



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:57 am BST

PDB ID : 1SKW  
Title : Binary 3' complex of T7 DNA polymerase with a DNA primer/template containing a disordered cis-syn thymine dimer on the template  
Authors : Li, Y.; Dutta, S.; Doublet, S.; Bdour, H.M.; Taylor, J.S.; Ellenberger, T.  
Deposited on : 2004-03-05  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

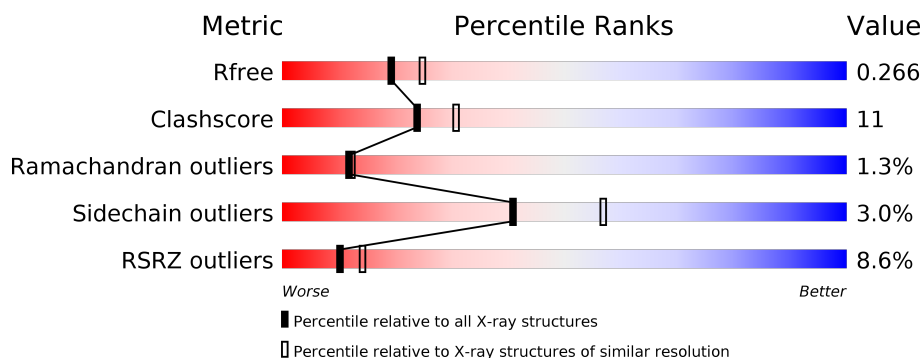
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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  $\leq 5\%$ . 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>29%</div> <div>10%</div> <div>62%</div> </div>
2	T	25	<div> <div>4%</div> <div>32%</div> <div>60%</div> </div>
3	A	698	<div> <div>9%</div> <div>74%</div> <div>21%</div> </div>
4	B	108	<div> <div>4%</div> <div>73%</div> <div>23%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6578 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\*C\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*(2DT))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	8	Total	C	N	O	P	0	0	0
			161	77	28	48	8			

- Molecule 2 is a DNA chain called 5'-D(\*CP\*CP\*CP\*(TTD)P\*AP\*GP\*GP\*CP\*AP\*CP\*T P\*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			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	678	Total	C	N	O	S	0	0	0
			5227	3331	904	968	24			

There are 6 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

- 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
			781	507	123	148	3			

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	8	Total 8	O 8	0	0
6	T	11	Total 11	O 11	0	0
6	A	167	Total 167	O 167	0	0
6	B	15	Total 15	O 15	0	0

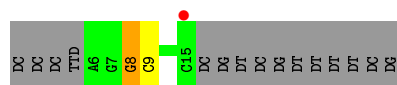
### 3 Residue-property plots

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 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.

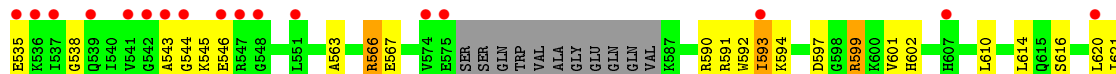
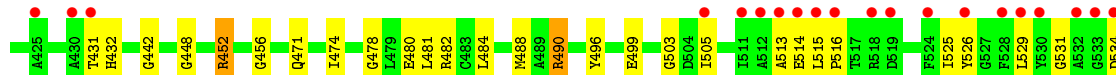
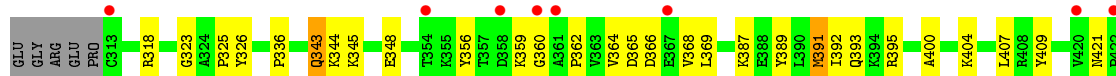
- Molecule 1: 5'-D(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*AP\*C\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*(2DT))-3'

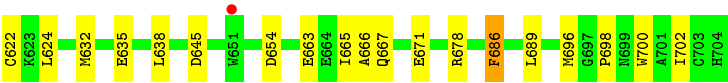


- Molecule 2: 5'-D(\*CP\*CP\*CP\*(TTD)P\*AP\*GP\*GP\*CP\*AP\*CP\*TP\*GP\*GP\*CP\*CP\*GP\*TP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*G)-3'

