



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:36 AM 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
<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

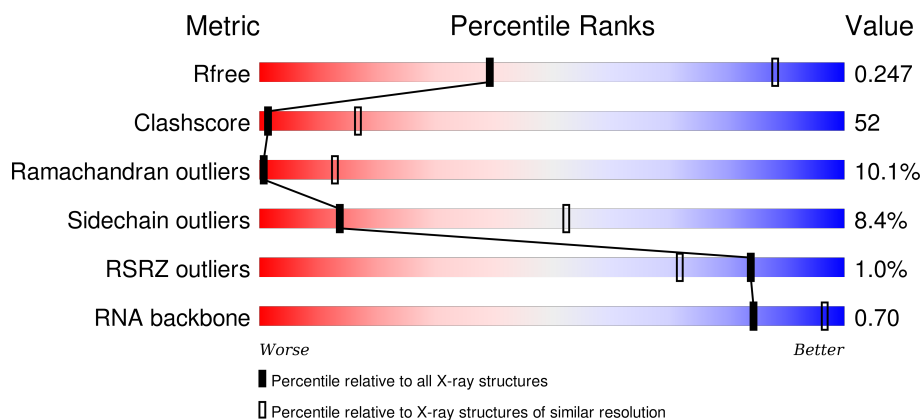
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.



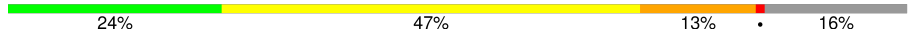
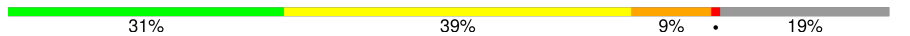




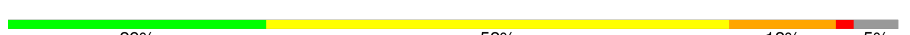
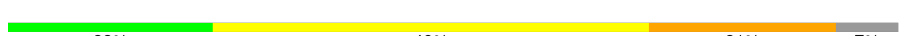


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

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 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>

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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

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		

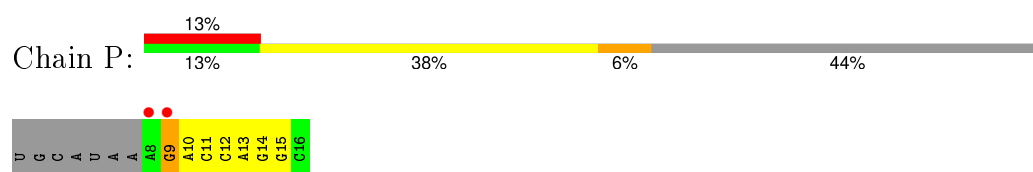
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

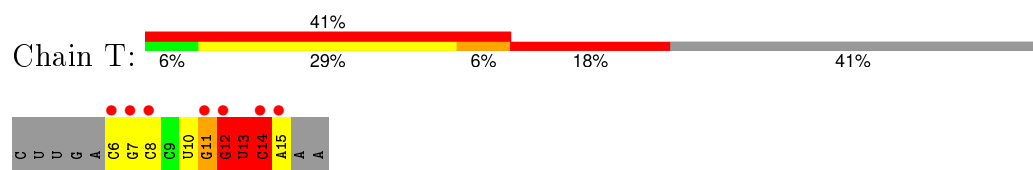
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

