



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 09:52 AM UTC

PDB ID : 3IKM / pdb_00003ikm
Title : Crystal structure of human mitochondrial DNA polymerase holoenzyme
Authors : Lee, Y.-S.; Kennedy, W.D.; Yin, Y.W.
Deposited on : 2009-08-06
Resolution : 3.24 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

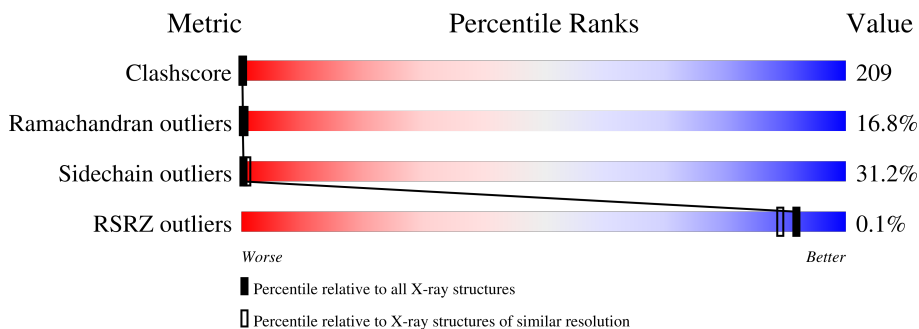
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1172	
1	D	1172	
2	B	427	
2	C	427	
2	E	427	
2	F	427	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29480 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 polymerase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1093	Total	C	N	O	S	0	0	0
			8681	5505	1537	1589	50			
1	D	1094	Total	C	N	O	S	0	0	0
			8695	5515	1540	1590	50			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ASN	-	SEE REMARK 999	UNP P54098
A	355	SER	-	SEE REMARK 999	UNP P54098
D	354	ASN	-	SEE REMARK 999	UNP P54098
D	354A	SER	-	SEE REMARK 999	UNP P54098

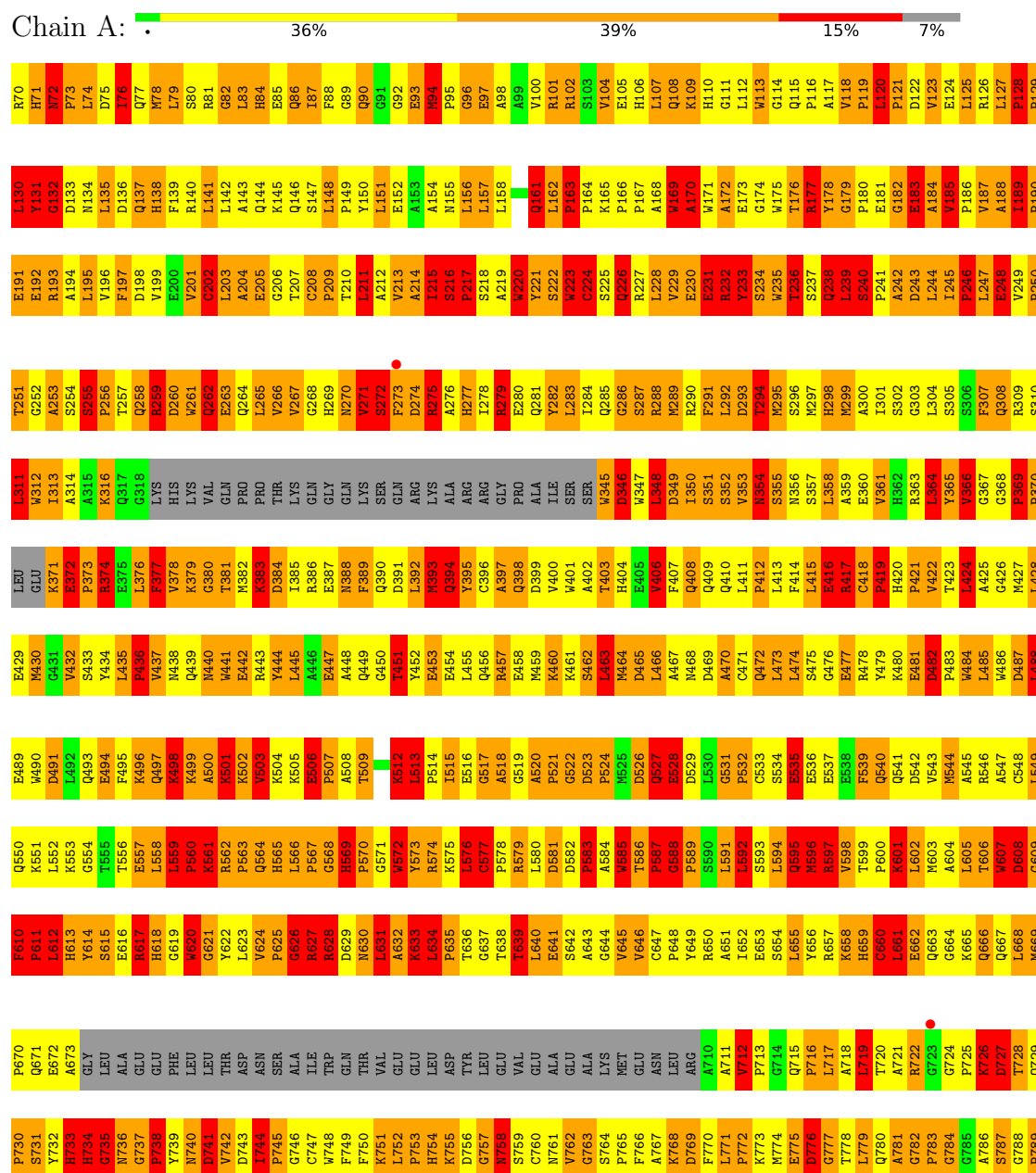
- Molecule 2 is a protein called DNA polymerase subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	355	Total	C	N	O	S	0	0	0
			2871	1840	504	511	16			
2	C	396	Total	C	N	O	S	0	0	0
			3181	2031	563	571	16			
2	E	355	Total	C	N	O	S	0	0	0
			2871	1840	504	511	16			
2	F	396	Total	C	N	O	S	0	0	0
			3181	2031	563	571	16			

