Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 05:57 AM EDT

PDB ID	:	3H4D
Title	:	Ternary complex of human DNA polymerase iota with template U/T and incoming dGTP
Authors	:	Jain, R.; Nair, D.T.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.
Deposited on	:	2009-04-18
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

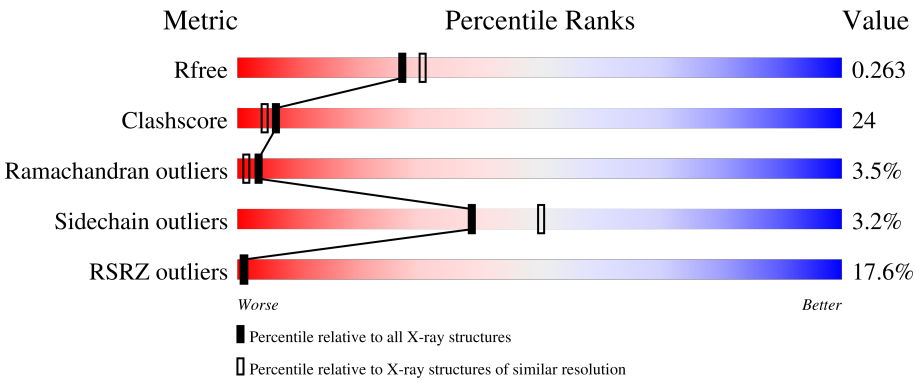
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	390	17%, 60%, 32%, ·, ·
2	P	7	14%, 57%, 29%
3	T	9	11%, 11%, 56%, 33%

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	T	875	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3489 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
			Total	C	N	O	S			
1	A	373	2844	1788	493	542	21	0	2	0

- Molecule 2 is a DNA chain called 5'-D(*AP*GP*GP*AP*CP*CP*(DOC)).

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

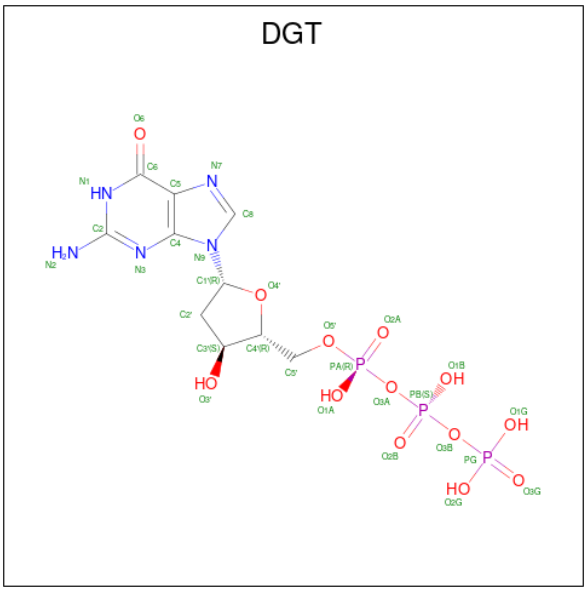
- Molecule 3 is a DNA chain called 5'-D(*TP*(BRU)P*GP*GP*GP*TP*CP*CP*T).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	P			
3	T	9	201	2	96	31	63	9	0	1	0

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

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

- 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
			Total	C	N	O	P		
5	T	1	31	10	5	13	3	0	0

- Molecule 6 is water.

