



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2017 – 04:31 PM EDT

PDB ID : 2R92
Title : Elongation complex of RNA polymerase II with artificial RdRP scaffold
Authors : Lehmann, E.; Brueckner, F.; Cramer, P.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

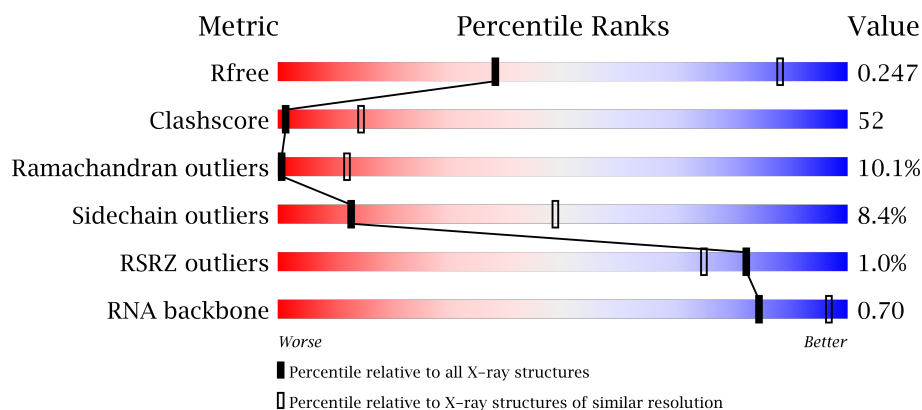
1 Overall quality at a glance

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.



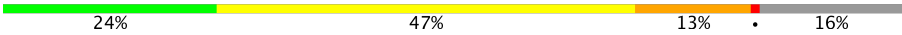
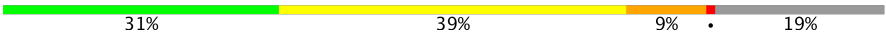


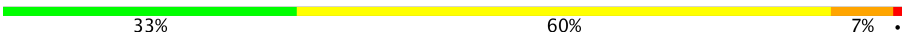
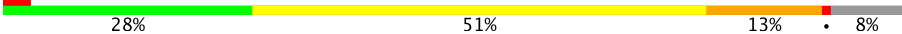
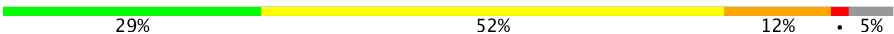
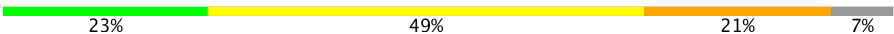
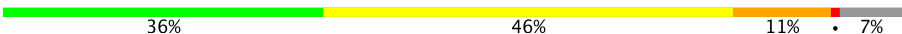

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)
RNA backbone	2435	1016 (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	<div> <div>13%</div> <div>13% 38% 6% 44%</div> </div>
2	T	17	<div> <div>41%</div> <div>6% 29% 6% 18% 41%</div> </div>
3	A	1733	<div> <div>27% 44% 9% 18%</div> </div>
4	B	1224	<div> <div>27% 53% 10% 9%</div> </div>

Continued on next page...

Continued from previous page...

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

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
1	P	9	Total	C	N	O	P	0	0	0
			192	87	39	58	8			

- 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
2	T	10	Total	C	N	O	P	0	0	0
			208	94	36	69	9			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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		

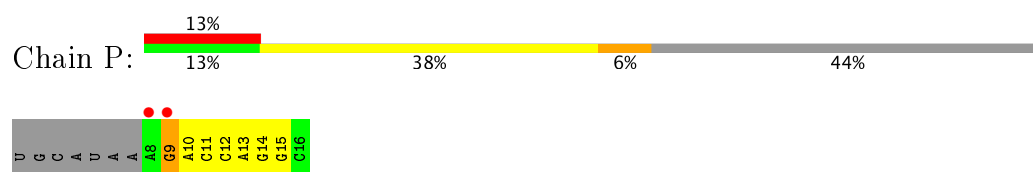
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

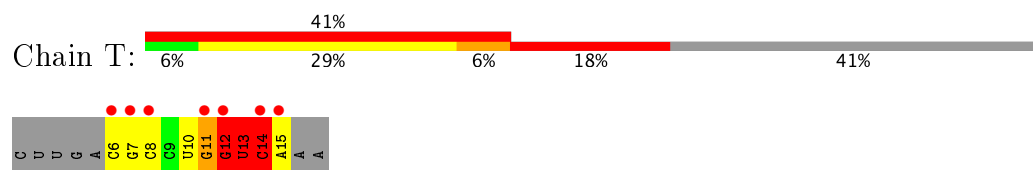
3 Residue-property plots

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.

