



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:24 AM GMT

PDB ID : 3IAY  
Title : Ternary complex of DNA polymerase delta  
Authors : Swan, M.K.; Aggarwal, A.K.  
Deposited on : 2009-07-15  
Resolution : 2.00 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 (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

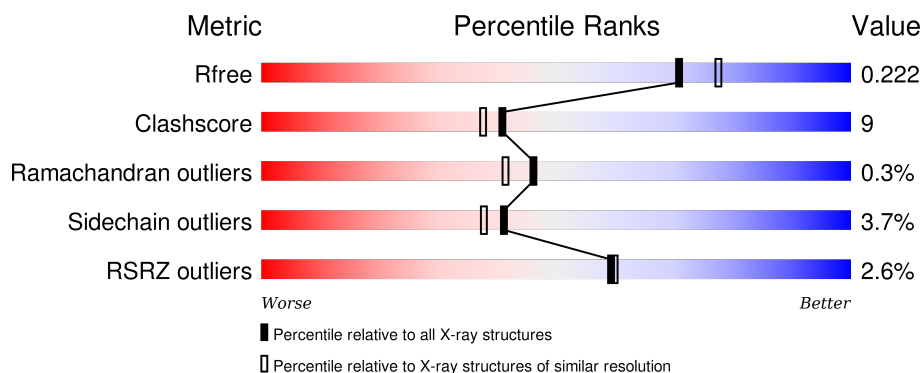
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	12	<div> <div>17%</div> <div>67%</div> <div>33%</div> </div>
2	T	16	<div> <div>75%</div> <div>25%</div> </div>
3	A	919	<div> <div>2%</div> <div>81%</div> <div>13%</div> <div>• •</div> </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	ACT	A	987	-	-	X	-
6	ACT	A	988	-	-	X	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8194 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(\*AP\*TP\*CP\*CP\*TP\*CP\*CP\*CP\*CP\*TP\*AP\*(D OC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	12	Total	C	N	O	P	0	0	0
			231	113	37	70	11			

- Molecule 2 is a DNA chain called 5'-D(\*TP\*AP\*AP\*GP\*GP\*TP\*AP\*GP\*GP\*GP\*GP\*A P\*GP\*GP\*AP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	16	Total	C	N	O	P	0	0	0
			338	160	71	92	15			

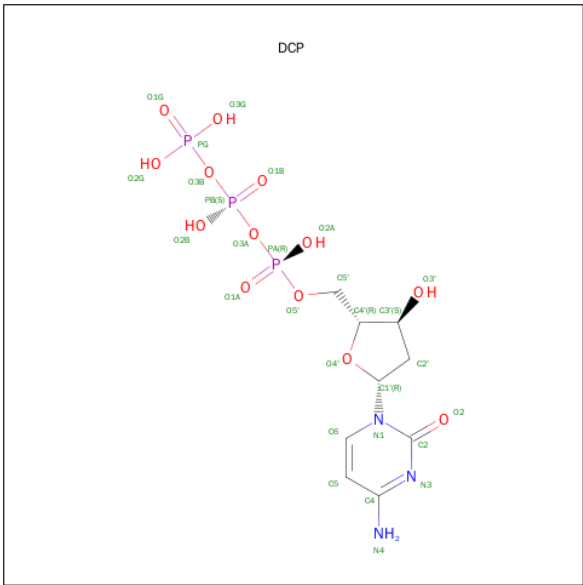
- Molecule 3 is a protein called DNA polymerase delta catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	885	Total	C	N	O	S	0	6	0
			7026	4487	1200	1307	32			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

