

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

#### Oct 15, 2023 – 03:33 AM EDT

PDB ID : 8DH4

Title : T7 RNA polymerase elongation complex with unnatural base dPa-DsTP pair

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Deposited on : 2022-06-24

Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

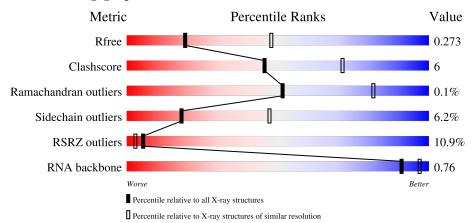
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 $(\# \mathrm{Entries})$	Similar resolution $(\# \text{Entries, resolution range}(\mathring{A}))$		
$R_{free}$	130704	3140 (2.80-2.80)		
Clashscore	141614	3569 (2.80-2.80)		
Ramachandran outliers	138981	3498 (2.80-2.80)		
Sidechain outliers	138945	3500 (2.80-2.80)		
RSRZ outliers	127900	3078 (2.80-2.80)		
RNA backbone	3102	1227 (3.10-2.50)		

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 chain		
1	В	883	81%	15%	
1	Е	883	11%	16%	• 7%
1	I	883	72%	20%	• 7%
1	M	883	70%	22%	• 7%

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Mol	Chain	Length	Quality of chain					
2	A	18	72%	11% 17%				
2	F	18	56%	39% 6%				
2	J	18		3% 22%				
2	N	18	6%	22% 17%				
3	С	12	75%	25%				
3	G	12	67%	33%				
3	K	12	8% 67%	33%				
3	О	12	33% 33%	33%				
4	D	9	44% 67%	33%				
4	Н	9		44% 11%				
4	L	9	11% 22%	67%				
4	Р	9	44% 67%	33%				

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:

$\mathbf{Mol}$	Type	Chain	$\operatorname{Res}$	Chirality	Geometry	Clashes	Electron density
6	MG	Ε	902	-	-	-	X



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 28446 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 T7 RNA polymerase.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	В	856	Total	С	N	О	S	0	0	0
1	Б	000	6728	4284	1169	1239	36	0	U	
1	Е	819	Total	С	N	О	S	0	0	0
1	<u> 1</u> 2	019	6397	4086	1097	1181	33	0		
1	Т	821	Total	С	N	О	S	0	0	0
1	1	021	6429	4106	1112	1176	35	0	U	
1	M	819	Total	С	N	О	S	0	0	0
1	1V1	019	6409	4090	1111	1176	32		U	0

• Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Λ	15	Total	С	N	О	Р	0	0	0
2	A	10	303	145	55	88	15	0	0	
2	F	17	Total	С	N	О	Р	0	0	0
2	I'	11	344	165	65	98	16	U		
2	Т	14	Total	С	N	О	Р	0	0	0
2	J	14	282	135	50	83	14	0		
2	N	15	Total	С	N	О	Р	0	0	0
	11	10	303	145	55	88	15	U	U	U

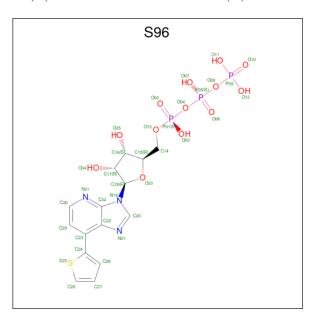
• Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	C	0	Total	С	N	О	Р	0	0	0
3		9	193	86	35	63	9	0	0	
3	G	8	Total	С	N	О	Р	0	0	0
3	G	8	173	77	33	55	8			
3	K	0	Total	С	N	О	Р	0	0	0
3	K	0	173	77	33	55	8	0		
2	0	Q	Total	С	N	О	Р	0	0	0
3	O	8	173	77	33	55	8		U	



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total C	N	О	Р	0	0	0
4	D	0	122 59	19	38	6	0	0	
1	Н	Q	Total C	N	О	Р	0	0	0
4	11	8	160 77	25	50	8	Ü		
1	Т	ર	Total C	N	О	Р	0	0	0
4	ь	3	63 30	12	18	3	0	0	
1	D	6	Total C	N	О	Р	0	0	0
4	1	0	122 59	19	38	6	U		

• Molecule 5 is (7P)-3-{5-O-[(R)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-D-ribofuranosyl}-7-(thiophen-2-yl)-3H-imidazo[4,5-b]pyridine (three-letter code: S96) (formula:  $C_{15}H_{18}N_3O_{13}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	С	N	О	Р	S	0	0
9	Ъ	1	35	15	3	13	3	1		0
5	E	1	Total	С	N	О	Р	S	0	0
9	12	1	35	15	3	13	3	1		

• Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

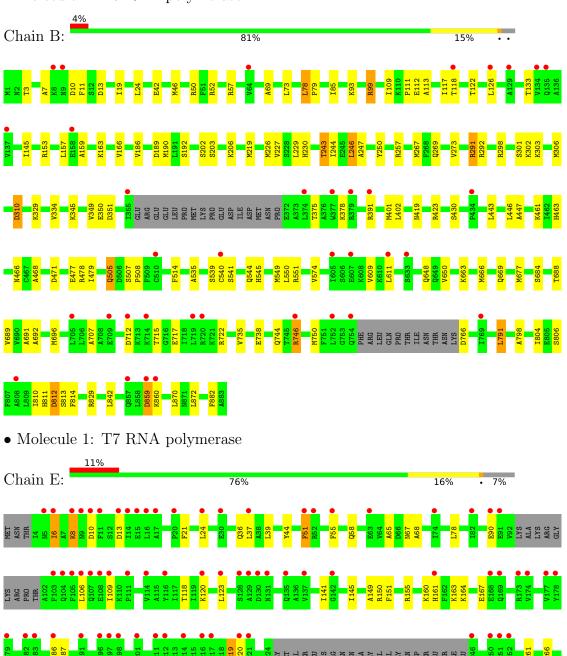
$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total Mg 1 1	0	0
6	E	1	Total Mg 1 1	0	0



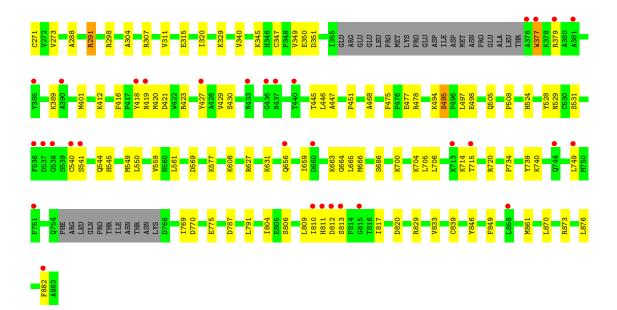
# 3 Residue-property plots (i)

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.

