



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:58 AM UTC

PDB ID : 1L9U / pdb_0000119u
Title : THERMUS AQUATICUS RNA POLYMERASE HOLOENZYME AT 4 Å
RESOLUTION
Authors : Murakami, K.S.; Masuda, S.; Darst, S.A.
Deposited on : 2002-03-26
Resolution : 4.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

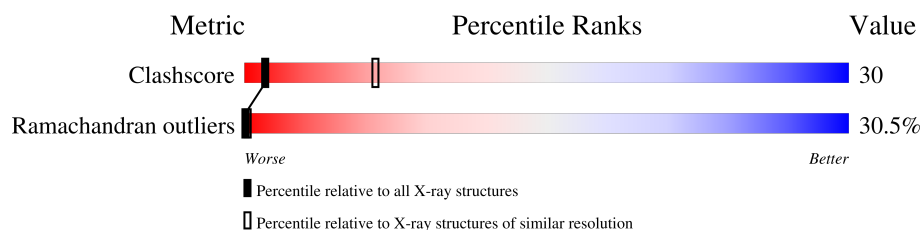
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	40% 29% . 29%
1	B	314	42% 25% . 30%
1	J	314	40% 29% . 29%
1	K	314	42% 25% . 30%
2	C	1118	51% 39% 6% .
2	L	1118	51% 39% 7% .
3	D	1524	35% 37% 6% 22%
3	M	1524	35% 37% 6% 22%
4	E	99	43% 44% 5% 7%

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Mol	Chain	Length	Quality of chain
4	N	99	43% 45% • 7%
5	H	332	73% 22% • •
5	Q	332	73% 22% • •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18756 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 RNA POLYMERASE, ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	0	0	0
			672	448	224			
1	B	220	Total	C	N	0	0	0
			660	440	220			
1	J	224	Total	C	N	0	0	0
			672	448	224			
1	K	220	Total	C	N	0	0	0
			660	440	220			

- Molecule 2 is a protein called RNA POLYMERASE, BETA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	1084	Total	C	N	0	0	0
			3252	2168	1084			
2	L	1084	Total	C	N	0	0	0
			3252	2168	1084			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP Q9KWU7
L	?	-	GLU	deletion	UNP Q9KWU7

- Molecule 3 is a protein called RNA POLYMERASE, BETA-PRIME SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	1183	Total	C	N	0	0	0
			3549	2366	1183			
3	M	1183	Total	C	N	0	0	0
			3549	2366	1183			

- Molecule 4 is a protein called RNA POLYMERASE, OMEGA SUBUNIT.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	92	Total	C	N	0	0	0
			276	184	92			
4	N	92	Total	C	N	0	0	0
			276	184	92			

- Molecule 5 is a protein called SIGMA FACTOR SIGA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	H	322	Total	C	N	0	0	0
			966	644	322			
5	Q	322	Total	C	N	0	0	0
			966	644	322			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ILE	deletion	UNP Q9EZJ8
H	?	-	GLN	deletion	UNP Q9EZJ8
H	?	-	LYS	deletion	UNP Q9EZJ8
H	?	-	ILE	deletion	UNP Q9EZJ8
H	?	-	PRO	deletion	UNP Q9EZJ8
H	?	-	GLY	deletion	UNP Q9EZJ8
H	?	-	LEU	deletion	UNP Q9EZJ8
H	?	-	LYS	deletion	UNP Q9EZJ8
H	?	-	GLU	deletion	UNP Q9EZJ8
H	?	-	LYS	deletion	UNP Q9EZJ8
H	?	-	PRO	deletion	UNP Q9EZJ8
H	?	-	ASP	deletion	UNP Q9EZJ8
H	?	-	PRO	deletion	UNP Q9EZJ8
H	?	-	LYS	deletion	UNP Q9EZJ8
H	?	-	THR	deletion	UNP Q9EZJ8
Q	?	-	ILE	deletion	UNP Q9EZJ8
Q	?	-	GLN	deletion	UNP Q9EZJ8
Q	?	-	LYS	deletion	UNP Q9EZJ8
Q	?	-	ILE	deletion	UNP Q9EZJ8
Q	?	-	PRO	deletion	UNP Q9EZJ8
Q	?	-	GLY	deletion	UNP Q9EZJ8
Q	?	-	LEU	deletion	UNP Q9EZJ8
Q	?	-	LYS	deletion	UNP Q9EZJ8
Q	?	-	GLU	deletion	UNP Q9EZJ8
Q	?	-	LYS	deletion	UNP Q9EZJ8
Q	?	-	PRO	deletion	UNP Q9EZJ8
Q	?	-	ASP	deletion	UNP Q9EZJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	PRO	deletion	UNP Q9EZJ8
Q	?	-	LYS	deletion	UNP Q9EZJ8
Q	?	-	THR	deletion	UNP Q9EZJ8

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	M	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

