



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:38 AM UTC

PDB ID : 3K5M / pdb_00003k5m
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

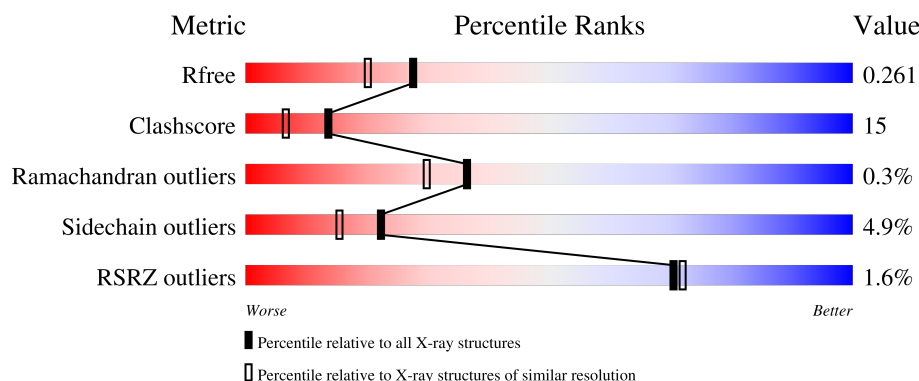
1 Overall quality at a glance

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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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	2% 67% 27% • •
2	T	20	30% 60% 10%
3	P	13	46% 54%

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

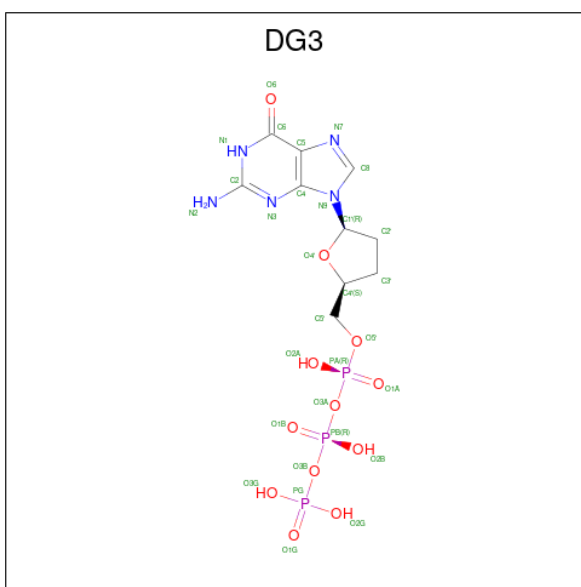
- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*TP*CP*CP*TP*GP*(3DR)P*AP*CP*GP*CP*TP*AP*GP*GP*CP*AP*CP*A)-3').

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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

