



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:58 AM UTC

PDB ID : 2JA6 / pdb\_00002ja6  
Title : CPD lesion containing RNA Polymerase II elongation complex B  
Authors : Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.  
Deposited on : 2006-11-23  
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](mailto: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>.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

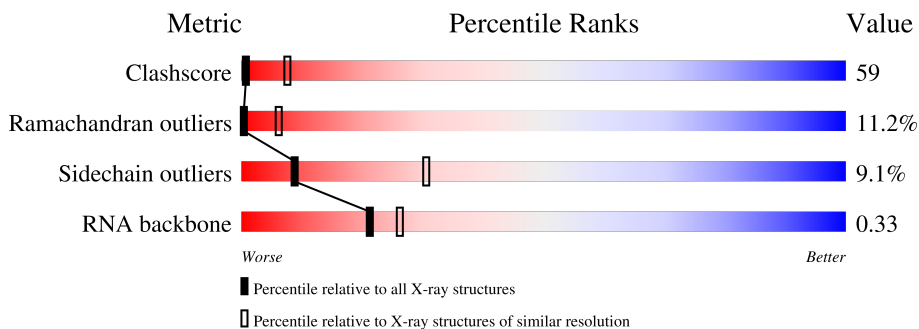
# 1 Overall quality at a glance

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))
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)


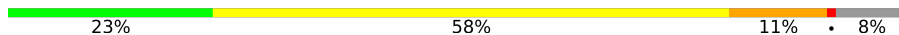

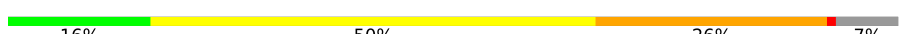
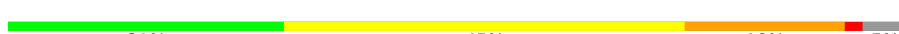

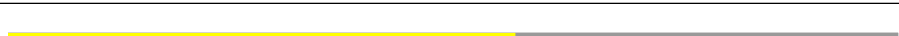
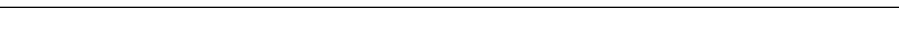
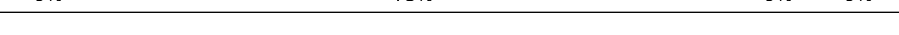
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1733	22% 44% 14% • 18%
2	B	1224	22% 54% 14% • 9%
3	C	318	22% 49% 11% • 16%
4	D	221	20% 42% 15% • 20%
5	E	215	36% 54% 9%
6	F	155	17% 30% 9% 44%

*Continued on next page...*

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Mol	Chain	Length	Quality of chain
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	11	
15	T	25	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	TT	T	17	-	-	X	-

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32010 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 LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1421	11186	7048	1958	2118	62	0	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1115	8866	5614	1553	1644	55	0	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE.

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE.

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

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23

## KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	87	705	451	119	132	3	0	0	0

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE.

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

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

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

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	N	8	165	79	29	49	8	0	0	0

- Molecule 14 is a RNA chain called 5'-R(\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
14	P	10	213	95	38	70	10	0	0	0

- Molecule 15 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*TTP\*TP\*CP\*CP\*BRUP\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	Br	C	N	O				P
15	T	19	403	1	196	62	125	19	0	0	0

