



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:34 PM GMT

PDB ID : 3LZJ
Title : RB69 DNA Polymerase (Y567A) ternary complex with dCTP Opposite 7,8-Dihydro-8-oxoguanine
Authors : Wang, M.; Beckman, J.; Blaha, G.; Wang, J.; Konigsberg, W.H.
Deposited on : 2010-03-01
Resolution : 2.05 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

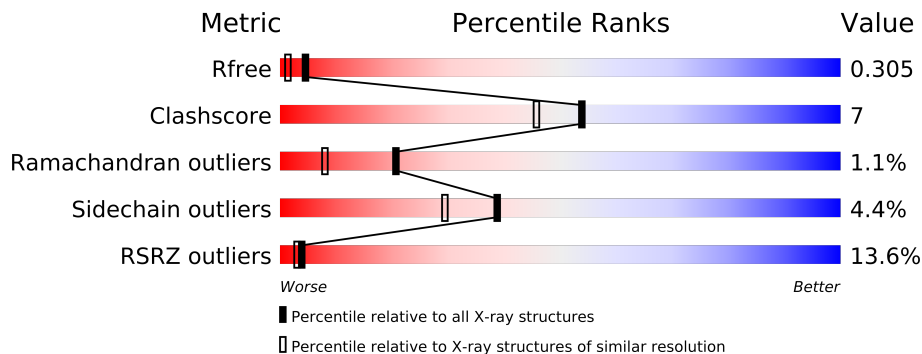
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.05 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}	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	903	
2	T	18	
3	P	13	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	CA	A	905	-	X
5	CA	A	907	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8619 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	2	0
			7385	4742	1232	1378	33			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED	UNP Q38087
A	327	ALA	ASP	ENGINEERED	UNP Q38087
A	567	ALA	TYR	ENGINEERED	UNP Q38087

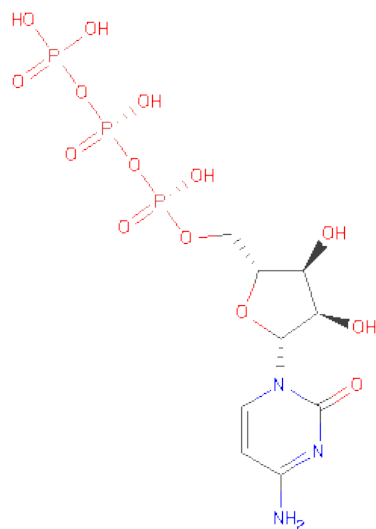
- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*CP*AP*(8OG)P*GP*TP*AP*AP*G P*CP*AP*GP*TP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	18	Total	C	N	O	P	0	0	0
			372	175	71	108	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			262	126	48	76	12			

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: C₉H₁₆N₃O₁₄P₃).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Ca	0	0
			4	4		

- Molecule 6 is water.