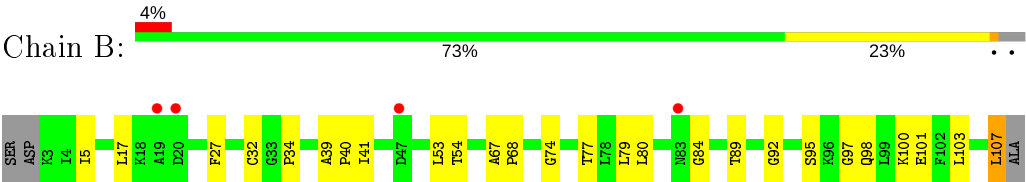


- Molecule 3: DNA polymerase





● Molecule 4: thioredoxin 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.72Å 211.49Å 52.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 41.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.30) 98.4 (41.94-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.32Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.239 , 0.278 0.230 , 0.266	Depositor DCC
$R_{free}$ test set	2539 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	0/158	0.83	0/241
2	T	0.52	0/232	0.84	0/356
3	A	0.36	0/5358	0.57	0/7280
4	B	0.32	0/796	0.58	0/1084
All	All	0.37	0/6544	0.59	0/8961

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
2	T	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	T	8	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	P	161	0	91	3	0
2	T	207	0	112	2	0
3	A	5227	0	4930	118	0
4	B	781	0	774	15	0
5	A	1	0	0	0	0
6	A	167	0	0	4	0
6	B	15	0	0	0	0
6	P	8	0	0	0	0
6	T	11	0	0	0	0
All	All	6578	0	5907	136	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 11.