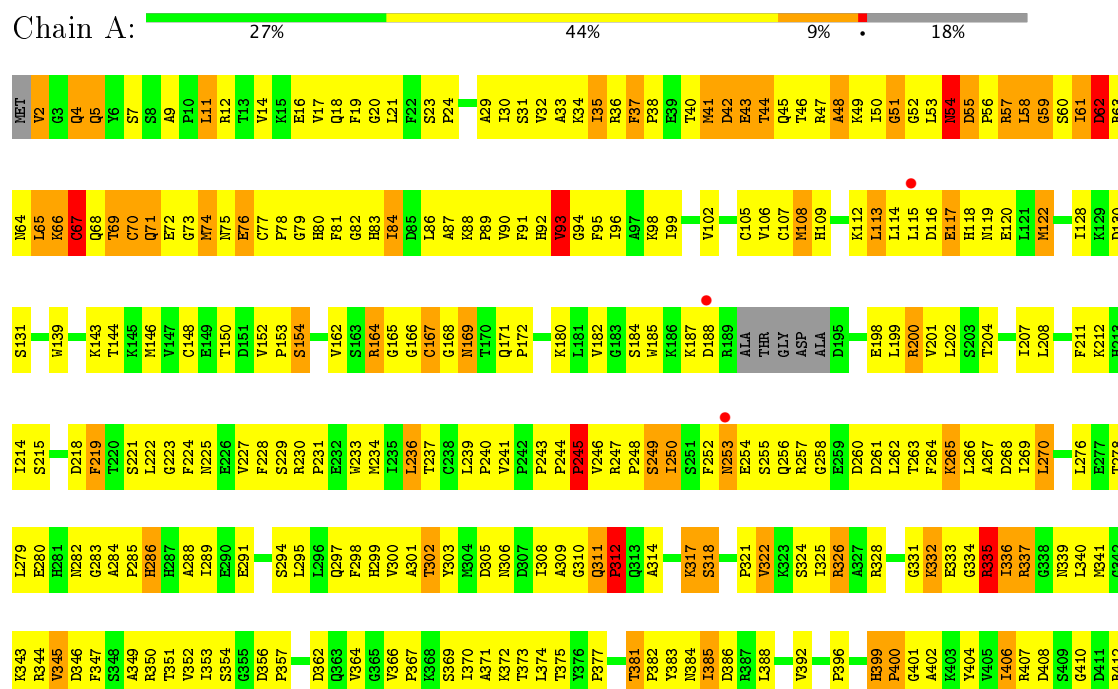
- Molecule 1: RNA (5'-R(*UP*GP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3')