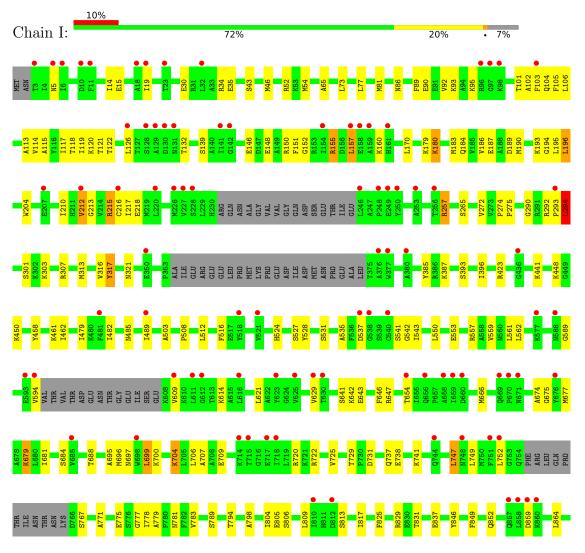
• Molecule 1: T7 RNA polymerase







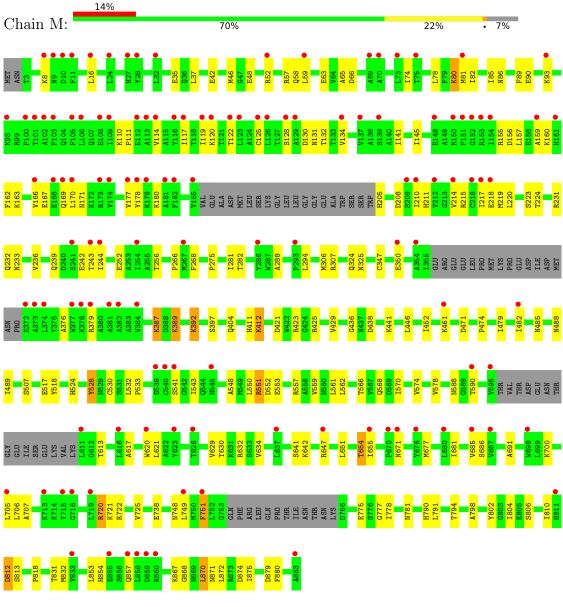
• Molecule 1: T7 RNA polymerase







 $\bullet$  Molecule 1: T7 RNA polymerase



• Molecule 2: Template strand DNA

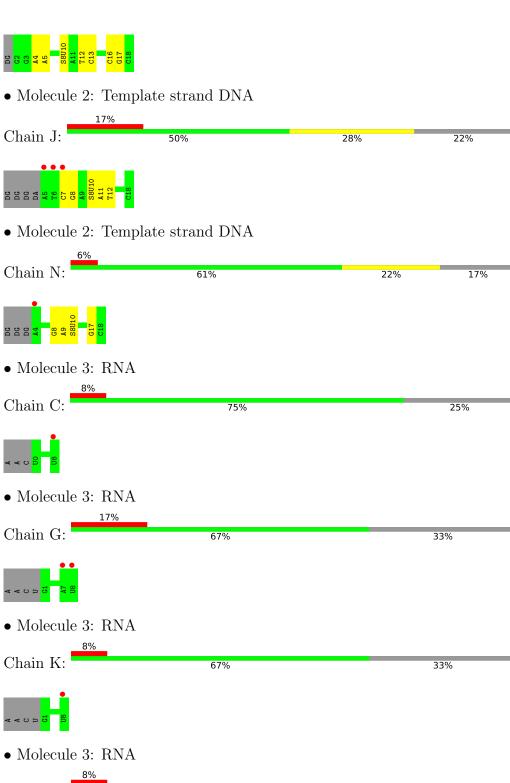
Chain A: 72% 11% 17%



• Molecule 2: Template strand DNA

Chain F: 56% 39% 6%



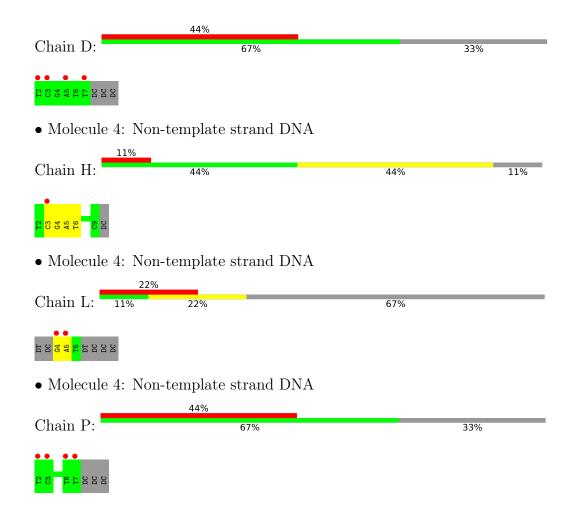


Chain O: 33% 33% 33%



• Molecule 4: Non-template strand DNA







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	78.78Å 86.23Å 201.46Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.85° 85.39° 69.59°	Depositor
Resolution (Å)	43.20 - 2.80	Depositor
Resolution (A)	43.20 - 2.80	EDS
% Data completeness	97.7 (43.20-2.80)	Depositor
(in resolution range)	97.7 (43.20-2.80)	EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
D D.	0.233 , 0.275	Depositor
$R, R_{free}$	0.231 , $0.273$	DCC
$R_{free}$ test set	1905 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.30, 69.6	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  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, S8U, S96

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		
WIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	В	0.28	0/6878	0.53	2/9304~(0.0%)	
1	Е	0.27	0/6542	0.52	1/8859 (0.0%)	
1	I	0.30	0/6575	0.56	3/8894 (0.0%)	
1	M	0.28	0/6553	0.56	4/8870 (0.0%)	
2	A	0.49	0/318	0.85	0/485	
2	F	0.48	0/365	0.86	0/559	
2	J	0.49	0/294	0.88	0/448	
2	N	0.48	0/318	0.93	0/485	
3	С	0.19	0/215	0.80	0/333	
3	G	0.17	0/193	0.75	0/299	
3	K	0.16	0/193	0.72	0/299	
3	O	0.19	0/193	0.84	0/299	
4	D	0.44	0/135	1.01	0/206	
4	Н	0.61	0/177	1.07	0/270	
4	L	0.45	0/70	0.90	0/106	
4	Р	0.61	0/135	1.06	0/206	
All	All	0.30	0/29154	0.59	10/39922 (0.0%)	

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	78	LEU	CB-CG-CD2	-12.44	89.86	111.00
1	I	699	LEU	CA-CB-CG	7.48	132.49	115.30
1	Е	787	ASP	CB-CG-OD2	7.19	124.77	118.30
1	M	130	ASP	CB-CG-OD1	7.09	124.68	118.30
1	M	870	LEU	CA-CB-CG	6.79	130.91	115.30

There are no chirality outliers.

