



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:13 PM GMT

PDB ID : 1SL0  
Title : Ternary 3' complex of T7 DNA polymerase with a DNA primer/template containing a disordered cis-syn thymine dimer on the template and an incoming nucleotide  
Authors : Li, Y.; Dutta, S.; Doublié, S.; Bdour, H.M.; Taylor, J.S.; Ellenberger, T.  
Deposited on : 2004-03-05  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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

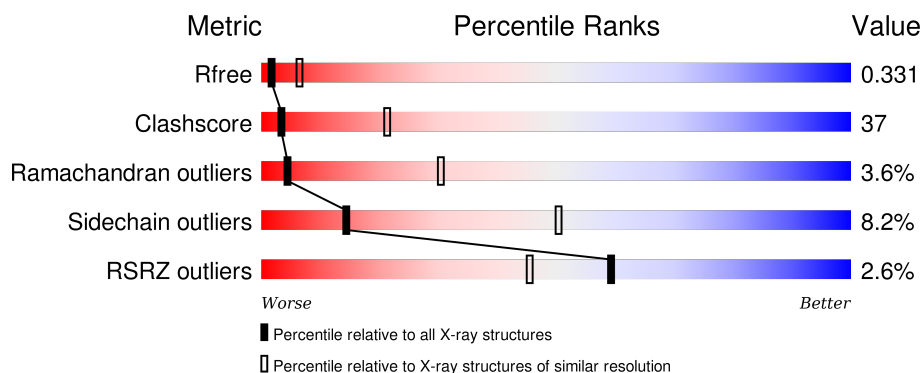
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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  $\geq 3$ , 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	P	21	<div> <div></div> <div>43%10%48%</div> </div>
1	Q	21	<div> <div>5%43%5%48%</div> </div>
2	T	25	<div> <div>28%12%60%</div> </div>
2	U	25	<div> <div>24%16%60%</div> </div>
3	A	698	<div> <div>2%46%43%5%6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	698	
4	B	108	
4	D	108	

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
5	MG	A	4003	-	-	-	X
6	DAD	A	4004	X	-	-	-
6	DAD	C	4005	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11904 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(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*(2DT))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	11	Total	C	N	O	P	0	0	0
			224	106	41	66	11			
1	Q	11	Total	C	N	O	P	0	0	0
			224	106	41	66	11			

- Molecule 2 is a DNA chain called 5'-D(\*CP\*CP\*CP\*(TTD)P\*AP\*GP\*GP\*CP\*AP\*CP\*TP\*GP\*GP\*CP\*CP\*GP\*TP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	10	Total	C	N	O	P	0	0	0
			207	97	41	59	10			
2	U	10	Total	C	N	O	P	0	0	0
			207	97	41	59	10			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	658	Total	C	N	O	S	0	0	0
			4782	3042	831	889	20			
3	C	658	Total	C	N	O	S	0	0	0
			4772	3031	830	891	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	DELETION	UNP P00581
A	?	-	ARG	DELETION	UNP P00581
A	?	-	PHE	DELETION	UNP P00581
A	?	-	GLY	DELETION	UNP P00581
A	?	-	SER	DELETION	UNP P00581
A	?	-	HIS	DELETION	UNP P00581

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LYS	DELETION	UNP P00581
C	?	-	ARG	DELETION	UNP P00581
C	?	-	PHE	DELETION	UNP P00581
C	?	-	GLY	DELETION	UNP P00581
C	?	-	SER	DELETION	UNP P00581
C	?	-	HIS	DELETION	UNP P00581

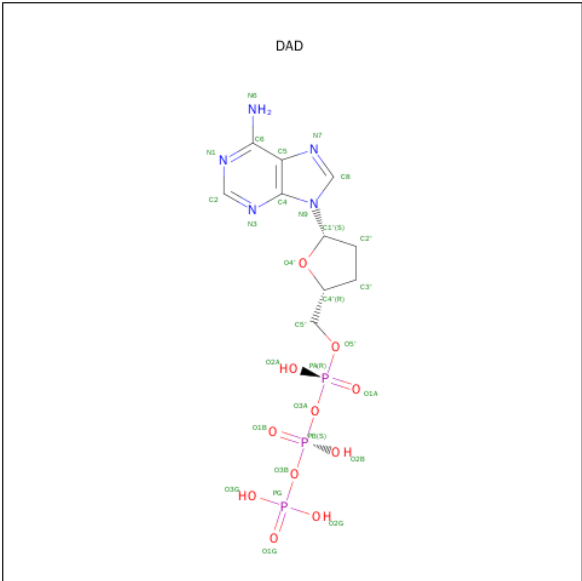
- Molecule 4 is a protein called Thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	105	Total	C	N	O	S	0	0	0
			716	461	118	135	2			
4	D	105	Total	C	N	O	S	0	0	0
			712	456	119	135	2			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 2',3'-DIDEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: DAD) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>11</sub>P<sub>3</sub>).



