



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:29 AM GMT

PDB ID : 3IKM
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
<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

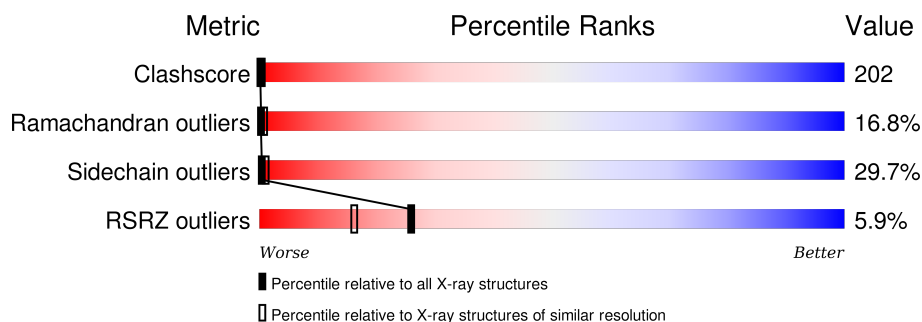
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (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 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	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

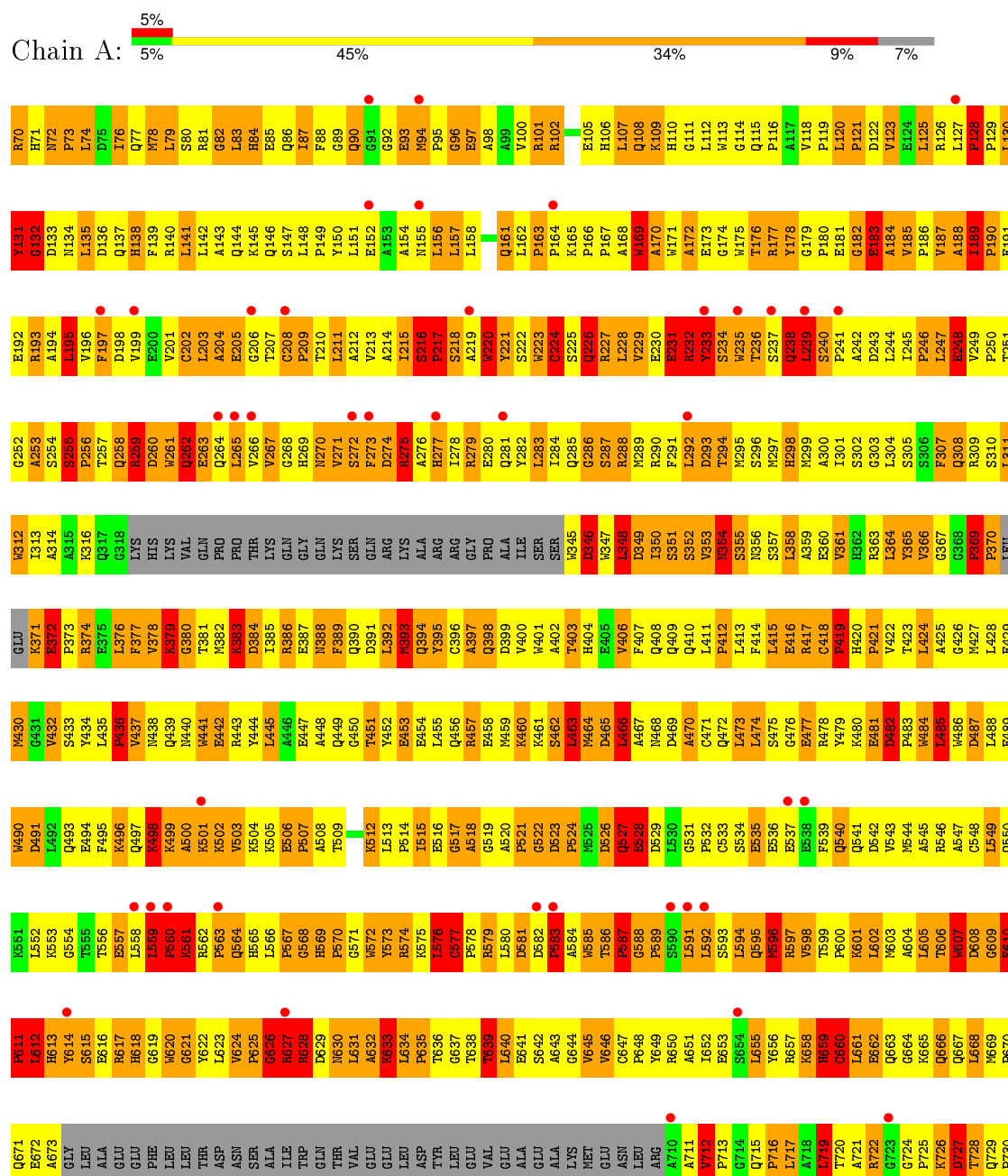
- Molecule 2 is a protein called DNA polymerase subunit gamma-2.

