

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 9, 2023 – 11:05 AM EDT

PDB ID	:	7KEF
Title	:	RNA polymerase II elongation complex with unnatural base dTPT3, rNaM in
		swing state
Authors	:	Oh, J.; Wang, D.
Deposited on	:	2020-10-10
Resolution	:	3.89 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35.1
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.89 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	$1002 \ (4.14-3.66)$
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

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 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 <=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	of chain		
1	А	1733	48%	30%	•	20%
2	В	1224	2% 51%	37%		• 10%
3	С	318	% <b>5</b> 3%	30%	•	16%
4	Е	215	5%		29%	·



Conti	nuea fron	i previous	page							
Mol	Chain	Length		C	Quality	of ch	ain			
5	F	155	32%		22%	•		46%		
6	Н	146	.% 	51%			38%	,	·	9%
7	Ι	122		59%				36%		••
8	J	70	41%				46%		6%	7%
9	K	120	.% 	67%				28%		• 5%
10	L	70	.% 		23	8%	•	34%		
11	R	10	10%		70%				20%	
12	Т	29	14%			79%				•••
13	Ν	16		56%			31	%	6%	6%



# 2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 29202 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 subunit RPB1.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
1	А	1390	Total 10920	C 6887	N 1913	O 2059	S 61	0	0	0

• Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
2	В	1106	Total 8792	C 5568	N 1538	O 1631	${ m S}{55}$	0	0	0

• Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
3	С	266	Total 2091	C 1315	N 348	0 415	S 13	0	0	0

• Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
4	Е	214	Total 1748	C 1108	N 308	0 321	S 11	0	0	0

• Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
5	F	84	Total 679	C 434	N 115	0 127	${ m S} { m 3}$	0	0	0

• Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues		At	$\mathbf{oms}$		ZeroOcc	AltConf	Trace	
6	Н	133	Total 1068	C 673	N 180	0 211	$\frac{S}{4}$	0	0	0



• Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
7	Ι	119	Total 971	C 596	N 179	0 186	S 10	0	0	0

• Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
8	J	65	Total	С	N	0	S	0	0	0
Ũ			532	339	93	94	6		Ŭ	Ŭ

• Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	K	114	Total 919	$\begin{array}{c} \mathrm{C} \\ 590 \end{array}$	N 156	0 171	${S \over 2}$	0	0	0

• Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
10	L	46	Total 359	C 221	N 71	O 63	${S \atop 4}$	0	0	0

• Molecule 11 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
11	R	10	Total 217	C 98	N 45	O 65	Р 9	0	0	0

• Molecule 12 is a DNA chain called Template strand DNA.

Mol	Chain	Residues			Atom	IS			ZeroOcc	AltConf	Trace
12	Т	28	Total 566	C 273	N 100	0 164	Р 27	${ m S} { m 2}$	0	0	0

• Molecule 13 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
13	N	15	Total 307	C 147	N 51	0 94	Р 15	0	0	0

• Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	А	2	Total Zn 2 2	0	0
14	В	1	Total Zn 1 1	0	0
14	С	1	Total Zn 1 1	0	0
14	Ι	2	Total Zn 2 2	0	0
14	J	1	Total Zn 1 1	0	0
14	L	1	Total Zn 1 1	0	0

• Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	А	1	Total Mg 1 1	0	0

• Molecule 16 is (1S)-1,4-anhydro-1-(3-methoxynaphthalen-2-yl)-5-O-phosphono-D-ri bitol (three-letter code: WC4) (formula: C<sub>16</sub>H<sub>19</sub>O<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	R	1	Total	C	0	P	0	0
			24	16	7	T		



# 3 Residue-property plots (i)

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: DNA-directed RNA polymerase II subunit RPB1





• Molecule 2: DNA-directed RNA polymerase II subunit RPB2





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• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1 5%



