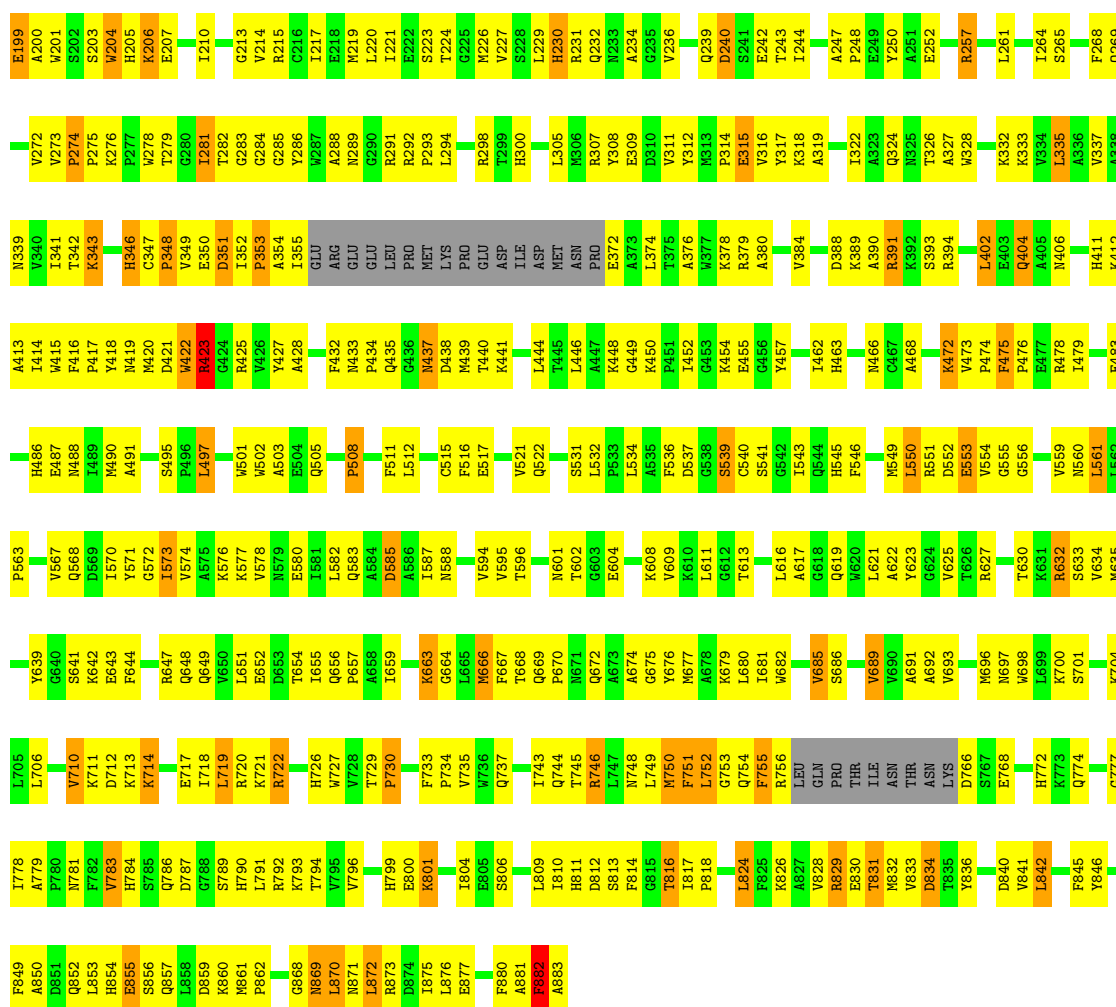
Chain B: 38% 49% 9%



• Molecule 1: DNA-DIRECTED RNA POLYMERASE

Chain C: 39% 49% 8%

ME1	N2	T3	I4	N5	I6	A7	K8	N9	D10	F11	S12	D13	I14	E15	L16	A17	I18	I19	P20	F21	T22	T23	L24	A25	Y28	G29	E30	Q36	L37	A38	E42	S43	Y44	E45	M46	G47	R50	F51	R52	K53	M54	F55	E56	R57	Q58	L59	K60	V64	A68																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
K71	P72	L73	L77	L78	A79	K80	M81	I82	A83	R84	I85	E158	A159	K160	H161	F162	K163	K164	N165	E168	Q169	L170	N171	K172	R173	H176	K179	K180	A181	F182	M183	Q184	V185	A188	D189	M190	L191	G194	L195	L196	L126	T127	S128	T132	T133	V134	H205	E207	D208	S209	I210																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
R143	A144	I145	D146	E147	A149	R150	F151	I154	R155	E158	A159	K160	H161	F162	K163	K164	N165	E168	Q169	L170	N171	K172	R173	H176	K179	K180	A181	F182	M183	Q184	V185	A188	D189	M190	L191	G194	L195	L196	L126	T127	S128	T132	T133	V134	H205	E207	D208	S209	I210																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
H211	V212	G213	V214	L217	E218	T221	E222	S223	T224	G225	K226	V227	L228	H229	K230	R231	Q232	N233	A234	G235	V236	Q239	D240	S241	E242	T243	L244	E245	Y250	R257	A258	G259	L261	N339	V340	L341	T342	K343	H346	C347	P348	V349	E350	D351	L352	I355	A360	A361	A362	A363	A364																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
G285	Y286	G287	A288	R291	R292	P293	L294	S301	K302	K303	A304	L305	M306	R307	V308	V311	Y312	M313	P314	G315	V316	Y317	N321	Q324	N325	T326	A327	K328	N410	H411	K412	A413	J414	W415	F416	P417	Y418	M419	M420	D421	W422	R423	G424	V425	V426	Y427	A428	V429	S430	K431	F432	N433	P434	Q435																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
LYS	PRO	GLU	ASP	ILE	ASP	MET	ASN	PRO	E372	A373	L374	W377	K378	R379	R386	R391	K392	R395	I396	S397	L398	E399	L402	P474	E403	Q404	K407	N410	H411	K412	A413	J414	W415	F416	P417	Y418	M419	M420	D421	W422	R423	G424	V425	V426	Y427	A428	V429	S430	K431	F432	N433	P434	Q435																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G436	M437	D438	T440	L444	L445	L446	K448	I452	G453	K454	E455	G456	Y457	Y458	W459	H463	N466	C467	A468	K472	V473	F475	P476	E477	R478	I479	K480	L481	I482	E483	E484	N485	H486	R487	N488	I489	M490	A491	C492	S495	N499	T500	W501	G502	L503	V504	A505	E506	D507	K508	L509	V510																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
