



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 10:59 AM EDT

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 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

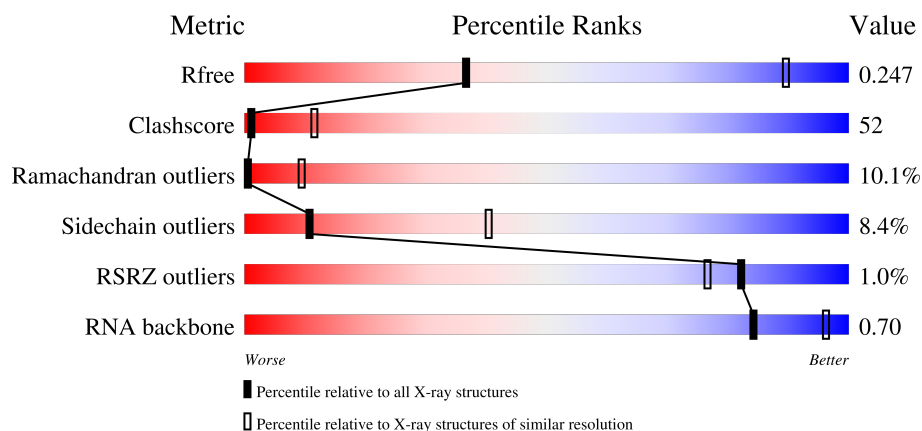
1 Overall quality at a glance

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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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 $\leq 5\%$. 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>12%</div> <div>12% 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	<div><div></div><div>24%47%13%16%</div></div>
6	D	221	<div><div></div><div>31%39%9%19%</div></div>
7	E	215	<div><div></div><div>2%36%55%8%</div></div>
8	F	155	<div><div></div><div>16%35%6%43%</div></div>
9	G	171	<div><div></div><div>33%60%7%</div></div>
10	H	146	<div><div></div><div>3%28%51%13%8%</div></div>
11	I	122	<div><div></div><div>29%52%12%5%</div></div>
12	J	70	<div><div></div><div>23%49%21%7%</div></div>
13	K	120	<div><div></div><div>36%46%11%7%</div></div>
14	L	70	<div><div></div><div>%14%30%20%34%</div></div>

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
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	A	2	Total	Zn	0	0
			2	2		
15	B	1	Total	Zn	0	0
			1	1		
15	C	1	Total	Zn	0	0
			1	1		
15	I	2	Total	Zn	0	0
			2	2		
15	J	1	Total	Zn	0	0
			1	1		
15	L	1	Total	Zn	0	0
			1	1		

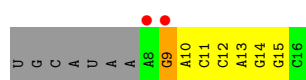
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

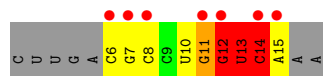
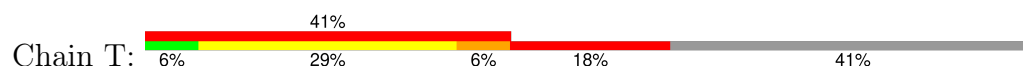
3 Residue-property plots

These plots are drawn for all protein, RNA, 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 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.

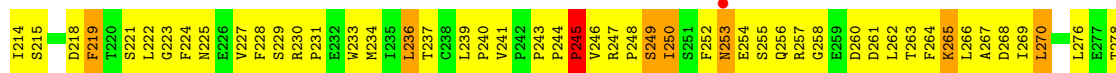
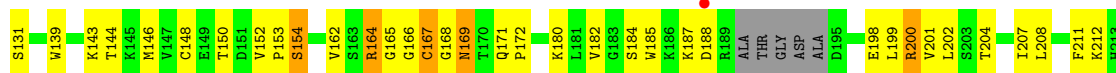
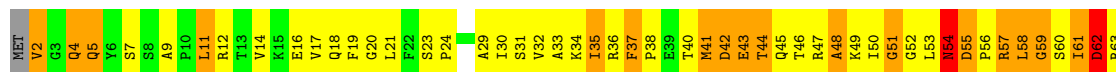
- Molecule 1: RNA (5'-R(*UP*GP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3')



