



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:11 PM UTC

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 : 9.0.010 (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

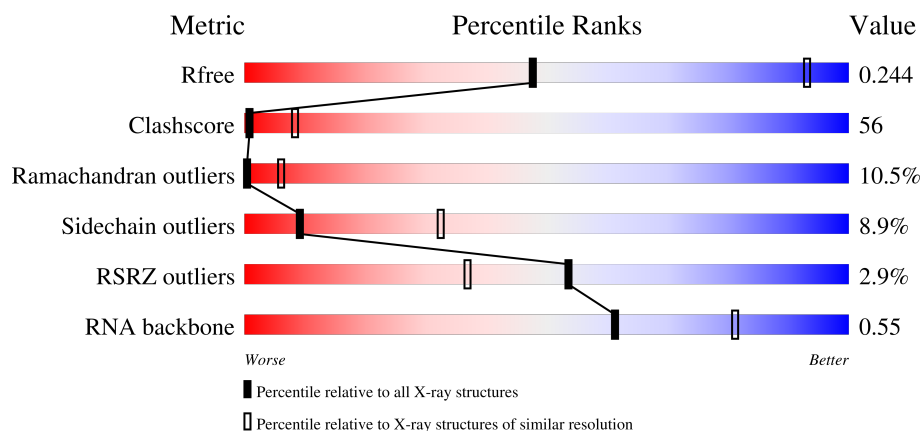
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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			

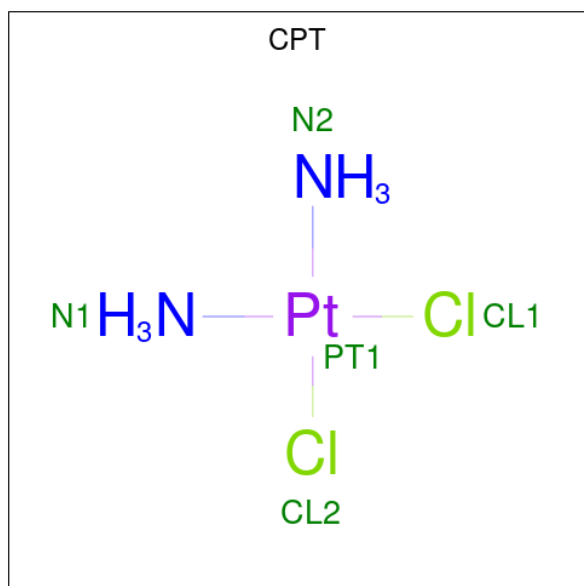
- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

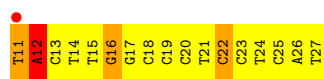
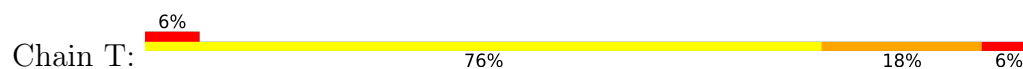
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

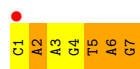
3 Residue-property plots

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',



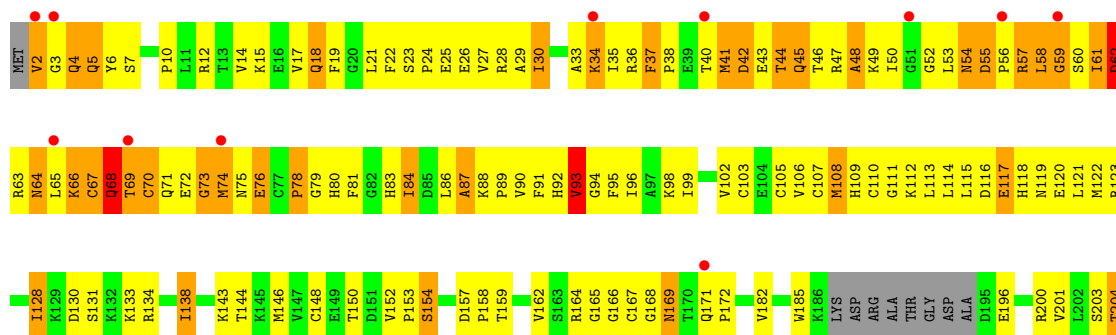
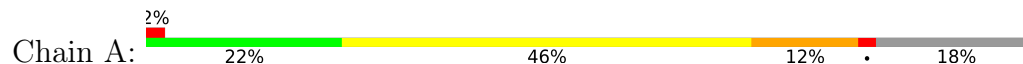
- Molecule 2: 5'-D(*CP*AP*AP*GP*TP*AP*G)-3'



