



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 09:38 AM EDT

PDB ID : 2R7Z / pdb_00002r7z
Title : Cisplatin lesion containing RNA polymerase II elongation complex
Authors : Damsma, G.E.; Alt, A.; Brueckner, F.; Carell, T.; Cramer, P.
Deposited on : 2007-09-10
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

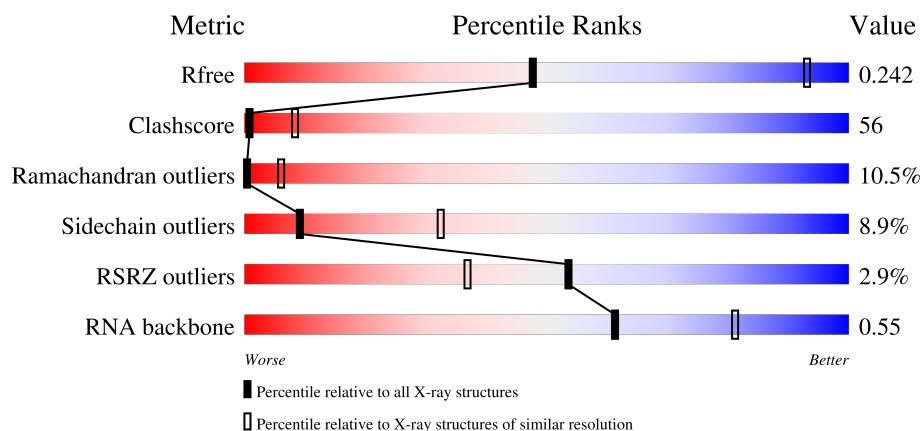
1 Overall quality at a glance

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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

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	T	17	6% 76% 18% 6%
2	N	7	14% 43% 57%
3	P	10	10% 20% 60% 10% 10%
4	A	1733	2% 22% 46% 12% 18%

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	D	221	
8	E	215	
9	F	155	
10	G	171	
11	H	146	
12	I	122	
13	J	70	
14	K	120	
15	L	70	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31804 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 DNA chain called 5'-D(*TP*AP*CP*TP*TP*GUP*CP*CP*CP*TP*CP*CP*TP*CP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	17	Total	C	N	O	P	0	0	0
			336	163	53	104	16			

- Molecule 2 is a DNA chain called 5'-D(*CP*AP*AP*GP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	7	Total	C	N	O	P	0	0	0
			143	69	30	38	6			

- Molecule 3 is a RNA chain called 5'-R(*UP*UP*UP*GP*AP*GP*GP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	P	0	0	0
			216	97	41	69	9			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

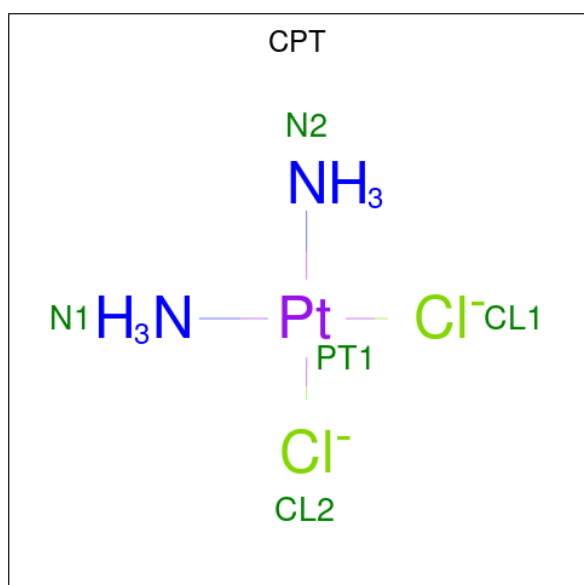
- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 16 is Cisplatin (CCD ID: CPT) (formula: $\text{Cl}_2\text{H}_6\text{N}_2\text{Pt}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	T	1	Total	N	Pt	0	0
			3	2	1		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Zn	0	0
			2	2		

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

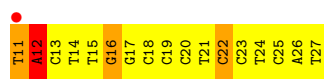
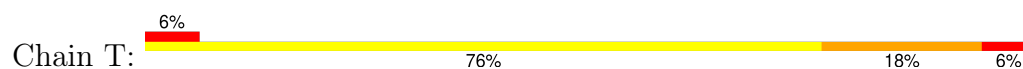
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

