Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 10:38 PM EST

PDB ID	:	3UXP
Title	:	Co-crystal Structure of Rat DNA polymerase beta Mutator I260Q: Enzyme-DNA-ddTTP
Authors	:	Gridley, C.L.; Jaeger, J.
Deposited on	:	2011-12-05
Resolution	:	2.72 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:

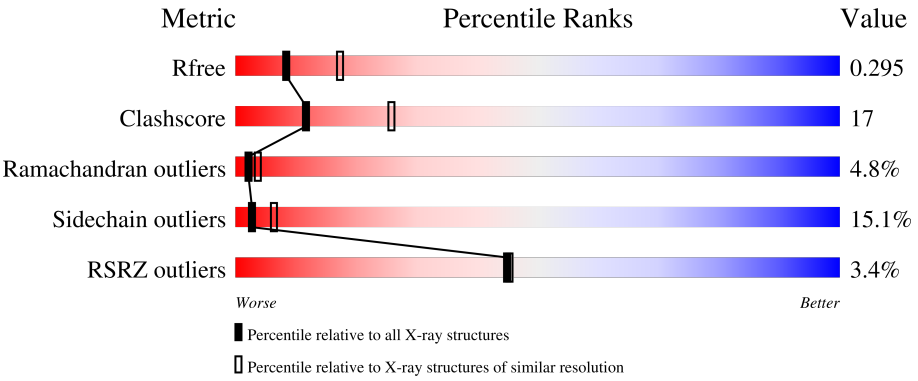
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	335	3% 56% 34% 7% .
1	B	335	4% 54% 35% 8% .
2	D	7	29% 71%
2	P	7	14% 14% 71%
3	E	9	22% 44% 33%

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Mol	Chain	Length	Quality of chain
3	T	9	33% 33% 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	NA	A	337	-	-	-	X
5	NA	B	339	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6010 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 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	9	2	0
			2641	1663	468	501	9			
1	B	326	Total	C	N	O	S	9	2	0
			2641	1663	468	501	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	GLN	ILE	engineered mutation	UNP P06766
B	260	GLN	ILE	engineered mutation	UNP P06766

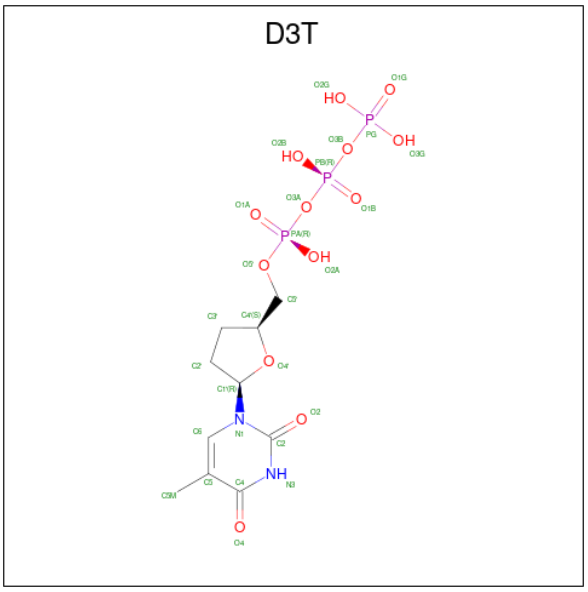
- Molecule 2 is a DNA chain called DNA 5'-D(P*AP*TP*GP*TP*GP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	1	0	0
			148	70	29	42	7			
2	D	7	Total	C	N	O	P	1	0	0
			148	70	29	42	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	9	Total	C	N	O	P	0	0	0
			164	77	28	50	9			
3	E	9	Total	C	N	O	P	0	0	0
			164	77	28	50	9			

- Molecule 4 is 2',3'-DIDEOXY-THYMIDINE-5'-TRIPHOSPHATE (three-letter code: D3T) (formula: $C_{10}H_{17}N_2O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 28 10 2 13 3	0	0
4	B	1	Total C N O P 28 10 2 13 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Na 4 4	0	0
5	B	3	Total Na 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	13	Total O 13 13	0	0
6	B	17	Total O 17 17	0	0
6	P	2	Total O 2 2	0	0
6	T	4	Total O 4 4	0	0
6	D	1	Total O 1 1	0	0

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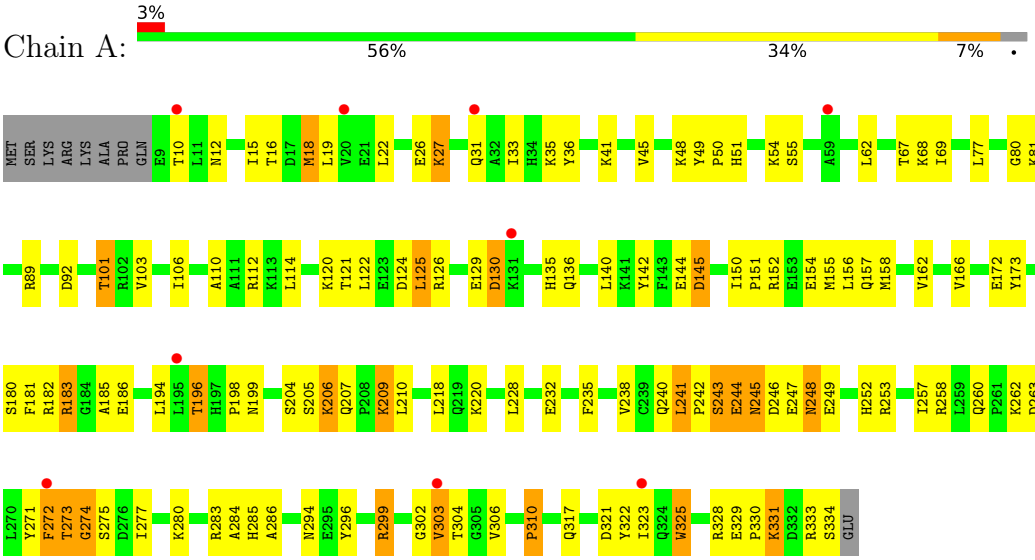
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	4	Total O 4 4	0	0

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.

