WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:00 AM GMT

PDB ID	:	3GV8
Title	:	Human DNA polymerase iota in complex with T template DNA and incoming dGTP
Authors	:	Kirouac, K.N.; Ling, H.
Deposited on	:	2009-03-30
Resolution	:	2.00 Å(reported)

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

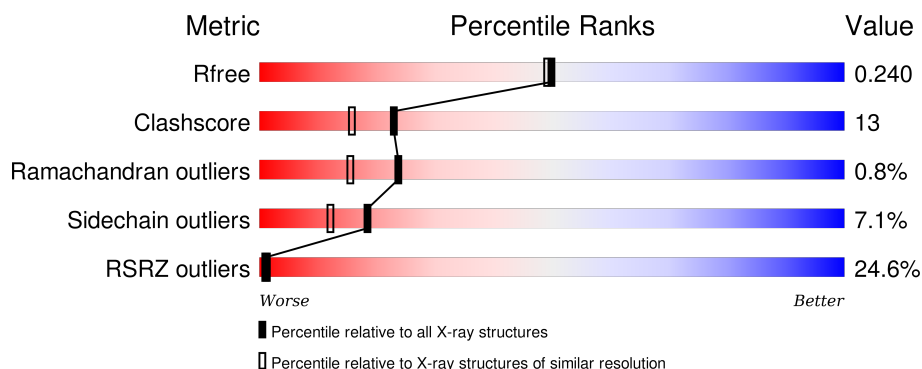|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.240
Clashscore		13
Ramachandran outliers		0.8%
Sidechain outliers		7.1%
RSRZ outliers		24.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	B	420	23% / 70% / 15% · · 11%
2	T	9	11% / 78% / 22%
3	P	7	29% / 29% / 43%

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
5	DGT	B	421	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3496 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 iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	374	Total	C	N	O	S	0	1	0
			2903	1845	504	533	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	9	Total	C	N	O	P	0	0	0
			181	88	32	53	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	7	Total	C	N	O	P	0	0	0
			139	67	29	37	6			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		

- Molecule 5 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
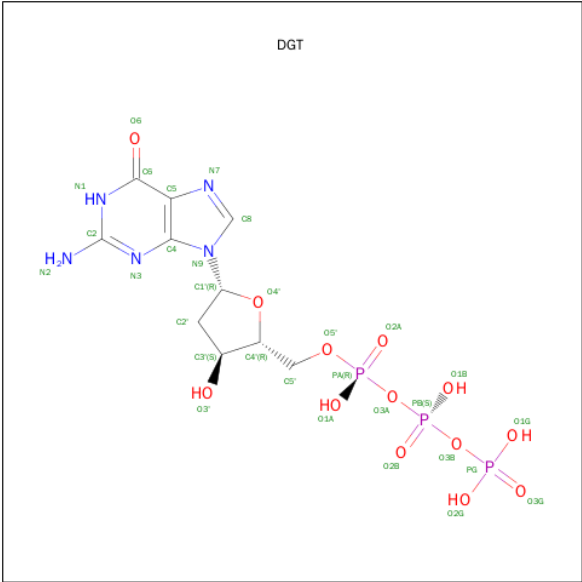
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	210	Total	O	0	0
			210	210		
6	T	19	Total	O	0	0
			19	19		
6	P	11	Total	O	0	0
			11	11		