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

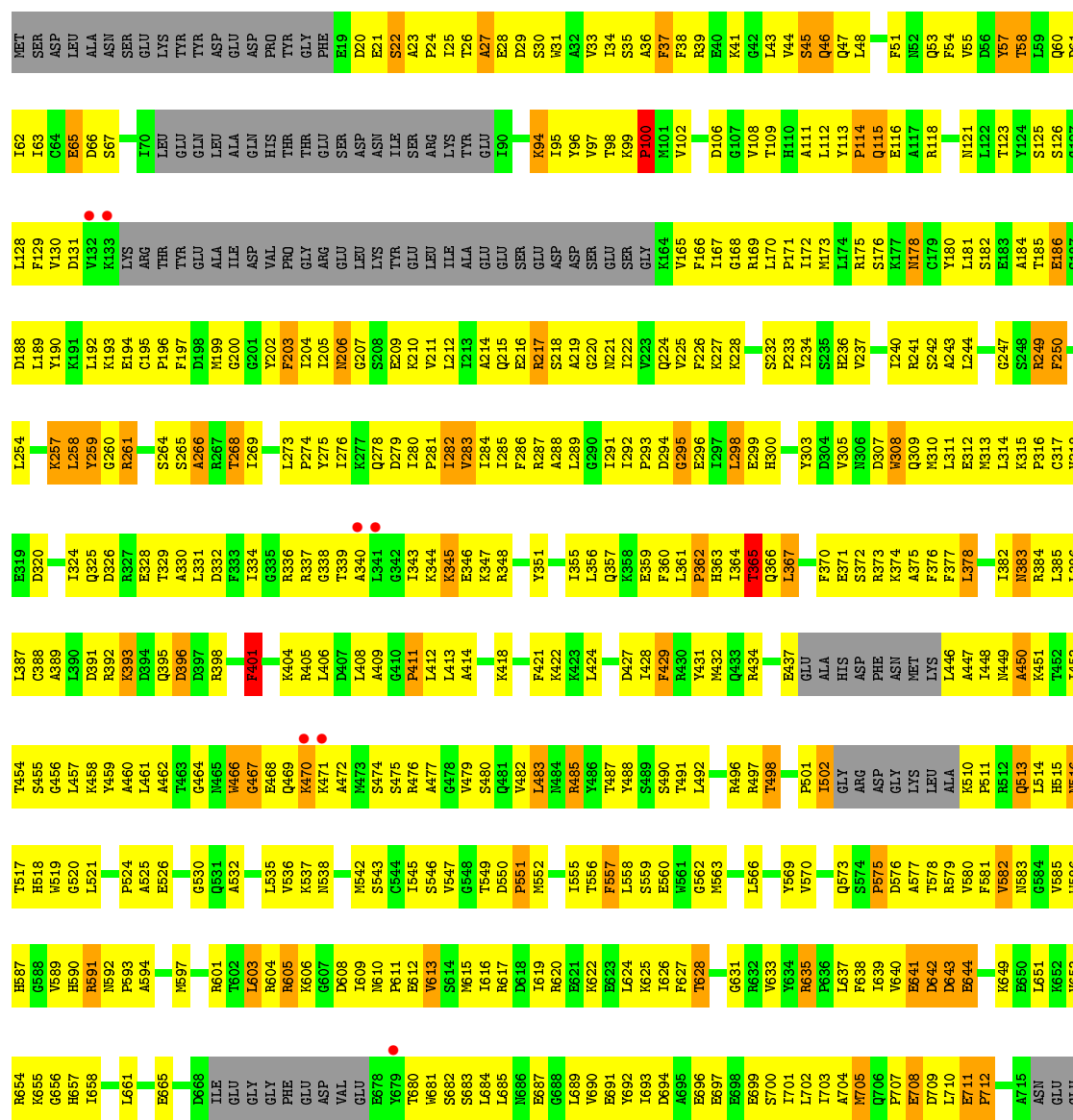


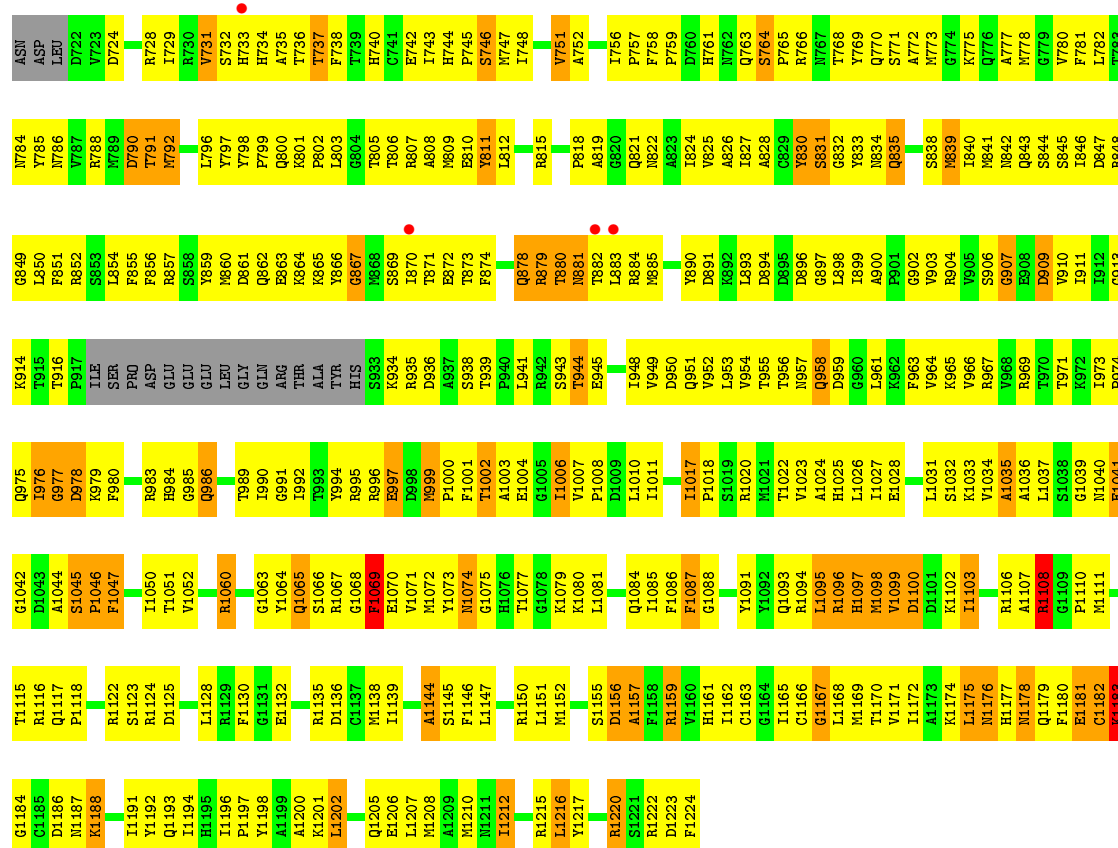
- Molecule 3: DNA-directed RNA polymerase II subunit RPB1