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	8	Total Zn 8 8	0	0




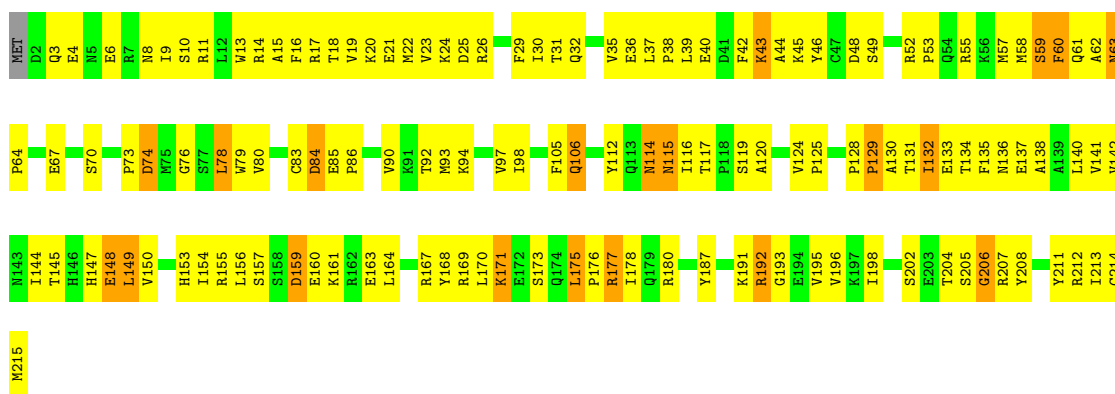


Chain B: 22% 54% 14% 9%

MET	D61	S125	T185	G247	M313	G379	N449	H515	V585	S645	F707	A772	R834	G897	D959
SER	I62	S126	E186	S248	L314	Y380	A450	M516	M586	L646	E708	A775	Q835	L898	G960
ASP	I63	G127	S187	R249	K315	M381	K451	T517	H588	K649	D709	Q776	E836	L899	L961
LEU	C64	L128	D188	F250	P316	I382	T454	H518	G588	E650	L710	Q777	D837	A900	K962
ALA	E85	F129	L189	I251	C317	N383	S455	G520	H590	E651	F711	M778	S838	P901	F963
ASN	D66	V130	Y190	L254	V318	R384	G456	L521	H591	K652	F712	Q779	M839	G902	V964
SER	S67	D131	K191	L254	L385	L386	G457	V522	R591	V653	A715	G779	I840	Y903	K965
GLU	I70	K133	L192	K257	V323	L387	K458	V522	M592	V654	A716	F780	M841	R904	V966
LYS	LEU	LYS	K193	L324	I324	L388	K459	E526	P593	M655	ASN	F781	R842	V905	
TYR	GLU	ARG	E194	C388	Q325	C388	A460	E527	A594	K656	GLU	L782	Q843	S906	R969
TRP	GLN	THR	C195	Y259	D326	A389	A461	T527	R595	G656	GLU	T783	S844	G907	T970
PRO	GLM	THR	P196	G260	R327	L390	L462	P528	M596	H657	ASN	N784	S845	E908	T971
ASP	LEU	THR	F197	R261	F328	D391	A463	E529	M597	L658	ASP	Y785	S846	K972	G972
GLU	ALA	GLU	D198	E262	T329	R392	T463	G530	E598	A659	LEU	N786	D847	V910	I973
ASP	ALA	ALA	M199	G263	A330	K393	G464	Q531	E599	R660	LEU	N787	R848	R911	Q974
PRO	GLN	ILE	K193	S264	L331	D394	N465	K537	L600	L661	ASN	F788	R849	V911	P914
THR	HIS	ASP	E194	S265	L332	H400	G467	M538	L601	M662	GLU	N789	C849	I912	Q975
GLY	THR	VAL	C195	A266	F333	F401	A472	M542	R606	A663	GLU	M790	R850	G913	I976
F18	THR	ASP	I204	R267	I334	G402	E468	L539	D608	T664	GLU	M791	F851	G914	I977
E19	GLU	PRO	I205	T268	G385	R398	Q469	S540	M609	E665	GLY	M792	R852	T915	D978
D20	LEU	GLY	N206	I269	R396	R399	K470	S541	M610	E666	GLY	M793	S853	T916	K979
E21	ASP	ARG	I212	I269	R337	H400	A471	L541	P611	D668	GLY	M794	S854	P917	F980
S22	ASN	ASN	I213	I270	R337	F401	K471	M542	E612	I668	PHE	N794	L854	R918	Q981
P24	ILE	LEU	A214	A214	G388	A472	S480	M543	V613	ILE	S732	L796	F855	I918	A981
I25	SER	LYS	Q215	Q215	G333	G402	Q481	S543	V614	ASP	S733	L797	F856	S919	S982
I26	ARG	TYR	E216	E216	I334	G402	M473	S544	M615	VAL	H740	H733	R857	PRO	R983
S26	LYS	GLU	R217	R217	A340	K403	S474	V547	M616	GLY	H734	Y798	S858	ASP	H984
A27	TYR	GLU	I212	I271	I343	K404	S475	V548	P617	GLY		P799	S859	GLU	G985
E28	GLU	ILE	I213	Q278	K344	R405	V479	G548	E617	PHE	T737	Q800	R860	GLU	Q986
D29	GLU	LEU	I213	Q278	K344	R405	S480	T549	E618	GLU	F738	R801	M861	GLU	K987
S30	ALA	ALA	A214	A214	K345	L408	Q481	D550	D618	ASP	F739	R802	R862	LEU	G988