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.
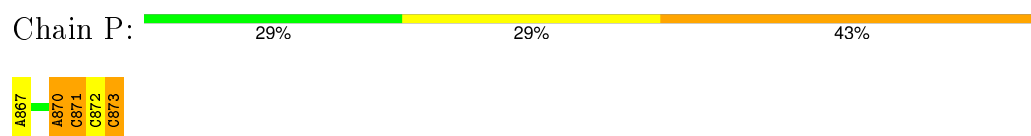
• Molecule 1: DNA polymerase iota
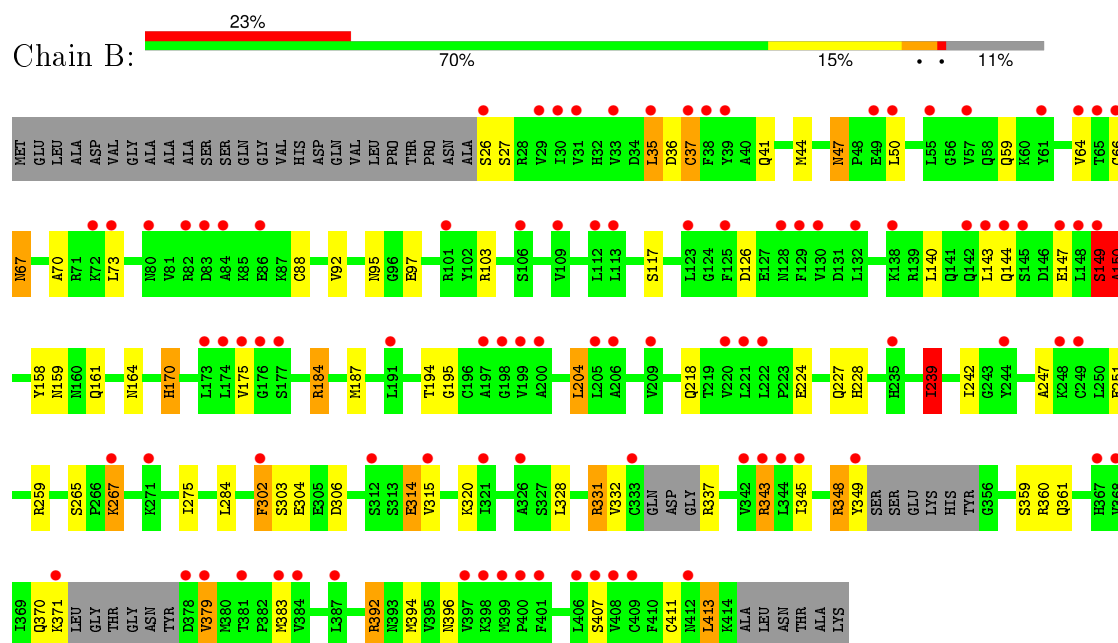
• Molecule 2: 5'-D(*AP*TP*GP*GP*GP*TP*CP*CP*T)-3'
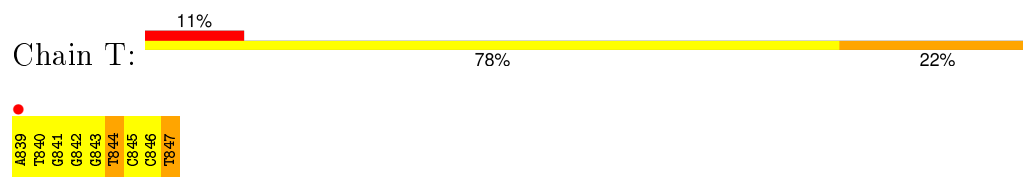
• Molecule 3: 5'-D(*AP*GP*GP*AP*CP*CP*C)-3'

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.07Å 98.07Å 203.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.84 – 2.00 23.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (23.84-2.00) 99.6 (23.83-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.56 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.218 , 0.248 0.215 , 0.240	Depositor DCC
R_{free} test set	826 reflections (2.13%)	DCC
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 39636 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3496	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DGT

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	B	0.88	4/2946 (0.1%)	0.98	16/3981 (0.4%)
2	T	1.42	0/202	2.24	14/311 (4.5%)
3	P	1.29	0/156	1.72	4/238 (1.7%)
All	All	0.94	4/3304 (0.1%)	1.16	34/4530 (0.8%)