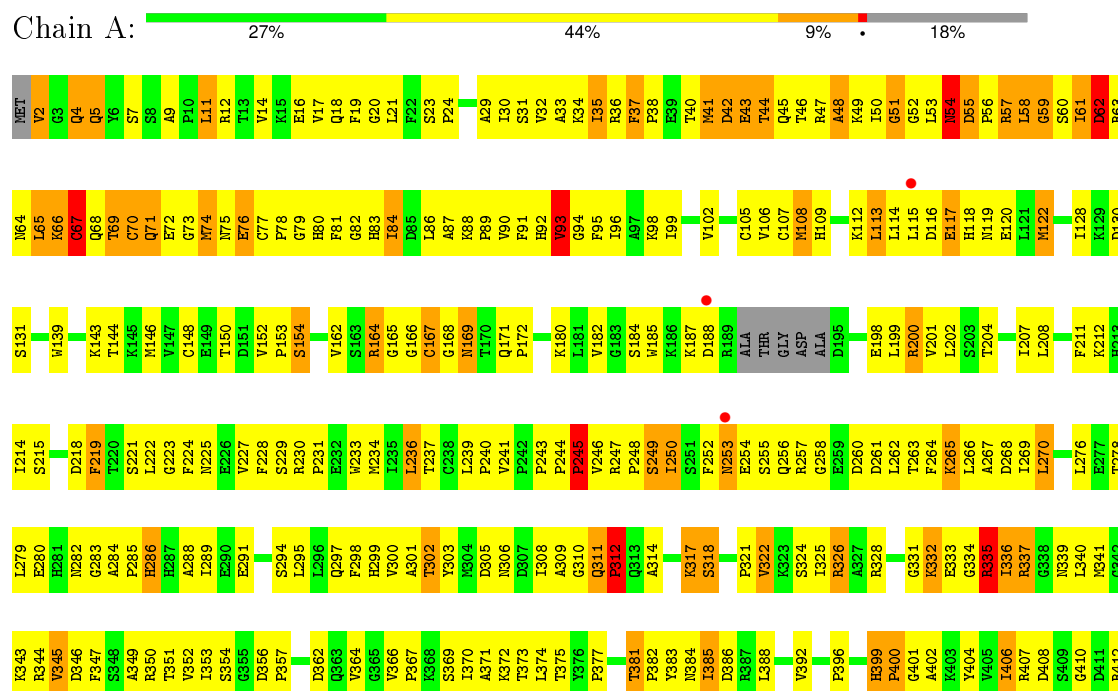
- Molecule 1: RNA (5'-R(*UP*GP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3')