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

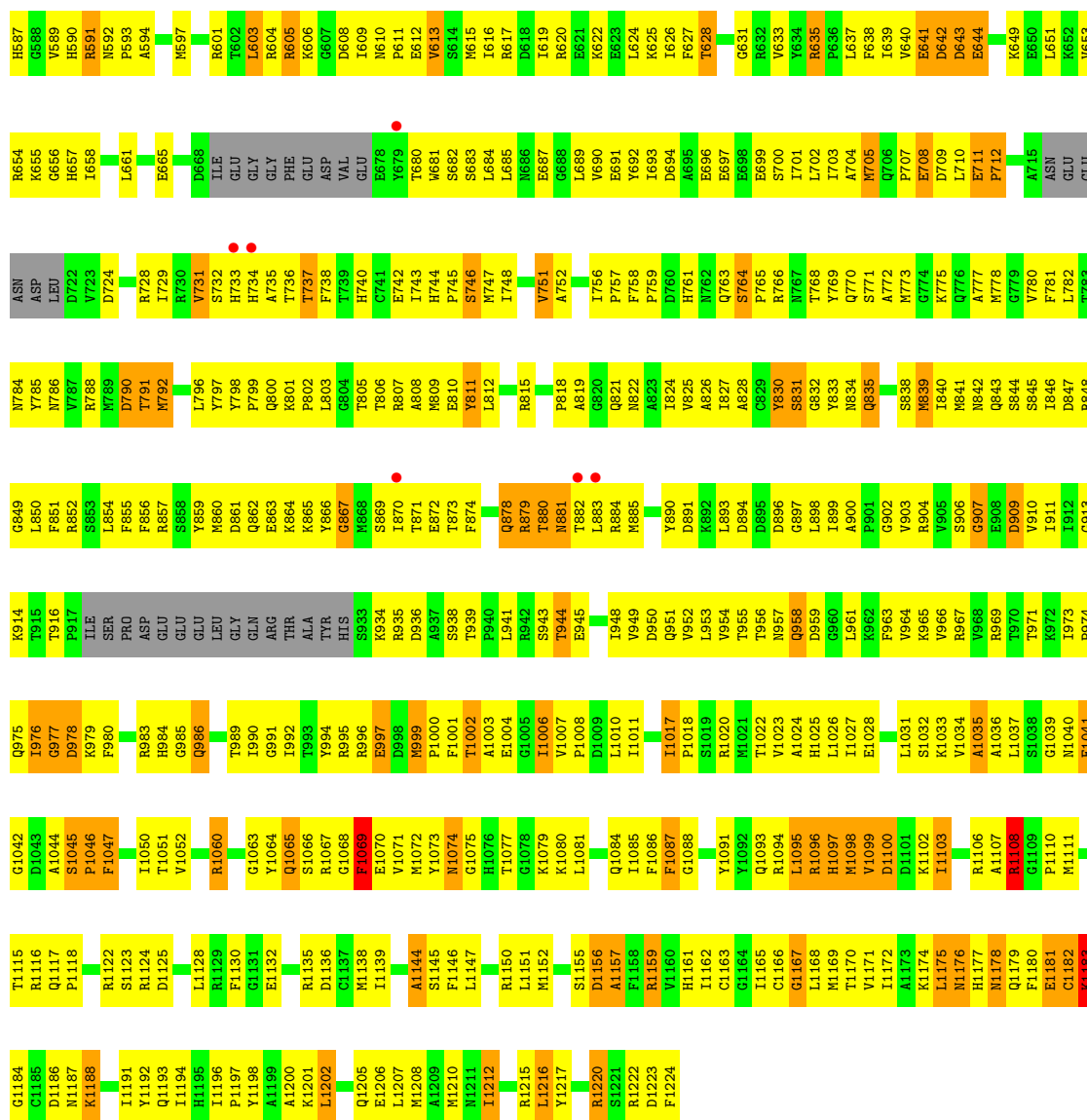


- Molecule 3: DNA-directed RNA polymerase II subunit RPB1



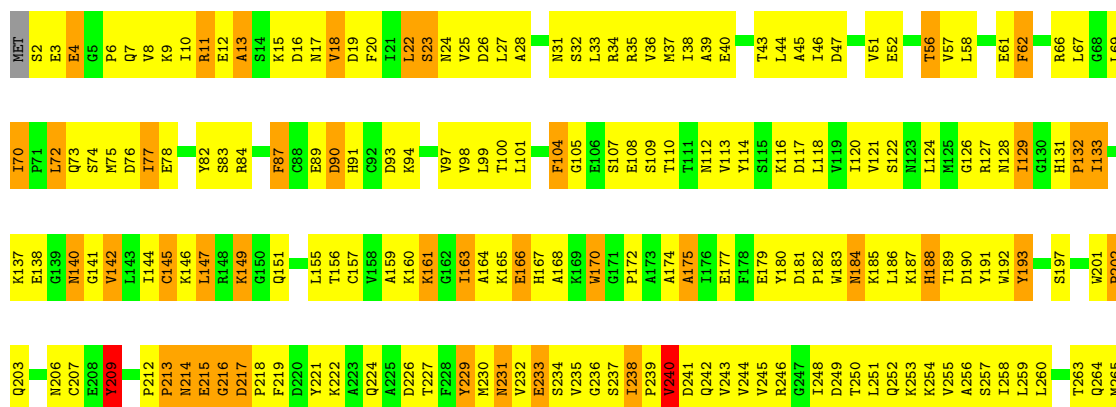
R1326	R1327	Y1119	P1190	L1260	K1261	Y1191	Q1052	D985	L901	G835	G784	K687	I612	E542	S476	L413	K343
I1327	Y1328	L1120	W1191	E1121	R1262	L1192	F1053	E986	L902	Y836	Y785	V693	I613	L543	P477	D414	R344
T1329	L1193	P1122	L1192	E1121	R1262	E1193	F1053	E987	T903	Q838	G786	T694	G615	V546	Y478	L415	D346
N1330	L1193	R1122	R1194	L1193	R1262	R1194	R1055	L988	D905	R839	Q787	K695	G616	V547	A480	R416	F347
E1264	R1123	H1124	R1194	L1193	R1262	H1124	R1055	R840	H906	R840	Q788	E696	V617	N548	D481	S418	S348
N1265	A1125	A1125	L1197	A1125	R1265	A1125	V1058	L841	T907	L841	R774	A697	E618	M549	K419	R420	A349
T1266	A1126	A1126	D1198	A1126	T1266	A1126	H1059	R842	L908	R842	I775	K698	K619	L550	K420	R350	R350
M1267	D1127	D1127	A1201	D1127	M1267	D1127	P1060	R843	L913	R843	F779	A699	K620	Y551	D423	T351	T351
L1268	Q1128	Q1128	A1201	Q1128	L1268	Q1128	G1061	A844	L913	A844	W780	W552	W621	W552	I424	I353	I353
M1269	Q1129	Q1129	A1202	Q1129	M1269	Q1129	E1062	L845	E914	L845	W780	W553	W622	W553	Q425	S354	S354
K1270	Q1130	Q1130	K1205	Q1130	K1270	Q1130	M1063	E846	I919	E846	D781	V559	G623	V559	L426	G355	G355
L1271	I1134	I1134	D1206	I1134	L1271	I1134	G1065	R846	L920	R846	R782	I560	S624	I560	Q427	D356	D356
L1273	R1135	R1135	D1206	R1135	L1273	R1135	V1066	R849	L920	R849	T783	P561	S625	P561	Y428	P357	P357
R1274	R1136	R1136	L1207	R1136	R1274	R1136	L1067	K1003	G921	K1003	L784	Q493	G627	T562	Q429	W430	D362
I1279	M1209	M1209	L1208	M1209	I1279	M1209	P1067	E1005	Q926	E1005	H786	P563	G628	P563	W431	K431	Q363
E1280	G1210	G1210	Q1211	E1280	E1280	G1210	S1071	I1007	L929	N854	F787	E712	L629	A564	V432	V364	V364
R1281	Q1211	Q1211	Q1211	R1281	R1281	Q1211	I1072	I1007	L929	N854	F787	E712	L629	A564	V432	V364	V364
V1282	Q1212	Q1212	Q1212	V1282	V1282	Q1212	I1072	I1007	L929	N854	F787	E712	L629	A564	V432	V364	V364
V1283	G1213	G1213	Q1213	V1283	V1283	G1213	I1072	I1007	L929	N854	F787	E712	L629	A564	V432	V364	V364
M1284	E1214	E1214	R1215	M1284	M1284	E1214	E1074	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
M1285	E1215	E1215	R1215	M1285	M1285	E1215	E1074	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
E1286	E1216	E1216	R1216	E1286	E1286	E1216	P1075	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
