



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 01:35 pm BST

PDB ID : 2JA6
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

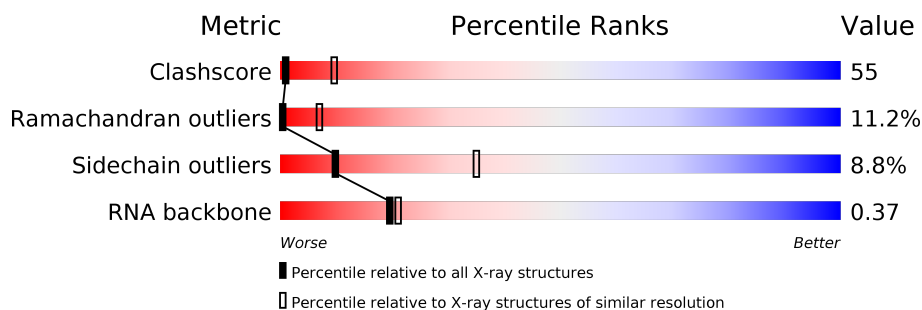
1 Overall quality at a glance

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	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RNA backbone	3102	1048 (5.00-3.00)

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 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	25% 45% 11% • 18%
2	B	1224	26% 54% 11% • 9%
3	C	318	25% 48% 10% • 16%
4	D	221	27% 40% 12% • 20%
5	E	215	40% 55% 5%
6	F	155	18% 34% • 44%
7	G	171	34% 57% 9% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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
1	A	1421	Total	C	N	O	S	0	0	0
			11186	7048	1958	2118	62			

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

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

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

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

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

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

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

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

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

KDA POLYPEPTIDE.

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

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

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

- 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
8	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

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

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

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

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

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

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

- 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
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- 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
13	N	8	Total	C	N	O	P	0	0	0
			165	79	29	49	8			

- 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
14	P	10	Total	C	N	O	P	0	0	0
			213	95	38	70	10			

- 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
15	T	19	Total	Br	C	N	O	P	0	0
			403	1	196	62	125	19		

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

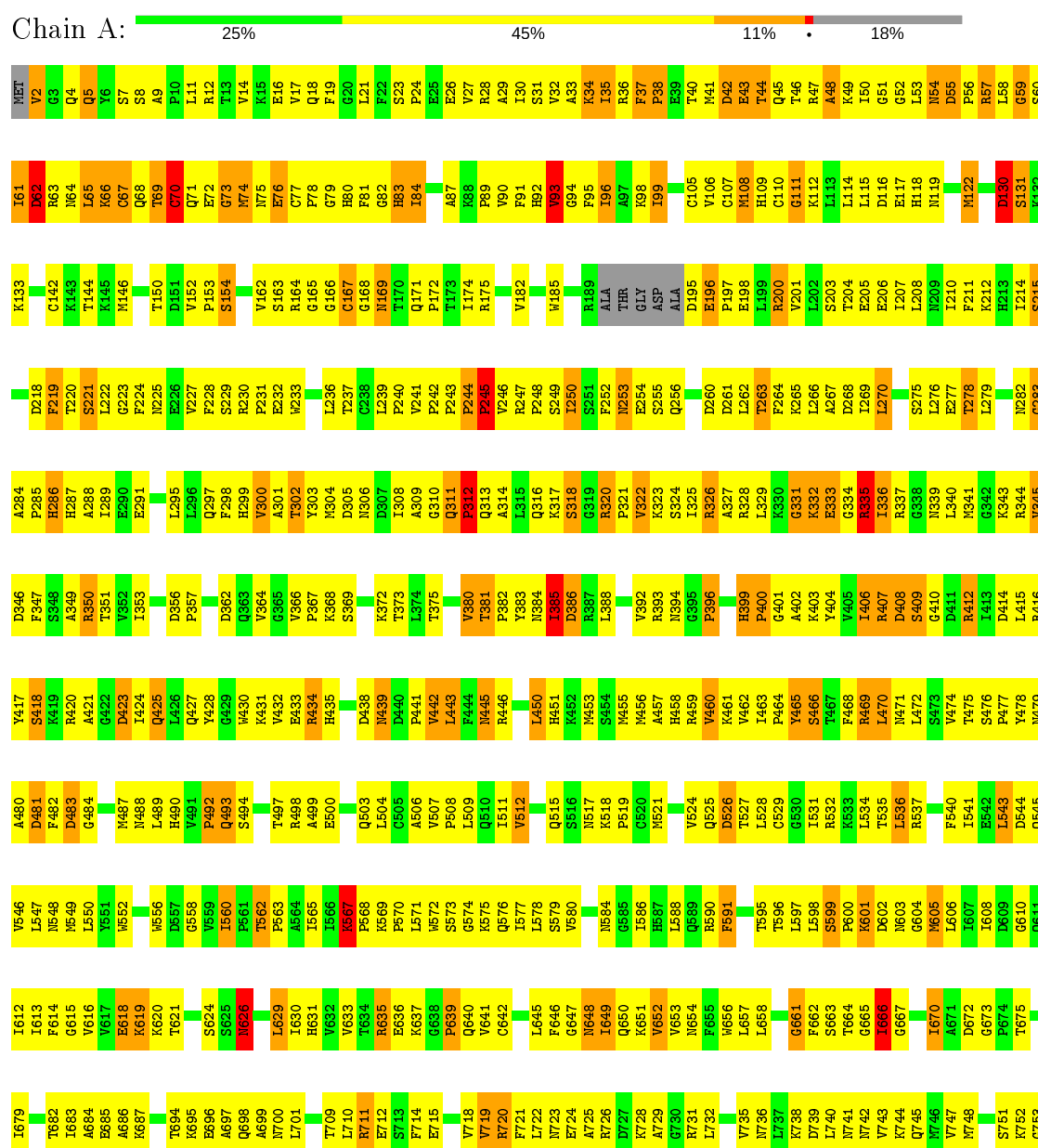
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	8	Total	Zn	0	0
			8	8		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

• Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT



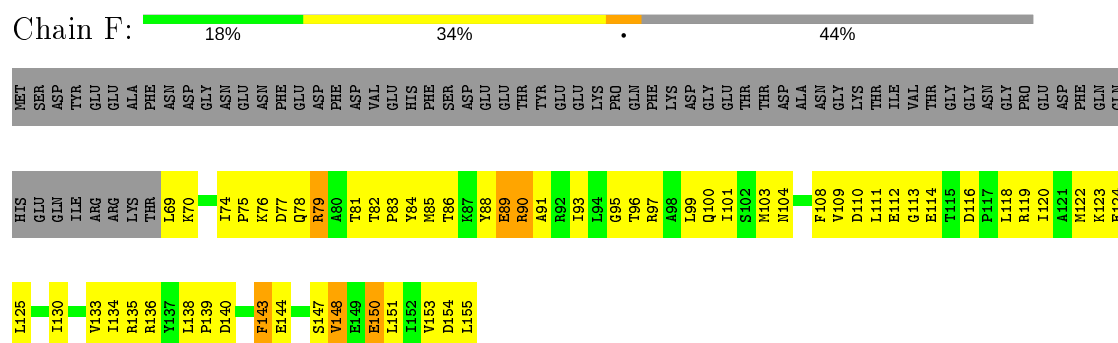
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE



• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE



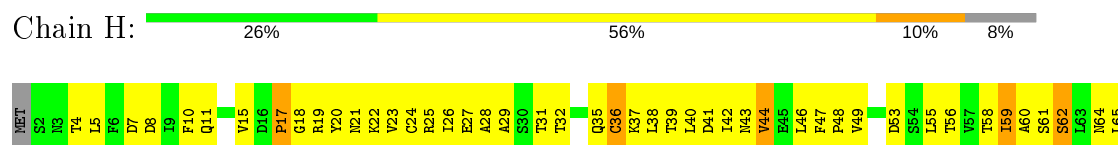
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE

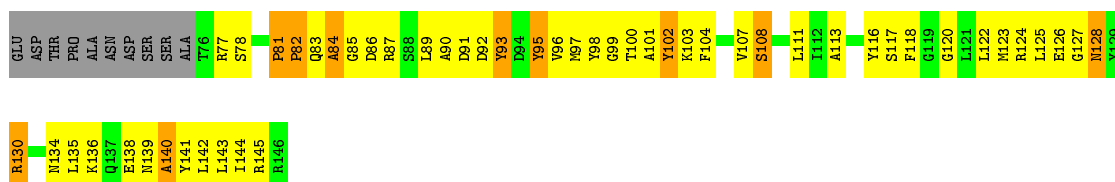


• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE



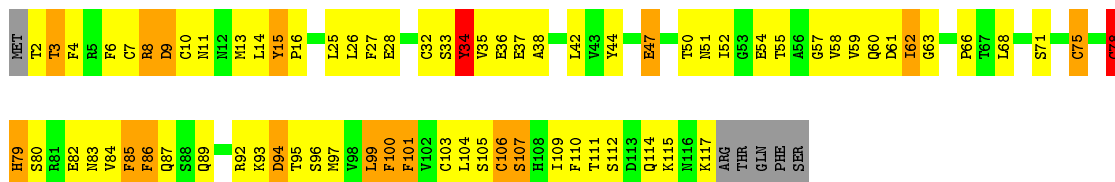
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE





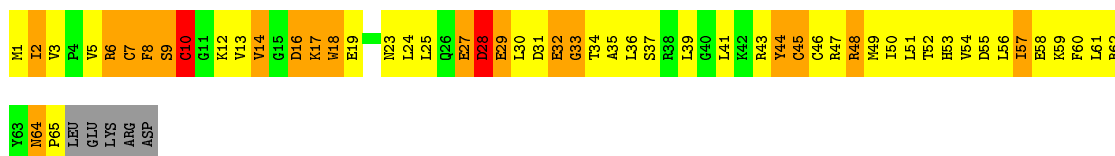
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9

Chain I: 34% 46% 13% • 5%



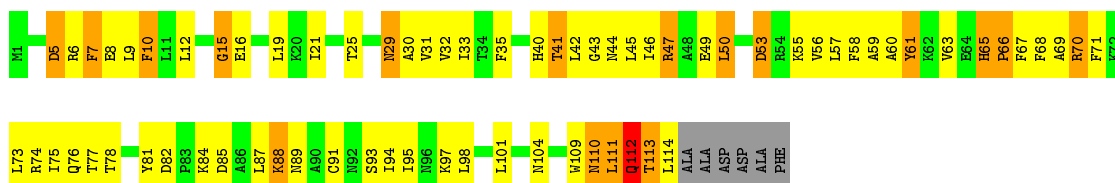
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10

Chain J: 16% 49% 26% • 7%



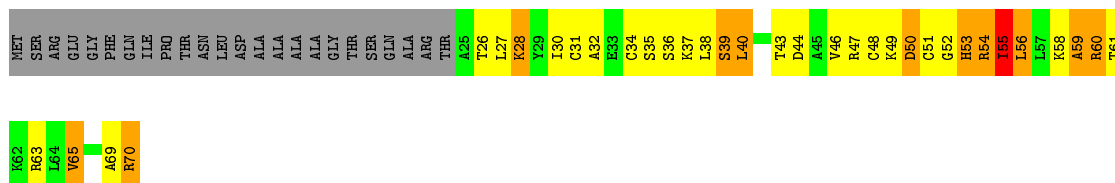
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

Chain K: 36% 44% 14% • 5%



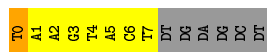
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE

Chain L: 17% 31% 16% • 34%

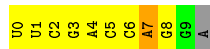


• Molecule 13: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'

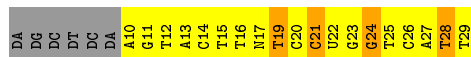
Chain N: 50% 7% 43%



- Molecule 14: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'



- 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'



4 Data and refinement statistics

Xtriage (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, α , β , γ	223.58 Å 393.49 Å 283.50 Å 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.	Xtriage
Total number of atoms	32010	wwPDB-VP
Average B, all atoms (Å ²)	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, ZN, BRU, TT

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	0.47	0/11385	0.73	2/15393 (0.0%)
2	B	0.47	0/9037	0.71	2/12181 (0.0%)
3	C	0.47	0/2138	0.72	0/2896
4	D	0.44	0/1437	0.68	1/1925 (0.1%)
5	E	0.43	0/1788	0.63	0/2406
6	F	0.54	0/716	0.76	0/964
7	G	0.50	0/1368	0.73	0/1844
8	H	0.39	0/1102	0.66	0/1492
9	I	0.39	0/962	0.67	0/1295
10	J	0.50	0/541	0.80	1/727 (0.1%)
11	K	0.54	0/937	0.76	1/1265 (0.1%)
12	L	0.45	0/366	0.71	0/485
13	N	1.16	1/184 (0.5%)	1.01	0/280
14	P	0.63	0/237	1.01	0/367
15	T	1.09	1/382 (0.3%)	1.24	3/582 (0.5%)
All	All	0.49	2/32580 (0.0%)	0.73	10/44102 (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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	0	DT	OP3-P	-6.79	1.53	1.61
15	T	21	DC	C3'-O3'	6.37	1.52	1.44

