



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 09:24 pm GMT

PDB ID : 2R92
Title : Elongation complex of RNA polymerase II with artificial RdRP scaffold
Authors : Lehmann, E.; Brueckner, F.; Cramer, P.
Deposited on : 2007-09-12
Resolution : 3.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

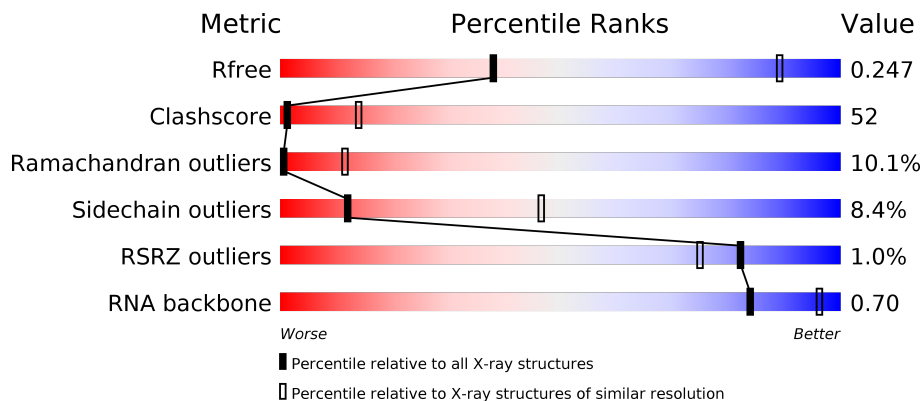
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.



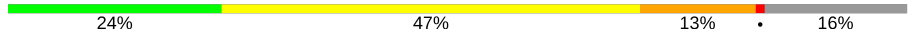
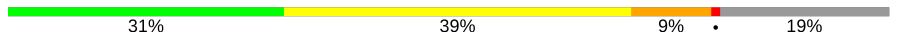
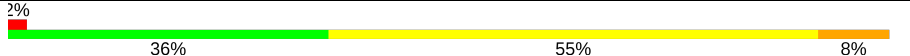


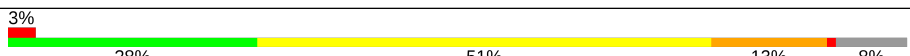
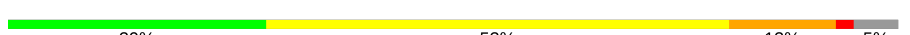
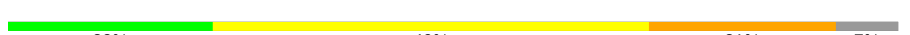


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1028 (4.02-3.58)
Clashscore	122126	1061 (4.00-3.60)
Ramachandran outliers	120053	1025 (4.00-3.60)
Sidechain outliers	120020	1019 (4.00-3.60)
RSRZ outliers	108989	1021 (4.06-3.54)
RNA backbone	2636	1083 (4.70-2.90)

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	P	16	
2	T	17	
3	A	1733	
4	B	1224	

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Mol	Chain	Length	Quality of chain
5	C	318	
6	D	221	
7	E	215	
8	F	155	
9	G	171	
10	H	146	
11	I	122	
12	J	70	
13	K	120	
14	L	70	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 31611 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 RNA chain called RNA (5'-R(*UP*GP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	P	9	192	87	39	58	8	0	0	0

- Molecule 2 is a RNA chain called RNA (5'-R(*CP*UP*UP*GP*AP*CP*GP*CP*CP*UP*GP*GP*UP*CP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	10	208	94	36	69	9	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	1422	11194	7054	1959	2119	62	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	1112	8841	5596	1550	1640	55	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	267	2101	1320	349	419	13	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	178	1434	887	257	288	2	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	E	214	1752	1111	309	321	11	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	F	88	712	455	120	134	3	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	G	171	1340	861	222	249	8	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	H	135	1084	683	183	214	4	0	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	I	116	944	581	172	181	10	0	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	J	65	532	339	93	94	6	0	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	112	Total	C	N	O	S	0	0	0
			904	580	154	168	2			

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	1	Total	Zn	0	0
			1	1		
15	B	1	Total	Zn	0	0
			1	1		
15	I	2	Total	Zn	0	0
			2	2		
15	C	1	Total	Zn	0	0
			1	1		
15	A	2	Total	Zn	0	0
			2	2		
15	L	1	Total	Zn	0	0
			1	1		

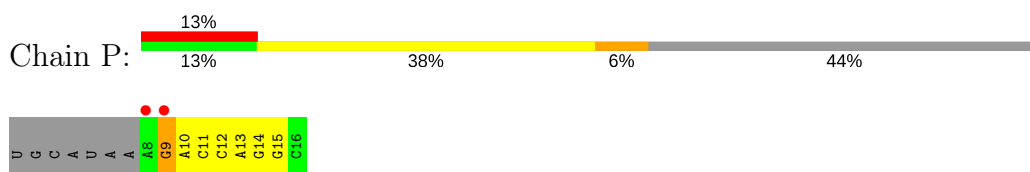
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