3 Residue-property plots

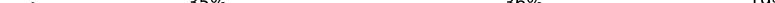
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA polymerase subunit gamma-1



G1211	L1151	E1091	E1031	H971	H911	T851	R790
I1212	A1152	F1092	T1032	R972	G912	R852	A791
P1213	L1153	M1093	A1033	L973	C913	R853	L792
Q1214	T1154	T1094	R1034	T974	T914	A854	E793
G1215	I1155	S1095	K1035	Q975	A915	V855	I794
A1216	L1156	R1096	S1036	Q976	F916	E856	N795
E1217	N1157	V1097	Q1037	E977	G917	R857	K796
L1218	L1158	M1098	M1038	A978	W918	T858	M797
L1219	L1159	W1099	K1039	A979	M919	R859	I798
I1220	T1160	V1100	K1040	E980	T920	L860	S799
V1221	R1161	V1101	W1041	K981	L921	T861	F800
Q1222	K1162	I1102	E1042	A982	Q922	A862	W801
I1223	M1163	S1103	V1043	Q983	G923	S863	R802
I1224	F1164	S1104	V1044	Q984	R924	R864	A803
E1225	A1165	A1105	A1045	M985	K925	A865	N804
L1226	V1166	V1106	E1046	Y986	S926	R866	R805
T1227	K1167	D1107	R1047	A987	E927	P867	K806
K1228	L1168	V1108	A1048	A988	G928	D868	R807
G1229	G1169	L1109	W1049	T989	T929	R869	L808
S1230	L1170	H1110	M1050	K990	D930	V870	S809
L1231	N1171	M1111	G1051	G991	L931	G871	S810
E1232	D1172	M1112	G1052	L992	H932	S872	Q811
K1233	L1173	L1113	T1053	R993	S933	E873	M812
R1234	P1174	V1114	E1054	W994	K934	L874	V813
S1235	Q1175	A1115	S1055	Y995	T935	K875	V814
Q1236	S1176	M1116	E1056	R996	A936	A876	W815
T1237	V1177	K1117	M1057	L997	T937	M877	L816
G1238	A1178	L1118	F1058	S998	T938	V878	R817
P1239	F1179	L1119	M1059	D999	V939	R879	R818
	F1180	F1120	K1060	E1000	G940	A880	
	S1181	E1121	L1061	G1001	I941	P881	
	A1182	E1122	E1062	E1002	S942	P882	
	V1183	F1123	S1063	W1003	R943	G883	
	D1184	A1124	L1064	L1004	E944	A884	
	L1185	I1125	A1065	V1005	H945	T885	
	D1186	D1126	T1066	R006	A946	L886	
	R1187	G1127	S1067	E1007	K947	V887	
	L1188	R1128	D1068	L1008	T948	G888	
	L1189	F1129	T1069	N1009	F949	A889	
	R1190	C1130	P1070	L1010	N950	D890	
	K1191	I1131	R1071	P1011	Y951	V891	
	E1192	S1132	T1072	V1012	G952	D892	
	V1193	L1133	F1073	D1013	R953	S893	
	T1194	H1134	V1074	R1014	I954	Q894	
	M1195	E1135	LEU	T1015	Y955	E895	
	L1196	E1136	GLY	E1016	G956	L896	
	G1197	V1137	CYS	G1017	A957	W897	
	K1198	R1138	CYS	G1018	G958	I898	
	T1199	Y1139	ILE	W1019	Q959	A899	
	P1200	L1140	SER	I1020	P960	A900	
	S1201	V1141	ARG	S1021	F961	V901	
	N1202	R1142	ALA	L1022	A962	L902	
	T1203	E1143	LEU	Q1023	F963	G903	
	T1204	E1144	GLU	D1024	R964	D904	
	M1205	D1145	PRO	L1025	L965	A905	
	K1206	R1146	SER	I1026	L966	H906	
	E1207	Y1147	ALA	K1027	M967	F907	
	R1208	L1148	VAL	V1028	Q968	A908	
	L1209	A1149	GLN	Q1029	F969	G909	
	K1210	A1150	E1030	L1030	M970	V910	

