



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:49 PM UTC

PDB ID : 2R93 / pdb_00002r93
Title : Elongation complex of RNA polymerase II with a hepatitis delta virus-derived RNA stem loop
Authors : Lehmann, E.; Brueckner, F.; Cramer, P.
Deposited on : 2007-09-12
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

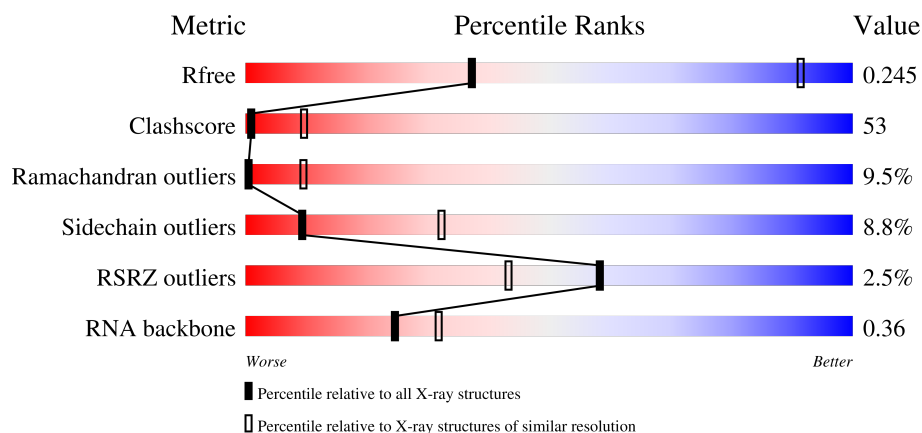
1 Overall quality at a glance

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	R	18	
2	A	1733	
3	B	1224	
4	C	318	

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31500 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*AP*UP*UP*CP*UP*CP*UP*AP*UP*CP*GP*GP*AP*AP*UP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	14	Total	C	N	O	P	0	0	0
			289	132	49	96	12			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB1.

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

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB2.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

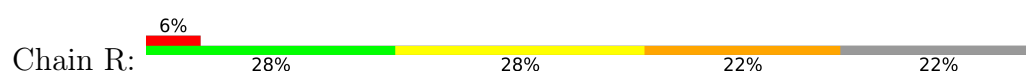
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