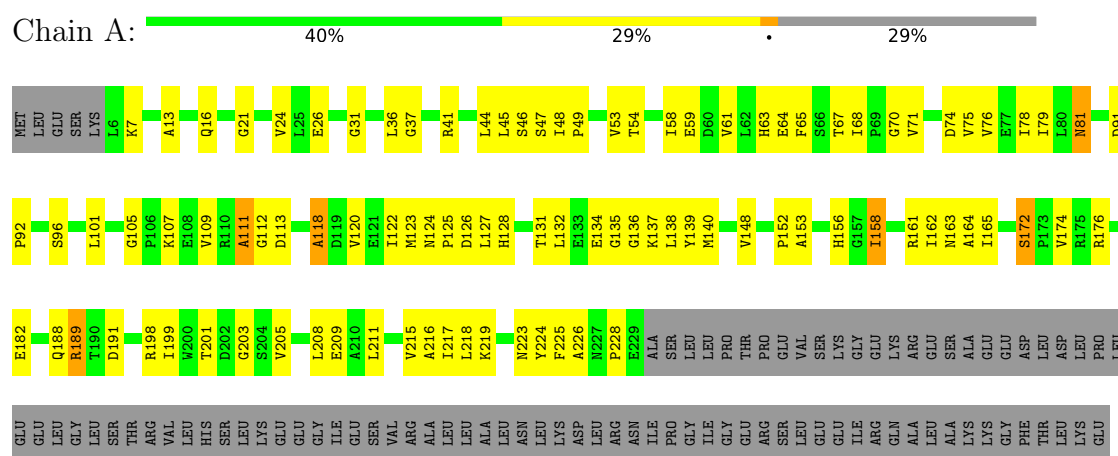
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	M	2	Total	Zn	0	0
			2	2		

3 Residue-property plots

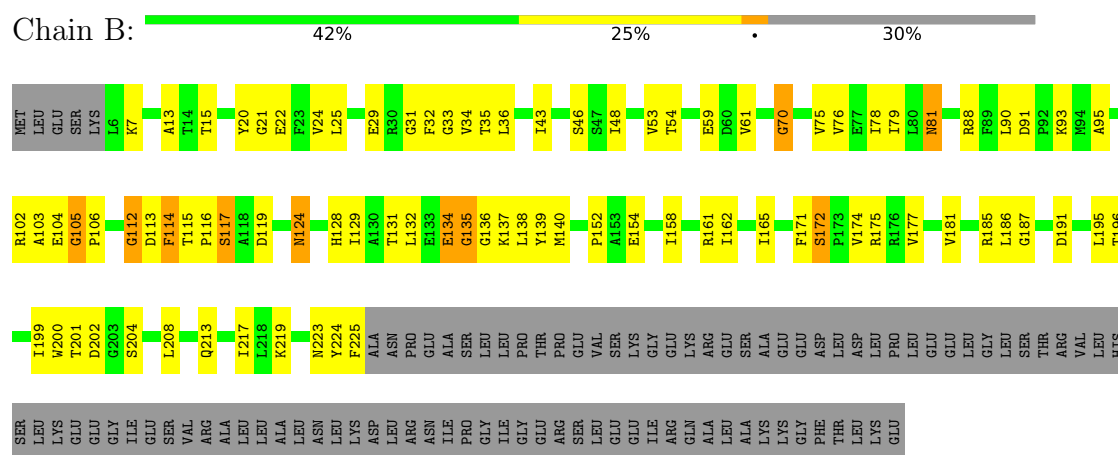
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

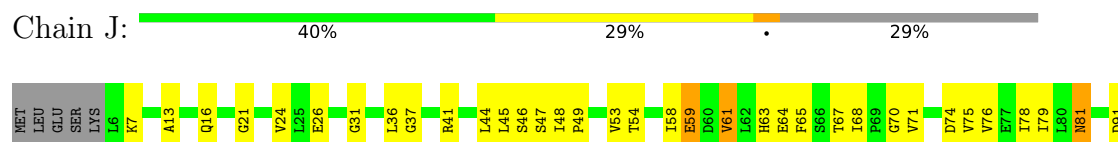
• Molecule 1: RNA POLYMERASE, ALPHA SUBUNIT