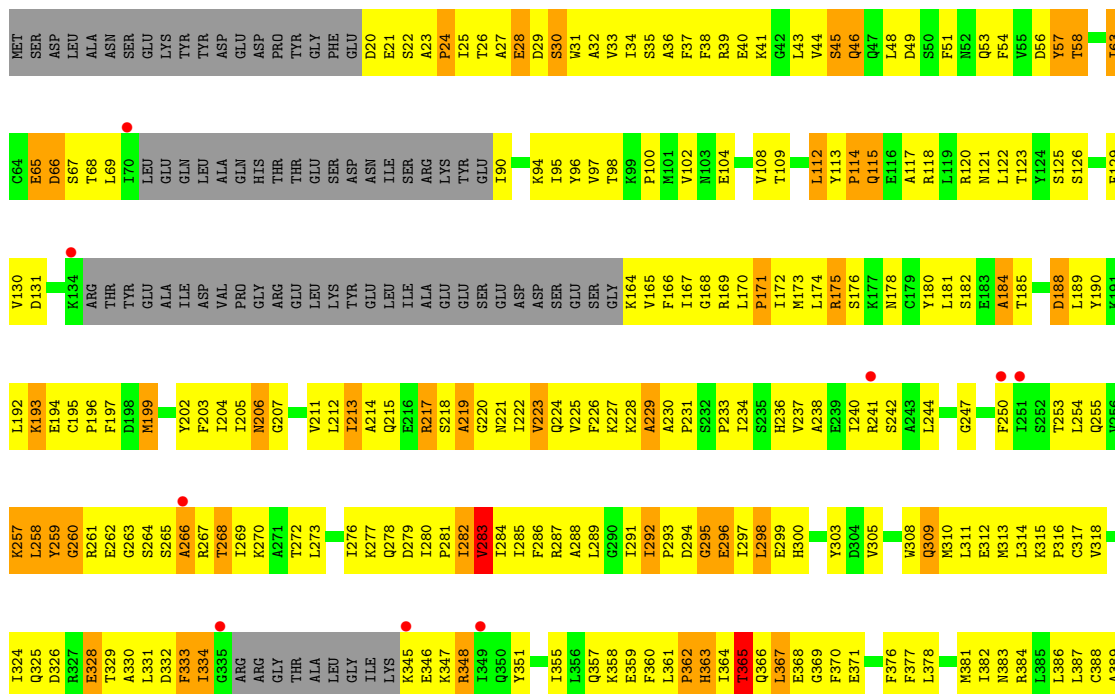
- Molecule 3: 5'-R(*UP*UP*UP*GP*AP*GP*GP*AP*GP*G)-3'