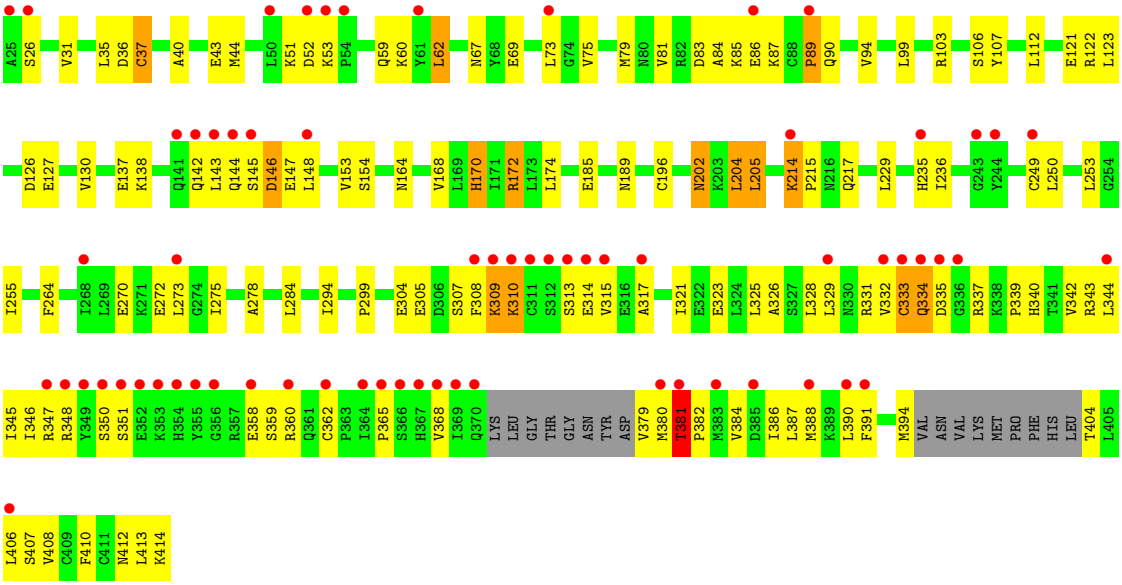
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	240	240	240	0	0
			Total	O		
6	P	9	9	9	0	0
			Total	O		
6	T	23	23	23	0	0

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.

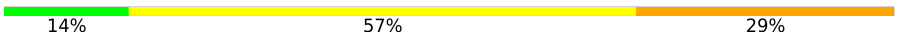
- Molecule 1: DNA polymerase iota

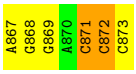
Chain A:



- Molecule 2: 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))

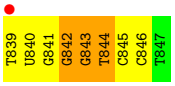
Chain P:





- Molecule 3: 5'-D(*TP*(BRU)P*GP*GP*GP*TP*CP*CP*T)

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	97.92Å 97.92Å 203.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.68 – 2.20 36.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (36.68-2.20) 95.9 (36.68-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	6.55 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.254 , 0.270 0.246 , 0.263	Depositor DCC
R_{free} test set	2306 reflections (7.68%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3489	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: DGT, BRU, MG, 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	0.34	0/2892	0.61	2/3913 (0.1%)
2	P	0.39	0/136	0.76	0/208
3	T	0.39	0/178	0.88	0/271
All	All	0.35	0/3206	0.64	2/4392 (0.0%)

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	P	0	2
3	T	0	3
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	LYS	N-CA-C	5.33	125.38	111.00
1	A	123	LEU	CB-CA-C	5.24	120.16	110.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	871	DC	Sidechain
2	P	872	DC	Sidechain
3	T	842	DG	Sidechain

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Mol	Chain	Res	Type	Group
3	T	843	DG	Sidechain
3	T	844	DT	Sidechain

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	A	2844	0	2815	120	0
2	P	139	0	79	7	0
3	T	201	0	111	23	0
4	A	2	0	0	0	0
5	T	31	0	11	10	0
6	A	240	0	0	5	0
6	P	9	0	0	3	0
6	T	23	0	0	3	0
All	All	3489	0	3016	150	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 24.