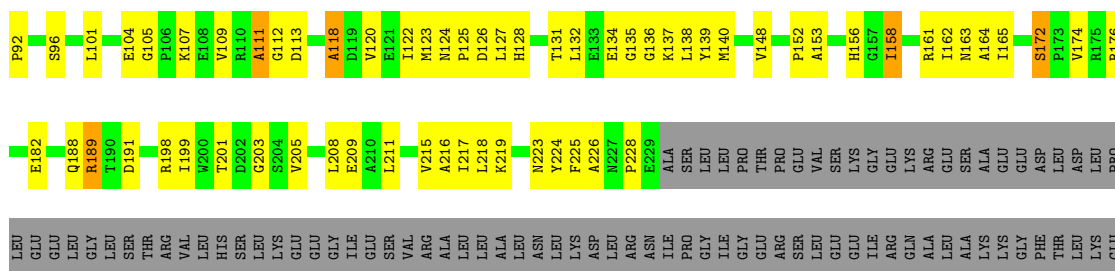


• Molecule 1: RNA POLYMERASE, ALPHA SUBUNIT

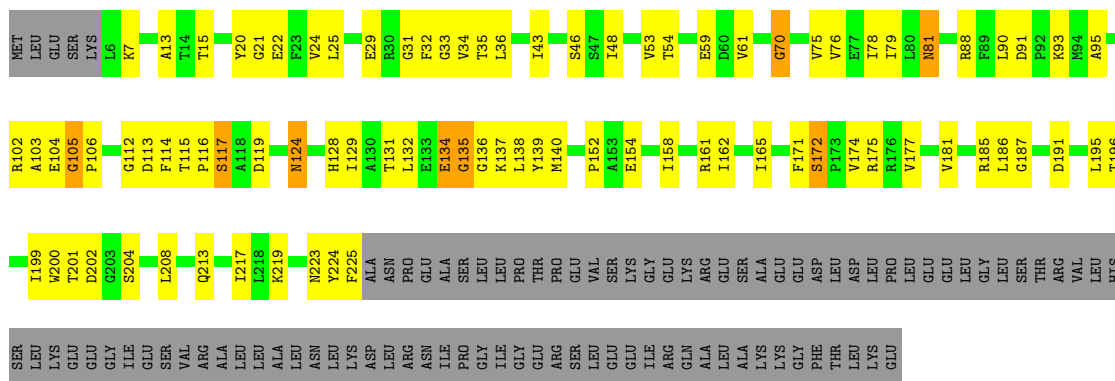


• Molecule 1: RNA POLYMERASE, ALPHA SUBUNIT