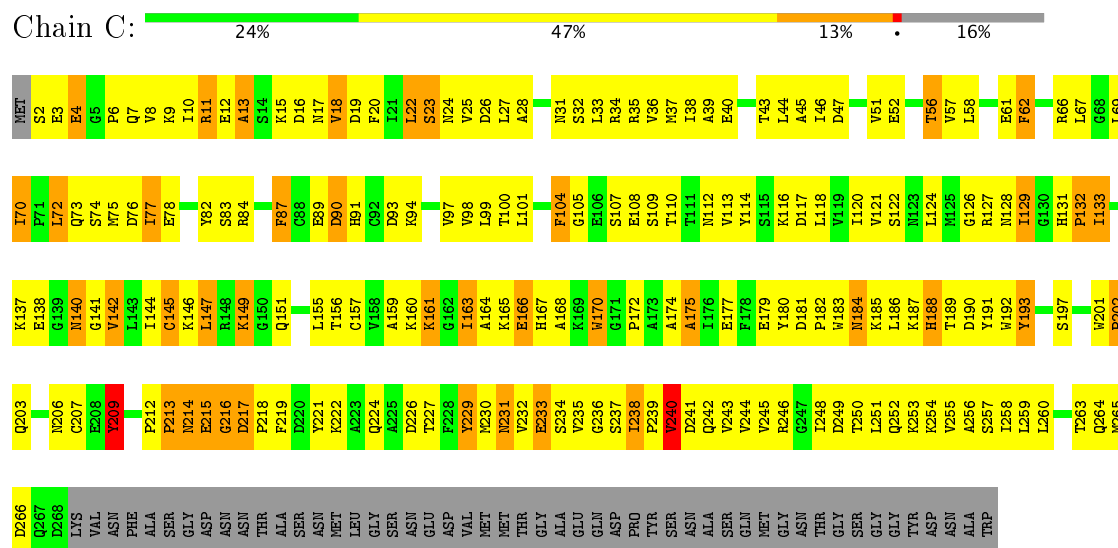
LYS	R1326	P1190	Y1119	Q1052	D985	L901	G835	C764	I687	I612	E542	S476	L413
ILE	I1327	W1191	L1120	Q1052	I986	L902	Y836	V765	I687	I613	E543	P477	D414
THR	Y1328	L1192	E1121	F1053	V987	N903	R837	G766	V693	G614	L543	P477	D415
GLU	T1329	L1193	P1122	L1054	L988	T904	Q838	Q767	T694	G615	Y546	N479	L416
ILE	N1330	R1194	G1123	R1055	D992	D905	R839	Q768	K695	V616	L547	A480	Y417
ASP	S1331	H1124	H1124	V1058	L993	H906	R840	R774	K696	V617	N548	D481	S418
GLY	F1332	D1197	A1125	R1059	L993	T907	L841	I775	K697	E618	K549	P482	K419
GLY	I1333	D1198	A1126	P1060	N996	L908	R842	I775	Q698	K619	L550	D483	K420
GLN	T1334	M1201	Q1128	G1061	L997	L913	A844	F779	Q699	K620	Y551	M487	D423
ASP	M1202	A1201	Q1128	E1062	L998	L914	L845	V780	N700	T621	Y552	N488	L424
GLY	V1406	E1129	M1063	E1062	L998	E914	L845	V780	N700	T621	Y552	N488	L424
GLY	E1307	Q1130	M1063	E1062	L998	E914	L845	V780	N700	T621	Y552	N488	L424
VAL	I1271	K1205	I1271	G1065	R1001	I919	E846	D781	H706	G623	V559	K490	Q425
THR	L1272	D1206	I1134	G1065	G1002	L920	D847	R782	H706	G623	V559	K490	Q425
PRO	L1273	L1207	R1135	L1066	R1003	L920	E848	T783	H706	G623	V559	K490	Q425
THR	R1274	T1208	S1136	L1067	R1004	G921	R849	L784	T709	G627	P561	P492	Q428
SER	I1279	M1209	A1137	L1067	E1005	Q926	Y852	H786	R711	G627	P561	P492	Q428
ASN	E1280	G1210	I1138	Q1070	I1006	Q926	D853	H786	R711	G627	P561	P492	Q428
GLU	R1281	Q1211	I1138	S1071	I1007	L929	N854	F787	E712	L629	A564	S494	K431
SER	V1282	V1212	T1141	I1072	Q1008	L929	T855	S788	S713	I630	I565	E496	V432
GLY	V1283	G1213	K1144	G1073	N1009	Y933	T856	Y792	N717	V632	K567	T497	E433
LEU	M1284	E1214	R1145	E1074	K934	K934	R857	S793	N718	V632	K567	T497	E433
VAL	M1285	R1215	P1075	P1075	Q935	Q935	N858	P794	V719	T634	P568	A499	K434
ASN	I1216	K1216	T1147	A1076	L936	L936	S859	P794	V719	T634	P568	A499	K434
ALA	R1289	K1217	I1148	HIS	D1013	L936	L860	E795	R720	R635	P570	Q503	D438
ASP	K1218	Q1218	A1149	PHE	A1014	D839	G861	S796	F721	G642	L571	L504	D440
LEU	V1291	T1219	S1150	PHE	T1080	R940	R862	K797	L722	G642	L571	L504	D440
ASP	P1292	P1220	E1151	ALA	T1016	K941	V863	G798	N723	L645	G574	C905	P441
VAL	S1293	K1221	ASN	ASN	T1017	F942	R864	F799	E724	L646	K575	A506	V442
VAL	P1294	N1222	THR	THR	F1018	L943	Q865	V800	A725	G647	K576	P507	L443