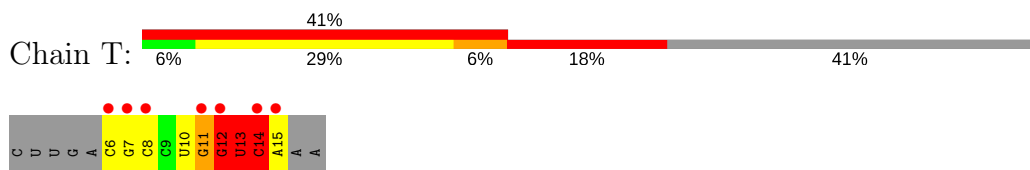
3 Residue-property plots

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

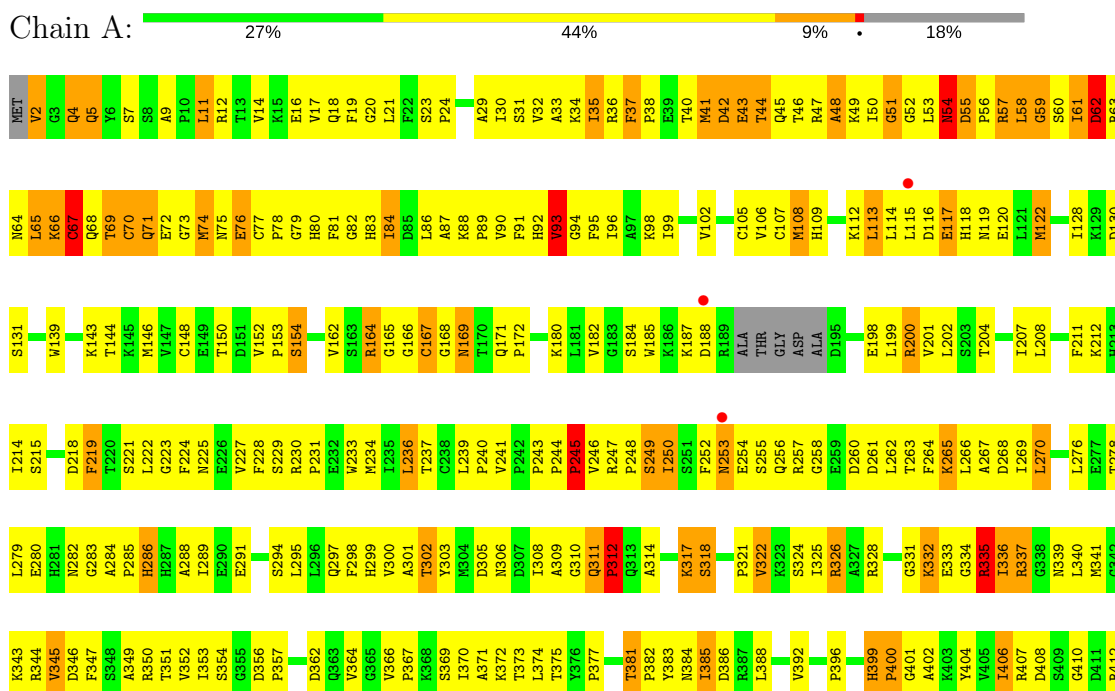
- Molecule 1: RNA (5'-R(*UP*GP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3')



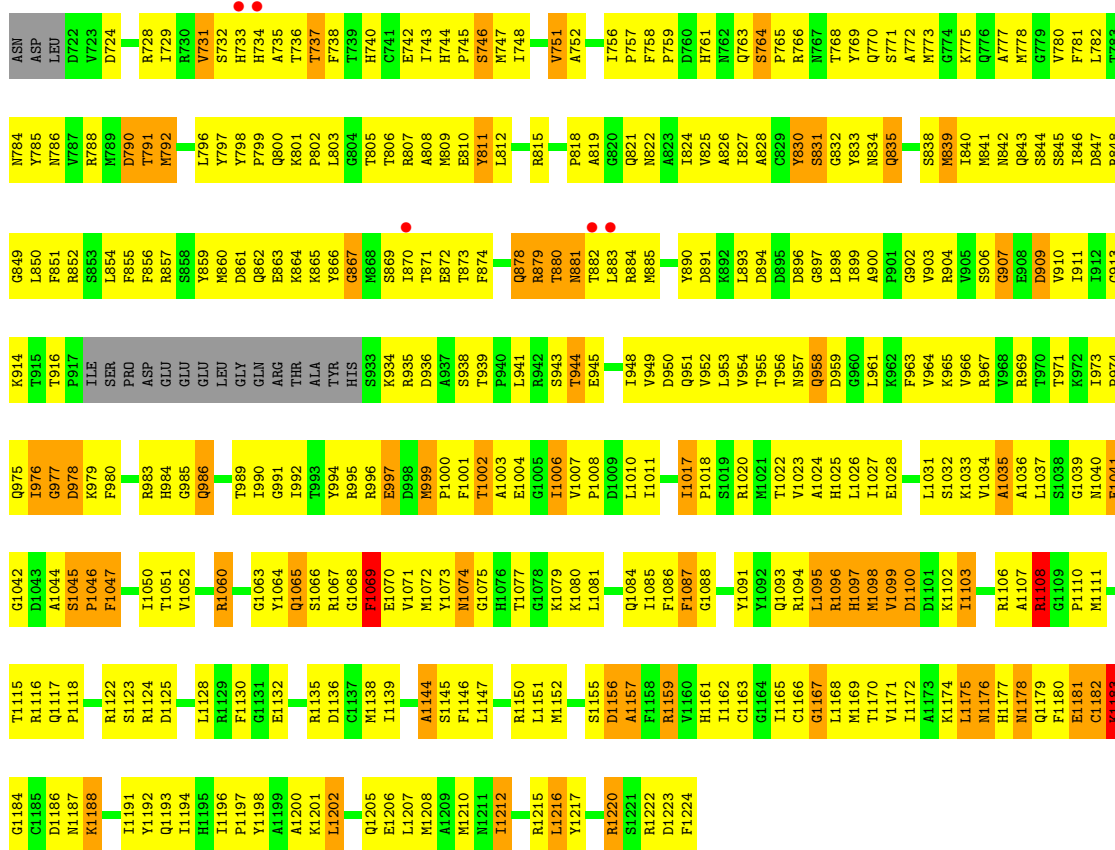
- Molecule 2: RNA (5'-R(*CP*UP*UP*GP*AP*CP*GP*CP*CP*UP*GP*GP*UP*CP*AP*AP*A)-3')