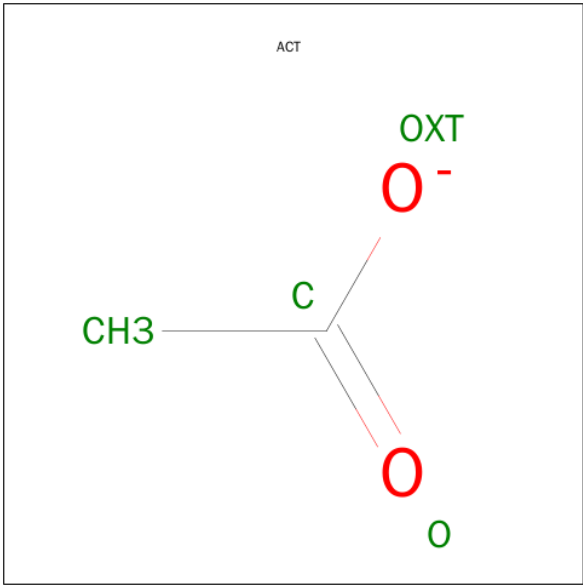
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Ca	0	0
			4	4		
4	T	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

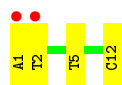
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	26	Total 26	O 26	0	0
7	T	63	Total 63	O 63	0	0
7	A	469	Total 469	O 469	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.

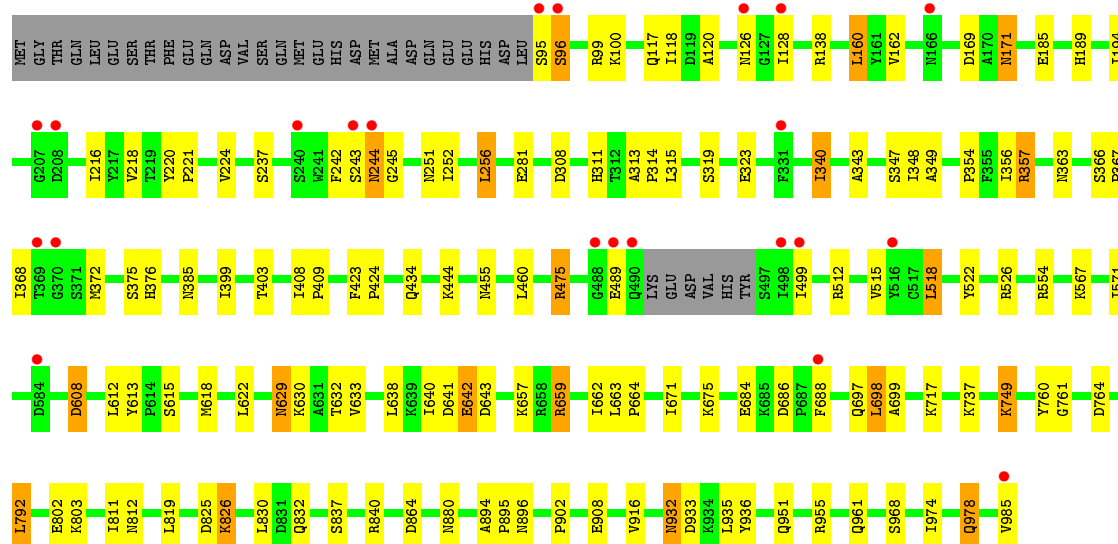
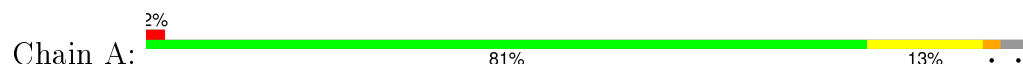
- Molecule 1: 5'-D(\*AP\*TP\*CP\*CP\*TP\*CP\*CP\*CP\*CP\*TP\*AP\*(DOC))-3'



- Molecule 2: 5'-D(\*TP\*AP\*AP\*GP\*GP\*TP\*AP\*GP\*GP\*GP\*GP\*AP\*GP\*GP\*AP\*T)-3',



- Molecule 3: DNA polymerase delta catalytic subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.08Å 85.95Å 86.87Å 90.00° 111.10° 90.00°	Depositor
Resolution (Å)	41.52 – 2.00 41.53 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (41.52-2.00) 98.2 (41.53-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.193 , 0.236 0.180 , 0.222	Depositor DCC
$R_{free}$ test set	3692 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 73549 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: DOC, CA, DCP, ACT

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	0.89	0/236	1.37	1/360 (0.3%)
2	T	0.96	0/382	1.42	3/591 (0.5%)
3	A	0.46	0/7191	0.58	0/9761
All	All	0.52	0/7809	0.69	4/10712 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	9	DG	O4'-C1'-N9	-8.38	102.13	108.00
2	T	8	DG	O4'-C1'-N9	6.64	112.64	108.00
1	P	5	DT	O4'-C1'-N1	-6.31	103.58	108.00
2	T	13	DG	O4'-C1'-N9	5.00	111.50	108.00

There are no chirality outliers.