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1096	ARG	NE-CZ-NH1	-11.17	114.72	120.30
15	T	24	DG	O4'-C1'-N9	7.13	112.99	108.00
10	J	10	CYS	CA-CB-SG	6.47	125.65	114.00
11	K	113	THR	N-CA-C	6.47	128.47	111.00
15	T	28	DT	O4'-C1'-N1	5.56	111.89	108.00

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

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	1369	0
2	B	8866	0	8898	1056	0
3	C	2101	0	2055	275	0
4	D	1427	0	1451	150	0
5	E	1752	0	1776	142	0
6	F	705	0	730	77	0
7	G	1340	0	1357	167	0
8	H	1084	0	1057	133	0
9	I	944	0	901	105	0
10	J	532	0	542	101	0
11	K	919	0	929	113	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	3528	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 55.

The worst 5 of 3528 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:53:LEU:HD23	1:A:54:ASN:H	0.94	1.09
7:G:138:THR:HG22	7:G:139:ILE:H	1.19	1.08

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	7
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	10
5	E	212/215 (99%)	153 (72%)	42 (20%)	17 (8%)	1	14
6	F	84/155 (54%)	65 (77%)	13 (16%)	6 (7%)	1	16
7	G	169/171 (99%)	128 (76%)	30 (18%)	11 (6%)	1	18
8	H	131/146 (90%)	87 (66%)	26 (20%)	18 (14%)	0	4
9	I	114/122 (93%)	77 (68%)	26 (23%)	11 (10%)	0	10
10	J	63/70 (90%)	34 (54%)	12 (19%)	17 (27%)	0	0
11	K	112/120 (93%)	82 (73%)	20 (18%)	10 (9%)	1	12
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	7

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 ⓘ

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%)	1123 (90%)	121 (10%)	8	30
2	B	967/1061 (91%)	886 (92%)	81 (8%)	11	37
3	C	235/274 (86%)	218 (93%)	17 (7%)	14	42
4	D	159/200 (80%)	138 (87%)	21 (13%)	4	21
5	E	196/197 (100%)	191 (97%)	5 (3%)	46	67
6	F	77/137 (56%)	71 (92%)	6 (8%)	12	39
7	G	152/152 (100%)	140 (92%)	12 (8%)	12	39
8	H	119/128 (93%)	112 (94%)	7 (6%)	19	48
9	I	110/116 (95%)	98 (89%)	12 (11%)	6	26
10	J	60/65 (92%)	52 (87%)	8 (13%)	4	21
11	K	99/102 (97%)	87 (88%)	12 (12%)	5	23
12	L	40/57 (70%)	36 (90%)	4 (10%)	7	29
All	All	3458/4009 (86%)	3152 (91%)	306 (9%)	10	35

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	396	ASP
2	B	878	GLN
10	J	7	CYS
2	B	429	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	635	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	465	ASN
2	B	821	GLN
9	I	90	GLN
2	B	515	HIS
2	B	538	ASN

5.3.3 RNA ⓘ

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 ⓘ

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	BRU	T	22	15,14	15,21,22	1.74	4 (26%)	17,30,33	4.11	4 (23%)
15	TT	T	17	15	40,43,44	4.79	9 (22%)	59,69,72	2.52	16 (27%)

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	BRU	T	22	15,14	-	2/4/21/22	0/2/2/2
15	TT	T	17	15	-	10/18/105/106	0/5/6/6

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	17	TT	C5T-C6T	-20.32	1.31	1.55
15	T	17	TT	C5-C6	-19.74	1.32	1.55
15	T	17	TT	C6T-N1T	-4.77	1.39	1.46
15	T	17	TT	C1'-N1	3.99	1.50	1.45
15	T	22	BRU	C4-C5	3.86	1.43	1.38

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C4-N3-C2	14.80	127.64	115.14
15	T	17	TT	C2R-C1R-N1T	8.38	126.91	115.59
15	T	17	TT	C5T-C5-C6	7.24	97.39	88.38
15	T	22	BRU	C5-C4-N3	-6.75	115.56	123.64
15	T	17	TT	C5-C6-C6T	-6.25	79.03	89.28

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	O4'-C4'-C5'-O5'
15	T	17	TT	O3'-C7-O5R-C5R
15	T	17	TT	C2'-C1'-N1-C6
15	T	17	TT	C2'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 26 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
1	A	1
3	C	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.