



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 06:39 PM UTC

PDB ID : 3H3V / pdb_00003h3v
Title : Yeast RNAP II containing poly(A)-signal sequence in the active site
Authors : Dengl, S.; Cramer, P.
Deposited on : 2009-04-17
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

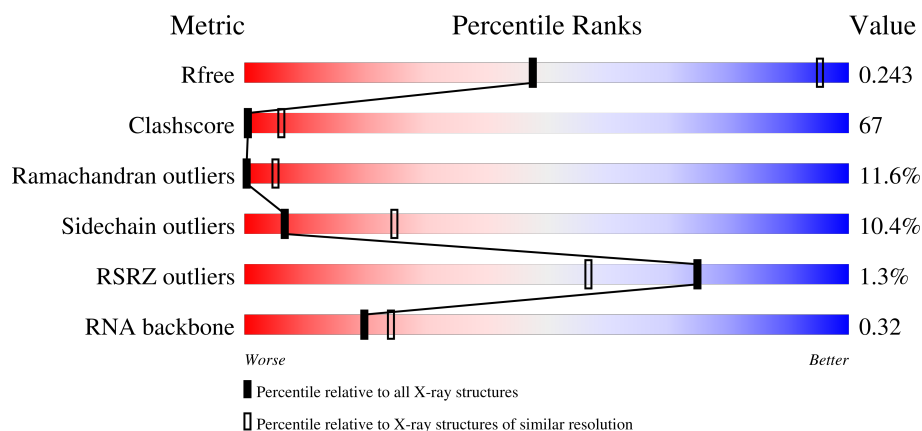
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



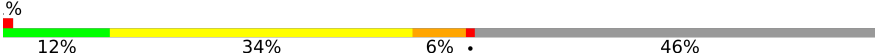
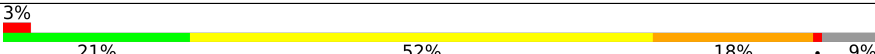
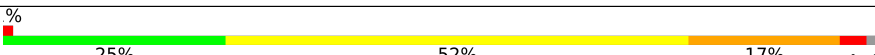
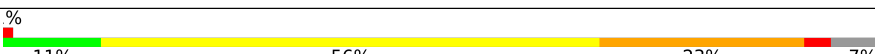
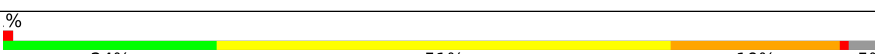
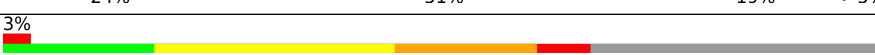
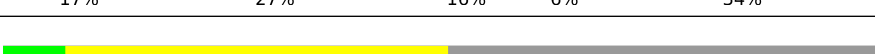
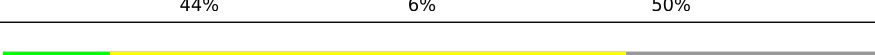
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

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	B	1733	
2	C	1224	
3	D	318	
4	E	221	

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Mol	Chain	Length	Quality of chain
5	F	215	
6	G	155	
7	H	171	
8	I	146	
9	J	122	
10	K	70	
11	L	120	
12	M	70	
13	N	14	
14	P	16	
15	T	26	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 31777 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1108	Total	C	N	O	S	0	0	0
			8810	5580	1541	1634	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 13 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*GP*C
P*TP*GP*CP*TP*TP*TP*AP*TP*TP*GP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	7	Total	C	N	O	P	11	0	0
			138	67	26	39	6			

- Molecule 14 is a RNA chain called 5'-D(*CP*AP*GP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	8	Total	C	N	O	P	0	0	0
			168	77	33	51	7			

- Molecule 15 is a DNA chain called 5'-R(*UP*GP*CP*AP*UP*UP*UP*CP*GP*CP*AP*AP*UP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	18	Total	C	N	O	P	8	0	0
			365	177	60	111	17			

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	B	2	Total	Zn	0	0
			2	2		
16	C	1	Total	Zn	0	0
			1	1		
16	D	1	Total	Zn	0	0
			1	1		
16	J	2	Total	Zn	0	0
			2	2		
16	K	1	Total	Zn	0	0
			1	1		
16	M	1	Total	Zn	0	0
			1	1		