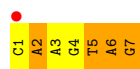
3 Residue-property plots

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: 5'-D(*TP*AP*CP*TP*TP*GUP*CP*CP*CP*TP*CP*CP*TP*CP*AP*T)-3',



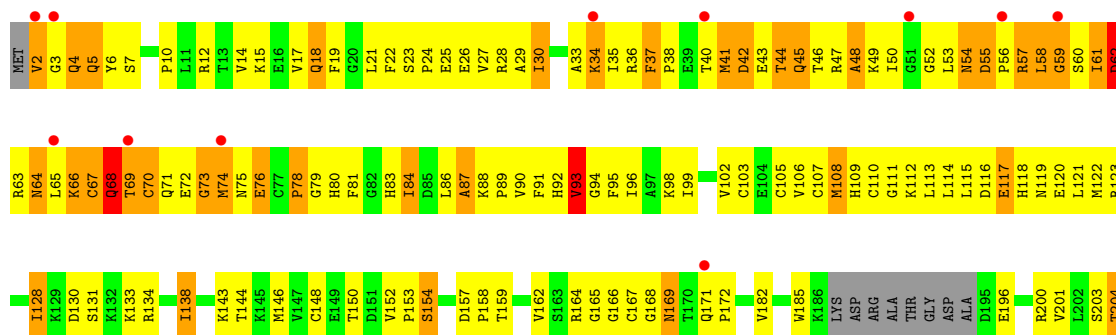
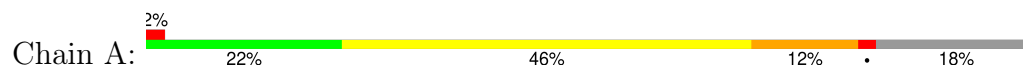
- Molecule 2: 5'-D(*CP*AP*AP*GP*TP*AP*G)-3'



- Molecule 3: 5'-R(*UP*UP*UP*GP*AP*GP*GP*AP*GP*G)-3'