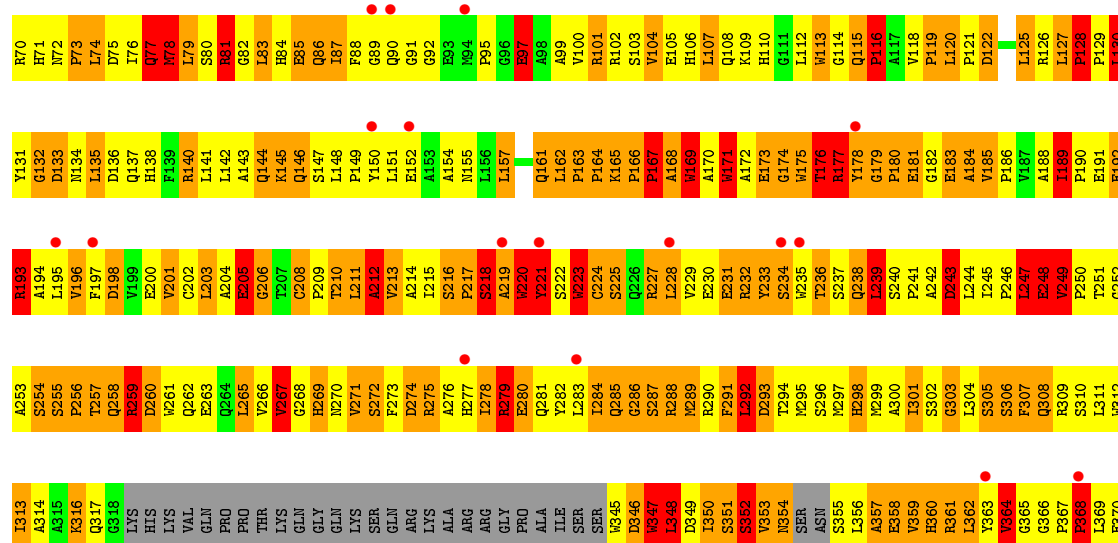
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	355	Total	C	N	O	S	0	0	0
			2871	1840	504	511	16			
2	C	396	Total	C	N	O	S	0	0	0
			3181	2031	563	571	16			
2	E	355	Total	C	N	O	S	0	0	0
			2871	1840	504	511	16			
2	F	396	Total	C	N	O	S	0	0	0
			3181	2031	563	571	16			

3 Residue-property plots

These plots are drawn for all protein, RNA 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.