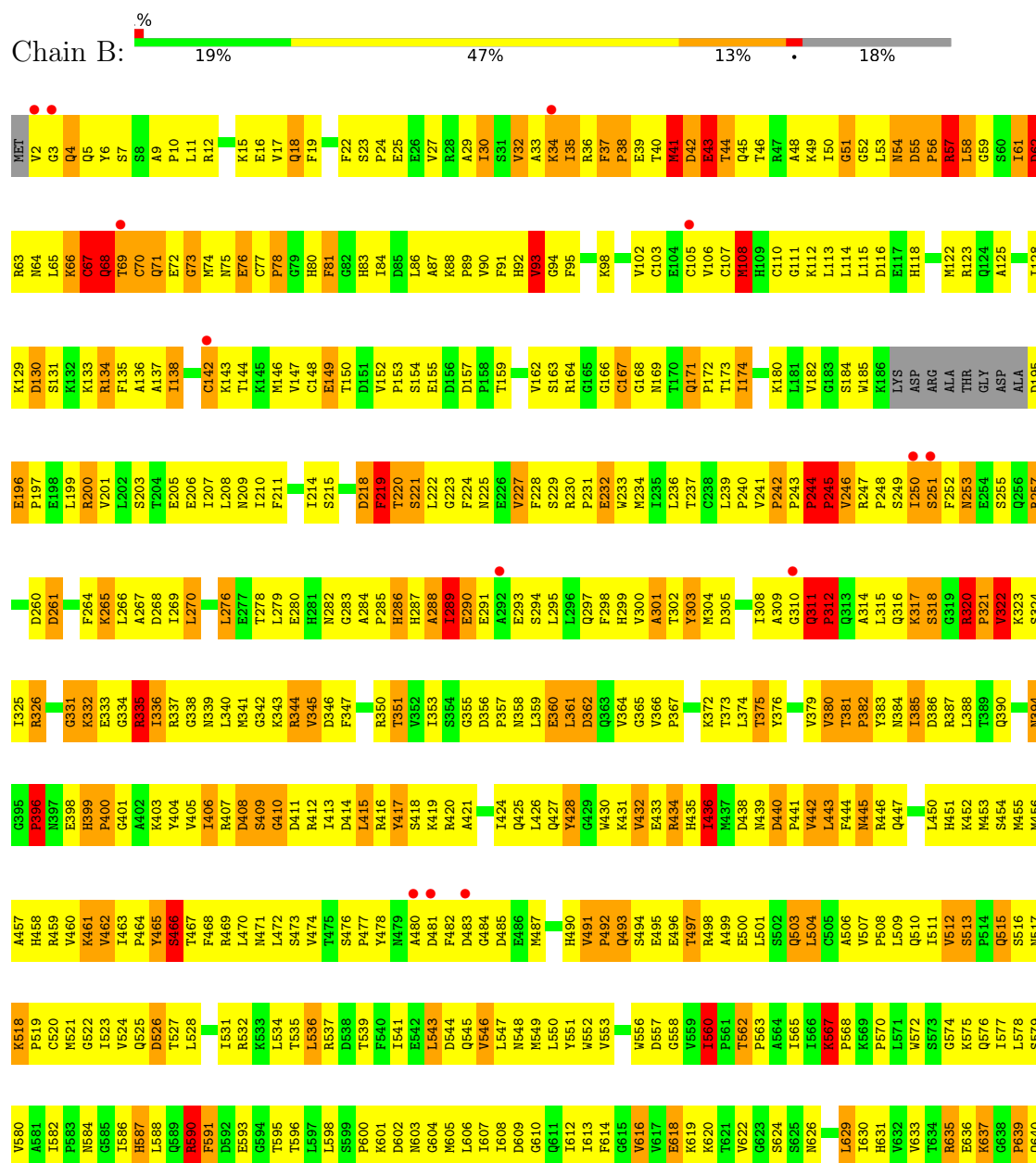
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	1	Total	Mg	0	0
			1	1		