P508	F509	C510	F511	L512	A513	F514	C515	F516	V521	O522	H523	L526	N529	G530	S531	L532	P533	L534	A535	F536	D537	E538	S539	S541	O544	H545	F546	M549	L550	R551	D552	E553	V554	G555	O556	R557	N560	L561	L562	P563	O568	B569	L570	Y571	G572	L573	V574	A575	K576	L577	V578																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L582	A586	I587	N588	V594	V595	T596	V597	N601	T602	G603	E604	L605	R606	G607	K608	V609	K610	L611	K614	A615	L616	Q619	W620	L621	A622	G623	G624	V625	V629	K631	R632	S633	G634	M635	T636	S641	K642	E643	F644	G645	F646	Q649	V650	G651	L652	V653	E654	L655	K656	Q657																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
P657	R663	G664	L665	M666	F667	T668	Q669	P670	R671	Q672	N673	V676	M677	A678	F679	L680	G681	V685	S686	V689	A691	A692	V693	E694	W698	L699	K700	S701	A702	K704	L705	L706	E709	V710	K711	R712	K713	E717	L718	L719	R720	H726	W727	V728	L729	P730	D731	P734	W735																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
Q736	Q737	E738	Y739	K740	K741	P742	I743	Q744	T745	R746	L747	N748	L749	M750	F751	L752	G753	Q754	R755	L756	GLN	THR	ILE	ASN	THR	LYS	D766	S767	E768	I769	Q774	G777	A779	P780	N781	F782	V783	H784	S785	Q786	D787	G788	S789	H790	L791	R792	K793	L794	F795	R796	W797	E800																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
K801	L804	E805	S806	F807	L808	L809	L810	S813	R814	G815	T816	L817	F818	A819	D820	N823	L824	F825	K826	A827	W828	R829	E830	T831	M832	W833	Y836	E837	S838	C839	D840	V841	L842	F845	Y846	D847	Q848	F849	A850	L853	H854	E855	S856	Q857	L858	D859	K860	H861	P862	P865	L866	G868																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
N869	L870	N871	L872	R873	D874	L875	L876	E877	A881	F882	A883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689



