



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2021 – 04:02 PM EDT

PDB ID : 3K5M
Title : Crystal structure of E.coli Pol II-abasic DNA-ddGTP Lt(-2, 2) ternary complex
Authors : Yang, W.; Wang, F.
Deposited on : 2009-10-07
Resolution : 2.04 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 : 2.23.2
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) : 2.23.2

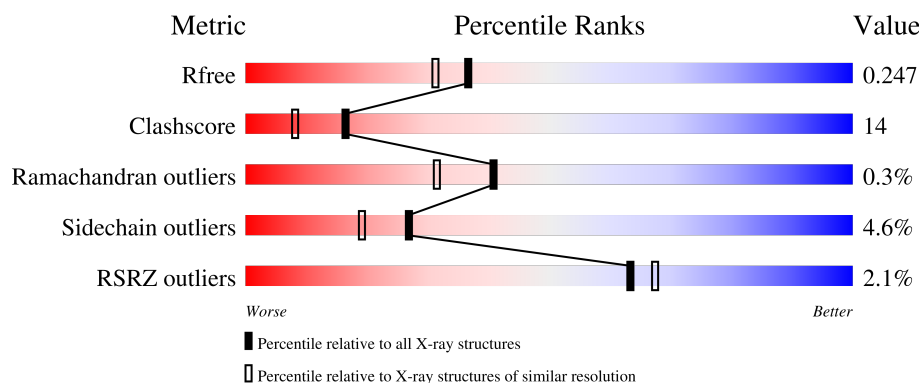
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 of 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	A	786	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>
2	T	20	<div> <div>40%</div> <div>50%</div> <div>10%</div> </div>
3	P	13	<div> <div>46%</div> <div>38%</div> <div>15%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7390 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	768	Total	C	N	O	S	0	0	0
			6204	3951	1109	1120	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P21189
A	-1	PRO	-	expression tag	UNP P21189
A	0	HIS	-	expression tag	UNP P21189
A	335	ASN	ASP	engineered mutation	UNP P21189

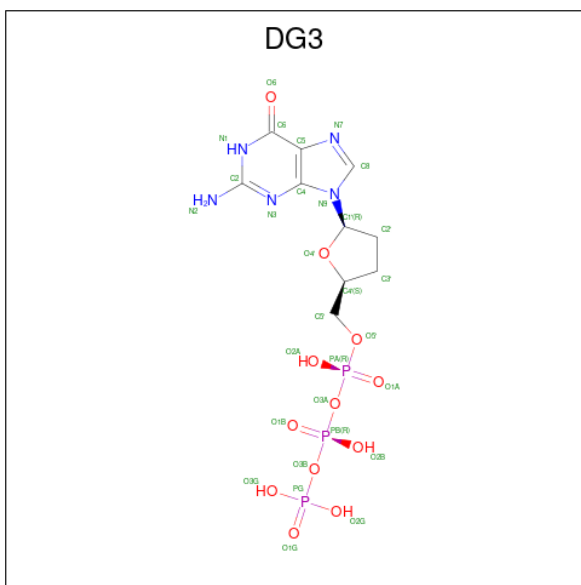
- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*TP*CP*CP*TP*GP*(3DR)P*AP*CP*GP*CP*TP*AP*GP*GP*CP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	20	Total	C	N	O	P	0	0	0
			397	189	74	115	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			266	127	50	77	12			

- Molecule 4 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DG3) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 30	C 10	N 5	O 12	P 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0