LYS	T1295	D1223	P1154	PHE	C1019	L943	R866	E801	K728	N648	I577	L569	N445
ASP	G1296	L1224	D1155	HIS	G1020	Y954	T867	N802	K728	L649	L578	Q510	R446
GLU	E1297	F1225	P1156	PHE	L1021	P955	T868	S803	K728	L649	L578	Q510	R446
MET	Y1362	V1226	T1161	ALA	L1022	P955	G869	N803	K728	L649	L578	Q510	R446
SER	N1363	I1227	V1162	ALA	R1023	L956	R870	Y804	R731	K651	V580	S512	L450
PRO	Y1364	N1228	V1163	ALA	S1024	V958	D871	R806	L732	V652	L584	P514	R451
LEU	R1366	D1233	P1164	SER	R1025	L960	G872	L808	V735	V653	L584	P514	R451
VAL	W1304	D1236	E1165	ALA	L1026	L960	R873	L808	N736	L657	L586	Q515	K452
ASP	V1305	L1237	D1166	K1093	A1027	R961	D874	T809	L737	L658	S516	S516	K453
GLY	L1306	I1237	T1170	K1093	T1028	R962	A875	T809	K738	L659	S517	S517	K454
SER	E1307	I1238	Q1171	V1094	R1029	I963	I878	E812	D739	S663	P591	P519	K455
ASN	T1308	R1239	Q1171	S1096	V1031	Q965	R883	F814	N741	T664	D592	C520	A457
ASP	D1309	G1240	F1174	G1097	L1032	N966	L883	F815	N742	G665	T595	G522	R458
ALA	G1310	R1241	S1175	R1100	Q1033	A967	D894	H816	V743	I666	T596	I523	V460
ALA	V1311	V1242	L1176	L1101	E1034	Q968	T885	A817	K744	G667	L597	V524	K461
MET	N1312	V1243	L1177	K1102	Y1035	Q969	I886	M818	Q745	G667	L597	V524	K461
ALA	M1444	R1244	L1177	K1102	R1036	T970	G887	A817	K745	G667	L597	V524	K461
GLY	Q1378	P1245	ASP	E1103	L1037	F971	G888	R821	N746	D672	P600	D526	L463
GLY	G1379	LYS	GLU	E1104	T1038	H972	S889	E822	N748	P674	P600	T527	L463
PHE	V1316	SER	GLU	L1105	K1039	I973	D890	E822	N748	P674	P600	T527	L463
THR	M1317	LEU	GLU	L1106	Q1040	I973	A891	I825	A749	T676	L602	L528	K465
ALA	T1385	ASP	ALA	V1107	A1041	K977	A891	I825	A749	T676	L602	L528	K465
ALA	R1386	ASP	GLU	V1107	A1041	K977	A891	I825	A749	T676	L602	L528	K465
THR	L1450	ASP	GLU	V1107	A1041	K977	A891	I825	A749	T676	L602	L528	K465
GLY	V1451	ALA	GLN	T1113	V1045	P978	E894	T827	G754	I679	K605	R532	F468
GLY	K1452	GLU	PHE	P1114	V1045	S979	K895	A828	G754	I679	K605	R532	F468
ALA	Y1453	THR	ASP	S1115	L1046	D980	R896	V829	N757	T832	L606	L534	L470
ALA	M1454	GLU	ASP	S1116	L1046	L981	R897	K830	N757	T832	L606	L534	L470
ASP	P1455	A1254	Q1187	L1116	S1047	T982	R898	T831	N761	I683	L608	L536	L472
THR	N1393	E1255	Q1188	T1117	N1048	I983	V899	T831	N761	I683	L608	L536	L472
GLY	T1394	E1256	S1189	V1118	I1049	K984	D900	T834	A763	A686	P611	I541	T475