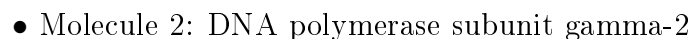
- Molecule 1: DNA polymerase subunit gamma-1

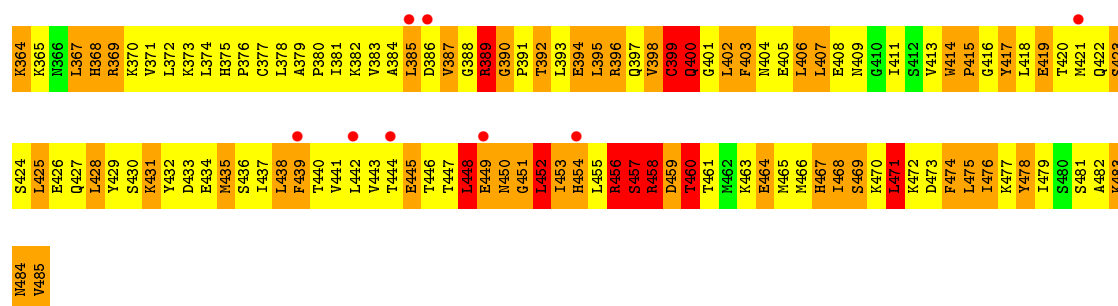




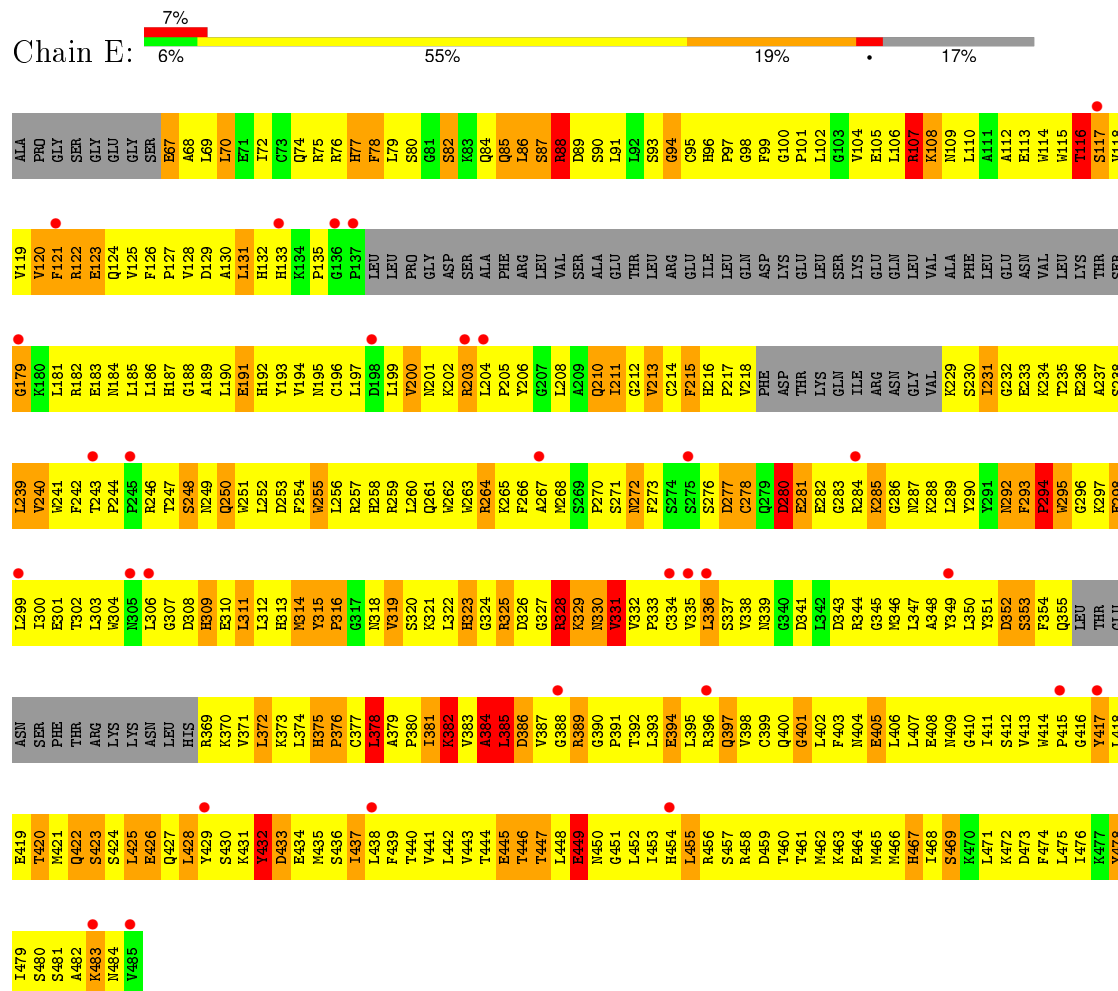
Q1214	Q1154	T1094	R1034	T974	T914	R853	E793	H733	A673	H613	K553	D491	G431	K371
I1155	I1155	S1095	K1035	Q775	A915	A854	I794	H734	GLY	Y614	G554	D492	V432	E372
E1215	T1156	R1096	S1036	Q776	F916	V855	K796	G735	LEU	S615	T595	Q493	S433	E373
A1217	M1157	V1097	Q1037	R977	G917	E856	K796	H736	ALA	R616	T556	E494	E434	R374
L1218	L1158	M1098	K1038	A978	N918	R857	I798	G737	GLU	R617	E557	F495	L435	E375
D1219	L1159	V1099	K1039	A979	N919	T858	S799	P738	GLU	H618	L558	K496	P436	L376
T1160	T1160	V1100	K1040	R980	T920	R859	S799	P739	PRO	Q497	L559	Q497	V437	F377
Y1220	T1161	V1101	W1041	R981	L921	L860	F800	N740	LEU	W620	P560	K498	Q438	V378
Q1222	C1162	V1102	E1042	A982	G922	S863	W801	D741	LEU	W621	P561	K499	Q439	R379
I1223	S1103	S1103	V1043	Q983	G923	N864	R802	V742	THR	G622	P562	A500	N440	G380
I1224	F1164	S1104	V1044	Q984	G924	A865	N803	D743	ASP	L623	P563	K501	W441	T381
E1225	A1105	A1045	N985	V985	G925	R866	H805	I744	ASN	A804	D564	E502	E442	K382
Y1166	V1106	V1106	E1046	N986	S926	R867	K806	P745	SER	P625	H565	K503	R443	K383
T1227	K1167	D1107	R1047	A987	A927	P867	K806	G746	ALA	G626	L566	K504	Y444	D384
L1168	L1168	Y1108	A1048	A988	G928	D868	R807	G747	ILE	R627	P567	K505	L445	T385
G1169	G1169	T989	R869	R989	T929	R869	R808	W748	TRP	R628	G568	E506	A446	R386
S1230	L1170	K1100	K1050	K990	D930	V870	S809	F749	GLN	D629	H569	GLN	E447	E387
L1231	G1051	L1111	G1051	G991	L931	G871	S810	F750	THR	N630	P570	T509	A448	N388
D1172	G1052	M1112	G1052	L992	H932	S872	Q811	K751	VAL	L631	G571	A510	Q449	F389