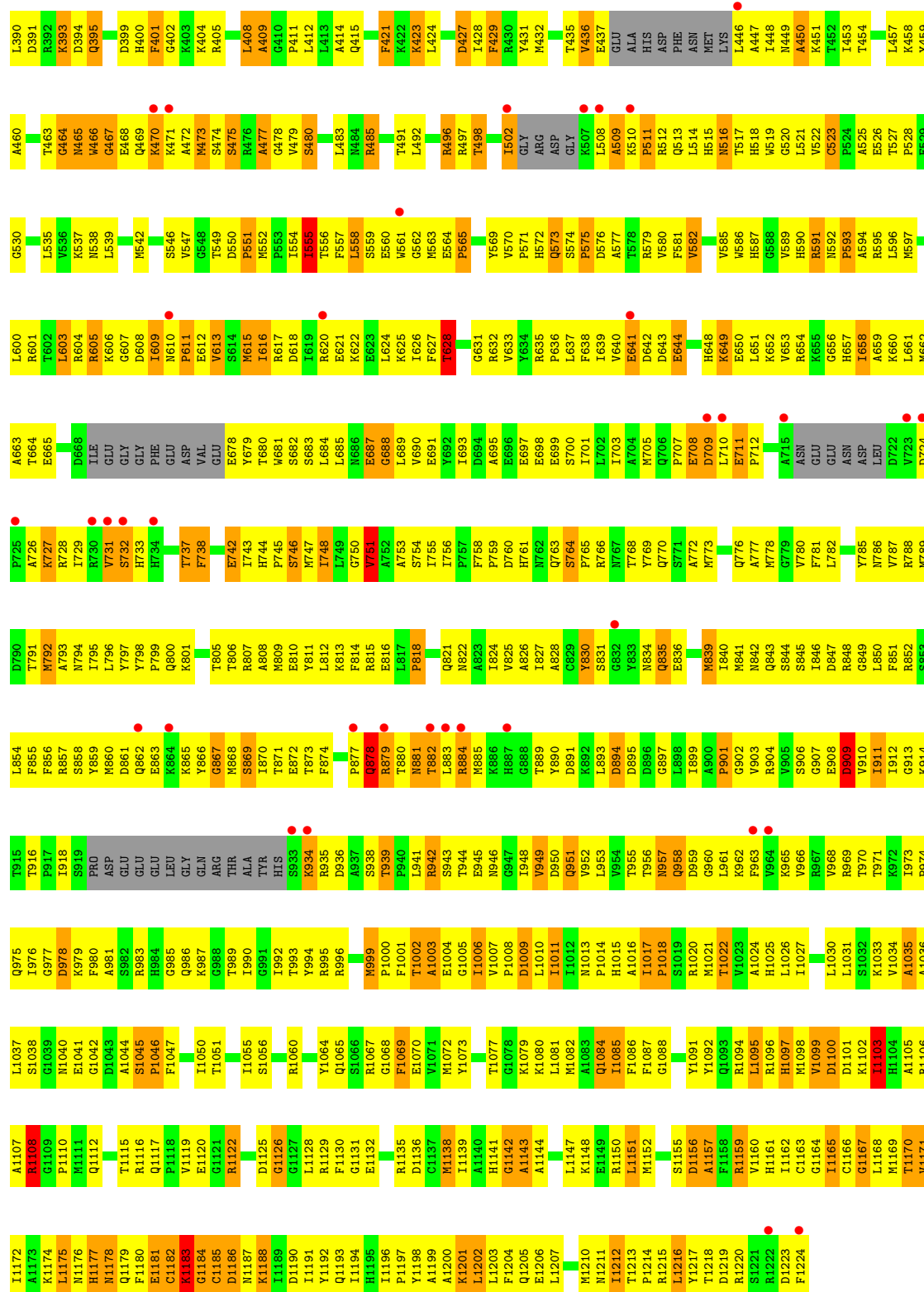


- Molecule 4: DNA-directed RNA polymerase II subunit RPB1



Q1130	A1069	G1002	K938	E870	G807	L737	I670	S599	L528	I463	G401	G334	D268	E205
A1131	Q1070	K1003	D939	D871	L808	K738	I671	P600	I531	P464	G401	K335	I269	E206
K1132	S1072	E1004	R940	M872	T909	D739	D672	K601	I531	Y465	Y404	I336	I270	I207
I1134	I1074	E1005	R941	M873	P810	L740	D673	D602	I534	S466	V405	R337	L267	L208
E1138	G1073	I1006	F942	D874	Q811	N741	N741	M605	L534	T467	I406	G338	L276	N209
A1139	E1074	Q1008	R943	A875	R812	N742	P674	L606	T535	F468	R407	N339	E277	I210
H1140	P1075	Q1009	E945	I878	F813	V743	T675	L607	L536	R469	D408	N340	T278	F211
T1076	A1076	A1010	V946	I879	F814	K744	M676	I608	R537	L470	S409	K341	L279	I214
Q1077	Q1078	Q1011	F947	S882	H816	K745	I679	D609	T539	N471	G410	G342	E280	I214
M1078	M1079	R1012	F947	L883	A817	V747	T680	I612	S473	L472	R412	K343	H281	S215
T1080	T1081	D1013	G950	T884	M818	N748	E681	T613	F540	S473	R413	K344	H282	I218
L1081	L1082	A1014	I886	T885	R821	K749	T682	F614	I542	T475	D414	R346	O283	F219
ASN	THR	V1015	N953	I886	R821	G750	I683	L543	I542	S476	L415	F347	P285	T220
THR	PHE	L1016	N954	G887	I825	S751	A884	G616	D544	Y477	R416	S348	H286	S221
PHE	THR	L1017	P955	G888	I826	K752	A885	G615	I544	Y478	R417	A349	L222	T220
HIS	HIS	F1018	L956	S889	D826	G753	E686	Q545	V546	N479	S418	R350	A288	G223
PHE	PHE	C1019	P957	D890	T927	S754	E687	E618	L547	A480	K419	T351	F224	F224
ALA	ALA	C1020	V958	A891	A828	I757	K688	K619	N548	O481	R420	V352	E290	N225
GLY	GLY	L1021	V959	R892	V829	I757	K689	K620	N549	F482	D423	I353	E291	E226
VAL	VAL	L1022	R960	R896	R830	M761	V690	T621	L550	D485	Q425	S354	A292	V227
ALA	ALA	R1025	R961	Y897	T831	M762	L691	G622	I551	D486	Q426	G355	E293	F228
SER	SER	R1026	R962	R898	A832	G767	D692	G623	M552	E486	I426	D356	I297	F229
K1092	K1093	R1029	T963	V899	E833	A763	V693	S624	I556	K487	Q427	P357	Q297	R230
V1094	V1095	R1030	T964	L901	G835	V765	K685	S625	D557	L489	Y428	E360	H299	P231
S1096	S1097	V1031	Q965	L902	I836	G766	E696	G627	G558	H490	Q429	L361	E232	E232
G1097	G1098	L1032	Q966	N903	I837	Q767	A697	G628	V559	V491	W430	I302	W233	W233
L1161	L1162	E1034	Q968	T904	Q838	Q768	Q698	L629	I560	P492	K431	G365	T302	M234
