



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:35 AM EDT

PDB ID : 3G6X / pdb_00003g6x
Title : Ternary complex of DNA Polymerase iota:DNA:dGTP with an abasic site at the templating position
Authors : Nair, D.T.; Aggarwal, A.K.
Deposited on : 2009-02-09
Resolution : 2.08 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

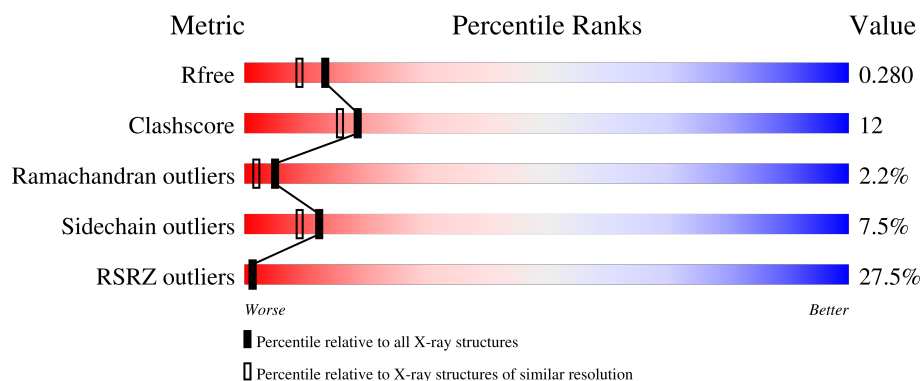
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	420	25% 65% 20% • 11%
2	P	7	29% 43% 29%
3	T	11	64% 9% 27%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3422 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	A	373	Total	C	N	O	S	0	0	0
			2876	1809	504	542	21			

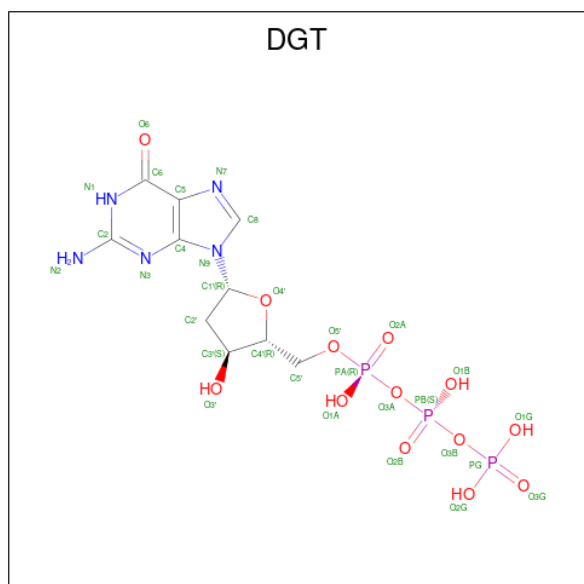
- Molecule 2 is a DNA chain called Primer DNA strand.

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

- Molecule 3 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	8	Total	C	N	O	P	0	0	0
			155	73	25	49	8			