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2









• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:	41%		46%	6% 7%	
M 12 12 12 12 12 12 12 12 12 12 12 12 12	D16 K17 W18 Y21 E27 E27 D28 D28 D28	S37         S37           R38         R38           L39         L39           L41         R42           R43         R43           Y44         C46           C46         C46           R47         R47	R48 M49 H52 H53 H53 D55 L55 L55 L55 L57	F60 L61 N64 P65 LEU GLU LYS ARG	ADF
• Molecule 9: DN	NA-directed RNA	polymerase II	subunit RPB	11	
Chain K:	67%		28	8% • 5%	I
M1 N2 A3 P4 A3 P4 D5 P7 F7 F1 F1 C119 K18 K18 K119 K119	121 121 124 130 430 430 133 133 141 141 142	643 145 145 146 146 146 147 150 150 157	459 465 766 764 175 177 777	195 195 195 198 108	L114 ALA ALA ASP
ASP ALA PHE					
• Molecule 10: D	NA-directed RNA	A polymerases	I, II, and III s	subunit RPAI	BC4
Chain L:	39%	23%	•	34%	
MET SER ARG CLU CLU CLU CLU THE PHE PRO ASN ASN	ALS ALA ALA ALA ALA ALA CLY THR SER ALA ALA ALA A26 A26	126 127 128 128 139 139 139 131 841 841	T43 D44 A45 A45 A45 C48 C48 K49 D50 B50 R54	155 L56 L64 L64 F67	
• Molecule 11: R	NA				
Chain R: 10%		70%		20%	
A1 U2 C3 C3 C3 C3 C3 C3 C9 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3					
• Molecule 12: Te	emplate strand D	NA			
Chain T: 14%		79%		• •	
C1 72 72 73 74 74 75 71 71 71 71 71 71 71 71 71 71 71 71 71	C16 C17 C17 C17 C20 C21 C21 C22 C23 C23 C23 C23 C23 C23 C25 C25 C25 C25 C25 C25 C25 C25 C25 C25	128 DG			
• Molecule 13: N	on-template stran	nd DNA			
Chain N:	56%		31%	6% 6%	
DG T3 C4 A10 A16 G17					



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	167.71Å 221.71Å 193.25Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $101.78^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	48.70 - 3.89	Depositor
Resolution (A)	48.70 - 3.89	EDS
% Data completeness	98.6 (48.70-3.89)	Depositor
(in resolution range)	98.6(48.70-3.89)	EDS
$R_{merge}$	1.01	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.03 (at 3.88 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.13	Depositor
B B.	0.268 , $0.326$	Depositor
$n, n_{free}$	0.268 , $0.325$	DCC
$R_{free}$ test set	1979 reflections $(3.17\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	107.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	0.26 , $58.5$	EDS
L-test for $twinning^2$	$ < L >=0.36, < L^2>=0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	29202	wwPDB-VP
Average B, all atoms $(Å^2)$	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MG, ZN, WC4, WC7

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).

Mal	Chain	Bond	lengths	Bo	ond angles
MOI	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.26	0/11113	0.48	1/15025~(0.0%)
2	В	0.26	0/8963	0.49	0/12086
3	С	0.26	0/2129	0.48	0/2886
4	Е	0.26	0/1784	0.46	0/2402
5	F	0.26	0/691	0.43	0/933
6	Н	0.26	0/1086	0.50	0/1470
7	Ι	0.27	0/989	0.47	0/1331
8	J	0.28	0/541	0.51	0/727
9	Κ	0.27	0/937	0.46	0/1265
10	L	0.25	0/361	0.57	0/481
11	R	0.41	0/244	1.08	1/380~(0.3%)
12	Т	0.62	0/609	1.06	1/934~(0.1%)
13	Ν	0.55	0/342	1.35	1/526~(0.2%)
All	All	0.28	0/29789	0.53	4/40446~(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	А	0	2
13	Ν	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	Ν	17	DG	C5-C6-O6	-20.52	116.29	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
12	Т	21	DC	O4'-C4'-C3'	-5.52	102.29	104.50
11	R	8	G	N3-C2-N2	-5.51	116.04	119.90
1	А	997	LEU	CA-CB-CG	5.40	127.71	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	332	LYS	Peptide
1	А	895	LYS	Peptide
13	Ν	17	DG	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	А	10920	0	11003	438	0
2	В	8792	0	8823	397	0
3	С	2091	0	2049	77	0
4	Е	1748	0	1765	50	0
5	F	679	0	701	27	0
6	Н	1068	0	1040	41	0
7	Ι	971	0	929	29	0
8	J	532	0	543	36	0
9	K	919	0	929	35	0
10	L	359	0	378	13	0
11	R	217	0	110	13	0
12	Т	566	0	305	34	0
13	Ν	307	0	172	6	1
14	А	2	0	0	0	0
14	В	1	0	0	0	0
14	С	1	0	0	0	0
14	Ι	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	R	24	0	0	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29202	0	28747	1036	1

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 18.