P1099	P1100	E1035	T970	D905	R839	I775	A699	T630	T562	S494	V432	V366	Y303	L236
R1100	R1101	R1036	F971	T907	R840	I775	N700	H631	P563	E495	R434	P367	N304	T237
L1101	L1102	L1037	R972	L908	V842	I775	L701	V632	A643	E496	R435	K368	D305	C238
E1165	E1166	T1038	1973	D909	K843	G778	L702	V633	I565	T497	I436	S369	N306	L239
I1103	I1104	K1039	K977	P910	A844	F779	T709	T634	I566	R498	W437	I307	I308	P240
L1105	L1106	Q1040	S911	S911	L845	D781	L710	P639	P568	A499	D438	T373	A309	V241
N1106	N1107	A1041	L912	L912	E846	R782	R711	Q640	K569	E500	N439	L374	P243	P243
F1042	F1043	F1042	S979	L913	D847	R783	E712	V641	I571	Q503	D440	T375	G310	P244
W1044	W1045	D1043	D980	S915	I848	L784	S713	C642	M572	L504	F441	I376	K311	P245
V1045	V1046	V1045	T982	G916	M849	F785	E715	F646	S573	Q503	V442	P377	K312	P246
L1046	L1047	L1046	T983	S917	V850	H786	D716	F646	Q574	L504	F444	I377	A314	R247
S1047	S1048	S1047	K984	E918	H851	F787	N717	F646	K575	V507	R445	T381	L315	P248
N1048	N1049	N1048	D985	I919	D853	S788	N718	N648	K575	I611	R446	P382	Q316	S249
I1049	I1050	I1049	T986	L920	N854	K789	V719	I649	Q676	V512	Q447	N384	K317	I250
E1050	E1051	E1050	V987	G921	T855	P794	R720	Q650	I577	S513	P448	I385	G319	S251
Q1052	Q1052	Q1052	G989	D922	R857	E795	L721	K651	L578	P514	S449	D386	R320	P252
V1058	V1058	V1058	V990	L925	N858	S796	N723	N654	V580	Q515	H451	R387	P321	N253
H1059	H1059	H1059	K991	Q926	S859	S796	E724	F655	I588	S516	K452	L388	V322	E254
E1121	E1121	E1121	D992	V927	L860	K797	A725	L658	Q689	K518	M453	I391	K323	Q256
G1123	G1123	G1123	L993	L928	G861	G798	R726	I658	Q689	P519	S454	V392	S324	E259
PHE	PHE	E1062	E995	L929	N862	F799	D727	I658	R590	C520	M455	R393	I325	D260
M1063	M1063	M1063	N996	E932	V863	V800	K728	G661	F591	M521	M456	N394	A327	D261
V1064	V1064	V1064	L997	E932	I864	E801	A729	F662	D592	G522	A457	G395	F328	T262
A1126	A1126	A1126	L993	Y933	Q865	N802	G730	S663	T595	I523	R459	P396	L329	T263
Q1187	Q1188	Q1188	L993	K934	F666	S803	R731	T664	T595	V524	R459	I397	K330	F264
S1189	S1189	S1189	V999	Q935	I867	Y804	L732	G665	T596	Q525	V460	E398	G331	K265
P1190	P1190	P1190	L1000	L1067	Y868	L805	L732	I666	I597	D526	K461	R399	K332	L266
W1191	W1191	W1191	R1001	V937	G969	R806	N736	G667	L598	T527	V462	P400	E333	A267

