



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2017 – 01:05 PM EST

PDB ID : 3C5G  
Title : Structure of a ternary complex of the R517K Pol lambda mutant  
Authors : Garcia-Diaz, M.; Bebenek, K.; Foley, M.C.; Pedersen, L.C.; Schlick, T.; Kunkel, T.A.  
Deposited on : 2008-01-31  
Resolution : 2.20 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

<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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

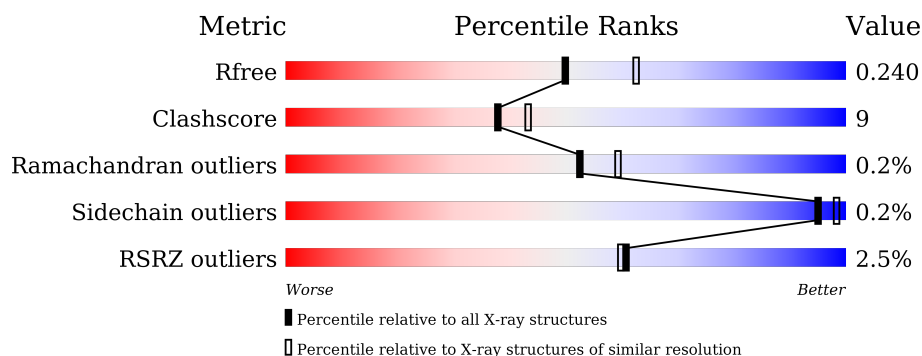
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	A	335	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div></div> </div> <div>.</div> </div>
1	B	335	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div></div> </div> <div>..</div> </div>
2	T	11	<div> <div>73%</div> <div>27%</div> </div>
2	U	11	<div> <div>73%</div> <div>27%</div> </div>
3	P	6	<div> <div>83%</div> <div>17%</div> </div>
3	Q	6	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	4	 <div>25% 75%</div>
4	E	4	 <div>50% 25% 25%</div>

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
6	NA	A	804	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6914 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 polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2534	1593	460	469	12			
1	B	329	Total	C	N	O	S	0	10	0
			2622	1645	480	485	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	expression tag	UNP Q9UGP5
A	517	LYS	ARG	engineered	UNP Q9UGP5
B	241	MET	-	expression tag	UNP Q9UGP5
B	517	LYS	ARG	engineered	UNP Q9UGP5

- Molecule 2 is a DNA chain called DNA (5'-D(\*DCP\*DGP\*DGP\*DCP\*DAP\*DAP\*DTP\*DAP\*DCP\*DTP\*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	11	Total	C	N	O	P	0	0	0
			223	107	43	63	10			
2	U	11	Total	C	N	O	P	0	0	0
			223	107	43	63	10			

- Molecule 3 is a DNA chain called DNA (5'-D(\*DCP\*DAP\*DGP\*DTP\*DAP\*(2DT))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	6	Total	C	N	O	P	0	0	0
			119	59	22	33	5			
3	Q	6	Total	C	N	O	P	0	0	0
			119	59	22	33	5			

- Molecule 4 is a DNA chain called DNA (5'-D(P\*DGP\*DCP\*DCP\*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
4	E	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			

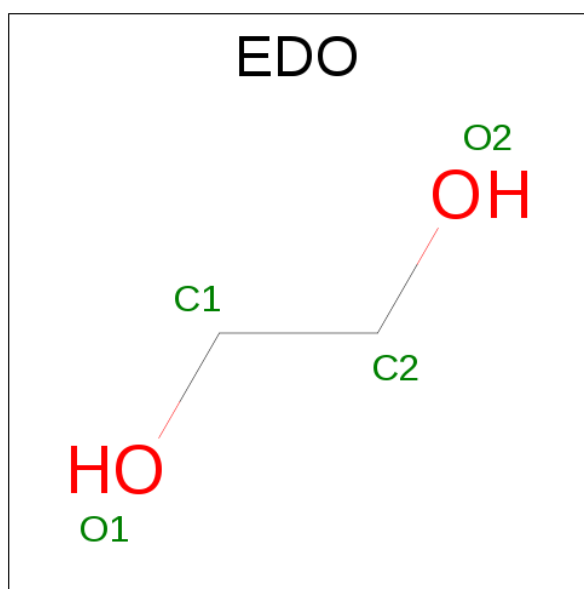
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