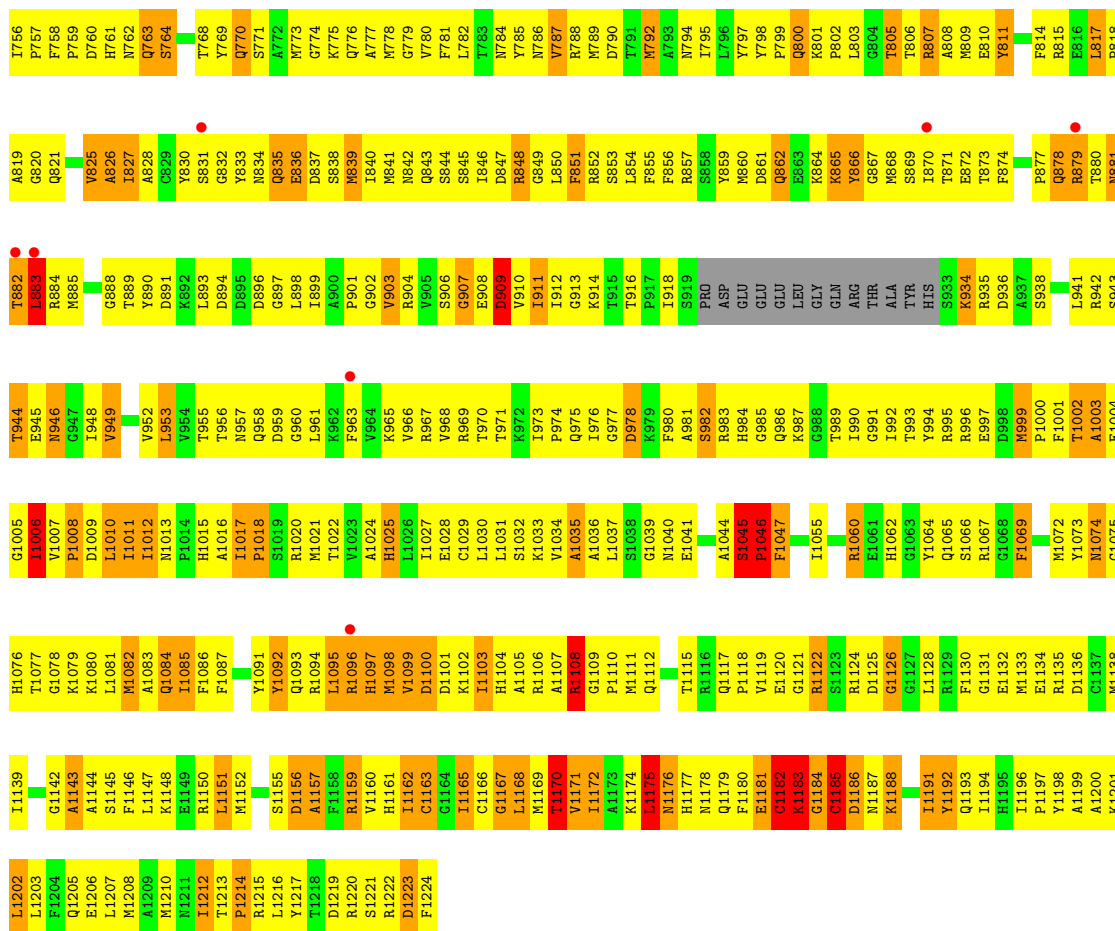
3 Residue-property plots

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.

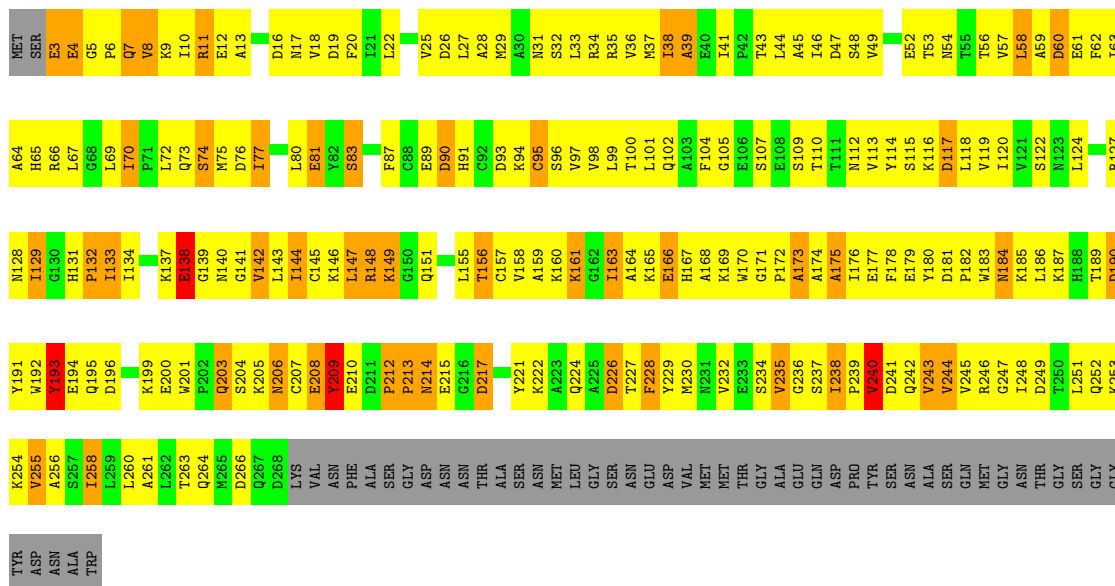
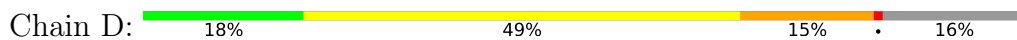
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