L1113	T1053	L1113	T1053	R993	S933	E873	H813	L752	GLU	A632	H572	A511	Q450	Q390
V1114	V1114	V1114	V1114	R994	H934	K874	H813	P753	GLU	R633	H573	K512	T451	D391
A1115	A1115	A1115	A1115	R995	T935	K875	H814	H754	LEU	L634	H574	L513	E453	L392
M1116	M1116	M1116	M1116	R996	A936	A876	W815	K755	ASP	P635	H575	P514	E453	K393
S1175	S1175	S1175	S1175	R997	T937	H877	L816	D756	TYR	T636	L576	I515	E454	D394
V1177	V1177	V1177	V1177	R998	T938	V878	P817	G757	LEU	G637	C577	E516	L455	K395
H1118	H1118	H1118	H1118	D999	V938	Q879	R818	H758	GLU	T638	P578	G517	Q456	C396
L1119	L1119	L1119	L1119	D999	V938	Q879	R818	H758	VAL	T639	H579	A518	R457	A397
F1180	F1180	F1180	F1180	G1000	G940	A880	S819	S759	VAL	T639	H579	G519	E458	K398
S1181	S1181	S1181	S1181	G1001	G941	P881	A820	C760	GLU	L640	H580	A519	E458	K399
A1182	A1182	A1182	A1182	E1002	S942	R882	L821	N761	ALA	A520	D581	P521	M459	D399
V1183	V1183	V1183	V1183	M1003	R943	G883	P822	V762	GLU	S642	D582	P521	K460	V400
L1184	L1184	L1184	L1184	L1004	E944	V884	R823	G763	ALA	A643	P583	G522	K461	H401
I1185	I1185	I1185	I1185	V1005	H945	T885	A824	S764	LVS	G644	A584	D523	S462	H402
D1186	D1186	D1186	D1186	R1006	A946	K886	R825	P765	MET	V645	H585	P524	L463	T403
G1127	G1127	G1127	G1127	E1007	K947	V887	I836	F766	GLU	V646	H586	D525	M464	H404
R1128	R1128	R1128	R1128	L1008	R948	G888	R837	A767	ASN	C647	P587	D526	D465	E405
L1189	L1189	L1189	L1189	I1069	F949	A889	H828	K768	LEU	P648	G588	Q527	L466	V406
R1190	R1190	R1190	R1190	P1070	N950	D890	P829	D769	R709	Y649	P589	E528	A467	F407
K1191	K1191	K1191	K1191	P1011	V951	H891	D830	F770	A710	R650	S590	D529	N468	Q408
E1192	E1192	E1192	E1192	D1012	G952	D892	H831	L771	A711	A651	L591	D530	D469	Q409