There are no planarity outliers.



#### 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	В	6728	0	6694	71	0
1	Е	6397	0	6304	68	0
1	I	6429	0	6372	99	0
1	M	6409	0	6347	108	0
2	A	303	0	157	1	0
2	F	344	0	180	4	0
2	J	282	0	146	3	0
2	N	303	0	157	2	0
3	С	193	0	96	0	0
3	G	173	0	86	0	0
3	K	173	0	86	0	0
3	О	173	0	86	2	0
4	D	122	0	70	0	0
4	Н	160	0	92	3	0
4	L	63	0	35	2	0
4	Р	122	0	70	0	0
5	В	35	0	0	1	0
5	Е	35	0	0	2	0
6	В	1	0	0	0	0
6	Е	1	0	0	0	0
All	All	28446	0	26978	356	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 6.

The worst 5 of 356 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
5:E:901:S96:C18	5:E:901:S96:O33	1.66	1.16
5:B:901:S96:C18	5:B:901:S96:O33	1.66	1.15
1:M:80:LYS:NZ	1:M:223:SER:O	1.96	0.99
1:B:78:LEU:HD21	1:B:746:ARG:HH12	1.47	0.78
1:E:700:LYS:HG2	1:E:775:GLU:HB2	1.67	0.76

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	Perce	$\mathbf{ntiles}$
1	В	850/883 (96%)	828 (97%)	21 (2%)	1 (0%)	51	81
1	E	809/883 (92%)	798 (99%)	11 (1%)	0	100	100
1	I	811/883 (92%)	796 (98%)	14 (2%)	1 (0%)	51	81
1	M	809/883 (92%)	797 (98%)	12 (2%)	0	100	100
All	All	$3279/3532 \ (93\%)$	3219 (98%)	58 (2%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	811	HIS
1	I	294	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	Perce	entiles
1	В	701/729 (96%)	661 (94%)	40 (6%)	20	50
1	E	660/729 (90%)	622 (94%)	38 (6%)	20	50
1	I	664/729 (91%)	618 (93%)	46 (7%)	15	41
1	M	662/729 (91%)	620 (94%)	42 (6%)	18	46
All	All	2687/2916 (92%)	2521 (94%)	166 (6%)	18	47

5 of 166 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	I	697	ASN
1	M	412	LYS
1	I	747	LEU
1	M	131	ASN
1	M	551	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	869	ASN
1	I	672	GLN
1	Е	781	ASN
1	Е	58	GLN
1	Е	869	ASN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	С	7/12 (58%)	0	0
3	G	6/12 (50%)	0	0
3	K	6/12 (50%)	0	0
3	O	6/12 (50%)	2 (33%)	0
All	All	25/48 (52%)	2 (8%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	$\operatorname{Res}$	$\mathbf{Type}$
3	О	2	С
3	О	4	G

There are no RNA pucker outliers to report.

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

4 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	Chain	Res	Link	Bond lengths			Bond angles		
		n Res	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	S8U	A	10	2	15,19,20	4.37	7 (46%)	16,26,29	1.27	2 (12%)
2	S8U	N	10	2	15,19,20	4.36	7 (46%)	16,26,29	1.37	2 (12%)
2	S8U	J	10	2	15,19,20	4.36	7 (46%)	16,26,29	1.39	2 (12%)
2	S8U	F	10	2	15,19,20	4.37	7 (46%)	16,26,29	1.40	2 (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
2	S8U	A	10	2	-	0/3/23/24	0/2/2/2
2	S8U	N	10	2	-	0/3/23/24	0/2/2/2
2	S8U	J	10	2	-	0/3/23/24	0/2/2/2
2	S8U	F	10	2	-	0/3/23/24	0/2/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}( ext{\AA})$
2	J	10	S8U	C2'-C3'	-11.29	1.23	1.52
2	A	10	S8U	C2'-C3'	-11.28	1.23	1.52
2	N	10	S8U	C2'-C3'	-11.27	1.23	1.52
2	F	10	S8U	C2'-C3'	-11.25	1.23	1.52
2	F	10	S8U	O4'-C4'	-8.10	1.26	1.45