All (150) 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:126:ASP:OD2	5:T:875:DGT:H5'	1.42	1.16
3:T:842:DG:H2"	3:T:843:DG:H5"	1.39	1.04
1:A:344:LEU:HD11	1:A:387:LEU:HD22	1.39	1.00
1:A:44:MET:HE2	1:A:51:LYS:HA	1.50	0.93
1:A:137:GLU:HG3	6:A:578:HOH:O	1.69	0.93
3:T:841:DG:H2"	3:T:842:DG:H5"	1.50	0.92
1:A:164:ASN:H	1:A:170:HIS:HD2	1.24	0.85
3:T:842:DG:H2"	3:T:843:DG:C5'	2.09	0.82
3:T:840[B]:BRU:O4	5:T:875:DGT:O6	1.99	0.80
3:T:841:DG:C2'	3:T:842:DG:H5"	2.12	0.80
1:A:44:MET:CE	1:A:67:ASN:HD22	1.99	0.76
1:A:365:PRO:O	1:A:368:VAL:HG22	1.87	0.75
1:A:79:MET:HE3	1:A:84:ALA:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD21	1:A:387:LEU:HB3	1.67	0.74
2:P:867:DA:H1'	2:P:868:DG:H5'	1.67	0.74
1:A:321:ILE:O	1:A:325:LEU:HD13	1.88	0.74
3:T:845:DC:H5"	6:T:176:HOH:O	1.86	0.74
3:T:840[B]:BRU:O4	5:T:875:DGT:C6	2.29	0.74
2:P:868:DG:N7	6:P:174:HOH:O	2.21	0.73
1:A:126:ASP:OD2	5:T:875:DGT:C5'	2.30	0.73
1:A:202:ASN:ND2	1:A:205:LEU:H	1.90	0.70
1:A:44:MET:HE1	1:A:67:ASN:HD22	1.57	0.69
3:T:839:DT:H2"	3:T:840[B]:BRU:O5'	1.93	0.67
3:T:841:DG:H2"	3:T:842:DG:C5'	2.25	0.67
1:A:106:SER:OG	1:A:122:ARG:NH2	2.29	0.66
2:P:869:DG:H1'	6:P:224:HOH:O	1.94	0.66
1:A:62:LEU:HD11	3:T:839:DT:O2	1.95	0.65
1:A:270:GLU:HG3	1:A:275:ILE:HA	1.78	0.65
1:A:325:LEU:HD11	1:A:387:LEU:CD1	2.29	0.63
1:A:331:ARG:HD2	6:A:457:HOH:O	1.97	0.63
1:A:347:ARG:HD2	1:A:404:THR:OG1	1.99	0.63
1:A:384:VAL:O	1:A:388:MET:HG2	1.99	0.63
1:A:202:ASN:HD21	1:A:205:LEU:H	1.47	0.62
1:A:315:VAL:C	1:A:317:ALA:H	2.02	0.62
1:A:51:LYS:O	1:A:53:LYS:N	2.33	0.62
1:A:335:ASP:OD2	1:A:337:ARG:HD3	2.00	0.61
1:A:43:GLU:HG3	1:A:94:VAL:HG21	1.83	0.61
1:A:164:ASN:H	1:A:170:HIS:CD2	2.13	0.61
1:A:51:LYS:C	1:A:53:LYS:H	2.04	0.60
1:A:386:ILE:O	1:A:390:LEU:HG	2.01	0.60
1:A:313:SER:O	1:A:314:GLU:HB2	2.01	0.59
1:A:107:TYR:OH	1:A:299:PRO:HG3	2.03	0.59
1:A:388:MET:O	1:A:391:PHE:HB3	2.02	0.59
1:A:79:MET:CE	1:A:84:ALA:HA	2.32	0.58
1:A:112:LEU:C	1:A:112:LEU:HD23	2.24	0.58
2:P:869:DG:N3	6:P:224:HOH:O	2.32	0.58
5:T:875:DGT:PB	5:T:875:DGT:H5'A	2.43	0.58
3:T:841:DG:H1'	3:T:842:DG:H5"	1.86	0.58
1:A:126:ASP:OD1	1:A:127:GLU:HG3	2.04	0.57
1:A:345:ILE:HG12	1:A:359:SER:HB3	1.86	0.57