- Molecule 4 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

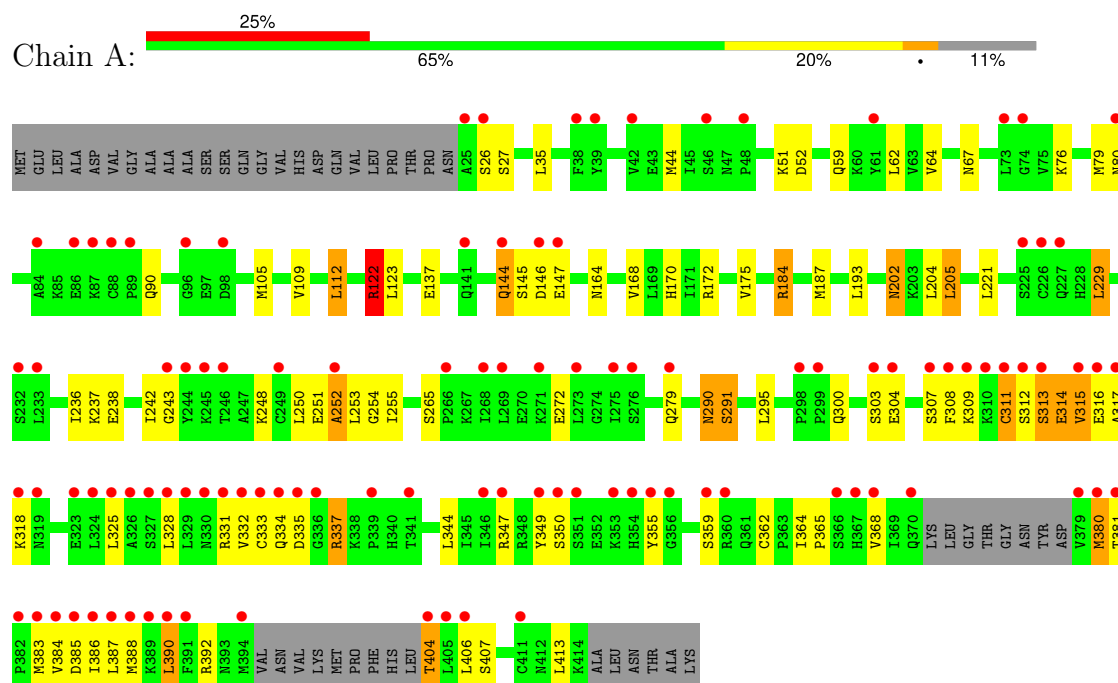
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	198	Total	O	0	0
			198	198		
6	P	6	Total	O	0	0
			6	6		
6	T	15	Total	O	0	0
			15	15		

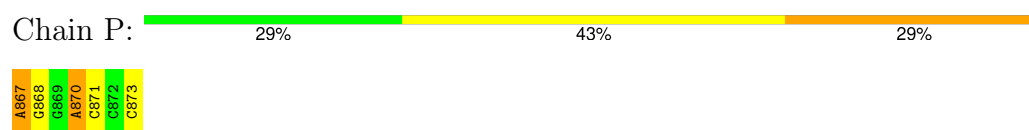
3 Residue-property plots [i](#)

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



- Molecule 2: Primer DNA strand



- Molecule 3: Template DNA strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.11Å 98.11Å 202.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.08 20.00 – 2.08	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.08) 96.0 (20.00-2.08)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.60 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.222 , 0.265 0.229 , 0.280	Depositor DCC
R_{free} test set	2813 reflections (8.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3422	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: 3DR, MG, DOC, 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	A	1.30	8/2914 (0.3%)	1.28	15/3934 (0.4%)
2	P	0.82	0/136	1.73	5/208 (2.4%)
3	T	1.00	0/160	1.85	5/245 (2.0%)
All	All	1.27	8/3210 (0.2%)	1.34	25/4387 (0.6%)

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	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	ARG	CZ-NH1	8.75	1.45	1.32
1	A	122	ARG	CD-NE	-7.43	1.35	1.46
1	A	242	ILE	CA-CB	7.42	1.62	1.53
1	A	184	ARG	CD-NE	-7.01	1.36	1.46
1	A	313	SER	CB-OG	6.46	1.55	1.42
1	A	26	SER	CA-C	6.34	1.58	1.53
1	A	390	LEU	C-O	5.65	1.31	1.24
1	A	386	ILE	CA-CB	5.09	1.60	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ARG	NE-CZ-NH2	-14.78	105.90	119.20
1	A	311	CYS	N-CA-C	9.52	124.72	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ARG	CD-NE-CZ	9.00	136.99	124.40
1	A	122	ARG	NE-CZ-NH1	8.49	129.99	121.50
3	T	843	DG	P-O5'-C5'	7.86	131.79	120.00
2	P	867	DA	O5'-C5'-C4'	7.03	121.34	110.80
1	A	122	ARG	CG-CD-NE	-6.97	96.66	112.00
1	A	238	GLU	CA-C-N	-6.45	117.94	122.59
1	A	238	GLU	C-N-CA	-6.45	117.94	122.59
3	T	842	DG	P-O5'-C5'	6.37	129.55	120.00
3	T	845	DC	P-O5'-C5'	6.12	129.18	120.00
1	A	184	ARG	NE-CZ-NH2	-6.06	113.75	119.20
1	A	291	SER	CA-C-N	5.74	125.64	119.85
1	A	291	SER	C-N-CA	5.74	125.64	119.85
2	P	870	DA	O4'-C1'-N9	5.72	116.97	108.40
3	T	846	DC	O3'-P-O5'	-5.48	95.78	104.00
1	A	381	THR	CA-C-N	-5.47	113.39	119.19
1	A	381	THR	C-N-CA	-5.47	113.39	119.19
1	A	175	VAL	N-CA-C	-5.41	105.25	110.72
1	A	349	TYR	N-CA-C	5.40	117.29	108.76
3	T	845	DC	P-O3'-C3'	5.23	128.04	120.20
2	P	870	DA	C3'-C2'-C1'	5.17	109.36	101.60
2	P	868	DG	P-O5'-C5'	5.13	127.70	120.00
2	P	867	DA	C4'-C3'-O3'	5.08	117.62	110.00
1	A	355	TYR	N-CA-C	5.00	116.80	109.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ARG	Sidechain