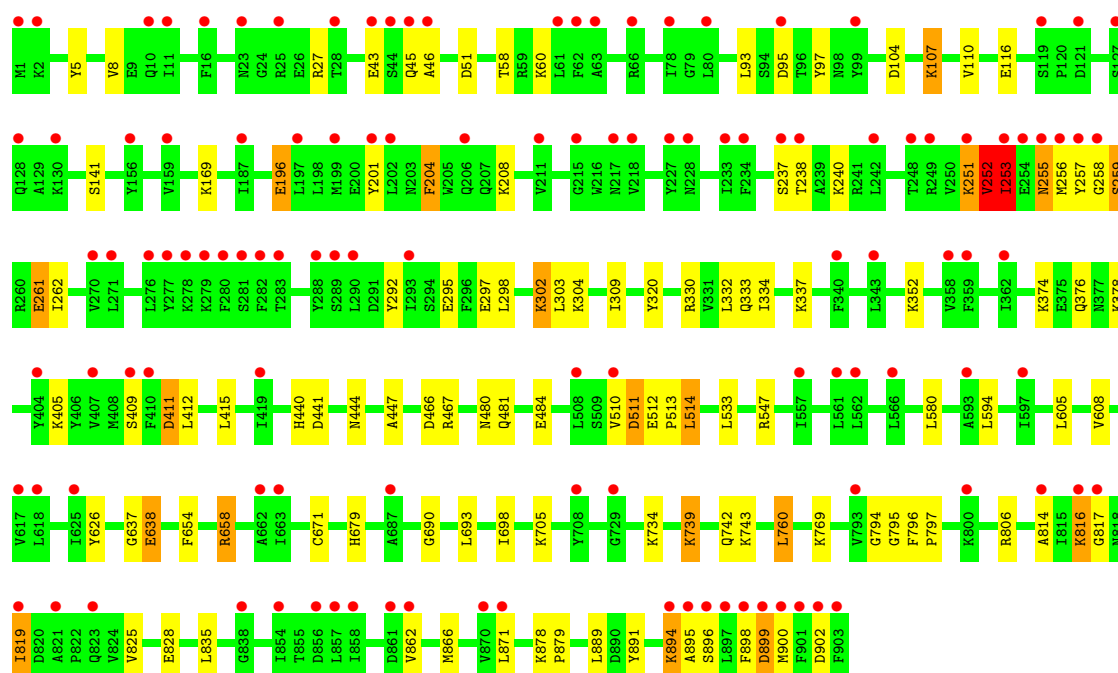
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	514	Total	O	0	0
			514	514		
6	T	38	Total	O	0	0
			38	38		
6	P	16	Total	O	0	0
			16	16		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

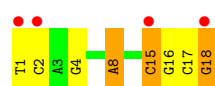
• Molecule 1: DNA polymerase

Chain A: 



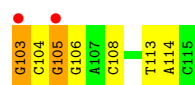
• Molecule 2: DNA (5'-D(P*TP*CP*AP*(8OG)P*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*C P*GP*CP*G)-3')

Chain T: 



• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*(DOC))-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	76.39Å 121.09Å 122.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.81 – 2.05 38.79 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.8 (38.81-2.05) 90.8 (38.79-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.205 , 0.251 0.266 , 0.305	Depositor DCC
R_{free} test set	3319 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	1.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 13.8	EDS
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 65493 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8619	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 8OG, CA, CTP, DOC

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	0.47	0/7569	0.57	0/10227
2	T	0.78	0/390	1.53	8/597 (1.3%)
3	P	0.77	0/273	1.41	5/420 (1.2%)
All	All	0.51	0/8232	0.71	13/11244 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	T	2	0

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	18	DG	O4'-C4'-C3'	-7.93	101.24	106.00
3	P	108	DC	O4'-C1'-N1	6.51	112.56	108.00
2	T	18	DG	O4'-C1'-N9	6.49	112.54	108.00
2	T	8	DA	O4'-C1'-N9	6.32	112.42	108.00
2	T	18	DG	C1'-O4'-C4'	-6.18	103.92	110.10
3	P	105	DG	P-O3'-C3'	6.08	126.99	119.70
2	T	2	DC	O4'-C1'-N1	5.86	112.10	108.00
2	T	15	DC	O4'-C1'-N1	5.79	112.06	108.00
2	T	1	DT	O4'-C1'-N1	5.69	111.99	108.00
3	P	103	DG	O4'-C4'-C3'	-5.61	102.26	104.50
2	T	17	DC	P-O3'-C3'	5.56	126.38	119.70
3	P	108	DC	O4'-C4'-C3'	-5.48	102.31	104.50
3	P	108	DC	C1'-O4'-C4'	-5.14	104.96	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	4	8OG	C4',C3'

