



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:29 pm BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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
buster-report : 1.1.7 (2018)
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

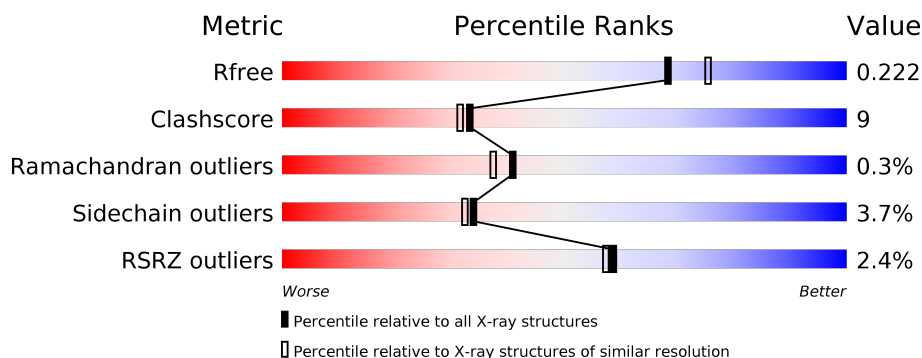
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 ≥ 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	12	<div> <div>17%</div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>
2	T	16	<div> <div>75%</div> <div>25%</div> </div>
3	A	919	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>13%</div> <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	-

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			

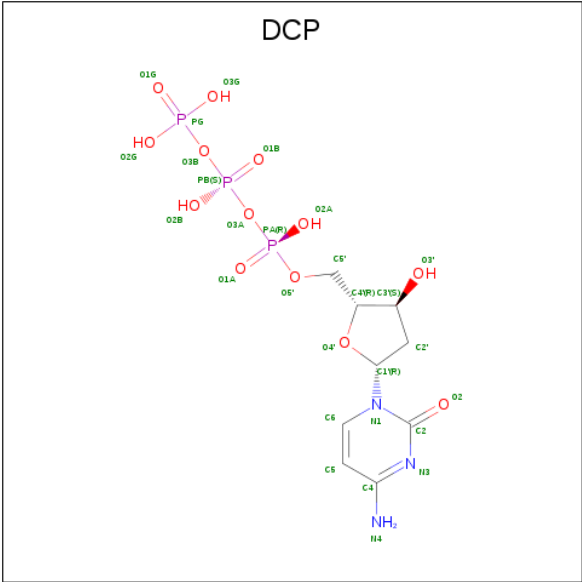
- Molecule 3 is a protein called DNA polymerase delta catalytic subunit.

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).

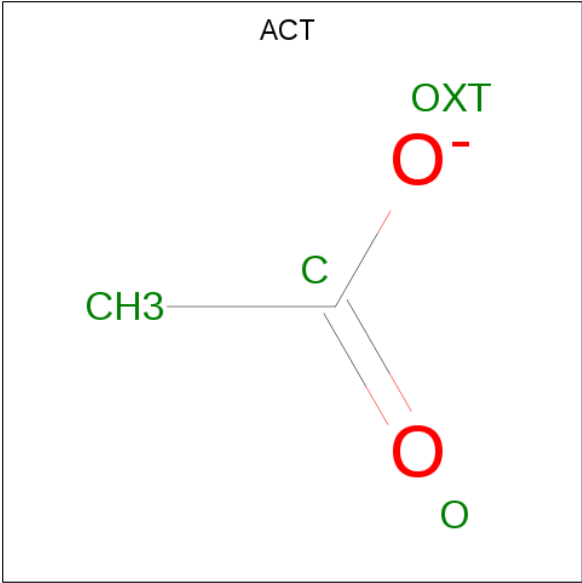
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Ca	0	0
			4	4		
4	T	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



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: C₂H₃O₂).



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		

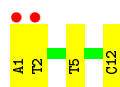
- Molecule 7 is water.

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

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.