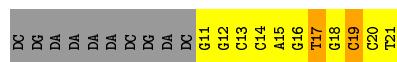
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			29	10	5	11	3		
6	A	1	Total	C	N	O	P	0	0
			29	10	5	11	3		

### 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 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(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*(2DT))-3'

Chain P: 



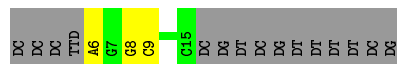
- Molecule 1: 5'-D(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*(2DT))-3'

Chain Q: 



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

Chain T: 



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

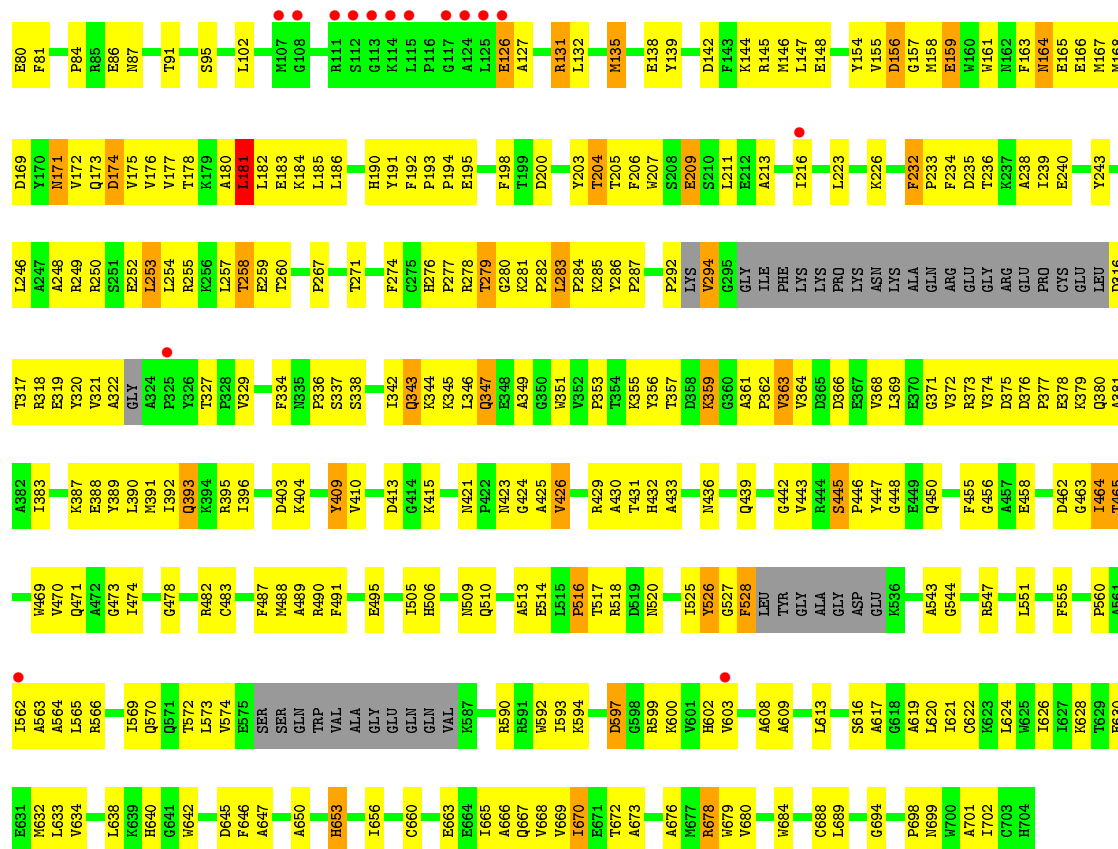
Chain U: 