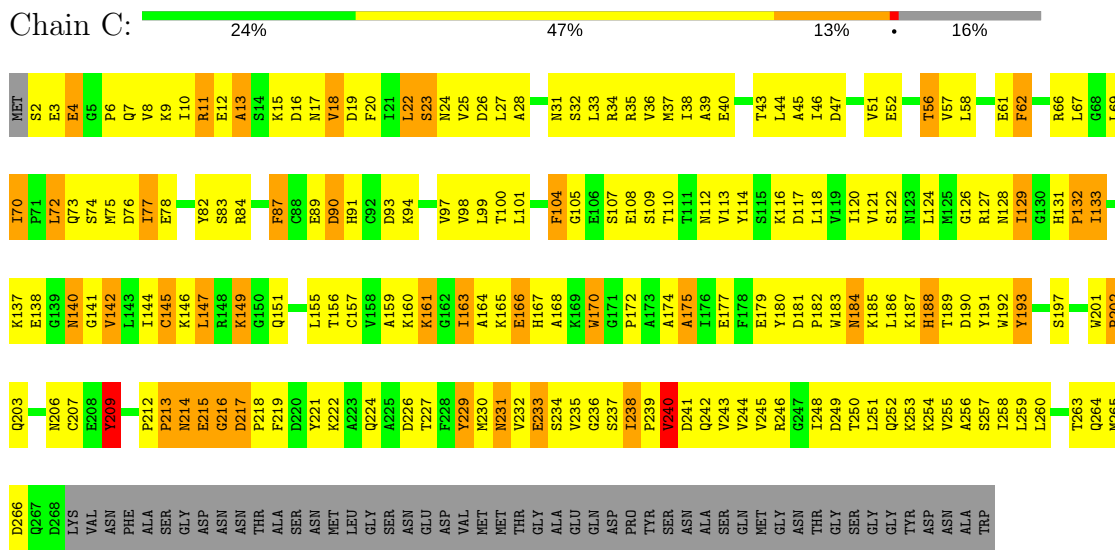
- Molecule 3: DNA-directed RNA polymerase II subunit RPB1