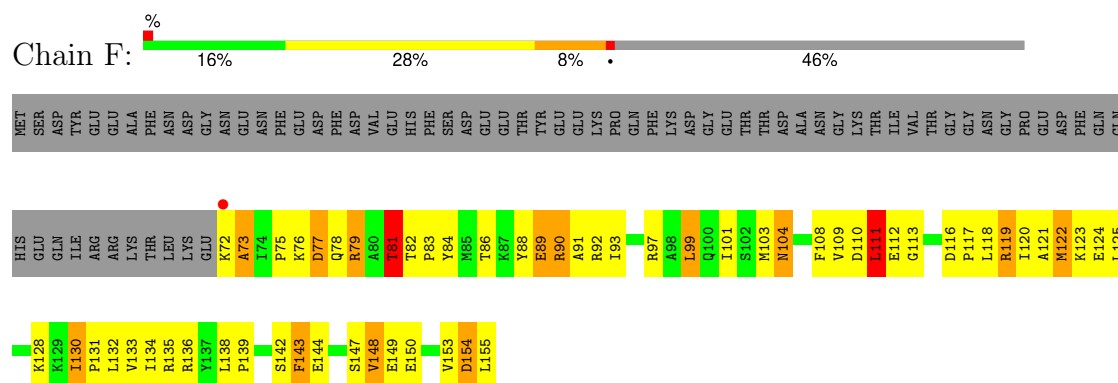




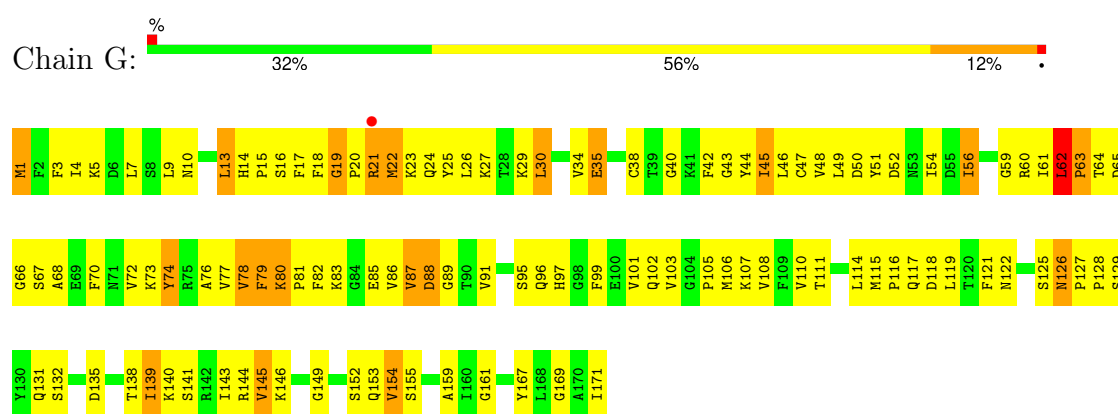
Chain C:



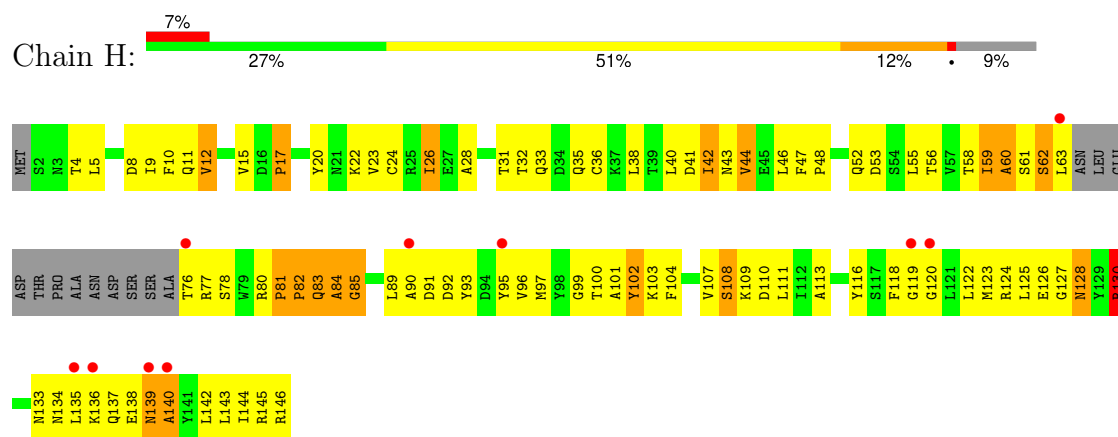
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2