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

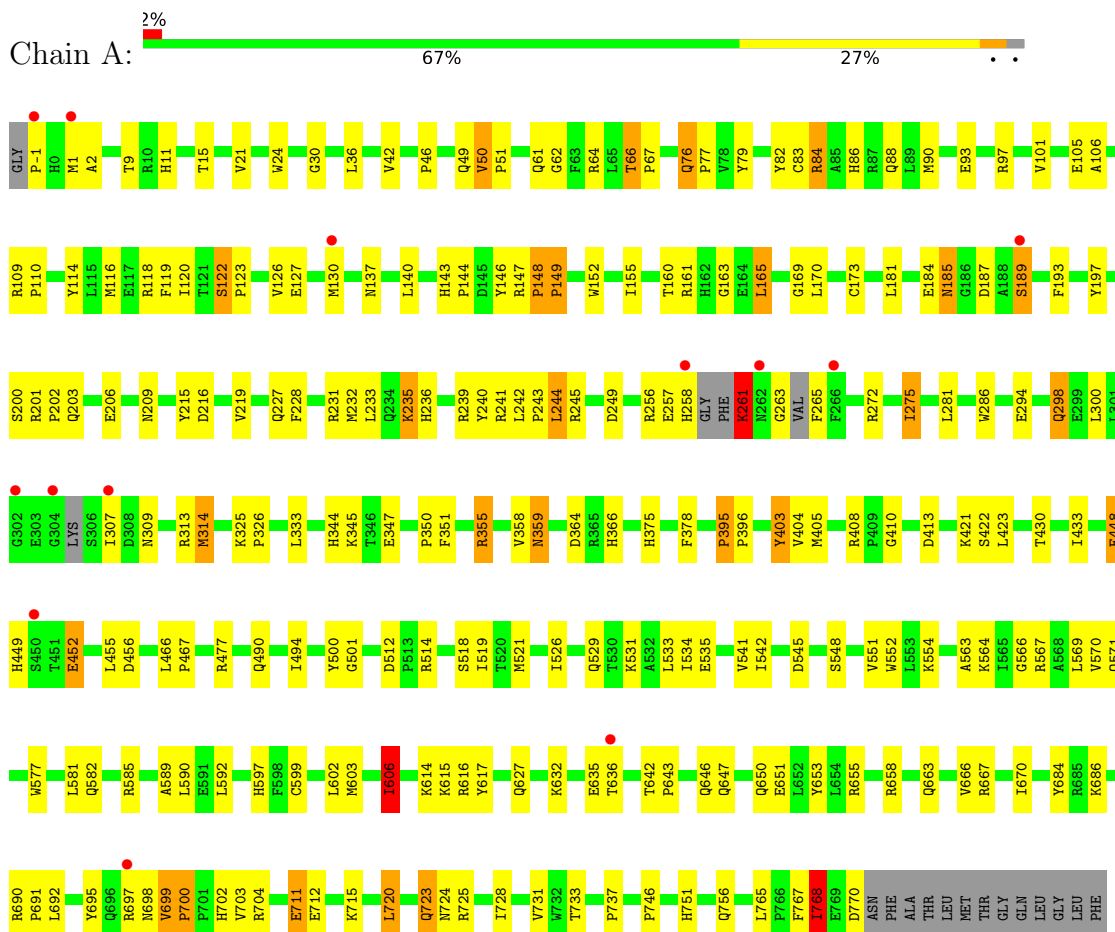
- Molecule 6 is water.

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

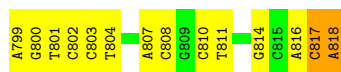
3 Residue-property plots

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')



G901	G902	G903	G904	G905	G906	T907	T908	T909	T910	T911	T912	T913

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 28.43 – 2.04	Depositor EDS
% Data completeness (in resolution range)	88.7 (28.43-2.04) 88.6 (28.43-2.04)	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 0.243 , 0.261	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)	0.35 , 41.7	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