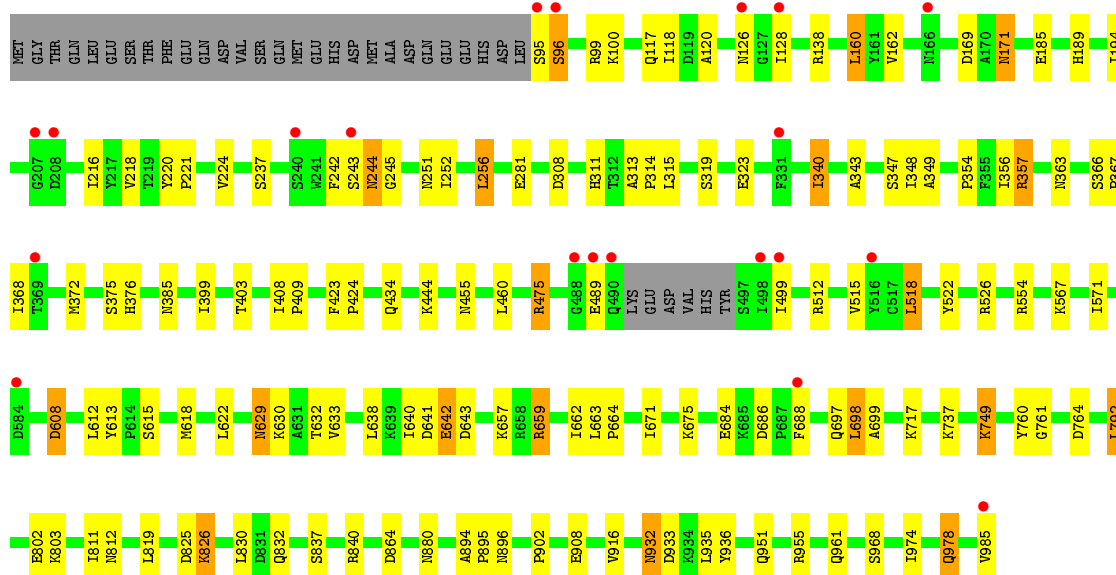
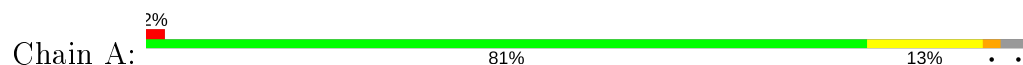
- Molecule 1: 5'-D(*AP*TP*CP*CP*TP*CP*CP*CP*CP*TP*AP*(DOC))-3'



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8194	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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
7:T:527:HOH:O	3:A:444:LYS:HE3	1.76	0.85
3:A:749:LYS:NZ	3:A:749:LYS:CB	2.38	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:CD	3:A:281:GLU:H	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:522:TYR:CE2	3:A:526:ARG:HD2	2.38	0.59
3:A:699:ALA:HB3	7:A:1394:HOH:O	2.03	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:95:SER:CA	3:A:372:MET:SD	2.91	0.57
3:A:749:LYS:HZ2	3:A:749:LYS:CB	2.17	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:252:ILE:HD11	3:A:256:LEU:HD13	1.87	0.55
3:A:629:ASN:HD22	3:A:632:THR:H	1.53	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:802:GLU:OE2	7:A:1271:HOH:O	2.19	0.51
3:A:932:ASN:ND2	3:A:932:ASN:O	2.43	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: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:819:LEU:HD23	3:A:830:LEU:CD2	2.42	0.48
3:A:363:ASN:O	3:A:375:SER:HB2	2.13	0.48
3:A:684:GLU:OE2	3:A:686:ASP:N	2.48	0.47
3:A:717:LYS:N	7:A:1284:HOH:O	2.09	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
3:A:802:GLU:CG	7:A:1271:HOH:O	2.60	0.44
1:P:1:DA:C2'	1:P:2:DT:OP2	2.43	0.44
3:A:218:VAL:HG21	3:A:224:VAL:HG23	1.99	0.44
3:A:319:SER:HB2	3:A:399:ILE:HD11	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
3:A:368:ILE:HD13	3:A:515:VAL:HG12	2.01	0.43
6:A:988:ACT:CH3	7:A:1406:HOH:O	2.62	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:118:ILE:HB	3:A:460:LEU:HD11	2.01	0.42
3:A:760:TYR:CG	3:A:761:GLY:N	2.88	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:220:TYR:HA	3:A:221:PRO:HD3	1.85	0.41
3:A:323:GLU:O	3:A:340:ILE:HD13	2.20	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:348:ILE:O	3:A:349:ALA:C	2.59	0.41
3:A:826:LYS:HB2	3:A:826:LYS:HE2	1.88	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: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
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

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%)	41	37

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%)	33	31

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	14,19,20	0.66	0	13,26,29	1.39	2 (15%)

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	-	0/4/18/19	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	C2-N3-C4	3.42	119.81	116.34
1	P	12	DOC	C3'-C2'-C1'	2.09	105.20	102.78