• Molecule 2: 5'-D(*GP*GP*GP*AP*AP*TP*CP*GP*AP*CP *AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain E: 61% 28% 6% 6%



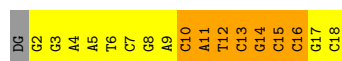
• Molecule 2: 5'-D(*GP*GP*GP*AP*AP*TP*CP*GP*AP*CP *AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain H: 17% 39% 39% 6%

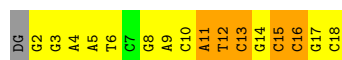


• Molecule 2: 5'-D(*GP*GP*GP*AP*AP*TP*CP*GP*AP*CP *AP*TP*CP*GP*CP*CP*GP*C)-3'

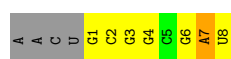
Chain K: 56% 39% 6%



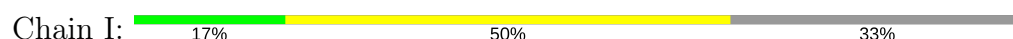
- Molecule 2: 5'-D(*GP*GP*GP*AP*AP*TP*CP*GP*AP*CP *AP*TP*CP*GP*CP*CP*GP*C)-3'



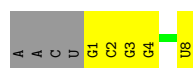
- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'



- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'



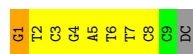
- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'



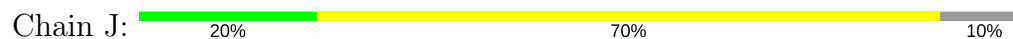
- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'



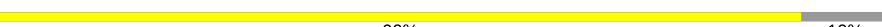
- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'



- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'




- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'

Chain M:  90% 10%

G1	T2	C3	G4	A5	T6	T7	C8	C9	DC
----	----	----	----	----	----	----	----	----	----

- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'

Chain P:  80% 10% 10%

G1	T2	C3	G4	A5	T6	T7	C8	C9	DC
----	----	----	----	----	----	----	----	----	----

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.91Å 84.97Å 202.00Å 90.36° 92.97° 109.94°	Depositor
Resolution (Å)	39.93 – 2.90	Depositor
% Data completeness (in resolution range)	98.0 (39.93-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	30948	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.89	9/6897 (0.1%)	0.85	5/9329 (0.1%)
1	B	0.93	2/6897 (0.0%)	0.87	9/9329 (0.1%)
1	C	0.64	0/6897	0.73	0/9329
1	D	0.58	0/6897	0.70	2/9329 (0.0%)
2	E	0.89	0/387	1.06	1/595 (0.2%)
2	H	0.94	0/412	1.03	1/634 (0.2%)
2	K	0.90	0/387	0.97	0/595
2	N	0.80	0/387	0.95	0/595
3	F	1.09	1/191 (0.5%)	0.85	0/297
3	I	0.94	0/191	0.81	0/297
3	L	0.81	0/191	0.79	0/297
3	O	0.61	0/191	0.74	0/297
4	G	0.88	0/199	0.84	0/305
4	J	0.77	0/199	0.93	0/305
4	M	0.68	0/199	0.85	0/305
4	P	0.74	0/199	1.05	0/305
All	All	0.78	12/30721 (0.0%)	0.81	18/42143 (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
2	E	0	6
2	H	0	8
2	K	0	7
2	N	0	6
4	G	0	1
4	J	0	1
4	P	0	1
All	All	0	30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	CYS	CB-SG	-8.42	1.68	1.82
1	A	573	ILE	CA-CB	7.10	1.71	1.54
1	A	654	THR	CA-CB	5.53	1.67	1.53
1	A	783	VAL	CA-CB	-5.40	1.43	1.54
3	F	7	A	C5-C6	-5.31	1.36	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	537	ASP	CB-CG-OD1	-8.22	110.90	118.30
1	A	557	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	829	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	B	549	MET	CB-CG-SD	-6.86	91.82	112.40
1	A	787	ASP	CB-CG-OD2	-6.55	112.41	118.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	11	DA	Sidechain
2	E	12	DT	Sidechain
2	E	13	DC	Sidechain
2	E	14	DG	Sidechain
2	E	15	DC	Sidechain