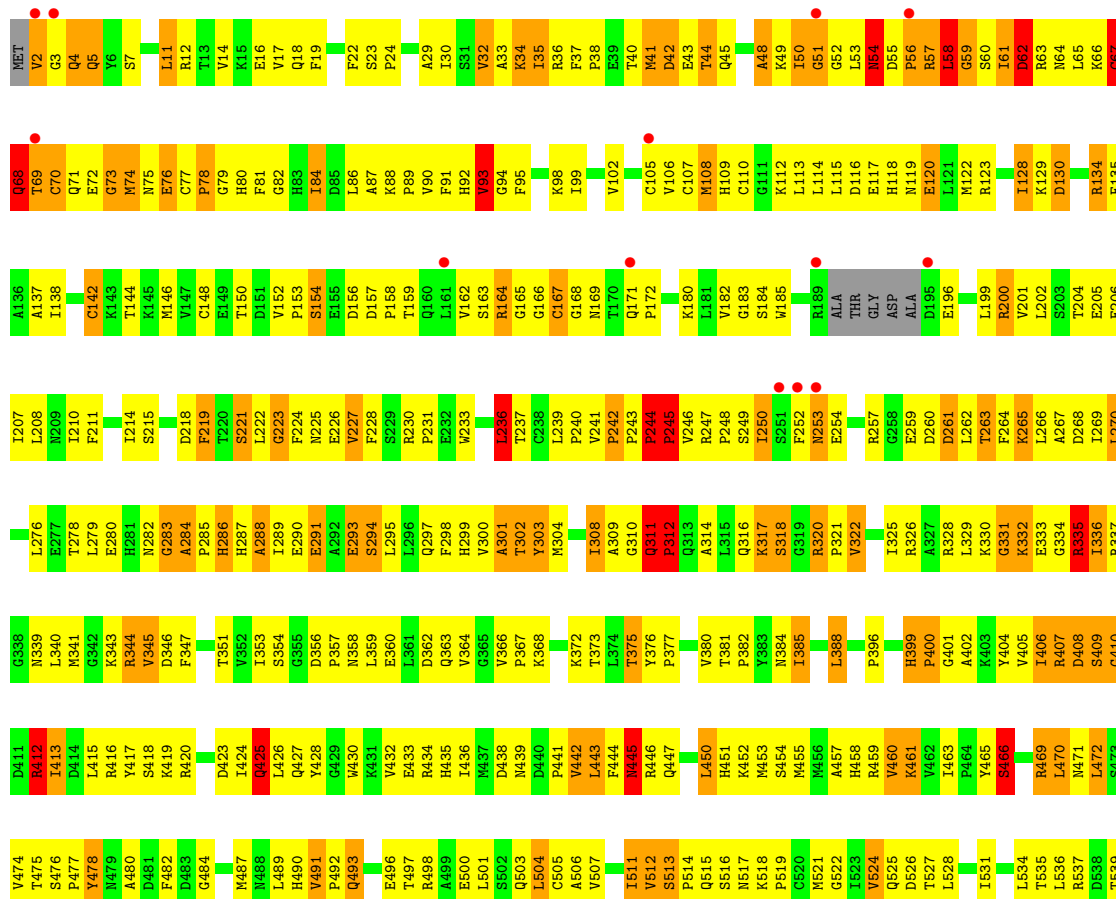
3 Residue-property plots

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*AP*UP*UP*CP*UP*CP*UP*AP*UP*CP*GP*GP*AP*AP*UP*C)-3')



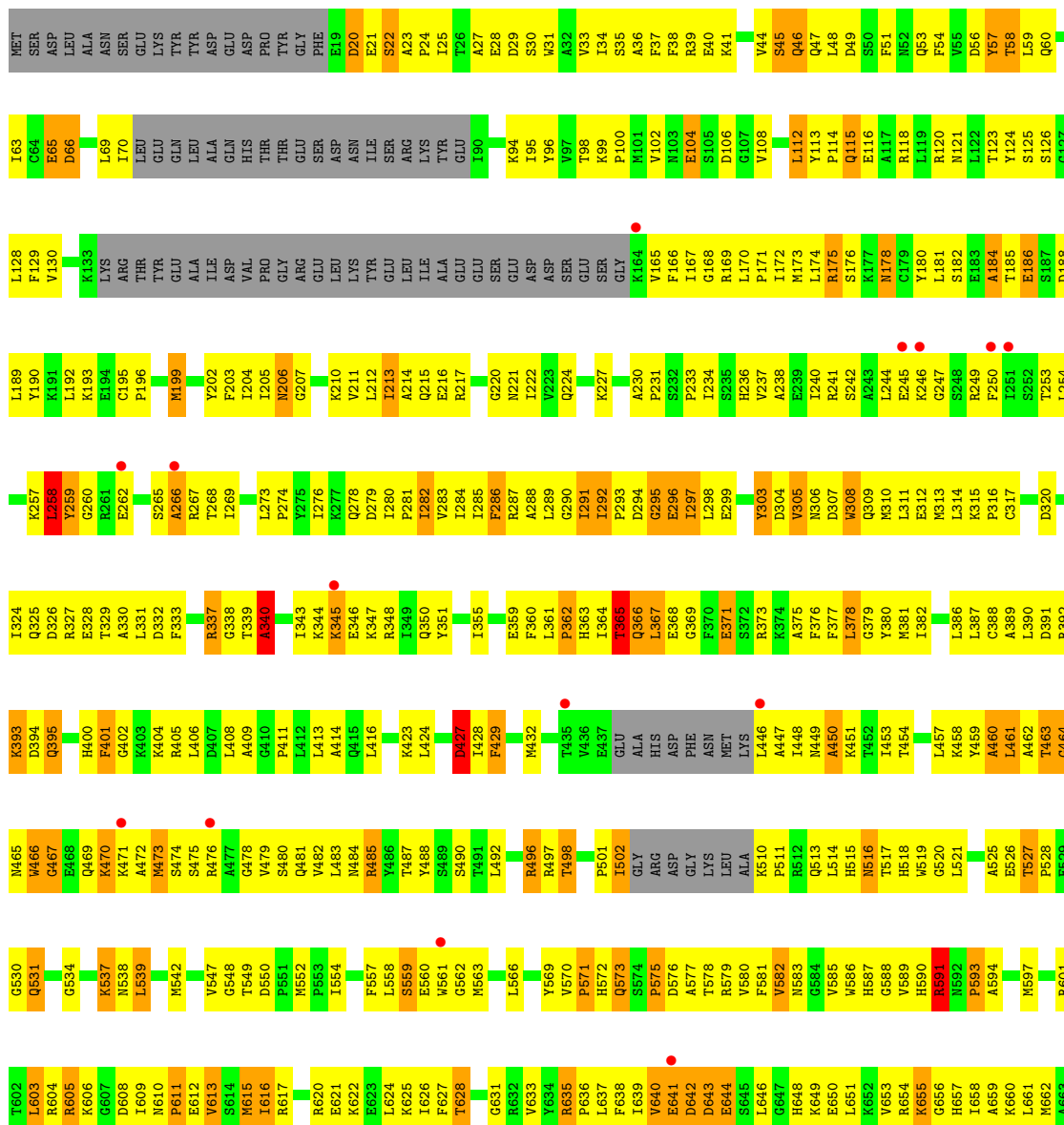
- Molecule 2: DNA-directed RNA polymerase II subunit RPB1