1:A:412:ASN:OD1	1:A:414:LYS:HE3	2.04	0.57
1:A:325:LEU:CD1	1:A:408:VAL:HG21	2.35	0.57
3:T:845:DC:C5'	6:T:176:HOH:O	2.48	0.56
1:A:196:CYS:SG	1:A:214:LYS:O	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:C	1:A:344:LEU:HD12	2.26	0.56
1:A:365:PRO:HB2	1:A:368:VAL:HG13	1.87	0.56
1:A:249:CYS:SG	1:A:273:LEU:HD21	2.46	0.55
1:A:44:MET:HE3	1:A:67:ASN:HD22	1.72	0.55
1:A:62:LEU:HD11	3:T:839:DT:C2	2.42	0.54
1:A:381:THR:OG1	1:A:382:PRO:HD3	2.07	0.54
1:A:308:PHE:O	1:A:310:LYS:N	2.40	0.54
1:A:344:LEU:CD1	1:A:387:LEU:HD22	2.27	0.53
1:A:137:GLU:CG	6:A:578:HOH:O	2.44	0.53
1:A:153:VAL:HB	1:A:174:LEU:HD22	1.91	0.53
1:A:144:GLN:NE2	6:A:523:HOH:O	2.41	0.52
1:A:305:GLU:HG3	1:A:407:SER:HB3	1.91	0.52
2:P:868:DG:H2"	2:P:869:DG:OP2	2.09	0.52
1:A:185:GLU:OE2	1:A:189[A]:ASN:ND2	2.41	0.52
3:T:839:DT:H2'	3:T:840[A]:BRU:BR	2.65	0.52
1:A:202:ASN:HD22	1:A:202:ASN:C	2.13	0.52
1:A:60:LYS:HE2	1:A:307:SER:O	2.09	0.51
1:A:414:LYS:HD3	6:A:586:HOH:O	2.10	0.51
3:T:839:DT:H2"	3:T:840[A]:BRU:O5'	2.10	0.51
5:T:875:DGT:H5'A	5:T:875:DGT:O2B	2.11	0.51
1:A:79:MET:HE3	1:A:84:ALA:CA	2.40	0.51
1:A:59:GLN:OE1	3:T:840[B]:BRU:H6	2.11	0.51
1:A:236:ILE:HD12	1:A:250:LEU:CD1	2.41	0.51
1:A:325:LEU:O	1:A:329:LEU:HD13	2.11	0.50
1:A:344:LEU:O	1:A:359:SER:HA	2.11	0.50
1:A:214:LYS:HZ1	5:T:875:DGT:PG	2.34	0.50
1:A:346:ILE:HG22	1:A:406:LEU:HD23	1.94	0.50
1:A:204:LEU:HG	1:A:284:LEU:HD22	1.94	0.49
2:P:872:DC:H2"	2:P:873:DOC:OP2	2.12	0.49
1:A:215:PRO:O	1:A:217:GLN:HG3	2.13	0.49
1:A:235:HIS:CD2	1:A:236:ILE:HG12	2.47	0.49
1:A:304:GLU:HG3	1:A:328:LEU:CD2	2.42	0.49
3:T:841:DG:C1'	3:T:842:DG:H5"	2.42	0.49
1:A:365:PRO:HB2	1:A:368:VAL:HG22	1.95	0.48
1:A:347:ARG:HG2	1:A:348:ARG:N	2.28	0.48
1:A:387:LEU:HA	1:A:390:LEU:HD12	1.94	0.48
1:A:309:LYS:O	1:A:310:LYS:C	2.52	0.48
1:A:36:ASP:O	1:A:37:CYS:C	2.52	0.48
1:A:138:LYS:O	1:A:142:GLN:HG2	2.14	0.48
1:A:332:VAL:CG1	1:A:339:PRO:HD3	2.44	0.47
1:A:345:ILE:HA	1:A:358:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLU:O	1:A:73:LEU:HD13	2.15	0.47
1:A:325:LEU:HD11	1:A:408:VAL:HG21	1.97	0.47
1:A:304:GLU:HG3	1:A:328:LEU:HD21	1.96	0.47
1:A:344:LEU:HD11	1:A:387:LEU:CD2	2.28	0.46
1:A:379:VAL:O	1:A:382:PRO:HD2	2.15	0.46
1:A:85:LYS:O	1:A:89:PRO:HG3	2.15	0.46