- Molecule 1: DNA polymerase subunit gamma-1

Chain D:  35% 36% 19% 7%

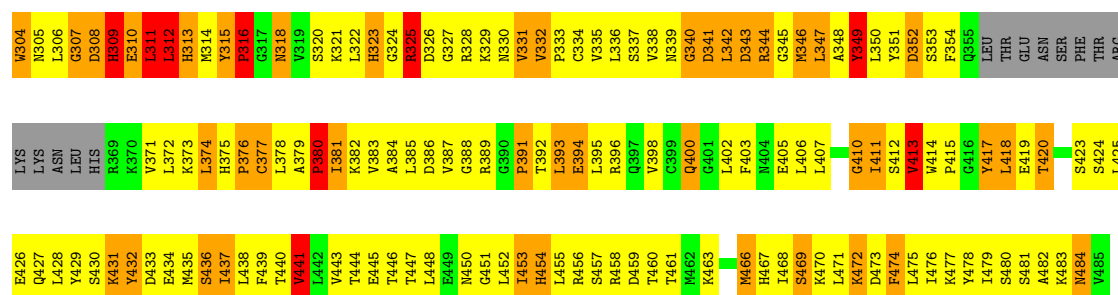
R70	R491	R431	K371	I313	A253	R183	Y131	R71
	L492	V432	E372	A314	S254	A194	G132	
	Q493	S433	P373	A315	S255	L195	D133	
	E494	Y434	R374	K316	P256	V196	N134	
	F495	L435	E375	K317	T257	F197	L135	
	K496	P436	L376	G318	Q258	D198	P136	
	Q497	V437	F377	LYS	R259	V199	Q137	
	K498	M438	P378	HIS	D260	E200	H138	
	R499	Q439	K379	LYS	W261	V201	F139	
	A500	N440	G380	VAL	Q262	C202	R140	
R72	K501	W441	T381	GLN	E263	L203	L141	R73
	F502	E442	K382	PRO	Q264	A204	L142	
	V503	R443	K383	PRO	L265	E205	A143	
	R504	L444	D384	THR	V266	G206	Q144	
	K505	L445	T385	LYS	V267	T207	K145	
	E506	A446	R386	GLN	G268	C208	Q146	
	P507	E447	E387	GLY	S269	P209	Q147	
	A508	A448	N388	GLN	W270	T210	L148	
	T509	Q449	F389	LYS	W271	L211	P149	
	A510	G450	G390	SER	S272	A212	Y150	
R73	S511	W451	D391	GLN	F273	W213	L151	R74
	K512	Y452	L392	ARG	D274	A214	E152	
	L513	E453	K393	LYS	R275	T215	A153	
	P514	K394	A394	ALA	A276	S216	A154	
	I515	L455	Y395	ARG	H277	P217	N155	
	E516	Q456	C396	ARG	L278	S218	L156	
	G517	R457	A397	GLY	R279	A219	L157	
	A518	E458	G398	PRO	E280	W220	Q161	
	G519	M459	D399	ALA	Q281	Y221	A162	
	A520	K460	V400	ILE	Y282	S222	L162	
R74	P521	E461	W401	SER	L283	W223	P163	R75
	G522	S462	A402	SER	T284	C224	P164	
	D523	L463	T403	W345	Q285	S225	K165	
	P524	M464	H404	D346	G286	Q226	P166	
	M525	D465	S405	W347	S287	R227	P167	
	D526	L466	V406	L348	R288	L228	A168	
	E527	A467	F407	D349	M289	V229	W169	
	E528	M468	Q408	I350	R290	E230	L170	
	D529	D469	Q409	S351	F291	E231	A171	
	L530	A470	Q410	S352	L292	R232	K172	
R75	G531	C471	L411	Y353	D293	Y233	E173	R76
	P532	Q472	P412	N354	T294	S234	G174	
	C533	L473	L413	SER	M295	W235	W175	
	S534	L474	F414	ASN	S296	T236	L176	
	E535	S475	L415	S355	M297	S237	R177	
	E536	G476	E416	L356	H298	Q238	Q115	
	E537	E477	R417	A357	W299	L239	G179	
	E538	R478	C418	E358	L300	S240	P180	
	F539	F419	P419	V359	L301	P241	E181	
	Q540	K480	H420	H360	S302	G242	G182	
R76	Q541	E481	P421	R361	G303	D243	E183	R77
	D542	D482	W422	L362	L304	L244	A184	
	P543	P483	T423	Y363	S305	T245	V185	
	M544	W484	L424	W364	S306	P246	P186	
	A545	L485	A425	G365	F307	L247	A187	
	R546	W486	G426	G366	Q308	E248	A188	
	A547	D487	W427	P367	R309	V249	H189	
	C548	L488	L428	P368	S310	P250	P190	
	L549	E489	E429	L369	L311	T251	E191	
	E550	W490	F430	E370	T252	G253	F192	