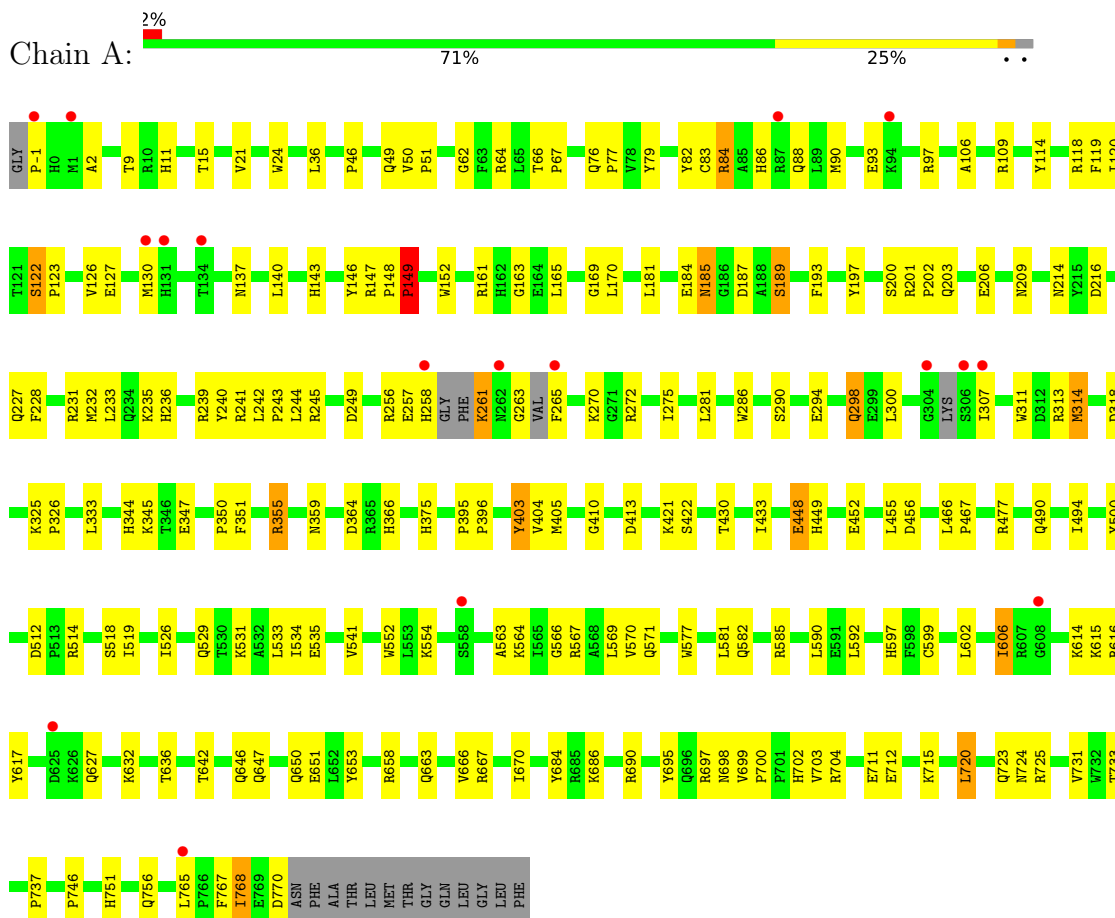
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	441	Total O 441 441	0	0
6	T	36	Total O 36 36	0	0
6	P	14	Total O 14 14	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: DNA polymerase II

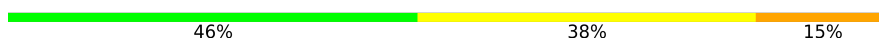


- Molecule 2: DNA (5'-D(*AP*GP*TP*CP*CP*TP*GP*(3DR)P*AP*CP*GP*CP*TP*AP*GP*GP*CP*AP*CP*A)-3')



- Molecule 3: DNA (5'-D(*GP*TP*GP*CP*CP*TP*AP*GP*CP*GP*TP*AP*G)-3')

Chain P:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.11Å 95.23Å 144.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.43 – 2.04 45.25 – 2.04	Depositor EDS
% Data completeness (in resolution range)	88.7 (28.43-2.04) 88.5 (45.25-2.04)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.03Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.260 0.227 , 0.247	Depositor DCC
R_{free} test set	1562 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7390	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DG3, CA, 3DR

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	0.61	0/6369	0.78	1/8638 (0.0%)
2	T	1.49	12/432 (2.8%)	1.61	5/662 (0.8%)
3	P	0.95	0/298	1.35	3/459 (0.7%)
All	All	0.71	12/7099 (0.2%)	0.90	9/9759 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	818	DA	C5-C6	-9.81	1.32	1.41
2	T	818	DA	N9-C4	-8.19	1.32	1.37
2	T	818	DA	C1'-N9	-7.77	1.36	1.47
2	T	818	DA	C4'-O4'	-6.97	1.38	1.45
2	T	818	DA	P-O5'	-6.82	1.52	1.59
2	T	818	DA	N3-C4	-6.59	1.30	1.34
2	T	818	DA	C5-C4	-6.41	1.34	1.38
2	T	818	DA	C2-N3	-6.19	1.27	1.33
2	T	818	DA	C8-N7	-6.11	1.27	1.31
2	T	818	DA	C6-N6	-5.70	1.29	1.33
2	T	818	DA	O4'-C1'	-5.02	1.36	1.42
2	T	817	DC	O3'-P	-5.00	1.55	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	818	DA	O4'-C1'-N9	-23.78	91.36	108.00
3	P	903	DG	O5'-P-OP2	-8.09	98.42	105.70
3	P	904	DC	O4'-C1'-N1	6.48	112.53	108.00
2	T	817	DC	OP2-P-O3'	5.86	118.08	105.20
2	T	818	DA	O5'-P-OP2	-5.47	100.77	105.70
3	P	913	DG	C1'-O4'-C4'	-5.37	104.73	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	818	DA	N1-C2-N3	-5.33	126.64	129.30
2	T	817	DC	C1'-O4'-C4'	-5.14	104.96	110.10
1	A	149	PRO	N-CA-C	-5.09	98.87	112.10

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	A	6204	0	6048	172	0
2	T	397	0	220	12	0
3	P	266	0	148	9	0
4	A	30	0	11	1	0
5	A	2	0	0	0	0
6	A	441	0	0	10	0
6	P	14	0	0	0	0
6	T	36	0	0	0	0
All	All	7390	0	6427	191	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 14.