R1289	K1217	K1217	Q1217	R1289	R1289	K1217	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
K1290	Q1218	Q1218	Q1218	K1290	K1290	Q1218	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
V1291	T1219	T1219	T1219	V1291	V1291	T1219	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
P1292	F1220	F1220	F1220	P1292	P1292	F1220	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
S1293	K1221	K1221	K1221	S1293	S1293	K1221	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
P1294	N1222	N1222	N1222	P1294	P1294	N1222	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
T1295	D1223	D1223	D1223	T1295	T1295	D1223	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
E1296	F1224	F1224	F1224	E1296	E1296	F1224	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
E1297	F1225	F1225	F1225	E1297	E1297	F1225	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
V1298	G1226	G1226	G1226	V1298	V1298	G1226	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
K1300	W1228	W1228	W1228	K1300	K1300	W1228	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
E1303	D1233	D1233	D1233	E1303	E1303	D1233	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
W1304	L1236	L1236	L1236	W1304	W1304	L1236	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
L1306	I1237	I1237	I1237	L1306	L1306	I1237	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
E1307	I1238	I1238	I1238	E1307	E1307	I1238	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
D1308	C1239	C1239	C1239	D1308	D1308	C1239	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
D1309	C1240	C1240	C1240	D1309	D1309	C1240	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
G1310	R1241	R1241	R1241	G1310	G1310	R1241	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
V1311	V1242	V1242	V1242	V1311	V1311	V1242	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
M1312	V1243	V1243	V1243	M1312	M1312	V1243	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
L1313	L1244	L1244	L1244	L1313	L1313	L1244	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
S1314	P1245	P1245	P1245	S1314	S1314	P1245	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
E1315	LYS	LYS	LYS	E1315	E1315	LYS	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
V1316	SER	SER	SER	V1316	V1316	SER	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
M1317	LEU	LEU	LEU	M1317	M1317	LEU	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