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

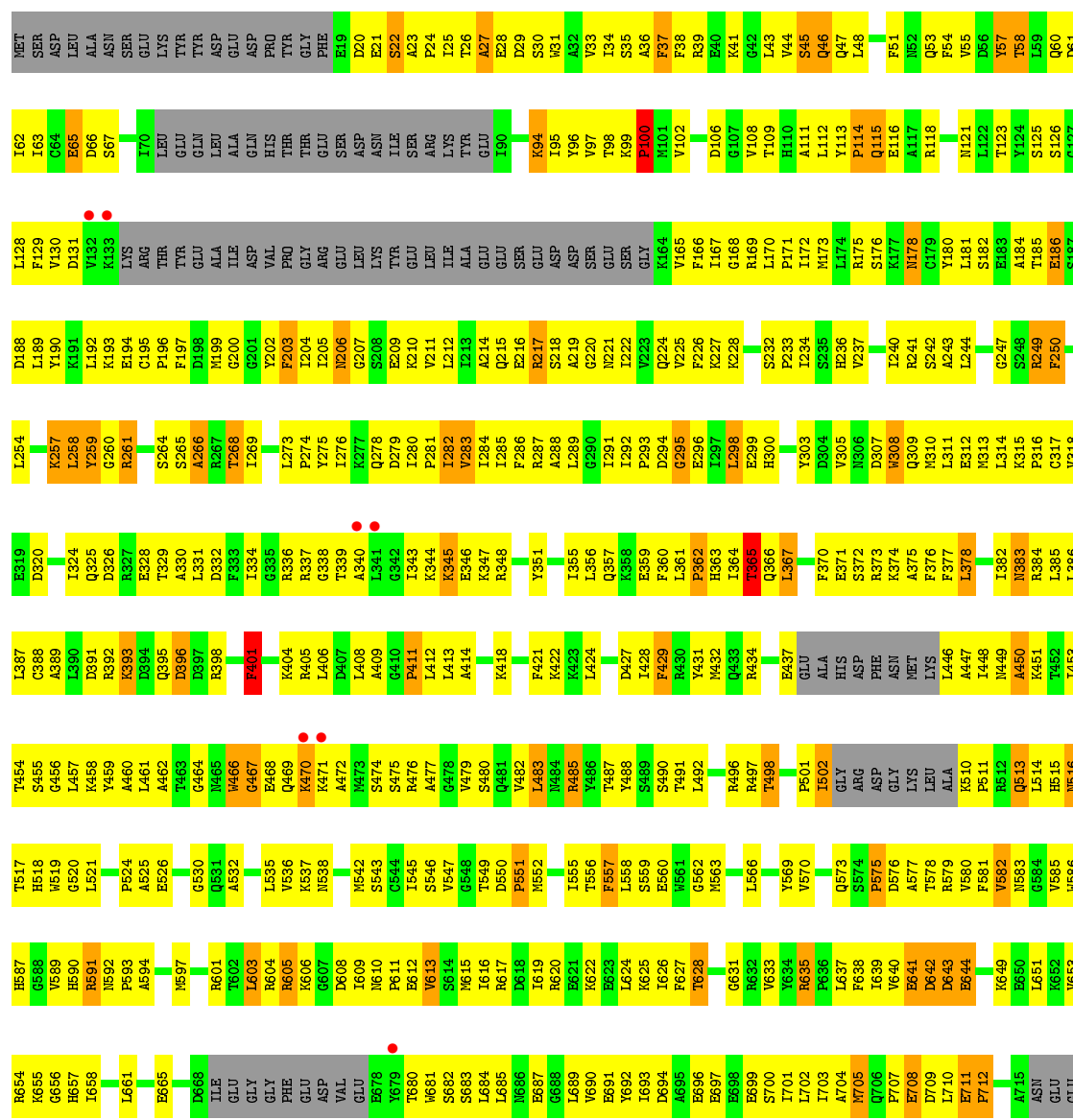


- Molecule 3: DNA-directed RNA polymerase II subunit RPB1

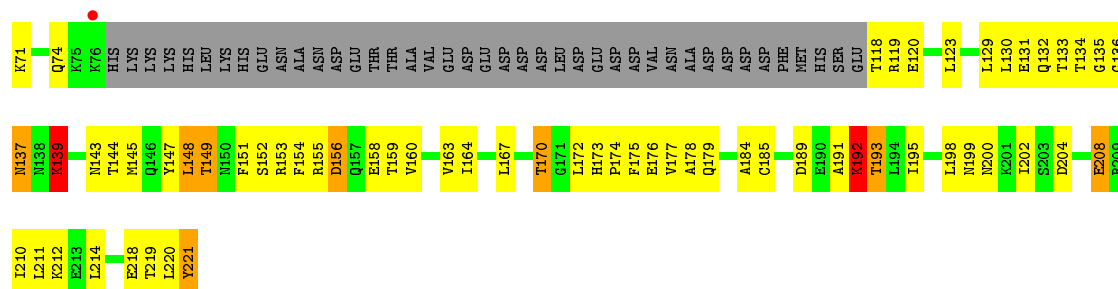


LYS	L1326	R1326	P1190	Y1119	Q1052	D985	L901	G835	C764	I687	I612	E542	S476	L413
ILE	I1327	I1327	W1191	L1120	Q1052	I986	L902	Y836	V765	I687	I613	E543	P477	D414
THR	Y1328	K1261	L1192	E1121	F1053	V987	N903	I837	G766	V693	G614	L543	Y478	L415
GLU	T1329	K1262	L1193	P1122	L1054	Q838	T904	Q838	Q767	T694	G615	V546	N479	L416
ILE	N1330	I1263	R1194	G1123	R1055	R839	D905	R840	Q768	K695	V616	L547	A480	Y417
GLU	S1331	E1264	H1124	H1124	V1058	R840	H906	R840	R774	K696	V617	N548	D481	S418
ASP	F1332	N1265	L1197	A1125	H1059	T907	T907	L841	R774	A697	E618	K549	P482	K419
GLY	I1333	T1266	D1198	A1126	R1059	L908	L908	V842	I775	Q698	K619	L550	D483	K420
GLN	T1334	T1267	D1127	D1127	P1060	N996	L913	R843	F779	A699	K620	Y551	M487	D423
ASP	L1335	L1268	Q1128	Q1128	G1061	L997	L914	A844	F780	N700	T621	V552	N488	L424
GLY	M1336	E1062	E1062	E1062	E1062	L998	E914	L345	V780	L701	G622	V553	K489	Q425
GLY	E1337	M1063	M1063	M1063	M1063	R1001	I919	E846	D781	H706	G623	V559	L490	Q426
VAL	I1338	I1138	Q1070	Q1070	G1065	L920	L920	D847	R782	H706	G624	V560	K490	L426
THR	I1339	L1273	G1065	G1065	G1065	G1002	L920	I843	T783	H706	G625	V560	V491	Q427
PRO	G1340	R1274	V1066	V1066	L1067	K921	G921	N849	L784	T709	G626	P561	P492	Y428
THR	I1341	T1208	L1067	L1067	L1067	M1004	Q926	Y852	P785	L710	G627	P562	Q493	G429
SER	E1342	M1209	E1005	E1005	E1005	E1005	Q926	R852	H786	R711	G628	P563	S494	W430
ASN	A1343	E1280	A1137	A1137	A1137	I1006	L929	D853	H787	E712	L629	A564	K431	K431
GLU	G1344	G1210	I1138	I1138	I1138	I1007	L929	N854	S788	S713	I630	I565	E496	V432
SER	R1345	V1282	S1071	S1071	S1071	Q1008	Q1008	T855	K789	F714	H631	I566	T497	E433
GLY	V1346	V1283	G1073	G1073	G1073	N1009	Y933	T856	Y792	N717	V632	K567	R498	E434
LEU	M1347	M1284	E1074	E1074	E1074	K934	K934	R857	S793	N718	V633	P568	A499	H435
VAL	L1348	M1285	P1075	P1075	P1075	Q935	Q935	N858	P794	V719	T634	K569	E500	
ASN	Y1349	I1216	A1076	A1076	A1076	L936	L936	S859	P794	R720	R635	K569		D438
ALA	K1350	K1217	I1148	I1148	I1148	D1013	D939	L860	E795	R720	G642	L571	Q503	N438
ASP	E1351	R1289	M1079	M1079	M1079	A1014	R940	G861	S796	F721		L572	L504	D440
LEU	V1352	K1290	T1080	T1080	T1080	V1015	R940	N862	K797	L722	L645	G574	C905	P441
ASP	P1291	T1219	E1151	E1151	E1151	T1016	K941	R863	G798	N723	L646	A506	A506	V442
ASP	P1292	P1220	A1081	A1081	A1081	T1017	F942	V863	F799	E724	F646	V507	V507	L443