All (191) 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:A:123:PRO:HB2	1:A:143:HIS:O	1.58	1.02
3:P:901:DG:H5'	3:P:901:DG:H8	1.24	1.00
1:A:62:GLY:HA3	1:A:84:ARG:HD3	1.49	0.95
1:A:534:ILE:HD13	1:A:569:LEU:HD22	1.52	0.91
1:A:2:ALA:HB2	1:A:127:GLU:HG2	1.57	0.87
3:P:901:DG:H2''	3:P:902:DT:H5'	1.55	0.86
1:A:185:ASN:HD21	1:A:325:LYS:H	1.24	0.85
3:P:905:DC:H2''	3:P:906:DT:OP2	1.77	0.82
3:P:901:DG:H5'	3:P:901:DG:C8	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:HIS:HB3	1:A:261:LYS:HG2	1.67	0.77
1:A:300:LEU:HD12	1:A:300:LEU:O	1.86	0.76
1:A:698:ASN:OD1	2:T:814:DG:H5'	1.86	0.75
1:A:582:GLN:HG3	6:A:1119:HOH:O	1.87	0.75
1:A:209:ASN:ND2	1:A:245:ARG:H	1.86	0.73
1:A:261:LYS:HD2	1:A:263:GLY:N	2.01	0.73
1:A:62:GLY:CA	1:A:84:ARG:HD3	2.19	0.73
1:A:200:SER:H	1:A:203:GLN:HE21	1.35	0.72
3:P:901:DG:H2''	3:P:902:DT:C5'	2.19	0.72
1:A:257:GLU:HB2	1:A:265:PHE:CE1	2.25	0.71
1:A:627:GLN:HE22	1:A:658:ARG:HD2	1.56	0.71
1:A:227:GLN:O	1:A:231:ARG:HD3	1.92	0.70
1:A:185:ASN:HD22	1:A:185:ASN:C	1.94	0.70
1:A:235:LYS:HG3	6:A:1082:HOH:O	1.90	0.70
1:A:765:LEU:HD23	1:A:768:ILE:HD11	1.74	0.68
1:A:209:ASN:HD21	1:A:245:ARG:H	1.38	0.68
1:A:552:TRP:CE2	1:A:554:LYS:HA	2.28	0.68
2:T:807:DA:H2''	2:T:808:DC:H5'	1.77	0.67
1:A:169:GLY:O	1:A:170:LEU:HD23	1.94	0.67
1:A:566:GLY:O	1:A:570:VAL:HG22	1.95	0.66
2:T:799:DA:H4'	2:T:800:DG:OP1	1.95	0.66
1:A:261:LYS:HD2	1:A:263:GLY:H	1.61	0.66
1:A:375:HIS:HD2	6:A:1032:HOH:O	1.78	0.65
1:A:410:GLY:HA2	1:A:767:PHE:CE1	2.32	0.64
1:A:404:VAL:HG11	1:A:614:LYS:HD2	1.78	0.64
1:A:355:ARG:NH1	1:A:359:ASN:HD21	1.96	0.63
1:A:529:GLN:O	1:A:533:LEU:HG	1.98	0.63
2:T:810:DC:H2'	2:T:811:DT:H71	1.81	0.63
1:A:161:ARG:NE	1:A:314:MET:HE2	2.15	0.62
1:A:704:ARG:CZ	1:A:737:PRO:HD2	2.29	0.62
1:A:161:ARG:HB3	1:A:314:MET:CE	2.29	0.62
1:A:366:HIS:HE1	6:A:941:HOH:O	1.82	0.61
1:A:765:LEU:O	1:A:768:ILE:HG13	2.01	0.61
1:A:62:GLY:HA3	1:A:84:ARG:CD	2.27	0.61
1:A:161:ARG:NE	1:A:314:MET:CE	2.64	0.61
1:A:83:CYS:HB3	1:A:88:GLN:OE1	2.02	0.60
1:A:602:LEU:HD23	1:A:653:TYR:CE2	2.37	0.60
1:A:216:ASP:HA	1:A:272:ARG:NH2	2.17	0.60
1:A:200:SER:H	1:A:203:GLN:NE2	2.00	0.58
1:A:314:MET:HE3	1:A:318:ASP:OD2	2.04	0.58
1:A:404:VAL:HG11	1:A:614:LYS:CD	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:O	1:A:232:MET:HG2	2.04	0.57
1:A:67:PRO:HD3	1:A:79:TYR:CE2	2.40	0.56
1:A:46:PRO:HB2	1:A:49:GLN:HG3	1.86	0.56
1:A:300:LEU:HD11	1:A:345:LYS:HG2	1.86	0.56
1:A:711:GLU:O	1:A:715:LYS:HE2	2.06	0.56
1:A:366:HIS:HD2	6:A:805:HOH:O	1.88	0.55
1:A:704:ARG:NH1	1:A:737:PRO:HD2	2.21	0.55
1:A:203:GLN:HA	1:A:206:GLU:HG3	1.89	0.55
3:P:901:DG:H2'	3:P:902:DT:C6	2.42	0.55
1:A:403:TYR:C	1:A:403:TYR:CD2	2.80	0.55
1:A:616:ARG:HA	1:A:632:LYS:O	2.07	0.55
1:A:161:ARG:HB3	1:A:314:MET:HE2	1.89	0.55
1:A:185:ASN:ND2	1:A:325:LYS:H	2.02	0.54
1:A:187:ASP:OD1	1:A:189:SER:HB2	2.08	0.53