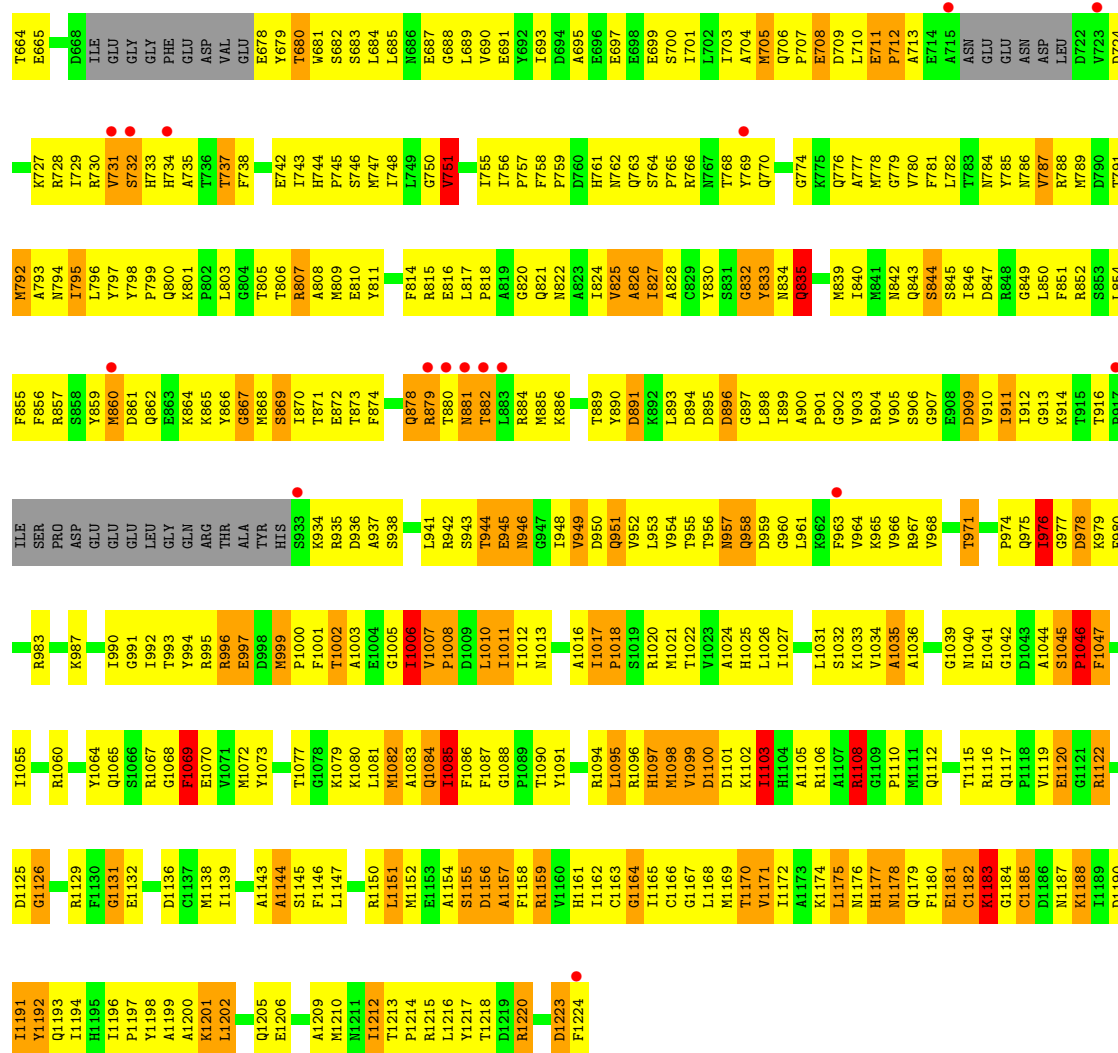


E1426	N1427	V1428	M1364	Y1365	E1429	L1430	G1431	Q1432	M1368	A1369	L1370	A1434	P1435	I1436	G1437	T1438	F1441	D1442	V1443	M1444	I1445	D1446	E1447	L1450	M1454	F1455	GLU	GLN	S1392	M1393	T1394	I1395	G1396	L1397	A1398	R1399	G1400	S1401	F1402	E1403	E1404	VAL	THR	PRO	TYR	SER	ASN	GLU	SER	GLY	GLY	LEU	VAL	ASN	ALA	ASP	D1419	L1420	C1421	ASP	VAL	LYS	ASP	GLU																																																																										
V1162	I1163	P1164	E1165	D1166	I1169	I1170	Q1171	L1172	H1173	F1174	S1175	L1176	L1177	ASP	GLU	GLU	ALA	GLU	GLN	SER	PHE	ASP	Q1187	Q1188	S1189	P1190	W1191	L1192	L1193	R1194	D1198	A1201	M1202	K1205	D1206	L1207	T1208	M1209	G1210	Q1211	V1212	G1213	E1214	R1215	Q1218	T1219	F1220	K1221	M1222	D1223	L1224	F1225	I1291	G1423	N1354	S1425																																																																																		
K1092	K1093	T1094	R1095	G1096	G1097	R1100	L1101	K1102	E1103	H1104	L1105	L1106	V1107	M1111	K1112	T1113	P1114	S1115	L1116	L1117	V1118	Y1119	L1120	E1121	P1122	G1123	H1124	D1127	Q1128	Q1129	Q1130	K1131	K1132	L1133	I1134	T1138	T1141	K1144	S1145	V1146	T1147	I1148	A1149	S1150	I1151	I1152	Y1153	Y1154	D1155	P1156	S1160	T1161																																																																																						
A1027	T1028	R1029	R1030	V1031	L1032	Q1033	E1034	Y1035	R1036	L1037	T1038	K1039	Q1040	A1041	F1042	V1045	L1046	S1047	N1048	I1049	E1050	A1051	Q1052	S1056	V1057	M1058	H1059	P1060	G1061	E1062	M1063	V1064	G1065	V1066	L1067	A1068	A1069	Q1070	S1071	E1074	P1075	A1076	M1079	T1080	L1081	ASN	THR	PHE	HIS	PHE	ALA	GLY	VAL	ALA	SER																																																																																			
R961	R962	T963	E964	Q965	R966	A967	Q968	Q969	T970	R971	H972	T973	D974	H975	T976	R977	Q978	R979	D980	L981	T982	T983	R984	D985	R986	R987	L988	L993	N996	L997	V998	V999	R1000	G1001	G1002	A1003	M1004	E1005	L1006	I1007	Q1008	N1009	A1010	Q1011	R1012	D1013	A1014	V1015	T1016	L1017	F1018	C1019	L1022	R1025	L1026																																																																																			