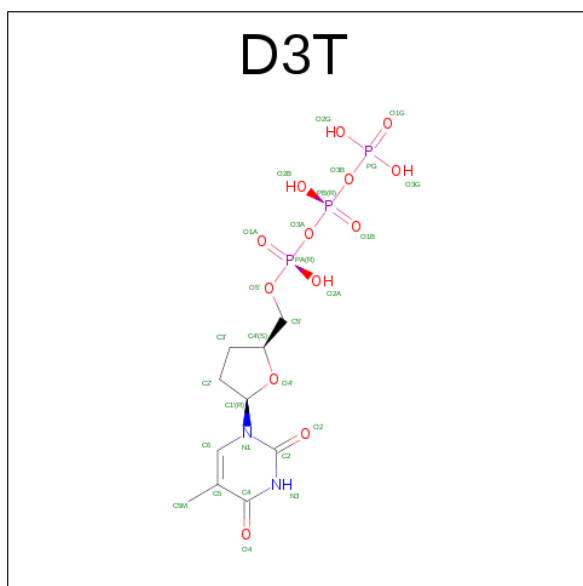
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	1	Total	Na	0	0
			1	1		
6	B	4	Total	Na	0	0
			4	4		
6	A	3	Total	Na	0	0
			3	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	T	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 2',3'-DIDEOXY-THYMIDINE-5'-TRIPHOSPHATE (three-letter code: D3T) (formula:  $C_{10}H_{17}N_2O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	2	13	3		
8	A	1	Total	C	N	O	P	0	0
			28	10	2	13	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	324	Total	O	0	0
			324	324		
9	T	49	Total	O	0	0
			49	49		
9	P	26	Total	O	0	0
			26	26		
9	D	13	Total	O	0	0
			13	13		
9	B	362	Total	O	0	0
			362	362		
9	U	31	Total	O	0	0
			31	31		

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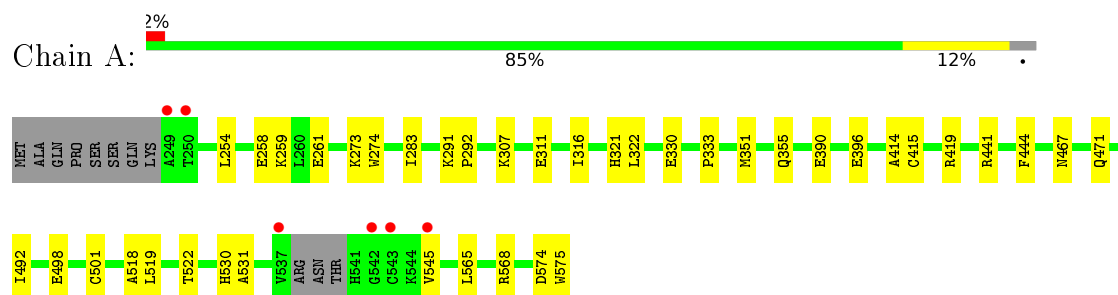
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	Q	24	Total 24	O 24	0	0
9	E	9	Total 9	O 9	0	0

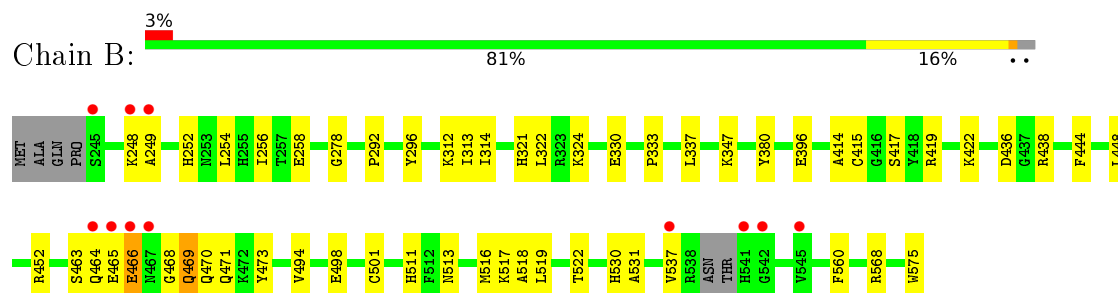
### 3 Residue-property plots [i](#)

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.