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
1	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	VAL	CA-CB	10.38	1.76	1.54
1	B	383	MET	CG-SD	6.96	1.99	1.81
1	B	314	GLU	CD-OE2	6.93	1.33	1.25
1	B	392	ARG	CG-CD	5.10	1.64	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH1	-16.52	112.04	120.30
1	B	184	ARG	NE-CZ-NH1	-15.29	112.66	120.30
1	B	184	ARG	NE-CZ-NH2	14.39	127.50	120.30
1	B	259	ARG	NE-CZ-NH2	14.30	127.45	120.30
1	B	331	ARG	NE-CZ-NH2	-11.24	114.68	120.30
2	T	847	DT	O4'-C1'-N1	-10.26	100.81	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	392	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	T	846	DC	O4'-C1'-N1	-7.08	103.04	108.00
2	T	842	DG	C4-C5-N7	-6.88	108.05	110.80
1	B	259	ARG	CD-NE-CZ	6.87	133.22	123.60
1	B	204	LEU	CB-CG-CD2	6.86	122.66	111.00
3	P	870	DA	O4'-C1'-N9	6.85	112.79	108.00
1	B	331	ARG	NE-CZ-NH1	6.39	123.49	120.30
3	P	872	DC	O4'-C4'-C3'	-6.07	102.07	104.50
3	P	871	DC	O4'-C4'-C3'	-5.90	102.14	104.50
3	P	873	DC	O4'-C1'-N1	5.88	112.11	108.00
2	T	842	DG	O5'-P-OP2	-5.84	100.44	105.70
2	T	842	DG	N1-C6-O6	-5.82	116.41	119.90
2	T	844	DT	O4'-C1'-N1	5.68	111.97	108.00
1	B	184	ARG	CD-NE-CZ	5.55	131.37	123.60
1	B	306	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	239	ILE	CG1-CB-CG2	5.53	123.56	111.40
2	T	841	DG	O4'-C1'-N9	5.51	111.86	108.00
2	T	844	DT	N3-C4-O4	-5.51	116.59	119.90
2	T	842	DG	O5'-P-OP1	5.45	117.24	110.70
1	B	150	ALA	N-CA-C	5.42	125.63	111.00
1	B	149	SER	N-CA-C	5.36	125.48	111.00
1	B	259	ARG	CG-CD-NE	-5.31	100.65	111.80
2	T	842	DG	C5-C6-O6	5.30	131.78	128.60
2	T	841	DG	P-O3'-C3'	5.12	125.85	119.70
1	B	315	VAL	O-C-N	-5.09	114.56	122.70
2	T	843	DG	C3'-C2'-C1'	-5.05	96.44	102.50
2	T	842	DG	O4'-C1'-C2'	5.05	109.94	105.90
2	T	844	DT	O4'-C1'-C2'	5.01	109.91	105.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	149	SER	Peptide

5.2 Too-close contacts (i)

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	B	2903	0	2942	67	0
2	T	181	0	101	8	1
3	P	139	0	77	4	0
4	B	2	0	0	0	0
5	B	31	0	12	13	0
6	B	210	0	0	12	0
6	P	11	0	0	1	1
6	T	19	0	0	0	0
All	All	3496	0	3132	86	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 13.