W31	GLU	GLU	Q215	Q215	A409	A409	S480	P551	V618	ASP	H740	P802	R863	GLY	T989
A32	GLU	GLU	E216	E216	K347	G410	Q481	M552	M615	VAL	H740	H733	E863	GLY	I990
A33	SER	SER	R217	R217	R348	P411	L412	E553	M616	GLY	E742	P799	K864	GLN	I991
A36	ASP	ASP	G220	G220	R348	L412	L412	E554	R617	GLY	E743	Q806	K865	ARG	G991
F37	GLU	GLU	N221	N221	Y351	L413	A414	I555	R618	P679	L743	T806	R866	THR	I992
F38	GLU	GLU	I222	I222	A352	L413	A414	I556	D618	F679	H744	R807	C867	ALA	I993
R39	SER	SER	V223	V223	A352	L413	A414	F557	M619	W681	F745	R808	R868	TYR	Y994
E40	GLY	GLY	Q224	Q224	K353	T419	S493	S559	R620	S682	S746	M809	S869	HIS	R995
E41	ASP	ASP	V225	V225	D354	L355	L424	E560	K622	L684	L748	E810	S870	ASP	R996
K41	ASP	ASP	F226	F226	L356	L356	L424	E561	E623	L684	L749	E811	T871	GLU	E997
G42	ASP	ASP	K227	K227	Q357	Q357	Q357	E562	S624	M686	G750	R812	E872	R935	D998
L43	ASP	ASP	K228	K228	K358	K358	L492	E563	L624	E687	F751	R813	F874	D936	P1000
V44	ASP	ASP	A229	A229	E359	E359	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
S45	ASP	ASP	A230	A230	F360	F360	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
Q46	ASP	ASP	A230	A230	L361	L361	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
Q47	ASP	ASP	A230	A230	P362	P362	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
L48	ASP	ASP	A230	A230	H363	H363	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
D49	ASP	ASP	A230	A230	I364	I364	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
S50	ASP	ASP	A230	A230	I364	I364	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
F51	ASP	ASP	A230	A230	H300	H300	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
M52	ASP	ASP	A230	A230	H236	H236	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
Q53	ASP	ASP	A230	A230	Y303	Y303	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
F54	ASP	ASP	A230	A230	D304	D304	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
V55	ASP	ASP	A230	A230	V305	V305	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
D56	ASP	ASP	A230	A230	N306	N306	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
Y57	ASP	ASP	A230	A230	D307	D307	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
T58	ASP	ASP	A230	A230	R373	R373	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
L59	ASP	ASP	A230	A230	M310	M310	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
L22	ASP	ASP	A230	A230	L244	L244	S493	M563	L626	E688	A752	R815	F874	F1001	F1001
Y124	ASP	ASP	A230	A230	K246	K246	S493	M563	L626	E688	A752	R815	F874	F1001	F1001