VAL	S1293	K1221	ASN	ASN	ASN	L1017	L942	I864	V800	A725	G647	K576	P508	F444
VAL	P1294	M1222	THR	THR	THR	F1018	L943	Q865	V800		N648	L577	L569	N445
LVS	I1355	D1223	PHE	PHE	PHE	C1019		R866	E801	K728	I649	L578	Q510	R446
ASP	T1356	L1224	HIS	HIS	HIS	G1020	W954	L867	N802				Q510	R446
GLU	D1359	F1225	PHE	PHE	PHE	L1021	P955	T868	S803				L511	Q447
LEU	F1225	P1156	PHE	PHE	PHE	L1021	P955	T868	S803				L511	Q447
MET	Y1362	Y1298	ALA	ALA	ALA	L1022	L956	G869	Y804	R731	K651	V580	S513	L450
SER	V1363	V1226	ALA	ALA	ALA	R1023	P957	E870	L805	L732	V652		S513	L450
PRO	M1364	I1227	VAL	VAL	VAL	S1024	V958	D871	R806		V653	N584	Q515	K451
LEU	Y1365	M1228	ALA	ALA	ALA	R1025	N959	G872	G807	V735	L657	G585	Q515	K452
VAL	R1366	D1233	SER	SER	SER	L1026	I960	N873	L808	N736	L658	L586	S516	N453
ASP	M1304	E1165	K1092	K1092	K1092	A1027	R961	D874	T809		L659	R590	M517	S454
ASP	V1305	D1166	K1093	K1093	K1093	T1028	R962	A875			H699	K518	K518	N455
GLY	L1306	I1237	V1094	V1094	V1094	R1029	I963	I878	E812	D739	S663	C520	C520	A457
SER	E1307	I1238	T1095	T1095	T1095	R1030	I964		F813	L740	T664	M521	M521	R458
SER	T1308	R1239	S1096	S1096	S1096	V1031	Q965	F814	F815	N742	G665	G522	G522	R459
ASN	D1309	G1240	G1097	G1097	G1097	L1032	N966	L883	H816	V743	I666	T596	I523	V460
ASP	G1310	R1241	G1097	G1097	G1097	Q1033	A967	D894			G667	T596	I523	V460
ALA	V1311	V1242	R1100	R1100	R1100	E1034	Q968	T885	M818	K744	G667	T596	I523	V460
ALA	N1312	V1243	L1101	L1101	L1101	Y1035	Q969	I886	A817	K744	G667	T596	I523	V460
ALA	M1444	R1244	K1102	K1102	K1102	R1036	T970	G887	M818	K744	G667	T596	I523	V460
GLY	S1314	P1245	ASP	ASP	ASP	L1037	F971	G888	R821	V747	D672	P600	D526	I463
GLY	Q1378	LVS	GLU	GLU	GLU	T1038	H972	S889	E822	N748	P674	L601	T527	P464
GLY	G1379	SER	GLU	GLU	GLU	K1039	I973	D890	E822	N748	P674	L601	T527	P464
PHE			GLU	GLU	GLU	L1105	I973	D890	E822	N748	P674	L601	T527	P464
THR	T1385	M1317	LEU	LEU	LEU	Q1040	A991	A891	I825	A749	T676	N603	I531	S466
ALA	R1386	ASP	ASP	ASP	ASP	A1041	K977	E894	D826	G753	M676	N603	I531	S466
ALA	H1387	ALA	GLU	GLU	GLU	V1107	P978	E894	T827	G754	I679	N605	R532	T467
GLY	F1388	GLU	GLN	GLN	GLN	T1113	S979	K895	A828	S754	I679	N605	R532	T467
GLY	F1389	THR	PHE	PHE	PHE	T1114	D980	K896	V829	N757	T832	L606	L534	L470
ALA		GLU	ASP	ASP	ASP	S1115	L981	K897	K830	N757	T832	L606	L534	L470
ASP	S1392	A1254	Q1187	Q1187	Q1187	L1116	T982	R898	T831	N761	I683	L608	L536	I471
GLU	M1393	E1255	Q1188	Q1188	Q1188	T1117	T982	R898	T831	N761	I683	L608	L536	I471
THR	T1394	E1256	S1189	S1189	S1189	V1118	K984	D900	T834	A763	A686	P609	R537	L472
GLY													I541	T475