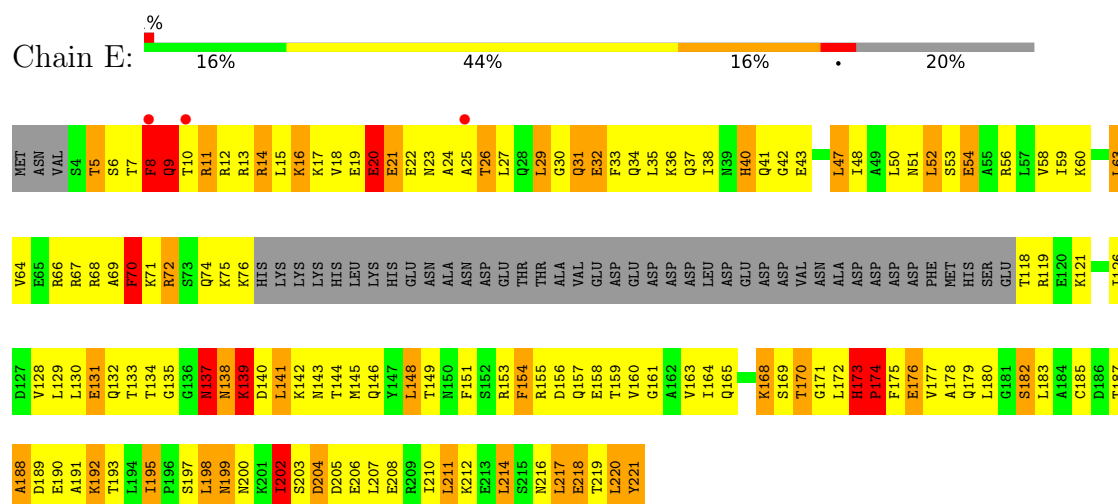
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GLY	TYR	A1412	A1346		D1223	D1157	S1096	E1034	H972	L908	K843	A776	M708	C642
PHE	ASN	G1413	A1347	Y1287	L1224	R1158	G1097	Y1035	D974		A844		L709	A643
GLY	GLU	A1414	L1348	D1288	F1225	R1159	V1098	R1036	D973	L912	L845	F779	L710	K644
VAL	SER	S1415	K1349	R1289	V1226	T1161	P1099	S1160	H975	E914	E846	D781	R711	L645
SER	GLY	A1416	K1350	K1290	I1227	T1162	R1100	T1037	T976	E915	D847	R782	E712	F646
SER	LEU	E1417	E1351	R1291	H1228	I1163	L1101	K1039	K977	G916	M848	T783	S713	G647
PRO	VAL	L1418	Y1352	P1292	S1229	I1163	K1102	Q1040	S978		V850	L784	E715	N648
GLY	ASN	D1419	Y1353	S1293	E1230	P1164	E1103	F1042	S979		H851	H785		I649
PHE	ALA	D1420	N1354	P1294	E1165	E1166	I1104	F1043	L981		L920	H786	V718	K651
SER	ASP	C1421	V1355	T1295	D1166	E1167	N1106	V1044	T982	G921	D853	F787	V652	V652
PRO	ASP	G1422		G1296	L1236		N1107	V1045	L983		M854	S788	R720	M653
THR	ASP	G1423	D1359	E1297	I1237	I1170	A1108	L1046	K984	L923	T855	K789	F721	M654
SER	VAL	V1424		Y1298	I1238		K1109	S1047	D986	A924	T856		L722	F655
PRO	VAL	E1425	V1363	V1299	I1239	H1173	N1110	I1049	L985		R857		N723	F656
THR	ASP	E1426	N1364	K1300	I1238	F1174	M1111	E1049	L986	G926	M858	P794	L722	L657
TYR	GLU	N1427	Y1365	E1301	C1240	S1175	K1112	T1050	L987	V927	S859	E795	R726	L658
SER	LEU	V1428	R1366	P1302	R1241	L1176	T1113	A1051	L988	L928	L860	S796	D727	M659
PRO	MET	I1429	H1367	E1303	V1242	LEU	P1114	Q1052	D992	L929	G861	K797	K728	M660
PRO	THR	L1430	M1368	W1304	V1243	ASP	S1115	F1053	L993		N862	G798	A729	G661
THR	PHE	G1431	A1369	V1305	ARG	GLU	T1116	R1054	Q994	E931	M863	F799	G730	F662
SER	SER	Q1432	L1370	L1306	PRO	GLU	L1117	R1055	E995	E932	I864	V800	R731	S663
PRO	PRO	M1433	L1371	E1307	LYS	GLU	T1117	S1056	N996	Y933	Q865	E801	L732	T664
ALA	ALA	A1434	V1372	T1308	SER	ALA	V1118	S1057	N996	K934	F866	N802		G665
TYR	VAL	P1435	D1373	D1309	LEU	GLN	L1120	V1058	L997	Q935	I867	S803	V735	I666
SER	ASP	I1436	V1374	G1310	ASP	SER	P1119	V1058	L998		T867	Y804	N736	G667
PRO	SER	G1437	M1375	V1311	ALA	PHE	E1121	H1059	V999	L986	G869	L805	L737	D668
THR	GLY	T1438	T1376	N1312	GLU	THR	P1122	P1060	V937		M868	R806	G738	
SER	SER	G1439	L1377	L1313	THR	GLU	G1123	G1061	R1001	K938	I867	G807	D739	D672
PRO	ASN	A1440	Q1378	S1314	GLU	GLU	H1124	M1062	Q1002	D939	D871	L808	L740	G673
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TYR	ALA	D1442	G1380	V1316	E1255	S1189	A1126	V1064	N1004	K941	M873		T675	
SER	MET	V1443	L1381	M1317	E1256	P1190	D1127	G1065	E1005	F942	D874	N742		
PRO	ALA	M1444		V1319	D1257	W1191	Q1128	V1066	I1006	R944	A876	E812	V743	I679
THR	GLY	I1445	V1394	P1320	M1258	L1192	L1129	L1067	Q1008	E945	H877	F814	M747	T680
SER	PHE	D1446	T1385	G1320	M1259	L1193	Q1130	A1068	N1009	V946	I878	F815	V748	E681
PRO	PRO	E1447	R1386	R1194	R1194		A1131		A1010			H816	M748	T682
SER	THR	E1448			K1261	L1197	K1132	I1072	A1010	F947	Q881	H816	S751	I683
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SER	TYR	L1450	N1390	P1324	I1263	D1198	T1134	E1074	R1012	D949	L883	M818	G753	E685
PRO	GLY	V1451	R1391	T1325	E1264			P1075	D1013	G950	L884	G819	S754	A686
THR	GLY		S1392	R1326	N1265	A1201	A1137	A1076	E951	A952	T885	R821	F755	K687
SER	ASP	M1454	N1393	I1327	T1266	M1202	I1138	T1077	V1015	N953	I886		I756	K688
SER	ASP	P1455	T1394	Y1328	M1267		E1139	Q1078	T1016	W954	Q887	I825	M757	K689
TYR	GLY	GLU	G1395	T1329	L1268	K1205	H1140	M1079	L1017			D826	I758	V690
TYR	GLY	LYS	A1396	M1330	E1269	D1206	T1141	T1080	F1018	P955		D827	A759	V693
PRO	ALA	ILE	L1397	S1331	N1270	L1207	T1142	ASN	C1019	L956		A828	Q760	T694
THR	THR	THR	R1398	F1332	I1271	T1208	L1143	GLY	C1020	P957			M761	K695
SER	SER	SER	R1399	I1333	T1272	M1209	K1144	THR	L1021	V958	E894	K830	S762	E896
PRO	PRO	ILE	C1400	D1334	L1273	G1210	S1145	PHE	L1022	N959	K895	T831	A763	A697
SER	PHE	GLU	S1401	I1335	R1274	Q1211	V1146	HIS	R1023	I960	R896		G764	Q698
TYR	GLY	ASP	F1402	M1336	G1275	V1212	T1147	PHE	R1024	R961	Y897	T834	V765	A699
TYR	GLY	ASP	E1403	L1337	V1276	G1213	I1148	ALA	R1025	R962	R898	G835	G766	K698
SER	ALA	GLY	E1404	V1338	E1277	G1214	A1149	GLY	L1026	I963	V899		Q767	N700
PRO	TYR	GLN	L1405	L1339	R1215	R1215	S1150	VAL	D900	L901	D900	Y836	Q768	L701
THR	GLY	ASP	V1406	G1340	I1279		E1151	ALA	T1028	Q965	L902	I837	Q769	L702
SER	GLY	GLY	E1407	I1341	E1280	Q1218	I1152	SER	R1029	Q968	L902	Q886	S769	
PRO	ALA	GLY	L1408	E1342	R1281	T1219	Y1153	K1092	R1030		T904	R839	K773	K705
SER	PRO	VAL	L1409	A1343	V1282	F1220	Y1154	K1093	V1031	G969		R840	R774	H706
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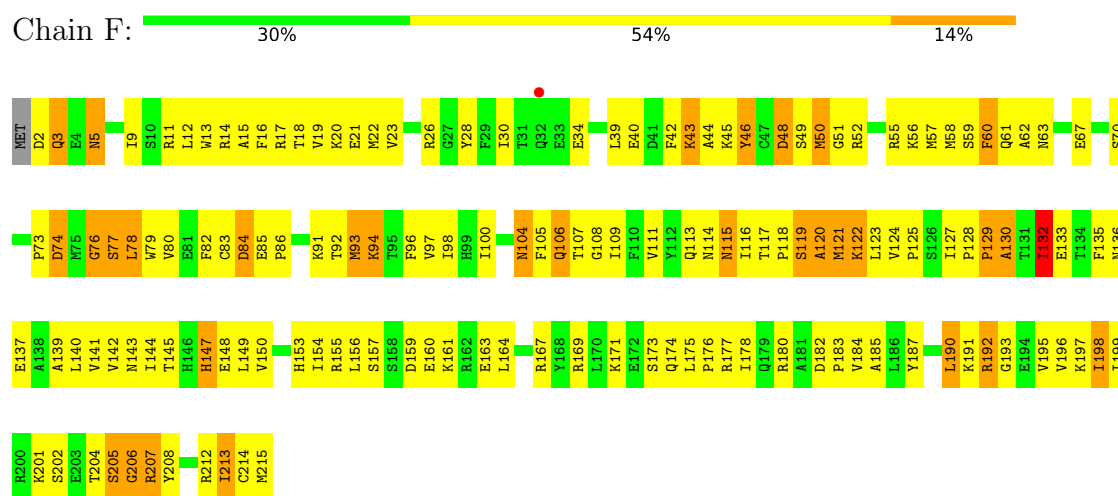
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