K551	K552	K553	K554	T555	T556	E557	L558	L559	K560	K561	P562	P563	Q564	R565	P567	G568	H569	P570	G571	W572	Y573	R574	K575	L576	C577	R578	R579	L580	D581	P582	P583	A584	W585	T586	P587	G588	P589	S590	L591	L592	S593	L594	Q595	M596	R597	V598	T599	P600	K601	L602	M603	A604	G605	L606	T607	D608	G609	F610																																																																																																																																																																																																																																																																																																																																																																																																																
P611	L612	H613	H614	S615	E616	H617	H618	G619	W620	L621	L622	Y623	V624	P625	L626	R627	R628	D629	M630	L631	A632	K633	L634	P635	T636	G637	T638	T639	L640	G641	S642	A643	G644	V645	V646	G647	P648	Y649	P650	A651	L652	P653	S654	L655	P656	R657	K658	H659	G660	L661	P662	Q663	G664	K665	L666	T667	D668	G669	F670																																																																																																																																																																																																																																																																																																																																																																																																															
G671	E672	A673	G674	L675	ALA	GLU	GLU	PHE	LEU	LEU	THR	ASP	ASN	SER	ALA	ILE	TRP	GLN	THR	VAL	GLU	GLU	LEU	ASP	TYR	LEU	GLU	VAL	GLU	ALA	GLU	ALA	LYS	GLU	ASN	LEU	R709	D709	A710	L711	P712	P713	G714	Q715	P716	L717	A718	L719	T720	A721	R722	G723	G724	G725	P726	D727	L728	G729	P730																																																																																																																																																																																																																																																																																																																																																																																																															
S731	Y732	H733	H734	R735	N736	G737	P738	S739	N740	D741	Y742	D743	L744	P745	C746	C747	F749	F750	F751	L752	P753	H754	K755	D756	G757	R758	R759	C760	N761	V762	G763	P764	P765	P766	A767	K768	D769	F770	L771	P772	K773	K774	E775	P776	G777	T778	L779	D780	A781	G782	P783	G784	G785	S786	G787	P788	R790																																																																																																																																																																																																																																																																																																																																																																																																																	
A791	L792	H793	L794	R795	R796	H797	L798	S799	R800	W801	R802	R803	A804	R805	R806	R807	L808	S809	S810	Q811	R812	R813	H814	R815	L816	R817	R818	R819	A820	L821	R822	R823	H824	R825	R826	R827	H828	P829	D830	Y831	D832	E833	E834	G835	L836	T837	G838	A839	L840	L841	P842	Q843	H844	G845	R846	A847	G848	T849	R850																																																																																																																																																																																																																																																																																																																																																																																																															
T851	R852	R853	A854	R855	E856	P857	T858	W859	L860	G861	S862	R863	R864	A865	R866	D868	R869	W870	G871	S872	E873	L874	R875	A876	R877	R878	R879	A880	P881	P882	G883	H884	T885	R886	Y887	G888	A889	D890	Y891	D892	S893	D894	E895	L896	W897	T898	A899	A900	Y901	L902	G903	D904	A905	L906	F907	A908	G909	M910	H911																																																																																																																																																																																																																																																																																																																																																																																																															