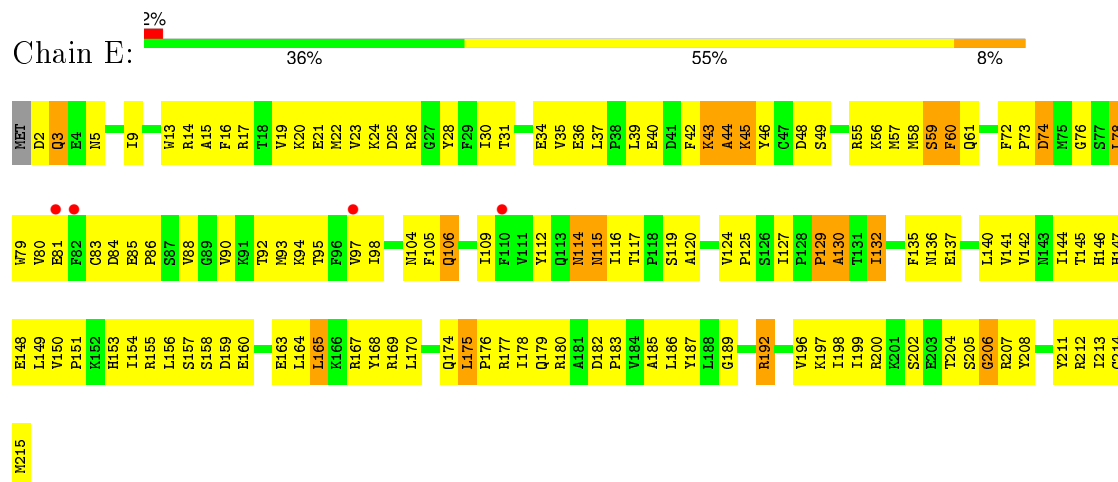
- Molecule 4: DNA-directed RNA polymerase II subunit RPB2