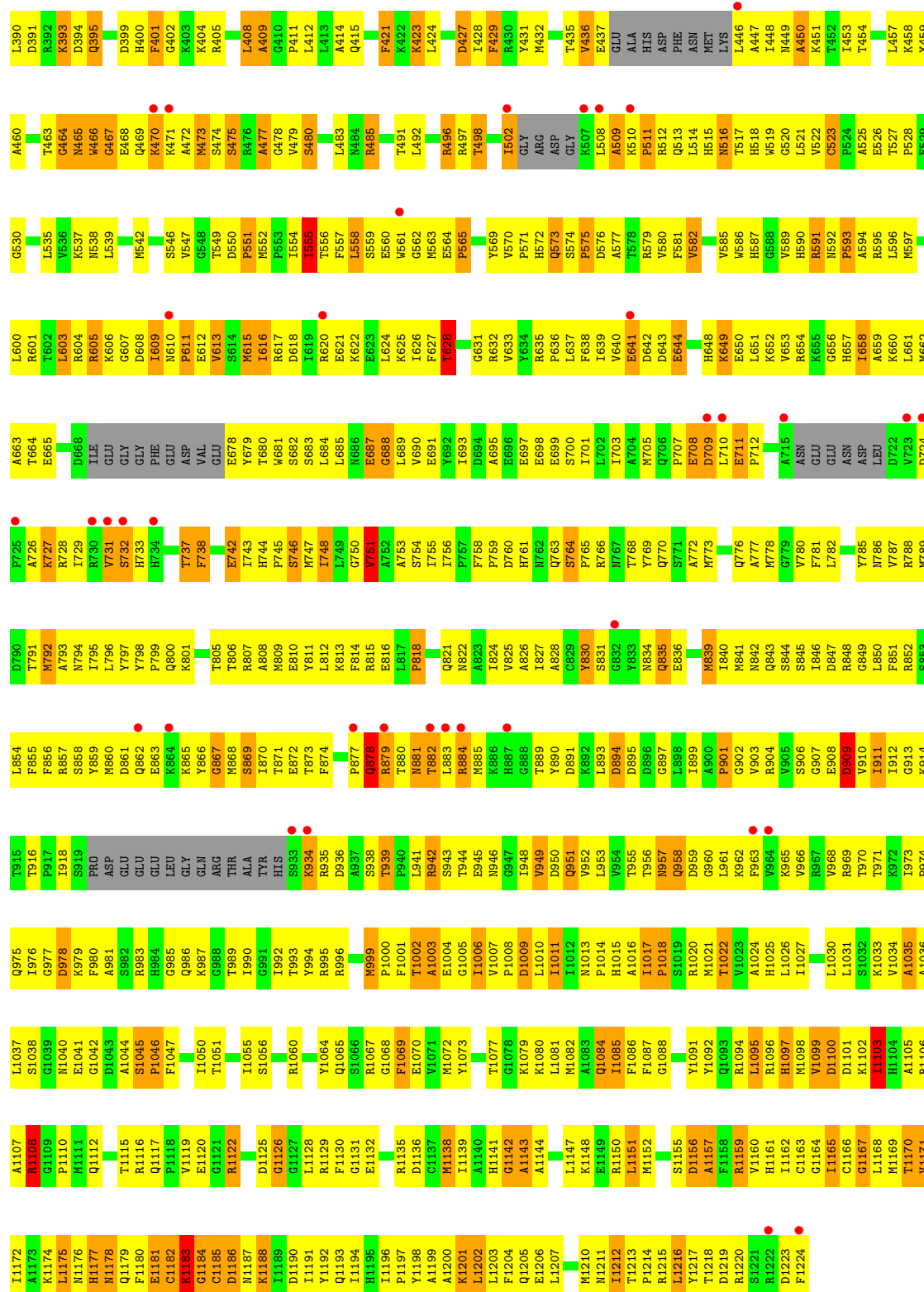


- Molecule 4: DNA-directed RNA polymerase II subunit RPB1



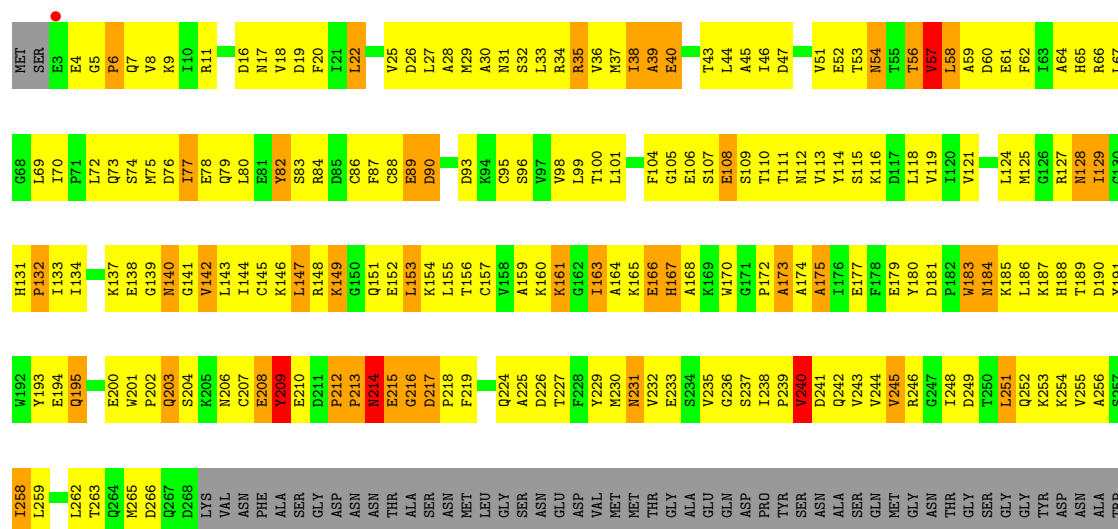
Q1130	A1069	G1002	K938	E870	G807	L737	L528	L463	G401	G334	D268	E205
A1131	Q1070	A1003	D939	D871	L808	K738	L531	P464	G401	R335	I269	E206
K1132	S1072	E1004	R940	M872	T809	D739	L531	Y465	Y404	R336	L270	I207
L1133	I1072	E1005	R941	M873	P810	L740	L534	S466	Y405	R337	L270	L208
I1134	G1073	I1006	F942	D874	Q811	N741	L534	T467	L406	G338	L276	M209
E1074	E1074	I1007	L943	A875	R812	N742	L535	F468	R407	N339	E277	I210
P1075	P1075	Q1008	R944	I876	F813	V743	L536	R469	D408	N340	T278	F211
A1009	A1009	Q1008	E945	I878	F814	K744	L537	L470	S409	K341	L279	
H1140	T1077	A1010	V946		F815	K745	L538	N471	G410	G342	E280	I214
Q1078	Q1078	Q1011	F947	S882	H816	Q746	L539	L472	D411	R343	I281	S215
I1079	I1079	R1012		L883	A817	V747	L540	S473	R412	R344	N282	
T1080	T1080	D1013	G950	T884	M818	N748	L541	V474	D413	V345	O283	D218
L1081	L1081	A1014		T885	R821	K749	L542	T475	D414	D346	O284	F219
ASN	THR	V1015	N953	I886		G750	L543	S476	F614	F347	P285	T220
THR	THR	L1016	N954	G887	I825	S751	L544	P477	L415	A348	H286	S221
PHE	PHE	L1017	P955	G888	A884	K752	L545	Y478	R416	G349	H287	L222
HIS	HIS	F1018	L956	S889	D826	G753	L546	Q545	Y417	R350	A288	G223
L956	L956	Q1019	P957	D890	A886	G754	L547	N479	S418	R351	F224	F224