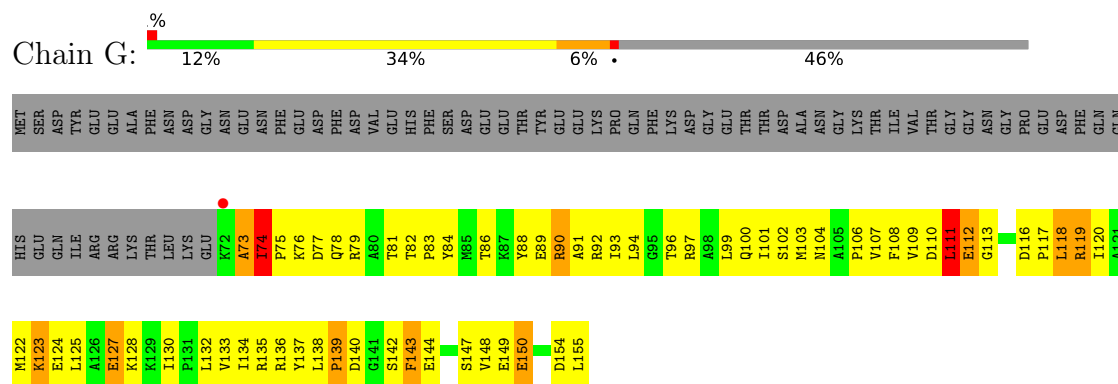
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