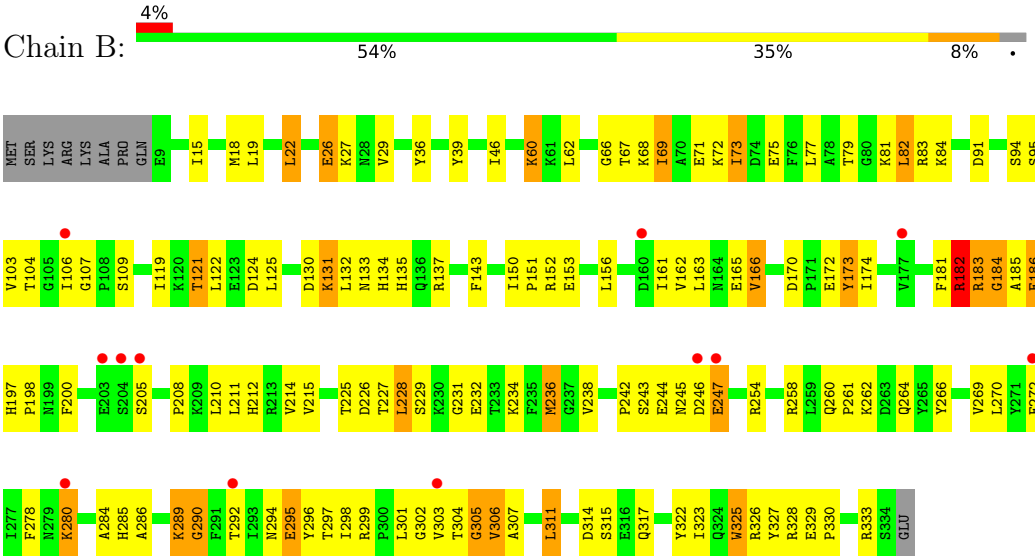
• Molecule 1: DNA polymerase beta

Chain A:



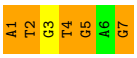
• Molecule 1: DNA polymerase beta

Chain B:



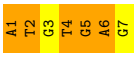
• Molecule 2: DNA 5'-D(P*AP*TP*GP*TP*GP*AP*G)-3'

Chain P:



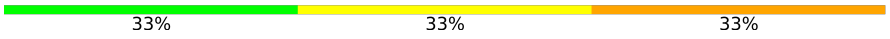
• Molecule 2: DNA 5'-D(P*AP*TP*GP*TP*GP*AP*G)-3'

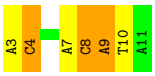
Chain D:



• Molecule 3: DNA 5'-D(P*AP*CP*TP*CP*AP*CP*AP*TP*A)-3'

Chain T:





• Molecule 3: DNA 5'-D(P*AP*CP*TP*CP*AP*CP*AP*TP*A)-3'

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.32Å 56.61Å 93.14Å 90.00° 102.04° 90.00°	Depositor
Resolution (Å)	27.20 – 2.72 49.06 – 2.72	Depositor EDS
% Data completeness (in resolution range)	90.1 (27.20-2.72) 90.1 (49.06-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.218 , 0.292 0.218 , 0.295	Depositor DCC
R_{free} test set	2012 reflections (8.03%)	wwPDB-VP
Wilson B-factor (Å^2)	61.7	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 44.9	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	0.94	EDS
Total number of atoms	6010	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, D3T

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	0.42	0/2692	0.62	0/3622
1	B	0.42	0/2692	0.66	2/3622 (0.1%)
2	D	1.27	2/166 (1.2%)	2.38	11/255 (4.3%)
2	P	1.16	0/166	2.63	14/255 (5.5%)
3	E	1.19	1/182 (0.5%)	1.96	8/278 (2.9%)
3	T	1.30	0/182	2.32	12/278 (4.3%)
All	All	0.57	3/6080 (0.0%)	1.03	47/8310 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	8	DC	C3'-O3'	6.30	1.52	1.44
2	D	1	DA	P-O5'	5.99	1.65	1.59
2	D	4	DT	N1-C2	5.17	1.42	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	DA	O4'-C4'-C3'	-15.62	96.62	106.00
2	P	4	DT	O4'-C4'-C3'	-13.06	98.16	106.00
3	T	8	DC	O4'-C4'-C3'	-11.89	98.86	106.00
2	P	1	DA	O4'-C4'-C3'	-10.40	99.76	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	5	DG	O4'-C1'-N9	10.14	115.10	108.00
2	P	4	DT	O4'-C1'-N1	10.13	115.09	108.00
2	D	4	DT	O4'-C4'-C3'	-9.92	100.05	106.00
2	P	5	DG	O4'-C4'-C3'	-9.81	100.12	106.00
3	T	7	DA	N1-C6-N6	9.51	124.31	118.60
2	D	5	DG	O4'-C1'-N9	9.24	114.47	108.00
3	T	10	DT	O4'-C4'-C3'	-9.04	100.57	106.00
3	E	4	DC	C1'-O4'-C4'	-8.05	102.05	110.10
3	E	8	DC	O4'-C1'-N1	7.99	113.60	108.00
2	D	4	DT	N3-C2-O2	-7.96	117.52	122.30
3	E	5	DT	O4'-C4'-C3'	-7.91	101.25	106.00
3	E	3	DA	O4'-C4'-C3'	-7.47	101.51	104.50
2	D	4	DT	O4'-C1'-N1	7.32	113.12	108.00
3	E	4	DC	O4'-C4'-C3'	-7.25	101.60	104.50
3	E	5	DT	O4'-C1'-N1	7.08	112.96	108.00
3	T	9	DA	N1-C6-N6	7.03	122.82	118.60
2	P	4	DT	N3-C2-O2	-6.96	118.13	122.30
2	D	5	DG	O4'-C4'-C3'	-6.91	101.74	104.50
2	P	7	DG	O4'-C1'-N9	-6.89	103.18	108.00
3	T	4	DC	N1-C2-O2	6.52	122.81	118.90
2	D	1	DA	P-O5'-C5'	6.51	131.32	120.90
2	P	4	DT	C1'-O4'-C4'	-6.46	103.64	110.10
3	T	4	DC	N3-C2-O2	-6.26	117.52	121.90
2	P	5	DG	P-O5'-C5'	-6.08	111.17	120.90
1	B	183	ARG	NE-CZ-NH1	5.96	123.28	120.30
3	E	4	DC	O4'-C1'-N1	5.76	112.03	108.00
3	T	8	DC	O4'-C1'-N1	5.66	111.96	108.00
3	E	10	DT	N3-C4-O4	5.64	123.28	119.90
2	P	5	DG	N3-C4-N9	-5.58	122.65	126.00
1	B	183	ARG	N-CA-C	-5.54	96.05	111.00
3	T	8	DC	N3-C2-O2	-5.48	118.06	121.90
2	D	4	DT	C1'-O4'-C4'	-5.36	104.75	110.10
2	P	2	DT	N3-C2-O2	-5.34	119.10	122.30
2	D	2	DT	N3-C2-O2	-5.33	119.10	122.30
2	D	6	DA	O4'-C4'-C3'	-5.29	102.38	104.50
2	P	2	DT	O4'-C1'-C2'	-5.21	101.73	105.90
2	P	1	DA	O4'-C1'-N9	5.21	111.64	108.00
3	T	7	DA	C5-C6-N6	-5.14	119.59	123.70
2	P	5	DG	O5'-P-OP2	-5.07	101.13	105.70
2	D	1	DA	O5'-P-OP1	5.07	116.78	110.70
3	T	9	DA	C5-C6-N6	-5.05	119.66	123.70
3	T	10	DT	N3-C4-O4	5.02	122.91	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	7	DA	N9-C4-C5	-5.00	103.80	105.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	GLN	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	A	2641	0	2656	83	0
1	B	2641	0	2656	96	0
2	D	148	0	80	11	0
2	P	148	0	80	11	0
3	E	164	0	90	7	0
3	T	164	0	90	10	0
4	A	28	0	13	1	0
4	B	28	0	13	0	0
5	A	4	0	0	0	0
5	B	3	0	0	0	0
6	A	13	0	0	0	0
6	B	17	0	0	0	0
6	D	1	0	0	1	0
6	E	4	0	0	1	0
6	P	2	0	0	0	0
6	T	4	0	0	0	0
All	All	6010	0	5678	201	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 17.