1:A:85:LYS:C	1:A:87:LYS:H	2.18	0.46
5:T:875:DGT:H8	5:T:875:DGT:O5'	2.16	0.46
1:A:325:LEU:HD11	1:A:387:LEU:HD11	1.98	0.46
2:P:871:DC:H2"	2:P:872:DC:OP2	2.16	0.46
1:A:99:LEU:HD12	3:T:842:DG:H4'	1.99	0.45
1:A:103:ARG:CZ	1:A:331:ARG:NH1	2.79	0.45
1:A:148:LEU:O	1:A:148:LEU:HD23	2.17	0.45
1:A:323:GLU:O	1:A:326:ALA:HB3	2.17	0.45
1:A:315:VAL:C	1:A:317:ALA:N	2.70	0.45
1:A:75:VAL:HA	1:A:79:MET:HE2	1.99	0.44
1:A:339:PRO:HG3	1:A:410:PHE:HD2	1.82	0.44
3:T:845:DC:H2"	3:T:846:DC:OP2	2.17	0.44
1:A:121:GLU:HB2	1:A:294:ILE:O	2.18	0.44
1:A:144:GLN:O	1:A:146:ASP:N	2.42	0.44
1:A:202:ASN:OD1	1:A:205:LEU:HD22	2.17	0.44
1:A:153:VAL:HG22	1:A:154:SER:N	2.33	0.44
1:A:270:GLU:HA	1:A:278:ALA:CB	2.48	0.44
1:A:315:VAL:O	1:A:317:ALA:N	2.50	0.43
3:T:840[A]:BRU:O2	5:T:875:DGT:N2	2.48	0.43
1:A:325:LEU:HD11	1:A:387:LEU:HD12	1.98	0.43
3:T:840[B]:BRU:H2'	3:T:840[B]:BRU:O2	2.19	0.43
1:A:196:CYS:HA	1:A:217:GLN:O	2.19	0.43
1:A:360:ARG:HG2	1:A:394:MET:CG	2.48	0.43
5:T:875:DGT:O1B	5:T:875:DGT:H3'	2.18	0.43
1:A:81:VAL:O	1:A:84:ALA:HB3	2.19	0.43
3:T:845:DC:P	6:T:176:HOH:O	2.77	0.42
1:A:168:VAL:HG22	1:A:172:ARG:HD2	2.01	0.42
1:A:236:ILE:HD12	1:A:250:LEU:HD12	2.00	0.42
1:A:40:ALA:O	1:A:44:MET:HG3	2.19	0.42
1:A:381:THR:CB	1:A:382:PRO:HD3	2.49	0.42
1:A:73:LEU:HD12	1:A:73:LEU:N	2.34	0.42
1:A:86:GLU:O	1:A:86:GLU:HG3	2.20	0.42
1:A:143:LEU:HA	1:A:147:GLU:OE2	2.18	0.42
1:A:255:ILE:HD11	1:A:264:PHE:CG	2.55	0.42
1:A:340:HIS:ND1	1:A:414:LYS:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:O	1:A:87:LYS:HB2	2.20	0.42
1:A:342:VAL:HG21	1:A:387:LEU:HD21	2.02	0.42
1:A:380:MET:O	1:A:381:THR:C	2.58	0.42
1:A:31:VAL:CG1	1:A:130:VAL:HB	2.50	0.42
1:A:35:LEU:HD12	1:A:35:LEU:N	2.35	0.41
1:A:51:LYS:C	1:A:53:LYS:N	2.71	0.41
1:A:112:LEU:HD23	1:A:112:LEU:O	2.20	0.41
1:A:253:LEU:HD21	1:A:272:GLU:OE2	2.20	0.41
1:A:137:GLU:OE2	1:A:172:ARG:NE	2.53	0.41
1:A:365:PRO:HB2	1:A:368:VAL:CG1	2.51	0.41
1:A:333:CYS:O	1:A:334:GLN:C	2.58	0.41
3:T:843:DG:H2'	3:T:844:DT:H72	2.02	0.41
1:A:343:ARG:HG2	1:A:344:LEU:N	2.35	0.40
1:A:337:ARG:HH21	1:A:413:LEU:HB2	1.86	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	369/390 (95%)	322 (87%)	34 (9%)	13 (4%)	3 1