1:A:64:ARG:HG2	1:A:82:TYR:HB2	1.90	0.53
1:A:193:PHE:CG	1:A:333:LEU:HD22	2.43	0.53
1:A:684:TYR:OH	1:A:751:HIS:HE1	1.92	0.53
1:A:-1:PRO:O	1:A:130:MET:HG3	2.07	0.53
1:A:700:PRO:HD2	1:A:703:VAL:HB	1.91	0.53
1:A:216:ASP:HA	1:A:272:ARG:HH21	1.72	0.53
1:A:146:TYR:O	1:A:147:ARG:HD3	2.09	0.52
1:A:642:THR:H	1:A:756:GLN:NE2	2.07	0.52
1:A:690:ARG:HB2	1:A:695:TYR:CZ	2.44	0.52
4:A:914:DG3:H5'1	3:P:913:DG:H2''	1.92	0.52
2:T:807:DA:H2'	2:T:808:DC:C6	2.44	0.52
1:A:300:LEU:HD11	1:A:345:LYS:HD3	1.92	0.52
1:A:404:VAL:HG12	1:A:405:MET:N	2.25	0.52
1:A:667:ARG:HG2	1:A:667:ARG:HH11	1.76	0.51
1:A:209:ASN:HD21	1:A:245:ARG:N	2.08	0.51
1:A:258:HIS:HB3	1:A:261:LYS:CG	2.39	0.51
2:T:810:DC:H2'	2:T:811:DT:C7	2.39	0.51
1:A:325:LYS:N	1:A:326:PRO:CD	2.73	0.51
1:A:512:ASP:OD2	1:A:514:ARG:HB2	2.11	0.51
1:A:765:LEU:CD2	1:A:768:ILE:HD11	2.41	0.51
1:A:181:LEU:HD22	1:A:201:ARG:HD3	1.93	0.51
1:A:232:MET:HE3	1:A:232:MET:HA	1.93	0.51
2:T:818:DA:C8	2:T:818:DA:H5'	2.45	0.51
1:A:200:SER:OG	1:A:203:GLN:HG3	2.11	0.50
1:A:240:TYR:HB2	1:A:242:LEU:CD2	2.42	0.50
1:A:152:TRP:CH2	1:A:344:HIS:CE1	3.01	0.49
1:A:161:ARG:CZ	1:A:314:MET:HE2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASN:ND2	1:A:245:ARG:N	2.58	0.49
1:A:724:ASN:O	1:A:725:ARG:HB2	2.13	0.49
1:A:240:TYR:HB2	1:A:242:LEU:HD23	1.93	0.49
1:A:120:ILE:O	1:A:375:HIS:HE1	1.94	0.49
1:A:201:ARG:N	1:A:202:PRO:HD2	2.28	0.49
1:A:490:GLN:O	1:A:494:ILE:HG12	2.13	0.49
1:A:114:TYR:CE1	1:A:118:ARG:CZ	2.96	0.48
1:A:185:ASN:C	1:A:185:ASN:ND2	2.65	0.48
1:A:712:GLU:HA	1:A:715:LYS:HE3	1.95	0.48
1:A:2:ALA:HA	1:A:126:VAL:O	2.13	0.48
1:A:122:SER:H	1:A:123:PRO:HD2	1.79	0.48
1:A:636:THR:HG21	1:A:650:GLN:HG3	1.96	0.48
1:A:50:VAL:HB	1:A:51:PRO:HD3	1.94	0.48
1:A:118:ARG:O	1:A:119:PHE:HB2	2.14	0.48
1:A:300:LEU:HD11	1:A:345:LYS:CG	2.44	0.48
1:A:433:ILE:HD12	1:A:518:SER:HB3	1.95	0.48
1:A:733:THR:HB	1:A:746:PRO:O	2.13	0.48
1:A:663:GLN:O	1:A:667:ARG:HG3	2.13	0.48
1:A:564:LYS:HE3	1:A:564:LYS:HB2	1.48	0.48
1:A:165:LEU:O	1:A:201:ARG:HD2	2.14	0.48
2:T:804:DT:H2''	2:T:807:DA:H5'	1.96	0.48
1:A:294:GLU:O	1:A:298:GLN:HB2	2.13	0.48
1:A:647:GLN:O	1:A:651:GLU:HG3	2.13	0.47
1:A:410:GLY:HA2	1:A:767:PHE:CD1	2.48	0.47
1:A:577:TRP:O	1:A:581:LEU:HD13	2.15	0.47
1:A:9:THR:OG1	1:A:11:HIS:CE1	2.67	0.47
1:A:249:ASP:HA	6:A:1176:HOH:O	2.15	0.47
1:A:21:VAL:HB	1:A:36:LEU:HD12	1.97	0.47
1:A:577:TRP:HE3	1:A:581:LEU:HD11	1.80	0.47
1:A:581:LEU:HD12	1:A:581:LEU:N	2.30	0.47
1:A:770:ASP:OD1	1:A:770:ASP:C	2.51	0.47
1:A:636:THR:CG2	1:A:650:GLN:HG3	2.45	0.47
1:A:233:LEU:HB3	1:A:244:LEU:HD21	1.97	0.46
1:A:636:THR:HA	1:A:646:GLN:HG2	1.98	0.46
1:A:684:TYR:OH	1:A:751:HIS:CE1	2.68	0.46
1:A:699:VAL:HA	1:A:700:PRO:HD3	1.83	0.46
1:A:711:GLU:O	1:A:715:LYS:CE	2.63	0.46
1:A:275:ILE:HD13	1:A:364:ASP:HB3	1.96	0.46
1:A:577:TRP:CG	1:A:590:LEU:HD12	2.50	0.46