All (201) 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)
2:P:3:DG:H1	3:T:8:DC:H42	1.16	0.92
2:P:3:DG:N2	3:T:8:DC:N3	2.24	0.84
1:B:323:ILE:HG23	1:B:325:TRP:HB2	1.58	0.84
2:P:7:DG:N2	3:T:4:DC:N3	2.27	0.82
1:A:294:ASN:HB3	1:A:296:TYR:H	1.44	0.82
2:P:1:DA:C8	2:P:1:DA:H5"	2.18	0.78
1:B:69:ILE:H	1:B:69:ILE:HD12	1.49	0.76
1:B:323:ILE:HD13	1:B:325:TRP:HD1	1.50	0.75
1:A:182:ARG:HH11	1:A:273:THR:HG21	1.51	0.75
1:A:125:LEU:HB3	1:A:140:LEU:HD11	1.70	0.74
2:D:2:DT:H2'	2:D:3:DG:C8	2.22	0.74
1:B:269:VAL:O	1:B:273:THR:HG22	1.86	0.74
1:B:183:ARG:NH2	1:B:274:GLY:O	2.22	0.72
2:D:3:DG:N7	6:D:19:HOH:O	2.22	0.72
2:D:1:DA:N7	6:E:17:HOH:O	2.22	0.71
1:A:92:ASP:OD2	1:A:120:LYS:NZ	2.24	0.70
1:B:258[B]:ARG:NH2	1:B:295:GLU:OE1	2.24	0.70
1:A:151:PRO:HG2	1:A:154:GLU:HB3	1.74	0.70
2:P:2:DT:H2"	2:P:3:DG:C8	2.29	0.68
2:D:1:DA:H5"	2:D:1:DA:C8	2.32	0.64
1:A:26:GLU:HG2	1:A:35:LYS:HB2	1.80	0.64
1:A:206:LYS:HG3	1:A:207[A]:GLN:H	1.63	0.64
1:B:245:ASN:O	1:B:247:GLU:N	2.30	0.64
1:A:206:LYS:HG3	1:A:207[B]:GLN:H	1.63	0.64
1:A:243:SER:O	1:A:245:ASN:N	2.32	0.63
2:D:6:DA:H2'	2:D:7:DG:C8	2.34	0.63
1:B:302:GLY:O	1:B:304:THR:N	2.26	0.63
1:A:272:PHE:O	1:A:274:GLY:N	2.33	0.62
1:B:27:LYS:HB2	1:B:36:TYR:CD1	2.35	0.62
1:A:241:LEU:HD23	1:A:242:PRO:HD2	1.82	0.61
1:A:10:THR:HG23	1:A:12:ASN:HB2	1.82	0.61
1:A:196:THR:HG23	1:A:262:LYS:HD2	1.83	0.61
1:B:286:ALA:HA	1:B:323:ILE:HG13	1.82	0.61
1:B:26:GLU:OE2	1:B:36:TYR:HA	2.02	0.60
3:E:4:DC:H2'	3:E:5:DT:C6	2.37	0.60
1:B:183:ARG:HH22	1:B:275:SER:HB3	1.67	0.60
1:B:292:THR:HG23	1:B:299:ARG:HD3	1.82	0.60
2:D:1:DA:H5"	2:D:1:DA:H8	1.67	0.59
1:A:283:ARG:HB3	3:T:3:DA:H4'	1.85	0.59
2:P:3:DG:H1	3:T:8:DC:N4	1.92	0.59
1:B:152:ARG:HH11	1:B:156:LEU:HD12	1.67	0.59
1:B:234:LYS:HB2	3:E:7:DA:OP1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLY:HA2	1:B:301:LEU:HD23	1.86	0.58
1:A:15:ILE:HD12	1:A:15:ILE:H	1.68	0.58
2:P:7:DG:N2	3:T:4:DC:C2	2.71	0.58
1:A:145:ASP:OD2	1:A:145:ASP:N	2.36	0.58
1:B:162:VAL:O	1:B:166:VAL:HB	2.04	0.57
2:D:1:DA:H61	3:E:10:DT:H3	1.52	0.57
1:A:121:THR:H	1:A:124:ASP:HB2	1.69	0.56
1:B:60:LYS:HD3	1:B:66:GLY:HA2	1.86	0.56
2:P:4:DT:H2"	2:P:5:DG:O5'	2.06	0.56
1:B:79:THR:HG22	1:B:81:LYS:H	1.70	0.56
1:A:182:ARG:HD3	1:A:273:THR:CG2	2.37	0.56
2:P:3:DG:H2"	2:P:4:DT:O5'	2.05	0.56
1:A:299:ARG:HB3	1:A:310:PRO:HA	1.88	0.55
1:A:273:THR:O	1:A:273:THR:OG1	2.24	0.55
1:B:69:ILE:H	1:B:69:ILE:CD1	2.18	0.55
1:B:66:GLY:H	1:B:69:ILE:HD13	1.72	0.55
1:A:244:GLU:OE1	1:A:244:GLU:N	2.37	0.54
1:B:323:ILE:HD13	1:B:325:TRP:CD1	2.36	0.54
1:B:330:PRO:HA	1:B:333:ARG:HG3	1.89	0.54
1:A:186:GLU:OE1	1:A:186:GLU:N	2.38	0.54
1:A:182:ARG:HD3	1:A:273:THR:HG21	1.90	0.54
1:A:152:ARG:O	1:A:155:MET:N	2.41	0.54
1:A:204:SER:HA	1:B:152:ARG:CZ	2.38	0.53
1:B:280:LYS:O	1:B:284:ALA:N	2.40	0.53
1:A:180:SER:HA	1:A:183:ARG:NH1	2.23	0.53
1:A:258[B]:ARG:HD2	1:A:272:PHE:CE1	2.44	0.53
1:A:126:ARG:HG2	1:A:140:LEU:HD21	1.91	0.53
1:A:180:SER:HA	1:A:183:ARG:HH11	1.73	0.53
1:B:258[A]:ARG:NH2	1:B:260:GLN:OE1	2.41	0.53
1:B:72:LYS:HG2	1:B:82:LEU:HD11	1.91	0.52
1:B:304:THR:OG1	1:B:305:GLY:N	2.42	0.52
1:A:272:PHE:O	1:A:273:THR:C	2.47	0.52
1:B:182:ARG:H	1:B:184:GLY:H	1.57	0.52
1:B:231:GLY:HA3	3:E:7:DA:H5"	1.92	0.52
1:A:182:ARG:NH1	1:A:273:THR:HG21	2.23	0.52
1:B:104:THR:HG23	1:B:135:HIS:CD2	2.44	0.52
1:A:156:LEU:HD23	1:A:181:PHE:HZ	1.75	0.51
1:B:183:ARG:O	1:B:185:ALA:N	2.44	0.51
1:B:266:TYR:HA	1:B:269:VAL:HG12	1.93	0.51
1:A:207[B]:GLN:HB3	1:A:210:LEU:HG	1.93	0.51
1:A:244:GLU:OE2	1:A:248:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLU:O	1:B:79:THR:HB	2.11	0.51
1:B:121:THR:HG23	1:B:124:ASP:H	1.75	0.51
1:A:330:PRO:HD3	1:A:333:ARG:HH21	1.74	0.51
1:A:27:LYS:HB2	1:A:36:TYR:CD1	2.46	0.51
1:B:289:LYS:NZ	1:B:323:ILE:HG12	2.26	0.50
1:B:228:LEU:HB2	1:B:236:MET:O	2.11	0.50
1:B:226:ASP:HB2	1:B:238:VAL:HG13	1.92	0.50
3:E:6:DC:H2"	3:E:7:DA:O5'	2.11	0.50
1:B:211:LEU:O	1:B:215:VAL:HG23	2.11	0.50
1:B:258[A]:ARG:NH1	1:B:296:TYR:OH	2.41	0.50
1:A:240:GLN:OE1	1:A:252:HIS:NE2	2.44	0.50
1:B:130:ASP:OD2	1:B:131:LYS:NZ	2.29	0.50
1:A:81:LYS:HE3	1:A:89:ARG:HH12	1.77	0.49
1:B:170:ASP:O	1:B:173:TYR:HB2	2.11	0.49
1:A:258[B]:ARG:NH2	1:A:271:TYR:OH	2.45	0.49
1:B:121:THR:OG1	1:B:122:LEU:N	2.45	0.49
3:T:8:DC:H2'	3:T:9:DA:C8	2.47	0.49
1:A:207[A]:GLN:HB3	1:A:210:LEU:HG	1.95	0.49
1:A:330:PRO:O	1:A:331:LYS:HB3	2.12	0.48
1:A:142:TYR:CE2	1:A:238:VAL:HG11	2.48	0.48