- Molecule 4: DNA-directed RNA polymerase II subunit RPB2

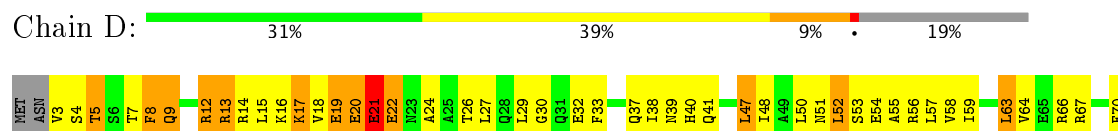


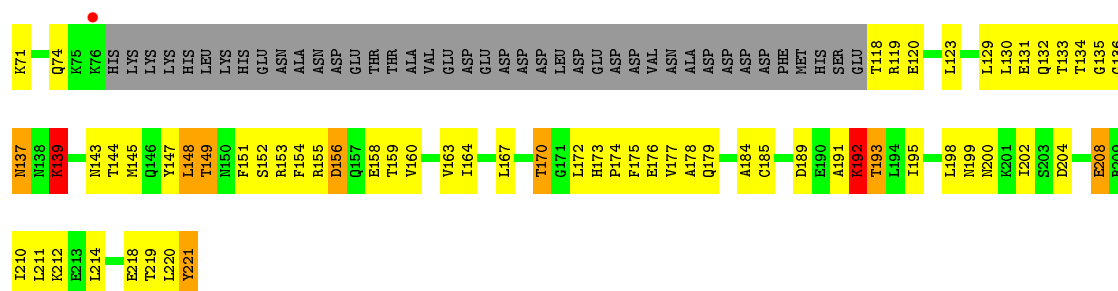


• Molecule 5: DNA-directed RNA polymerase II subunit RPB3

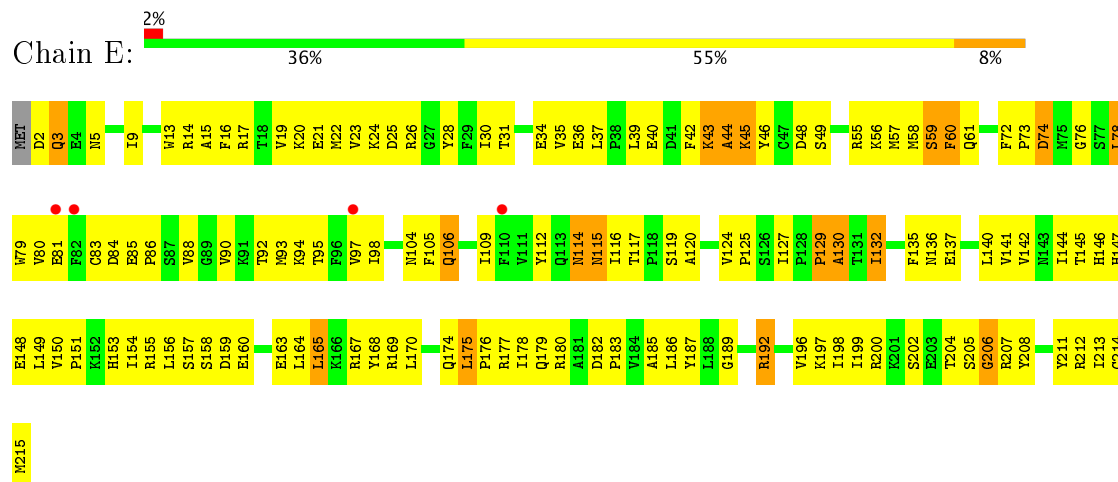


• Molecule 6: DNA-directed RNA polymerase II subunit RPB4

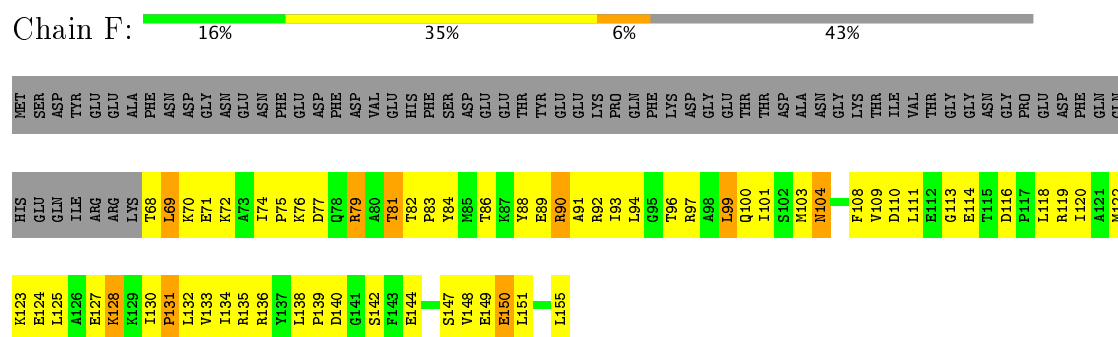




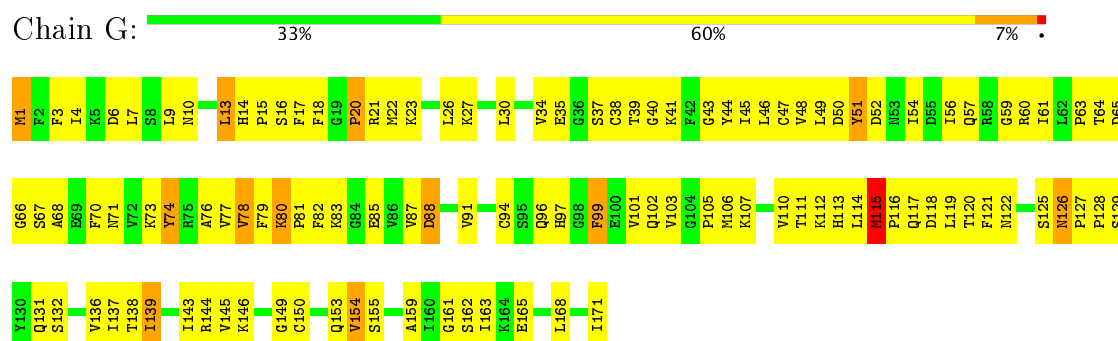
