



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:02 AM GMT

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

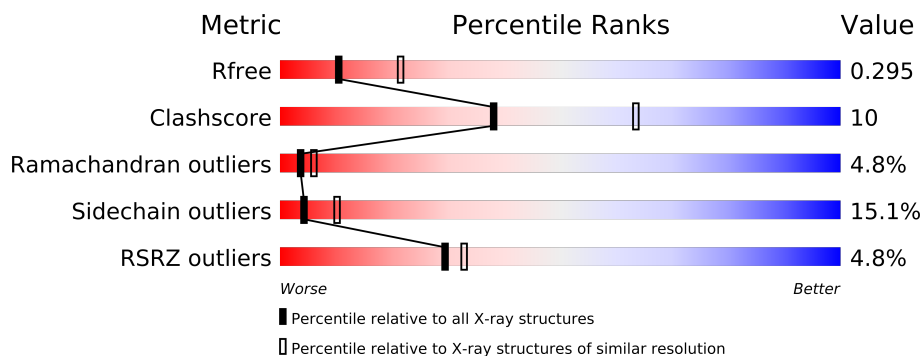
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.72 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}	66092	1770 (2.74-2.70)
Clashscore	79885	2183 (2.74-2.70)
Ramachandran outliers	78287	2147 (2.74-2.70)
Sidechain outliers	78261	2148 (2.74-2.70)
RSRZ outliers	66119	1772 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	335	
1	B	335	
2	D	7	
2	P	7	
3	E	9	
3	T	9	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	NA	A	337	-	X
5	NA	B	339	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6010 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase 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

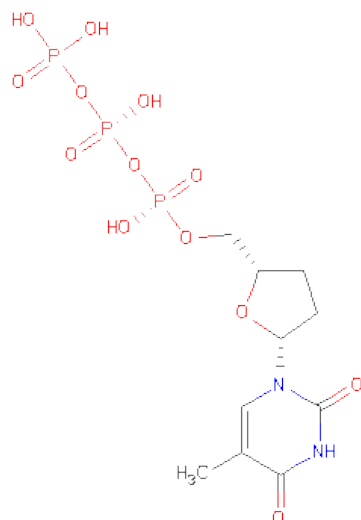
- Molecule 2 is a DNA chain called DNA 5'-D(P*AP*TP*GP*TP*GP*AP*G)-3'.

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: C₁₀H₁₇N₂O₁₃P₃).



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

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

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

- Molecule 6 is water.

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

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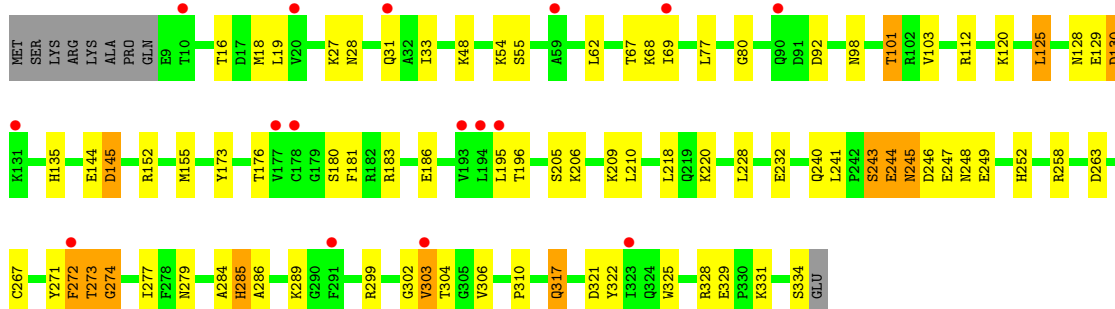
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	4	Total	O	0	0
			4	4		

3 Residue-property plots

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

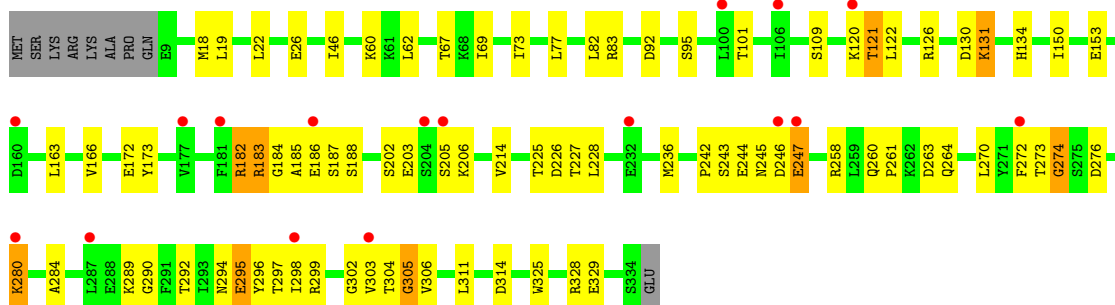
- Molecule 1: DNA polymerase beta

Chain A: 