1:A:18:MET:O	1:A:22:LEU:HB2	2.14	0.48
1:A:284:ALA:C	1:A:286:ALA:H	2.15	0.48
1:B:134:HIS:NE2	1:B:227:THR:O	2.45	0.48
1:B:173:TYR:CE1	1:B:197:HIS:HB2	2.49	0.48
3:T:8:DC:H2"	3:T:9:DA:O5'	2.13	0.48
1:A:158:MET:O	1:A:162:VAL:HG23	2.14	0.48
1:B:161:ILE:O	1:B:165:GLU:HG2	2.14	0.48
2:P:1:DA:H5"	2:P:1:DA:H8	1.75	0.48
1:A:50:PRO:HG2	1:A:51:HIS:CE1	2.49	0.48
1:A:82:LEU:HD12	1:A:83:ARG:N	2.30	0.47
1:A:130:ASP:OD1	1:A:130:ASP:N	2.43	0.47
1:A:106:ILE:HG13	1:A:136:GLN:HG2	1.97	0.46
1:A:157:GLN:HB3	1:A:241:LEU:HD21	1.97	0.46
1:B:196:THR:HB	1:B:262:LYS:HG3	1.97	0.46
1:A:330:PRO:HD3	1:A:333:ARG:NH2	2.31	0.46
1:B:151:PRO:HA	1:B:186:GLU:O	2.15	0.46
1:A:26:GLU:HG2	1:A:35:LYS:CB	2.44	0.46
1:A:110:ALA:O	1:A:114:LEU:HG	2.15	0.46
1:A:269:VAL:O	1:A:273:THR:HG23	2.16	0.46
1:A:209:LYS:HE3	1:A:209:LYS:HB3	1.74	0.46
1:B:266:TYR:CD1	1:B:315:SER:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:VAL:HG21	1:B:94:SER:HB2	1.96	0.46
1:B:285:HIS:HB3	1:B:323:ILE:HD11	1.97	0.46
1:B:132:LEU:HB2	1:B:137:ARG:HG2	1.98	0.46
1:B:69:ILE:HD12	1:B:69:ILE:N	2.24	0.45
1:B:91:ASP:HB3	1:B:94:SER:OG	2.16	0.45
1:A:81:LYS:HG2	1:A:82:LEU:H	1.82	0.45
1:B:225:THR:OG1	1:B:226:ASP:OD2	2.23	0.45
1:A:22:LEU:HD13	1:A:85:LEU:HD13	1.97	0.45
1:B:82:LEU:HD22	1:B:84:LYS:H	1.82	0.45
1:B:200:PHE:CE2	1:B:210:LEU:HD12	2.52	0.44
1:B:236:MET:HE3	1:B:254:ARG:NH2	2.31	0.44
1:B:302:GLY:H	1:B:307:ALA:HA	1.83	0.44
1:A:162:VAL:O	1:A:166:VAL:HB	2.16	0.44
1:A:280:LYS:HD2	3:T:3:DA:C5	2.51	0.44
1:A:280:LYS:HD2	3:T:3:DA:C6	2.52	0.44
1:B:294:ASN:OD1	1:B:296:TYR:HB2	2.18	0.44
2:D:7:DG:H8	2:D:7:DG:O5'	2.00	0.44
1:A:150:ILE:HG12	1:A:253:ARG:CZ	2.48	0.44
1:B:294:ASN:C	1:B:296:TYR:H	2.21	0.44
1:A:323:ILE:HG13	1:A:325:TRP:HB2	1.98	0.44
1:B:107:GLY:N	2:D:5:DG:H5"	2.32	0.44
1:A:178:CYS:HB3	1:A:272:PHE:HB3	2.00	0.44
1:B:103:VAL:HG22	1:B:143:PHE:CD1	2.52	0.44
1:B:182:ARG:N	1:B:184:GLY:H	2.14	0.44
1:B:22:LEU:HD22	1:B:39:TYR:CE1	2.52	0.44
1:B:296:TYR:HE1	3:E:6:DC:OP1	2.01	0.44
1:B:133:ASN:O	1:B:137:ARG:HG3	2.17	0.44
1:B:317:GLN:OE1	1:B:327:TYR:HB2	2.18	0.43
1:A:122:LEU:O	1:A:126:ARG:HG3	2.18	0.43
1:A:85:LEU:O	1:A:89:ARG:HD3	2.18	0.43
1:B:229:SER:HB2	3:E:7:DA:O3'	2.19	0.43
1:A:263:ASP:OD1	1:A:263:ASP:N	2.47	0.43
1:A:274:GLY:HA3	1:A:275:SER:HA	1.86	0.43
1:A:41:LYS:O	1:A:45:VAL:HG13	2.19	0.43
1:A:166:VAL:HG13	1:A:173:TYR:HB3	1.99	0.43
1:B:119:ILE:HA	1:B:124:ASP:HB3	2.01	0.43
1:B:323:ILE:HG12	1:B:323:ILE:O	2.19	0.43
1:B:236:MET:HE3	1:B:254:ARG:HH22	1.84	0.43
1:A:194:LEU:HD11	1:A:260:GLN:HB2	2.01	0.43
1:B:27:LYS:HD3	1:B:36:TYR:CE1	2.54	0.43
1:B:68:LYS:HA	1:B:71:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PRO:HB2	1:B:212:HIS:CD2	2.54	0.43
1:A:155:MET:HG2	1:A:181:PHE:HD1	1.84	0.42
2:D:2:DT:H4'	2:D:3:DG:OP1	2.18	0.42
1:A:235:PHE:HD2	1:A:257:ILE:HG13	1.84	0.42
1:B:174:ILE:HB	1:B:196:THR:OG1	2.19	0.42
1:B:150:ILE:O	1:B:187:SER:HA	2.19	0.42
1:A:152:ARG:NH2	1:A:181:PHE:O	2.53	0.42
1:A:150:ILE:HD13	1:A:158:MET:HE1	2.02	0.42
1:B:183:ARG:C	1:B:185:ALA:N	2.73	0.42
1:B:278:PHE:HB2	1:B:333:ARG:O	2.19	0.42
1:B:81:LYS:HE2	1:B:81:LYS:HB2	1.81	0.42
1:B:294:ASN:O	1:B:296:TYR:N	2.52	0.42
1:B:311:LEU:HD13	1:B:322:TYR:CZ	2.54	0.42
1:A:121:THR:HG22	1:A:124:ASP:OD1	2.20	0.41
1:A:172:GLU:HB3	1:A:198:PRO:HD2	2.02	0.41
1:A:199:ASN:O	1:B:156:LEU:HD21	2.20	0.41
1:B:208:PRO:HB3	1:B:232:GLU:HA	2.02	0.41
1:B:181:PHE:O	1:B:182:ARG:HB2	2.20	0.41
4:A:336:D3T:C6	2:P:7:DG:H2'	2.51	0.41
2:D:4:DT:H2"	2:D:5:DG:O5'	2.20	0.41
1:B:242:PRO:O	1:B:244:GLU:N	2.54	0.41
1:A:49:TYR:HA	1:A:50:PRO:HD2	1.83	0.41
1:A:204:SER:HA	1:B:152:ARG:NE	2.35	0.41
1:A:284:ALA:O	1:A:286:ALA:N	2.54	0.41
1:B:103:VAL:HB	1:B:106:ILE:HD12	2.02	0.41
1:B:125:LEU:HD23	1:B:125:LEU:HA	1.82	0.41
1:B:150:ILE:N	1:B:188:SER:O	2.50	0.41
1:A:180:SER:HB3	1:A:185:ALA:HB3	2.03	0.40
1:B:15:ILE:HG12	1:B:73:ILE:HG12	2.03	0.40
1:A:198:PRO:HA	1:A:262:LYS:HD3	2.02	0.40
1:B:234:LYS:HG2	1:B:258[B]:ARG:HG3	2.04	0.40
1:B:289:LYS:HZ2	1:B:323:ILE:HG12	1.86	0.40
1:B:197:HIS:CG	1:B:198:PRO:HD2	2.56	0.40
1:B:306:VAL:HG12	1:B:307:ALA:H	1.86	0.40
1:A:144:GLU:OE1	1:A:144:GLU:N	2.52	0.40
1:B:325:TRP:HE3	1:B:326:ARG:H	1.69	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	326/335 (97%)	280 (86%)	28 (9%)	18 (6%)	2	3
1	B	326/335 (97%)	275 (84%)	38 (12%)	13 (4%)	3	5
All	All	652/670 (97%)	555 (85%)	66 (10%)	31 (5%)	2	4