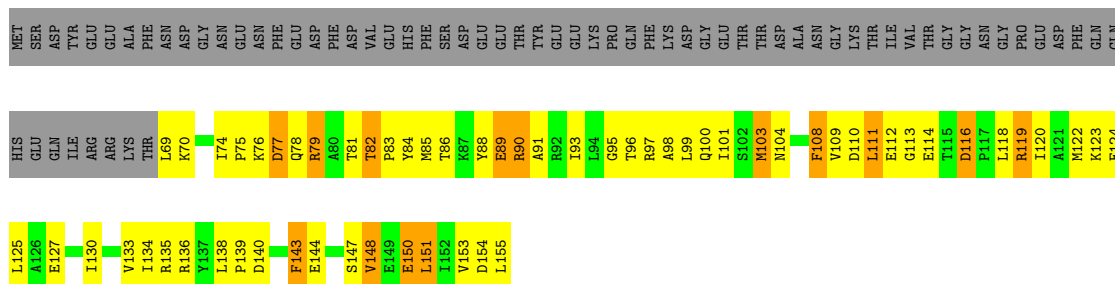


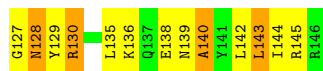
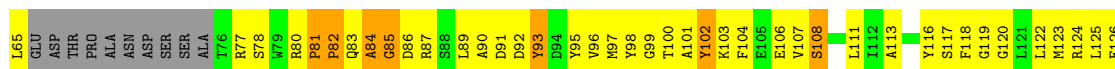
Chain E:  36% 54% 9%



- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE

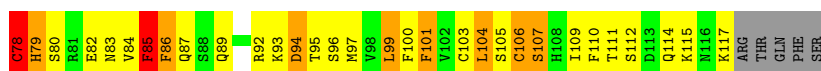
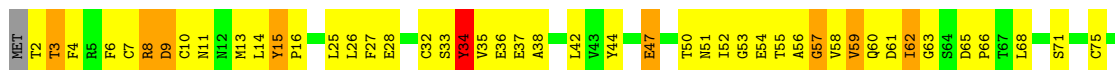
Chain F:  17% 30% 9% 44%





- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9

Chain I: 32% 48% 13% • 5%



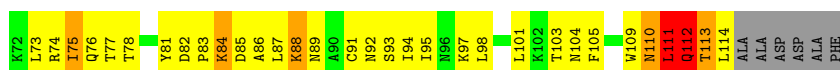
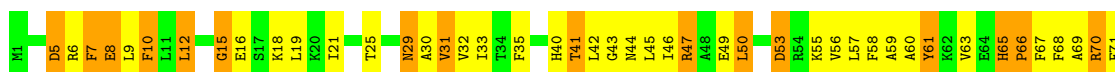
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10

Chain J: 16% 50% 26% • 7%



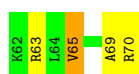
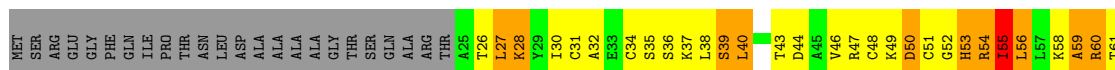
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

Chain K: 31% 45% 18% • 5%



- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE

Chain L: 17% 31% 16% • 34%

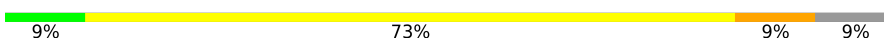


- Molecule 13: 5'-D(\*TP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*GP \*AP\*GP\*CP\*T)-3'

Chain N: 57% 43%

T0	A1	A2	G3	T4	A5	C6	T7	DT	DG	DA	DG	DC	DT
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- Molecule 14: 5'-R(\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*AP)-3'