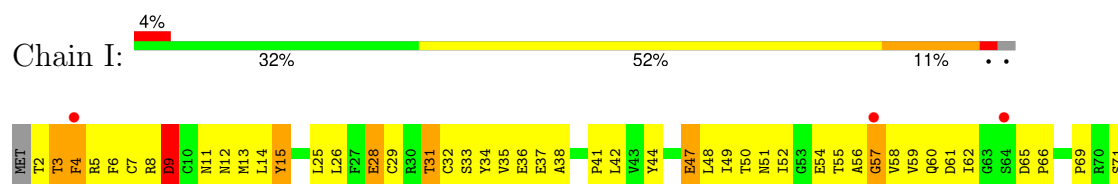
• Molecule 10: DNA-directed RNA polymerase II subunit RPB7

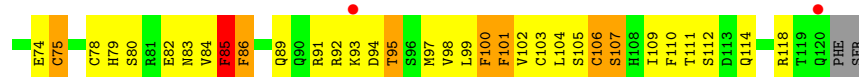


• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

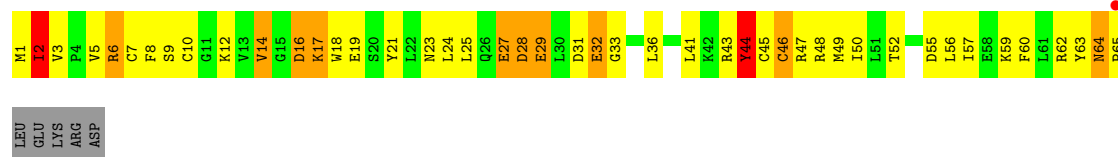


• Molecule 12: DNA-directed RNA polymerase II subunit RPB9

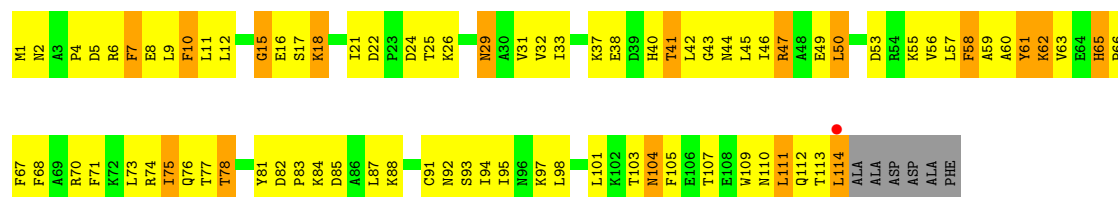




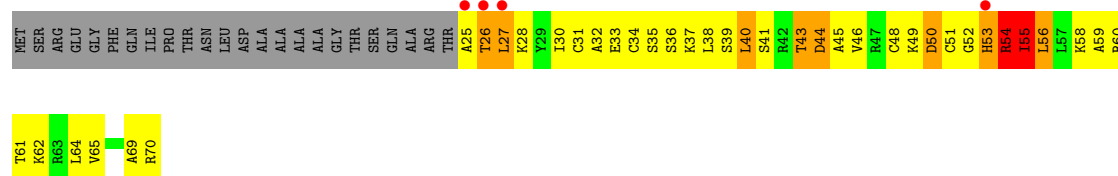
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 14: DNA-directed RNA polymerase II subunit RPB11



- Molecule 15: 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	222.06Å 393.12Å 283.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 99.7 (50.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.240 0.216 , 0.242	Depositor DCC
R_{free} test set	2410 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	106.6	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.045 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.045 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	31804	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, CPT