R815	R816	R817	R818	R821	R825	D826	T827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	T855	T856	R857	R858	S859	L860	R861	R862	R863	F866	T867	Y868	C869	E870	D871	R872	R873	D874	R875	A876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960
F540	I541	E542	L543	D544	G545	V546	L547	N548	M549	L550	Y551	W552	V553	T560	P561	T562	P563	A564	I565	I566	K567	P568	K569	P570	L571	W572	S573	G574	K575	Q576	L577	L578	S579	V580	H587	L588	Q589	R590	F591	D592	T595	T596	L597	L598	S599	P600	K601	D602	N603	G604	M605	L606	I607	L608	D609	G610																																																																																		
Q611	I612	F613	F614	G615	G616	V617	L618	K619	K620	T621	V622	G623	S624	G628	L629	L630	H631	V632	V633	T634	G635	E636	K637	W638	T639	P639	V641	F646	G647	K648	T649	Q650	K651	N654	L657	L658	H659	D660	G661	F662	S663	T664	G665	T666	G667	D668	T669	G673	M674	L675	M676	T679	T680																																																																																					
E681	T682	A683	A684	E685	A686	K687	K688	K689	V690	V693	T694	K695	E696	A697	Q698	A699	T700	L701	L702	K705	H706	E636	K637	W638	T639	P639	V641	F646	G647	K648	T649	Q650	K651	N654	L657	L658	H659	D660	G661	F662	S663	T664	G665	T666	G667	D668	T669	G673	M674	L675	M676	T679	T680																																																																																					
W746	V747	M748	S751	K752	G753	S754	S755	T756	N757	T758	A759	Q760	S761	T762	A763	G764	W765	G766	Q767	Q768	R774	R775	A776	F777	G778	F779	W780	D781	R782	T783	L784	P785	H786	F787	S788	K789	P794	E795	S796	K797	G798	F799	E800	E801	N802	S803	Y804	L805	R806	G807	L808	D809	E812	R813	F814																																																																																			

[illegible]

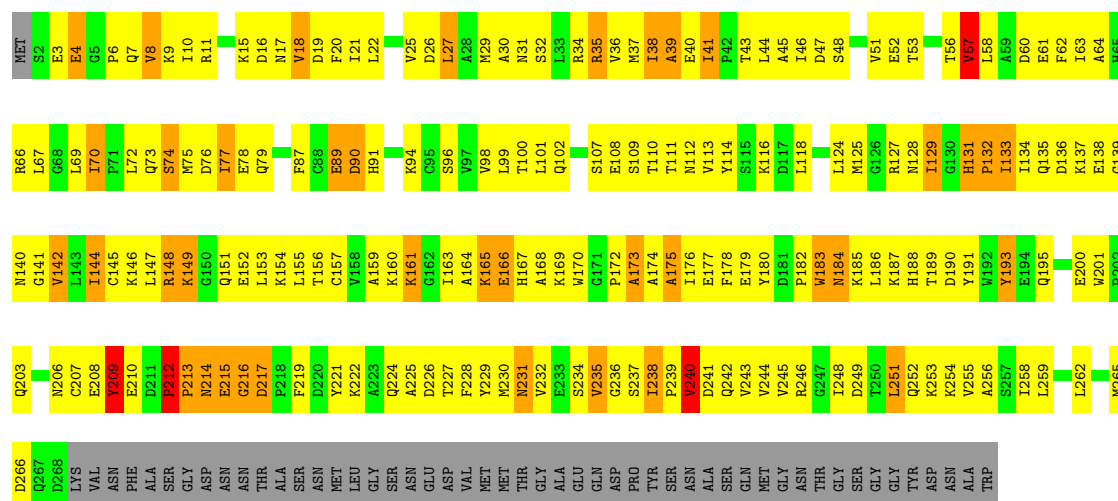
- Molecule 3: DNA-directed RNA polymerase II subunit RPB2