Chain P: 

U0	U1	C2	G3	A4	C5	C6	A7	G8	G9	A
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- Molecule 15: 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP \*CP\*TP\*TP\*TTP\*TP\*CP\*CP \*BRUP\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'

Chain T: 

DA	DG	DC	DT	DC	DA	A10	G11	T12	A13	C14	T15	T16	M17	T19	C20	C21	U22	G23	G24	T25	C26	A27	T28	T29
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## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.58Å 393.49Å 283.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00	Depositor
% Data completeness (in resolution range)	99.3 (50.00-4.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.292 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	32010	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.60	0/11385	1.11	93/15393 (0.6%)
2	B	0.56	0/9037	1.05	53/12181 (0.4%)
3	C	0.58	0/2138	1.10	13/2896 (0.4%)
4	D	0.50	0/1437	1.09	15/1925 (0.8%)
5	E	0.50	0/1788	1.01	15/2406 (0.6%)
6	F	0.67	0/716	1.15	6/964 (0.6%)
7	G	0.59	0/1368	1.14	17/1844 (0.9%)
8	H	0.48	0/1102	1.00	7/1492 (0.5%)
9	I	0.46	0/962	1.03	5/1295 (0.4%)
10	J	0.61	0/541	0.99	1/727 (0.1%)
11	K	0.66	1/937 (0.1%)	1.20	11/1265 (0.9%)
12	L	0.56	0/366	0.92	0/485
13	N	0.61	0/184	0.91	0/280
14	P	0.45	0/237	0.92	0/367
15	T	0.63	0/382	1.21	5/582 (0.9%)
All	All	0.57	1/32580 (0.0%)	1.08	241/44102 (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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	113	THR	CA-C	5.60	1.59	1.53

The worst 5 of 241 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	113	THR	N-CA-C	15.33	128.47	108.24
1	A	56	PRO	N-CA-C	-12.29	101.90	114.68
4	D	26	THR	N-CA-C	-11.82	96.65	112.26
2	B	1185	CYS	N-CA-C	-10.78	100.13	113.18
2	B	473	MET	N-CA-C	-10.72	99.86	113.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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	A	11186	0	11266	1469	0
2	B	8866	0	8898	1140	0
3	C	2101	0	2055	288	0
4	D	1427	0	1451	161	0
5	E	1752	0	1776	155	0
6	F	705	0	730	82	0
7	G	1340	0	1357	172	0
8	H	1084	0	1057	139	0
9	I	944	0	901	110	0
10	J	532	0	542	107	0
11	K	919	0	929	122	0
12	L	364	0	386	49	0
13	N	165	0	92	14	0
14	P	213	0	109	22	0
15	T	403	0	229	56	0
16	A	1	0	0	0	0
17	A	8	0	0	0	0
All	All	32010	0	31778	3778	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 59.

The worst 5 of 3778 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)
8:H:100:THR:HG23	8:H:138:GLU:HA	1.33	1.11
2:B:343:ILE:HG23	2:B:347:LYS:HB2	1.13	1.11
1:A:34:LYS:HD3	1:A:57:ARG:HH22	1.07	1.10
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.32	1.09
15:T:16:DT:C5	15:T:17:TT:H5A1	1.88	1.09

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	A	1410/1733 (81%)	947 (67%)	306 (22%)	157 (11%)	0	6
2	B	1096/1224 (90%)	754 (69%)	222 (20%)	120 (11%)	0	7
3	C	264/318 (83%)	164 (62%)	62 (24%)	38 (14%)	0	3
4	D	173/221 (78%)	118 (68%)	38 (22%)	17 (10%)	0	9
5	E	212/215 (99%)	153 (72%)	42 (20%)	17 (8%)	1	12
6	F	84/155 (54%)	65 (77%)	13 (16%)	6 (7%)	1	14
7	G	169/171 (99%)	128 (76%)	30 (18%)	11 (6%)	1	15
8	H	131/146 (90%)	87 (66%)	26 (20%)	18 (14%)	0	3
9	I	114/122 (93%)	77 (68%)	26 (23%)	11 (10%)	0	9
10	J	63/70 (90%)	34 (54%)	12 (19%)	17 (27%)	0	0
11	K	112/120 (93%)	82 (73%)	20 (18%)	10 (9%)	0	10
12	L	44/70 (63%)	18 (41%)	13 (30%)	13 (30%)	0	0
All	All	3872/4565 (85%)	2627 (68%)	810 (21%)	435 (11%)	0	6