V1193	V1193	V1193	V1193	D1013	R953	S893	D832	P772	V712	L652	L592	G531	A470	Q410
T1194	T1194	T1194	T1194	R1014	I954	Q894	E833	K773	R713	S653	S593	P532	C471	L411
M1195	M1195	M1195	M1195	T1015	V955	E895	E834	N774	G714	S654	L594	G533	Q472	P412
D1196	D1196	D1196	D1196	E1016	G956	L896	G835	E775	Q715	L655	D595	D542	L473	L413
C1197	C1197	C1197	C1197	G1017	A957	H897	L836	D776	P716	Y656	H596	D542	L474	L414
K1198	K1198	K1198	K1198	G1018	G958	I898	H837	G777	L717	R657	R597	E537	S475	L415
T1199	T1199	T1199	T1199	W1019	Q959	A899	G838	T778	A718	K658	V598	E538	G476	E416
P1200	P1200	P1200	P1200	I1020	F960	A900	G839	L779	R719	H659	T599	F539	E477	R417
S1201	S1201	S1201	S1201	ARG	F961	V901	I840	Q780	T720	C660	P600	Q540	R478	C418
N1202	N1202	N1202	N1202	ALA	A962	L902	L841	A781	A721	L661	K601	Q541	Y479	P419
P1203	P1203	P1203	P1203	LEU	E963	G903	P842	G782	R722	E662	L602	D542	K480	H420
T1204	T1204	T1204	T1204	D1024	R964	D904	Q843	P783	G723	Q663	H603	V543	E481	P421
G1205	G1205	G1205	G1205	L1025	L965	A905	H843	G784	G724	G664	A604	V544	D482	V422
M1206	M1206	M1206	M1206	R1026	L966	H906	V845	G785	P725	K665	L605	A545	P483	T423
E1207	E1207	E1207	E1207	ALA	N967	F907	T846	A786	K726	Q666	T606	R546	W484	L424
R1208	R1208	R1208	R1208	VAL	Q968	A908	A847	S787	D727	Q667	H607	A547	L485	A425
C1209	C1209	C1209	C1209	GLN	P969	G909	G848	S788	T728	L668	D608	C548	W486	A426
A1150	A1150	A1150	A1150	R1030	N970	H910	T849	P789	Q729	M669	G609	L549	D487	M427
G1211	G1211	G1211	G1211	E1031	H971	H911	I850	R790	P730	P670	F611	Q550	L488	L428
I1212	I1212	I1212	I1212	T1032	R972	G912	T851	A791	S731	Q671	P611	Q551	E489	E429
P1213	P1213	P1213	P1213	A1033	L973	C913	R852	L792	Y732	E672	L612	L552	W490	M430