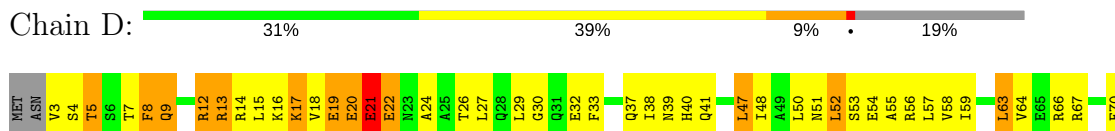
LYS	L1387	R1326	P1190	Y1119	Q1052	D985	L901	G835	C764	K687	I612	E542	S476	L413
ILE	L1327	I1327	W1191	L1120	F1053	I986	L902	Y836	V765	V693	I613	L543	P477	D414
THR	M1398	Y1328	L1192	E1121	R1054	V987	N903	I837	G766	T694	G615	V546	Y478	L415
GLU	C1400	M1330	L1193	P1122	L1055	L988	T904	Q838	Q767	T694	G616	L547	N479	R416
ASP	S1401	M1331	R1194	H1124	R1055	D992	D905	R839	Q768	K695	V617	N548	A480	S418
GLY	F1402	F1332	E1264	H1124	V1058	L993	R907	R840	R774	A697	E618	E549	F482	K419
GLN	E1403	I1333	A1125	A1126	V1059	N996	L908	V842	I775	Q698	K619	L550	D483	R420
ASP	T1405	M1266	D1127	D1127	P1060	L997	L913	R943	F779	A699	K620	Y551	M487	D423
GLY	V1406	L1268	Q1128	Q1128	G1061	L998	E914	A844	V780	N700	T621	V552	M488	L424
VAL	E1407	I1271	Q1130	Q1130	M1063	R1001	I919	E846	D781	H706	G623	V659	R490	Q425
THR	L1409	D1206	I1134	I1134	G1865	G1002	L920	D847	R782	H706	S624	V660	R491	L426
PRO	F1410	L1274	R1135	R1135	V1066	R1003	G921	V849	T783	T709	M626	P561	P492	Q428
THR	E1411	L1208	S1136	S1136	L1067	N1004	R940	R943	R784	L710	G627	V662	P492	Y429
SER	G1412	M1209	A1137	A1137	Q1070	E1005	Q926	Y852	H786	R711	G628	P563	Q493	G429
ASN	A1413	E1280	I1138	I1138	G1073	I1006	R926	R853	H786	R711	G629	P563	S494	W430
GLU	A1414	R1281	T1141	T1141	P1075	I1007	L929	N854	F787	E712	G630	V565	A495	K431
SER	S1415	V1282	T1141	T1141	A1076	Q1008	Y933	T855	K789	F714	H631	V566	T497	E433
GLY	A1416	V1283	K1144	K1144	G1073	N1009	R934	Y792	Y792	M717	V632	P568	R498	E433
LEU	L1417	M1284	R1144	R1144	E1074	A1010	Q935	N858	P794	V718	V633	P568	A499	R434
VAL	L1418	M1285	T1147	T1147	P1075	I1011	L936	N854	P794	V719	T634	P568	A499	H435
ASN	Y1349	R1216	T1147	T1147	A1076	R1012	L936	S859	E801	V720	R635	P570	E500	D438
ALA	K1350	K1217	T1148	T1148	H1079	D1013	D939	L860	E802	R728	C642	L571	L504	D440
ASP	E1351	Q1218	A1149	A1149	M1079	A1014	R940	G861	S796	F721	C642	L572	L504	P441
LEU	V1352	T1219	S1150	S1150	T1080	V1015	R940	N862	K797	L722	C642	L572	L504	P441
ASP	G1423	F1220	E1151	E1151	L1081	T1016	R940	V863	G798	M722	L645	G574	A506	V442
VAL	V1424	K1221	I1152	I1152	ASN	L1017	F942	R864	F799	E724	F646	K575	V507	L443
LYS	S1425	P1294	Y1153	Y1153	THR	F1018	L943	Q865	V800	A725	G647	Q576	P508	F444
ASP	E1426	D1223	T1154	T1154	PHE	C1019	Y854	F866	E801	K728	N648	V577	V569	N445
GLU	I1429	L1224	D1155	D1155	HIS	C1020	P954	I867	N802	K728	L649	L578	Q510	R446
MET	G1430	V1226	P1156	P1156	PHE	L1021	P955	Y868	S803	Q650	L650	S879	I511	Q447
SER	M1431	I1227	T1161	T1161	ALA	R1022	L956	G869	Y804	R731	L658	V580	V512	L450
PRO	M1433	W1228	V1162	V1162	GLY	L1023	P957	E870	R805	L732	L658	V580	V512	L450
LEU	A1434	D1233	I1163	I1163	VAL	S1024	V958	D871	R806	V735	L657	V580	V512	L450
VAL	P1435	D1233	P1164	P1164	SER	L1026	R960	G872	G807	V735	L657	V580	V512	L450
ASP	I1436	L1236	E1165	E1165	K1092	A1027	R961	D874	T809	L737	L657	V580	V512	L450
ASP	I1436	W1304	D1166	D1166	K1093	T1028	R962	A875	E812	K738	L659	V580	V512	L450
ASP	I1436	V1305	I1170	I1170	V1094	R1029	I963	I878	F812	D739	S663	D592	P519	R451
SER	G1437	L1306	Q1171	Q1171	T1095	R1030	I964	I878	F814	L740	S663	D592	P519	R451
GLY	G1438	E1307	Q1171	Q1171	S1096	V1031	Q965	F815	N742	N742	T664	G652	M521	R458
SER	G1439	T1308	F1174	F1174	G1097	L1032	N966	L883	F815	N742	G665	T696	G652	R459
ASN	A1440	D1309	ASP	ASP	GLU	Q1033	A967	D884	H816	V743	I668	V596	I523	V460
ASP	F1441	R1240	GLU	GLU	L1105	D1038	H972	D884	H816	V743	I668	V596	I523	V460
ALA	D1442	R1242	ALA	ALA	L1105	K1039	I973	D884	H816	V743	I668	V596	I523	V460
ALA	V1443	V1242	ALA	ALA	L1106	Q1040	A1041	D884	H816	V743	I668	V596	I523	V460
ALA	M1444	V1244	L1176	L1176	V1107	A1041	K977	D826	G753	G753	M676	N603	I531	T467
ALA	I1445	R1244	L1177	L1177	V1107	V1045	P978	D826	G753	G753	M676	N603	I531	T467
GLY	Q1378	P1245	ASP	ASP	L1114	W1044	S979	D826	G753	G753	M676	N603	I531	T467
GLY	D1446	LYS	GLU	GLU	S1115	V1045	R980	D826	G753	G753	M676	N603	I531	T467
PHE	E1447	SER	GLU	GLU	S1115	L1046	L981	D826	G753	G753	M676	N603	I531	T467
THR	T1385	M1317	GLU	GLU	L1116	S1047	T962	D826	G753	G753	M676	N603	I531	T467
ALA	R1386	M1317	LEU	LEU	L1116	S1047	T962	D826	G753	G753	M676	N603	I531	T467
ALA	R1386	M1317	ASP	ASP	Q1187	T1117	R989	D826	G753	G753	M676	N603	I531	T467
ALA	V1451	V1319	ASP	ASP	Q1187	T1117	R989	D826	G753	G753	M676	N603	I531	T467
GLY	G1388	V1319	GLU	GLU	S1115	L1046	L981	D826	G753	G753	M676	N603	I531	T467
GLY	F1389	P1320	THR	THR	S1115	L1046	L981	D826	G753	G753	M676	N603	I531	T467
ALA	M1454	G1321	PHE	PHE	S1115	L1046	L981	D826	G753	G753	M676	N603	I531	T467
ASP	P1455	I1322	GLU	GLU	L1116	S1047	T962	D826	G753	G753	M676	N603	I531	T467
TRP	M1393	D1323	GLU	GLU	L1116	S1047	T962	D826	G753	G753	M676	N603	I531	T467
GLY	L1394	T1325	E1254	E1254	V1118	I1049	K984	D826	G753	G753	M676	N603	I531	T467