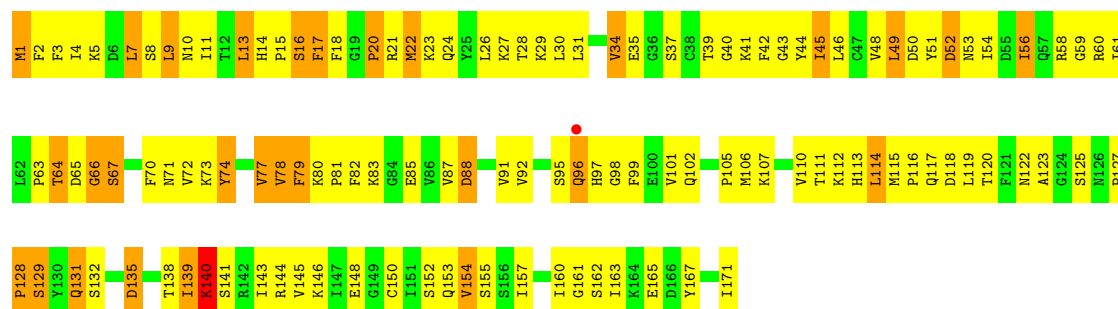


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

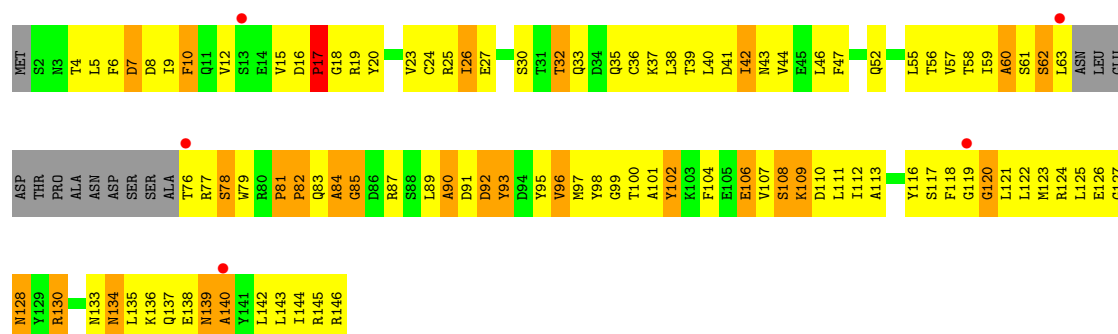
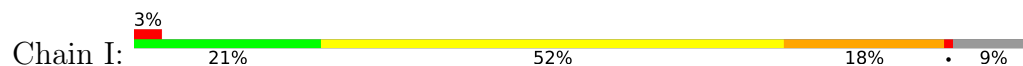


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

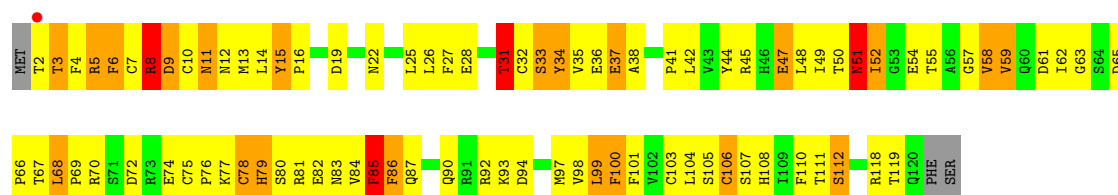




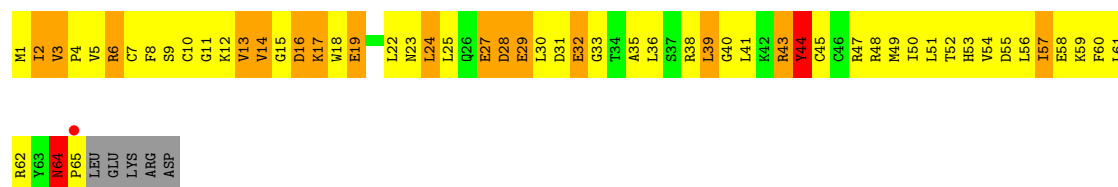
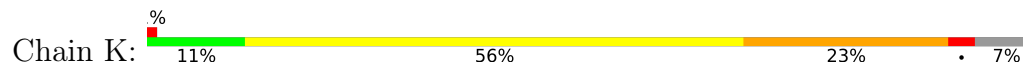
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