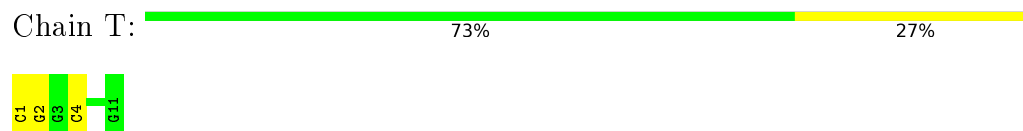
- Molecule 1: DNA polymerase lambda



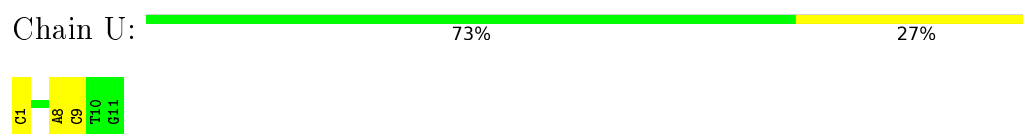
- Molecule 1: DNA polymerase lambda



- Molecule 2: DNA (5'-D(\*DCP\*DGP\*DGP\*DCP\*DAP\*DAP\*DTP\*DAP\*DCP\*DTP\*DG)-3')




- Molecule 2: DNA (5'-D(\*DCP\*DGP\*DGP\*DCP\*DAP\*DAP\*DTP\*DAP\*DCP\*DTP\*DG)-3')



- Molecule 3: DNA (5'-D(\*DCP\*DAP\*DGP\*DTP\*DAP\*(2DT))-3')

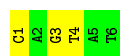


Chain P:  83% 17%




- Molecule 3: DNA (5'-D(\*DCP\*DAP\*DGP\*DTP\*DAP\*(2DT))-3')

Chain Q:  50% 50%



- Molecule 4: DNA (5'-D(P\*DGP\*DCP\*DCP\*DG)-3')

Chain D:  25% 75%



- Molecule 4: DNA (5'-D(P\*DGP\*DCP\*DCP\*DG)-3')

Chain E:  50% 25% 25%



## 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, $\alpha$ , $\beta$ , $\gamma$	94.33 Å   150.82 Å   85.82 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 2.20 37.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.2 (50.00-2.20) 88.6 (37.81-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.20 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.201   ,   0.236 0.206   ,   0.240	Depositor DCC
$R_{free}$ test set	2806 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.61 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.5655e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2DT, MG, EDO, D3T, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.37	0/2585	0.59	0/3487
1	B	2.79	2/2678 (0.1%)	0.72	4/3613 (0.1%)
2	T	0.35	0/250	0.74	0/384
2	U	0.33	0/250	0.69	0/384
3	P	0.42	0/112	0.79	0/171
3	Q	0.40	0/112	0.75	0/171
4	D	0.94	1/92 (1.1%)	0.73	0/138
4	E	0.91	1/92 (1.1%)	0.74	0/138
All	All	1.86	4/6171 (0.1%)	0.67	4/8486 (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	B	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466[A]	GLU	CB-CG	101.11	3.44	1.52
1	B	466[B]	GLU	CB-CG	101.11	3.44	1.52
4	D	1	DG	OP3-P	-7.31	1.52	1.61
4	E	1	DG	OP3-P	-6.94	1.52	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466[A]	GLU	CA-CB-CG	-16.33	77.47	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466[B]	GLU	CA-CB-CG	-16.33	77.47	113.40
1	B	466[A]	GLU	N-CA-C	5.61	126.15	111.00
1	B	466[B]	GLU	N-CA-C	5.61	126.15	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	469[B]	GLN	Mainchain
1	B	511[B]	HIS	Mainchain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2534	0	2522	38	0
1	B	2622	0	2584	68	0
2	T	223	0	125	3	0
2	U	223	0	125	16	0
3	P	119	0	70	1	0
3	Q	119	0	70	3	0
4	D	83	0	45	1	0
4	E	83	0	45	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	3	0	0	0	0
6	B	4	0	0	0	0
6	P	1	0	0	0	0
7	T	4	0	6	0	0
8	A	28	0	13	0	0
8	B	28	0	13	0	0
9	A	324	0	0	3	0
9	B	362	0	0	2	0
9	D	13	0	0	0	0
9	E	9	0	0	0	0
9	P	26	0	0	0	0
9	Q	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	T	49	0	0	0	0
9	U	31	0	0	0	0
All	All	6914	0	5618	107	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 9.