PHE	PHE	L957	P958	A891	T927	S754	L548	A480	K419	T352	I289	N225
ALA	ALA	C1020	V958		K688		L549	N481	R420	V352	E290	E226
GLY	GLY	L1021	V959		K689	N757	L550	P482	D423	S353	E291	V227
VAL	VAL	L1022	R896	R896	R830	M761	L551	D485	Q425	G355	E292	F228
ALA	ALA	R1025	Y897	R898	T831	M762	L552	E486	Q426	D356	E293	S229
SER	SER		R899	R899	A832	G763		K487	L426	P357		R230
K1092	K1092	R1029	D900	D900	T833	A763	L556	N488	Q427	E297		P231
V1094	V1094	R1030	L901	L901	G835	V765	L557	L489	Y428	E360		E232
S1095	S1095	V1031	L902	L902	Y836	G766	L558	H490	Q429	L361		E233
S1096	S1096	L1032	N903	N903	I837	Q767	L559	V491	W430	A301		M234
G1097	G1097	Q1033	T904	T904	Q898	Q768	L560	P492	K431	T302		I235
L1161	L1161	E1034	D905	D905	A699	H631	L561	Q493	V432	G365		L236
P1099	P1099	V1035	H906	H906	N700	H631	L562	S494	W433	V366		T237
R1100	R1100	R1036	T907	T907	L701	V632	L563	E495	R434	P367		N304
L1101	L1101	L1037	L908	L908	L702	V633	L565	T497	L436	K368		D305
E1165	E1165	T1038	D909	D909	K843		L566	R498	W437	S369		N306
P1166	P1166	K1039	P910	P910	T709	G778	L567	A499	D438	D307		P240
E1167	E1167	Q1040	S911	S911	L710	F779	L568	E500	K372	I308		V241
L1105	L1105	A1041	L912	L912	R711	D781	L569		T373	A309		P242
N1106	N1106	F1042	L913	L913	E712	R782	L570		L374	G310		P243
V1107	V1107	D1043	S979	S979	S713	L783	L571	Q503	D440	K311		P244
