



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:35 AM GMT

PDB ID : 2R7Z
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

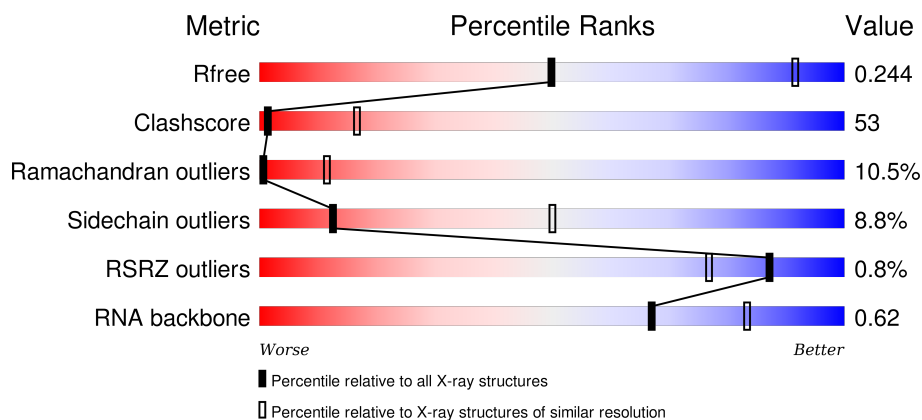
1 Overall quality at a glance

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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
2	N	7	
3	P	10	
4	A	1733	

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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			

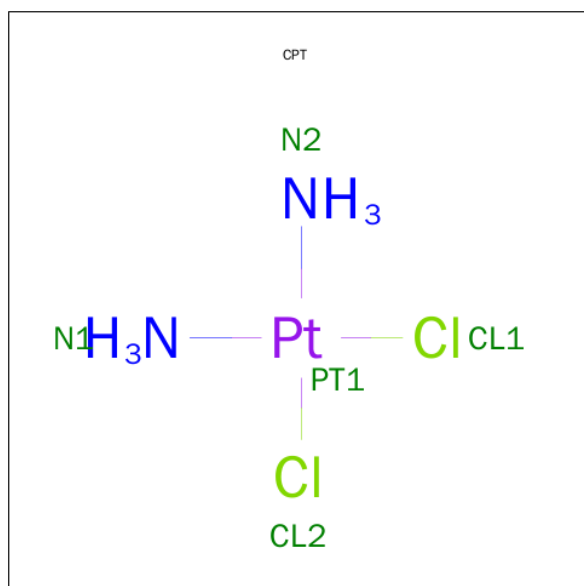
- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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 (three-letter code: 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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total	Zn	0	0
			1	1		

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

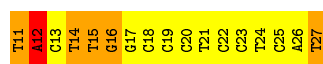
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total 1	Mg 1	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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',

Chain T: 



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

Chain N: 



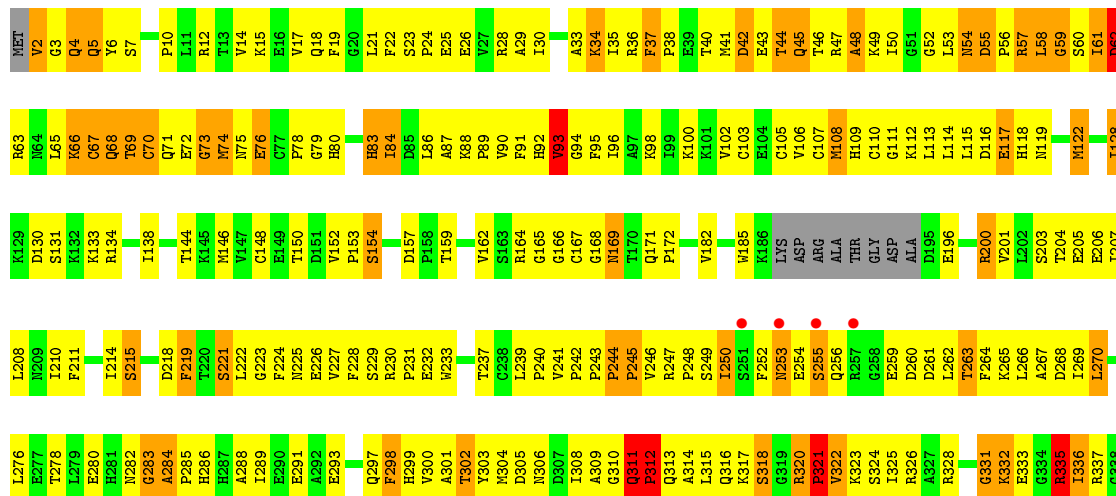
- Molecule 3: 5'-R(*UP*UP*UP*GP*AP*GP*GP*AP*GP*G)-3'