T1318	ASP	ASP	ASP	T1318	T1318	ASP	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
V1319	ALA	ALA	ALA	V1319	V1319	ALA	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
G1320	THR	THR	THR	G1320	G1320	THR	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
P1321	THR	THR	THR	P1321	P1321	THR	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
I1322	GLU	GLU	GLU	I1322	I1322	GLU	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
D1323	ASP	ASP	ASP	D1323	D1323	ASP	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
P1324	ASP	ASP	ASP	P1324	P1324	ASP	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
S1332	ASP	ASP	ASP	S1332	S1332	ASP	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
N1333	ASP	ASP	ASP	N1333	N1333	ASP	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
T1334	ASP	ASP	ASP	T1334	T1334	ASP	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
S1339	ASP	ASP	ASP	S1339	S1339	ASP	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
S1392	ASP	ASP	ASP	S1392	S1392	ASP	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
N1393	ASP	ASP	ASP	N1393	N1393	ASP	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
T1394	ASP	ASP	ASP	T1394	T1394	ASP	A1076	N855	Y933	R857	W792	W717	L646	K575	E433	E433	G365
K343	R344	V345	D346	F347	S348	A349	R350	T351	I353	S354	G355	D356	P357	K358	S359	I370	A371
L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388
L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406
L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424
L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442
L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460
L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478
L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496
L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514
L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532
L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550
L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568
L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586
L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604
L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622
L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640
L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658
L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676
L677	L678	L679	L680	L681	L682	L683	L684	L685									