All (136) 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:A:276:HIS:HD2	3:A:278:ARG:H	1.27	0.83
3:A:566:ARG:HB2	3:A:566:ARG:HH11	1.43	0.83
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.68	0.74
3:A:663:GLU:HG3	3:A:696:MET:SD	2.29	0.72
3:A:145:ARG:O	3:A:149:GLU:HB2	1.90	0.71
1:P:16:DG:H1'	1:P:17:DT:H5''	1.74	0.69
4:B:95:SER:OG	4:B:98:GLN:HG3	1.93	0.69
3:A:49:GLU:HA	3:A:52:ARG:NH1	2.09	0.68
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.29	0.67
3:A:566:ARG:CB	3:A:566:ARG:HH11	2.07	0.67
3:A:173:GLN:O	3:A:176:VAL:HG22	1.95	0.65
3:A:343:GLN:HG3	3:A:362:PRO:CG	2.25	0.65
3:A:276:HIS:CD2	3:A:278:ARG:H	2.13	0.65
3:A:391:MET:HE2	3:A:391:MET:O	1.97	0.65
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.78	0.64
3:A:366:ASP:OD1	3:A:387:LYS:HD2	1.99	0.63
3:A:481:LEU:HD21	3:A:525:ILE:HG12	1.80	0.62
3:A:496:TYR:CZ	3:A:505:ILE:HD11	2.35	0.62
3:A:79:ARG:HD3	6:A:5042:HOH:O	1.99	0.61
3:A:147:LEU:C	3:A:149:GLU:H	2.04	0.61
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.82	0.61
3:A:290:LYS:HD3	3:A:291:THR:N	2.15	0.60
3:A:343:GLN:HG3	3:A:362:PRO:HG3	1.81	0.60
3:A:667:GLN:O	3:A:671:GLU:HG3	2.01	0.60
3:A:499:GLU:OE1	3:A:503:GLY:HA3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.84	0.58
3:A:35:ARG:HB3	3:A:36:PRO:CD	2.34	0.57
3:A:484:LEU:HD22	3:A:529:LEU:HD21	1.87	0.57
3:A:496:TYR:CE1	3:A:505:ILE:HD11	2.40	0.57
3:A:391:MET:HE3	3:A:395:ARG:HG3	1.86	0.57
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.05	0.56
3:A:94:LEU:HB3	3:A:185:LEU:HD13	1.86	0.56
2:T:8:DG:H2''	2:T:9:DC:H5'	1.87	0.56
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.45	0.56
3:A:131:ARG:O	3:A:135:MET:HG2	2.05	0.56
3:A:663:GLU:O	3:A:696:MET:HE1	2.05	0.56
3:A:144:LYS:HB3	3:A:144:LYS:NZ	2.21	0.56
3:A:478:GLY:O	3:A:482:ARG:HG3	2.06	0.55
3:A:632:MET:O	3:A:635:GLU:HG2	2.05	0.55
3:A:538:GLY:HA3	3:A:544:GLY:O	2.06	0.55
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.06	0.55
3:A:49:GLU:HA	3:A:52:ARG:HH11	1.71	0.55
4:B:53:LEU:HD12	4:B:107:LEU:HD11	1.88	0.55
3:A:130:TYR:CZ	3:A:134:GLU:HG3	2.42	0.54
3:A:566:ARG:HB2	3:A:566:ARG:NH1	2.18	0.54
4:B:5:ILE:HD12	4:B:54:THR:HG21	1.90	0.54
3:A:391:MET:CE	3:A:395:ARG:HG3	2.37	0.54
3:A:85:ARG:HG3	3:A:222:TRP:CG	2.43	0.54
3:A:513:ALA:O	3:A:515:LEU:N	2.41	0.54
3:A:666:ALA:HB3	3:A:696:MET:HE2	1.90	0.54
3:A:336:PRO:HB2	3:A:389:TYR:CE1	2.43	0.53
1:P:16:DG:H2''	1:P:17:DT:H5'	1.91	0.53
3:A:344:LYS:O	3:A:348:GLU:HG3	2.09	0.53
3:A:525:ILE:HG23	3:A:526:TYR:N	2.24	0.53
3:A:698:PRO:CG	3:A:702:ILE:HD12	2.39	0.52
3:A:474:ILE:N	3:A:474:ILE:HD12	2.25	0.52
3:A:326:TYR:HB3	4:B:92:GLY:HA2	1.92	0.52
2:T:9:DC:H4'	3:A:432:HIS:O	2.09	0.52
3:A:356:TYR:HD2	3:A:360:GLY:O	1.93	0.51
3:A:343:GLN:CG	3:A:362:PRO:HG3	2.41	0.51
3:A:368:VAL:HG23	3:A:369:LEU:N	2.26	0.51
3:A:666:ALA:HB3	3:A:696:MET:CE	2.41	0.51
3:A:143:PHE:HE2	3:A:158:MET:HG3	1.75	0.50
3:A:173:GLN:NE2	3:A:176:VAL:HG21	2.25	0.50
1:P:16:DG:H2''	1:P:17:DT:C5'	2.42	0.50
4:B:74:GLY:O	4:B:77:THR:OG1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:484:LEU:O	3:A:488:MET:HG2	2.11	0.50