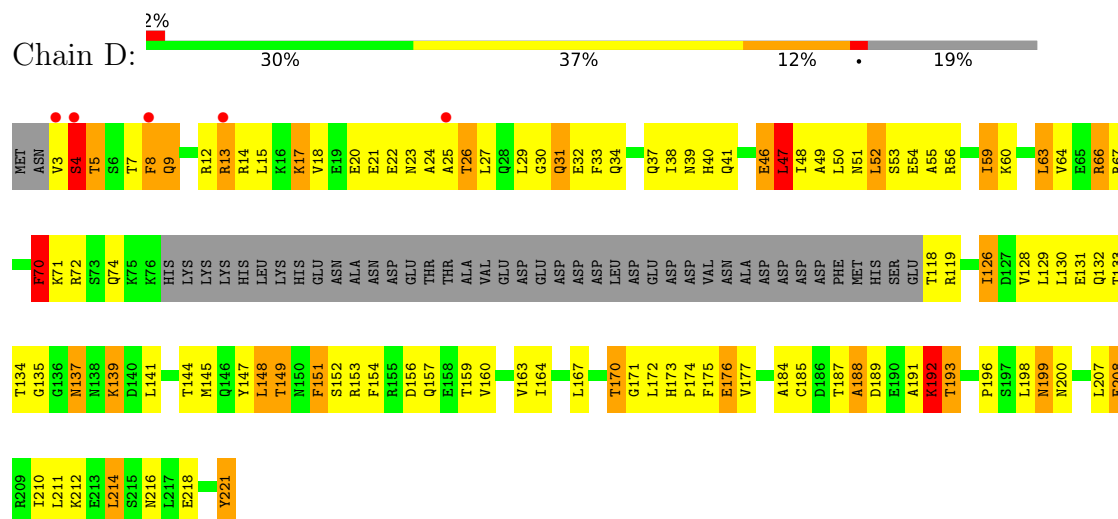


• Molecule 4: DNA-directed RNA polymerase II subunit RPB3

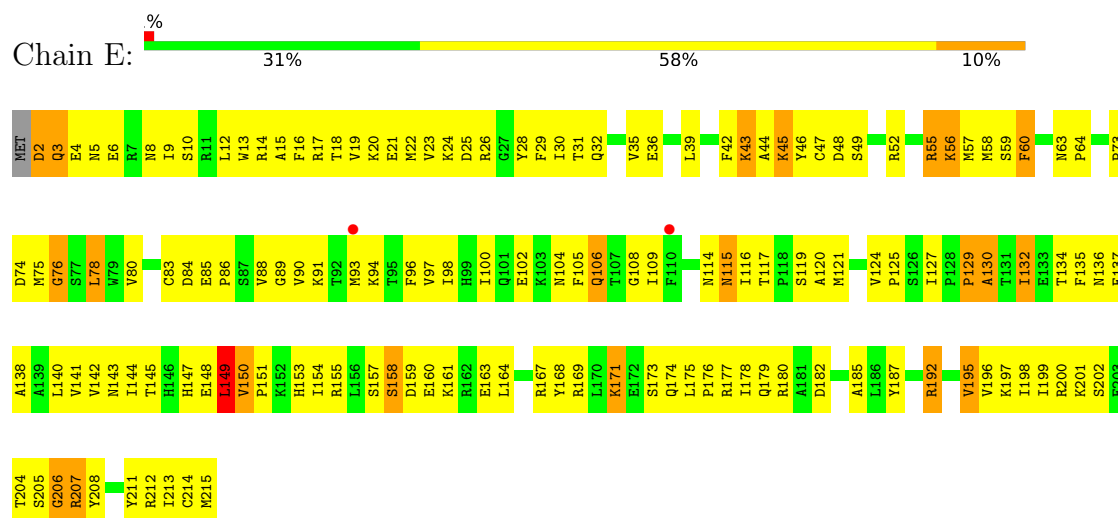
Chain C: 23% 48% 12% 16%



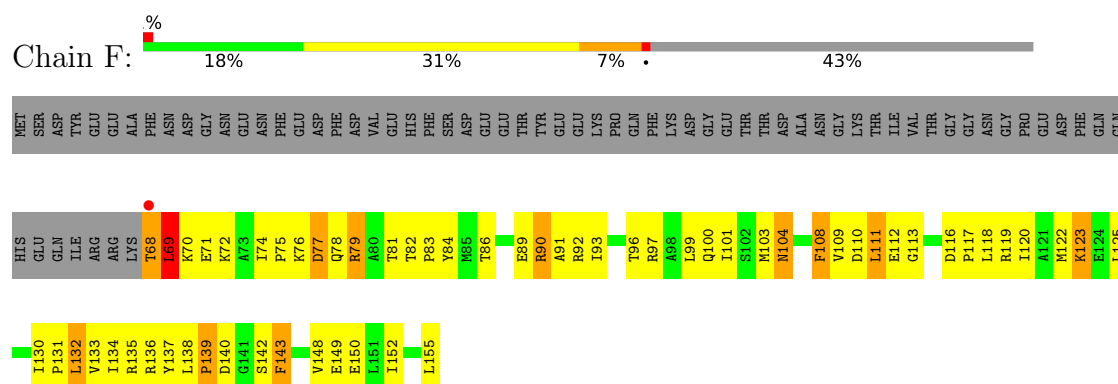
• Molecule 5: DNA-directed RNA polymerase II subunit RPB4



• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC1

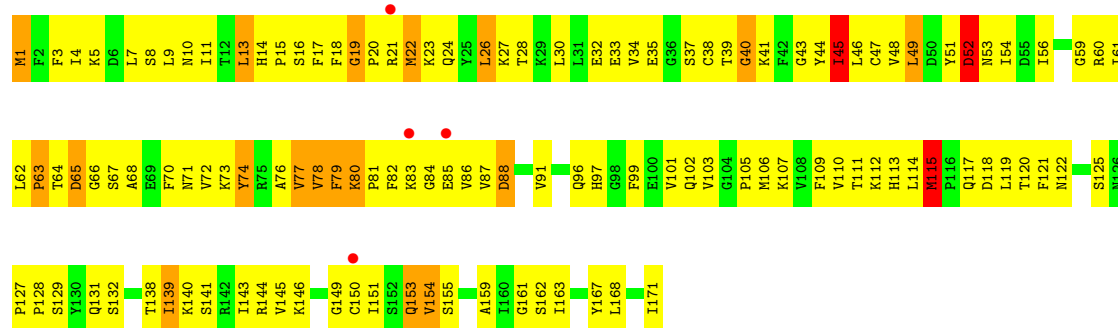


• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC2

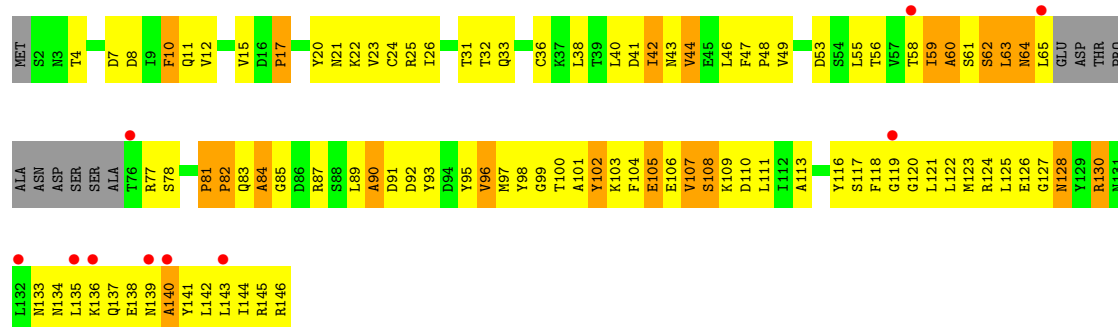


• Molecule 8: DNA-directed RNA polymerase II subunit RPB7

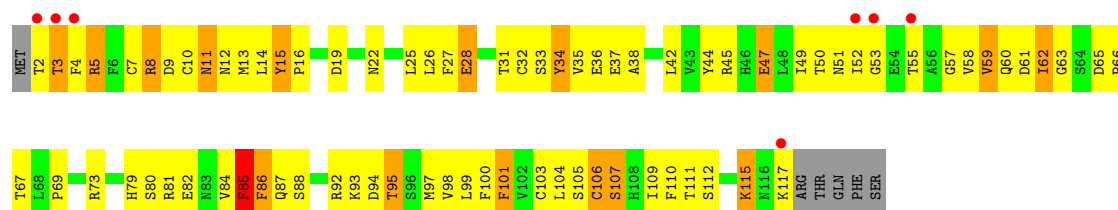




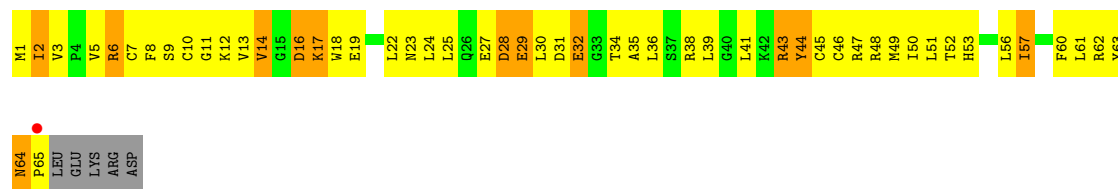
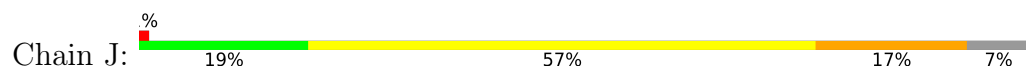
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 10: DNA-directed RNA polymerase II subunit RPB9