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	THR
1	A	244	GLU
1	A	246	ASP
1	A	249	GLU
1	A	273	THR
1	A	310	PRO
1	A	331	LYS
1	B	182	ARG
1	B	243	SER
1	B	246	ASP
1	B	303	VAL
1	A	80	GLY
1	A	243	SER
1	A	272	PHE
1	A	274	GLY
1	B	205	SER
1	B	274	GLY
1	A	285	HIS
1	A	304	THR
1	B	184	GLY
1	B	247	GLU
1	A	206	LYS
1	A	245	ASN
1	A	302	GLY
1	B	276	ASP

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Mol	Chain	Res	Type
1	B	295	GLU
1	B	305	GLY
1	A	303	VAL
1	A	317	GLN
1	B	261	PRO
1	B	290	GLY

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	290/296 (98%)	246 (85%)	44 (15%)	3 6
1	B	290/296 (98%)	247 (85%)	43 (15%)	3 7
All	All	580/592 (98%)	493 (85%)	87 (15%)	3 6

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	18	MET
1	A	19	LEU
1	A	27	LYS
1	A	33	ILE
1	A	48	LYS
1	A	54	LYS
1	A	55	SER
1	A	62	LEU
1	A	67	THR
1	A	68	LYS
1	A	69	ILE
1	A	77	LEU
1	A	101	THR
1	A	103	VAL
1	A	112	ARG
1	A	125	LEU