3:A:593:ILE:HG22	3:A:601:VAL:HB	1.93	0.50
3:A:678:ARG:NH2	3:A:689:LEU:HD11	2.26	0.49
3:A:456:GLY:HA2	3:A:471:GLN:OE1	2.12	0.49
3:A:49:GLU:OE2	3:A:54:GLY:HA3	2.13	0.49
3:A:593:ILE:HD13	3:A:594:LYS:H	1.77	0.49
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.47	0.49
3:A:233:PRO:HB2	3:A:456:GLY:O	2.13	0.49
3:A:323:GLY:O	3:A:325:PRO:HD3	2.13	0.48
3:A:112:SER:OG	3:A:130:TYR:HE1	1.97	0.48
3:A:448:GLY:O	3:A:452:ARG:HB2	2.14	0.48
3:A:144:LYS:HG2	3:A:154:TYR:CD1	2.49	0.48
3:A:264:TRP:CZ3	3:A:345:LYS:HE2	2.49	0.48
3:A:282:PRO:O	3:A:284:PRO:HD3	2.14	0.48
3:A:145:ARG:HH11	3:A:145:ARG:HG3	1.79	0.47
3:A:158:MET:HA	3:A:161:TRP:CE2	2.50	0.47
3:A:698:PRO:HG2	3:A:702:ILE:HD12	1.96	0.47
3:A:196:ILE:HB	3:A:198:PHE:CE1	2.50	0.47
3:A:91:THR:HB	3:A:181:LEU:HD13	1.96	0.47
3:A:480:GLU:HB3	3:A:529:LEU:HD13	1.97	0.47
3:A:391:MET:HE1	3:A:392:ILE:HA	1.96	0.46
3:A:365:ASP:O	3:A:368:VAL:HG22	2.16	0.46
3:A:442:GLY:O	3:A:448:GLY:HA3	2.16	0.45
3:A:143:PHE:CE2	3:A:158:MET:HG3	2.52	0.45
3:A:404:LYS:HA	3:A:409:TYR:HE2	1.81	0.45
3:A:203:TYR:CE1	3:A:204:THR:HG22	2.51	0.45
3:A:282:PRO:C	3:A:284:PRO:HD3	2.37	0.45
3:A:534:ASP:C	3:A:545:LYS:HA	2.37	0.45
3:A:135:MET:HG3	3:A:174:ASP:OD1	2.16	0.45
4:B:41:ILE:N	4:B:41:ILE:HD12	2.32	0.44
3:A:155:VAL:O	3:A:156:ASP:C	2.55	0.44
3:A:195:GLU:HG3	3:A:195:GLU:H	1.46	0.44
3:A:622:CYS:SG	3:A:654:ASP:HA	2.57	0.44
3:A:38:ASP:HA	6:A:5104:HOH:O	2.17	0.44
3:A:563:ALA:O	3:A:567:GLU:HG3	2.18	0.43
3:A:400:ALA:CB	3:A:407:LEU:HD12	2.49	0.43
3:A:159:GLU:HG2	3:A:160:TRP:CD1	2.53	0.43
3:A:666:ALA:CB	3:A:696:MET:HE2	2.48	0.43
3:A:590:ARG:HD3	3:A:592:TRP:CZ2	2.54	0.43
3:A:53:GLY:HA2	6:A:5034:HOH:O	2.18	0.43
3:A:145:ARG:CZ	3:A:145:ARG:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:391:MET:HE2	3:A:391:MET:C	2.39	0.43
3:A:452:ARG:HG3	3:A:700:TRP:HB3	2.00	0.43
3:A:616:SER:O	3:A:620:LEU:HG	2.19	0.43
4:B:67:ALA:HB3	4:B:68:PRO:HD3	2.00	0.43
3:A:147:LEU:C	3:A:149:GLU:N	2.72	0.42
3:A:490:ARG:CB	3:A:490:ARG:HH11	2.33	0.42
4:B:103:LEU:O	4:B:107:LEU:HB2	2.19	0.42
3:A:261:PHE:HB3	3:A:345:LYS:HE3	2.01	0.42
3:A:176:VAL:HG23	3:A:177:VAL:N	2.35	0.42
3:A:391:MET:CE	3:A:395:ARG:CG	2.97	0.42
3:A:400:ALA:HB2	3:A:407:LEU:HD12	2.01	0.42
3:A:525:ILE:CG2	3:A:526:TYR:N	2.82	0.42
3:A:276:HIS:CD2	3:A:278:ARG:HB3	2.55	0.42
3:A:610:LEU:O	3:A:614:LEU:HG	2.20	0.42
4:B:100:LYS:HB3	4:B:100:LYS:NZ	2.34	0.42
3:A:236:THR:O	3:A:240:GLU:HG3	2.20	0.41
3:A:621:ILE:HD11	3:A:686:PHE:CZ	2.55	0.41
3:A:79:ARG:HG2	3:A:80:GLU:N	2.35	0.41
3:A:452:ARG:NH2	6:A:5040:HOH:O	2.45	0.41
3:A:638:LEU:N	3:A:638:LEU:CD1	2.83	0.41
3:A:47:GLU:HG3	3:A:81:PHE:HE1	1.85	0.41
3:A:591:ARG:HG2	3:A:602:HIS:CE1	2.56	0.41
4:B:97:GLY:O	4:B:101:GLU:HG3	2.21	0.41
3:A:158:MET:HA	3:A:161:TRP:CD2	2.56	0.41
3:A:22:VAL:HB	3:A:175:VAL:HG21	2.03	0.40
4:B:27:PHE:HE1	4:B:79:LEU:HD22	1.86	0.40
3:A:364:VAL:O	3:A:364:VAL:HG12	2.20	0.40
4:B:77:THR:HG22	4:B:79:LEU:HD13	2.01	0.40
4:B:17:LEU:HA	4:B:84:GLY:HA2	2.03	0.40