All (107) 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)
1:B:464[B]:GLN:NE2	2:U:8:DA:H4'	1.55	1.20
2:U:1:DC:H6	2:U:1:DC:HO5'	1.10	0.97
1:B:464[B]:GLN:HE22	2:U:8:DA:H4'	1.07	0.95
1:B:444:PHE:CE1	1:B:465[B]:GLU:CB	2.52	0.93
1:A:568:ARG:HH12	1:A:575:TRP:HE1	1.20	0.85
1:B:464[B]:GLN:CD	2:U:8:DA:H4'	2.06	0.75
1:B:254:LEU:O	1:B:258:GLU:HG2	1.88	0.72
3:P:1:DC:H5''	1:B:537:VAL:HG22	1.71	0.72
1:B:438:ARG:HG3	1:B:438:ARG:HH11	1.57	0.69
1:A:574:ASP:HB3	9:A:1061:HOH:O	1.94	0.68
1:B:444:PHE:CD1	1:B:465[B]:GLU:CB	2.76	0.68
1:A:441:ARG:NH2	1:B:466[B]:GLU:OE2	2.27	0.67
1:B:312:LYS:NZ	1:B:324:LYS:NZ	2.43	0.67
1:B:464[B]:GLN:HB2	2:U:9:DC:H5'	1.78	0.65
1:B:464[B]:GLN:HB2	2:U:9:DC:C5'	2.26	0.65
1:A:396:GLU:HG3	1:A:414:ALA:HB2	1.79	0.64
1:B:464[B]:GLN:OE1	2:U:8:DA:H5''	2.00	0.62
1:A:568:ARG:NH1	1:A:575:TRP:CZ2	2.68	0.61
1:A:441:ARG:NE	1:B:466[B]:GLU:OE2	2.33	0.61
1:A:351:MET:O	1:A:355:GLN:HG3	2.03	0.58
1:A:575:TRP:N	1:A:575:TRP:CD1	2.66	0.58
2:T:1:DC:H2''	2:T:2:DG:H5'	1.87	0.57
1:A:498:GLU:HG2	1:A:530:HIS:O	2.05	0.57
1:A:330:GLU:O	1:A:333:PRO:HD2	2.05	0.56
1:A:519:LEU:HD22	1:A:565:LEU:HD21	1.88	0.56
1:B:498:GLU:HG2	1:B:530:HIS:O	2.05	0.56
4:E:1:DG:H2''	4:E:2:DC:H5'	1.88	0.56
1:B:465[B]:GLU:HA	1:B:471:GLN:HB3	1.88	0.55
1:B:252:HIS:HB3	1:B:292:PRO:HG3	1.87	0.55
1:A:519:LEU:HD22	1:A:565:LEU:HD11	1.89	0.55
1:A:441:ARG:CZ	1:B:465[A]:GLU:CB	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:ARG:HD2	9:B:872:HOH:O	2.06	0.54
1:A:575:TRP:H	1:A:575:TRP:HD1	1.55	0.54
1:B:248:LYS:HG3	1:B:249:ALA:N	2.23	0.54
1:A:471:GLN:NE2	9:A:1062:HOH:O	2.40	0.53
1:B:312:LYS:HZ1	1:B:324:LYS:HZ2	1.56	0.53
1:B:470:GLN:HG2	1:B:494:VAL:HG12	1.91	0.53
1:B:464[B]:GLN:CD	2:U:8:DA:O3'	2.47	0.52
1:B:417:SER:HB2	1:B:422:LYS:HG3	1.92	0.52
1:A:441:ARG:CZ	1:B:466[B]:GLU:OE2	2.57	0.52
1:B:312:LYS:NZ	1:B:324:LYS:HZ1	2.08	0.52
1:B:422:LYS:HE2	1:B:422:LYS:HA	1.93	0.51
1:B:448:LEU:O	1:B:452:ARG:HG3	2.10	0.51
2:T:1:DC:H2'	2:T:2:DG:C8	2.45	0.51
1:B:330:GLU:O	1:B:333:PRO:HD2	2.11	0.51
1:B:464[B]:GLN:O	1:B:471:GLN:HA	2.10	0.51
1:A:501:CYS:SG	1:A:531:ALA:HA	2.51	0.50
1:B:464[A]:GLN:HG2	1:B:465[A]:GLU:H	1.77	0.50
1:B:312:LYS:HZ3	1:B:324:LYS:HZ1	1.60	0.49
1:B:312:LYS:NZ	1:B:324:LYS:HZ2	2.10	0.49
1:A:467:ASN:ND2	1:B:469[A]:GLN:HG2	2.28	0.49
1:B:518:ALA:O	1:B:522:THR:HG23	2.12	0.49
1:A:259:LYS:HB2	1:A:316:ILE:HD13	1.93	0.49
1:B:464[B]:GLN:O	1:B:464[B]:GLN:HG2	2.13	0.48
1:A:568:ARG:NH1	1:A:575:TRP:HZ2	2.09	0.48