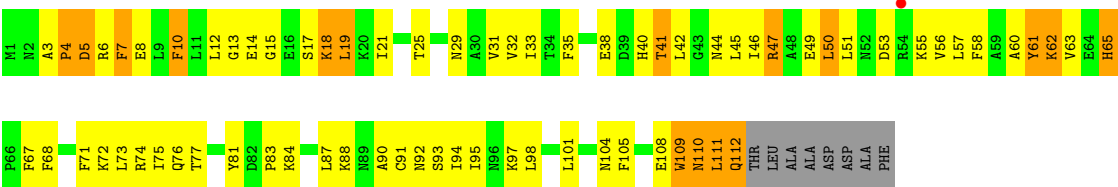


• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

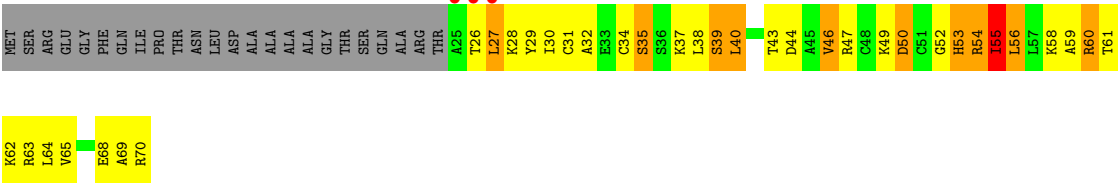


• Molecule 12: DNA-directed RNA polymerase II subunit RPB11





● Molecule 13: 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	223.34Å 394.88Å 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) 97.1 (50.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 4.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.216 , 0.241 0.224 , 0.245	Depositor DCC
R_{free} test set	2129 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	103.2	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.010 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31500	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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	R	0.59	0/321	1.05	2/496 (0.4%)
2	A	0.52	1/11394 (0.0%)	1.10	91/15407 (0.6%)
3	B	0.50	0/9013	1.02	45/12152 (0.4%)
4	C	0.51	0/2139	1.10	16/2899 (0.6%)
5	D	0.47	0/1444	1.08	10/1935 (0.5%)
6	E	0.47	0/1788	1.04	12/2406 (0.5%)
7	F	0.64	0/723	1.36	5/974 (0.5%)
8	G	0.50	0/1368	1.13	13/1844 (0.7%)
9	H	0.48	0/1102	0.94	2/1492 (0.1%)
10	I	0.44	0/962	0.98	5/1295 (0.4%)
11	J	0.53	0/541	0.94	0/727
12	K	0.48	0/922	1.01	6/1244 (0.5%)
13	L	0.58	0/366	0.96	1/485 (0.2%)
All	All	0.51	1/32083 (0.0%)	1.06	208/43356 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	50	ILE	CA-CB	5.13	1.59	1.54

The worst 5 of 208 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	70	LYS	N-CA-C	-23.01	82.14	114.12
2	A	452	LYS	N-CA-C	-12.61	96.17	111.69
3	B	1185	CYS	N-CA-C	-11.44	99.43	113.50
5	D	26	THR	N-CA-C	-11.23	99.88	112.57
2	A	56	PRO	N-CA-C	-10.89	101.97	114.92

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	R	289	0	153	11	0
2	A	11194	0	11279	1259	0
3	B	8841	0	8875	1079	0
4	C	2101	0	2056	276	0
5	D	1434	0	1460	129	0
6	E	1752	0	1776	165	0
7	F	712	0	737	111	0
8	G	1340	0	1357	169	0
9	H	1084	0	1057	134	0
10	I	944	0	901	110	0
11	J	532	0	543	94	0
12	K	904	0	911	110	0
13	L	364	0	387	50	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31500	0	31492	3359	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 53.