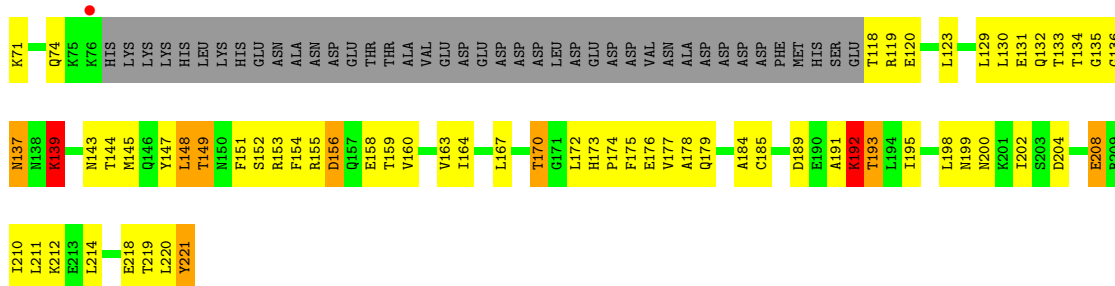


● Molecule 5: DNA-directed RNA polymerase II subunit RPB3

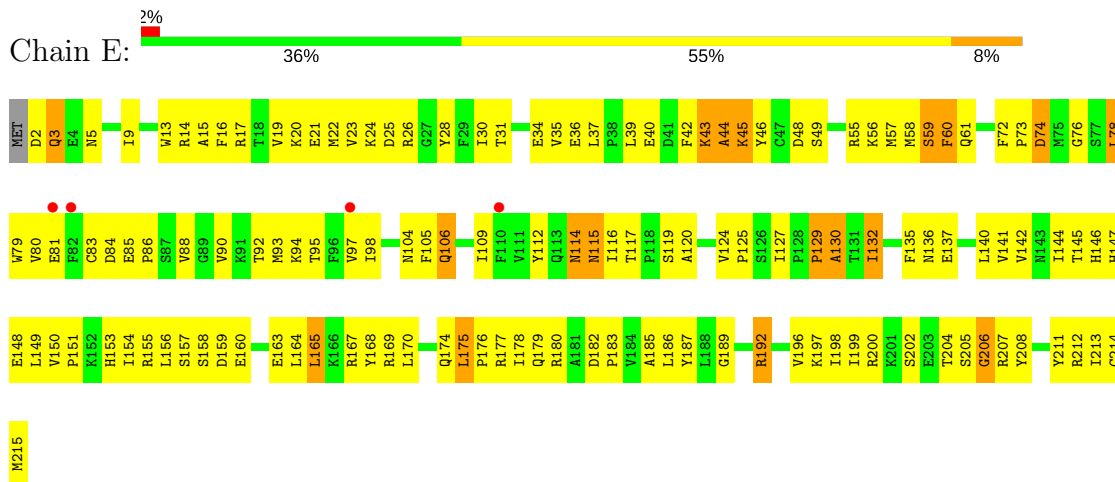


● Molecule 6: DNA-directed RNA polymerase II subunit RPB4

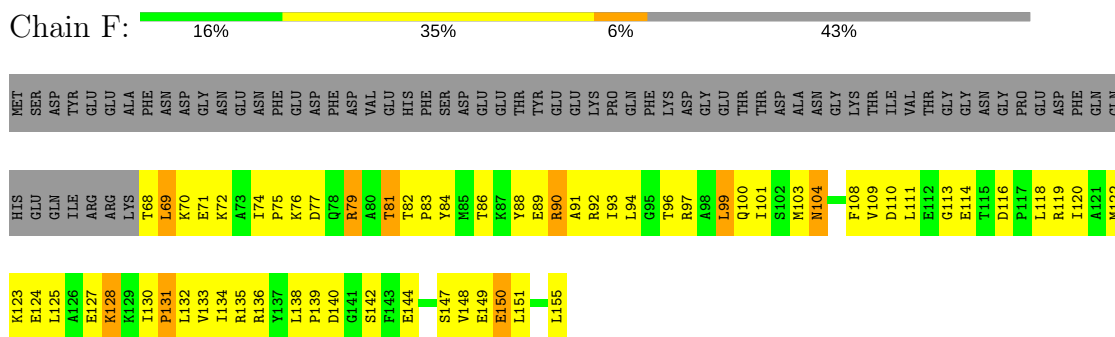




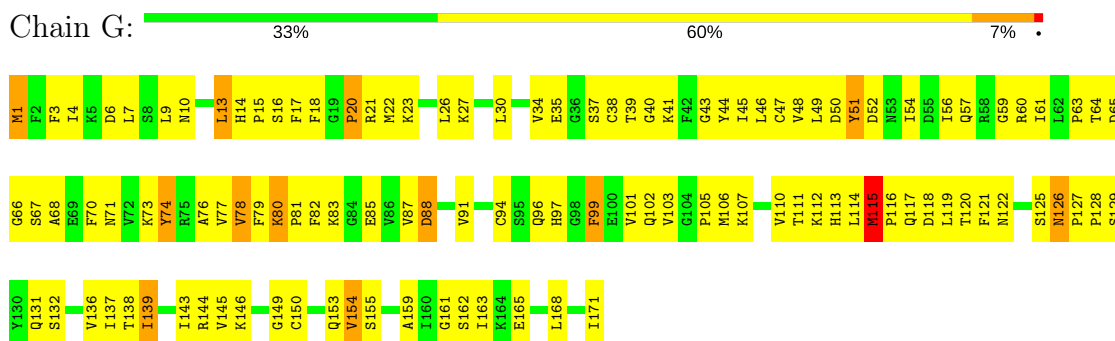
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