1:A:575:TRP:N	1:A:575:TRP:HD1	2.09	0.48
1:B:468[A]:GLY:HA3	9:B:1081:HOH:O	2.14	0.48
1:B:296:TYR:N	1:B:314:ILE:HD11	2.28	0.48
1:B:438:ARG:HH11	1:B:438:ARG:CG	2.24	0.47
1:A:471:GLN:O	1:A:492:ILE:HA	2.14	0.47
1:B:312:LYS:HZ1	1:B:324:LYS:NZ	2.10	0.47
1:A:441:ARG:NH2	1:B:465[A]:GLU:CB	2.78	0.47
1:B:463[A]:SER:HB2	1:B:473:TYR:CD1	2.50	0.46
1:B:464[B]:GLN:HB2	2:U:9:DC:H5''	1.96	0.46
1:B:464[B]:GLN:OE1	2:U:8:DA:C5'	2.63	0.46
1:A:518:ALA:O	1:A:522:THR:HG23	2.16	0.46
1:B:278:GLY:HA3	4:E:1:DG:H1'	1.98	0.46
1:B:501:CYS:SG	1:B:531:ALA:HA	2.56	0.45
1:B:436:ASP:OD1	1:B:436:ASP:C	2.54	0.45
4:D:3:DC:H2''	4:D:4:DG:C8	2.52	0.45
1:A:307:LYS:O	1:A:311:GLU:HG3	2.17	0.45
1:B:396:GLU:HG3	1:B:414:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:MET:HE1	1:B:560:PHE:CZ	2.51	0.45
1:A:568:ARG:NH1	1:A:575:TRP:CE2	2.86	0.44
1:B:513:ASN:O	1:B:517:LYS:HG3	2.17	0.44
9:A:1049:HOH:O	3:Q:1:DC:H5'	2.16	0.44
1:A:261:GLU:HG2	1:A:283:ILE:HD13	1.99	0.44
1:A:321:HIS:CG	1:A:322:LEU:N	2.86	0.44
3:Q:3:DG:H2''	3:Q:4:DT:O5'	2.17	0.44
1:B:321:HIS:CG	1:B:322:LEU:N	2.86	0.44
1:A:254:LEU:O	1:A:258:GLU:HB2	2.18	0.43
1:B:463[A]:SER:HB2	1:B:473:TYR:HD1	1.82	0.43
1:B:256:ILE:HD13	1:B:313:ILE:HG23	1.99	0.43
1:A:568:ARG:NH1	1:A:575:TRP:NE1	2.58	0.43
1:A:291:LYS:HB2	1:A:292:PRO:HD2	2.00	0.43
1:A:467:ASN:CG	1:B:469[A]:GLN:HG2	2.38	0.43
1:B:464[B]:GLN:OE1	2:U:8:DA:C4'	2.67	0.43
1:B:575:TRP:N	1:B:575:TRP:CD1	2.86	0.43
1:B:519:LEU:C	1:B:519:LEU:HD13	2.39	0.42
1:A:390:GLU:CD	1:A:390:GLU:H	2.22	0.42
1:A:261:GLU:CG	1:A:283:ILE:HD13	2.50	0.42
1:B:464[B]:GLN:OE1	2:U:8:DA:H4'	2.20	0.42
1:B:347:LYS:HB2	3:Q:4:DT:OP2	2.19	0.42
1:B:438:ARG:NH1	1:B:438:ARG:CG	2.81	0.42
1:B:337:LEU:HD12	1:B:380:TYR:OH	2.20	0.41
1:B:470:GLN:CG	1:B:494:VAL:HG12	2.49	0.41
1:A:415:CYS:HA	1:A:419:ARG:HB2	2.01	0.41
2:U:8:DA:H2''	2:U:9:DC:OP2	2.19	0.41
1:B:415:CYS:HA	1:B:419:ARG:HB2	2.01	0.41
1:B:464[B]:GLN:HE22	2:U:8:DA:C4'	2.01	0.41
1:A:519:LEU:CD2	1:A:565:LEU:HD11	2.50	0.41
1:B:296:TYR:HB2	1:B:314:ILE:HG13	2.03	0.41
1:B:464[B]:GLN:CD	2:U:8:DA:C4'	2.83	0.41
1:A:274:TRP:CZ3	2:T:4:DC:H2''	2.56	0.40
1:B:464[B]:GLN:NE2	2:U:8:DA:C4'	2.50	0.40
1:B:464[A]:GLN:HE21	1:B:464[A]:GLN:HB3	1.72	0.40
1:A:273:LYS:HB2	1:A:273:LYS:HE3	1.97	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/335 (96%)	309 (97%)	10 (3%)	1 (0%)	46	50
1	B	335/335 (100%)	326 (97%)	9 (3%)	0	100	100
All	All	655/670 (98%)	635 (97%)	19 (3%)	1 (0%)	52	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	545	VAL