5.1 Standard geometry

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

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	0.79	3/6369 (0.0%)	1.14	50/8638 (0.6%)
2	T	0.78	1/432 (0.2%)	1.19	6/662 (0.9%)
3	P	0.56	0/298	1.23	1/459 (0.2%)
All	All	0.78	4/7099 (0.1%)	1.15	57/9759 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	PRO	CA-C	-6.02	1.46	1.52
1	A	50	VAL	CA-CB	5.40	1.57	1.53
1	A	144	PRO	CA-C	-5.38	1.44	1.52
2	T	818	DA	C1'-N9	-5.04	1.36	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	818	DA	O4'-C1'-N9	-11.36	91.36	108.40
1	A	110	PRO	N-CA-C	9.80	122.66	110.70
2	T	818	DA	C4'-C3'-O3'	-7.94	98.09	110.00
1	A	589	ALA	N-CA-C	-7.52	103.19	112.88
1	A	603	MET	CA-C-N	7.42	127.38	120.03
1	A	603	MET	C-N-CA	7.42	127.38	120.03
1	A	149	PRO	N-CA-C	-7.28	98.87	111.32
1	A	148	PRO	N-CA-C	7.27	119.57	110.70
1	A	699	VAL	CA-C-N	7.07	124.75	119.66
1	A	699	VAL	C-N-CA	7.07	124.75	119.66
1	A	309	ASN	N-CA-C	6.86	119.38	109.84
1	A	66	THR	CA-C-N	6.83	126.82	119.78
1	A	66	THR	C-N-CA	6.83	126.82	119.78
1	A	692	LEU	N-CA-C	6.71	119.45	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	691	PRO	N-CA-C	-6.59	100.86	111.14
1	A	261	LYS	CA-C-N	-6.51	111.58	120.44
1	A	261	LYS	C-N-CA	-6.51	111.58	120.44
1	A	215	TYR	N-CA-C	6.41	120.31	112.23
1	A	711	GLU	N-CA-C	-6.10	104.71	111.36
1	A	723	GLN	N-CA-C	6.08	117.98	111.36
1	A	768	ILE	N-CA-C	-6.03	105.49	111.88
1	A	643	PRO	N-CA-C	-6.03	105.51	113.65
1	A	551	VAL	N-CA-C	5.87	116.32	107.80
1	A	30	GLY	CA-C-N	5.86	125.62	119.76
1	A	30	GLY	C-N-CA	5.86	125.62	119.76
1	A	728	ILE	N-CA-C	5.84	116.28	108.11
2	T	817	DC	O3'-P-O5'	-5.73	95.40	104.00
3	P	911	DT	N1-C1'-C2'	-5.72	104.92	113.50
1	A	452	GLU	N-CA-C	5.62	118.42	110.50
1	A	700	PRO	CA-C-N	5.58	125.68	119.32
1	A	700	PRO	C-N-CA	5.58	125.68	119.32
1	A	359	ASN	N-CA-C	5.40	119.86	113.16
1	A	395	PRO	CA-C-N	5.40	125.16	119.76
1	A	395	PRO	C-N-CA	5.40	125.16	119.76
1	A	148	PRO	CB-CA-C	-5.38	104.36	110.92
1	A	542	ILE	N-CA-C	5.32	117.73	111.09
1	A	606	ILE	N-CA-C	-5.31	102.72	109.58
1	A	219	VAL	N-CA-C	5.30	115.76	108.12
1	A	165	LEU	N-CA-C	5.26	117.94	110.10
1	A	423	LEU	N-CA-C	5.26	116.69	111.07
1	A	548	SER	N-CA-C	5.25	117.97	109.40
1	A	42	VAL	N-CA-C	5.25	116.22	108.45
1	A	408	ARG	CB-CA-C	-5.23	104.99	110.17
2	T	818	DA	C5'-C4'-C3'	5.23	122.75	114.90
1	A	545	ASP	N-CA-C	5.19	116.65	107.61
1	A	101	VAL	N-CA-C	5.18	115.37	108.11
1	A	501	GLY	N-CA-C	5.17	118.94	112.73
2	T	803	DC	N1-C1'-C2'	-5.17	105.75	113.50
1	A	275	ILE	N-CA-C	5.16	115.48	107.28
1	A	358	VAL	N-CA-C	5.16	115.82	110.82
1	A	105	GLU	N-CA-C	5.13	119.12	112.86
1	A	173	CYS	N-CA-C	-5.05	105.77	112.24
2	T	802	DC	N1-C1'-C2'	-5.05	105.93	113.50
1	A	378	PHE	N-CA-C	5.04	120.95	109.81
1	A	76	GLN	CA-C-N	5.04	124.97	119.78
1	A	76	GLN	C-N-CA	5.04	124.97	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	THR	N-CA-C	-5.01	104.24	110.41

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	176	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	9	0
6	P	14	0	0	0	0
6	T	36	0	0	0	0
All	All	7390	0	6427	195	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 15.

All (195) 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:161:ARG:HB3	1:A:314:MET:HE2	1.44	0.97
1:A:62:GLY:HA3	1:A:84:ARG:HD3	1.49	0.95
1:A:90:MET:HE3	1:A:109:ARG:NH2	1.84	0.93
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:185:ASN:HD22	1:A:185:ASN:C	1.94	0.74
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:235:LYS:HG3	6:A:1082:HOH:O	1.90	0.70
1:A:116:MET:HE2	1:A:375:HIS:HA	1.74	0.69
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:704:ARG:CZ	1:A:737:PRO:HD2	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:403:TYR:C	1:A:403:TYR:CD2	2.80	0.59
1:A:200:SER:H	1:A:203:GLN:NE2	2.00	0.58
1:A:404:VAL:HG11	1:A:614:LYS:CD	2.33	0.57
1:A:228:PHE:O	1:A:232:MET:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:MET:HE3	1:A:232:MET:HA	1.86	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:161:ARG:NE	1:A:314:MET:HE2	2.20	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:161:ARG:NH2	1:A:314:MET:HE3	2.22	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:CE	2.29	0.54
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
1:A:770:ASP:OD1	1:A:770:ASP:C	2.51	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
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