The worst 5 of 3359 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)
7:F:68:THR:HG21	7:F:69:LEU:N	1.59	1.16
7:F:69:LEU:HD23	7:F:71:GLU:CB	1.77	1.14
7:F:69:LEU:HD23	7:F:71:GLU:HB2	1.17	1.12
2:A:58:LEU:HD12	2:A:59:GLY:N	1.65	1.11
2:A:34:LYS:NZ	2:A:57:ARG:HH12	1.50	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
2	A	1412/1733 (82%)	1032 (73%)	252 (18%)	128 (9%)	0	10
3	B	1096/1224 (90%)	781 (71%)	206 (19%)	109 (10%)	0	8
4	C	265/318 (83%)	169 (64%)	66 (25%)	30 (11%)	0	5
5	D	174/221 (79%)	133 (76%)	27 (16%)	14 (8%)	1	12
6	E	212/215 (99%)	166 (78%)	32 (15%)	14 (7%)	1	15
7	F	85/155 (55%)	70 (82%)	11 (13%)	4 (5%)	2	19
8	G	169/171 (99%)	128 (76%)	32 (19%)	9 (5%)	1	18
9	H	131/146 (90%)	78 (60%)	33 (25%)	20 (15%)	0	3
10	I	114/122 (93%)	76 (67%)	26 (23%)	12 (10%)	0	7
11	J	63/70 (90%)	37 (59%)	16 (25%)	10 (16%)	0	3
12	K	110/120 (92%)	88 (80%)	15 (14%)	7 (6%)	1	15
13	L	44/70 (63%)	20 (46%)	12 (27%)	12 (27%)	0	0
All	All	3875/4565 (85%)	2778 (72%)	728 (19%)	369 (10%)	0	9

5 of 369 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	42	ASP
2	A	48	ALA
2	A	54	ASN
2	A	57	ARG
2	A	62	ASP

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	
2	A	1245/1520 (82%)	1126 (90%)	119 (10%)	8	28
3	B	964/1061 (91%)	877 (91%)	87 (9%)	9	31
4	C	235/274 (86%)	217 (92%)	18 (8%)	12	35
5	D	160/200 (80%)	137 (86%)	23 (14%)	3	17
6	E	196/197 (100%)	188 (96%)	8 (4%)	27	49
7	F	78/137 (57%)	70 (90%)	8 (10%)	7	25
8	G	152/152 (100%)	135 (89%)	17 (11%)	6	22
9	H	119/128 (93%)	114 (96%)	5 (4%)	26	49
10	I	110/116 (95%)	105 (96%)	5 (4%)	24	47
11	J	60/65 (92%)	56 (93%)	4 (7%)	15	39
12	K	97/102 (95%)	89 (92%)	8 (8%)	10	34
13	L	40/57 (70%)	38 (95%)	2 (5%)	22	45
All	All	3456/4009 (86%)	3152 (91%)	304 (9%)	9	32

5 of 304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	47	LEU
10	I	34	TYR
5	D	149	THR
7	F	123	LYS
12	K	61	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	516	ASN
10	I	12	ASN
3	B	1015	HIS
10	I	11	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	K	76	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	12/18 (66%)	4 (33%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	6	C
1	R	7	U
1	R	13	G
1	R	17	U

There are no RNA pucker outliers to report.

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 oligosaccharides 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
7	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	68:THR	C	69:LEU	N	4.50

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	14/18 (77%)	0.56	1 (7%) 22 21	128, 147, 176, 188	0
2	A	1422/1733 (82%)	0.06	33 (2%) 61 45	57, 116, 171, 200	0
3	B	1112/1224 (90%)	0.18	30 (2%) 56 41	61, 126, 184, 200	0
4	C	267/318 (83%)	0.04	0 100 100	73, 111, 159, 176	0
5	D	178/221 (80%)	0.28	5 (2%) 55 40	88, 133, 179, 192	0
6	E	214/215 (99%)	0.18	2 (0%) 81 64	93, 154, 191, 199	0
7	F	88/155 (56%)	-0.16	1 (1%) 78 60	61, 93, 130, 153	0
8	G	171/171 (100%)	0.10	4 (2%) 61 45	88, 116, 155, 163	0
9	H	135/146 (92%)	0.67	10 (7%) 20 20	131, 161, 187, 196	0
10	I	116/122 (95%)	0.50	7 (6%) 27 24	110, 161, 191, 196	0
11	J	65/70 (92%)	-0.00	1 (1%) 72 54	79, 109, 145, 149	0
12	K	112/120 (93%)	-0.10	1 (0%) 81 64	76, 115, 140, 158	0
13	L	46/70 (65%)	0.77	3 (6%) 25 23	107, 170, 191, 193	0
All	All	3940/4583 (85%)	0.14	98 (2%) 58 43	57, 122, 182, 200	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1081	LEU	7.0
5	D	3	VAL	6.8
10	I	2	THR	4.9
2	A	69	THR	4.2
3	B	883	LEU	4.1

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
14	ZN	I	204	1/1	0.96	0.09	190,190,190,190	0
15	MG	A	1	1/1	0.98	0.08	68,68,68,68	0
14	ZN	L	105	1/1	0.99	0.04	156,156,156,156	0
14	ZN	A	1506	1/1	0.99	0.05	119,119,119,119	0
14	ZN	I	203	1/1	1.00	0.08	113,113,113,113	0
14	ZN	A	1508	1/1	1.00	0.06	79,79,79,79	0
14	ZN	J	101	1/1	1.00	0.04	86,86,86,86	0
14	ZN	B	1307	1/1	1.00	0.06	78,78,78,78	0
14	ZN	C	302	1/1	1.00	0.07	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.