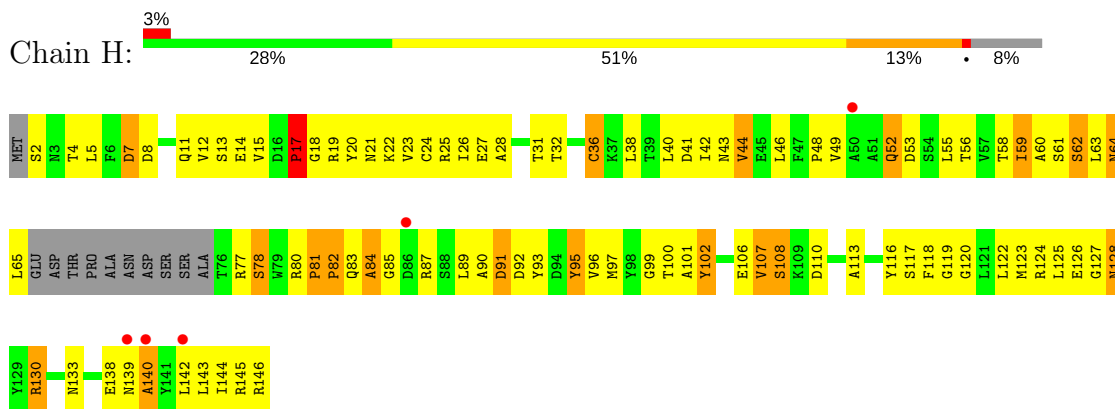
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



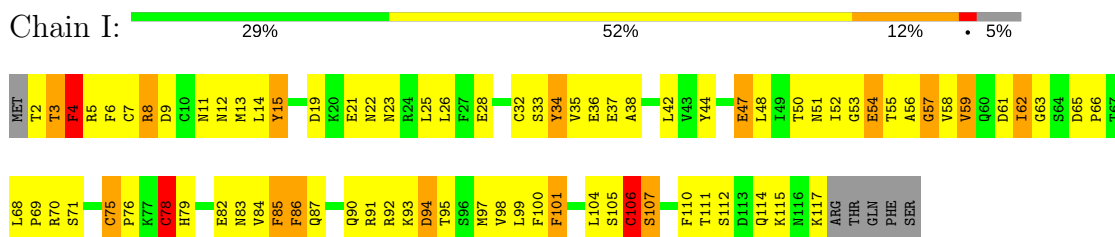
- Molecule 9: DNA-directed RNA polymerase II subunit RPB7



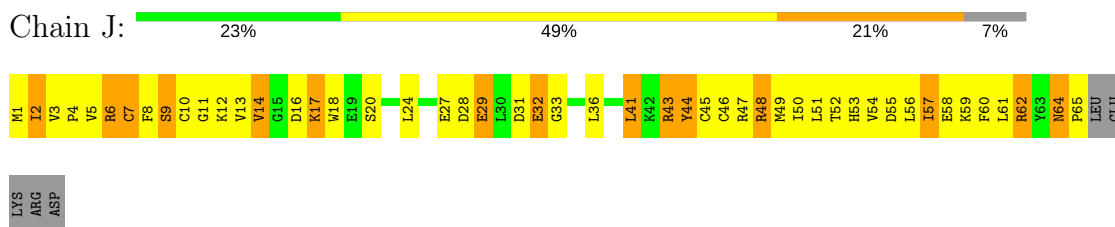
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3