The worst 5 of 1036 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)
2:B:1094:ARG:NH2	2:B:1098:MET:SD	2.09	1.23
16:R:11:WC4:O06	16:R:11:WC4:C05	1.66	1.19
2:B:1094:ARG:HH12	2:B:1098:MET:HE2	0.98	1.11
2:B:1094:ARG:HH12	2:B:1098:MET:CE	1.65	1.10
1:A:508:PRO:HA	1:A:511:ILE:HG13	1.35	1.05

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:17:DG:C6	13:N:17:DG:O6[2_856]	1.25	0.95

#### 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	Perce	ntiles
1	А	1378/1733~(80%)	1285~(93%)	93~(7%)	0	100	100
2	В	1088/1224~(89%)	1021 (94%)	67~(6%)	0	100	100
3	С	264/318~(83%)	242 (92%)	22 (8%)	0	100	100
4	Е	212/215~(99%)	206 (97%)	6 (3%)	0	100	100
5	F	82/155~(53%)	80 (98%)	2 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	Н	129/146~(88%)	121 (94%)	8 (6%)	0	100 100
7	Ι	117/122~(96%)	111 (95%)	6~(5%)	0	100 100
8	J	63/70~(90%)	62~(98%)	1 (2%)	0	100 100
9	Κ	112/120~(93%)	108 (96%)	4 (4%)	0	100 100
10	L	44/70~(63%)	43~(98%)	1 (2%)	0	100 100
All	All	3489/4173~(84%)	3279 (94%)	210 (6%)	0	100 100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	entiles
1	А	1210/1520~(80%)	1123 (93%)	87 (7%)	14	44
2	В	960/1061~(90%)	898 (94%)	62~(6%)	17	46
3	С	233/274~(85%)	225~(97%)	8 (3%)	37	62
4	Ε	195/197~(99%)	180 (92%)	15 (8%)	13	42
5	F	74/137~(54%)	70~(95%)	4(5%)	22	52
6	Н	117/128~(91%)	105 (90%)	12 (10%)	7	30
7	Ι	113/116~(97%)	106 (94%)	7~(6%)	18	48
8	J	60/65~(92%)	54 (90%)	6 (10%)	7	30
9	Κ	99/102~(97%)	97~(98%)	2(2%)	55	74
10	L	39/57~(68%)	33~(85%)	6 (15%)	2	17
All	All	3100/3657~(85%)	2891 (93%)	209 (7%)	16	46

 $5~{\rm of}~209$  residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	В	560	GLU
2	В	1148	LYS



Continued from previous page...

Mol	Chain	Res	Type
8	J	48	ARG
2	В	678	GLU
2	В	935	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
6	Н	52	GLN
9	Κ	112	GLN
7	Ι	22	ASN
2	В	1025	HIS
6	Н	11	GLN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	9/10~(90%)	2(22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	5	А
11	R	10	А

There are no RNA pucker outliers to report.

#### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is 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 Cha	Chain	Dog	Tink	Bo	ond leng	ths	B	ond ang	les	
	Unain	I nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
12	WC7	Т	18	12	16,23,24	1.39	3 (18%)	17,33,36	1.39	3 (17%)

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
12	WC7	Т	18	12	-	3/7/21/22	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
12	Т	18	WC7	C5-S1	-3.19	1.59	1.66
12	Т	18	WC7	C1-C2	3.00	1.40	1.33
12	Т	18	WC7	C3-C2	-2.44	1.39	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
12	Т	18	WC7	C6-C3-C4	3.67	113.60	107.10
12	Т	18	WC7	C2-C1-N1	2.40	124.41	121.25
12	Т	18	WC7	C3'-C2'-C1'	2.02	107.60	102.54

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	Т	18	WC7	C3'-C4'-C5'-O5'
12	Т	18	WC7	O4'-C4'-C5'-O5'
12	Т	18	WC7	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides 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).