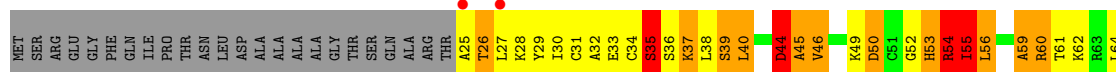


• Molecule 11: DNA-directed RNA polymerase II subunit RPB11





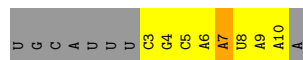
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



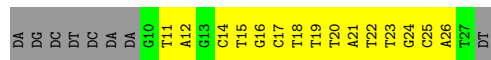
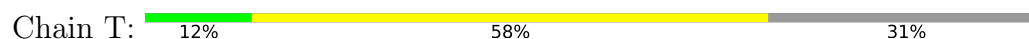
- Molecule 13: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*GP*CP*TP*GP*CP*TP*TP*TP*AP*TP*TP*GP*CP*AP*TP*T)-3'



- Molecule 14: 5'-D(*CP*AP*GP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'



- Molecule 15: 5'-R(*UP*GP*CP*AP*UP*UP*UP*CP*GP*CP*AP*AP*UP*AP*AP*A)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.47Å 391.62Å 284.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 50.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 99.9 (50.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 4.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.205 , 0.241 0.215 , 0.243	Depositor DCC
R_{free} test set	16372 reflections (8.09%)	wwPDB-VP
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 106.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31777	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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	B	0.54	0/11339	1.08	97/15334 (0.6%)
2	C	0.51	0/8981	1.04	52/12108 (0.4%)
3	D	0.53	0/2133	1.09	15/2891 (0.5%)
4	E	0.48	0/1437	1.14	17/1925 (0.9%)
5	F	0.48	0/1788	1.03	9/2406 (0.4%)
6	G	0.58	0/691	1.10	3/933 (0.3%)
7	H	0.52	0/1368	1.08	9/1844 (0.5%)
8	I	0.47	0/1086	1.03	4/1470 (0.3%)
9	J	0.48	0/989	1.02	8/1331 (0.6%)
10	K	0.53	0/541	0.96	1/727 (0.1%)
11	L	0.50	0/937	1.05	10/1265 (0.8%)
12	M	0.56	0/366	0.95	1/485 (0.2%)
13	N	0.42	0/154	0.78	0/235
14	P	0.40	0/188	0.96	0/291
15	T	0.10	0/407	0.30	0/627
All	All	0.51	0/32405	1.05	226/43872 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	K	0	1

There are no bond length outliers.

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	PRO	N-CA-C	-16.32	97.71	114.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	173	HIS	CA-C-N	11.00	133.59	119.84
4	E	173	HIS	C-N-CA	11.00	133.59	119.84
2	C	574	SER	CA-C-N	9.87	129.24	118.97
2	C	574	SER	C-N-CA	9.87	129.24	118.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	K	44	TYR	Sidechain

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	B	11140	0	11215	1592	0
2	C	8810	0	8847	1339	0
3	D	2095	0	2051	319	0
4	E	1427	0	1451	186	0
5	F	1752	0	1776	189	0
6	G	679	0	701	108	0
7	H	1340	0	1357	192	0
8	I	1068	0	1040	167	0
9	J	971	0	929	129	0
10	K	532	0	542	131	0
11	L	919	0	929	140	0
12	M	364	0	388	57	0
13	N	138	0	80	8	0
14	P	168	0	88	15	0
15	T	365	0	208	48	0
16	B	2	0	0	0	0
16	C	1	0	0	0	0
16	D	1	0	0	0	0
16	J	2	0	0	0	0
16	K	1	0	0	0	0
16	M	1	0	0	0	0
17	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31777	0	31602	4227	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 67.