1:A:50:VAL:N	1:A:51:PRO:CD	2.78	0.46
1:A:563:ALA:O	1:A:567:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:THR:OG1	1:A:11:HIS:HE1	2.00	0.45
1:A:90:MET:CE	1:A:109:ARG:NH2	2.79	0.45
1:A:666:VAL:O	1:A:670:ILE:HG13	2.16	0.45
1:A:615:LYS:HD2	2:T:808:DC:O4'	2.16	0.45
1:A:430:THR:CG2	1:A:581:LEU:HD23	2.46	0.45
1:A:617:TYR:CZ	1:A:632:LYS:HG3	2.51	0.45
1:A:126:VAL:HG23	1:A:140:LEU:HD23	1.98	0.45
1:A:300:LEU:CD1	1:A:345:LYS:HD3	2.47	0.45
1:A:270:LYS:NZ	6:A:1172:HOH:O	2.47	0.44
1:A:686:LYS:HD2	1:A:702:HIS:CG	2.53	0.44
1:A:410:GLY:CA	1:A:767:PHE:CE1	3.00	0.44
1:A:355:ARG:NH1	1:A:359:ASN:ND2	2.64	0.44
1:A:636:THR:HG21	1:A:650:GLN:CG	2.47	0.44
1:A:76:GLN:HA	1:A:77:PRO:HD3	1.85	0.44
1:A:731:VAL:O	1:A:737:PRO:HA	2.18	0.44
1:A:286:TRP:HA	6:A:1163:HOH:O	2.18	0.44
1:A:161:ARG:HE	1:A:314:MET:CE	2.30	0.44
1:A:448:GLU:HG2	1:A:449:HIS:CE1	2.53	0.44
1:A:413:ASP:HA	1:A:599:CYS:O	2.19	0.43
1:A:433:ILE:HG13	1:A:519:ILE:HG12	2.00	0.43
2:T:799:DA:C4'	2:T:800:DG:OP1	2.63	0.43
1:A:351:PHE:CD2	1:A:351:PHE:C	2.92	0.43
1:A:455:LEU:O	1:A:456:ASP:HB2	2.19	0.43
1:A:606:ILE:HD13	1:A:606:ILE:HA	1.77	0.43
1:A:11:HIS:CE1	1:A:24:TRP:HD1	2.36	0.43
1:A:261:LYS:HD2	1:A:263:GLY:CA	2.48	0.43
1:A:421:LYS:O	1:A:422:SER:C	2.57	0.42
1:A:690:ARG:HB2	1:A:695:TYR:CE2	2.54	0.42
1:A:723:GLN:HB2	6:A:808:HOH:O	2.19	0.42
1:A:50:VAL:N	1:A:51:PRO:HD2	2.35	0.42
2:T:816:DA:H2''	2:T:817:DC:O5'	2.19	0.42
1:A:477:ARG:HG2	6:A:1046:HOH:O	2.20	0.42
1:A:720:LEU:HB3	1:A:723:GLN:HG2	2.01	0.42
1:A:570:VAL:HG12	1:A:592:LEU:HG	2.00	0.41
1:A:93:GLU:HG3	1:A:106:ALA:HB3	2.01	0.41
1:A:257:GLU:HB2	1:A:265:PHE:CD1	2.55	0.41
1:A:93:GLU:HG3	1:A:106:ALA:CB	2.50	0.41
1:A:355:ARG:HE	1:A:355:ARG:HB3	1.43	0.41
1:A:466:LEU:N	1:A:467:PRO:CD	2.84	0.41
1:A:697:ARG:O	1:A:698:ASN:C	2.56	0.41
3:P:902:DT:H2''	3:P:903:DG:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:TRP:CZ3	1:A:554:LYS:HG2	2.56	0.41
1:A:395:PRO:HA	1:A:396:PRO:HD3	1.74	0.41
1:A:86:HIS:NE2	1:A:109:ARG:HD3	2.36	0.41
1:A:90:MET:HE2	1:A:109:ARG:NH2	2.36	0.41
1:A:347:GLU:O	1:A:350:PRO:HD2	2.21	0.41
1:A:430:THR:HG21	1:A:581:LEU:HD23	2.03	0.41
1:A:577:TRP:HE3	1:A:581:LEU:CD1	2.33	0.41
1:A:581:LEU:N	1:A:581:LEU:CD1	2.83	0.41
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.74	0.41
3:P:905:DC:C2'	3:P:906:DT:OP2	2.51	0.41
1:A:148:PRO:HA	1:A:149:PRO:HD3	1.97	0.40
1:A:531:LYS:HG3	1:A:541:VAL:HG11	2.04	0.40
1:A:184:GLU:HA	1:A:197:TYR:CE1	2.56	0.40
1:A:163:GLY:O	1:A:236:HIS:HE1	2.04	0.40
1:A:243:PRO:HG3	1:A:245:ARG:NH2	2.37	0.40
1:A:526:ILE:HG23	1:A:577:TRP:CZ2	2.56	0.40
1:A:531:LYS:HE2	1:A:535:GLU:OE2	2.21	0.40
2:T:799:DA:C8	2:T:801:DT:O4'	2.74	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
1	A	760/786 (97%)	745 (98%)	13 (2%)	2 (0%)	41 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	SER
1	A	307	ILE