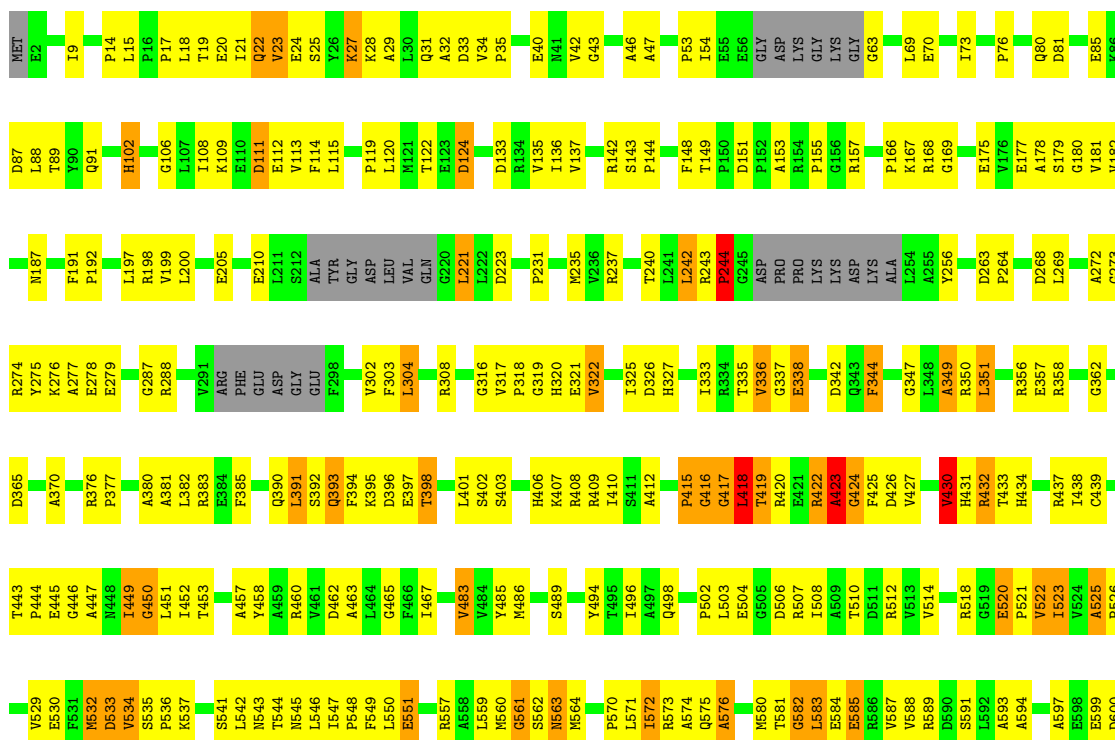


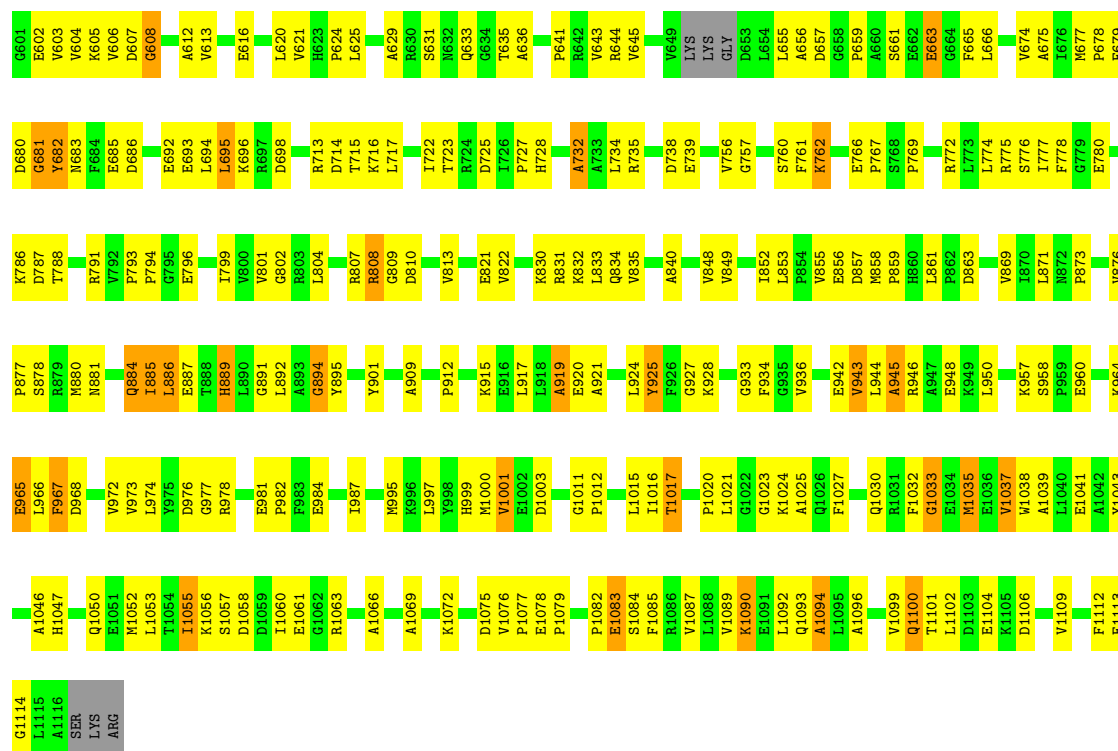


• Molecule 1: RNA POLYMERASE, ALPHA SUBUNIT



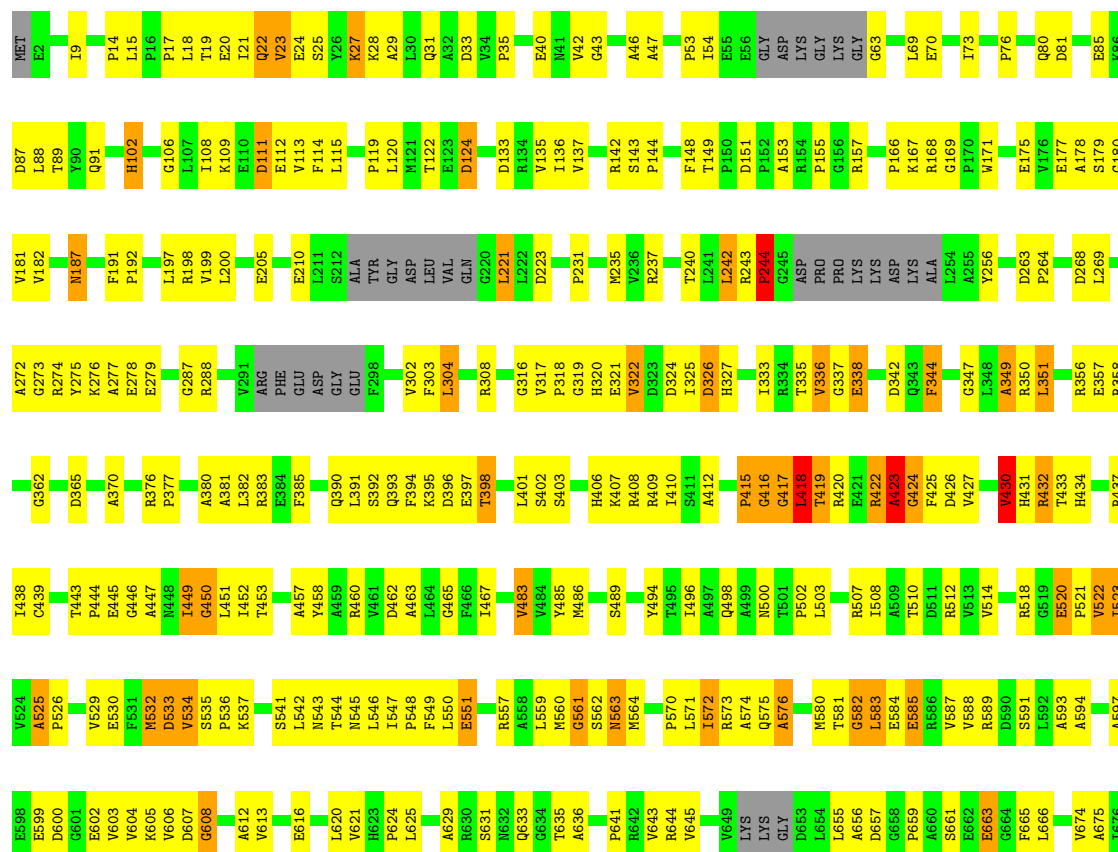
• Molecule 2: RNA POLYMERASE, BETA SUBUNIT