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	23,29,29	0.65	0	30,45,45	1.31	3 (10%)
6	ACT	A	987	-	1,3,3	2.37	1 (100%)	0,3,3	0.00	-
6	ACT	A	988	-	1,3,3	1.45	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	-	4/19/34/34	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	987	ACT	CH3-C	2.37	1.51	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	986	DCP	C2-N3-C4	3.96	120.36	116.34
5	A	986	DCP	C2'-C1'-N1	-3.47	106.26	114.27
5	A	986	DCP	O3G-PG-O2G	2.37	116.69	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

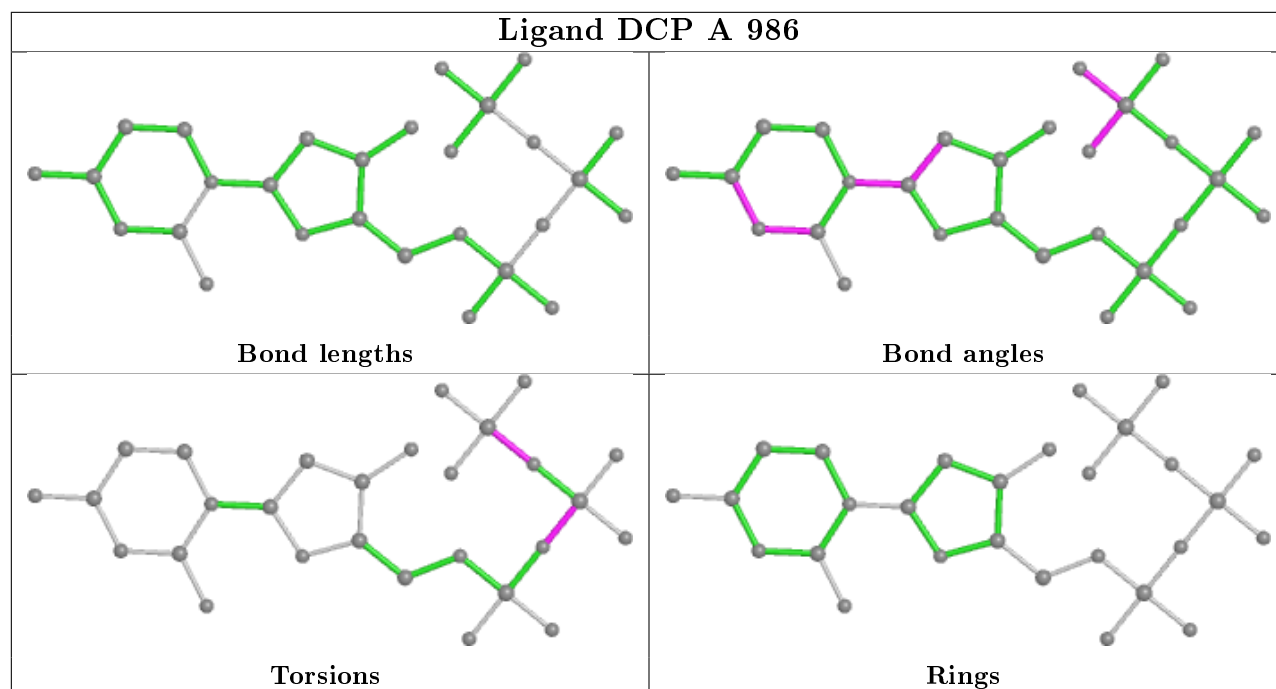
Mol	Chain	Res	Type	Atoms
5	A	986	DCP	PB-O3B-PG-O3G
5	A	986	DCP	PA-O3A-PB-O1B
5	A	986	DCP	PB-O3B-PG-O1G
5	A	986	DCP	PA-O3A-PB-O2B

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th 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 ²)	Q<0.9
1	P	11/12 (91%)	0.45	2 (18%) 1 1	17, 22, 68, 76	0
2	T	16/16 (100%)	-0.20	0 100 100	17, 27, 40, 50	0
3	A	885/919 (96%)	-0.15	20 (2%) 60 59	18, 27, 38, 47	0
All	All	912/947 (96%)	-0.14	22 (2%) 59 57	17, 27, 38, 76	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	243	SER	5.1
3	A	95	SER	4.6
3	A	490	GLN	4.3
1	P	1	DA	3.8
3	A	488	GLY	3.5
3	A	516	TYR	3.5
3	A	985	VAL	3.0
3	A	166	ASN	2.8
3	A	96	SER	2.8
3	A	499	ILE	2.8
3	A	207	GLY	2.7
3	A	331	PHE	2.7
3	A	489	GLU	2.6
3	A	128	ILE	2.6
3	A	498	ILE	2.6
3	A	240	SER	2.4
3	A	208	ASP	2.3
3	A	688	PHE	2.2
1	P	2	DT	2.1
3	A	369	THR	2.1
3	A	126	ASN	2.0
3	A	584	ASP	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, 95th 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 ²)	Q<0.9
1	DOC	P	12	18/19	0.98	0.15	12,14,17,17	0