- Molecule 2: DNA polymerase subunit gamma-2

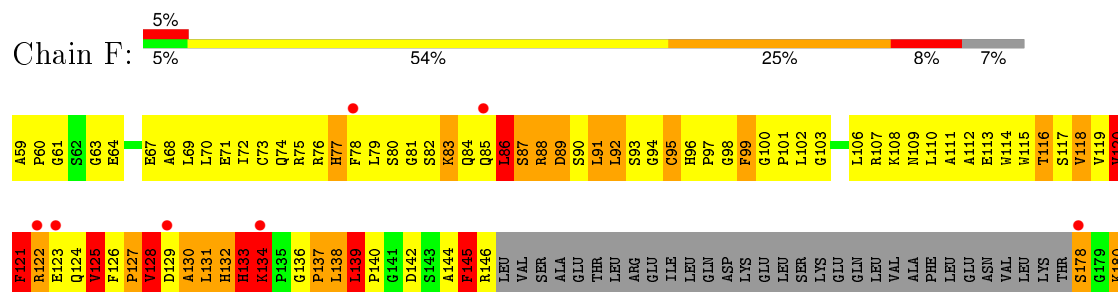




• Molecule 2: DNA polymerase subunit gamma-2



• Molecule 2: DNA polymerase subunit gamma-2



A482	K483 M484 V485	Q422	●	R363 R364 R365 R366 R367 R368 R369 R370 R371 R372 R373 R374 R375 R376 R377 R378 R379 R380 R381 R382 R383 R384 R385 R386 R387 R388 R389 R390 R391 R392 R393 R394 R395 R396 R397 R398 R399 Q400 G401 L402 F403 M404 E405 L406 L407 E408 M409 G410 I411 S412 V413 F414 L415 L416 L417 L418 S469 K470	E301 T302 L303 M304 T305 L306 G307 D308 E309 H310 E310 L311 L312 H313 M314 V315 P316 P317 G318 M318 V319 S320 K321 L322 H323 G324 L325 D326 G327 K328 R328 K329 M330 V331 V332 P333 C334 V335 L336 S337 V338 R339 Q339 G401 L402 F403 M404 E405 L406 L407 E408 M409 G410 I411 S412 V413 F414 L415 L416 L417 L418 S469 K470	W241 F242 L243 P244 T245 R246 T247 S248 N249 Q250 W251 L252 D253 F254 W255 L256 R257 H258 L259 S260 Q261 W262 W263 R264 K265 F266 G267 M268 K268 S269 P270 L271 M272 F273 S274 S275 S276 D277 P278 Q279 R279 D280 T221 E281 E282 G283 R284 K285 G286 M287 K288 L289 V290 Y291 D292 S293 F294 W295 G296 M297 K298 L299 S300	L181 L182 E183 N184 L185 L186 H187 G188 A189 L190 E191 H192 Y193 M194 N195 G196 L197 D198 L199 V200 N201 K202 K203 L204 P205 Y206 G207 L208 A209 Q210 L211 G212 V213 G214 F215 H216 V218 F219 D220 T221 K222 Q223 L224 R225 N226 G227 V228 K229 S230 L231 D232 E233 K234 E235 G236 T237 A237 S238 L239 V240
		●					
		●					
		●					
		●					