Chain P: 

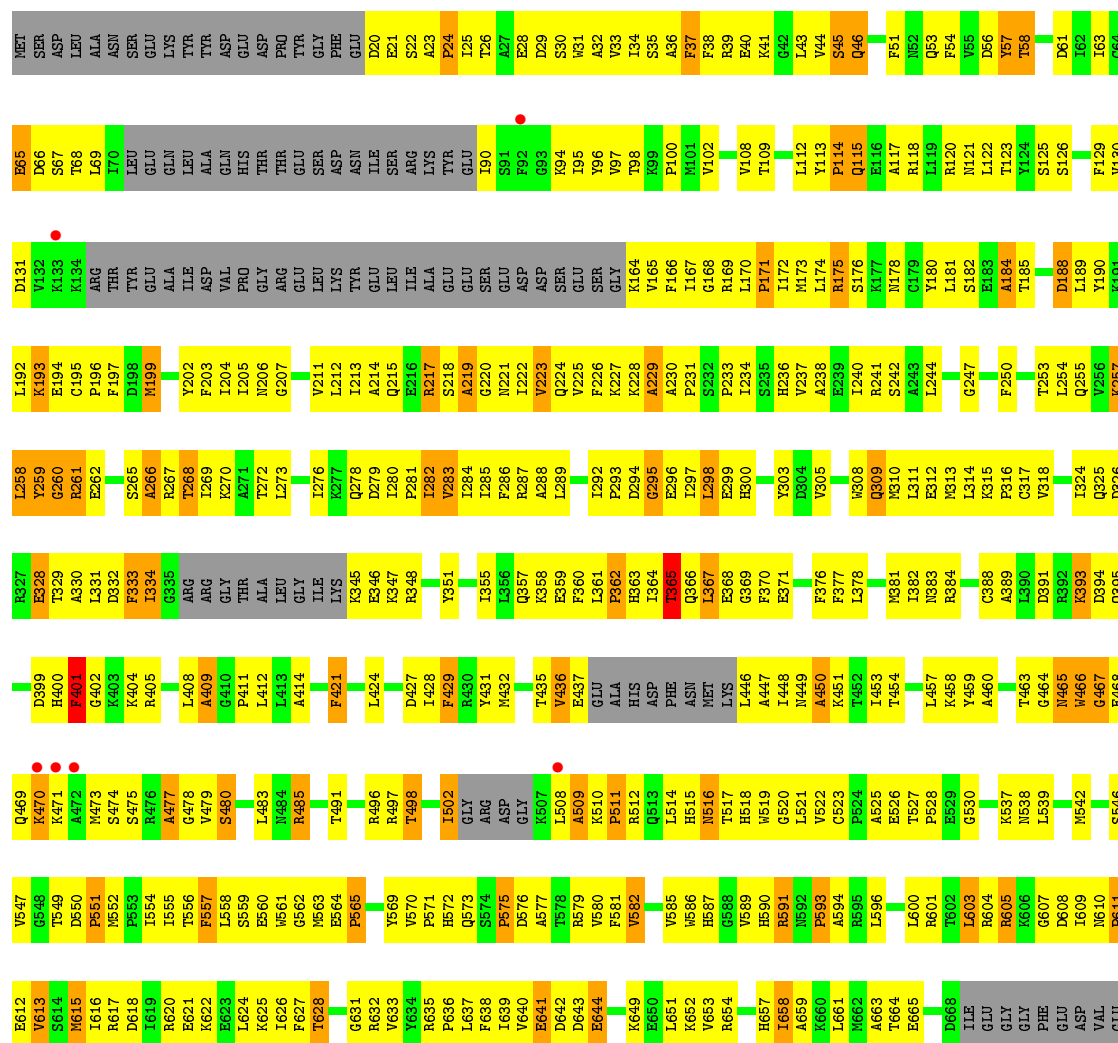


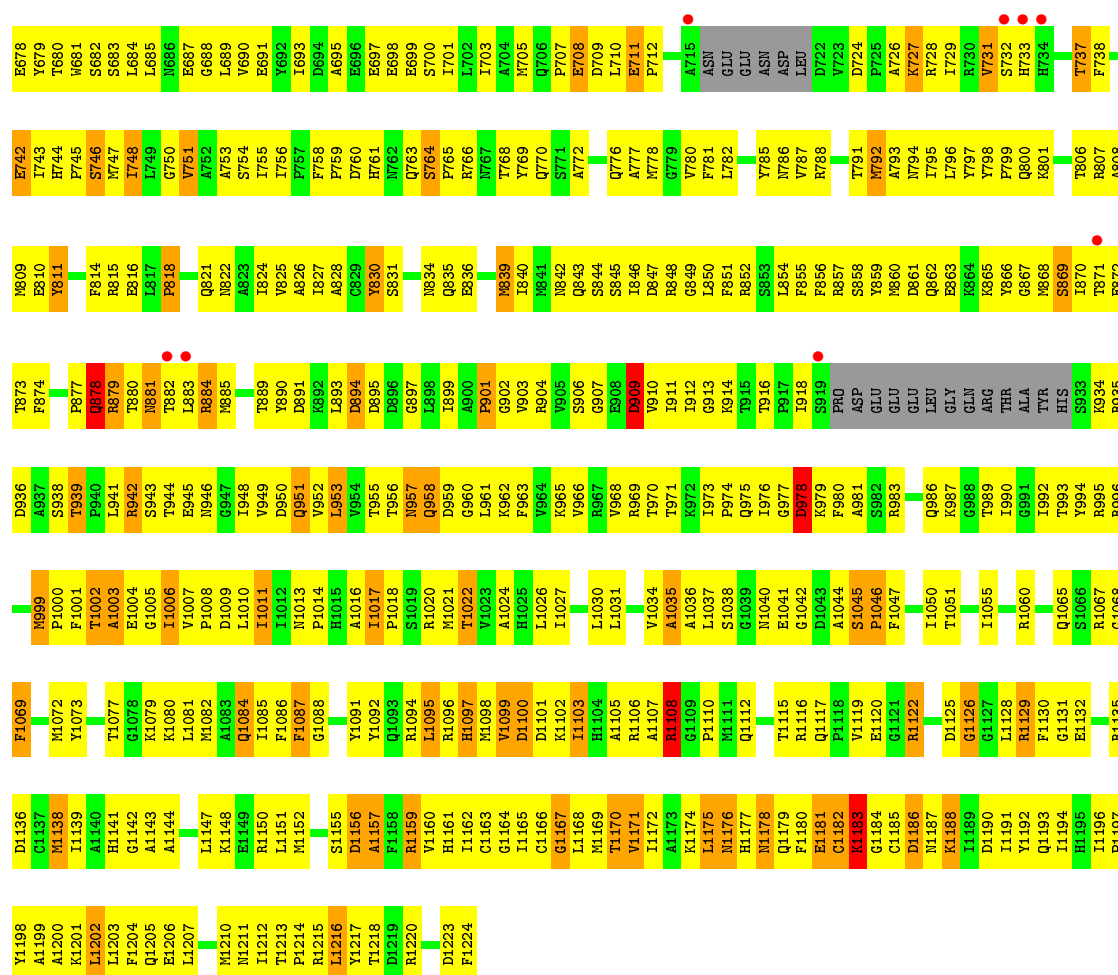
- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain A: 












- Chain H:
-
- 2% 27% 52% 12% 9%
- MET
- ASP THR PRO ALA ASN ASP SER SER ALA T76 R77 S78 P81 P82 Q83 Q85 Q86 L89 A90 D91 D92 Y93 D94 Y95 Y96 Y97 Y98 G99 T100 A101 Y102 K103 F104 V107 S108 K109 D110 L111 I112 A113 Y116 S117 F118 G119 G120 L121 L122 M123 R124 L125 E126 G127 M128 Y129 P130
- N133 N134 K135 K136 Q137 E138 N139 A140 Y141 L142 L143 I144 R145 R146