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7385	0	7282	102	0
2	T	372	0	200	3	0
3	P	262	0	148	5	0
4	A	28	0	10	0	0
5	A	4	0	0	0	0
6	A	514	0	0	11	0
6	P	16	0	0	0	0
6	T	38	0	0	0	0
All	All	8619	0	7640	108	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (108) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:251:LYS:HB3	1:A:252:VAL:HA	1.16	1.15
1:A:898:PHE:HA	1:A:899:ASP:HB3	1.29	1.15
1:A:510:VAL:HA	1:A:511:ASP:CB	1.95	0.97
1:A:251:LYS:HB3	1:A:252:VAL:CA	1.96	0.95
1:A:258:GLY:HA3	1:A:259:SER:HB2	1.46	0.94
1:A:794:GLY:HA3	1:A:796:PHE:H	1.31	0.94
1:A:895:ALA:HB3	1:A:896:SER:HA	1.47	0.94
1:A:794:GLY:HA3	1:A:796:PHE:N	1.82	0.92
1:A:894:LYS:HD3	1:A:896:SER:HB3	1.53	0.90
1:A:330[B]:ARG:HH11	1:A:333:GLN:HE22	1.23	0.86
1:A:898:PHE:HA	1:A:899:ASP:CB	2.06	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:794:GLY:CA	1:A:796:PHE:H	1.92	0.82
1:A:510:VAL:HA	1:A:511:ASP:HB2	1.65	0.78
1:A:251:LYS:CB	1:A:252:VAL:HA	2.07	0.78
1:A:510:VAL:CA	1:A:511:ASP:HB2	2.16	0.76
1:A:201:TYR:O	6:A:1079:HOH:O	2.04	0.75
1:A:510:VAL:HA	1:A:511:ASP:HB3	1.67	0.73
1:A:895:ALA:CB	1:A:896:SER:HA	2.21	0.71
1:A:252:VAL:HG21	1:A:262:ILE:N	2.09	0.68
1:A:258:GLY:CA	1:A:259:SER:HB2	2.22	0.68
1:A:512:GLU:HG3	1:A:513:PRO:HD2	1.73	0.68
1:A:898:PHE:HB3	1:A:900:MET:H	1.58	0.67
1:A:480:ASN:O	1:A:484:GLU:HG2	1.94	0.67
1:A:251:LYS:CB	1:A:252:VAL:CA	2.70	0.66
1:A:898:PHE:CA	1:A:899:ASP:HB3	2.18	0.65
1:A:252:VAL:HG11	1:A:261:GLU:HA	1.79	0.65
1:A:441:ASP:HB3	1:A:447:ALA:HB2	1.79	0.64
1:A:895:ALA:HB3	1:A:896:SER:CA	2.23	0.64
1:A:739:LYS:HE2	1:A:742:GLN:OE1	1.98	0.64
1:A:196:GLU:HG2	6:A:1405:HOH:O	1.97	0.63
1:A:825:VAL:HB	1:A:828:GLU:HG3	1.81	0.63
1:A:894:LYS:CD	1:A:896:SER:HB3	2.26	0.61
1:A:894:LYS:HD3	1:A:896:SER:CB	2.30	0.61
1:A:816:LYS:HG2	1:A:817:GLY:N	2.16	0.61
1:A:376:GLN:HB2	1:A:378:LYS:HG3	1.84	0.60
1:A:330[B]:ARG:HH11	1:A:333:GLN:NE2	1.98	0.60
1:A:794:GLY:N	1:A:796:PHE:H	2.00	0.59
1:A:60:LYS:HD3	6:A:1559:HOH:O	2.02	0.58
1:A:201:TYR:C	6:A:1079:HOH:O	2.38	0.58
1:A:510:VAL:CA	1:A:511:ASP:CB	2.70	0.56
1:A:637:GLY:O	1:A:638:GLU:CB	2.53	0.56
1:A:412:LEU:HD13	1:A:415:LEU:HD13	1.90	0.54
1:A:292:TYR:OH	1:A:739:LYS:NZ	2.40	0.54
1:A:256:MET:HB3	1:A:257:TYR:HB2	1.89	0.54
1:A:698:ILE:HG21	1:A:889:LEU:HD11	1.89	0.54
1:A:894:LYS:CD	1:A:896:SER:CB	2.87	0.53
1:A:204:PHE:CE1	1:A:208:LYS:HD2	2.44	0.53
1:A:240:LYS:HG3	6:A:1546:HOH:O	2.09	0.53
1:A:252:VAL:CG1	1:A:261:GLU:HA	2.39	0.52
1:A:251:LYS:HB2	1:A:252:VAL:HB	1.91	0.52
1:A:898:PHE:HB3	1:A:900:MET:N	2.24	0.51
1:A:816:LYS:HG2	1:A:817:GLY:H	1.75	0.51