		W1044	D980	D980	F714	L784	L572	L504	F441	P312		P245
N1110	N1110	V1045	T982	T982	E715	F785	L573		L443	Q313		V246
M1111	M1111	L1046	L983	L983	H851	H786	L574		F444	A314		R247
K1112	K1112	S1047	L984	L984	N717	F787	L575	V507	R445	L315		P248
T1113	T1113	N1048	D985	D985	N718	N718	L576		P382	Q316		S249
P1114	P1114	I1049	L986	L986	A719	K789	L577		Y383	K317		I250
S1115	S1115	E1050	V987	V987	R720		L578		N384	S318		S251
G1117	G1117	Q1052	G989	G989	L721		L579		D386	G319		P252
V1118	V1118		L925	L925	N723		L580		R387	R320		N253
Y1119	Y1119	V1058	Q926	Q926	E724		L581		L388	P321		E254
L1120	L1120	H1059	V927	V927	A725		L582		L391	V322		S255
E1121	E1121	P1060	L928	L928	R726		L583		V392	S324		Q256
G1123	G1123	G1061	N929	N929	K727		L584		S454	E259		E259
N995	N995	E1062	V963	V963	D728		L585		R393	I325		D260
M1063	M1063	L964	N865	N865	N729		L586		N394	R326		D261
V1064	V1064	I965	I864	I864	A729		L587		A457	A327		L262
A1125	A1125	Q933	N802	N802	G730		L588		P396	L328		T263
A1126	A1126	K934	S803	S803	R731		L589		N397	K330		F264
Q1187	Q1187	G1065	F868	F868	L732		L590		E398	G331		K265
G1188	G1188	V1066	I867	I867	L732		L591		S399	L266		L266
S1189	S1189	L1067	L805	L805	L732		L592		V460	K332		E333
P1190	P1190	Q1128	L1000	L1000	N736		L593		Y462	P400		
W1191	W1191	R1001	R806	R806			L594					