- Chain I:
-
- | Amino Acid | Percentage |
|------------|------------|
| MET | 2% |
| T2 | 34% |
| T3 | 52% |
| F4 | 11% |
| P66 | .. |
| P69 | .. |
| S71 | .. |
| S74 | .. |

- Chain J: 
- | Residue | Category | Percentage |
|---------|----------|------------|
| M1 | Yellow | 29% |
| I2 | Yellow | 29% |
| V3 | Yellow | 29% |
| P4 | Green | 29% |
| V5 | Orange | 29% |
| C7 | Yellow | 29% |
| F8 | Yellow | 29% |
| S9 | Yellow | 29% |
| C10 | Yellow | 29% |
| G11 | Green | 29% |
| K12 | Yellow | 29% |
| V13 | Green | 29% |
| V14 | Yellow | 29% |
| G15 | Yellow | 29% |
| D16 | Orange | 29% |
| K17 | Orange | 29% |
| W18 | Orange | 29% |
| E19 | Orange | 29% |
| S20 | Orange | 29% |
| Y21 | Yellow | 29% |
| L22 | Yellow | 29% |
| N23 | Yellow | 29% |
| L24 | Yellow | 29% |
| L25 | Yellow | 29% |
| Q26 | Green | 29% |
| E27 | Orange | 29% |
| D28 | Orange | 29% |
| E29 | Orange | 29% |
| L30 | Yellow | 29% |
| D31 | Yellow | 29% |
| E32 | Yellow | 29% |
| G33 | Yellow | 29% |
| L36 | Yellow | 47% |
| L41 | Yellow | 47% |
| K42 | Green | 47% |
| R43 | Green | 47% |
| Y44 | Red | 47% |
| C45 | Orange | 47% |
| C46 | Orange | 47% |
| R47 | Orange | 47% |
| R48 | Orange | 47% |
| M49 | Yellow | 47% |
| I50 | Yellow | 47% |
| L51 | Green | 47% |
| T52 | Yellow | 47% |
| D55 | Yellow | 16% |
| L56 | Yellow | 16% |
| I57 | Yellow | 16% |
| E58 | Green | 16% |
| K59 | Orange | 16% |
| F60 | Yellow | 16% |
| L61 | Green | 16% |
| R62 | Yellow | 16% |
| Y63 | Orange | 16% |
| D64 | Orange | 16% |
| D65 | Grey | 7% |
- LEU
GLU
LYS
ARG
ASP

- Chain K: 

Chain K	Category 1 (28%)	Category 2 (57%)	Category 3 (11%)	Category 4 (5%)
M1				
M2				
A3				
P4				
D5				
R6				
F7				
E8				
L9				
F10				
L11				
L12				
G15				
E16				
S17				
K18				
T21				
D24				
T25				
K26				
M29				
A30				
V31				
V32				
I33				
K37				
E38				
T41				
L42				
G43				
N44				
L45				
L46				
R47				
A48				
E49				
L50				
D53				
A54				
K55				
V56				
L57				
F58				
A59				
A60				
Y61				
K62				
V63				
E64				
H65				
P66				
F67				
F68				
A69				
R70				
F71				
K72				
L73				
N74				
L75				
Q76				
T77				
T78				
Y81				
D82				
K83				
K84				
D85				
A86				
L87				
K88				
G91				
N92				
S93				
I94				
I95				
N96				
K97				
L98				
L101				
K102				
T103				
N104				
F105				
E106				
T107				
E108				
N109				
N110				
Q112				
T113				
L114				
ALA				
ALA				
ASP				
ASP				
ALA				
PHE				