5 of 435 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	48	ALA
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU

### 5.3.2 Protein sidechains [i](#)

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	A	1244/1520 (82%)	1124 (90%)	120 (10%)	8	28
2	B	967/1061 (91%)	885 (92%)	82 (8%)	10	33
3	C	235/274 (86%)	216 (92%)	19 (8%)	11	34
4	D	159/200 (80%)	134 (84%)	25 (16%)	2	15
5	E	196/197 (100%)	189 (96%)	7 (4%)	31	53
6	F	77/137 (56%)	69 (90%)	8 (10%)	7	25
7	G	152/152 (100%)	139 (91%)	13 (9%)	10	33
8	H	119/128 (93%)	112 (94%)	7 (6%)	18	42
9	I	110/116 (95%)	99 (90%)	11 (10%)	7	26
10	J	60/65 (92%)	54 (90%)	6 (10%)	7	26
11	K	99/102 (97%)	87 (88%)	12 (12%)	5	21
12	L	40/57 (70%)	36 (90%)	4 (10%)	7	26
All	All	3458/4009 (86%)	3144 (91%)	314 (9%)	9	30

5 of 314 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	139	LYS
9	I	78	CYS
4	D	174	PRO
6	F	153	VAL
11	K	12	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	734	HIS
2	B	1176	ASN
10	J	53	HIS
2	B	763	GLN
2	B	975	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/11 (81%)	1 (11%)	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 [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
15	TT	T	17	15	40,43,44	5.03	10 (25%)	58,69,72	2.62	16 (27%)
15	BRU	T	22	15,14	18,21,22	0.81	1 (5%)	25,30,33	1.00	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	TT	T	17	15	-	10/18/105/106	0/5/6/6
15	BRU	T	22	15,14	-	2/7/21/22	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	17	TT	C5T-C6T	-21.42	1.31	1.55
15	T	17	TT	C5-C6	-20.81	1.32	1.55
15	T	17	TT	C6T-N1T	-4.83	1.39	1.46
15	T	17	TT	C1'-N1	3.95	1.50	1.45
15	T	17	TT	C6-N1	-3.85	1.40	1.46

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	17	TT	C2R-C1R-N1T	8.38	126.91	115.59
15	T	17	TT	C5T-C5-C6	7.72	97.39	88.36
15	T	17	TT	C5-C6-C6T	-6.66	79.03	89.26
15	T	17	TT	C5-C6-N1	6.29	123.99	115.65
15	T	17	TT	N3T-C2T-N1T	-4.65	111.92	116.78

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	17	TT	C3R-C4R-C5R-O5R
15	T	17	TT	O3'-C7-O5R-C5R
15	T	17	TT	C2'-C1'-N1-C6
15	T	17	TT	C2'-C1'-N1-C2
15	T	17	TT	O4'-C1'-N1-C6

There are no ring outliers.

2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	17	TT	23	0
15	T	22	BRU	4	0

## 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
2	B	2
3	C	1
1	A	1
6	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	18:PHE	C	19:GLU	N	3.98
1	C	2:SER	C	3:GLU	N	3.88
1	A	1175:SER	C	1176:LEU	N	3.69
1	F	69:LEU	C	70:LYS	N	3.59
1	B	337:ARG	C	338:GLY	N	2.64

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.