All (86) 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:B:379:VAL:CB	1:B:379:VAL:CA	1.76	1.56
5:B:421:DGT:H5'A	5:B:421:DGT:H8	1.25	1.16
5:B:421:DGT:H5'A	5:B:421:DGT:C8	1.76	1.16
5:B:421:DGT:O2A	6:B:632:HOH:O	1.68	1.10
5:B:421:DGT:H4'	6:B:631:HOH:O	1.60	0.99
3:P:867:DA:O5'	6:P:115:HOH:O	1.61	0.91
1:B:164:ASN:H	1:B:170:HIS:HD2	1.17	0.91
5:B:421:DGT:H8	5:B:421:DGT:C5'	2.04	0.86
1:B:41:GLN:HE22	1:B:194:THR:H	1.25	0.82
1:B:239:ILE:CD1	1:B:284:LEU:HB3	2.10	0.81
5:B:421:DGT:N2	2:T:840:DT:O2	2.14	0.81
5:B:421:DGT:C4'	6:B:631:HOH:O	2.23	0.77
1:B:239:ILE:HD12	1:B:284:LEU:HB3	1.68	0.76
1:B:267:LYS:H	1:B:267:LYS:HD2	1.49	0.76
1:B:117:SER:OG	6:B:626:HOH:O	2.05	0.75
1:B:161:GLN:NE2	1:B:224:GLU:HG2	2.03	0.73
1:B:331:ARG:CD	6:B:544:HOH:O	2.39	0.71
1:B:247:ALA:O	1:B:251:GLU:HG3	1.94	0.68
1:B:379:VAL:CG1	1:B:379:VAL:CA	2.72	0.67
1:B:164:ASN:H	1:B:170:HIS:CD2	2.08	0.67
1:B:331:ARG:HD2	6:B:544:HOH:O	1.96	0.66
1:B:304:GLU:OE2	6:B:457:HOH:O	2.12	0.66
1:B:343:ARG:HH21	1:B:361:GLN:HE22	1.46	0.64
1:B:302[A]:PHE:N	1:B:302[A]:PHE:HD1	1.97	0.62
1:B:302[A]:PHE:CD1	1:B:302[A]:PHE:N	2.69	0.61
1:B:67:ASN:HD22	1:B:67:ASN:C	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:VAL:CG2	1:B:379:VAL:CA	2.73	0.60
1:B:379:VAL:N	1:B:379:VAL:CB	2.59	0.59
1:B:184:ARG:HH11	1:B:218:GLN:HE21	1.49	0.58
5:B:421:DGT:C8	3:P:873:DC:H2'	2.33	0.58
1:B:267:LYS:H	1:B:267:LYS:CD	2.16	0.58
2:T:839:DA:H3'	2:T:840:DT:H72	1.86	0.57
1:B:328:LEU:O	1:B:332:VAL:HG23	2.05	0.57
1:B:345:ILE:HB	1:B:407:SER:HB3	1.86	0.57
1:B:239:ILE:CD1	1:B:284:LEU:CB	2.83	0.57
1:B:239:ILE:HD11	1:B:284:LEU:CB	2.35	0.57
1:B:348:ARG:O	1:B:349:TYR:HB2	2.05	0.57
1:B:159:ASN:OD1	6:B:497:HOH:O	2.17	0.56
1:B:239:ILE:HD11	1:B:284:LEU:HB3	1.87	0.56
1:B:144:GLN:O	1:B:147:GLU:HG2	2.06	0.55
1:B:170:HIS:HE1	1:B:224:GLU:OE2	1.91	0.54
5:B:421:DGT:H8	3:P:873:DC:H2'	1.89	0.53
1:B:337:ARG:NH2	1:B:413:LEU:HD23	2.23	0.53
1:B:239:ILE:HG12	1:B:242:ILE:HD12	1.91	0.53
1:B:161:GLN:HE22	1:B:224:GLU:HG2	1.71	0.53
1:B:348:ARG:O	1:B:349:TYR:CB	2.56	0.53
5:B:421:DGT:C2	2:T:840:DT:O2	2.58	0.52
1:B:50:LEU:HD22	1:B:92:VAL:HG11	1.92	0.52
1:B:343:ARG:HH21	1:B:361:GLN:NE2	2.06	0.51
5:B:421:DGT:H16	2:T:840:DT:H3	1.59	0.51
1:B:331:ARG:HD3	6:B:544:HOH:O	2.06	0.51
1:B:158:TYR:OH	1:B:228:HIS:HD2	1.94	0.50
1:B:35:LEU:HD23	6:B:442:HOH:O	2.12	0.50
1:B:184:ARG:HA	1:B:187:MET:HE3	1.94	0.49
1:B:149:SER:HB3	6:B:598:HOH:O	2.11	0.49
1:B:184:ARG:HD2	1:B:195:GLY:O	2.13	0.49
1:B:95:ASN:HD21	1:B:97:GLU:HB2	1.77	0.49
1:B:379:VAL:C	1:B:379:VAL:CB	2.74	0.48
5:B:421:DGT:N1	2:T:840:DT:O2	2.47	0.48
2:T:839:DA:H2'	2:T:840:DT:C6	2.49	0.48
1:B:73:LEU:HD12	1:B:88:CYS:SG	2.54	0.47
1:B:67:ASN:ND2	1:B:70:ALA:H	2.13	0.47
1:B:44:MET:HE1	1:B:67:ASN:OD1	2.14	0.46
1:B:303:SER:O	1:B:331:ARG:NH2	2.48	0.46
1:B:59:GLN:OE1	1:B:64:VAL:HG11	2.16	0.46
3:P:870:DA:H2'	3:P:871:DC:C6	2.51	0.46
1:B:47:ASN:HD22	1:B:47:ASN:C	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:421:DGT:C5'	5:B:421:DGT:C8	2.68	0.45
1:B:36:ASP:O	1:B:37:CYS:C	2.55	0.45
1:B:184:ARG:HA	1:B:187:MET:CE	2.46	0.45
2:T:844:DT:H2"	2:T:845:DC:H5'	1.98	0.45
1:B:103:ARG:CZ	1:B:331:ARG:HD3	2.48	0.44
1:B:147:GLU:H	1:B:147:GLU:HG2	1.68	0.44
1:B:66:CYS:HB2	1:B:70:ALA:HB3	2.00	0.43
1:B:95:ASN:ND2	1:B:97:GLU:H	2.16	0.43
1:B:314:GLU:OE1	1:B:392:ARG:NH1	2.52	0.43
1:B:302[B]:PHE:CE2	1:B:413:LEU:HD21	2.53	0.42
1:B:73:LEU:HD23	1:B:73:LEU:N	2.35	0.42
1:B:147:GLU:O	1:B:150:ALA:HB3	2.20	0.41
1:B:359:SER:O	1:B:360:ARG:HD3	2.20	0.41
1:B:44:MET:CE	1:B:67:ASN:OD1	2.68	0.41
2:T:844:DT:H2'	2:T:845:DC:C6	2.56	0.41
1:B:140:LEU:HD21	1:B:175:VAL:HG21	2.02	0.41
1:B:35:LEU:CD2	6:B:442:HOH:O	2.69	0.40
1:B:302[B]:PHE:HE2	1:B:413:LEU:HD21	1.87	0.40
1:B:67:ASN:ND2	1:B:67:ASN:C	2.73	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)
2:T:847:DT:O3'	6:P:115:HOH:O[12_544]	1.80	0.40