G912	C913	T914	A915	F916	R917	G918	H919	T920	L921	Q922	G923	R924	X925	S926	R927	G928	T929	D930	L931	H932	S933	L934	T935	A936	T937	T938	V939	G940	L941	R942	R943	E944	H945	A946	K947	T948	F949	L950	Y951	G952	D953	R954	L955	G956	A957	G958	Q959	P960	F961	A962	Q963	R964	L965	L966	R967	Q968	P969	T970	H971																																																																																																																																																																																																																																																																																																																																																																																																															
R972	L973	T974	Q975	Q976	Q977	A978	S979	E980	K981	A982	Q983	Q984	M985	Y986	A987	A988	T989	K990	G991	L992	R993	W994	Y995	R996	L997	S998	D999	E1000	G1001	E1002	H1003	L1004	V1005	A1006	E1007	L1008	N1009	L1010	P1011	G1012	D1013	R1014	T1015	E1016	G1017	L1018	W1019	P1020	S1021	A1022	Q1023	D1024	L1025	L1026	R1027	V1028	Q1029	T1030	E1031																																																																																																																																																																																																																																																																																																																																																																																																															
T1032	A1033	R1034	K1035	T1036	Q1037	W1038	K1039	E1040	W1041	E1042	V1043	V1044	A1045	E1046	R1047	A1048	W1049	K1050	G1051	T1052	E1053	E1054	S1055	E1056	H1057	F1058	N1059	K1060	L1061	S1062	S1063	T1064	A1065	T1066	S1067	D1068	T1069	P1070	T1071	S1072	P1073	P1074	LEU	GLY	CYS	CYS	ILE	SER	ARG	ALA	LEU	GLU	PRO	SER	ALA	VAL	GLN	E1090	E1091																																																																																																																																																																																																																																																																																																																																																																																																															
F1092	M1093	T1094	S1095	T1096	V1097	M1098	W1099	V1100	R1101	Q1102	S1103	S1104	A1105	V1106	D1107	L1108	L1109	H1110	L1111	M1112	L1113	V1114	A1115	M1116	K1117	W1118	L1119	F1120	E1121	E1122	F1123	A1124	I1125	D1126	G1127	R1128	C1129	F1129	L1129	P1130	L1131	S1132	L1133	H1134	D1135	E1136	V1137	R1138	Y1139	L1140	V1141	R1142	E1143	E1144	D1145	G1205	L1146	Y1147	R1148	A1149	A1150	L1151																																																																																																																																																																																																																																																																																																																																																																																																												
A1152	L1153	Q1154	T1155	L1156	N1157	L1158	L1159	T1160	R1161	C1162	M1163	F1164	A1165	Y1166	K1167	L1168	G1169	L1170	R1171	D1172	L1173	P1174	Q1175	S1176	V1177	A1178	F1179	P1180	S1181	A1182	V1183	D1184	I1185	R1186	R1187	C1188	L1189	L1190	K1191	E1192	V1193	T1194	M1195	D1196	K1197	K1198	P1200	S1201	N1202	P1203	L1204	G1205	M1206	E1207	R1208	Y1209	Y1210	G1211																																																																																																																																																																																																																																																																																																																																																																																																																
L1212	P1213	Q1214	G1215	E1216	L1217	L1218	D1219	L1220	Q1221	Q1222	L1223	L1224	E1225	L1226	T1227	K1228	G1229	S1230	L1231	E1232	K1233	R1234	L1235	G1236	P1237	G1238	P1239	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