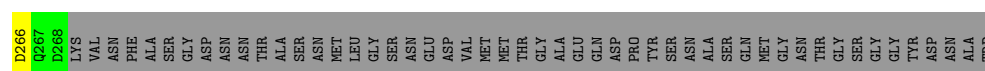




• Molecule 5: DNA-directed RNA polymerase II subunit RPB3

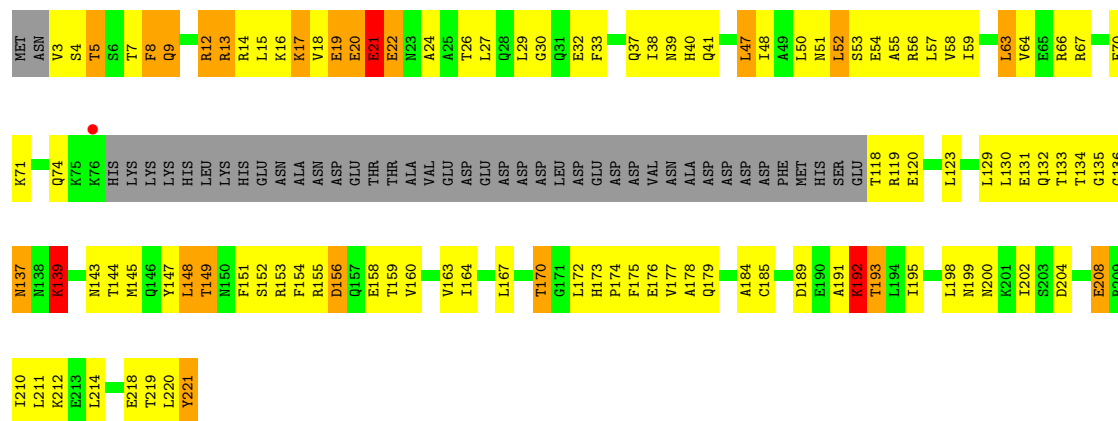
Chain C: 24% 47% 13% 16%





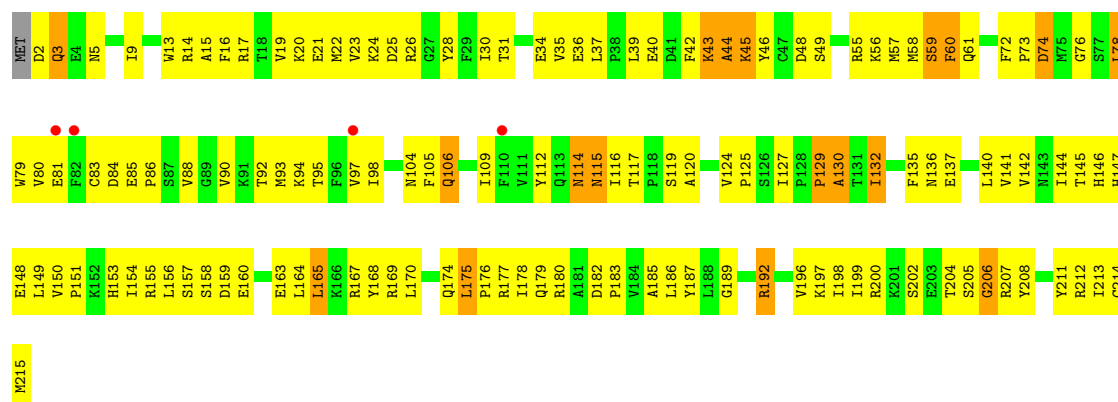
• Molecule 6: DNA-directed RNA polymerase II subunit RPB4

Chain D: 31% 39% 9% 19%



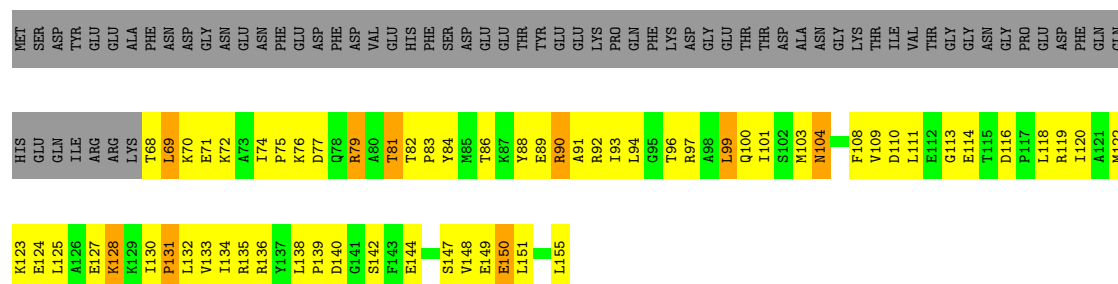
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 2% 36% 55% 8%