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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:232:MET:HE1	1:A:235:LYS:HE2	1.95	0.49
1:A:114:TYR:CE1	1:A:118:ARG:CZ	2.96	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: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:351:PHE:CD2	1:A:351:PHE:C	2.92	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:300:LEU:HD12	1:A:300:LEU:C	2.38	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:421:LYS:O	1:A:422:SER:C	2.57	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: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:118:ARG:O	1:A:119:PHE:HB2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ARG:O	1:A:698:ASN:C	2.56	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
1:A:9:THR:OG1	1:A:11:HIS:HE1	2.00	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: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: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:232:MET:HE3	1:A:232:MET:CA	2.47	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:161:ARG:CZ	1:A:314:MET:HE3	2.49	0.42
1:A:347:GLU:C	1:A:350:PRO:HD2	2.44	0.42
1:A:635:GLU:H	1:A:635:GLU:CD	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LEU:N	1:A:467:PRO:CD	2.84	0.41
3:P:902:DT:H2''	3:P:903:DG:H8	1.85	0.41
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:455:LEU:HD21	1:A:521:MET:HE1	2.01	0.41
1:A:86:HIS:NE2	1:A:109:ARG:HD3	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 [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	760/786 (97%)	745 (98%)	13 (2%)	2 (0%)	36 30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	SER

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Mol	Chain	Res	Type
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%)	616 (95%)	32 (5%)	22	15

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	15	THR
1	A	61	GLN
1	A	66	THR
1	A	84	ARG
1	A	97	ARG
1	A	137	ASN
1	A	155	ILE
1	A	185	ASN
1	A	189	SER
1	A	235	LYS
1	A	239	ARG
1	A	241	ARG
1	A	244	LEU
1	A	256	ARG
1	A	261	LYS
1	A	281	LEU
1	A	298	GLN
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

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Mol	Chain	Res	Type
1	A	571	GLN
1	A	585	ARG
1	A	597	HIS
1	A	606	ILE
1	A	655	ARG
1	A	720	LEU
1	A	768	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) 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	268	GLN
1	A	298	GLN
1	A	341	GLN
1	A	344	HIS
1	A	359	ASN
1	A	366	HIS
1	A	375	HIS
1	A	464	HIS
1	A	472	ASN
1	A	475	HIS
1	A	571	GLN
1	A	597	HIS
1	A	622	GLN
1	A	627	GLN
1	A	659	ASN
1	A	721	GLN
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	0.63	0	7,14,17	0.91	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	31,32,32	1.11	1 (3%)	44,50,50	2.29	19 (43%)

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	-	6/22/31/31	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	914	DG3	C5-N7	-2.46	1.34	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	914	DG3	O2A-PA-O3A	-6.12	90.72	107.27
4	A	914	DG3	C2-N3-C4	4.98	120.88	112.30
4	A	914	DG3	C5-C4-N3	-4.16	121.77	128.39
4	A	914	DG3	C2'-C1'-N9	-3.97	104.87	112.40
4	A	914	DG3	O5'-PA-O1A	3.94	124.54	108.94
4	A	914	DG3	O3A-PB-O1B	3.77	122.05	110.70
4	A	914	DG3	PA-O5'-C5'	3.51	141.48	121.35
4	A	914	DG3	C2-N1-C6	-3.22	119.27	125.11
4	A	914	DG3	O4'-C1'-N9	3.10	113.37	107.86
4	A	914	DG3	N9-C4-N3	2.94	131.83	125.95
4	A	914	DG3	O2G-PG-O3B	2.35	112.50	104.64
4	A	914	DG3	C8-N7-C5	2.30	108.36	104.26
4	A	914	DG3	C3'-C2'-C1'	-2.25	100.28	102.87
4	A	914	DG3	C2'-C3'-C4'	-2.24	98.59	102.75
4	A	914	DG3	N9-C8-N7	-2.16	109.39	113.40
4	A	914	DG3	C5-C6-N1	2.13	118.68	113.25
4	A	914	DG3	O6-C6-C5	-2.12	120.95	126.53
4	A	914	DG3	O4'-C4'-C5'	2.08	113.09	109.34
4	A	914	DG3	C4-C5-N7	-2.07	107.39	110.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