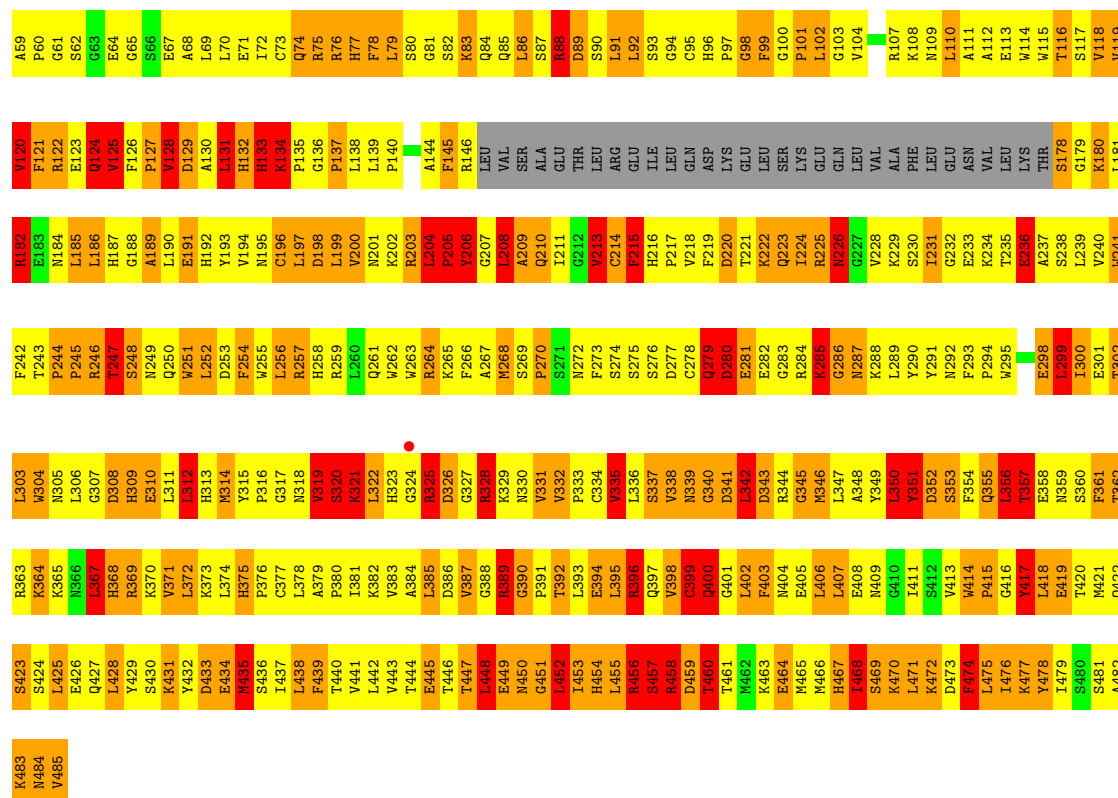
• Molecule 2: DNA polymerase subunit gamma-2