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	2876	0	2899	73	0
2	P	139	0	79	3	1
3	T	155	0	88	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	31	0	12	0	0
5	A	2	0	0	0	0
6	A	198	0	0	4	0
6	P	6	0	0	0	0
6	T	15	0	0	0	0
All	All	3422	0	3078	75	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 12.

All (75) 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:137:GLU:HG2	6:A:614:HOH:O	1.46	1.12
1:A:44:MET:HE2	1:A:51:LYS:HA	1.40	1.03
1:A:164:ASN:H	1:A:170:HIS:HD2	1.11	0.95
1:A:344:LEU:CD1	1:A:387:LEU:HD22	2.03	0.89
1:A:308:PHE:HE1	1:A:312:SER:HB2	1.38	0.88
1:A:318:LYS:HB2	1:A:388:MET:HE2	1.59	0.85
1:A:308:PHE:HB2	1:A:311:CYS:HB2	1.62	0.82
1:A:236:ILE:HD12	1:A:250:LEU:HD13	1.63	0.80
1:A:331:ARG:HD2	6:A:597:HOH:O	1.81	0.78
1:A:164:ASN:H	1:A:170:HIS:CD2	2.00	0.77
1:A:344:LEU:HD11	1:A:387:LEU:HD22	1.66	0.77
1:A:44:MET:CE	1:A:67:ASN:HD22	2.00	0.73
1:A:308:PHE:HE1	1:A:312:SER:CB	2.07	0.68
1:A:44:MET:HE3	1:A:67:ASN:HD22	1.58	0.67
1:A:308:PHE:CE1	1:A:312:SER:HB2	2.27	0.67
1:A:318:LYS:HB2	1:A:388:MET:CE	2.24	0.67
1:A:308:PHE:O	1:A:404:THR:HA	1.94	0.67
1:A:112:LEU:C	1:A:112:LEU:HD23	2.20	0.66
1:A:290:ASN:HD22	1:A:290:ASN:C	2.04	0.65
1:A:59:GLN:OE1	1:A:64:VAL:HG11	1.97	0.64
1:A:325:LEU:HD23	1:A:380:MET:HE1	1.80	0.64
1:A:304:GLU:HG3	1:A:328:LEU:HG	1.81	0.62
1:A:365:PRO:O	1:A:368:VAL:HG22	1.99	0.62
1:A:300:GLN:NE2	6:A:512:HOH:O	2.33	0.60
1:A:362:CYS:SG	1:A:390:LEU:HD21	2.41	0.60
1:A:202:ASN:ND2	1:A:205:LEU:H	2.00	0.58
1:A:313:SER:O	1:A:314:GLU:HB2	2.04	0.58
1:A:44:MET:HE3	1:A:67:ASN:ND2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD23	1:A:380:MET:CE	2.34	0.57
1:A:236:ILE:HD12	1:A:250:LEU:CD1	2.34	0.56
1:A:335:ASP:OD2	1:A:337:ARG:HD3	2.06	0.56
1:A:221:LEU:HD22	1:A:229:LEU:HD12	1.86	0.55
1:A:347:ARG:HD2	1:A:404:THR:CG2	2.37	0.54
1:A:251:GLU:O	1:A:252:ALA:C	2.50	0.54
1:A:168:VAL:HG22	1:A:172:ARG:HD2	1.91	0.53
1:A:308:PHE:HB2	1:A:311:CYS:CB	2.37	0.53
1:A:308:PHE:CD1	1:A:311:CYS:HB2	2.43	0.53
1:A:76:LYS:HB2	1:A:79:MET:HE3	1.92	0.52
1:A:308:PHE:HD1	1:A:311:CYS:HB2	1.74	0.52
1:A:347:ARG:NH1	1:A:404:THR:OG1	2.43	0.52
1:A:164:ASN:N	1:A:170:HIS:HD2	1.94	0.52
1:A:335:ASP:CG	1:A:337:ARG:HD3	2.35	0.52
1:A:105:MET:CG	1:A:193:LEU:HD11	2.40	0.51