The worst 5 of 8 bond angle outliers are listed below:

Mo	l Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(^{\scriptscriptstyle o})$	$  \ \mathbf{Ideal}(^o)  $
2	J	10	S8U	O14-C13-C12	-2.96	119.98	124.17
2	N	10	S8U	O14-C13-C12	-2.94	120.01	124.17
2	A	10	S8U	O14-C13-C12	-2.89	120.07	124.17
2	F	10	S8U	O14-C13-C12	-2.88	120.09	124.17
2	J	10	S8U	C2'-C3'-C4'	2.68	108.35	102.76

There are no chirality outliers.

There are no torsion outliers.

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	Trus	Chain	Res	Link	Bond lengths				ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	S96	Е	901	6	31,38,38	6.95	16 (51%)	35,59,59	1.68	7 (20%)
5	S96	В	901	6	31,38,38	6.94	16 (51%)	35,59,59	1.67	6 (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
5	S96	Е	901	6	-	6/20/42/42	0/4/4/4
5	S96	В	901	6	-	4/20/42/42	0/4/4/4

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(Å)	$Ideal(\AA)$
5	Е	901	S96	O33-C18	18.34	1.66	1.41
5	В	901	S96	O33-C18	18.29	1.66	1.41
5	В	901	S96	C24-S25	-16.82	1.56	1.72
5	Е	901	S96	C24-S25	-16.72	1.56	1.72
5	Е	901	S96	C17-C18	-16.27	1.29	1.53

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



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
5	Ε	901	S96	C27-C26-S25	-6.24	107.92	112.98
5	В	901	S96	C27-C26-S25	-6.07	108.05	112.98
5	Ε	901	S96	C29-C30-N31	-3.19	119.64	124.58
5	В	901	S96	C29-C30-N31	-3.07	119.83	124.58
5	Е	901	S96	C30-N31-C32	2.96	120.44	116.77

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	901	S96	C14-O13-P01-O03
5	В	901	S96	C14-O13-P01-O04
5	Е	901	S96	O13-C14-C15-O33
5	Е	901	S96	C14-O13-P01-O04
5	Е	901	S96	O13-C14-C15-C16

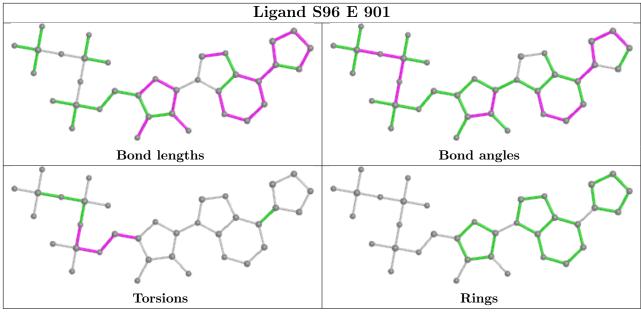
There are no ring outliers.

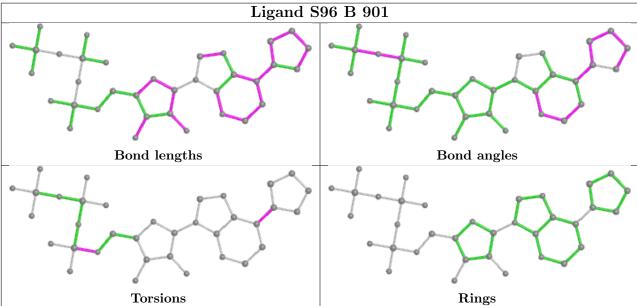
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Е	901	S96	2	0
5	В	901	S96	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,  $95^{th}$  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>	#RSRZ>	>2	$ ext{OWAB}( ext{Å}^2)$	Q<0.9
1	В	856/883 (96%)	0.32	36 (4%) 36	26	46, 79, 149, 207	0
1	E	819/883 (92%)	0.66	101 (12%) 4	2	51, 91, 194, 254	0
1	I	821/883 (92%)	0.60	89 (10%) 5	3	65, 116, 181, 226	0
1	M	819/883 (92%)	0.83	125 (15%) 2	1	79, 130, 209, 268	0
2	A	14/18 (77%)	0.76	2 (14%) 2	1	57, 83, 257, 270	0
2	F	16/18 (88%)	0.27	0 100 1	00	74, 128, 257, 274	0
2	J	13/18 (72%)	1.00	3 (23%) 0	0	82, 92, 293, 308	0
2	N	14/18 (77%)	0.53	1 (7%) 16	9	102, 150, 228, 260	0
3	С	9/12 (75%)	0.94	1 (11%) 5	3	65, 75, 116, 168	0
3	G	8/12 (66%)	0.93	2 (25%) 0	0	77, 92, 140, 155	0
3	K	8/12 (66%)	0.60	1 (12%) 3	2	96, 100, 125, 152	0
3	О	8/12 (66%)	0.61	1 (12%) 3	2	114, 124, 185, 194	0
4	D	6/9 (66%)	2.30	4 (66%) 0	0	217, 228, 252, 264	0
4	Н	8/9 (88%)	1.38	1 (12%) 3	2	224, 231, 239, 254	0
4	L	3/9 (33%)	2.40	2 (66%) 0	0	251, 251, 273, 277	0
4	Р	6/9 (66%)	2.37	4 (66%) 0	0	244, 258, 263, 277	0
All	All	3428/3688 (92%)	0.61	373 (10%) 5	3	46, 106, 197, 308	0