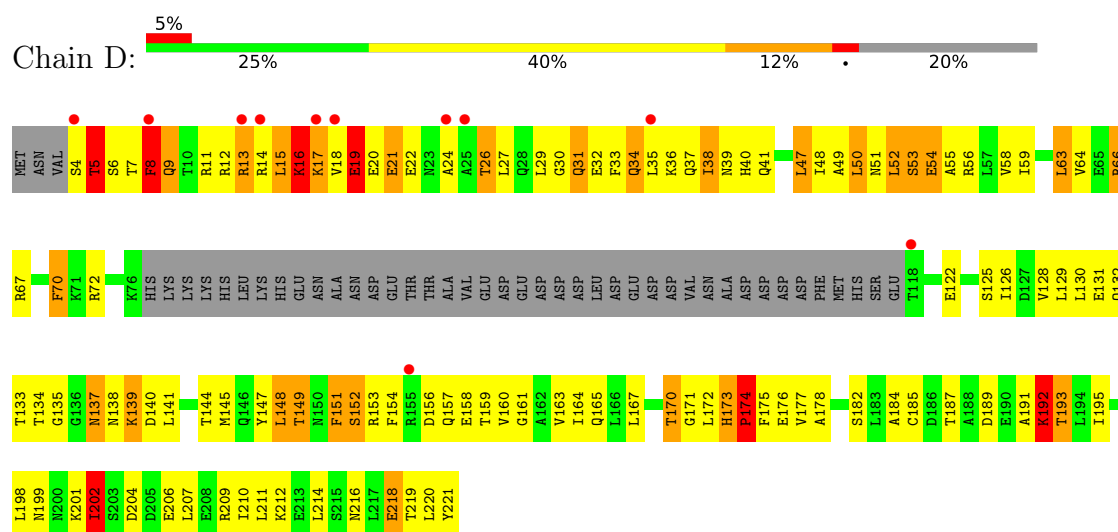


• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

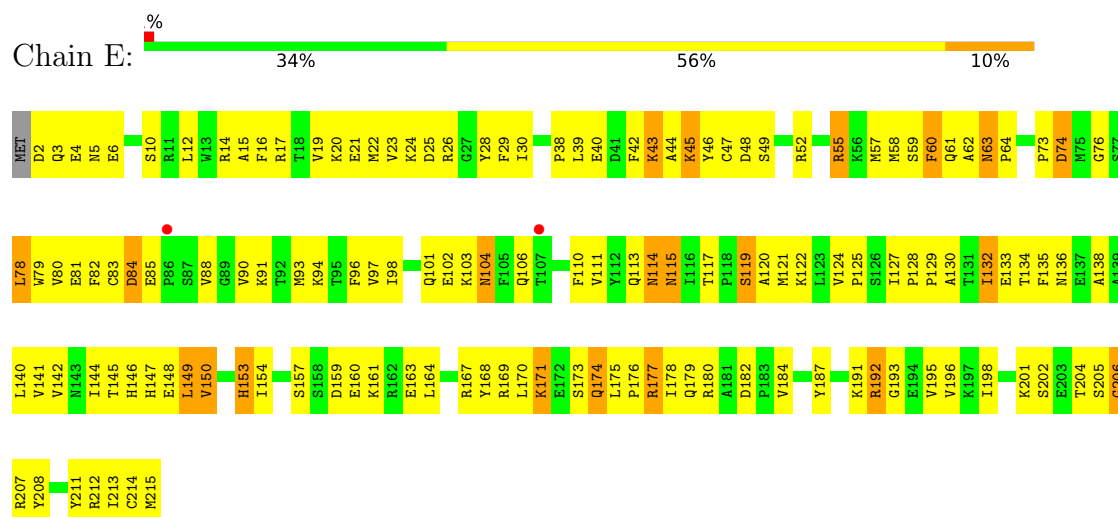
Chain C: 20% 49% 13% 16%



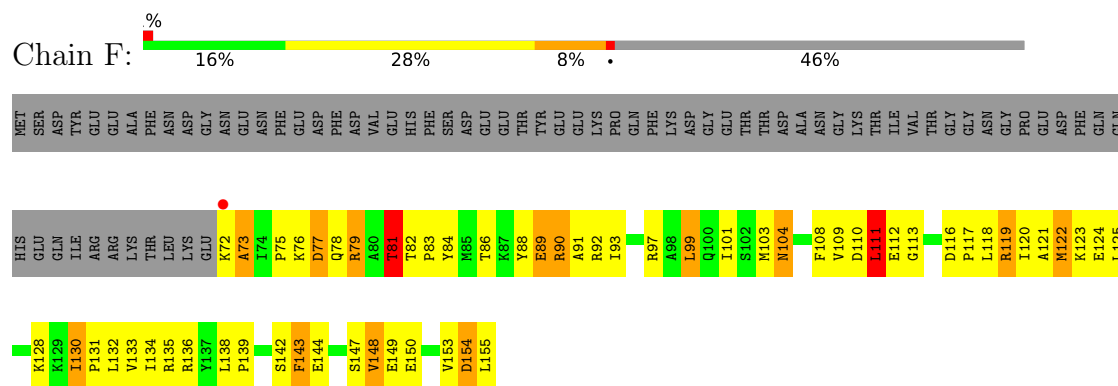