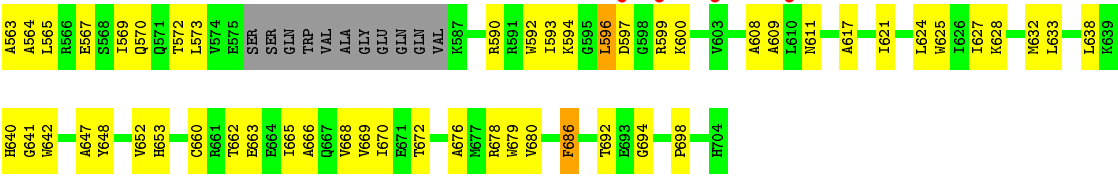
- Molecule 3: DNA polymerase

Chain A: 

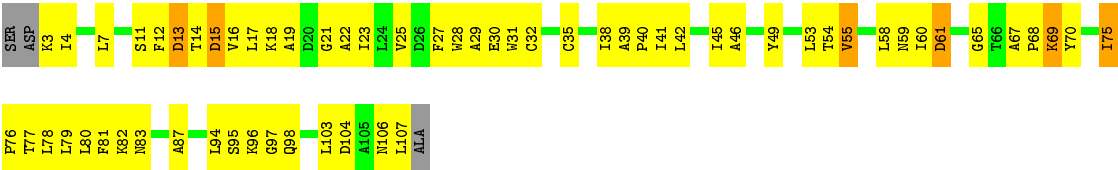




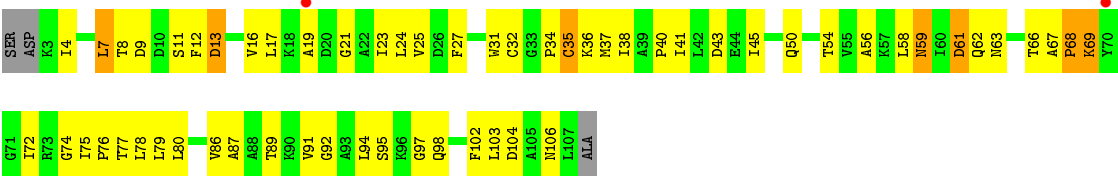




• Molecule 4: Thioredoxin 1



• Molecule 4: Thioredoxin 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.27Å 105.47Å 213.93Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 39.63 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-3.20) 91.7 (39.63-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.37 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.282 , 0.351 0.272 , 0.331	Depositor DCC
$R_{free}$ test set	1987 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	87.3	Xtriage
Anisotropy	0.771	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.9	EDS
Estimated twinning fraction	0.136 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 39684 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAD, 2DT, 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	P	0.73	0/229	0.84	0/351
1	Q	0.54	0/229	0.86	0/351
2	T	0.67	0/232	0.82	0/356
2	U	0.54	0/232	0.74	0/356
3	A	0.46	0/4899	0.68	1/6701 (0.0%)
3	C	0.42	0/4887	0.66	0/6685
4	B	0.39	0/730	0.65	0/1006
4	D	0.38	0/725	0.63	0/998
All	All	0.45	0/12163	0.68	1/16804 (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	P	0	2
1	Q	0	1
3	A	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	181	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	409	TYR	Sidechain
1	P	17	DT	Sidechain
1	P	19	DC	Sidechain
1	Q	20	DC	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	P	224	0	124	18	0
1	Q	224	0	124	17	0
2	T	207	0	112	5	0
2	U	207	0	112	6	0
3	A	4782	0	4271	326	0
3	C	4772	0	4237	333	0
4	B	716	0	647	76	0
4	D	712	0	647	73	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	29	0	12	0	0
6	C	29	0	12	0	0
All	All	11904	0	10298	818	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 37.

The worst 5 of 818 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)
3:C:391:MET:HE1	3:C:392:ILE:HD13	1.38	1.02
3:C:131:ARG:HH11	3:C:131:ARG:HA	1.21	1.01
3:A:131:ARG:HH11	3:A:131:ARG:HA	1.21	1.00
3:A:164:ASN:HD21	3:A:167:MET:H	1.12	0.97
3:C:126:GLU:HG2	3:C:127:ALA:H	1.26	0.96

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	
3	A	646/698 (93%)	513 (79%)	111 (17%)	22 (3%)	5	31
3	C	645/698 (92%)	505 (78%)	117 (18%)	23 (4%)	4	30
4	B	103/108 (95%)	76 (74%)	23 (22%)	4 (4%)	4	28
4	D	103/108 (95%)	77 (75%)	21 (20%)	5 (5%)	3	22
All	All	1497/1612 (93%)	1171 (78%)	272 (18%)	54 (4%)	4	30