There are no planarity outliers.

### 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	231	0	137	3	0
2	T	338	0	181	2	0
3	A	7026	0	6981	121	1
4	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	1	0	0	0	0
5	A	28	0	12	2	0
6	A	8	0	6	9	1
7	A	469	0	0	21	0
7	P	26	0	0	0	0
7	T	63	0	0	2	0
All	All	8194	0	7317	128	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (128) 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:697:GLN:NE2	3:A:698:LEU:HD13	1.54	1.21
3:A:185:GLU:HG2	6:A:988:ACT:H2	1.28	1.15
3:A:717:LYS:HE3	7:A:63:HOH:O	1.48	1.14
3:A:749:LYS:HZ3	3:A:749:LYS:HB3	1.14	1.06
3:A:571:ILE:HD11	3:A:662:ILE:HD11	1.32	1.04
3:A:749:LYS:HB3	3:A:749:LYS:NZ	1.71	1.01
3:A:308:ASP:O	3:A:311[A]:HIS:CE1	2.18	0.96
1:P:1:DA:H2"	1:P:2:DT:OP2	1.63	0.95
3:A:812:ASN:OD1	7:A:1212:HOH:O	1.83	0.95
3:A:932:ASN:HB3	7:A:1371:HOH:O	1.68	0.92
3:A:185:GLU:HG2	6:A:988:ACT:CH3	1.98	0.92
3:A:171:ASN:HD22	3:A:171:ASN:H	1.07	0.91
3:A:697:GLN:NE2	3:A:698:LEU:CD1	2.34	0.91
3:A:243:SER:HA	3:A:244:ASN:CB	2.02	0.89
3:A:242:PHE:O	3:A:244:ASN:HA	1.74	0.86
3:A:749:LYS:NZ	3:A:749:LYS:CB	2.38	0.85
7:T:527:HOH:O	3:A:444:LYS:HE3	1.76	0.85
3:A:615:SER:HA	3:A:618:MET:HE3	1.58	0.85
6:A:987:ACT:C	7:A:1388:HOH:O	2.24	0.84
3:A:961:GLN:NE2	7:A:1211:HOH:O	2.09	0.83
3:A:171:ASN:ND2	3:A:171:ASN:H	1.78	0.82
3:A:160:LEU:C	3:A:160:LEU:HD12	2.00	0.82
3:A:571:ILE:CD1	3:A:662:ILE:HD11	2.11	0.81
3:A:832:GLN:NE2	3:A:837:SER:OG	2.14	0.79
3:A:659:ARG:HD2	7:A:1089:HOH:O	1.83	0.78
3:A:185:GLU:CG	6:A:988:ACT:H2	2.12	0.77
3:A:697:GLN:HE22	3:A:698:LEU:CD1	1.97	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:281:GLU:N	3:A:281:GLU:OE2	2.15	0.74
3:A:95:SER:HA	3:A:372:MET:SD	2.28	0.73
3:A:629:ASN:ND2	3:A:632:THR:H	1.87	0.73
3:A:864:ASP:OD1	7:A:1332:HOH:O	2.07	0.73
3:A:512:ARG:O	3:A:515:VAL:HG22	1.88	0.72
3:A:171:ASN:HD22	3:A:171:ASN:N	1.77	0.71
3:A:308:ASP:O	3:A:311[A]:HIS:HE1	1.72	0.71
3:A:802:GLU:HG3	7:A:1271:HOH:O	1.91	0.71
3:A:281:GLU:H	3:A:281:GLU:CD	1.92	0.71
3:A:717:LYS:CE	7:A:63:HOH:O	2.19	0.69