1:A:330[B]:ARG:NH1	1:A:333:GLN:HE22	2.02	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:605:LEU:HA	1:A:608:VAL:HG22	1.93	0.51
1:A:97:TYR:O	1:A:352:LYS:HE2	2.11	0.51
1:A:878:LYS:HB3	1:A:879:PRO:HD3	1.94	0.50
1:A:251:LYS:CB	1:A:252:VAL:HB	2.43	0.49
1:A:794:GLY:H	1:A:796:PHE:H	1.60	0.49
1:A:252:VAL:HG21	1:A:262:ILE:H	1.78	0.49
1:A:411:ASP:C	1:A:411:ASP:OD1	2.50	0.49
2:T:15:DC:H2''	2:T:16:DG:C8	2.47	0.49
1:A:8:VAL:HG11	1:A:93:LEU:HD11	1.95	0.48
1:A:256:MET:HB3	1:A:257:TYR:CB	2.44	0.47
1:A:797:PRO:HG2	1:A:806:ARG:NH1	2.29	0.47
1:A:862:VAL:O	1:A:866:MET:HG3	2.15	0.47
1:A:898:PHE:HD1	1:A:899:ASP:HB3	1.80	0.47
1:A:510:VAL:N	1:A:511:ASP:HB2	2.30	0.47
1:A:679:HIS:HE1	6:A:1562:HOH:O	1.98	0.46
1:A:252:VAL:HG11	1:A:261:GLU:HG3	1.97	0.46
3:P:105:DG:H4'	3:P:106:DG:OP1	2.16	0.45
1:A:5:TYR:HB3	1:A:97:TYR:CE1	2.52	0.45
3:P:113:DT:H2''	3:P:114:DA:H5'	1.99	0.45
1:A:104:ASP:HB3	1:A:107:LYS:HG3	1.97	0.45
1:A:237:SER:N	6:A:1546:HOH:O	2.49	0.45
1:A:252:VAL:O	1:A:253:ILE:C	2.56	0.45
1:A:252:VAL:HG11	1:A:262:ILE:H	1.83	0.44
1:A:255:ASN:HB2	1:A:256:MET:HA	1.99	0.44
1:A:734:LYS:HG2	3:P:113:DT:H5'	1.99	0.44
1:A:760:LEU:HD13	1:A:891:TYR:HA	1.99	0.44
1:A:895:ALA:CB	1:A:896:SER:CA	2.91	0.44
1:A:116:GLU:HB3	1:A:320:TYR:OH	2.18	0.44
1:A:705:LYS:HD3	2:T:8:DA:H5''	2.00	0.43
1:A:654:PHE:O	1:A:658:ARG:HB2	2.19	0.43
1:A:794:GLY:CA	1:A:796:PHE:N	2.59	0.43
1:A:440[A]:HIS:CE1	1:A:444:ASN:HD21	2.36	0.43
3:P:104:DC:H2''	3:P:105:DG:C8	2.53	0.43
1:A:297:GLU:O	1:A:337:LYS:NZ	2.47	0.43
3:P:103:DG:H2''	3:P:104:DC:C6	2.54	0.42
1:A:169:LYS:HG2	6:A:1284:HOH:O	2.19	0.42
1:A:819:ILE:HG13	1:A:819:ILE:H	1.56	0.42
2:T:18:DG:H3'	2:T:18:DG:OP1	2.19	0.42
1:A:51:ASP:HB2	6:A:1047:HOH:O	2.19	0.42
1:A:898:PHE:CA	1:A:899:ASP:CB	2.87	0.42
1:A:409:SER:HB3	1:A:626:TYR:CD2	2.55	0.42
1:A:816:LYS:H	1:A:816:LYS:HD2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:298:LEU:HD11	1:A:334:ILE:HG13	2.01	0.41
1:A:481:GLN:HG2	6:A:1169:HOH:O	2.19	0.41
1:A:302:LYS:HG2	1:A:304:LYS:HG3	2.02	0.41
1:A:110:VAL:HB	1:A:141:SER:HB3	2.03	0.41
1:A:671:CYS:SG	6:A:1560:HOH:O	2.33	0.41
1:A:258:GLY:HA3	1:A:259:SER:CB	2.24	0.41
1:A:405:LYS:O	1:A:690:GLY:HA2	2.21	0.41
1:A:898:PHE:CB	1:A:900:MET:H	2.32	0.40
1:A:547:ARG:HD3	1:A:547:ARG:HA	1.90	0.40
1:A:637:GLY:O	1:A:638:GLU:HB2	2.21	0.40
1:A:256:MET:HB3	1:A:257:TYR:CA	2.51	0.40
1:A:95:ASP:OD2	1:A:374:LYS:HE3	2.22	0.40
1:A:514:LEU:HD22	1:A:533:LEU:HD11	2.04	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	903/903 (100%)	855 (95%)	38 (4%)	10 (1%)	21 8