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



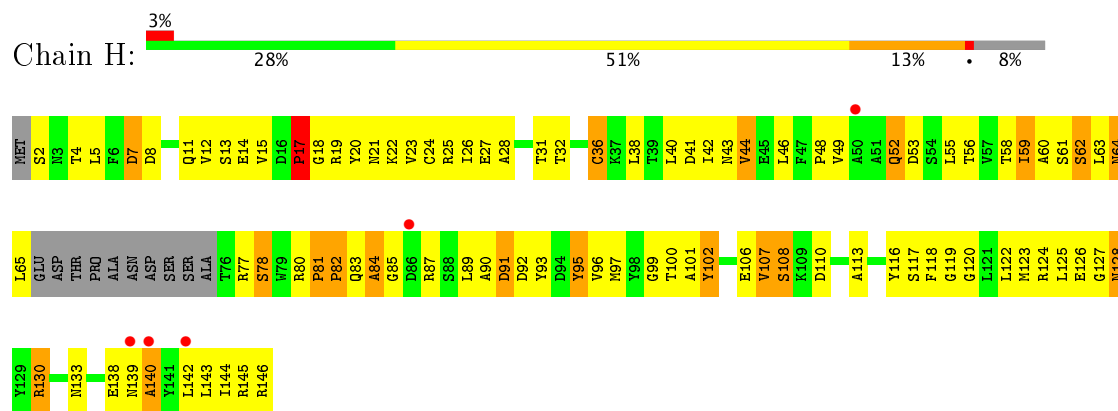
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



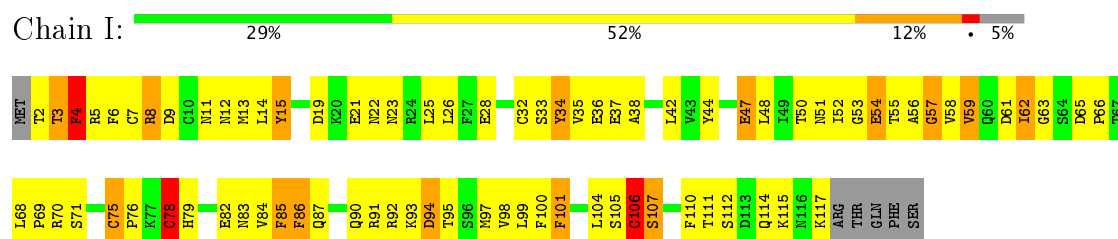
- Molecule 9: DNA-directed RNA polymerase II subunit RPB7



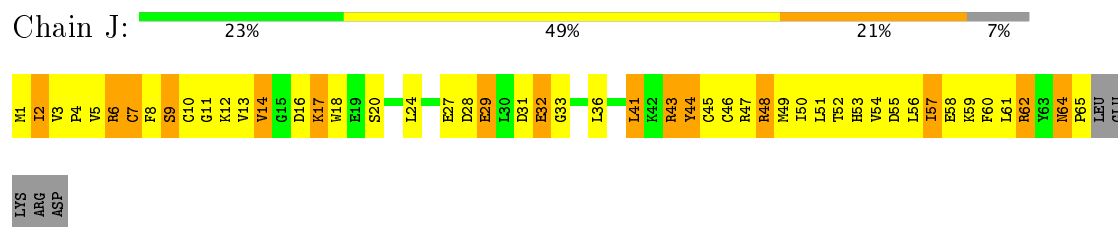
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3