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	
1	A	648/672 (96%)	618 (95%)	30 (5%)	27	19

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	66	THR
1	A	84	ARG
1	A	97	ARG
1	A	137	ASN
1	A	149	PRO
1	A	185	ASN
1	A	189	SER
1	A	214	ASN
1	A	239	ARG
1	A	241	ARG
1	A	256	ARG
1	A	261	LYS
1	A	281	LEU
1	A	290	SER
1	A	298	GLN
1	A	311	TRP
1	A	313	ARG
1	A	314	MET
1	A	355	ARG
1	A	403	TYR
1	A	448	GLU
1	A	452	GLU
1	A	500	TYR
1	A	571	GLN
1	A	585	ARG
1	A	597	HIS
1	A	606	ILE
1	A	720	LEU
1	A	768	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	17	GLN
1	A	61	GLN
1	A	185	ASN
1	A	203	GLN
1	A	209	ASN
1	A	214	ASN
1	A	298	GLN
1	A	366	HIS
1	A	375	HIS
1	A	397	HIS
1	A	472	ASN
1	A	475	HIS
1	A	571	GLN
1	A	597	HIS
1	A	627	GLN
1	A	713	ASN
1	A	735	ASN
1	A	751	HIS
1	A	756	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	$\# Z > 2$
2	3DR	T	806	2	8,11,12	0.78	0	9,14,17	0.81	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
2	3DR	T	806	2	-	0/3/15/16	0/1/1/1