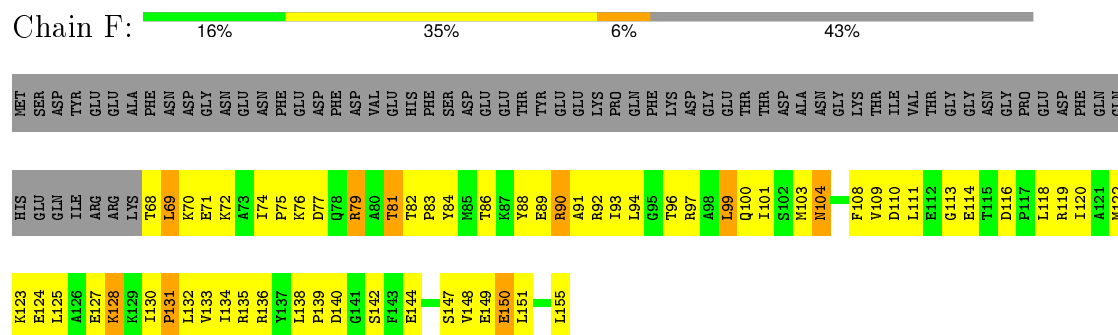




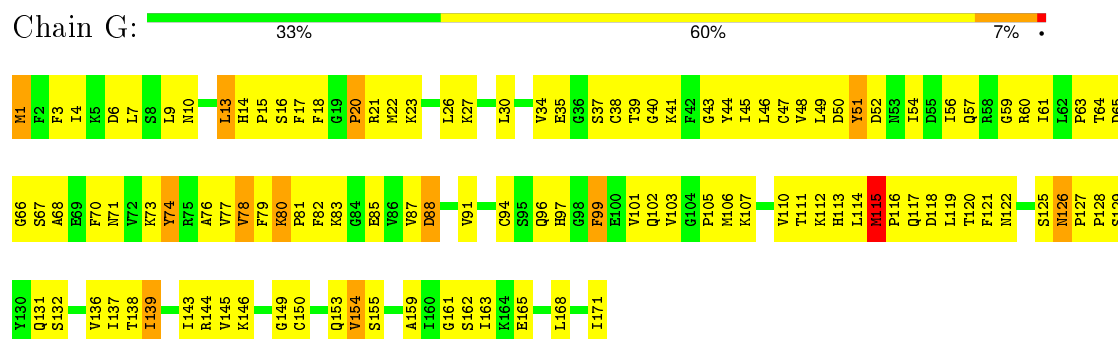
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