- Chain L: 
- | Amino Acid | Percentage |
|------------|------------|
| Met | 11% |
| Ser | 11% |
| Arg | 11% |
| Glu | 11% |
| Phe | 11% |
| Gln | 11% |
| Ile | 11% |
| Pro | 11% |
| Thr | 11% |
| Asn | 11% |
| Leu | 11% |
| Asp | 11% |
| Ala | 11% |
| Ala | 11% |
| Ala | 11% |
| Ala | 11% |
| Gly | 11% |
| Thr | 11% |
| Gln | 11% |
| Arg | 11% |
| Thr | 11% |
| A25 | 11% |
| T26 | 11% |
| L27 | 11% |
| K28 | 11% |
| Y29 | 11% |
| I30 | 11% |
| C31 | 11% |
| A32 | 11% |
| E33 | 11% |
| C34 | 11% |
| S35 | 11% |
| S36 | 11% |
| K37 | 11% |
| L38 | 11% |
| S39 | 11% |
| L40 | 11% |
| K41 | 11% |
| K42 | 11% |
| T43 | 11% |
| D44 | 11% |
| A45 | 11% |
| V46 | 11% |
| R47 | 11% |
| C48 | 11% |
| K49 | 11% |
| D50 | 11% |
| C51 | 11% |
| G52 | 11% |
| H53 | 11% |
| R54 | 11% |
| L55 | 11% |
| L56 | 11% |
| L57 | 11% |
| K58 | 11% |
| A59 | 11% |
| P60 | 11% |



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 49.14 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 99.8 (49.14-3.80)	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%)	DCC
Wilson B-factor (Å ²)	106.6	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 58.8	EDS
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
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 121417 reflections	Xtriage
F_o, F_c correlation	0.91	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, 0.375 respectively for untwinned datasets, and 0.333, 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, CPT, 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	T	1.41	5/373 (1.3%)	1.79	11/572 (1.9%)
2	N	1.38	0/161	1.10	0/247
3	P	0.95	0/242	0.98	0/377
4	A	0.43	0/11339	0.72	4/15334 (0.0%)
5	B	0.42	0/8981	0.68	0/12108
6	C	0.44	0/2133	0.72	0/2891
7	D	0.42	0/1437	0.69	1/1925 (0.1%)
8	E	0.41	0/1788	0.65	0/2406
9	F	0.49	0/691	0.77	0/933
10	G	0.45	0/1368	0.72	0/1844
11	H	0.38	0/1086	0.65	0/1470
12	I	0.36	0/989	0.65	0/1331
13	J	0.47	0/541	0.74	0/727
14	K	0.45	0/937	0.68	0/1265
15	L	0.47	0/366	0.71	0/485
All	All	0.46	5/32432 (0.0%)	0.73	16/43915 (0.0%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	16	DG	N3-C4	8.85	1.41	1.35
1	T	17	DG	N3-C4	7.68	1.40	1.35
1	T	17	DG	C2-N3	6.93	1.38	1.32
1	T	16	DG	N1-C2	5.71	1.42	1.37
1	T	14	DT	O3'-P	5.20	1.67	1.61

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	17	DG	O4'-C1'-N9	11.85	116.29	108.00
1	T	16	DG	O4'-C1'-N9	9.50	114.65	108.00
1	T	17	DG	N3-C2-N2	7.61	125.22	119.90
4	A	567	LYS	C-N-CD	6.05	141.11	128.40
1	T	16	DG	N1-C2-N3	-5.93	120.34	123.90

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	1294	0
5	B	8810	0	8847	1025	0
6	C	2095	0	2052	253	0
7	D	1427	0	1451	136	0
8	E	1752	0	1776	149	0
9	F	679	0	701	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	G	1340	0	1357	152	0
11	H	1068	0	1040	131	0
12	I	971	0	930	102	0
13	J	532	0	543	106	0
14	K	919	0	929	115	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	3347	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 3347 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%)	1	13
5	B	1090/1224 (89%)	754 (69%)	217 (20%)	119 (11%)	0	11
6	C	264/318 (83%)	181 (69%)	50 (19%)	33 (12%)	0	8
7	D	173/221 (78%)	125 (72%)	28 (16%)	20 (12%)	0	9
8	E	212/215 (99%)	157 (74%)	38 (18%)	17 (8%)	1	19
9	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	2	27
10	G	169/171 (99%)	131 (78%)	30 (18%)	8 (5%)	3	33
11	H	129/146 (88%)	90 (70%)	19 (15%)	20 (16%)	0	5
12	I	117/122 (96%)	84 (72%)	23 (20%)	10 (8%)	1	17
13	J	63/70 (90%)	36 (57%)	15 (24%)	12 (19%)	0	3
14	K	112/120 (93%)	86 (77%)	20 (18%)	6 (5%)	2	30
15	L	44/70 (63%)	17 (39%)	14 (32%)	13 (30%)	0	0
All	All	3861/4565 (85%)	2711 (70%)	746 (19%)	404 (10%)	1	11