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.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
4	DG3	A	914	5	25,32,32	1.41	2 (8%)	28,50,50	2.44	12 (42%)

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
4	DG3	A	914	5	-	5/18/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	914	DG3	C6-N1	4.61	1.41	1.33
4	A	914	DG3	C2-N1	2.42	1.39	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	914	DG3	N3-C2-N1	-5.32	120.12	127.22
4	A	914	DG3	C2-N3-C4	4.84	120.88	115.36
4	A	914	DG3	C2'-C1'-N9	-4.04	104.87	112.48
4	A	914	DG3	O5'-PA-O1A	3.96	124.54	109.07
4	A	914	DG3	PB-O3B-PG	-3.64	120.34	132.83
4	A	914	DG3	C5-C6-N1	-3.47	118.68	123.43
4	A	914	DG3	PA-O5'-C5'	3.38	141.48	121.68
4	A	914	DG3	O2G-PG-O3B	2.35	112.50	104.64
4	A	914	DG3	C2'-C3'-C4'	-2.21	98.59	102.72
4	A	914	DG3	O4'-C4'-C5'	2.17	113.09	109.52
4	A	914	DG3	C3'-C2'-C1'	-2.16	100.28	102.78
4	A	914	DG3	C6-N1-C2	2.10	119.27	115.93

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	914	DG3	PB-O3A-PA-O5'
4	A	914	DG3	C5'-O5'-PA-O3A
4	A	914	DG3	C5'-O5'-PA-O2A
4	A	914	DG3	C4'-C5'-O5'-PA
4	A	914	DG3	O4'-C4'-C5'-O5'

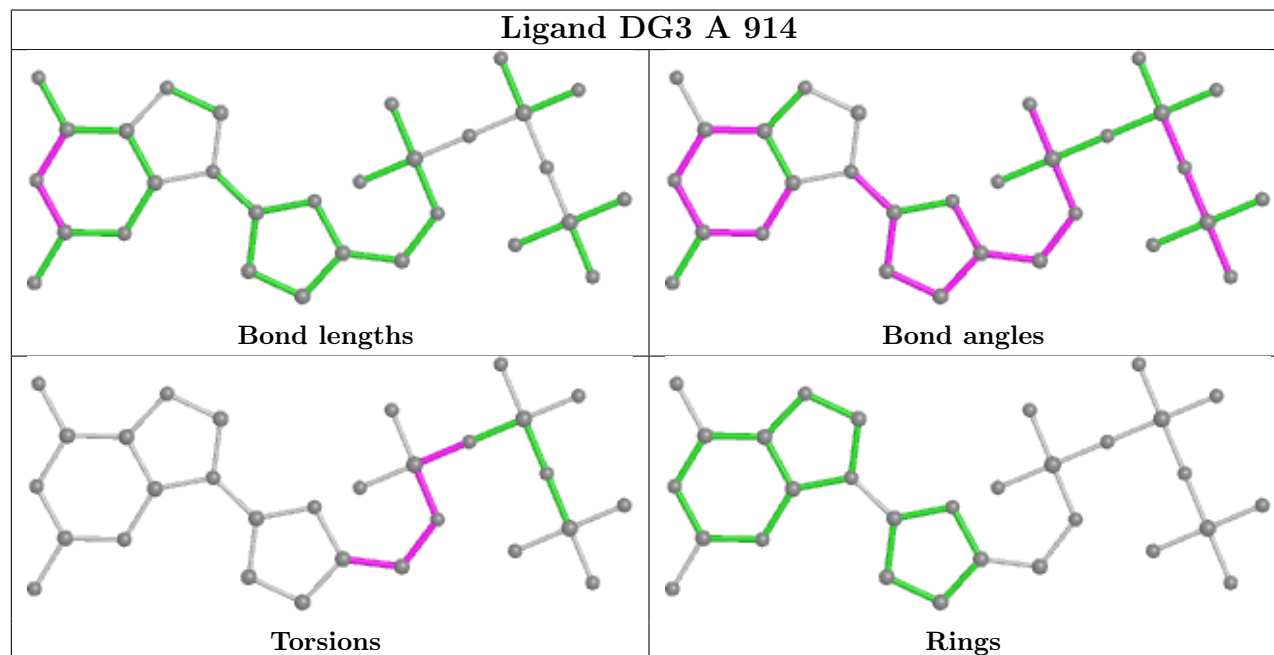
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	914	DG3	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	768/786 (97%)	0.38	17 (2%) 62 66	22, 31, 45, 67	0
2	T	19/20 (95%)	0.35	0 100 100	26, 33, 64, 81	0
3	P	13/13 (100%)	0.23	0 100 100	25, 35, 56, 57	0
All	All	800/819 (97%)	0.37	17 (2%) 63 67	22, 31, 47, 81	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	ASN	6.0
1	A	307	ILE	5.0
1	A	304	GLY	3.5
1	A	94	LYS	3.1
1	A	1	MET	3.0
1	A	-1	PRO	2.7
1	A	131	HIS	2.6
1	A	87	ARG	2.6
1	A	130	MET	2.5
1	A	625	ASP	2.5
1	A	306	SER	2.4
1	A	258	HIS	2.4
1	A	608	GLY	2.4
1	A	765	LEU	2.3
1	A	558	SER	2.3
1	A	265	PHE	2.2
1	A	134	THR	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(\AA^2)	Q<0.9
2	3DR	T	806	11/12	0.94	0.13	29,32,32,33	0