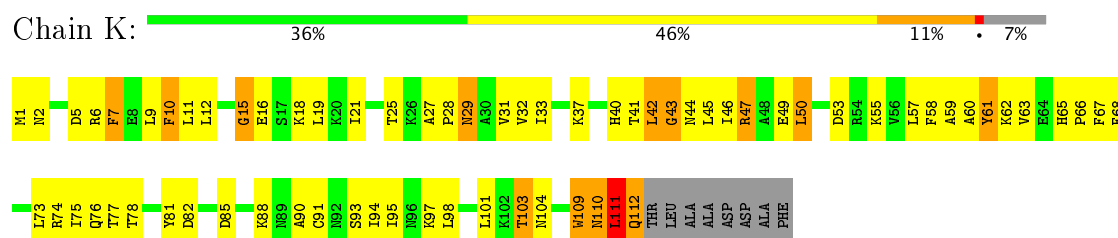
- Molecule 11: DNA-directed RNA polymerase II subunit RPB9



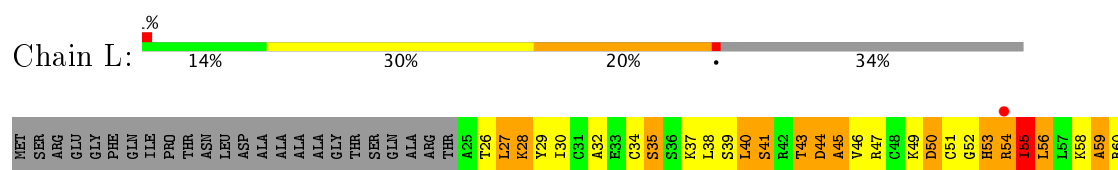
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



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



T61	
RG2	
RG3	
LG4	
VG5	
LG9	
RG0	

4 Data and refinement statistics

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)	Xtriage
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%)	DCC
Wilson B-factor (Å ²)	114.7	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
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	Xtriage
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

Xtriage'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

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	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 ⓘ

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	14
4	B	1094/1224 (89%)	780 (71%)	214 (20%)	100 (9%)	1	15
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	16
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	37
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	6
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	21
14	L	44/70 (63%)	18 (41%)	10 (23%)	16 (36%)	0	0
All	All	3873/4565 (85%)	2744 (71%)	736 (19%)	393 (10%)	1	12

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 ⓘ

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	43
4	B	964/1061 (91%)	890 (92%)	74 (8%)	15	52
5	C	235/274 (86%)	212 (90%)	23 (10%)	9	40
6	D	160/200 (80%)	142 (89%)	18 (11%)	7	34
7	E	196/197 (100%)	188 (96%)	8 (4%)	35	69
8	F	78/137 (57%)	75 (96%)	3 (4%)	38	70
9	G	152/152 (100%)	140 (92%)	12 (8%)	14	51
10	H	119/128 (93%)	113 (95%)	6 (5%)	28	65
11	I	110/116 (95%)	99 (90%)	11 (10%)	9	39
12	J	60/65 (92%)	55 (92%)	5 (8%)	13	49
13	K	97/102 (95%)	87 (90%)	10 (10%)	8	38
14	L	40/57 (70%)	36 (90%)	4 (10%)	9	39
All	All	3456/4009 (86%)	3166 (92%)	290 (8%)	13	49

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

Continued on next page...

Continued from previous page...

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	1.99	2 (22%) 1 1	194, 200, 200, 200	0
2	T	10/17 (58%)	2.20	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%)	-0.19	11 (0%) 82 75	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 85	87, 133, 184, 198	0
7	E	214/215 (99%)	-0.25	4 (1%) 67 58	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%) 42 34	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%)	0.01	1 (2%) 62 53	111, 166, 194, 196	0
All	All	3945/4598 (85%)	-0.21	38 (0%) 82 75	56, 123, 187, 200	0

The worst 5 of 38 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	3.7
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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
15	ZN	B	1307	1/1	1.00	0.22	0.80	83,83,83,83	0
15	ZN	I	203	1/1	0.99	0.16	0.27	120,120,120,120	0
15	ZN	C	302	1/1	1.00	0.13	-0.56	82,82,82,82	0
15	ZN	A	1508	1/1	1.00	0.14	-0.96	83,83,83,83	0
15	ZN	J	101	1/1	1.00	0.25	-0.97	100,100,100,100	0
15	ZN	L	105	1/1	0.97	0.10	-1.12	155,155,155,155	0
15	ZN	I	204	1/1	0.99	0.04	-1.70	181,181,181,181	0
15	ZN	A	1506	1/1	0.95	0.08	-2.66	121,121,121,121	0
16	MG	A	1	1/1	0.97	0.18	-	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.