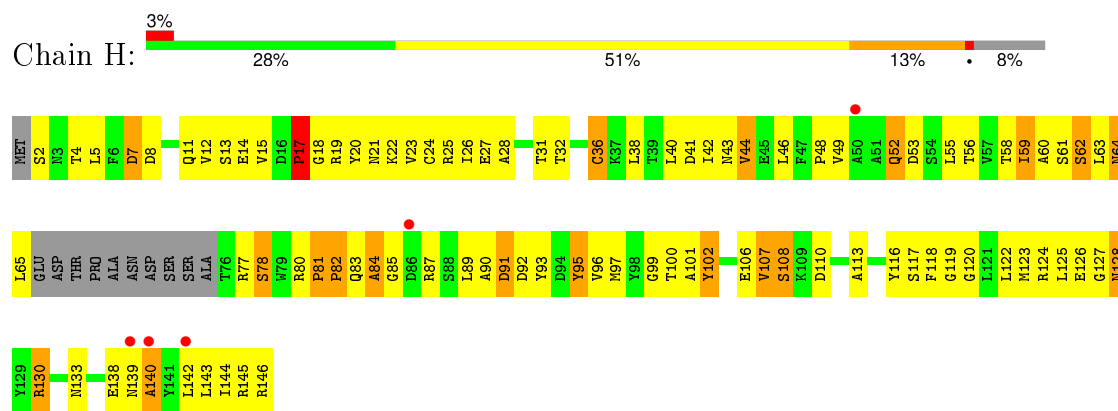
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



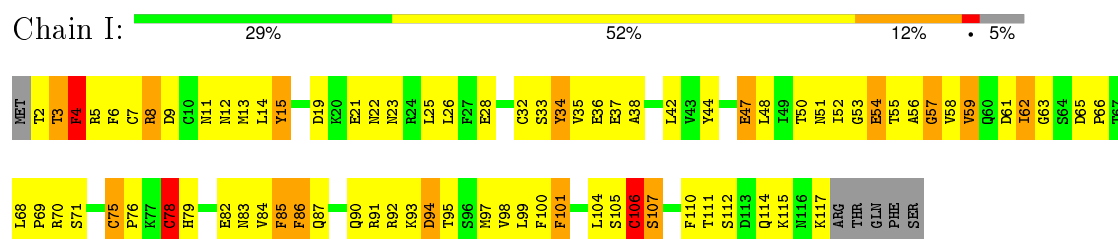
- Molecule 9: DNA-directed RNA polymerase II subunit RPB7



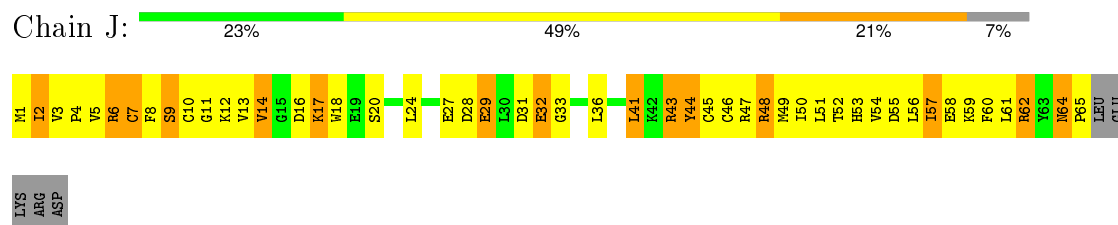
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3



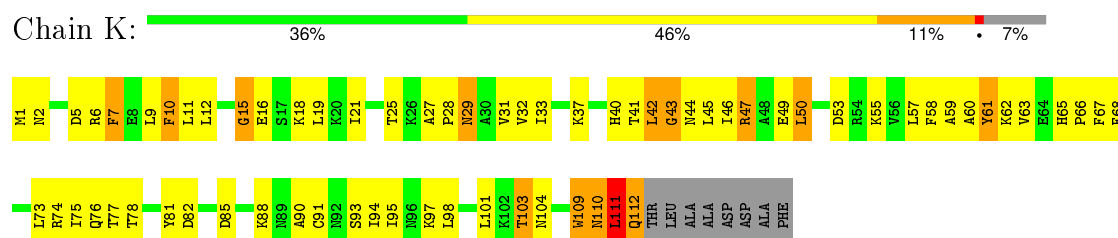
- Molecule 11: DNA-directed RNA polymerase II subunit RPB9