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	309	LYS
1	A	350	SER
1	A	26	SER
1	A	37	CYS
1	A	145	SER
1	A	146	ASP

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Mol	Chain	Res	Type
1	A	310	LYS
1	A	334	GLN
1	A	333	CYS
1	A	351	SER
1	A	89	PRO
1	A	381	THR

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	A	313/354 (88%)	303 (97%)	10 (3%)	39 50

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	90	GLN
1	A	170	HIS
1	A	172	ARG
1	A	202	ASN
1	A	204	LEU
1	A	205	LEU
1	A	229	LEU
1	A	362	CYS
1	A	381	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	67	ASN
1	A	90	GLN
1	A	170	HIS
1	A	202	ASN

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Mol	Chain	Res	Type
1	A	235	HIS
1	A	262	GLN
1	A	334	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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	BRU	T	840[B]	3	18,21,22	0.53	0	26,30,33	0.73	0
2	DOC	P	873	2,3	16,19,20	0.38	0	20,26,29	0.65	0
3	BRU	T	840[A]	3	18,21,22	0.50	0	26,30,33	0.68	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
3	BRU	T	840[B]	3	-	4/7/21/22	0/2/2/2
2	DOC	P	873	2,3	-	0/7/18/19	0/2/2/2
3	BRU	T	840[A]	3	-	4/7/21/22	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	840[B]	BRU	C2'-C1'-N1-C2
3	T	840[B]	BRU	O4'-C1'-N1-C6
3	T	840[B]	BRU	C2'-C1'-N1-C6
3	T	840[B]	BRU	O4'-C1'-N1-C2
3	T	840[A]	BRU	C2'-C1'-N1-C6
3	T	840[A]	BRU	O4'-C1'-N1-C6
3	T	840[A]	BRU	O4'-C1'-N1-C2
3	T	840[A]	BRU	C2'-C1'-N1-C2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	840[B]	BRU	5	0
2	P	873	DOC	1	0
3	T	840[A]	BRU	3	0

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	$\#\|Z\| > 2$
5	DGT	T	875	-	26,33,33	1.72	7 (26%)	32,52,52	1.42	8 (25%)

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	T	875	-	-	4/18/34/34	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	875	DGT	O4'-C4'	-4.27	1.35	1.45
5	T	875	DGT	C1'-N9	-3.12	1.40	1.49
5	T	875	DGT	PG-O3G	3.02	1.60	1.50
5	T	875	DGT	PA-O1A	-2.95	1.41	1.55
5	T	875	DGT	PB-O2B	2.41	1.59	1.50
5	T	875	DGT	C2-N1	2.11	1.42	1.37
5	T	875	DGT	PB-O1B	-2.09	1.45	1.55

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	T	875	DGT	C4'-O4'-C1'	2.94	116.56	109.45
5	T	875	DGT	C2'-C1'-N9	2.50	120.05	114.27
5	T	875	DGT	O5'-C5'-C4'	2.50	117.60	108.99
5	T	875	DGT	O3B-PG-O3G	-2.27	98.60	111.19
5	T	875	DGT	O1B-PB-O2B	-2.20	101.38	112.24
5	T	875	DGT	O2G-PG-O1G	2.15	115.84	107.64
5	T	875	DGT	O6-C6-N1	2.08	123.11	120.65
5	T	875	DGT	O1G-PG-O3B	2.06	111.55	104.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	T	875	DGT	O4'-C4'-C5'-O5'
5	T	875	DGT	C3'-C4'-C5'-O5'
5	T	875	DGT	PB-O3B-PG-O3G
5	T	875	DGT	PB-O3B-PG-O1G

There are no ring outliers.