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	T	0.77	0/373	1.53	4/572 (0.7%)
2	N	0.71	0/161	1.19	2/247 (0.8%)
3	P	0.55	0/242	0.89	2/377 (0.5%)
4	A	0.54	0/11339	1.09	84/15334 (0.5%)
5	B	0.50	1/8981 (0.0%)	1.04	48/12108 (0.4%)
6	C	0.53	0/2133	1.07	11/2891 (0.4%)
7	D	0.49	0/1437	1.12	10/1925 (0.5%)
8	E	0.48	0/1788	1.06	13/2406 (0.5%)
9	F	0.60	0/691	1.15	6/933 (0.6%)
10	G	0.51	0/1368	1.12	13/1844 (0.7%)
11	H	0.47	0/1086	0.99	5/1470 (0.3%)
12	I	0.43	0/989	0.99	5/1331 (0.4%)
13	J	0.53	0/541	0.99	1/727 (0.1%)
14	K	0.51	0/937	1.06	8/1265 (0.6%)
15	L	0.55	0/366	0.90	0/485
All	All	0.52	1/32432 (0.0%)	1.07	212/43915 (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
1	T	0	2
2	N	0	2
6	C	0	1
13	J	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	292	ILE	CA-CB	5.17	1.57	1.53

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	452	LYS	N-CA-C	-12.53	97.62	111.28
5	B	1185	CYS	N-CA-C	-12.31	98.93	114.56
7	D	26	THR	N-CA-C	-12.05	97.33	112.88
5	B	1177	HIS	N-CA-C	-10.70	101.63	112.97
10	G	62	LEU	CA-C-N	-10.21	107.08	119.84

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	82	TYR	Sidechain
2	N	5	DT	Sidechain
2	N	6	DA	Sidechain
1	T	11	DT	Sidechain
1	T	12	DA	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	T	336	0	195	46	0
2	N	143	0	80	20	0
3	P	216	0	108	13	0
4	A	11140	0	11217	1389	0
5	B	8810	0	8847	1093	0
6	C	2095	0	2052	269	0
7	D	1427	0	1451	145	0
8	E	1752	0	1776	166	0
9	F	679	0	701	82	0
10	G	1340	0	1357	167	0
11	H	1068	0	1040	136	0
12	I	971	0	930	106	0
13	J	532	0	543	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	K	919	0	929	121	0
15	L	364	0	388	57	0
16	T	3	0	0	1	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	31804	0	31614	3579	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 56.

The worst 5 of 3579 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)
11:H:100:THR:HG23	11:H:138:GLU:HA	1.26	1.16
10:G:138:THR:HG22	10:G:139:ILE:H	1.09	1.12
4:A:53:LEU:HD23	4:A:54:ASN:H	0.99	1.12
4:A:1094:VAL:HG13	4:A:1113:THR:HG21	1.32	1.11
5:B:510:LYS:HG3	5:B:511:PRO:HD3	1.12	1.11

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
4	A	1406/1733 (81%)	988 (70%)	277 (20%)	141 (10%)	0 7
5	B	1090/1224 (89%)	754 (69%)	217 (20%)	119 (11%)	0 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	264/318 (83%)	181 (69%)	50 (19%)	33 (12%)	0	4
7	D	173/221 (78%)	125 (72%)	28 (16%)	20 (12%)	0	4
8	E	212/215 (99%)	157 (74%)	38 (18%)	17 (8%)	1	10
9	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	1	14
10	G	169/171 (99%)	131 (78%)	30 (18%)	8 (5%)	2	18
11	H	129/146 (88%)	90 (70%)	19 (15%)	20 (16%)	0	2
12	I	117/122 (96%)	84 (72%)	23 (20%)	10 (8%)	0	9
13	J	63/70 (90%)	36 (57%)	15 (24%)	12 (19%)	0	1
14	K	112/120 (93%)	86 (77%)	20 (18%)	6 (5%)	1	16
15	L	44/70 (63%)	17 (39%)	14 (32%)	13 (30%)	0	0
All	All	3861/4565 (85%)	2711 (70%)	746 (19%)	404 (10%)	0	6