3:A:160:LEU:O	3:A:160:LEU:HD12	1.94	0.68
3:A:95:SER:O	3:A:96:SER:CB	2.41	0.67
3:A:819:LEU:HD23	3:A:830:LEU:HD23	1.77	0.66
3:A:376:HIS:CE1	3:A:385:ASN:HD22	2.14	0.66
6:A:987:ACT:O	7:A:1388:HOH:O	2.12	0.65
6:A:988:ACT:H1	7:A:1406:HOH:O	1.95	0.65
3:A:916:VAL:O	7:A:1027:HOH:O	2.14	0.65
3:A:567:LYS:NZ	7:A:57:HOH:O	2.29	0.64
3:A:308:ASP:O	3:A:311[A]:HIS:ND1	2.30	0.64
3:A:629:ASN:HD22	3:A:629:ASN:C	2.02	0.62
3:A:243:SER:CA	3:A:244:ASN:CB	2.76	0.62
3:A:819:LEU:CD2	3:A:830:LEU:HD23	2.31	0.60
3:A:160:LEU:CD1	3:A:160:LEU:C	2.70	0.60
3:A:955:ARG:HH22	3:A:985:VAL:HB	1.66	0.60
3:A:811:ILE:HD12	3:A:968:SER:O	2.02	0.59
3:A:699:ALA:HB3	7:A:1394:HOH:O	2.03	0.59
3:A:522:TYR:CE2	3:A:526:ARG:HD2	2.38	0.59
3:A:376:HIS:HE1	3:A:385:ASN:HD22	1.49	0.58
3:A:825:ASP:CB	3:A:826:LYS:HD3	2.33	0.58
3:A:825:ASP:HB2	3:A:826:LYS:HD3	1.86	0.58
3:A:749:LYS:HZ2	3:A:749:LYS:CB	2.17	0.57
3:A:95:SER:CA	3:A:372:MET:SD	2.91	0.57
3:A:615:SER:HA	3:A:618:MET:CE	2.33	0.57
7:T:527:HOH:O	3:A:444:LYS:CE	2.43	0.56
3:A:189:HIS:NE2	6:A:988:ACT:OXT	2.33	0.56
3:A:629:ASN:HD22	3:A:632:THR:H	1.53	0.55
3:A:252:ILE:HD11	3:A:256:LEU:HD13	1.87	0.55
3:A:475:ARG:HD3	3:A:840:ARG:HG2	1.89	0.55
3:A:880[B]:ASN:ND2	3:A:951:GLN:HE22	2.05	0.54
3:A:737:LYS:HE2	3:A:792:LEU:HB3	1.89	0.53
3:A:880[B]:ASN:HD21	3:A:951:GLN:HE22	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:408:ILE:HB	3:A:409:PRO:HD3	1.90	0.52
3:A:640:ILE:O	3:A:641:ASP:HB2	2.10	0.52
3:A:902:PRO:HG3	3:A:936:TYR:HA	1.91	0.52
3:A:612:LEU:HD22	3:A:764:ASP:HB3	1.92	0.51
3:A:932:ASN:ND2	3:A:932:ASN:O	2.43	0.51
3:A:802:GLU:OE2	7:A:1271:HOH:O	2.19	0.51
1:P:12:DOC:H5''	7:A:1270:HOH:O	2.10	0.51
3:A:686:ASP:OD1	3:A:688:PHE:N	2.44	0.51
2:T:1:DT:H2'	3:A:717:LYS:HD3	1.93	0.51
3:A:242:PHE:O	3:A:245:GLY:HA2	2.12	0.49
3:A:313:ALA:HB1	3:A:314:PRO:HD2	1.95	0.49
3:A:819:LEU:HD23	3:A:830:LEU:CD2	2.42	0.48
3:A:638:LEU:HB3	3:A:643:ASP:HB2	1.95	0.48
3:A:671:ILE:O	3:A:675:LYS:HG3	2.13	0.48
3:A:363:ASN:O	3:A:375:SER:HB2	2.13	0.48