6.3 Carbohydrates [i](#)

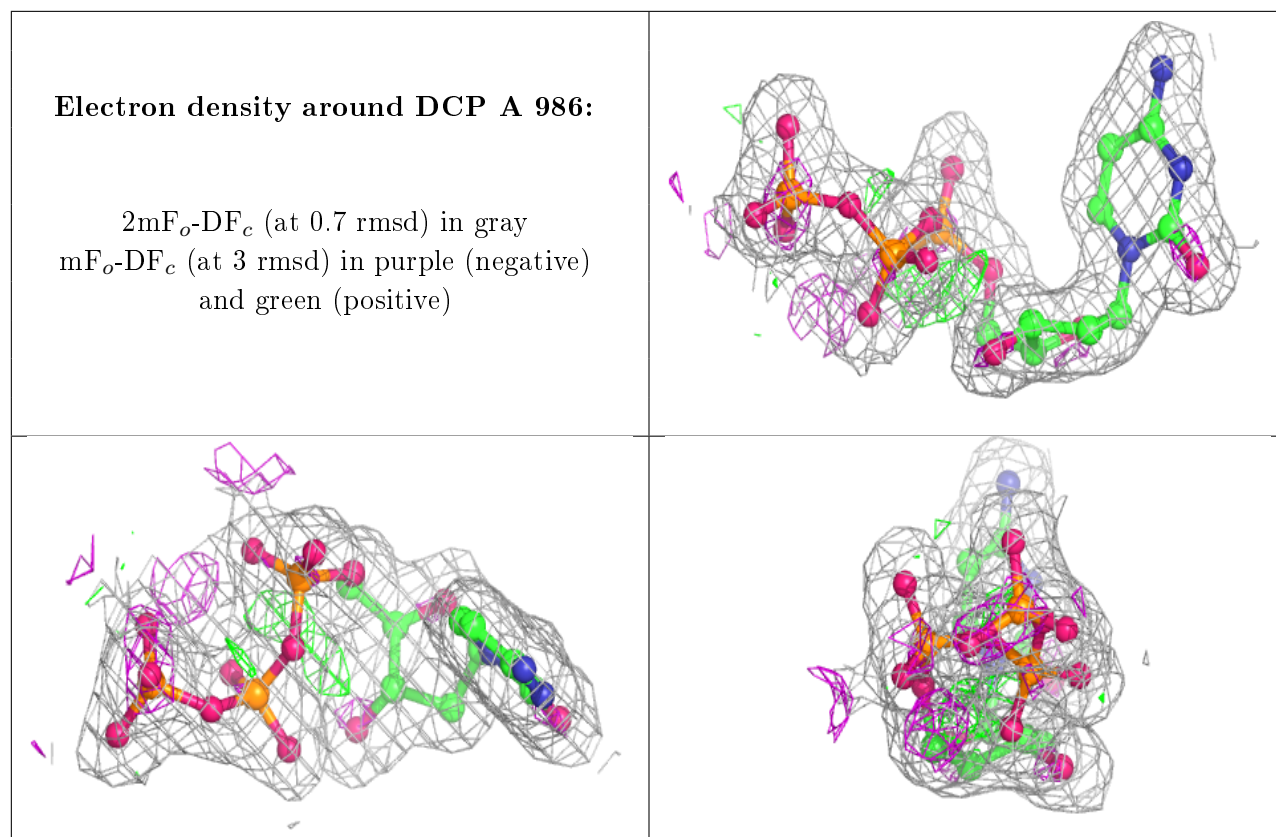
There are no carbohydrates in this entry.

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. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
6	ACT	A	987	4/4	0.92	0.10	33,33,34,34	0
4	CA	A	2	1/1	0.94	0.19	43,43,43,43	0
6	ACT	A	988	4/4	0.94	0.23	52,53,53,53	0
4	CA	A	4	1/1	0.95	0.08	55,55,55,55	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
5	DCP	A	986	28/28	0.99	0.06	15,20,22,22	0
4	CA	A	1	1/1	0.99	0.01	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.