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ILE
1	A	259	SER
1	A	511	ASP
1	A	638	GLU
1	A	251	LYS
1	A	252	VAL
1	A	795	GLY
1	A	814	ALA
1	A	899	ASP
1	A	46	ALA

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	801/799 (100%)	766 (96%)	35 (4%)	39 29

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	43	GLU
1	A	45	GLN
1	A	58	THR
1	A	107	LYS
1	A	196	GLU
1	A	204	PHE
1	A	238	THR
1	A	252	VAL
1	A	253	ILE
1	A	255	ASN
1	A	261	GLU
1	A	295	GLU
1	A	302	LYS
1	A	303	LEU
1	A	309	ILE
1	A	332	LEU
1	A	411	ASP
1	A	466	ASP
1	A	467	ARG
1	A	514	LEU
1	A	580	LEU
1	A	594	LEU
1	A	658	ARG
1	A	693	LEU
1	A	739	LYS
1	A	743	LYS
1	A	760	LEU
1	A	769	LYS
1	A	816	LYS
1	A	819	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	835	LEU
1	A	871	LEU
1	A	894	LYS
1	A	902	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	112	ASN
1	A	131	HIS
1	A	173	GLN
1	A	255	ASN
1	A	333	GLN
1	A	339	GLN
1	A	376	GLN
1	A	444	ASN
1	A	564	ASN
1	A	679	HIS
1	A	761	GLN
1	A	773	GLN
1	A	823	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DOC	P	115	3,2	17,19,20	1.58	2 (11%)	20,26,29	3.85	7 (35%)
2	8OG	T	4	2	23,25,26	5.20	8 (34%)	27,37,40	3.72	14 (51%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DOC	P	115	3,2	-	0/5/18/19	0/2/2/2
2	8OG	T	4	2	2/2/4/4	0/6/21/22	0/1/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	4	8OG	P-OP1	18.41	1.67	1.46
2	T	4	8OG	O8-C8	11.35	1.47	1.23
2	T	4	8OG	C3'-C4'	-6.87	1.33	1.53
2	T	4	8OG	O6-C6	5.93	1.36	1.24
2	T	4	8OG	C5'-C4'	-5.74	1.33	1.51
2	T	4	8OG	O3'-C3'	-4.45	1.33	1.43
3	P	115	DOC	C2-N1	4.43	1.43	1.38
3	P	115	DOC	P-OP1	4.26	1.51	1.46
2	T	4	8OG	C4-N9	-2.85	1.33	1.37
2	T	4	8OG	C2-N2	2.06	1.35	1.32