5 of 404 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	42	ASP
4	A	44	THR
4	A	48	ALA
4	A	54	ASN
4	A	55	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	
4	A	1239/1520 (82%)	1123 (91%)	116 (9%)	8	30
5	B	962/1061 (91%)	883 (92%)	79 (8%)	10	35
6	C	234/274 (85%)	210 (90%)	24 (10%)	7	27
7	D	159/200 (80%)	130 (82%)	29 (18%)	2	12
8	E	196/197 (100%)	188 (96%)	8 (4%)	27	51
9	F	74/137 (54%)	64 (86%)	10 (14%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	G	152/152 (100%)	140 (92%)	12 (8%)	11	36
11	H	117/128 (91%)	113 (97%)	4 (3%)	32	55
12	I	113/116 (97%)	104 (92%)	9 (8%)	11	36
13	J	60/65 (92%)	56 (93%)	4 (7%)	15	41
14	K	99/102 (97%)	90 (91%)	9 (9%)	9	32
15	L	40/57 (70%)	37 (92%)	3 (8%)	12	38
All	All	3445/4009 (86%)	3138 (91%)	307 (9%)	9	32

5 of 307 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	D	126	ILE
12	I	84	VAL
7	D	170	THR
9	F	111	LEU
14	K	50	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	763	GLN
12	I	89	GLN
5	B	1084	GLN
12	I	60	GLN
8	E	147	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	3	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 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CPT	T	67	1	0,2,4	-	-	-		

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	67	CPT	1	0

5.7 Other polymers [i](#)

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	T	17/17 (100%)	0.88	1 (5%) 28 23	110, 139, 169, 175	0
2	N	7/7 (100%)	1.14	1 (14%) 6 9	148, 156, 169, 171	0
3	P	10/10 (100%)	0.80	1 (10%) 12 15	118, 128, 165, 172	0
4	A	1416/1733 (81%)	0.00	28 (1%) 65 44	44, 103, 161, 199	0
5	B	1108/1224 (90%)	0.21	45 (4%) 41 30	47, 116, 176, 199	0
6	C	266/318 (83%)	-0.05	1 (0%) 88 74	64, 100, 144, 162	0
7	D	177/221 (80%)	0.33	11 (6%) 26 22	70, 120, 177, 190	0
8	E	214/215 (99%)	0.25	2 (0%) 81 60	79, 144, 185, 197	0
9	F	84/155 (54%)	-0.28	1 (1%) 76 54	53, 81, 115, 132	0
10	G	171/171 (100%)	0.07	1 (0%) 85 68	82, 103, 141, 150	0
11	H	133/146 (91%)	0.64	10 (7%) 20 18	119, 149, 180, 188	0
12	I	119/122 (97%)	0.49	5 (4%) 40 29	94, 150, 183, 199	0
13	J	65/70 (92%)	0.01	1 (1%) 72 50	71, 96, 131, 140	0
14	K	114/120 (95%)	-0.22	1 (0%) 81 60	64, 101, 130, 149	0
15	L	46/70 (65%)	0.60	4 (8%) 16 16	96, 154, 172, 178	0
All	All	3947/4599 (85%)	0.13	113 (2%) 53 37	44, 111, 175, 199	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1176	LEU	7.7
4	A	1081	LEU	4.6
7	D	25	ALA	4.5
11	H	63	LEU	4.3
5	B	883	LEU	4.2

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
16	CPT	T	67	3/5	0.95	0.30	131,131,131,132	0
17	ZN	I	204	1/1	0.95	0.13	196,196,196,196	0
18	MG	A	1736	1/1	0.98	0.10	58,58,58,58	0
17	ZN	L	105	1/1	0.99	0.05	127,127,127,127	0
17	ZN	A	1734	1/1	0.99	0.05	108,108,108,108	0
17	ZN	I	203	1/1	1.00	0.07	113,113,113,113	0
17	ZN	A	1735	1/1	1.00	0.03	65,65,65,65	0
17	ZN	J	101	1/1	1.00	0.03	68,68,68,68	0
17	ZN	B	1307	1/1	1.00	0.04	71,71,71,71	0
17	ZN	C	319	1/1	1.00	0.06	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.