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	279	THR
3	A	359	LYS
3	A	426	VAL
3	A	543	ALA

### 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	
3	A	430/579 (74%)	397 (92%)	33 (8%)	16	54
3	C	427/579 (74%)	388 (91%)	39 (9%)	12	42
4	B	62/87 (71%)	58 (94%)	4 (6%)	21	61
4	D	62/87 (71%)	58 (94%)	4 (6%)	21	61
All	All	981/1332 (74%)	901 (92%)	80 (8%)	14	50

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	75	ILE
3	C	150	GLN
3	C	678	ARG
3	C	5	ASP
3	C	91	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	509	ASN
3	A	611	ASN
4	D	50	GLN
3	A	510	GLN
3	A	683	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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	$\# Z  > 2$
1	2DT	P	21	1,2	11,20,21	1.38	3 (27%)	12,28,31	4.93	3 (25%)
1	2DT	Q	21	1,2	11,20,21	1.37	3 (27%)	12,28,31	4.86	3 (25%)

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
1	2DT	P	21	1,2	-	0/3/18/19	0/2/2/2
1	2DT	Q	21	1,2	-	0/3/18/19	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	21	2DT	C6-C5	-2.28	1.33	1.40
1	Q	21	2DT	C6-C5	-2.26	1.34	1.40
1	P	21	2DT	C6-N1	2.28	1.38	1.35
1	Q	21	2DT	C6-N1	2.34	1.38	1.35
1	P	21	2DT	C4-N3	2.91	1.38	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	21	2DT	C5-C4-N3	-8.99	115.13	125.14
1	Q	21	2DT	C5-C4-N3	-8.98	115.14	125.14
1	Q	21	2DT	C5M-C5-C6	2.08	122.80	118.62
1	P	21	2DT	C5M-C5-C6	2.19	123.03	118.62
1	Q	21	2DT	C4-N3-C2	13.97	127.32	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	21	2DT	2	0
1	Q	21	2DT	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	DAD	A	4004	-	23,31,31	0.73	0	28,48,48	1.06	2 (7%)
6	DAD	C	4005	-	23,31,31	0.72	0	28,48,48	1.02	2 (7%)

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
6	DAD	A	4004	-	2/2/5/5	0/18/31/31	0/3/3/3
6	DAD	C	4005	-	2/2/5/5	0/18/31/31	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4004	DAD	PA-O3A-PB	-2.19	126.58	132.73
6	C	4005	DAD	C2'-C1'-N9	2.08	116.69	112.49
6	A	4004	DAD	O2G-PG-O1G	2.79	119.55	110.58
6	C	4005	DAD	O2G-PG-O1G	2.81	119.61	110.58

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	4004	DAD	C4'
6	A	4004	DAD	C1'
6	C	4005	DAD	C4'
6	C	4005	DAD	C1'

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](#)

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, 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	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	P	10/21 (47%)	-0.14	0 100 100	53, 64, 118, 140	0
1	Q	10/21 (47%)	-0.36	0 100 100	70, 95, 153, 171	0
2	T	10/25 (40%)	0.01	0 100 100	43, 56, 91, 100	0
2	U	10/25 (40%)	-0.32	0 100 100	65, 95, 116, 139	0
3	A	658/698 (94%)	0.04	15 (2%) 64 49	23, 65, 125, 182	0
3	C	658/698 (94%)	-0.02	23 (3%) 48 32	35, 76, 130, 198	0
4	B	105/108 (97%)	-0.08	0 100 100	48, 80, 127, 163	0
4	D	105/108 (97%)	-0.10	2 (1%) 70 55	53, 92, 122, 155	0
All	All	1566/1704 (91%)	-0.01	40 (2%) 59 45	23, 74, 130, 198	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	124	ALA	12.8
3	A	112	SER	12.6
3	A	113	GLY	11.1
3	A	114	LYS	7.9
3	C	275	CYS	7.7

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

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	2DT	Q	21	19/20	0.89	0.20	-	70,70,70,70	0
1	2DT	P	21	19/20	0.95	0.21	-	70,70,70,70	0

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	MG	A	4003	1/1	0.89	0.42	3.47	70,70,70,70	0
6	DAD	A	4004	29/29	0.77	0.20	0.09	131,131,207,207	0
6	DAD	C	4005	29/29	0.74	0.18	-	132,132,188,188	0
5	MG	C	4004	1/1	0.88	0.45	-	70,70,70,70	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.