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%)	1124 (91%)	115 (9%)	11	47
5	B	962/1061 (91%)	887 (92%)	75 (8%)	16	55
6	C	234/274 (85%)	211 (90%)	23 (10%)	10	44
7	D	159/200 (80%)	129 (81%)	30 (19%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	E	196/197 (100%)	190 (97%)	6 (3%)	47 80
9	F	74/137 (54%)	65 (88%)	9 (12%)	6 34
10	G	152/152 (100%)	139 (91%)	13 (9%)	13 51
11	H	117/128 (91%)	112 (96%)	5 (4%)	35 74
12	I	113/116 (97%)	104 (92%)	9 (8%)	15 54
13	J	60/65 (92%)	56 (93%)	4 (7%)	20 62
14	K	99/102 (97%)	89 (90%)	10 (10%)	9 43
15	L	40/57 (70%)	36 (90%)	4 (10%)	9 43
All	All	3445/4009 (86%)	3142 (91%)	303 (9%)	12 50

5 of 303 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	463	THR
5	B	978	ASP
12	I	75	CYS
5	B	498	THR
5	B	737	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	734	HIS
5	B	1179	GLN
12	I	60	GLN
5	B	763	GLN
5	B	1015	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 carbohydrates 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	0.00	-	0,1,6	0.00	-

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
16	CPT	T	67	1	-	0/0/0/0	0/0/0/0

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 [i](#)

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%)	-0.39	0 100 100	110, 139, 169, 175	0
2	N	7/7 (100%)	0.40	0 100 100	148, 156, 169, 171	0
3	P	10/10 (100%)	-0.21	0 100 100	118, 128, 165, 172	0
4	A	1416/1733 (81%)	-0.29	8 (0%) 90 82	44, 103, 161, 199	0
5	B	1108/1224 (90%)	-0.23	14 (1%) 79 65	47, 116, 176, 199	0
6	C	266/318 (83%)	-0.37	0 100 100	64, 100, 144, 162	0
7	D	177/221 (80%)	-0.17	2 (1%) 82 69	70, 120, 177, 190	0
8	E	214/215 (99%)	-0.21	2 (0%) 85 74	79, 144, 185, 197	0
9	F	84/155 (54%)	-0.51	0 100 100	53, 81, 115, 132	0
10	G	171/171 (100%)	-0.28	0 100 100	82, 103, 141, 150	0
11	H	133/146 (91%)	0.18	3 (2%) 64 48	119, 149, 180, 188	0
12	I	119/122 (97%)	-0.08	2 (1%) 73 58	94, 150, 183, 199	0
13	J	65/70 (92%)	-0.57	0 100 100	71, 96, 131, 140	0
14	K	114/120 (95%)	-0.37	0 100 100	64, 101, 130, 149	0
15	L	46/70 (65%)	-0.09	0 100 100	96, 154, 172, 178	0
All	All	3947/4599 (85%)	-0.26	31 (0%) 87 77	44, 111, 175, 199	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1176	LEU	10.4
4	A	1175	SER	5.1
5	B	471	LYS	4.8
4	A	1455	PRO	3.7
5	B	470	LYS	3.6

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
17	ZN	B	1307	1/1	0.99	0.19	-0.08	71,71,71,71	0
17	ZN	J	101	1/1	0.99	0.22	-0.22	68,68,68,68	0
17	ZN	I	203	1/1	0.99	0.14	-0.24	113,113,113,113	0
17	ZN	C	319	1/1	0.99	0.14	-0.28	60,60,60,60	0
17	ZN	L	105	1/1	0.99	0.10	-1.15	127,127,127,127	0
17	ZN	I	204	1/1	0.99	0.07	-1.32	196,196,196,196	0
17	ZN	A	1735	1/1	1.00	0.12	-1.37	65,65,65,65	0
17	ZN	A	1734	1/1	0.98	0.09	-2.80	108,108,108,108	0
18	MG	A	1736	1/1	0.97	0.21	-	58,58,58,58	0
16	CPT	T	67	3/5	0.96	0.23	-	131,131,131,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.