The worst 5 of 4227 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)
15:T:21:DA:C2'	15:T:22:DT:H5'	1.58	1.32
15:T:21:DA:H2''	15:T:22:DT:C5'	1.65	1.25
15:T:20:DT:C2'	15:T:21:DA:H5'	1.73	1.18
11:L:47:ARG:HB3	11:L:47:ARG:HH11	1.11	1.15
15:T:20:DT:H2'	15:T:21:DA:H5'	1.13	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1406/1733 (81%)	965 (69%)	284 (20%)	157 (11%)	0	6
2	C	1090/1224 (89%)	719 (66%)	243 (22%)	128 (12%)	0	5
3	D	264/318 (83%)	163 (62%)	70 (26%)	31 (12%)	0	5
4	E	173/221 (78%)	107 (62%)	43 (25%)	23 (13%)	0	3
5	F	212/215 (99%)	154 (73%)	36 (17%)	22 (10%)	0	7
6	G	82/155 (53%)	62 (76%)	13 (16%)	7 (8%)	0	11
7	H	169/171 (99%)	129 (76%)	26 (15%)	14 (8%)	0	11
8	I	129/146 (88%)	79 (61%)	30 (23%)	20 (16%)	0	3
9	J	117/122 (96%)	80 (68%)	24 (20%)	13 (11%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	63/70 (90%)	38 (60%)	12 (19%)	13 (21%)	0	1
11	L	112/120 (93%)	81 (72%)	24 (21%)	7 (6%)	1	15
12	M	44/70 (63%)	22 (50%)	8 (18%)	14 (32%)	0	0
All	All	3861/4565 (85%)	2599 (67%)	813 (21%)	449 (12%)	0	5

5 of 449 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	GLN
1	B	41	MET
1	B	48	ALA
1	B	54	ASN
1	B	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	
1	B	1239/1520 (82%)	1117 (90%)	122 (10%)	7	27
2	C	962/1061 (91%)	860 (89%)	102 (11%)	6	24
3	D	234/274 (85%)	212 (91%)	22 (9%)	8	29
4	E	159/200 (80%)	132 (83%)	27 (17%)	2	13
5	F	196/197 (100%)	181 (92%)	15 (8%)	12	35
6	G	74/137 (54%)	67 (90%)	7 (10%)	8	28
7	H	152/152 (100%)	134 (88%)	18 (12%)	5	21
8	I	117/128 (91%)	106 (91%)	11 (9%)	8	29
9	J	113/116 (97%)	103 (91%)	10 (9%)	9	32
10	K	60/65 (92%)	53 (88%)	7 (12%)	5	21
11	L	99/102 (97%)	86 (87%)	13 (13%)	4	19
12	M	40/57 (70%)	36 (90%)	4 (10%)	7	26
All	All	3445/4009 (86%)	3087 (90%)	358 (10%)	7	25

5 of 358 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	138	GLU
5	F	207	ARG
3	D	209	TYR
4	E	126	ILE
7	H	45	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	538	ASN
9	J	90	GLN
2	C	1065	GLN
9	J	12	ASN
5	F	147	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	7/16 (43%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	7	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	1416/1733 (81%)	-0.10	17 (1%) 76 59	76, 129, 175, 200	0
2	C	1108/1224 (90%)	0.07	18 (1%) 70 52	79, 140, 185, 200	0
3	D	266/318 (83%)	-0.11	0 100 100	93, 126, 168, 188	0
4	E	177/221 (80%)	0.05	3 (1%) 69 51	106, 142, 182, 190	0
5	F	214/215 (99%)	0.02	1 (0%) 87 73	99, 160, 187, 200	0
6	G	84/155 (54%)	-0.23	1 (1%) 76 59	73, 107, 138, 147	0
7	H	171/171 (100%)	0.03	1 (0%) 85 71	98, 127, 164, 174	0
8	I	133/146 (91%)	0.35	5 (3%) 44 34	134, 165, 186, 196	0
9	J	119/122 (97%)	0.18	1 (0%) 82 65	122, 165, 189, 200	0
10	K	65/70 (92%)	-0.14	1 (1%) 72 54	92, 121, 158, 169	0
11	L	114/120 (95%)	-0.11	1 (0%) 81 64	94, 128, 156, 170	0
12	M	46/70 (65%)	0.36	2 (4%) 40 31	120, 172, 195, 198	0
13	N	7/14 (50%)	0.98	0 100 100	84, 199, 200, 200	1 (14%)
14	P	8/16 (50%)	0.29	0 100 100	198, 199, 200, 200	0
15	T	18/26 (69%)	0.87	0 100 100	116, 198, 200, 200	1 (5%)
All	All	3946/4621 (85%)	-0.00	51 (1%) 75 57	73, 136, 184, 200	2 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1081	LEU	4.8
2	C	335	GLY	4.5
2	C	882	THR	3.5
10	K	65	PRO	3.4
8	I	63	LEU	3.3

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
17	MG	B	1736	1/1	0.83	0.12	153,153,153,153	0
16	ZN	J	124	1/1	0.97	0.06	200,200,200,200	0
16	ZN	M	71	1/1	0.99	0.04	174,174,174,174	0
16	ZN	D	319	1/1	1.00	0.06	98,98,98,98	0
16	ZN	J	123	1/1	1.00	0.08	136,136,136,136	0
16	ZN	B	1734	1/1	1.00	0.04	149,149,149,149	0
16	ZN	K	71	1/1	1.00	0.03	113,113,113,113	0
16	ZN	B	1735	1/1	1.00	0.05	110,110,110,110	0
16	ZN	C	1225	1/1	1.00	0.08	104,104,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.