6.3 Carbohydrates [i](#)

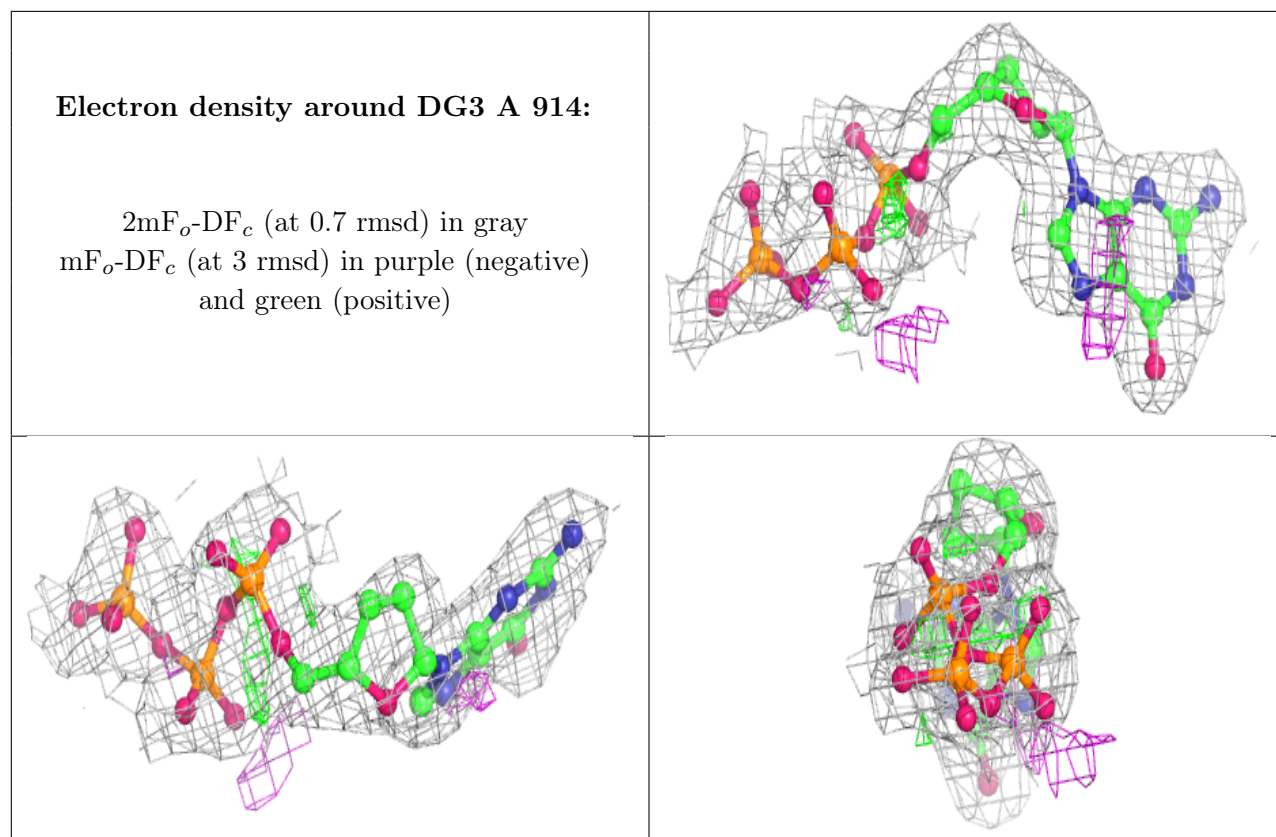
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
5	CA	A	1002	1/1	0.84	0.09	59,59,59,59	0
4	DG3	A	914	30/30	0.90	0.16	23,33,43,44	0
5	CA	A	1001	1/1	0.99	0.10	32,32,32,32	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.