### 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	Percentiles	
1	A	268/281 (95%)	267 (100%)	1 (0%)	93	97
1	B	274/281 (98%)	274 (100%)	0	100	100
All	All	542/562 (96%)	541 (100%)	1 (0%)	95	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	444	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	511	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	$\# Z  > 2$
3	2DT	P	6	3,2	11,20,21	1.23	2 (18%)	12,28,31	5.41	3 (25%)
3	2DT	Q	6	3,2	11,20,21	1.21	2 (18%)	12,28,31	5.43	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
3	2DT	P	6	3,2	-	0/3/18/19	0/2/2/2
3	2DT	Q	6	3,2	-	0/3/18/19	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	6	2DT	C6-C5	-2.17	1.34	1.40
3	P	6	2DT	C6-C5	-2.11	1.34	1.40
3	Q	6	2DT	C4-N3	3.09	1.38	1.33
3	P	6	2DT	C4-N3	3.28	1.39	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	6	2DT	C5-C4-N3	-11.98	115.30	125.35
3	Q	6	2DT	C5-C4-N3	-11.89	115.36	125.35
3	P	6	2DT	C5M-C5-C6	2.16	123.01	118.63
3	Q	6	2DT	C5M-C5-C6	2.24	123.16	118.63
3	P	6	2DT	C4-N3-C2	14.06	126.89	115.16
3	Q	6	2DT	C4-N3-C2	14.18	126.99	115.16