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) 89.5 (46.92-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.25Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.284 , 0.303 0.362 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	93.9	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.7	EDS
Estimated twinning fraction	0.008 for -h,-k,l 0.459 for h,-h-k,-l 0.009 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 76508 reflections	Xtriage
F_o, F_c correlation	0.83	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 2.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.72	10/8913 (0.1%)	1.33	149/12100 (1.2%)
1	D	0.81	18/8927 (0.2%)	1.45	161/12118 (1.3%)
2	B	0.60	2/2944 (0.1%)	0.99	16/3981 (0.4%)
2	C	0.68	0/3262	1.31	47/4411 (1.1%)
2	E	0.67	6/2944 (0.2%)	1.11	23/3981 (0.6%)
2	F	0.64	0/3262	1.28	37/4411 (0.8%)
All	All	0.72	36/30252 (0.1%)	1.31	433/41002 (1.1%)

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 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	358	GLU	CG-CD	12.87	1.71	1.51
2	E	385	LEU	CA-CB	-11.49	1.27	1.53
1	D	352	SER	N-CA	9.45	1.65	1.46
1	A	232	ARG	N-CA	-8.85	1.28	1.46
2	E	382	LYS	N-CA	-8.69	1.28	1.46

The worst 5 of 433 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	382	LYS	N-CA-C	16.56	155.72	111.00
2	E	385	LEU	N-CA-C	16.34	155.11	111.00
1	D	248	GLU	CA-C-N	-14.80	84.64	117.20
2	B	280	ASP	C-N-CA	14.32	157.51	121.70
1	A	1212	ILE	C-N-CD	-12.99	92.03	120.60

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	3592	8
1	D	8695	0	8540	3900	7
2	B	2871	0	2862	809	0
2	C	3181	0	3168	1419	1
2	E	2871	0	2862	945	0
2	F	3181	0	3168	1467	4
All	All	29480	0	29121	11814	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 202.

The worst 5 of 11814 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:C	1:D:352:SER:CA	1.74	1.55
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	2
All	All	3657/4052 (90%)	2203 (60%)	838 (23%)	616 (17%)	0	1

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%)	611 (67%)	307 (33%)	0	0
1	D	919/988 (93%)	584 (64%)	335 (36%)	0	0
2	B	317/380 (83%)	259 (82%)	58 (18%)	2	10
2	C	350/380 (92%)	260 (74%)	90 (26%)	0	2
2	E	317/380 (83%)	270 (85%)	47 (15%)	4	17
2	F	350/380 (92%)	245 (70%)	105 (30%)	0	1
All	All	3171/3496 (91%)	2229 (70%)	942 (30%)	0	1

5 of 942 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	369	ARG
1	D	308	GLN
2	F	231	ILE
2	C	407	LEU
1	D	145	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	454	HIS
1	D	394	GLN
2	F	84	GLN
1	D	86	GLN

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Mol	Chain	Res	Type
1	D	155	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 carbohydrates 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%)	0.23	61 (5%) 28 18	27, 80, 112, 124	0
1	D	1094/1172 (93%)	0.15	53 (4%) 34 23	27, 81, 113, 124	0
2	B	355/427 (83%)	0.44	31 (8%) 13 8	81, 111, 129, 141	0
2	C	396/427 (92%)	0.31	20 (5%) 32 21	42, 85, 113, 127	1 (0%)
2	E	355/427 (83%)	0.41	30 (8%) 13 9	64, 108, 129, 144	0
2	F	396/427 (92%)	0.20	22 (5%) 28 18	42, 87, 114, 128	0
All	All	3689/4052 (91%)	0.25	217 (5%) 26 16	27, 88, 120, 144	1 (0%)

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	267	ALA	7.6
1	D	583	PRO	7.0
2	F	327	GLY	6.9
1	D	277	HIS	6.2
1	A	563	PRO	6.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.