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	115	DOC	C4'-O4'-C1'	-14.96	103.81	110.05
2	T	4	8OG	C8-N9-C1'	10.25	130.86	125.17
2	T	4	8OG	C2'-C1'-N9	-10.14	105.49	115.79
2	T	4	8OG	C5-C4-N9	4.77	108.37	106.00
2	T	4	8OG	C8-N7-C5	-4.23	103.19	107.48
2	T	4	8OG	O4'-C1'-N9	3.95	111.83	108.15
3	P	115	DOC	C2-N3-C4	3.86	121.15	115.57
3	P	115	DOC	C6-C5-C4	3.76	119.03	117.47
2	T	4	8OG	O3'-C3'-C4'	3.71	125.38	110.14
3	P	115	DOC	O4'-C4'-C5'	3.59	114.68	109.67
2	T	4	8OG	O3'-C3'-C2'	3.57	124.23	110.78
3	P	115	DOC	O4'-C1'-N1	3.52	114.30	107.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	4	8OG	C2'-C3'-C4'	3.39	110.32	102.73
2	T	4	8OG	C2-N3-C4	3.30	119.72	115.09
2	T	4	8OG	O4'-C4'-C5'	3.24	120.91	109.36
2	T	4	8OG	C4-C5-N7	3.17	108.78	106.14
2	T	4	8OG	N3-C4-N9	2.75	131.26	127.09
2	T	4	8OG	O4'-C4'-C3'	2.74	112.62	105.66
2	T	4	8OG	C5-C4-N3	-2.45	120.36	125.70
3	P	115	DOC	C3'-C2'-C1'	2.13	105.16	102.80
3	P	115	DOC	C2'-C1'-N1	-2.09	108.49	112.66

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	4	8OG	C4'
2	T	4	8OG	C3'

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 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	CTP	A	904	5	28,29,30	0.96	0	38,45,47	1.54	7 (18%)