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 13 ligands modelled in this entry, 10 are monoatomic - leaving 3 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
8	D3T	A	576	5,6	20,29,29	1.15	1 (5%)	22,45,45	4.18	4 (18%)
8	D3T	B	577	5,6	20,29,29	1.13	1 (5%)	22,45,45	4.15	4 (18%)
7	EDO	T	2801	-	3,3,3	0.53	0	2,2,2	0.49	0

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
8	D3T	A	576	5,6	-	0/18/31/31	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	D3T	B	577	5,6	-	0/18/31/31	0/2/2/2
7	EDO	T	2801	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	576	D3T	C4-N3	3.09	1.38	1.33
8	B	577	D3T	C4-N3	3.13	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	576	D3T	C5-C4-N3	-12.32	115.01	125.35
8	B	577	D3T	C5-C4-N3	-12.11	115.18	125.35
8	A	576	D3T	C5M-C5-C6	2.24	123.16	118.63
8	B	577	D3T	C5M-C5-C6	2.25	123.18	118.63
8	B	577	D3T	O2G-PG-O1G	2.56	118.97	110.63
8	A	576	D3T	O2G-PG-O1G	2.58	119.05	110.63
8	A	576	D3T	C4-N3-C2	14.52	127.27	115.16
8	B	577	D3T	C4-N3-C2	14.52	127.28	115.16

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	A	324/335 (96%)	-0.32	6 (1%) 70 68	13, 25, 43, 79	0
1	B	329/335 (98%)	-0.31	11 (3%) 50 49	12, 24, 46, 77	1 (0%)
2	T	11/11 (100%)	-0.71	0 100 100	20, 28, 38, 40	0
2	U	11/11 (100%)	-0.38	0 100 100	23, 35, 43, 46	0
3	P	5/6 (83%)	-0.50	0 100 100	17, 19, 35, 48	0
3	Q	5/6 (83%)	-0.61	0 100 100	19, 23, 40, 47	0
4	D	4/4 (100%)	-0.90	0 100 100	22, 24, 31, 41	0
4	E	4/4 (100%)	-0.89	0 100 100	25, 28, 33, 38	0
All	All	693/712 (97%)	-0.33	17 (2%) 61 60	12, 25, 44, 79	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	542	GLY	6.3
1	B	464[A]	GLN	5.2
1	A	250	THR	4.5
1	B	467[A]	ASN	4.1
1	A	545	VAL	4.1
1	B	541	HIS	3.8
1	A	249	ALA	3.7
1	A	542	GLY	3.6
1	A	537	VAL	3.6
1	B	545	VAL	3.1
1	B	465[A]	GLU	3.1
1	B	249	ALA	3.0
1	B	245	SER	2.9
1	B	248	LYS	2.8
1	B	537	VAL	2.6
1	A	543	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	466[A]	GLU	2.1

## 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. 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(Å <sup>2</sup> )	Q<0.9
3	2DT	Q	6	19/20	0.99	0.13	-	14,18,21,26	0
3	2DT	P	6	19/20	0.98	0.14	-	14,16,19,21	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(Å <sup>2</sup> )	Q<0.9
6	NA	A	804	1/1	0.98	0.14	3.41	22,22,22,22	0
7	EDO	T	2801	4/4	0.85	0.13	0.73	38,39,41,41	0
8	D3T	A	576	28/28	0.98	0.13	0.71	7,15,19,23	0
6	NA	B	801	1/1	0.97	0.10	0.59	18,18,18,18	0
6	NA	B	806	1/1	0.91	0.10	0.11	30,30,30,30	0
6	NA	A	805	1/1	0.97	0.12	0.07	28,28,28,28	0
8	D3T	B	577	28/28	0.97	0.12	-0.03	12,16,18,19	0
6	NA	B	808	1/1	0.95	0.11	-0.12	36,36,36,36	0
5	MG	A	602	1/1	0.97	0.06	-	14,14,14,14	0
6	NA	B	802	1/1	0.98	0.20	-	22,22,22,22	0
6	NA	P	807	1/1	0.97	0.16	-	38,38,38,38	0
6	NA	A	803	1/1	0.98	0.11	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	B	601	1/1	0.93	0.09	-	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.