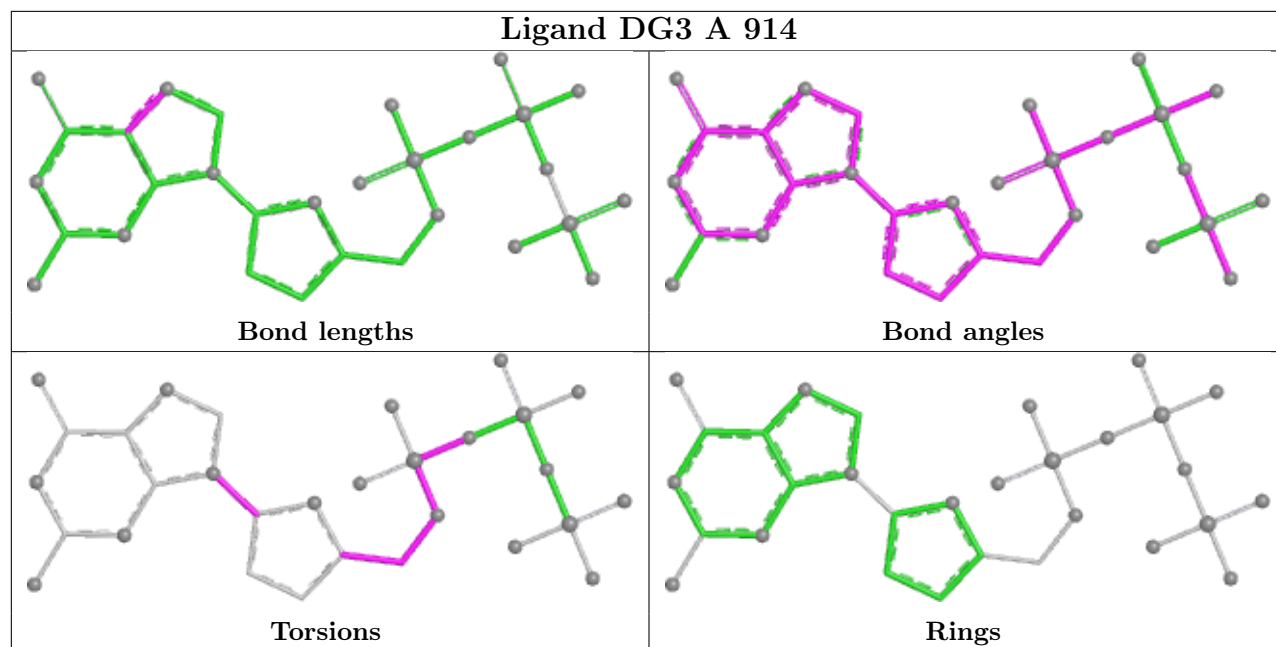
Mol	Chain	Res	Type	Atoms
4	A	914	DG3	PB-O3A-PA-O5'
4	A	914	DG3	C5'-O5'-PA-O3A
4	A	914	DG3	C5'-O5'-PA-O2A
4	A	914	DG3	C4'-C5'-O5'-PA
4	A	914	DG3	O4'-C4'-C5'-O5'
4	A	914	DG3	O4'-C1'-N9-C4

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%)	0.37	13 (1%) 69 70	22, 31, 45, 67	0
2	T	19/20 (95%)	0.07	0 100 100	26, 33, 64, 81	0
3	P	13/13 (100%)	0.15	0 100 100	25, 35, 56, 57	0
All	All	800/819 (97%)	0.36	13 (1%) 70 72	22, 31, 47, 81	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	MET	3.0
1	A	-1	PRO	2.8
1	A	307	ILE	2.6
1	A	450	SER	2.4
1	A	636	THR	2.4
1	A	302	GLY	2.3
1	A	304	GLY	2.3
1	A	262	ASN	2.3
1	A	266	PHE	2.3
1	A	258	HIS	2.2
1	A	697	ARG	2.1
1	A	1	MET	2.1
1	A	189	SER	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($\text{\AA}^2$)	Q<0.9
2	3DR	T	806	11/12	0.93	0.10	29,32,32,33	0