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Mol	Chain	Res	Type
1	A	129	GLU
1	A	130	ASP
1	A	135	HIS
1	A	145	ASP
1	A	176	THR
1	A	183	ARG
1	A	196	THR
1	A	205	SER
1	A	209	LYS
1	A	218	LEU
1	A	220	LYS
1	A	228	LEU
1	A	232	GLU
1	A	241	LEU
1	A	247	GLU
1	A	248	ASN
1	A	267	CYS
1	A	277	ILE
1	A	299	ARG
1	A	303	VAL
1	A	306	VAL
1	A	321	ASP
1	A	322	TYR
1	A	325	TRP
1	A	328	ARG
1	A	329	GLU
1	A	334	SER
1	B	18	MET
1	B	19	LEU
1	B	22	LEU
1	B	26	GLU
1	B	46	ILE
1	B	60	LYS
1	B	62	LEU
1	B	67	THR
1	B	69	ILE
1	B	73	ILE
1	B	77	LEU
1	B	82	LEU
1	B	83	ARG
1	B	95	SER
1	B	101	THR

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Mol	Chain	Res	Type
1	B	109	SER
1	B	121	THR
1	B	131	LYS
1	B	153	GLU
1	B	163	LEU
1	B	166	VAL
1	B	172	GLU
1	B	173	TYR
1	B	182	ARG
1	B	186	GLU
1	B	187	SER
1	B	214	VAL
1	B	228	LEU
1	B	236	MET
1	B	264	GLN
1	B	270	LEU
1	B	272	PHE
1	B	273	THR
1	B	280	LYS
1	B	289	LYS
1	B	297	THR
1	B	298	ILE
1	B	306	VAL
1	B	311	LEU
1	B	314	ASP
1	B	325	TRP
1	B	328	ARG
1	B	329	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	264	GLN
1	B	294	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	D3T	A	336	5	25,29,29	1.32	4 (16%)	35,45,45	2.15	11 (31%)
4	D3T	B	336	5	25,29,29	1.31	3 (12%)	35,45,45	2.32	12 (34%)

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	D3T	A	336	5	-	9/22/31/31	0/2/2/2
4	D3T	B	336	5	-	6/22/31/31	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	336	D3T	C6-C5	3.52	1.40	1.34
4	B	336	D3T	C4-C5	2.75	1.49	1.44
4	A	336	D3T	C6-N1	-2.60	1.33	1.38
4	A	336	D3T	C6-C5	2.46	1.38	1.34
4	A	336	D3T	C4-C5	2.43	1.48	1.44
4	B	336	D3T	C4-N3	-2.39	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	336	D3T	C4-N3	-2.28	1.34	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	336	D3T	C4-N3-C2	-5.29	120.50	127.35
4	B	336	D3T	N3-C2-N1	5.17	121.75	114.89
4	B	336	D3T	PB-O3A-PA	-4.74	116.55	132.83
4	A	336	D3T	C4-N3-C2	-4.73	121.22	127.35
4	B	336	D3T	C5-C4-N3	4.46	119.12	115.31
4	A	336	D3T	O4-C4-C5	-4.38	119.82	124.90
4	B	336	D3T	C5-C6-N1	-4.14	119.08	123.34
4	B	336	D3T	O4-C4-C5	-4.03	120.23	124.90
4	A	336	D3T	N3-C2-N1	3.97	120.16	114.89
4	A	336	D3T	C5-C6-N1	-3.96	119.27	123.34
4	A	336	D3T	C5-C4-N3	3.82	118.57	115.31
4	A	336	D3T	PB-O3A-PA	-3.68	120.20	132.83
4	B	336	D3T	O2-C2-N1	-3.58	118.03	122.79
4	A	336	D3T	O2-C2-N1	-3.39	118.27	122.79
4	B	336	D3T	C2'-C1'-N1	-3.26	106.22	112.40
4	B	336	D3T	C3'-C2'-C1'	3.16	106.43	102.78
4	A	336	D3T	PB-O3B-PG	-3.07	122.30	132.83
4	B	336	D3T	O3G-PG-O3B	2.32	112.42	104.64
4	B	336	D3T	O4'-C1'-N1	2.26	111.90	107.86
4	A	336	D3T	C2'-C1'-N1	-2.25	108.14	112.40
4	A	336	D3T	C5M-C5-C4	2.21	121.20	118.77
4	B	336	D3T	O4'-C4'-C3'	2.16	108.39	104.80
4	A	336	D3T	C5M-C5-C6	-2.11	120.03	122.85

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	336	D3T	C5'-O5'-PA-O1A
4	A	336	D3T	C5'-O5'-PA-O2A
4	B	336	D3T	C5'-O5'-PA-O1A
4	B	336	D3T	PB-O3B-PG-O2G
4	A	336	D3T	C3'-C4'-C5'-O5'
4	B	336	D3T	C5'-O5'-PA-O3A
4	A	336	D3T	PG-O3B-PB-O1B
4	B	336	D3T	C5'-O5'-PA-O2A
4	A	336	D3T	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	B	336	D3T	PG-O3B-PB-O2B
4	A	336	D3T	C5'-O5'-PA-O3A
4	A	336	D3T	PB-O3A-PA-O1A
4	A	336	D3T	PB-O3A-PA-O2A
4	A	336	D3T	PA-O3A-PB-O2B
4	B	336	D3T	PG-O3B-PB-O1B

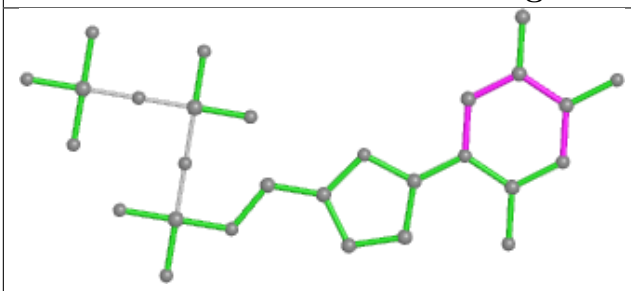
There are no ring outliers.