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	B	367/420 (87%)	357 (97%)	7 (2%)	3 (1%)	24	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	ALA
1	B	370	GLN
1	B	37	CYS

5.3.2   Protein sidechains (i)

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	B	324/376 (86%)	300 (93%)	24 (7%)	17 11

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	26	SER
1	B	27	SER
1	B	35	LEU
1	B	47	ASN
1	B	67	ASN
1	B	126	ASP
1	B	143	LEU
1	B	170	HIS
1	B	204	LEU
1	B	227	GLN
1	B	239	ILE
1	B	265	SER
1	B	267	LYS
1	B	275	ILE
1	B	302[A]	PHE
1	B	302[B]	PHE
1	B	320	LYS
1	B	343	ARG
1	B	348	ARG
1	B	371	LYS
1	B	394	MET
1	B	396	ASN

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Mol	Chain	Res	Type
1	B	411	CYS
1	B	413	LEU

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

Mol	Chain	Res	Type
1	B	41	GLN
1	B	47	ASN
1	B	95	ASN
1	B	156	HIS
1	B	170	HIS
1	B	189	ASN
1	B	217	GLN
1	B	218	GLN
1	B	228	HIS
1	B	361	GLN
1	B	396	ASN
1	B	402	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#|Z| > 2$
5	DGT	B	421	4	25,33,33	1.07	2 (8%)	35,52,52	1.74	8 (22%)

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	DGT	B	421	4	-	0/18/34/34	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	421	DGT	C2-N1	2.59	1.40	1.35
5	B	421	DGT	C6-N1	3.16	1.39	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	421	DGT	N3-C2-N1	-4.21	121.03	127.44
5	B	421	DGT	C5-C6-N1	-3.96	118.17	123.59
5	B	421	DGT	PB-O3B-PG	-2.34	124.81	132.67
5	B	421	DGT	O1B-PB-O3A	2.09	114.55	105.09
5	B	421	DGT	O4'-C4'-C3'	2.11	110.97	105.67
5	B	421	DGT	O1B-PB-O3B	2.69	117.31	105.09
5	B	421	DGT	C6-N1-C2	3.40	120.65	115.94
5	B	421	DGT	O3'-C3'-C2'	3.74	123.12	110.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	421	DGT	13	0