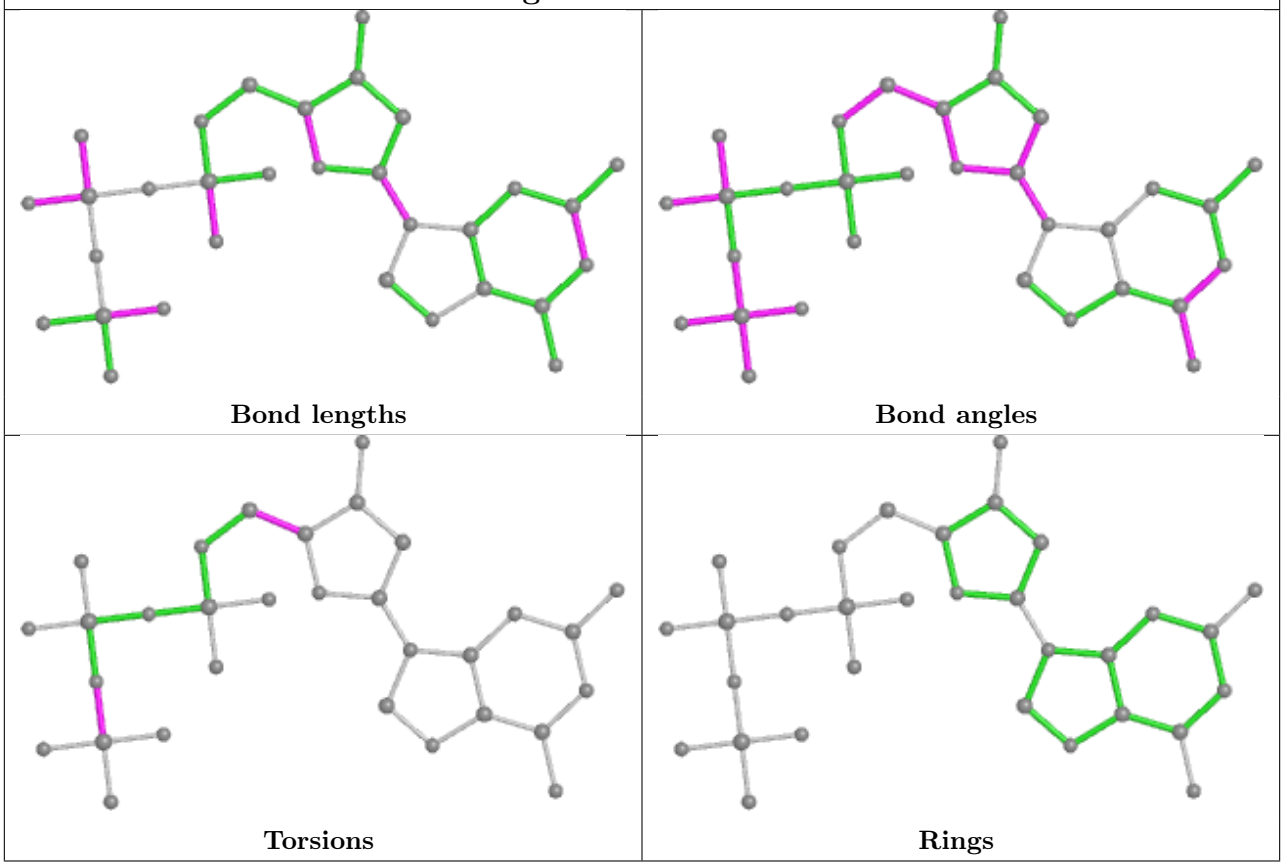
1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	875	DGT	10	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 then 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.