The worst 5 of 373 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ε	174	VAL	6.9
1	I	377	TRP	6.5
1	${ m E}$	106	LEU	6.4
1	M	159	ALA	6.1
1	M	620	TRP	5.9



#### 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	S8U	N	10	18/19	0.90	0.23	133,140,152,158	0
2	S8U	J	10	18/19	0.94	0.22	102,109,130,139	0
2	S8U	F	10	18/19	0.95	0.20	78,87,103,108	0
2	S8U	A	10	18/19	0.97	0.21	62,75,87,89	0

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

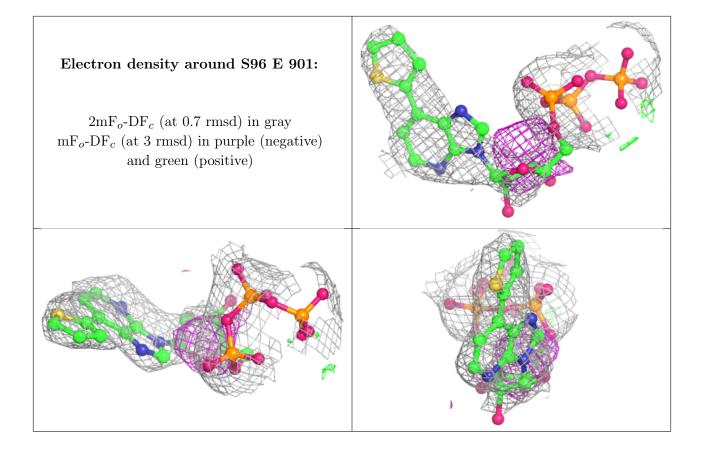
#### 6.4 Ligands (i)

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.

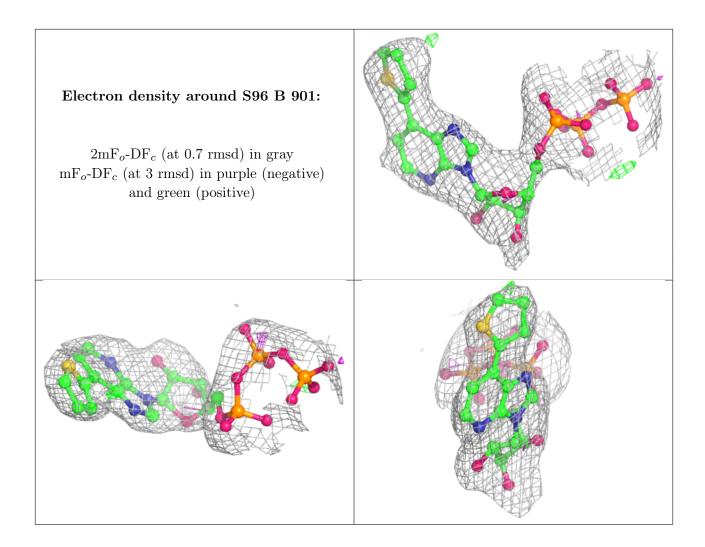
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
6	MG	E	902	1/1	0.80	0.61	103,103,103,103	0
5	S96	Е	901	35/35	0.90	0.22	76,122,135,140	0
5	S96	В	901	35/35	0.92	0.21	68,102,129,134	0
6	MG	В	902	1/1	0.94	0.40	79,79,79,79	0

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.