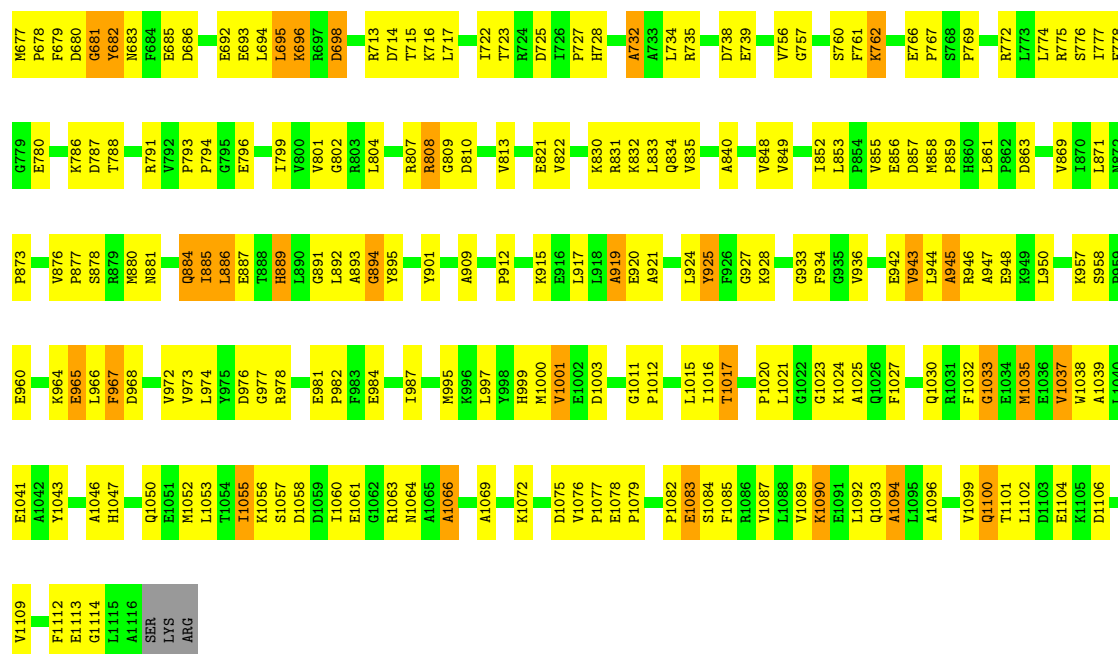




• Molecule 2: RNA POLYMERASE, BETA SUBUNIT

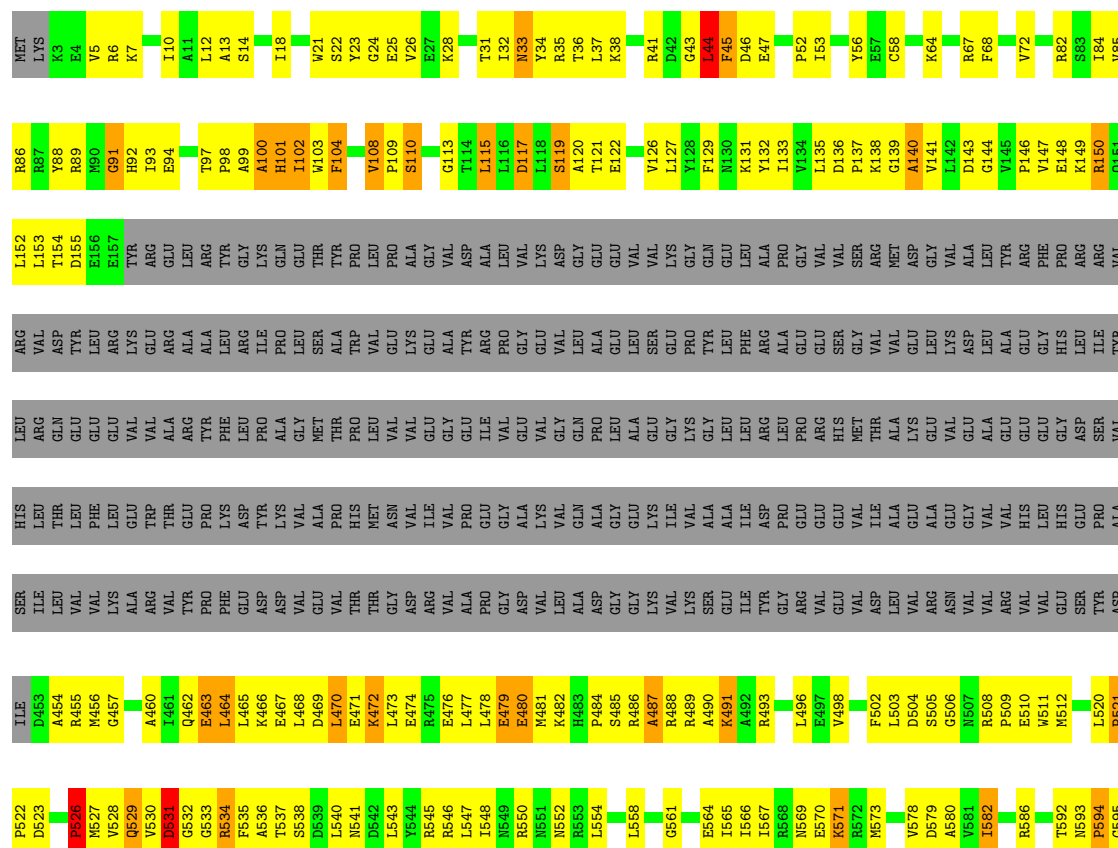
Chain L: 51% 39% 7% •





• Molecule 3: RNA POLYMERASE, BETA-PRIME SUBUNIT

Chain D: 35% 37% 6% 22%



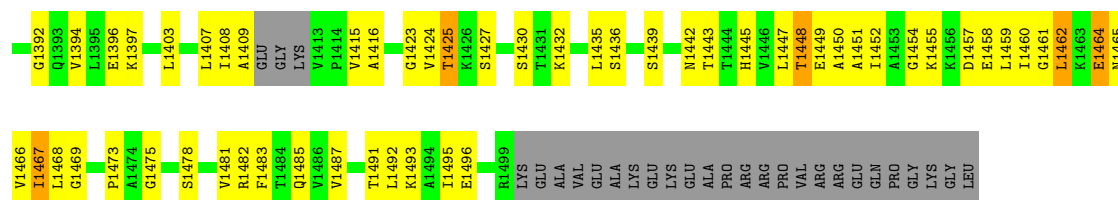
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• Molecule 3: RNA POLYMERASE, BETA-PRIME SUBUNIT