● Molecule 7: DNA-directed RNA polymerase II subunit RPB4



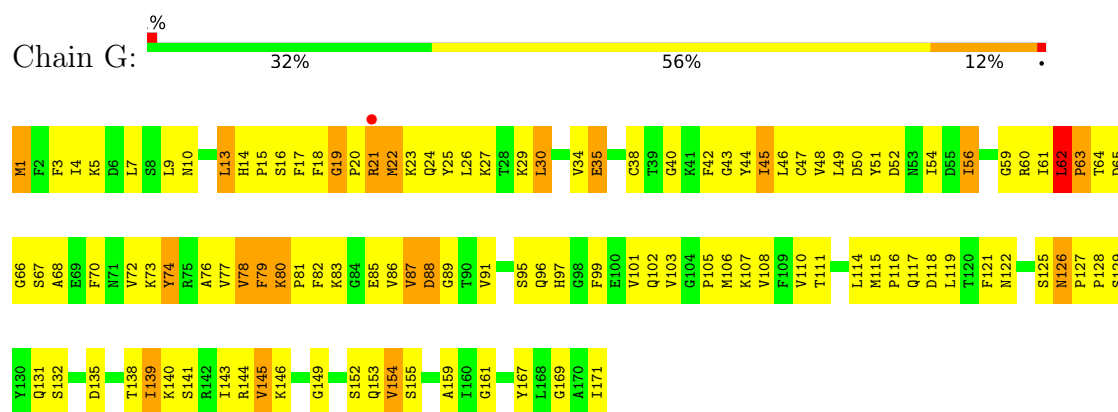
● Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1



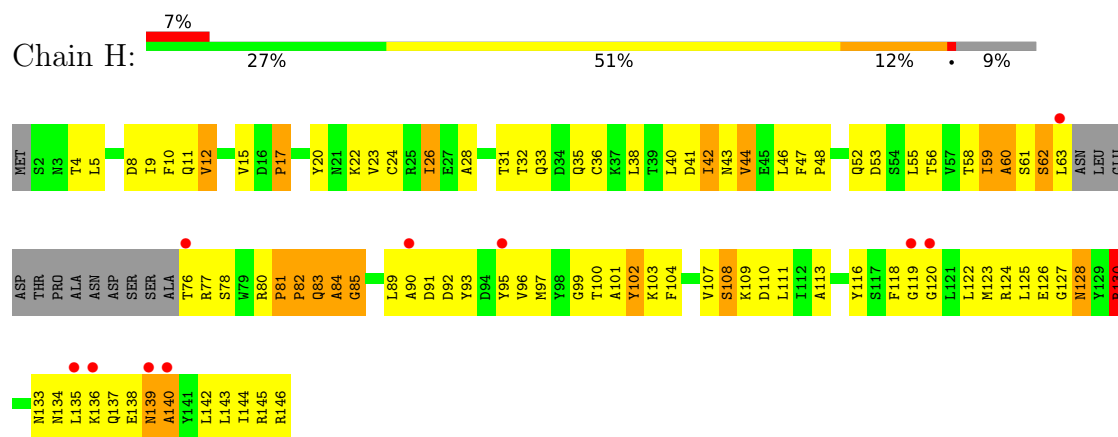
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2