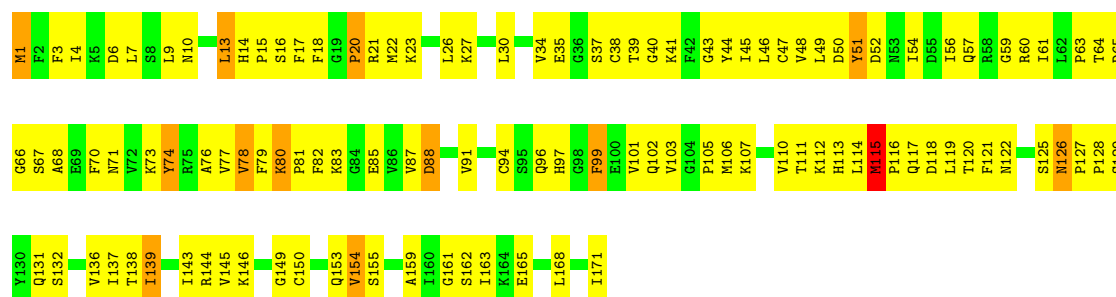
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 16% 35% 6% 43%



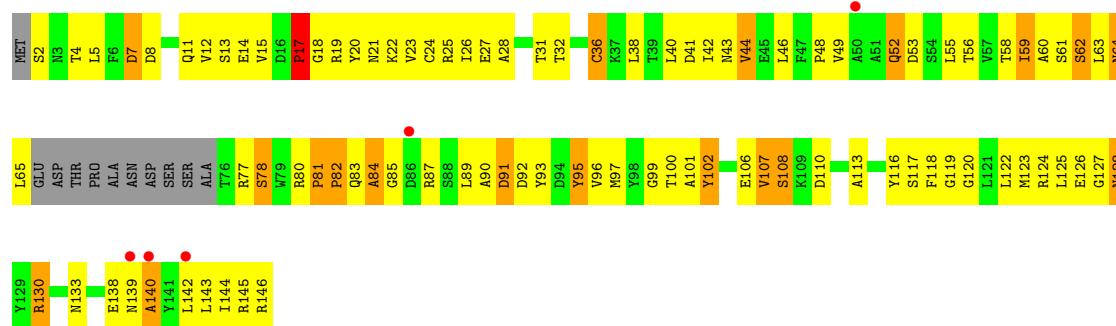
• Molecule 9: DNA-directed RNA polymerase II subunit RPB7

Chain G:  33% 60% 7%



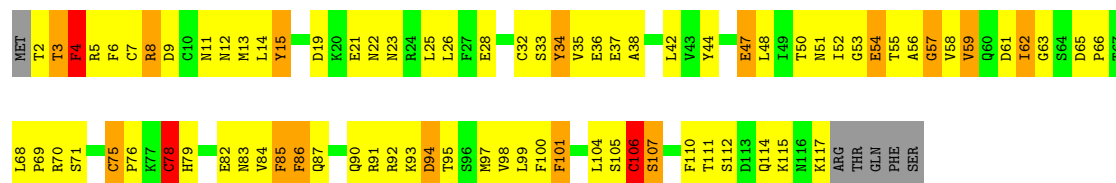
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  3% 28% 51% 13% 8%

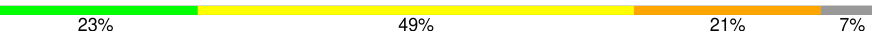


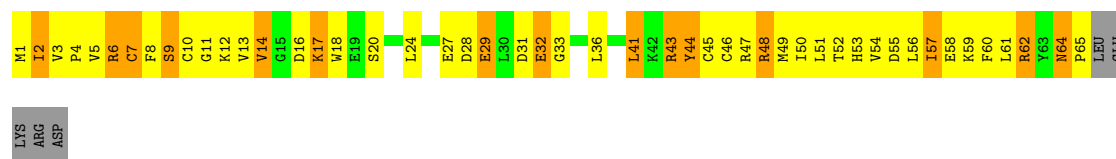
• Molecule 11: DNA-directed RNA polymerase II subunit RPB9

Chain I:  29% 52% 12% 5%



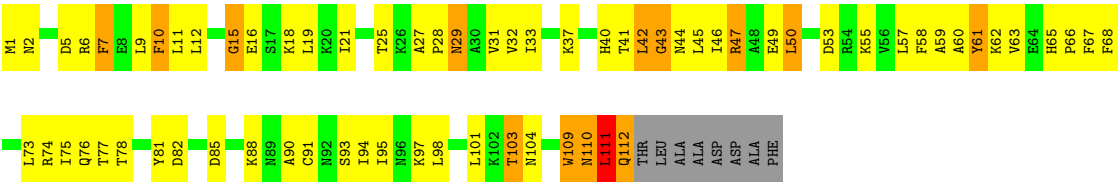
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  23% 49% 21% 7%