Chain M: 35% 37% 6% 22%

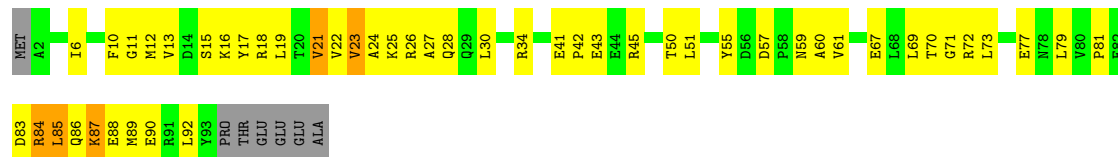
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R86	R87	Y88	R89	G90	H91	H92	I93	E94	T97	P98	A99	A100	H101	I102	W103	F104	V108	P109	S110	G113	T114	L115	D117	L118	S119	A120	T121	E122	V126	L127	Y128	F129	R130	K131	Y132	I133	V134	L135	D136	P137	K138	G139	A140	V141	L142	D143	G144	V145	P146	V147	E148	K149	R150

Y1318	T1237	L1072	P996	P929	D847	L770	D685	G595	P521	ILE	SER	HIS	LEU	L152
V1319	M1238	S1073	T997	L930	E848	L770	E686	G595	P522	D453	ILE	THR	GLN	L153
A1320	R1239	K1079	E998	L931	A849	S771	W688	R601	P523	A454	VAL	LEU	GLU	T154
A1321	PHE	H1172	T999	D932	A853	S774	D689	S602		R455	VAL	PHE	GLU	D155
G1322	HIS	F1173	K1000	L934	A854	G775	A690	T604	P526	M456	VAL	LEU	GLU	E156
P1324	THR	G1081	E1001	K935	H855	E776	L691	D605	N527	G457	VAL	GLU	VAL	E157
	GLY	T1084	A1006	Y936	G856		E692	L606	Q529	A460	VAL	GLU	VAL	TYR
G1328	GLY	A1085	V1007	Y937	L857	S782	E693	L607	W530	I461	VAL	THR	ALA	ARG
A1329	VAL	L1086	F1008	G938	L858	R783	W694	S608	Q532	Q462	THR	GLU	ARG	GLU
I1330	ALA	R1087	K1009	F939	L859	D784	L695	G609	D531	E463	PRO	ARG	ALA	LEU
D1331	VAL	T1088	N1010	T940	D862	I785	H696	G533	E464	L464	PHE	LYS	PHE	ARG
P1332	GLY	A1089	N1010	L941	W663		G697	L619	R534	L465	ASP	LYS	LEU	GLY
H1333	THR	D1090	E1012	S942	W664	I792	K698	G620	R535	K466	ASP	TYR	PRO	LYS
Q1334	ASP	S1091	ASP	T943	T865	I793		G621	F536	K467	ASP	THR	ALA	GLN
	ILE	R1189	P1016	T944	T866	Q794	L702	R622	A536	E467	VAL	VAL	GLU	GLU
K1339	THR	L1093	P1019	S945	R872	W795		W623	T537	L468	VAL	ALA	PRO	THR
G1340	GLN	L1094	P1191	G946	T875	R796	R710	D624	S538	D469	VAL	ALA	SER	THR
P1341	GLY	T1095	L1020	T947	T876	K797	L711	W625	L540	L470	VAL	PRO	ALA	PRO
E1342	LEU	R1096	Y1021	T948	S876	E798	G712	S626	N541	E471	THR	HIS	THR	PRO
A1343		C1194	Y1022	T949	P877	K799	L713		P542	K472	GLY	MET	VAL	LEU
R1344	P1257	Q1195	M1023	G950	R878	E799	Q714	W630	L543	L473	ASP	VAL	VAL	PRO
E1345	R1258	L1098	A1024	L951	R879	G803	A715	W631	W544	R475	ARG	ILE	GLU	ALA
G1346	V1259	V1099	A1024	L951	R879	G803	A715	W631	W544	R475	ARG	ILE	GLU	GLY
R1347	E1260	D1100		D952	F882	Q716	G716	W632	R545	E476	VAL	VAL	GLY	VAL
Y1347	E1261	V1101	A1028	D953	A883	Q717	Q717	W633	R546	L477	ALA	PRO	GLY	ASP
	L1262	A1102	R1029	A954	A883	Q718	Q718	W633	L547	L478	PRO	GLU	ILE	ALA
D1350	F1263	H1103	G1030	P955	A884	P809	W719	L637	E479	GLY	GLY	VAL	VAL	LEU
E1351		E1104	N1031	P956	R884	E810	L720	K638	E480	ASP	ALA	ALA	GLY	GLU
P1268	P1268	L1105	P1032	P957	R885	E811	W721	L639	N481	VAL	VAL	GLY	GLY	VAL
K1269	K1269	V1106	Q1033	E958	G887	E811	W721	H640	N482	VAL	VAL	GLY	VAL	ASP
A1270	A1270	V1107	G1034	F959	G887	E811	W721	H640	N482	VAL	VAL	GLY	VAL	ASP
E1271	E1271	R1108	I1035	K960	D892	E815	Q723	G641	N552	R483	ALA	GLN	GLY	GLY
A1272	A1272	E1109	R1036	K961	E893	Y816	Q724	G642	R484	P484	ASP	ALA	PRO	GLU
V1273	V1273	A1110	Q1037	R962	K894	Y817	S725	Q643	S485	S485	GLY	GLY	GLU	GLU
G1274	G1274	D1111	G1040	L964	K894	Y817	Q727	Q644	R486	R486	GLY	GLY	VAL	VAL
E1276	E1276	G1113	M1041	E965	K894	Y817	Q727	Q645	R487	R487	LYS	LYS	GLY	VAL
I1277	I1277	T1114	R1042	E966	K894	Y817	Q727	Q646	R488	R488	VAL	ILE	GLY	LYS
		T1115		E967	K894	Y817	Q727	Q647	R489	R489	VAL	ILE	GLY	LYS
V1280	V1280	M1116	M1045	A967	K894	Y817	Q727	Q648	A490	A490	SER	ALA	GLY	GLN
V1281	V1281	Q1124	Q1046	R972	K894	Y817	Q727	Q649	K491	K491	GLY	ALA	LEU	GLU
			K1047	R973	K894	Y817	Q727	Q650	A492	A492	TYR	ILE	LEU	LEU
E1287	E1287	V1128	K1048	Q975	K894	Y817	Q727	Q651	R493	R493	GLY	ALA	ARG	ALA
D1288	D1288	T1129	P1049	E975	K894	Y817	Q727	Q652	L496	L496	ARG	GLY	PRO	GLY
R1289	R1289	R1130	S1049	E975	K894	Y817	Q727	Q653	E570	E570	VAL	GLY	VAL	VAL
L1290	L1290	T1131	F1053	Q976	K894	Y817	Q727	Q654	R571	R571	VAL	HIS	ARG	SER
S1291	S1291	L1132	E1054	Q976	K894	Y817	Q727	Q655	B572	B572	VAL	THR	THR	GLY
Q1374	Q1374	R1133	P1055	Q976	K894	Y817	Q727	Q656	F502	F502	VAL	ILE	MET	VAL
M1375	M1375	L1134	P1056	Q976	K894	Y817	Q727	Q657	L503	L503	VAL	ALA	ALA	VAL
L1376	L1376	R1135	P1057	Q976	K894	Y817	Q727	Q658	D504	D504	VAL	LYS	GLY	ASP
K1377	K1377	K1136	S1059	Q976	K894	Y817	Q727	Q659	S505	S505	VAL	ALA	GLY	VAL
		K1137	S1060	Q976	K894	Y817	Q727	Q660	G506	G506	VAL	GLY	VAL	VAL
V1381	V1381	E1141	F1061	R988	K894	Y817	Q727	Q661	R508	R508	VAL	ALA	ALA	ALA
P1386	P1386	S1142	R1062	Q990	K894	Y817	Q727	Q662	P509	P509	VAL	GLY	GLY	LEU
G1385	G1385	G1143	V1067	Q991	K894	Y817	Q727	Q663	E510	E510	VAL	HIS	GLY	ARG
D1386	D1386	G1146	L1068	V992	K894	Y817	Q727	Q664	W511	W511	VAL	GLY	GLY	PHE
S1387	S1387	Q1235	E1069	V993	K894	Y817	Q727	Q665	W512	W512	VAL	HIS	GLY	PRO
R1388	R1388	L1236	Y1070	V994	K894	Y817	Q727	Q666	T592	T592	SER	GLY	LEU	ARG
L1389	L1389	L1149	F1071	L995	K894	Y817	Q727	Q667	N593	N593	TYR	ASP	ASP	VAL