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	672/698 (96%)	634 (94%)	28 (4%)	10 (2%)	10	10
4	B	103/108 (95%)	103 (100%)	0	0	100	100
All	All	775/806 (96%)	737 (95%)	28 (4%)	10 (1%)	12	12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	516	PRO
3	A	318	ARG
3	A	514	GLU
3	A	531	GLY
3	A	543	ALA
3	A	148	GLU
3	A	546	GLU
3	A	359	LYS
3	A	535	GLU

### 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	513/579 (89%)	498 (97%)	15 (3%)	42	58
4	B	79/87 (91%)	76 (96%)	3 (4%)	33	47
All	All	592/666 (89%)	574 (97%)	18 (3%)	41	57

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	171	ASN
3	A	181	LEU
3	A	195	GLU
3	A	232	PHE
3	A	249	ARG
3	A	343	GLN

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Mol	Chain	Res	Type
3	A	391	MET
3	A	393	GLN
3	A	452	ARG
3	A	490	ARG
3	A	566	ARG
3	A	593	ILE
3	A	599	ARG
3	A	624	LEU
3	A	686	PHE
4	B	80	LEU
4	B	89	THR
4	B	107	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	173	GLN
3	A	276	HIS
3	A	502	ASN
3	A	602	HIS
3	A	667	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2DT	P	21	1,2	14,20,21	1.18	1 (7%)	12,28,31	4.28	1 (8%)

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	-	0/4/18/19	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	21	2DT	C4-N3	3.13	1.38	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	21	2DT	C4-N3-C2	14.47	127.36	115.14

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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](#)

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	7/21 (33%)	-0.09	0 100 100	29, 34, 50, 57	0
2	T	10/25 (40%)	0.24	1 (10%) 7 10	28, 40, 55, 59	0
3	A	678/698 (97%)	0.41	64 (9%) 8 11	18, 35, 61, 67	0
4	B	105/108 (97%)	0.14	4 (3%) 40 47	28, 43, 55, 59	0
All	All	800/852 (93%)	0.37	69 (8%) 10 14	18, 36, 61, 67	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	535	GLU	5.2
3	A	294	VAL	5.0
3	A	541	VAL	4.8
3	A	542	GLY	4.6
3	A	358	ASP	4.4
3	A	533	GLY	4.1
3	A	537	ILE	4.1
3	A	529	LEU	3.9
3	A	519	ASP	3.7
3	A	515	LEU	3.7
3	A	543	ALA	3.5
3	A	360	GLY	3.5
3	A	528	PHE	3.5
3	A	313	CYS	3.5
3	A	513	ALA	3.4
3	A	607	HIS	3.4
3	A	532	ALA	3.4
3	A	298	PHE	3.4
3	A	536	LYS	3.4
3	A	548	GLY	3.3
3	A	575	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
3	A	524	PHE	3.2
3	A	430	ALA	3.2
3	A	551	LEU	3.1
3	A	514	GLU	3.1
3	A	512	ALA	3.0
3	A	530	TYR	2.9
3	A	534	ASP	2.9
3	A	505	ILE	2.9
3	A	148	GLU	2.8
3	A	354	THR	2.7
3	A	544	GLY	2.7
3	A	547	ARG	2.7
3	A	539	GLN	2.7
3	A	301	PRO	2.6
3	A	156	ASP	2.6
3	A	153	GLU	2.6
4	B	47	ASP	2.5
2	T	15	DC	2.5
3	A	422	PRO	2.4
3	A	111	ARG	2.4
3	A	511	ILE	2.4
3	A	574	VAL	2.3
3	A	361	ALA	2.3
3	A	300	LYS	2.3
3	A	221	ALA	2.3
3	A	620	LEU	2.3
3	A	425	ALA	2.3
3	A	135	MET	2.2
3	A	420	VAL	2.2
3	A	147	LEU	2.2
3	A	516	PRO	2.2
3	A	173	GLN	2.2
3	A	367	GLU	2.2
3	A	302	LYS	2.1
3	A	224	LEU	2.1
3	A	272	GLU	2.1
3	A	593	ILE	2.1
3	A	518	ARG	2.1
4	B	20	ASP	2.1
3	A	431	THR	2.1
3	A	145	ARG	2.1
3	A	278	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
4	B	83	ASN	2.1
3	A	295	GLY	2.1
3	A	526	TYR	2.1
4	B	19	ALA	2.0
3	A	546	GLU	2.0
3	A	651	TRP	2.0

## 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
1	2DT	P	21	19/20	0.97	0.14	26,29,32,32	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	A	4003	1/1	0.86	0.23	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.