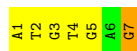
- Molecule 1: DNA polymerase beta

Chain B: 



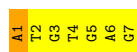
- Molecule 2: DNA 5'-D(P*AP*TP*GP*TP*GP*AP*G)-3'

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

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) 90.2 (49.06-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	2009 reflections (8.02%)	DCC
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 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25068 reflections	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2641	0	0	25	0
1	B	2641	0	0	23	0
2	D	148	0	0	3	0
2	P	148	0	0	3	0
3	E	164	0	90	3	0
3	T	164	0	90	5	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	2	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	206	58	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:3:DG:N2	3:T:8:DC:N3	2.24	0.84
2:P:7:DG:N2	3:T:4:DC:N3	2.27	0.83
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:B:302:GLY:O	1:B:304:THR:N	2.26	0.69
1:B:130:ASP:OD2	1:B:131:LYS:NZ	2.29	0.66
1:B:280:LYS:N	6:B:340:HOH:O	2.29	0.66
1:B:245:ASN:O	1:B:247:GLU:N	2.30	0.64
1:A:243:SER:O	1:A:245:ASN:N	2.32	0.63
1:A:173:TYR:OH	1:A:210:LEU:O	2.18	0.62
1:A:272:PHE:O	1:A:274:GLY:N	2.33	0.62
3:E:4:DC:H2'	3:E:5:DT:C6	2.37	0.60
2:P:7:DG:N2	3:T:4:DC:C2	2.71	0.58
1:A:145:ASP:N	1:A:145:ASP:OD2	2.36	0.58
1:A:244:GLU:N	1:A:244:GLU:OE1	2.37	0.57
1:A:186:GLU:OE1	1:A:186:GLU:N	2.38	0.57
1:B:225:THR:OG1	1:B:226:ASP:OD2	2.23	0.57
1:B:292:THR:N	1:B:299:ARG:O	2.39	0.56
1:A:273:THR:O	1:A:273:THR:OG1	2.24	0.55
1:B:258[A]:ARG:NH1	1:B:296:TYR:OH	2.41	0.54
1:B:280:LYS:O	1:B:284:ALA:N	2.40	0.54
1:A:152:ARG:O	1:A:155:MET:N	2.41	0.54
1:B:258[A]:ARG:NH2	1:B:260:GLN:OE1	2.41	0.53
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
2:D:7:DG:N2	3:E:4:DC:N3	2.56	0.52
1:A:271:TYR:O	1:A:279:ASN:ND2	2.42	0.52
1:A:130:ASP:N	1:A:130:ASP:OD1	2.43	0.51
1:B:183:ARG:O	1:B:185:ALA:N	2.44	0.51
1:B:126:ARG:NE	6:B:351:HOH:O	2.42	0.51
1:A:180:SER:OG	4:A:336:D3T:O1G	2.29	0.50
3:E:6:DC:H2''	3:E:7:DA:O5'	2.11	0.50
1:A:240:GLN:OE1	1:A:252:HIS:NE2	2.44	0.50
1:B:134:HIS:NE2	1:B:227:THR:O	2.45	0.49
1:A:317:GLN:OE1	1:A:317:GLN:N	2.46	0.49
3:T:8:DC:H2'	3:T:9:DA:C8	2.47	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
1:A:263:ASP:N	1:A:263:ASP:OD1	2.47	0.48
3:T:8:DC:H2''	3:T:9:DA:O5'	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:92:ASP:OD1	1:B:120:LYS:NZ	2.47	0.47
1:A:285:HIS:O	1:A:289:LYS:NZ	2.49	0.46
1:B:150:ILE:N	1:B:188:SER:O	2.50	0.45
1:A:28:ASN:ND2	1:A:98:ASN:OD1	2.50	0.44
1:A:125:LEU:O	1:A:128:ASN:N	2.51	0.44
1:B:203:GLU:O	1:B:206:LYS:NZ	2.52	0.43
1:A:144:GLU:OE1	1:A:144:GLU:N	2.52	0.43
1:A:152:ARG:NH2	1:A:181:PHE:O	2.53	0.42
1:B:183:ARG:C	1:B:185:ALA:N	2.73	0.42
1:B:294:ASN:O	1:B:296:TYR:N	2.52	0.42
1:A:195:LEU:N	1:A:258[B]:ARG:O	2.53	0.41
1:B:242:PRO:O	1:B:244:GLU:N	2.54	0.41
1:A:284:ALA:O	1:A:286:ALA:N	2.54	0.41
1:A:195:LEU:N	1:A:258[A]:ARG:O	2.54	0.40
1:B:202:SER:OG	1:B:263:ASP:OD1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/335 (97%)	280 (86%)	28 (9%)	18 (6%)	3	4
1	B	326/335 (97%)	275 (84%)	38 (12%)	13 (4%)	5	9
All	All	652/670 (97%)	555 (85%)	66 (10%)	31 (5%)	4	6