Mal	Mol Type Chain F		Dog	Tink	Bond lengths			Bond angles		
	туре	Ullalli	lain nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	WC4	R	11	15,11	23,26,27	7.11	18 (78%)	33,37,40	1.53	4 (12%)

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	WC4	R	11	15,11	-	9/9/27/28	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	R	11	WC4	C16-C05	-16.02	1.35	1.54
16	R	11	WC4	O06-C05	14.76	1.66	1.44
16	R	11	WC4	C25-C03	11.16	1.56	1.36
16	R	11	WC4	C18-C04	10.46	1.54	1.36
16	R	11	WC4	C23-C24	8.24	1.55	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
16	R	11	WC4	C14-C16-C05	4.14	106.70	101.93
16	R	11	WC4	O02-C03-C25	-3.87	120.23	125.24
16	R	11	WC4	O02-C03-C04	3.83	119.49	115.83
16	R	11	WC4	C01-O02-C03	-2.51	113.74	117.53

There are no chirality outliers.

5 of 9 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
16	R	11	WC4	C03-C04-C05-C16
16	R	11	WC4	C18-C04-C05-C16
16	R	11	WC4	C14-C07-C08-O5'
16	R	11	WC4	O06-C07-C08-O5'
16	R	11	WC4	C25-C03-O02-C01

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	R	11	WC4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

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, 95<sup>th</sup> 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	1390/1733~(80%)	-0.05	24 (1%) 70 60	56,105,169,216	0
2	В	1106/1224~(90%)	-0.04	22 (1%) 65 55	65, 108, 158, 199	0
3	С	266/318~(83%)	-0.17	3 (1%) 80 73	66, 105, 134, 156	0
4	Е	214/215~(99%)	-0.03	10 (4%) 31 25	68, 126, 185, 214	0
5	F	84/155~(54%)	-0.25	0 100 100	81, 107, 128, 139	0
6	Н	133/146~(91%)	-0.05	2 (1%) 73 64	95, 126, 164, 190	0
7	Ι	119/122~(97%)	-0.13	0 100 100	83, 117, 144, 172	0
8	J	65/70~(92%)	-0.14	0 100 100	74, 101, 130, 149	0
9	K	114/120~(95%)	-0.17	1 (0%) 84 77	75, 107, 132, 142	0
10	L	46/70~(65%)	0.13	1 (2%) 62 51	90, 143, 170, 183	0
11	R	10/10~(100%)	0.38	0 100 100	101, 121, 165, 172	0
12	Т	27/29~(93%)	-0.10	0 100 100	109, 164, 257, 265	0
13	N	15/16~(93%)	-0.09	0 100 100	149, 224, 249, 252	0
All	All	3589/4228~(84%)	-0.07	63 (1%) 68 59	56, 109, 167, 265	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	258	GLY	5.9
4	Е	126	SER	5.6
4	Е	125	PRO	4.6
4	Е	83	CYS	4.5
4	Е	123	LEU	4.5



#### 6.2 Non-standard residues in protein, DNA, RNA chains (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,  $95^{th}$  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	$B-factors(Å^2)$	Q<0.9
12	WC7	Т	18	21/22	0.88	0.21	110,121,135,140	0

#### 6.3 Carbohydrates (i)

There are no monosaccharides 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
14	ZN	В	1307	1/1	0.79	0.10	179,179,179,179	0
14	ZN	L	105	1/1	0.79	0.08	179,179,179,179	0
16	WC4	R	11	24/25	0.90	0.25	96,109,119,123	0
14	ZN	С	319	1/1	0.92	0.10	91,91,91,91	0
14	ZN	J	101	1/1	0.92	0.21	107,107,107,107	0
14	ZN	А	1735	1/1	0.93	0.04	134,134,134,134	0
14	ZN	Ι	204	1/1	0.94	0.08	131,131,131,131	0
14	ZN	Ι	203	1/1	0.97	0.07	98,98,98,98	0
15	MG	А	2001	1/1	0.98	0.09	88,88,88,88	0
14	ZN	А	1734	1/1	0.98	0.21	206,206,206,206	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers (i)

There are no such residues in this entry.