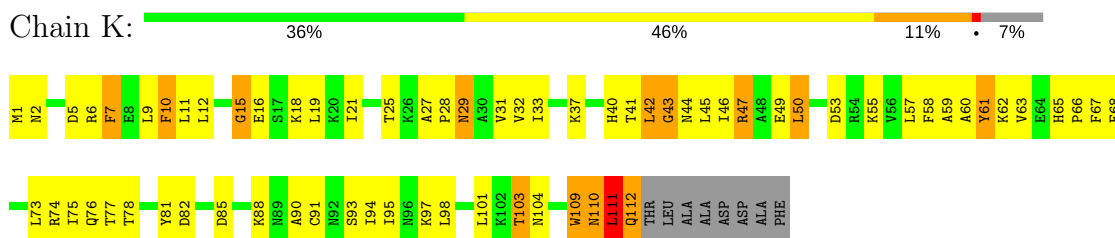
- Molecule 11: DNA-directed RNA polymerase II subunit RPB9



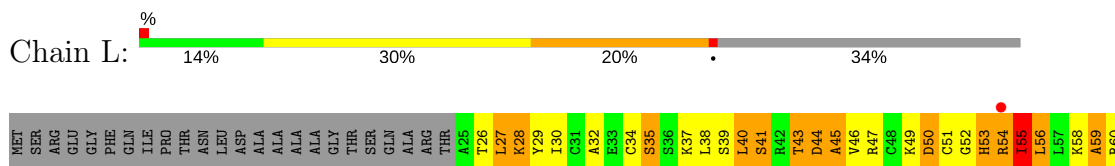
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 13: DNA-directed RNA polymerase II subunit RPB11



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC4



T61	✓
RG2	✓
RG3	✓
L64	✓
V65	✓
A69	✓
R70	✓

4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.68Å 393.85Å 283.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 48.51 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 99.9 (48.51-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.44 (at 3.77Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.246 0.217 , 0.247	Depositor DCC
R_{free} test set	2431 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	114.7	Xtrriage
Anisotropy	0.449	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.038 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31611	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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 [i](#)

5.1 Standard geometry [i](#)

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	P	0.63	0/215	0.81	0/334
2	T	0.71	0/231	1.32	5/358 (1.4%)
3	A	0.42	0/11394	0.73	7/15407 (0.0%)
4	B	0.41	0/9012	0.68	1/12149 (0.0%)
5	C	0.43	0/2138	0.71	0/2896
6	D	0.39	0/1444	0.66	0/1935
7	E	0.39	0/1788	0.63	0/2406
8	F	0.45	0/724	0.76	0/977
9	G	0.45	0/1368	0.72	0/1844
10	H	0.37	0/1102	0.62	0/1492
11	I	0.38	0/962	0.65	0/1295
12	J	0.47	0/541	0.75	0/727
13	K	0.45	0/922	0.68	0/1244
14	L	0.46	0/366	0.69	0/485
All	All	0.42	0/32207	0.71	13/43549 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1176	LEU	CA-CB-CG	13.45	146.23	115.30
2	T	12	G	N9-C1'-C2'	9.04	125.76	114.00
2	T	12	G	O4'-C1'-N9	8.14	114.72	108.20
2	T	13	U	O4'-C1'-N1	7.87	114.50	108.20
3	A	1176	LEU	CB-CA-C	-7.05	96.81	110.20

There are no chirality outliers.

There are no planarity outliers.

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	P	192	0	101	6	0
2	T	208	0	110	16	0
3	A	11194	0	11278	1259	0
4	B	8841	0	8874	1006	0
5	C	2101	0	2055	275	0
6	D	1434	0	1460	146	0
7	E	1752	0	1776	163	0
8	F	712	0	738	89	0
9	G	1340	0	1357	182	0
10	H	1084	0	1057	140	0
11	I	944	0	903	120	0
12	J	532	0	542	90	0
13	K	904	0	911	93	0
14	L	364	0	388	54	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	1	0	0	0	0
All	All	31611	0	31550	3310	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 52.

The worst 5 of 3310 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:A:58:LEU:HD12	3:A:59:GLY:H	0.99	1.11
4:B:343:ILE:HG23	4:B:347:LYS:HB2	1.25	1.09
4:B:510:LYS:HG2	4:B:511:PRO:HD3	1.22	1.08
3:A:53:LEU:HD23	3:A:54:ASN:N	1.68	1.08
5:C:43:THR:HG22	5:C:44:LEU:H	0.98	1.07