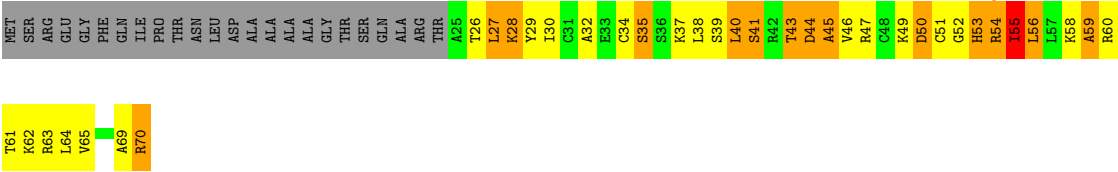


• Molecule 13: DNA-directed RNA polymerase II subunit RPB11

Chain K:  36% 46% 11% 7%



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



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%)	wwPDB-VP
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: MG, ZN

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%)	0	11
4	B	1094/1224 (89%)	780 (71%)	214 (20%)	100 (9%)	1	12
5	C	264/318 (83%)	164 (62%)	64 (24%)	36 (14%)	0	4
6	D	174/221 (79%)	126 (72%)	30 (17%)	18 (10%)	0	9
7	E	212/215 (99%)	158 (74%)	36 (17%)	18 (8%)	1	12
8	F	86/155 (56%)	69 (80%)	9 (10%)	8 (9%)	0	11
9	G	169/171 (99%)	130 (77%)	33 (20%)	6 (4%)	3	30
10	H	131/146 (90%)	74 (56%)	36 (28%)	21 (16%)	0	3
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	16
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	9

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%)	9	35
4	B	964/1061 (91%)	890 (92%)	74 (8%)	13	43
5	C	235/274 (86%)	212 (90%)	23 (10%)	8	33
6	D	160/200 (80%)	142 (89%)	18 (11%)	6	28
7	E	196/197 (100%)	188 (96%)	8 (4%)	30	59
8	F	78/137 (57%)	75 (96%)	3 (4%)	33	61
9	G	152/152 (100%)	140 (92%)	12 (8%)	12	42
10	H	119/128 (93%)	113 (95%)	6 (5%)	24	55
11	I	110/116 (95%)	99 (90%)	11 (10%)	7	32
12	J	60/65 (92%)	55 (92%)	5 (8%)	11	40
13	K	97/102 (95%)	87 (90%)	10 (10%)	7	31
14	L	40/57 (70%)	36 (90%)	4 (10%)	7	32
All	All	3456/4009 (86%)	3166 (92%)	290 (8%)	11	40

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

Mol	Chain	Res	Type
7	E	60	PHE
14	L	27	LEU
7	E	175	LEU
11	I	4	PHE
3	A	1332	PHE

Sometimes 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	1065	GLN
6	D	179	GLN
4	B	1176	ASN
5	C	167	HIS

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Mol	Chain	Res	Type
7	E	114	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 monosaccharides 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
5	C	1
4	B	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%)	2.02	2 (22%) 0 0	194, 200, 200, 200	0
2	T	10/17 (58%)	2.22	7 (70%) 0 0	180, 190, 200, 200	0
3	A	1422/1733 (82%)	-0.26	8 (0%) 89 85	56, 116, 175, 200	0
4	B	1112/1224 (90%)	-0.19	12 (1%) 80 74	57, 126, 188, 200	0
5	C	267/318 (83%)	-0.28	0 100 100	74, 110, 158, 180	0
6	D	178/221 (80%)	-0.25	1 (0%) 89 85	87, 133, 184, 198	0
7	E	214/215 (99%)	-0.24	4 (1%) 66 59	90, 159, 197, 200	0
8	F	88/155 (56%)	-0.51	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%)	0.35	5 (3%) 41 34	139, 166, 190, 200	0
11	I	116/122 (95%)	0.07	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%)	0.03	1 (2%) 62 54	111, 166, 194, 196	0
All	All	3945/4598 (85%)	-0.21	40 (1%) 82 76	56, 123, 187, 200	0

The worst 5 of 40 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 monosaccharides 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	0.10	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	B	1307	1/1	1.00	0.22	83,83,83,83	0
15	ZN	J	101	1/1	1.00	0.25	100,100,100,100	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

6.5 Other polymers [i](#)

There are no such residues in this entry.