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	B	374/420 (89%)	1.19	95 (25%)	1	1	28, 42, 60, 65	0
2	T	9/9 (100%)	0.28	1 (11%)	7	8	33, 39, 62, 84	0
3	P	7/7 (100%)	-0.09	0	100	100	34, 39, 50, 54	0
All	All	390/436 (89%)	1.15	96 (24%)	1	1	28, 42, 60, 84	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	MET	7.9
1	B	333	CYS	6.5
1	B	244	TYR	5.9
1	B	349	TYR	5.9
1	B	199	VAL	5.9
1	B	401	PHE	5.6
1	B	398	LYS	5.4
1	B	173	LEU	4.9
1	B	387	LEU	4.9
1	B	221	LEU	4.6
1	B	33	VAL	4.6
1	B	345	ILE	4.5
1	B	400	PRO	4.5
1	B	26	SER	4.3
1	B	83	ASP	4.2
1	B	220	VAL	4.2
1	B	61	TYR	4.1
2	T	839	DA	4.1
1	B	148	LEU	4.1
1	B	31	VAL	4.0
1	B	109	VAL	4.0
1	B	86	GLU	4.0
1	B	367	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	82	ARG	4.0
1	B	381	THR	3.8
1	B	315	VAL	3.5
1	B	38	PHE	3.5
1	B	397	VAL	3.5
1	B	409	CYS	3.5
1	B	49	GLU	3.5
1	B	84	ALA	3.4
1	B	408	VAL	3.3
1	B	50	LEU	3.3
1	B	147	GLU	3.3
1	B	312	SER	3.3
1	B	200	ALA	3.2
1	B	176	GLY	3.2
1	B	39	TYR	3.2
1	B	342	VAL	3.2
1	B	145	SER	3.1
1	B	406	LEU	3.1
1	B	29	VAL	3.1
1	B	175	VAL	3.1
1	B	344	LEU	3.1
1	B	371	LYS	3.0
1	B	144	GLN	2.9
1	B	209	VAL	2.9
1	B	65	THR	2.9
1	B	198	GLY	2.9
1	B	138	LYS	2.9
1	B	66	CYS	2.9
1	B	249	CYS	2.8
1	B	222	LEU	2.8
1	B	407	SER	2.8
1	B	321	ILE	2.7
1	B	206	ALA	2.7
1	B	132	LEU	2.7
1	B	379	VAL	2.6
1	B	30	ILE	2.6
1	B	142	GLN	2.6
1	B	123	LEU	2.6
1	B	35	LEU	2.5
1	B	343	ARG	2.5
1	B	191	LEU	2.5
1	B	248	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	125	PHE	2.4
1	B	57	VAL	2.4
1	B	64	VAL	2.4
1	B	80	ASN	2.4
1	B	412	ASN	2.4
1	B	326	ALA	2.4
1	B	101	ARG	2.3
1	B	235	HIS	2.3
1	B	271	LYS	2.3
1	B	113	LEU	2.3
1	B	55	LEU	2.3
1	B	174	LEU	2.3
1	B	106	SER	2.2
1	B	302[A]	PHE	2.2
1	B	130	VAL	2.2
1	B	197	ALA	2.2
1	B	368	VAL	2.2
1	B	205	LEU	2.2
1	B	267	LYS	2.2
1	B	112	LEU	2.1
1	B	384	VAL	2.1
1	B	378	ASP	2.1
1	B	72	LYS	2.1
1	B	177	SER	2.1
1	B	128	ASN	2.1
1	B	37	CYS	2.1
1	B	143	LEU	2.1
1	B	73	LEU	2.0
1	B	149	SER	2.0
1	B	129	PHE	2.0
1	B	383	MET	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
5	DGT	B	421	31/31	0.93	0.21	0.56	37,49,51,53	0
4	MG	B	871	1/1	0.96	0.14	-1.19	40,40,40,40	0
4	MG	B	422	1/1	0.92	0.33	-	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.