1 monomer is involved in 1 short contact:

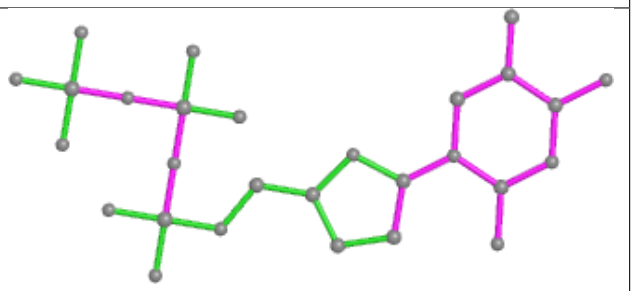
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	336	D3T	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

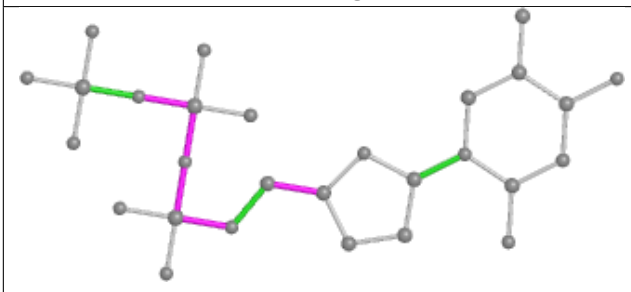
Ligand D3T A 336



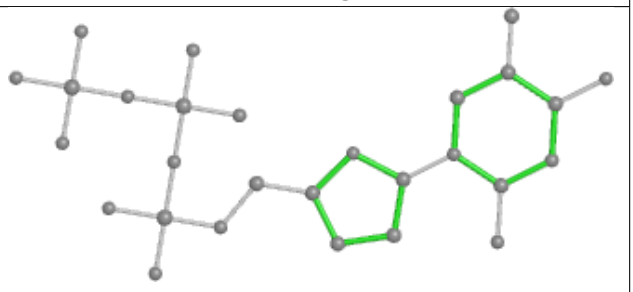
Bond lengths



Bond angles

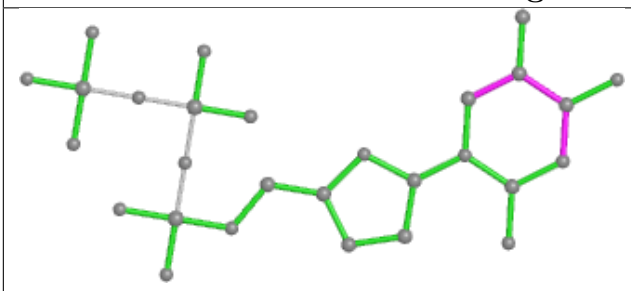


Torsions

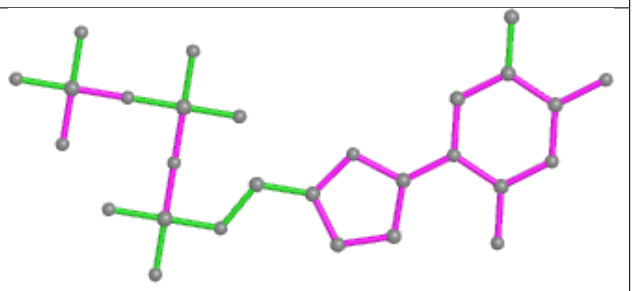


Rings

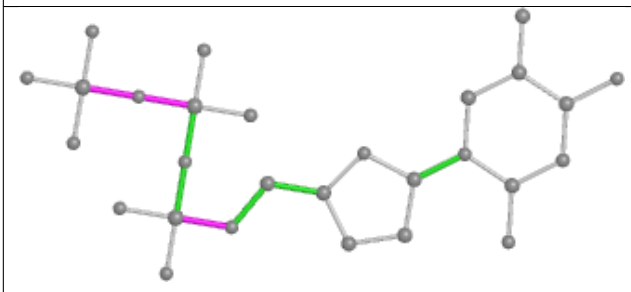
Ligand D3T B 336



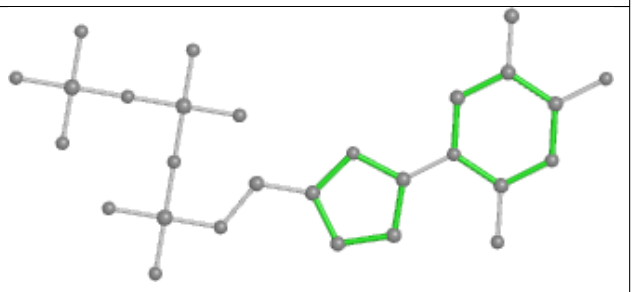
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	325/335 (97%)	0.11	10 (3%) 49 50	47, 85, 134, 168	0
1	B	325/335 (97%)	0.17	13 (4%) 38 37	57, 89, 159, 202	0
2	D	7/7 (100%)	0.05	0 100 100	69, 91, 122, 140	0
2	P	7/7 (100%)	-0.01	0 100 100	56, 81, 107, 109	0
3	E	9/9 (100%)	-0.37	0 100 100	69, 88, 95, 102	0
3	T	9/9 (100%)	-0.46	0 100 100	46, 71, 90, 100	0
All	All	682/702 (97%)	0.12	23 (3%) 45 45	46, 88, 148, 202	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	VAL	6.1
1	A	10	THR	5.1
1	B	205	SER	4.4
1	B	204	SER	4.4
1	B	246	ASP	4.2
1	B	177	VAL	3.7
1	A	272	PHE	3.2
1	B	272	PHE	2.9
1	A	323	ILE	2.8
1	B	247	GLU	2.8
1	A	177	VAL	2.8
1	B	106	ILE	2.8
1	B	280	LYS	2.8
1	A	131	LYS	2.6
1	B	100	LEU	2.4
1	A	195	LEU	2.4
1	A	303	VAL	2.4
1	B	160	ASP	2.3
1	A	31	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	59	ALA	2.3
1	B	203	GLU	2.2
1	B	292	THR	2.1
1	A	20	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