3:A:717:LYS:N	7:A:1284:HOH:O	2.09	0.47
3:A:684:GLU:OE2	3:A:686:ASP:N	2.48	0.47
3:A:434:GLN:HG3	3:A:455:ASN:O	2.16	0.46
3:A:638:LEU:HB3	3:A:643:ASP:CB	2.46	0.46
3:A:423:PHE:N	3:A:424:PRO:CD	2.80	0.45
3:A:518:LEU:HA	3:A:518:LEU:HD23	1.83	0.45
3:A:613:TYR:CD2	5:A:986:DCP:H2'2	2.52	0.45
3:A:613:TYR:CG	5:A:986:DCP:H2'2	2.53	0.44
1:P:1:DA:C2'	1:P:2:DT:OP2	2.43	0.44
3:A:802:GLU:CG	7:A:1271:HOH:O	2.60	0.44
3:A:319:SER:HB2	3:A:399:ILE:HD11	1.99	0.44
3:A:218:VAL:HG21	3:A:224:VAL:HG23	1.99	0.44
3:A:171:ASN:ND2	3:A:171:ASN:N	2.45	0.44
3:A:347:SER:HB3	3:A:354:PRO:HA	1.98	0.44
3:A:237:SER:HA	3:A:243:SER:HB3	1.99	0.44
3:A:554:ARG:NH1	7:A:1282:HOH:O	2.38	0.43
3:A:194:ILE:HG12	3:A:216:ILE:HG12	2.00	0.43
3:A:663:LEU:HB2	3:A:664:PRO:HD3	2.00	0.43
6:A:988:ACT:CH3	7:A:1406:HOH:O	2.62	0.43
3:A:368:ILE:HD13	3:A:515:VAL:HG12	2.01	0.43
3:A:608:ASP:OD2	3:A:802:GLU:CD	2.58	0.43
3:A:244:ASN:HA	3:A:245:GLY:HA2	1.73	0.43
3:A:356:ILE:C	3:A:357[A]:ARG:HG3	2.40	0.43
3:A:974:ILE:HD12	3:A:978:GLN:HB3	2.01	0.42
3:A:99:ARG:HG3	7:A:1369:HOH:O	2.18	0.42
3:A:169:ASP:N	3:A:169:ASP:OD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:343:ALA:HB1	3:A:518:LEU:HD23	2.01	0.42
3:A:760:TYR:CG	3:A:761:GLY:N	2.88	0.42
3:A:118:ILE:HB	3:A:460:LEU:HD11	2.01	0.42
3:A:281:GLU:CD	3:A:281:GLU:N	2.67	0.42
3:A:894:ALA:HB1	3:A:895:PRO:HD2	2.02	0.41
3:A:323:GLU:O	3:A:340:ILE:HD13	2.20	0.41
3:A:220:TYR:HA	3:A:221:PRO:HD3	1.85	0.41
3:A:185:GLU:HG2	6:A:988:ACT:C	2.51	0.41
3:A:323:GLU:OE1	3:A:499:ILE:HD13	2.21	0.41
3:A:826:LYS:HB2	3:A:826:LYS:HE2	1.88	0.41
3:A:348:ILE:O	3:A:349:ALA:C	2.59	0.41
3:A:642:GLU:OE2	3:A:657:LYS:HE3	2.21	0.41
2:T:1:DT:N3	3:A:251:ASN:O	2.47	0.40
3:A:630:LYS:O	3:A:633:VAL:CG2	2.69	0.40
3:A:160:LEU:CD1	3:A:162:VAL:HG13	2.51	0.40
3:A:629:ASN:ND2	3:A:629:ASN:C	2.74	0.40
3:A:688:PHE:CD1	3:A:688:PHE:C	2.95	0.40
3:A:120:ALA:HA	3:A:138:ARG:O	2.21	0.40
3:A:366:SER:HA	3:A:367:PRO:HD3	1.92	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:933:ASP:OD2	6:A:988:ACT:OXT[2_555]	2.12	0.08