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	4	10
1	B	290/296 (98%)	247 (85%)	43 (15%)	4	11
All	All	580/592 (98%)	493 (85%)	87 (15%)	4	10

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	B	328	ARG
1	B	329	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	29,29,29	1.06	2 (6%)	40,45,45	1.63	7 (17%)
4	D3T	B	336	5	29,29,29	0.98	2 (6%)	40,45,45	2.07	9 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	D3T	A	336	5	-	0/19/31/31	0/2/2/2
4	D3T	B	336	5	-	0/19/31/31	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	336	D3T	C4-C5	2.96	1.49	1.42
4	A	336	D3T	C4-C5	2.72	1.48	1.42
4	A	336	D3T	C2-N1	2.62	1.41	1.38
4	B	336	D3T	C2-N1	2.43	1.41	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	336	D3T	N3-C2-N1	6.92	121.75	115.97
4	B	336	D3T	PB-O3A-PA	-5.16	116.55	131.68
4	A	336	D3T	N3-C2-N1	5.01	120.16	115.97
4	B	336	D3T	C6-N1-C2	-4.76	121.05	122.41
4	A	336	D3T	PB-O3A-PA	-3.91	120.20	131.68
4	A	336	D3T	C4'-O4'-C1'	3.67	111.58	110.05
4	B	336	D3T	C3'-C2'-C1'	3.28	106.43	102.80
4	B	336	D3T	C2'-C1'-N1	-3.22	106.22	112.66
4	A	336	D3T	PB-O3B-PG	-3.20	122.30	131.68
4	B	336	D3T	C5-C6-N1	-2.58	119.08	121.59
4	A	336	D3T	C5-C6-N1	-2.38	119.27	121.59
4	B	336	D3T	C4-N3-C2	-2.38	120.50	125.39
4	A	336	D3T	C2'-C1'-N1	-2.26	108.14	112.66
4	B	336	D3T	O4'-C1'-N1	2.24	111.90	107.68
4	B	336	D3T	O4'-C4'-C3'	2.14	108.39	104.80
4	A	336	D3T	C4-N3-C2	-2.03	121.22	125.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	325/335 (97%)	0.20	16 (4%)	28 32	47, 85, 134, 168	0
1	B	325/335 (97%)	0.24	17 (5%)	26 29	57, 89, 159, 202	0
2	D	7/7 (100%)	0.03	0	100 100	69, 91, 122, 140	0
2	P	7/7 (100%)	-0.04	0	100 100	56, 81, 107, 109	0
3	E	9/9 (100%)	-0.32	0	100 100	69, 88, 95, 102	0
3	T	9/9 (100%)	-0.37	0	100 100	47, 71, 90, 100	0
All	All	682/702 (97%)	0.20	33 (4%)	29 33	47, 88, 148, 202	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	VAL	6.3
1	A	10	THR	5.2
1	B	177	VAL	4.3
1	A	131	LYS	4.0
1	A	272	PHE	3.7
1	B	246	ASP	3.6
1	B	205	SER	3.5
1	B	106	ILE	3.3
1	B	204	SER	3.3
1	B	186	GLU	3.0
1	B	272	PHE	2.9
1	A	177	VAL	2.9
1	B	181	PHE	2.8
1	B	100	LEU	2.7
1	A	323	ILE	2.7
1	A	59	ALA	2.6
1	B	247	GLU	2.4
1	A	178	CYS	2.4
1	A	291	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	120	LYS	2.3
1	A	69	ILE	2.2
1	A	31	GLN	2.2
1	A	303	VAL	2.2
1	A	20	VAL	2.1
1	B	280	LYS	2.1
1	A	195	LEU	2.1
1	A	194	LEU	2.1
1	B	232	GLU	2.1
1	A	90	GLN	2.0
1	B	298	ILE	2.0
1	A	193	VAL	2.0
1	B	287	LEU	2.0
1	B	160	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NA	A	337	1/1	0.42	11.10	81,81,81,81	0
5	NA	B	339	1/1	0.55	4.27	80,80,80,80	0
5	NA	B	337	1/1	0.22	0.68	84,84,84,84	0
5	NA	A	340	1/1	0.23	0.35	86,86,86,86	0
4	D3T	A	336	28/28	0.17	-0.23	41,57,91,99	0
4	D3T	B	336	28/28	0.17	-0.40	47,65,81,85	0
5	NA	A	339	1/1	0.15	-1.05	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NA	B	338	1/1	0.09	-1.32	89,89,89,89	0
5	NA	A	338	1/1	0.06	-1.97	80,80,80,80	0

6.5 Other polymers ⓘ

There are no such residues in this entry.