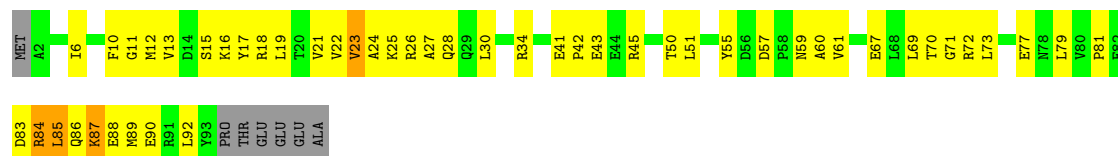
• Molecule 4: RNA POLYMERASE, OMEGA SUBUNIT

Chain E: 43% 44% 5% 7%



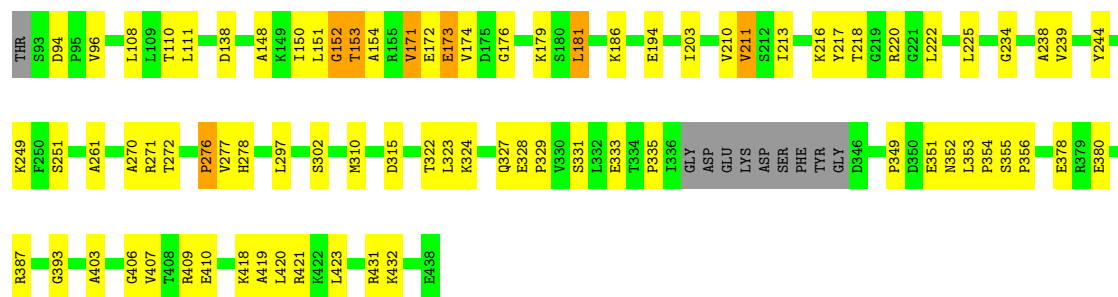
• Molecule 4: RNA POLYMERASE, OMEGA SUBUNIT