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	CTP	A	904	5	-	0/19/34/38	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	CTP	C2-N3-C4	4.67	122.33	115.57
4	A	904	CTP	O2B-PB-O3A	3.42	121.34	105.14
4	A	904	CTP	C2'-C1'-N1	-2.83	110.38	113.39
4	A	904	CTP	O4'-C1'-N1	2.79	113.95	108.06
4	A	904	CTP	C6-C5-C4	2.62	118.56	117.47
4	A	904	CTP	O4'-C4'-C3'	2.10	105.97	102.67
4	A	904	CTP	C5-C4-N3	-2.09	118.85	121.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	903/903 (100%)	1.16	120 (13%) 4 3	2, 7, 27, 125	0
2	T	18/18 (100%)	0.67	4 (22%) 1 1	2, 5, 83, 105	0
3	P	13/13 (100%)	0.67	2 (15%) 3 2	2, 5, 33, 38	0
All	All	934/934 (100%)	1.14	126 (13%) 4 3	2, 7, 28, 125	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	901	PHE	19.1
1	A	900	MET	15.6
1	A	898	PHE	14.4
1	A	903	PHE	13.1
1	A	897	LEU	11.9
1	A	902	ASP	11.8
1	A	899	ASP	9.5
1	A	510	VAL	6.7
1	A	895	ALA	6.3
1	A	253	ILE	6.2
1	A	857	LEU	6.1
1	A	896	SER	5.7
1	A	99	TYR	5.5
1	A	817	GLY	5.4
1	A	11	ILE	4.8
1	A	257	TYR	4.7
1	A	858	ILE	4.6
1	A	233	ILE	4.4
1	A	16	PHE	4.3
1	A	1	MET	4.2
1	A	816	LYS	4.2
1	A	821	ALA	4.1
1	A	819	ILE	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	1	DT	4.0
1	A	43	GLU	4.0
1	A	793	VAL	3.9
1	A	234	PHE	3.8
1	A	862	VAL	3.6
1	A	2	LYS	3.6
1	A	46	ALA	3.6
2	T	2	DC	3.5
1	A	63	ALA	3.5
1	A	227	TYR	3.5
1	A	130	LYS	3.4
1	A	28	THR	3.3
1	A	45	GLN	3.2
1	A	199	MET	3.2
1	A	277	TYR	3.2
1	A	258	GLY	3.2
1	A	156	TYR	3.1
1	A	861	ASP	3.1
1	A	358	VAL	3.0
1	A	814	ALA	3.0
1	A	121	ASP	2.9
1	A	282	PHE	2.9
1	A	289	SER	2.9
1	A	127	SER	2.9
1	A	800	LYS	2.9
1	A	251	LYS	2.8
1	A	271	LEU	2.8
1	A	238	THR	2.8
1	A	128	GLN	2.7
1	A	249	ARG	2.7
1	A	290	LEU	2.7
1	A	78	ILE	2.7
1	A	557	ILE	2.7
1	A	340	PHE	2.7
1	A	25	ARG	2.7
1	A	242	LEU	2.7
1	A	854	ILE	2.6
1	A	407	VAL	2.6
2	T	15	DC	2.6
3	P	103	DG	2.6
1	A	279	LYS	2.5
1	A	23	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	708	TYR	2.5
1	A	838	GLY	2.5
1	A	597	ILE	2.5
1	A	566	LEU	2.5
1	A	278	LYS	2.5
1	A	276	LEU	2.5
1	A	44	SER	2.5
1	A	211	VAL	2.5
1	A	248	THR	2.4
1	A	894	LYS	2.4
1	A	187	ILE	2.4
1	A	255	ASN	2.4
1	A	508	LEU	2.4
1	A	871	LEU	2.4
1	A	359	PHE	2.4
1	A	625	ILE	2.4
1	A	288	TYR	2.4
1	A	410	PHE	2.4
1	A	343	LEU	2.4
1	A	206	GLN	2.4
1	A	201	TYR	2.4
1	A	61	LEU	2.3
1	A	66	ARG	2.3
1	A	562	LEU	2.3
1	A	218	VAL	2.3
1	A	280	PHE	2.3
1	A	95	ASP	2.3
1	A	270	VAL	2.3
1	A	617	VAL	2.3
1	A	215	GLY	2.2
1	A	62	PHE	2.2
1	A	119	SER	2.2
1	A	687	ALA	2.2
1	A	159	VAL	2.2
1	A	256	MET	2.2
1	A	237	SER	2.2
1	A	561	LEU	2.2
1	A	870	VAL	2.2
1	A	217	ASN	2.2
1	A	281	SER	2.2
1	A	618	LEU	2.2
1	A	362	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	293	ILE	2.1
1	A	729	GLY	2.1
1	A	662	ALA	2.1
2	T	18	DG	2.1
1	A	202	LEU	2.1
1	A	254	GLU	2.1
1	A	409	SER	2.1
1	A	80	LEU	2.1
1	A	283	THR	2.1
1	A	419	ILE	2.1
1	A	663	ILE	2.1
3	P	105	DG	2.1
1	A	10	GLN	2.1
1	A	197	LEU	2.1
1	A	593	ALA	2.1
1	A	823	GLN	2.1
1	A	404	TYR	2.1
1	A	856	ASP	2.1
1	A	228	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	DOC	P	115	18/19	0.09	-1.74	2,2,7,8	0
2	8OG	T	4	23/24	0.08	-2.04	2,2,4,4	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	CA	A	907	1/1	0.29	8.96	69,69,69,69	0
5	CA	A	905	1/1	0.25	4.73	31,31,31,31	0
5	CA	A	908	1/1	0.09	-2.51	59,59,59,59	0
5	CA	A	906	1/1	0.07	-2.71	54,54,54,54	0
4	CTP	A	904	28/29	0.10	-2.78	2,2,2,4	0

6.5 Other polymers ⓘ

There are no such residues in this entry.