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	
3	A	1412/1733 (82%)	1030 (73%)	249 (18%)	133 (9%)	1	13
4	B	1094/1224 (89%)	780 (71%)	214 (20%)	100 (9%)	1	14
5	C	264/318 (83%)	164 (62%)	64 (24%)	36 (14%)	0	5
6	D	174/221 (79%)	126 (72%)	30 (17%)	18 (10%)	0	11
7	E	212/215 (99%)	158 (74%)	36 (17%)	18 (8%)	1	15
8	F	86/155 (56%)	69 (80%)	9 (10%)	8 (9%)	1	14
9	G	169/171 (99%)	130 (77%)	33 (20%)	6 (4%)	4	35
10	H	131/146 (90%)	74 (56%)	36 (28%)	21 (16%)	0	4
11	I	114/122 (93%)	69 (60%)	30 (26%)	15 (13%)	0	5
12	J	63/70 (90%)	39 (62%)	10 (16%)	14 (22%)	0	1
13	K	110/120 (92%)	87 (79%)	15 (14%)	8 (7%)	1	20
14	L	44/70 (63%)	18 (41%)	10 (23%)	16 (36%)	0	0
All	All	3873/4565 (85%)	2744 (71%)	736 (19%)	393 (10%)	0	11

5 of 393 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	4	GLN
3	A	44	THR
3	A	48	ALA
3	A	54	ASN
3	A	57	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	1245/1520 (82%)	1129 (91%)	116 (9%)	10	40
4	B	964/1061 (91%)	890 (92%)	74 (8%)	14	49
5	C	235/274 (86%)	212 (90%)	23 (10%)	9	38
6	D	160/200 (80%)	142 (89%)	18 (11%)	6	32
7	E	196/197 (100%)	188 (96%)	8 (4%)	33	66
8	F	78/137 (57%)	75 (96%)	3 (4%)	36	68
9	G	152/152 (100%)	140 (92%)	12 (8%)	13	48
10	H	119/128 (93%)	113 (95%)	6 (5%)	27	62
11	I	110/116 (95%)	99 (90%)	11 (10%)	8	37
12	J	60/65 (92%)	55 (92%)	5 (8%)	12	46
13	K	97/102 (95%)	87 (90%)	10 (10%)	8	36
14	L	40/57 (70%)	36 (90%)	4 (10%)	8	37
All	All	3456/4009 (86%)	3166 (92%)	290 (8%)	12	46

5 of 290 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	393	LYS
4	B	909	ASP
11	I	94	ASP
4	B	429	PHE
4	B	628	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	366	GLN
4	B	957	ASN
11	I	90	GLN
4	B	513	GLN

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Mol	Chain	Res	Type
4	B	538	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	P	8/16 (50%)	1 (12%)	0
2	T	9/17 (52%)	5 (55%)	2 (22%)
All	All	17/33 (51%)	6 (35%)	2 (11%)

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	P	9	G
2	T	11	G
2	T	12	G
2	T	13	U
2	T	14	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	T	12	G
2	T	13	U

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](#)

Of 9 ligands modelled in this entry, 9 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
4	B	1
5	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2:SER	C	3:GLU	N	3.04
1	B	337:ARG	C	338:GLY	N	2.61

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	P	9/16 (56%)	2.00	2 (22%) 0 0	194, 200, 200, 200	0
2	T	10/17 (58%)	2.21	7 (70%) 0 0	180, 190, 200, 200	0
3	A	1422/1733 (82%)	-0.26	7 (0%) 90 86	56, 116, 175, 200	0
4	B	1112/1224 (90%)	-0.20	12 (1%) 80 72	57, 126, 188, 200	0
5	C	267/318 (83%)	-0.29	0 100 100	74, 110, 158, 180	0
6	D	178/221 (80%)	-0.26	1 (0%) 89 84	87, 133, 184, 198	0
7	E	214/215 (99%)	-0.24	4 (1%) 66 57	90, 159, 197, 200	0
8	F	88/155 (56%)	-0.52	0 100 100	65, 91, 129, 140	0
9	G	171/171 (100%)	-0.30	0 100 100	88, 112, 155, 163	0
10	H	135/146 (92%)	0.34	5 (3%) 41 32	139, 166, 190, 200	0
11	I	116/122 (95%)	0.06	0 100 100	114, 163, 191, 200	0
12	J	65/70 (92%)	-0.49	0 100 100	79, 108, 146, 153	0
13	K	112/120 (93%)	-0.31	0 100 100	81, 114, 139, 167	0
14	L	46/70 (65%)	0.02	1 (2%) 62 51	111, 166, 194, 196	0
All	All	3945/4598 (85%)	-0.21	39 (0%) 82 75	56, 123, 187, 200	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	471	LYS	5.2
1	P	9	G	4.6
3	A	1092	LYS	3.8
1	P	8	A	3.5
2	T	15	A	3.5

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	ZN	A	1506	1/1	0.95	0.08	121,121,121,121	0
15	ZN	L	105	1/1	0.97	0.11	155,155,155,155	0
16	MG	A	1	1/1	0.97	0.18	79,79,79,79	0
15	ZN	I	203	1/1	0.99	0.16	120,120,120,120	0
15	ZN	I	204	1/1	0.99	0.04	181,181,181,181	0
15	ZN	C	302	1/1	1.00	0.13	82,82,82,82	0
15	ZN	A	1508	1/1	1.00	0.14	83,83,83,83	0
15	ZN	J	101	1/1	1.00	0.25	100,100,100,100	0
15	ZN	B	1307	1/1	1.00	0.22	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.