1:A:144:GLN:HG3	1:A:147:GLU:OE2	2.11	0.51
1:A:304:GLU:O	1:A:407:SER:HB2	2.10	0.51
1:A:308:PHE:HZ	1:A:406:LEU:HD23	1.76	0.50
1:A:359:SER:O	2:P:867:DA:H3'	2.12	0.50
1:A:307:SER:HB2	3:T:841:DG:OP2	2.13	0.49
1:A:304:GLU:HG2	1:A:331:ARG:HH21	1.78	0.49
1:A:335:ASP:OD1	1:A:337:ARG:HD3	2.13	0.48
1:A:202:ASN:HD22	1:A:202:ASN:C	2.22	0.48
3:T:844:DT:H2''	3:T:845:DC:H5'	1.96	0.48
1:A:105:MET:HE2	1:A:105:MET:HA	1.97	0.47
1:A:251:GLU:O	1:A:254:GLY:N	2.42	0.47
1:A:290:ASN:C	1:A:290:ASN:ND2	2.73	0.47
1:A:248:LYS:HD3	1:A:248:LYS:HA	1.56	0.47
1:A:290:ASN:HD22	1:A:291:SER:N	2.12	0.47
1:A:347:ARG:HD2	1:A:404:THR:HG23	1.97	0.47
1:A:122:ARG:HD3	6:A:425:HOH:O	2.15	0.47
1:A:105:MET:HE2	1:A:105:MET:CA	2.45	0.46
1:A:144:GLN:C	1:A:146:ASP:H	2.23	0.45
1:A:184:ARG:HA	1:A:187:MET:HE3	1.99	0.45
1:A:315:VAL:C	1:A:317:ALA:H	2.25	0.44
1:A:364:ILE:HG23	1:A:383:MET:HE1	2.00	0.44
1:A:380:MET:HE2	1:A:384:VAL:HG23	2.01	0.43
1:A:347:ARG:HD2	1:A:404:THR:HG21	2.00	0.42
1:A:251:GLU:O	1:A:253:LEU:N	2.52	0.42
1:A:236:ILE:HD13	1:A:255:ILE:HG22	2.01	0.41
1:A:243:GLY:CA	2:P:871:DC:OP1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:SER:O	1:A:331:ARG:NH2	2.53	0.41
1:A:253:LEU:HD11	1:A:272:GLU:HG2	2.03	0.41
1:A:325:LEU:HD21	1:A:383:MET:HB3	2.02	0.41
1:A:144:GLN:HG3	1:A:144:GLN:H	1.63	0.40
2:P:870:DA:H2''	2:P:871:DC:O4'	2.21	0.40
1:A:35:LEU:HD11	1:A:109:VAL:HG21	2.02	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:P:867:DA:O5'	3:T:847:DT:O3'[10_665]	1.87	0.33

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	367/420 (87%)	341 (93%)	18 (5%)	8 (2%)	5 2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	VAL
1	A	334	GLN
1	A	252	ALA
1	A	314	GLU
1	A	316	GLU
1	A	333	CYS
1	A	52	ASP
1	A	350	SER

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	321/376 (85%)	297 (92%)	24 (8%)	12 9

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

Mol	Chain	Res	Type
1	A	27	SER
1	A	62	LEU
1	A	80	ASN
1	A	90	GLN
1	A	112	LEU
1	A	123	LEU
1	A	144	GLN
1	A	145	SER
1	A	202	ASN
1	A	204	LEU
1	A	205	LEU
1	A	229	LEU
1	A	237	LYS
1	A	265	SER
1	A	279	GLN
1	A	290	ASN
1	A	295	LEU
1	A	309	LYS
1	A	332	VAL
1	A	337	ARG
1	A	380	MET
1	A	385	ASP
1	A	404	THR
1	A	413	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN

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Mol	Chain	Res	Type
1	A	170	HIS
1	A	202	ASN
1	A	216	ASN
1	A	256	ASN
1	A	262	GLN
1	A	282	GLN
1	A	290	ASN
1	A	334	GLN
1	A	393	ASN
1	A	412	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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$
2	DOC	P	873	2,3	16,19,20	1.10	2 (12%)	20,26,29	1.75	5 (25%)
3	3DR	T	840	3	8,11,12	1.11	1 (12%)	7,14,17	1.97	3 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	P	873	2,3	-	0/7/18/19	0/2/2/2
3	3DR	T	840	3	-	2/3/15/16	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	873	DOC	C2-N1	2.61	1.45	1.40
3	T	840	3DR	O4'-C4'	-2.34	1.40	1.44
2	P	873	DOC	C6-C5	2.25	1.40	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	840	3DR	O4'-C1'-C2'	-3.78	98.91	106.34
2	P	873	DOC	O4'-C4'-C3'	3.52	110.61	104.81
2	P	873	DOC	C3'-C2'-C1'	3.52	106.93	102.87
2	P	873	DOC	O4'-C1'-N1	3.43	113.95	107.86
2	P	873	DOC	C2'-C1'-N1	-2.42	107.82	112.40
2	P	873	DOC	O2-C2-N3	-2.29	118.72	122.33
3	T	840	3DR	C1'-C2'-C3'	-2.20	100.90	103.26
3	T	840	3DR	O3'-C3'-C2'	-2.05	106.64	111.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	840	3DR	C3'-C4'-C5'-O5'
3	T	840	3DR	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	DGT	A	875	5	32,33,33	2.04	8 (25%)	48,52,52	1.89	7 (14%)

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	DGT	A	875	5	-	2/22/34/34	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	875	DGT	PA-O3A	6.26	1.66	1.59
4	A	875	DGT	PB-O3B	5.25	1.65	1.59
4	A	875	DGT	C5-C4	3.68	1.48	1.38
4	A	875	DGT	O3'-C3'	2.97	1.49	1.43
4	A	875	DGT	C5-N7	-2.46	1.34	1.39
4	A	875	DGT	C6-N1	-2.28	1.34	1.38
4	A	875	DGT	C8-N7	2.14	1.38	1.32
4	A	875	DGT	C2-N1	-2.07	1.32	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	875	DGT	C5-C4-N3	-6.10	118.69	128.39
4	A	875	DGT	O3A-PA-O2A	-5.12	95.29	110.70
4	A	875	DGT	C2-N3-C4	4.54	120.11	112.30
4	A	875	DGT	N9-C4-N3	4.52	134.99	125.95
4	A	875	DGT	O1A-PA-O2A	3.01	126.44	112.44
4	A	875	DGT	C6-C5-N7	2.72	135.24	130.29
4	A	875	DGT	O3A-PB-O2B	2.01	116.74	110.70