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	6746	0	6708	722	0
1	B	6746	0	6708	733	0
1	C	6746	0	6708	680	0
1	D	6746	0	6708	653	0
2	E	345	0	191	30	0
2	H	367	0	202	28	0
2	K	345	0	191	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	345	0	191	21	0
3	F	171	0	89	7	0
3	I	171	0	89	11	0
3	L	171	0	89	9	0
3	O	171	0	89	5	0
4	G	179	0	104	14	0
4	J	179	0	104	8	0
4	M	179	0	104	18	0
4	P	179	0	104	11	0
5	A	310	0	0	102	0
5	B	352	0	0	133	0
5	C	185	0	0	79	0
5	D	177	0	0	105	0
5	E	13	0	0	2	0
5	F	16	0	0	2	0
5	G	12	0	0	5	0
5	H	20	0	0	6	0
5	I	11	0	0	4	0
5	J	9	0	0	4	0
5	K	17	0	0	7	0
5	L	5	0	0	2	0
5	M	8	0	0	1	0
5	N	12	0	0	4	0
5	O	6	0	0	0	0
5	P	9	0	0	3	0
All	All	30948	0	28379	2933	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 50.

The worst 5 of 2933 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:A:668:THR:HG22	1:A:669:GLN:NE2	1.51	1.24
1:C:428:ALA:H	1:C:435:GLN:NE2	1.44	1.15
1:B:50:ARG:HG2	1:B:50:ARG:HH11	1.01	1.14
1:C:133:THR:HA	1:C:243:THR:HG22	1.28	1.10
1:A:120:LYS:HE3	1:A:752:LEU:HD21	1.31	1.10

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	851/883 (96%)	740 (87%)	94 (11%)	17 (2%)	9	31
1	B	851/883 (96%)	736 (86%)	98 (12%)	17 (2%)	9	31
1	C	851/883 (96%)	737 (87%)	93 (11%)	21 (2%)	6	25
1	D	851/883 (96%)	735 (86%)	96 (11%)	20 (2%)	7	27
All	All	3404/3532 (96%)	2948 (87%)	381 (11%)	75 (2%)	8	29

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	GLY
1	A	199	GLU
1	A	539	SER
1	A	663	LYS
1	A	755	PHE

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	703/729 (96%)	615 (88%)	88 (12%)	5	16
1	B	703/729 (96%)	619 (88%)	84 (12%)	6	18
1	C	703/729 (96%)	623 (89%)	80 (11%)	7	20
1	D	703/729 (96%)	628 (89%)	75 (11%)	8	23
All	All	2812/2916 (96%)	2485 (88%)	327 (12%)	6	19

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	668	THR
1	C	120	LYS
1	D	689	VAL
1	B	725	VAL
1	B	829	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	786	GLN
1	C	289	ASN
1	D	744	GLN
1	B	823	ASN
1	C	171	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	F	7/12 (58%)	0	0
3	I	7/12 (58%)	0	0
3	L	7/12 (58%)	0	0
3	O	7/12 (58%)	0	0
All	All	28/48 (58%)	0	0

There are no RNA backbone outliers to report.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.