6.3 Carbohydrates [i](#)

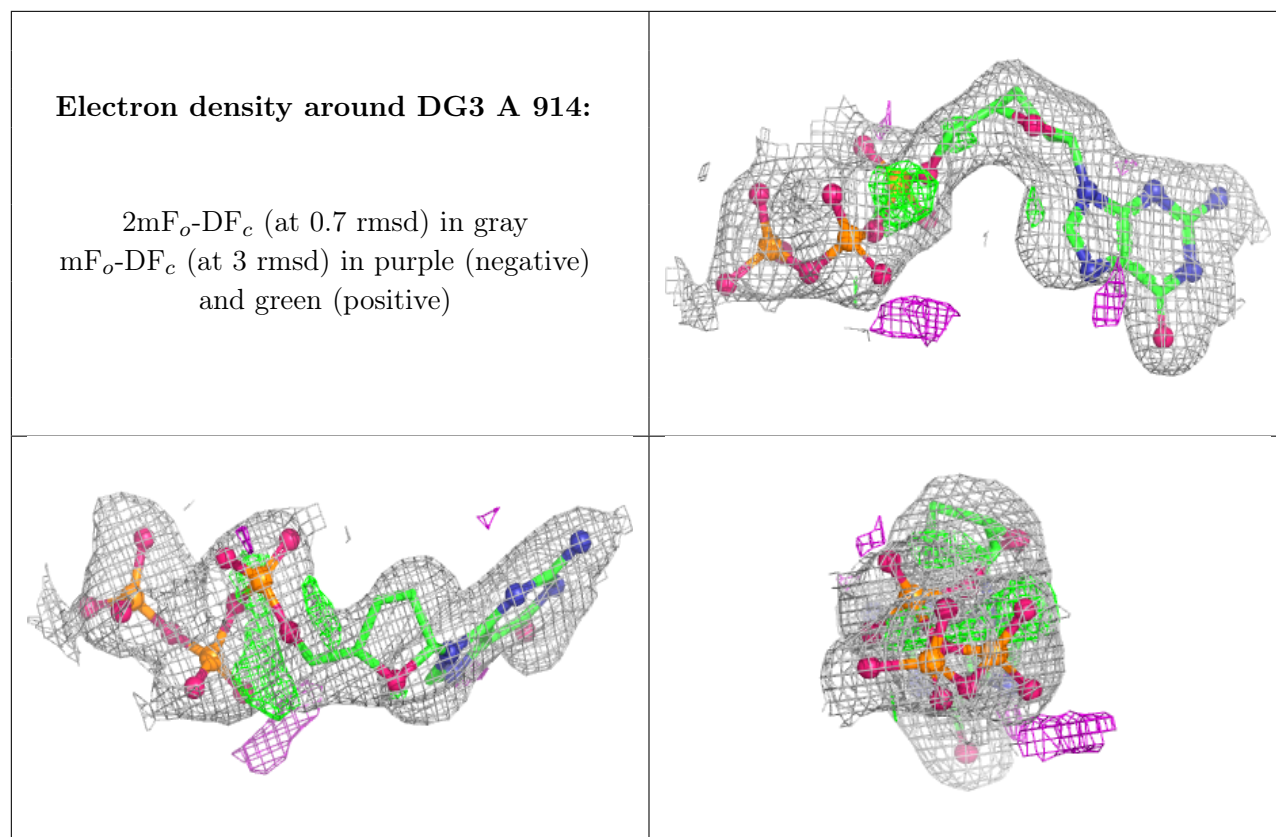
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
5	CA	A	1002	1/1	0.89	0.12	59,59,59,59	0
4	DG3	A	914	30/30	0.91	0.11	23,33,43,44	0
5	CA	A	1001	1/1	0.98	0.04	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.