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	875	DGT	PA-O3A-PB-O2B

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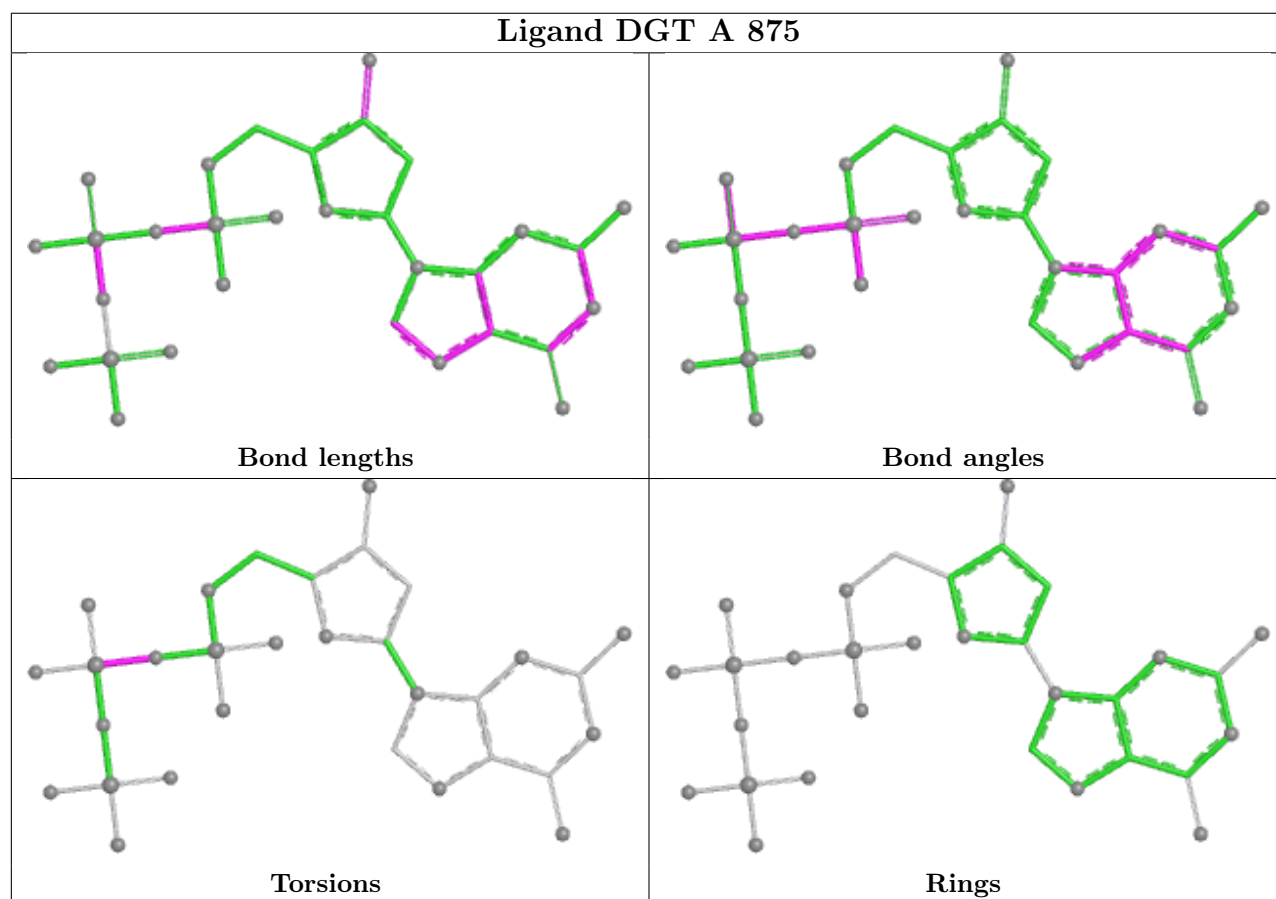
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Mol	Chain	Res	Type	Atoms
4	A	875	DGT	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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