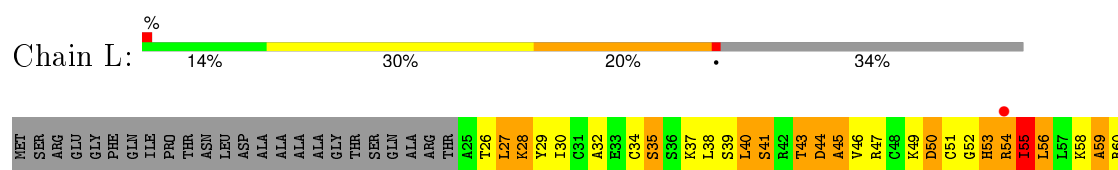
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- 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	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
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
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 122098 reflections	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	15
4	B	1094/1224 (89%)	780 (71%)	214 (20%)	100 (9%)	1	16
5	C	264/318 (83%)	164 (62%)	64 (24%)	36 (14%)	0	6
6	D	174/221 (79%)	126 (72%)	30 (17%)	18 (10%)	1	12
7	E	212/215 (99%)	158 (74%)	36 (17%)	18 (8%)	1	17
8	F	86/155 (56%)	69 (80%)	9 (10%)	8 (9%)	1	15
9	G	169/171 (99%)	130 (77%)	33 (20%)	6 (4%)	4	41
10	H	131/146 (90%)	74 (56%)	36 (28%)	21 (16%)	0	5
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	22
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	13

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%)	11	47
4	B	964/1061 (91%)	890 (92%)	74 (8%)	16	56
5	C	235/274 (86%)	212 (90%)	23 (10%)	10	44
6	D	160/200 (80%)	142 (89%)	18 (11%)	7	38
7	E	196/197 (100%)	188 (96%)	8 (4%)	37	74
8	F	78/137 (57%)	75 (96%)	3 (4%)	40	76
9	G	152/152 (100%)	140 (92%)	12 (8%)	15	55
10	H	119/128 (93%)	113 (95%)	6 (5%)	30	70
11	I	110/116 (95%)	99 (90%)	11 (10%)	9	43
12	J	60/65 (92%)	55 (92%)	5 (8%)	14	52
13	K	97/102 (95%)	87 (90%)	10 (10%)	9	42
14	L	40/57 (70%)	36 (90%)	4 (10%)	9	43
All	All	3456/4009 (86%)	3166 (92%)	290 (8%)	14	52

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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%)	1.97	2 (22%) 1 1	194, 200, 200, 200	0
2	T	10/17 (58%)	2.17	7 (70%) 0 1	180, 190, 200, 200	0
3	A	1422/1733 (82%)	-0.24	8 (0%) 90 82	56, 116, 175, 200	0
4	B	1112/1224 (90%)	-0.17	11 (0%) 84 72	57, 126, 188, 200	0
5	C	267/318 (83%)	-0.26	0 100 100	74, 110, 158, 180	0
6	D	178/221 (80%)	-0.23	1 (0%) 90 82	87, 133, 184, 198	0
7	E	214/215 (99%)	-0.22	4 (1%) 70 54	90, 159, 197, 200	0
8	F	88/155 (56%)	-0.49	0 100 100	65, 91, 129, 140	0
9	G	171/171 (100%)	-0.28	0 100 100	88, 112, 155, 163	0
10	H	135/146 (92%)	0.37	5 (3%) 45 30	139, 166, 190, 200	0
11	I	116/122 (95%)	0.09	0 100 100	114, 163, 191, 200	0
12	J	65/70 (92%)	-0.46	0 100 100	79, 108, 146, 153	0
13	K	112/120 (93%)	-0.28	0 100 100	81, 114, 139, 167	0
14	L	46/70 (65%)	0.04	1 (2%) 65 50	111, 166, 194, 196	0
All	All	3945/4598 (85%)	-0.18	39 (0%) 84 72	56, 123, 187, 200	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	471	LYS	5.1
1	P	9	G	4.5
3	A	1092	LYS	3.7
1	P	8	A	3.5
2	T	15	A	3.4

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.