Chain B: 9% 45% 22% 7% 17%

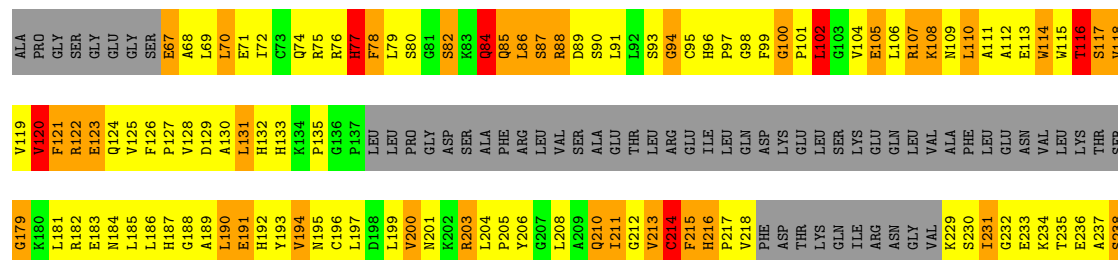
ALA	PRO	GLY	SER	GLY	GLU	GLY	SER	GLY	E67	A68	L69	R70	L71	I72	C73	T77	S80	G81	S82	K83	Q84	Q85	L86	S87	R88	D89	S90	L91	L92	S93	C94	C95	H96	P97	G98	G99	F100	P101	L102	G103	V104	E105	L106	R107	K108	M109	L110	A111	A112	E113	V114	V115	T116	S117	V118			
V119	V120	F121	R122	E123	Q124	V125	F126	P127	V128	D129	A130	L131	H132	H133	K134	P137	LEU	PRO	GLY	ASP	SER	ALA	PHE	ARG	LEU	VAL	SER	ALA	GLU	THR	L91	ARG	GLU	ILE	LEU	GLN	ASP	LYS	GLU	GLN	LEU	VAL	VAL	ALA	PHE	L110	LEU	GLU	ASN	VAL	VAL	LEU	LYS	THR	THR	SER	C179	
K180	L181	R182	E183	M184	L185	L186	H187	G188	A189	L190	E191	H192	Y193	V194	N195	C196	L197	D198	L199	N200	N201	K202	R203	L204	P205	Y206	G207	L208	A209	Q210	T211	G212	V213	C214	F215	G216	H216	V218	PHE	ASP	THR	LYS	GLN	ILE	ARG	ASN	GLY	VAL	K229	S230	G232	E233	K234	T235	E236	A237	S238	L239
W240	W241	T242	T243	P244	P245	R246	T247	S248	N249	Q250	L251	L252	D253	F254	W255	L256	R257	H258	L259	L260	W261	W262	W263	R264	K265	F266	G267	M268	L269	S269	T270	T271	N272	F273	D277	C278	Q279	D280	E281	E282	G283	R284	K285	G286	N287	K288	L289	F293	P294	W295	Q296	K297	E298	L299	T300	E301	T302	L303



• Molecule 2: DNA polymerase subunit gamma-2



• Molecule 2: DNA polymerase subunit gamma-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	138.39Å 138.39Å 226.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.92 – 3.24 46.92 – 3.25	Depositor EDS
% Data completeness (in resolution range)	89.5 (46.92-3.24) 89.6 (46.92-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.25Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.284 , 0.303 0.361 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	91.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 336.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l 0.468 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29480	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.94	18/8913 (0.2%)	2.06	406/12100 (3.4%)
1	D	1.03	30/8927 (0.3%)	2.18	471/12118 (3.9%)
2	B	0.78	6/2944 (0.2%)	1.43	67/3981 (1.7%)
2	C	0.92	11/3262 (0.3%)	1.95	114/4411 (2.6%)
2	E	0.92	12/2944 (0.4%)	1.59	75/3981 (1.9%)
2	F	0.85	2/3262 (0.1%)	1.88	128/4411 (2.9%)
All	All	0.94	79/30252 (0.3%)	1.97	1261/41002 (3.1%)

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	4
1	D	1	3
2	B	0	1
2	C	0	1
2	E	1	2
2	F	0	1
All	All	2	12

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	352	SER	CA-C	16.23	1.74	1.52
2	E	385	LEU	CA-CB	-15.47	1.27	1.53
1	D	352	SER	N-CA	14.78	1.65	1.46
1	A	232	ARG	N-CA	-13.60	1.28	1.46
2	B	280	ASP	C-O	-13.58	1.06	1.24