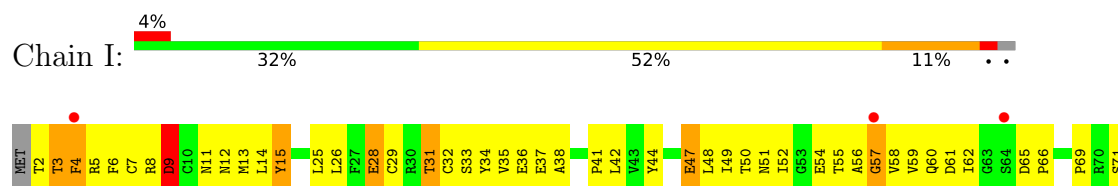
• Molecule 10: DNA-directed RNA polymerase II subunit RPB7

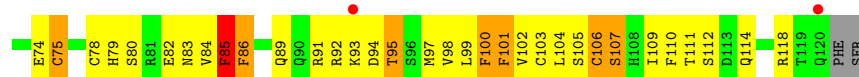


• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

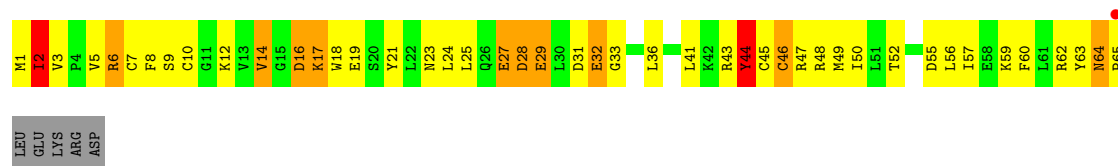


• Molecule 12: DNA-directed RNA polymerase II subunit RPB9

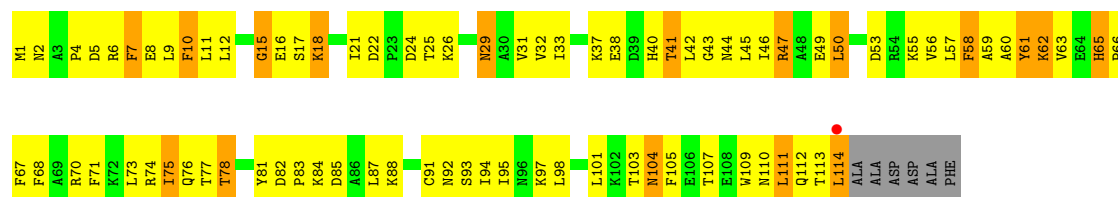




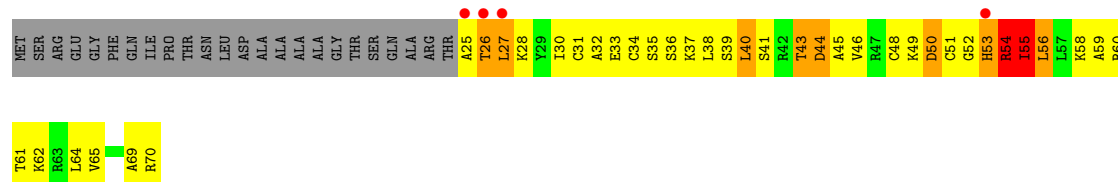
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- 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 0.225 , 0.244	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

5.1 Standard geometry

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	105	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	3578	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 3578 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.