Chain N: 43% 45% 7%



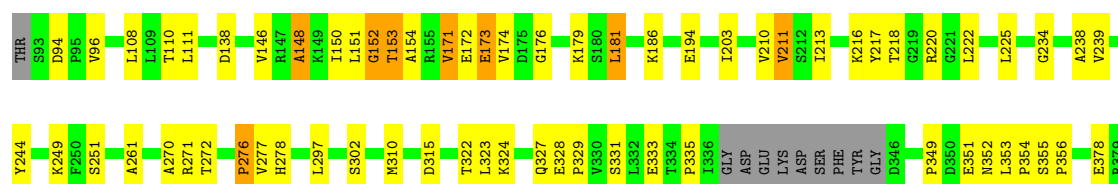
• Molecule 5: SIGMA FACTOR SIGA

Chain H: 73% 22% 5%



• Molecule 5: SIGMA FACTOR SIGA

Chain Q: 73% 22% 5%



E380	
R387	
G393	
A403	
G406	
V407	
T408	
R409	
E410	
K418	
A419	
L420	
R421	
K422	
L423	
K431	
K432	
E438	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	155.00Å 271.20Å 155.30Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 4.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-4.00)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18756	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.57	0/671	1.81	25/670 (3.7%)
1	B	0.54	0/659	1.88	21/658 (3.2%)
1	J	0.57	0/671	1.81	26/670 (3.9%)
1	K	0.54	0/659	1.88	21/658 (3.2%)
2	C	1.29	11/3246 (0.3%)	2.20	94/3240 (2.9%)
2	L	1.29	11/3246 (0.3%)	2.21	94/3240 (2.9%)
3	D	1.47	32/3545 (0.9%)	2.23	126/3541 (3.6%)
3	M	1.47	32/3545 (0.9%)	2.23	126/3541 (3.6%)
4	E	0.52	0/275	1.65	5/274 (1.8%)
4	N	0.52	0/275	1.65	5/274 (1.8%)
5	H	0.96	4/964 (0.4%)	1.60	11/962 (1.1%)
5	Q	0.95	4/964 (0.4%)	1.60	11/962 (1.1%)
All	All	1.24	94/18720 (0.5%)	2.10	565/18690 (3.0%)

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	C	0	8
2	L	0	8
3	D	0	7
3	M	0	7
All	All	0	30

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	91	GLY	C-N	-30.07	0.92	1.33
3	M	91	GLY	C-N	-30.07	0.92	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	244	PRO	C-N	-28.93	0.92	1.33
2	L	244	PRO	C-N	-28.90	0.92	1.33
2	C	417	GLY	C-N	-27.09	0.95	1.33

The worst 5 of 565 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	417	GLY	CA-C-N	27.12	173.35	121.54
2	L	417	GLY	C-N-CA	27.12	173.35	121.54
2	C	417	GLY	CA-C-N	27.12	173.34	121.54
2	C	417	GLY	C-N-CA	27.12	173.34	121.54
2	C	419	THR	CA-C-N	25.46	170.16	121.54

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	242	LEU	Peptide
2	C	244	PRO	Peptide
2	C	416	GLY	Peptide
2	C	417	GLY	Peptide
2	C	418	LEU	Peptide

5.2 Too-close contacts [i](#)

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	672	0	241	17	0
1	B	660	0	238	16	0
1	J	672	0	241	18	0
1	K	660	0	238	16	0
2	C	3252	0	1190	140	0
2	L	3252	0	1190	141	0
3	D	3549	0	1281	177	0
3	M	3549	0	1281	182	0
4	E	276	0	96	20	0
4	N	276	0	96	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	966	0	342	17	0
5	Q	966	0	342	19	0
6	D	1	0	0	0	0
6	M	1	0	0	0	0
7	D	2	0	0	0	0
7	M	2	0	0	0	0
All	All	18756	0	6776	768	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 30.

The worst 5 of 768 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)
3:M:44:LEU:C	3:M:45:PHE:N	1.70	1.46
3:D:44:LEU:C	3:D:45:PHE:N	1.70	1.45
3:M:933:ALA:C	3:M:935:LYS:H	1.80	0.88
2:L:542:LEU:C	2:L:544:THR:H	1.83	0.86
3:M:44:LEU:C	3:M:46:ASP:H	1.85	0.85

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%)	95 (43%)	65 (29%)	62 (28%)	0	0
1	B	218/314 (69%)	110 (50%)	53 (24%)	55 (25%)	0	1
1	J	222/314 (71%)	95 (43%)	65 (29%)	62 (28%)	0	0
1	K	218/314 (69%)	110 (50%)	53 (24%)	55 (25%)	0	1
2	C	1072/1118 (96%)	439 (41%)	296 (28%)	337 (31%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	1072/1118 (96%)	439 (41%)	294 (27%)	339 (32%)	0	0
3	D	1175/1524 (77%)	456 (39%)	307 (26%)	412 (35%)	0	0
3	M	1175/1524 (77%)	456 (39%)	309 (26%)	410 (35%)	0	0
4	E	90/99 (91%)	40 (44%)	24 (27%)	26 (29%)	0	0
4	N	90/99 (91%)	40 (44%)	24 (27%)	26 (29%)	0	0
5	H	318/332 (96%)	209 (66%)	57 (18%)	52 (16%)	0	3
5	Q	318/332 (96%)	209 (66%)	57 (18%)	52 (16%)	0	3
All	All	6190/7402 (84%)	2698 (44%)	1604 (26%)	1888 (30%)	0	0

5 of 1888 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	64	GLU
1	A	76	VAL
1	A	125	PRO
1	A	137	LYS

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	11
3	M	11
2	C	8
2	L	8
5	H	1
5	Q	1

The worst 5 of 40 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	44:LEU	C	45:PHE	N	1.70
1	M	44:LEU	C	45:PHE	N	1.70
1	D	532:GLY	C	533:GLY	N	1.61
1	M	532:GLY	C	533:GLY	N	1.61
1	C	416:GLY	C	417:GLY	N	1.19

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.