## 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
3	A	887/919 (96%)	860 (97%)	24 (3%)	3 (0%)	46 41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	96	SER
3	A	128	ILE
3	A	244	ASN

### 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	767/818 (94%)	738 (96%)	29 (4%)	40	36

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	100	LYS
3	A	117	GLN
3	A	126	ASN
3	A	160	LEU
3	A	171	ASN
3	A	256	LEU
3	A	315	LEU
3	A	340	ILE
3	A	357[A]	ARG
3	A	357[B]	ARG
3	A	403	THR
3	A	475	ARG
3	A	489	GLU
3	A	518	LEU
3	A	608	ASP
3	A	622	LEU
3	A	629	ASN
3	A	642	GLU
3	A	659	ARG
3	A	698	LEU
3	A	749	LYS
3	A	792	LEU

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Mol	Chain	Res	Type
3	A	803	LYS
3	A	826	LYS
3	A	896	ASN
3	A	908	GLU
3	A	932	ASN
3	A	935	LEU
3	A	978	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	117	GLN
3	A	171	ASN
3	A	200	GLN
3	A	284	ASN
3	A	376	HIS
3	A	388	ASN
3	A	466	GLN
3	A	557	GLN
3	A	629	ASN
3	A	832	GLN
3	A	851	ASN
3	A	932	ASN

### 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	DOC	P	12	1,2	11,19,20	0.42	0	14,26,29	1.32	2 (14%)

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	DOC	P	12	1,2	-	0/3/18/19	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	12	DOC	C3'-C2'-C1'	2.23	105.20	102.71
1	P	12	DOC	C2-N3-C4	2.98	119.81	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	12	DOC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 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	$\# Z  > 2$
5	DCP	A	986	4	21,29,29	0.65	0	33,45,45	1.28	4 (12%)
6	ACT	A	987	-	1,3,3	2.13	1 (100%)	0,3,3	0.00	-
6	ACT	A	988	-	1,3,3	1.27	0	0,3,3	0.00	-

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	DCP	A	986	4	-	0/18/34/34	0/2/2/2
6	ACT	A	987	-	-	0/0/0/0	0/0/0/0
6	ACT	A	988	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	987	ACT	CH3-C	2.13	1.51	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	986	DCP	C2'-C1'-N1	-3.25	106.26	114.16
5	A	986	DCP	O3G-PG-O2G	2.45	116.69	107.38
5	A	986	DCP	O2B-PB-O3A	2.53	116.58	105.09
5	A	986	DCP	C2-N3-C4	3.37	120.36	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	986	DCP	2	0
6	A	987	ACT	2	0
6	A	988	ACT	7	1

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	11/12 (91%)	0.47	2 (18%) 2 2	17, 22, 68, 76	0
2	T	16/16 (100%)	-0.18	0 100 100	17, 27, 40, 50	0
3	A	885/919 (96%)	-0.10	22 (2%) 61 61	18, 27, 38, 47	0
All	All	912/947 (96%)	-0.09	24 (2%) 59 60	17, 27, 38, 76	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	243	SER	5.3
3	A	95	SER	4.8
3	A	490	GLN	4.5
1	P	1	DA	3.9
3	A	488	GLY	3.7
3	A	516	TYR	3.6
3	A	985	VAL	3.3
3	A	166	ASN	3.0
3	A	499	ILE	3.0
3	A	96	SER	2.9
3	A	331	PHE	2.8
3	A	498	ILE	2.8
3	A	207	GLY	2.8
3	A	128	ILE	2.8
3	A	489	GLU	2.7
3	A	240	SER	2.5
3	A	208	ASP	2.4
3	A	688	PHE	2.3
1	P	2	DT	2.2
3	A	369	THR	2.2
3	A	584	ASP	2.2
3	A	126	ASN	2.1
3	A	370	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	244	ASN	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
1	DOC	P	12	18/19	0.98	0.15	-	12,14,17,17	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	ACT	A	988	4/4	0.94	0.24	6.91	52,53,53,53	0
5	DCP	A	986	28/28	0.99	0.06	-3.33	15,20,22,22	0
4	CA	A	1	1/1	0.99	0.02	-6.76	20,20,20,20	0
4	CA	A	3	1/1	0.98	0.10	-	40,40,40,40	0
4	CA	T	17	1/1	0.98	0.03	-	47,47,47,47	0
4	CA	A	4	1/1	0.95	0.08	-	55,55,55,55	0
4	CA	A	2	1/1	0.94	0.19	-	43,43,43,43	0
6	ACT	A	987	4/4	0.92	0.11	-	33,33,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.