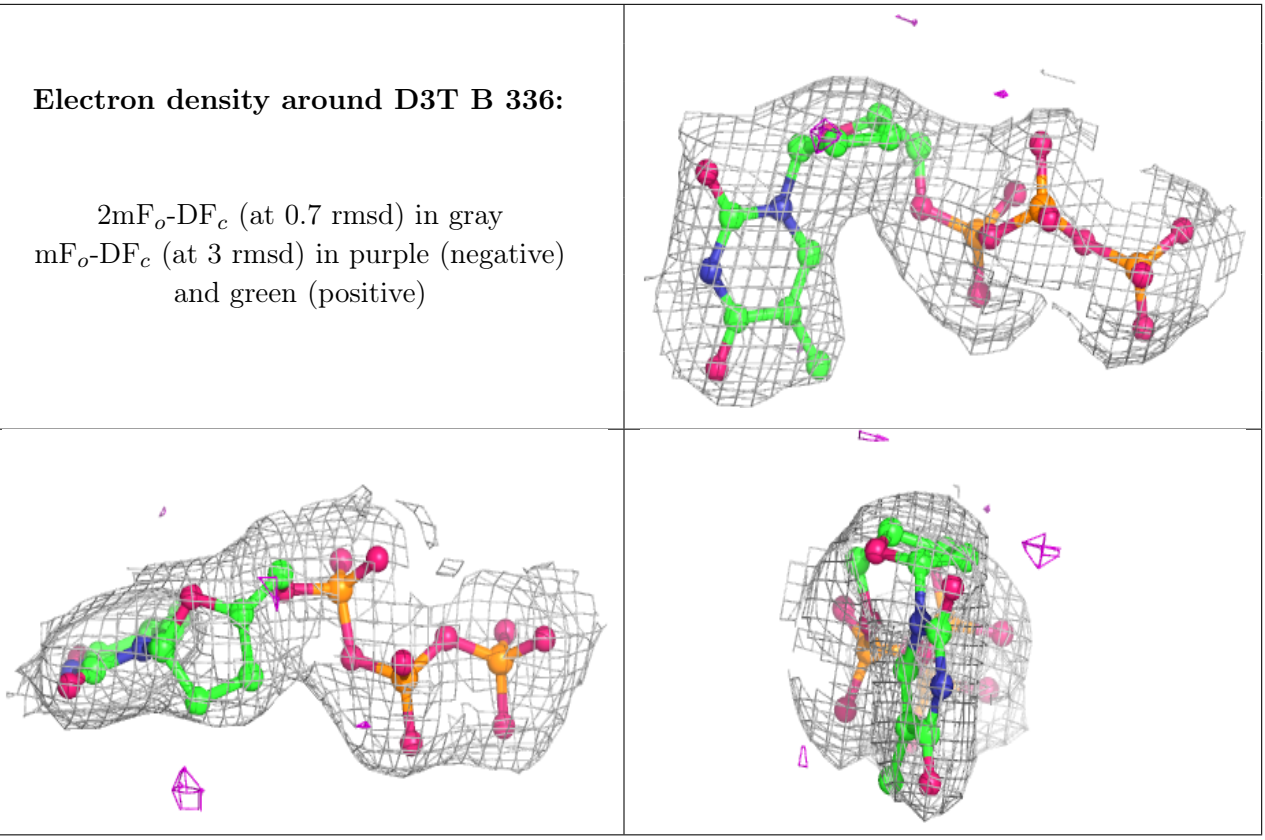
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	NA	A	340	1/1	0.70	0.18	86,86,86,86	0
5	NA	A	337	1/1	0.71	0.43	81,81,81,81	0
5	NA	A	339	1/1	0.76	0.14	81,81,81,81	0
5	NA	B	339	1/1	0.77	0.58	80,80,80,80	0
5	NA	B	337	1/1	0.81	0.23	84,84,84,84	0
5	NA	B	338	1/1	0.84	0.09	89,89,89,89	0
5	NA	A	338	1/1	0.96	0.05	80,80,80,80	0
4	D3T	B	336	28/28	0.97	0.17	47,65,81,85	0
4	D3T	A	336	28/28	0.97	0.17	41,57,91,99	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.

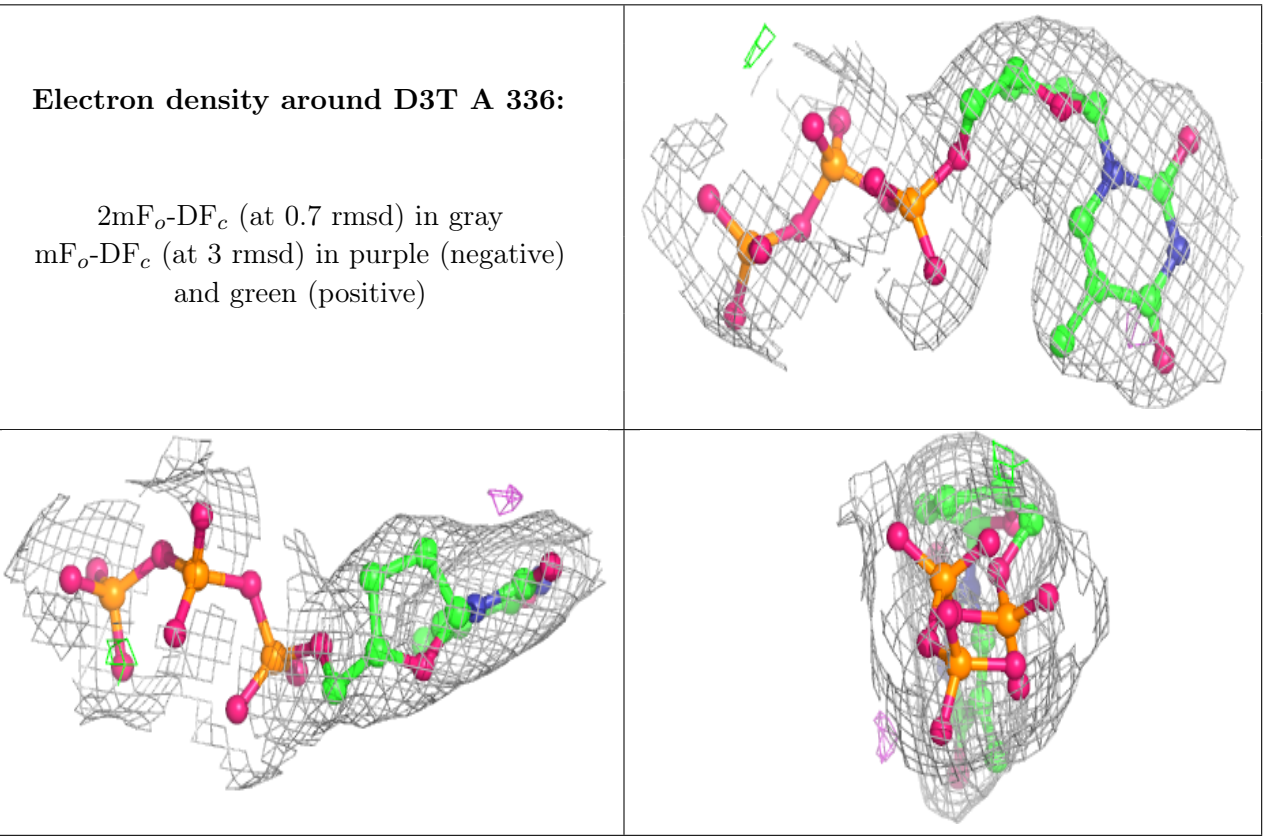
Electron density around D3T B 336:

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



Electron density around D3T A 336:

$2mF_o$-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.