The worst 5 of 1261 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	347	TRP	N-CA-C	25.37	145.20	109.18
1	A	274	ASP	N-CA-C	-25.20	82.79	114.04
1	D	274	ASP	N-CA-C	-23.61	83.85	114.31
1	D	351	SER	N-CA-C	-22.78	84.80	112.59
1	D	721	ALA	N-CA-C	-21.86	77.17	110.17

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	249	VAL	CA
2	E	385	LEU	CA

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1179	PHE	Sidechain
1	A	221	TYR	Sidechain
1	A	239	LEU	Mainchain
1	A	395	TYR	Sidechain
2	B	417	TYR	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	8681	0	8521	3706	8
1	D	8695	0	8540	4055	7
2	B	2871	0	2862	852	0
2	C	3181	0	3168	1455	1
2	E	2871	0	2863	978	0
2	F	3181	0	3168	1512	4
All	All	29480	0	29122	12233	10

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 209.

The worst 5 of 12233 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:D:352:SER:CA	1:D:352:SER:C	1.74	1.59
1:D:460:LYS:HE2	1:D:460:LYS:N	1.20	1.48
2:E:432:TYR:HB2	2:E:437:ILE:CD1	1.51	1.39
1:D:352:SER:CA	1:D:358:GLU:OE2	1.73	1.36
1:D:914:THR:O	1:D:918:TRP:HB3	1.24	1.35

The worst 5 of 10 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ALA:O	2:F:318:ASN:O[2_734]	1.91	0.29
1:A:673:ALA:C	2:F:318:ASN:O[2_734]	1.98	0.22
1:A:1034:ARG:NE	2:F:450:ASN:ND2[1_545]	2.04	0.16
1:A:994:TRP:NE1	1:D:522:GLY:N[1_545]	2.06	0.14
1:D:1232:GLU:OE2	2:F:223:GLN:OE1[2_844]	2.11	0.09

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	1085/1172 (93%)	629 (58%)	254 (23%)	202 (19%)	0	0
1	D	1086/1172 (93%)	645 (59%)	234 (22%)	207 (19%)	0	0
2	B	349/427 (82%)	205 (59%)	94 (27%)	50 (14%)	0	1
2	C	394/427 (92%)	254 (64%)	84 (21%)	56 (14%)	0	1
2	E	349/427 (82%)	219 (63%)	79 (23%)	51 (15%)	0	1
2	F	394/427 (92%)	251 (64%)	93 (24%)	50 (13%)	0	1
All	All	3657/4052 (90%)	2203 (60%)	838 (23%)	616 (17%)	0	0

5 of 616 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	76	ILE
1	A	96	GLY
1	A	163	PRO
1	A	169	TRP

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	918/988 (93%)	590 (64%)	328 (36%)	0	0
1	D	919/988 (93%)	572 (62%)	347 (38%)	0	0
2	B	317/380 (83%)	260 (82%)	57 (18%)	2	8
2	C	350/380 (92%)	253 (72%)	97 (28%)	0	2
2	E	317/380 (83%)	265 (84%)	52 (16%)	2	10
2	F	350/380 (92%)	242 (69%)	108 (31%)	0	1
All	All	3171/3496 (91%)	2182 (69%)	989 (31%)	0	1

5 of 989 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	402	LEU
2	F	91	LEU
1	D	384	ASP
2	E	453	ILE
2	F	357	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	450	ASN
2	F	187	HIS
2	B	313	HIS
2	B	305	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	201	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1093/1172 (93%)	-1.20	2 (0%) 91 85	27, 80, 112, 124	0
1	D	1094/1172 (93%)	-1.22	1 (0%) 92 89	27, 81, 113, 124	0
2	B	355/427 (83%)	-1.12	0 100 100	81, 111, 129, 141	0
2	C	396/427 (92%)	-1.19	1 (0%) 90 81	42, 85, 113, 127	1 (0%)
2	E	355/427 (83%)	-1.07	0 100 100	64, 108, 129, 144	0
2	F	396/427 (92%)	-1.20	0 100 100	42, 87, 114, 128	0
All	All	3689/4052 (91%)	-1.18	4 (0%) 92 89	27, 88, 120, 144	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	723	GLY	3.6
1	D	723	GLY	2.9
2	C	324	GLY	2.8
1	A	273	PHE	2.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.