Ligand DGT T 875



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	373/390 (95%)	0.93	67 (17%) 1 1	18, 44, 96, 113	0
2	P	6/7 (85%)	1.17	0 100 100	45, 54, 60, 64	0
3	T	8/9 (88%)	0.80	1 (12%) 3 3	32, 37, 52, 82	0
All	All	387/406 (95%)	0.93	68 (17%) 1 1	18, 45, 95, 113	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	TYR	15.4
1	A	354	HIS	13.3
1	A	25	ALA	8.9
1	A	349	TYR	7.3
1	A	336	GLY	7.0
1	A	312	SER	7.0
1	A	244	TYR	7.0
1	A	368	VAL	6.9
1	A	350	SER	6.8
1	A	353	LYS	6.4
1	A	311	CYS	6.2
1	A	352	GLU	6.1
1	A	313	SER	4.8
1	A	348	ARG	4.7
1	A	26	SER	4.6
1	A	351	SER	4.6
1	A	333	CYS	4.6
1	A	388	MET	4.4
1	A	366	SER	3.9
1	A	145	SER	3.9
1	A	391	PHE	3.9
1	A	356	GLY	3.8
1	A	385	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	310	LYS	3.5
1	A	315	VAL	3.4
3	T	839	DT	3.4
1	A	334	GLN	3.3
1	A	249	CYS	3.3
1	A	308	PHE	3.2
1	A	364	ILE	3.2
1	A	329	LEU	3.1
1	A	390	LEU	3.1
1	A	335	ASP	3.0
1	A	370	GLN	3.0
1	A	50	LEU	2.9
1	A	383	MET	2.9
1	A	317	ALA	2.9
1	A	314	GLU	2.9
1	A	347	ARG	2.9
1	A	406	LEU	2.9
1	A	141	GLN	2.8
1	A	61	TYR	2.8
1	A	243	GLY	2.8
1	A	214	LYS	2.7
1	A	358	GLU	2.7
1	A	332	VAL	2.6
1	A	54	PRO	2.6
1	A	142	GLN	2.6
1	A	144	GLN	2.6
1	A	365	PRO	2.5
1	A	360	ARG	2.4
1	A	235	HIS	2.4
1	A	52	ASP	2.4
1	A	367	HIS	2.4
1	A	369	ILE	2.3
1	A	148	LEU	2.3
1	A	309	LYS	2.3
1	A	344	LEU	2.3
1	A	73	LEU	2.2
1	A	86	GLU	2.2
1	A	380	MET	2.2
1	A	381	THR	2.2
1	A	268	ILE	2.2
1	A	143	LEU	2.2
1	A	273	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	362	CYS	2.1
1	A	53	LYS	2.1
1	A	89	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BRU	T	840[A]	20/21	0.85	0.19	49,58,73,98	20
3	BRU	T	840[B]	20/21	0.85	0.19	48,54,71,80	20
2	DOC	P	873	18/19	0.96	0.18	30,36,40,41	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

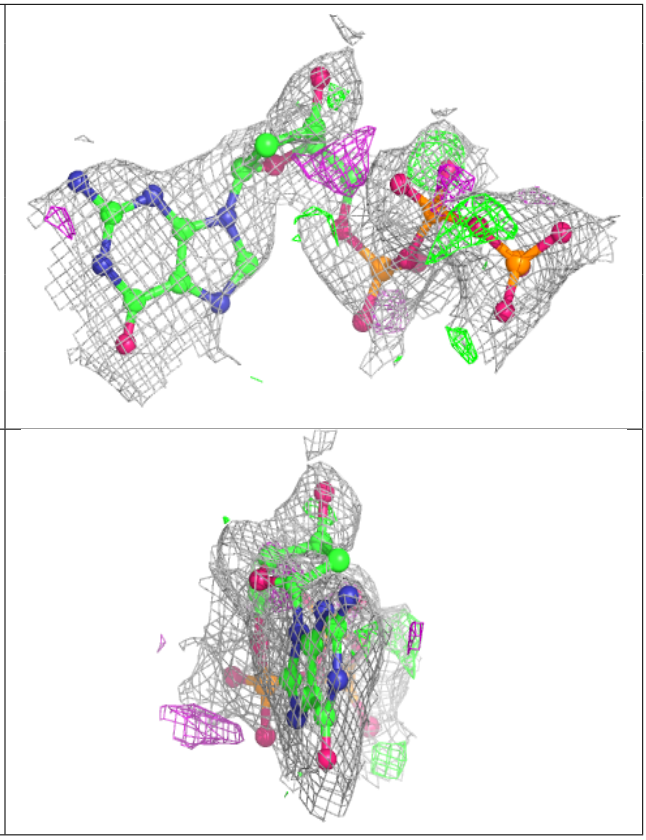
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	871	1/1	0.66	0.12	64,64,64,64	0
5	DGT	T	875	31/31	0.80	0.23	40,46,50,51	31
4	MG	A	872	1/1	0.89	0.34	58,58,58,58	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.

Electron density around DGT T 875:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.