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	373/420 (88%)	1.12	106 (28%)  	10, 27, 49, 62	0
2	P	6/7 (85%)	0.96	0  	23, 29, 33, 35	0
3	T	7/11 (63%)	0.10	0  	15, 17, 23, 23	0
All	All	386/438 (88%)	1.10	106 (27%)  	10, 27, 49, 62	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	ALA	8.0
1	A	249	CYS	7.3
1	A	379	VAL	7.0
1	A	354	HIS	6.5
1	A	317	ALA	6.1
1	A	350	SER	5.9
1	A	381	THR	5.5
1	A	276	SER	5.4
1	A	367	HIS	5.4
1	A	89	PRO	4.6
1	A	312	SER	4.6
1	A	298	PRO	4.3
1	A	244	TYR	4.3
1	A	315	VAL	4.3
1	A	388	MET	4.1
1	A	88	CYS	4.1
1	A	349	TYR	4.0
1	A	404	THR	3.9
1	A	385	ASP	3.9
1	A	309	LYS	3.7
1	A	334	GLN	3.7
1	A	386	ILE	3.7
1	A	391	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	405	LEU	3.6
1	A	316	GLU	3.6
1	A	252	ALA	3.6
1	A	333	CYS	3.5
1	A	382	PRO	3.5
1	A	146	ASP	3.5
1	A	271	LYS	3.5
1	A	308	PHE	3.4
1	A	42	VAL	3.4
1	A	299	PRO	3.4
1	A	313	SER	3.4
1	A	368	VAL	3.4
1	A	394	MET	3.3
1	A	268	ILE	3.2
1	A	390	LEU	3.2
1	A	310	LYS	3.1
1	A	39	TYR	3.1
1	A	356	GLY	3.1
1	A	38	PHE	3.1
1	A	387	LEU	3.1
1	A	80	ASN	3.0
1	A	226	CYS	3.0
1	A	26	SER	2.9
1	A	73	LEU	2.9
1	A	384	VAL	2.9
1	A	225	SER	2.9
1	A	330	ASN	2.9
1	A	144	GLN	2.9
1	A	275	ILE	2.9
1	A	380	MET	2.8
1	A	147	GLU	2.8
1	A	360	ARG	2.8
1	A	98	ASP	2.8
1	A	328	LEU	2.8
1	A	406	LEU	2.8
1	A	74	GLY	2.7
1	A	326	ALA	2.7
1	A	346	ILE	2.7
1	A	339	PRO	2.6
1	A	366	SER	2.6
1	A	353	LYS	2.6
1	A	269	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	245	LYS	2.6
1	A	355	TYR	2.5
1	A	318	LYS	2.5
1	A	335	ASP	2.5
1	A	327	SER	2.5
1	A	86	GLU	2.5
1	A	389	LYS	2.5
1	A	311	CYS	2.5
1	A	325	LEU	2.5
1	A	336	GLY	2.4
1	A	279	GLN	2.4
1	A	351	SER	2.4
1	A	246	THR	2.4
1	A	273	LEU	2.4
1	A	141	GLN	2.4
1	A	304	GLU	2.4
1	A	303	SER	2.4
1	A	347	ARG	2.4
1	A	227	GLN	2.3
1	A	324	LEU	2.3
1	A	329	LEU	2.3
1	A	307	SER	2.3
1	A	332	VAL	2.3
1	A	84	ALA	2.2
1	A	370	GLN	2.2
1	A	359	SER	2.2
1	A	61	TYR	2.2
1	A	96	GLY	2.1
1	A	243	GLY	2.1
1	A	233	LEU	2.1
1	A	46	SER	2.1
1	A	266	PRO	2.1
1	A	319	ASN	2.1
1	A	323	GLU	2.1
1	A	48	PRO	2.1
1	A	232	SER	2.1
1	A	411	CYS	2.0
1	A	331	ARG	2.0
1	A	341	THR	2.0
1	A	87	LYS	2.0
1	A	383	MET	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
3	3DR	T	840	11/12	0.90	0.10	22,31,46,47	0
2	DOC	P	873	18/19	0.93	0.11	10,16,19,21	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

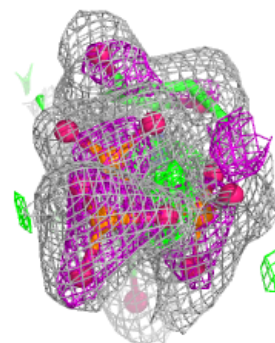
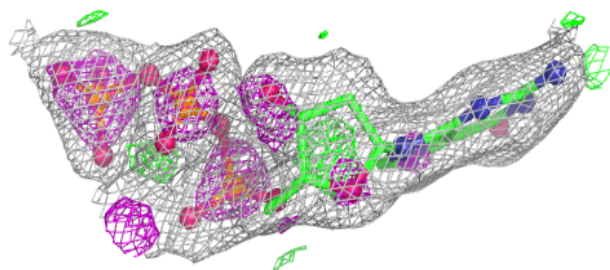
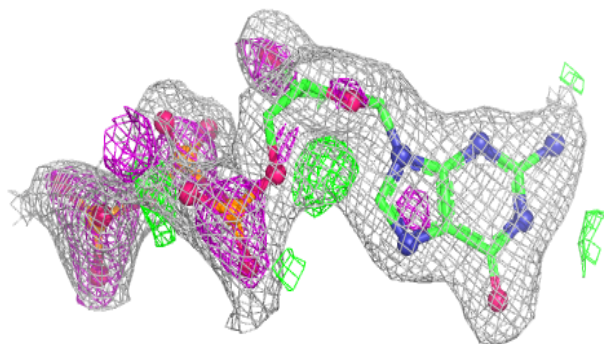
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	A	872	1/1	0.84	0.35	59,59,59,59	0
4	DGT	A	875	31/31	0.96	0.09	8,16,21,22	0
5	MG	A	871	1/1	0.97	0.14	2,2,2,2	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 A 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.