



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:08 AM UTC

PDB ID : 5ULX / pdb_00005ulx
Title : Structure of human DNA polymerase iota bound to template 1-methyl-deoxy adenosine crystallized in the presence of dCTP
Authors : Jain, R.; Aggarwal, A.K.
Deposited on : 2017-01-25
Resolution : 1.96 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
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

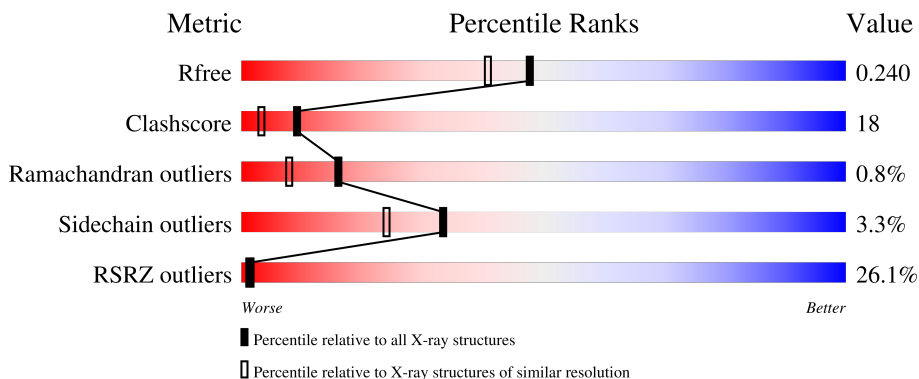
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	P	7	29% 57% 14%
2	T	11	36% 36% 9% 18%
3	A	420	24% 65% 22% • 11%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3442 atoms, of which 26 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 DNA chain called DNA (5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	P	7	Total	C	H	N	O	P	0	0	0
			151	67	12	29	37	6			

- Molecule 2 is a DNA chain called DNA (5'-D(P*(MA7)P*GP*GP*GP*TP*CP*CP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	T	9	Total	C	H	N	O	P	0	0	1
			181	79	14	30	50	8			

- Molecule 3 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	373	Total	C	N	O	S	0	3	0
			2818	1789	490	518	21			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

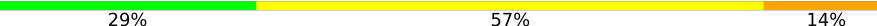
- Molecule 5 is water.

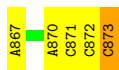
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	13	Total	O	0	0
			13	13		
5	T	21	Total	O	0	0
			21	21		
5	A	257	Total	O	0	0
			257	257		

3 Residue-property plots

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.

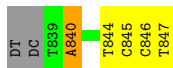
- Molecule 1: DNA (5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3')

Chain P: 



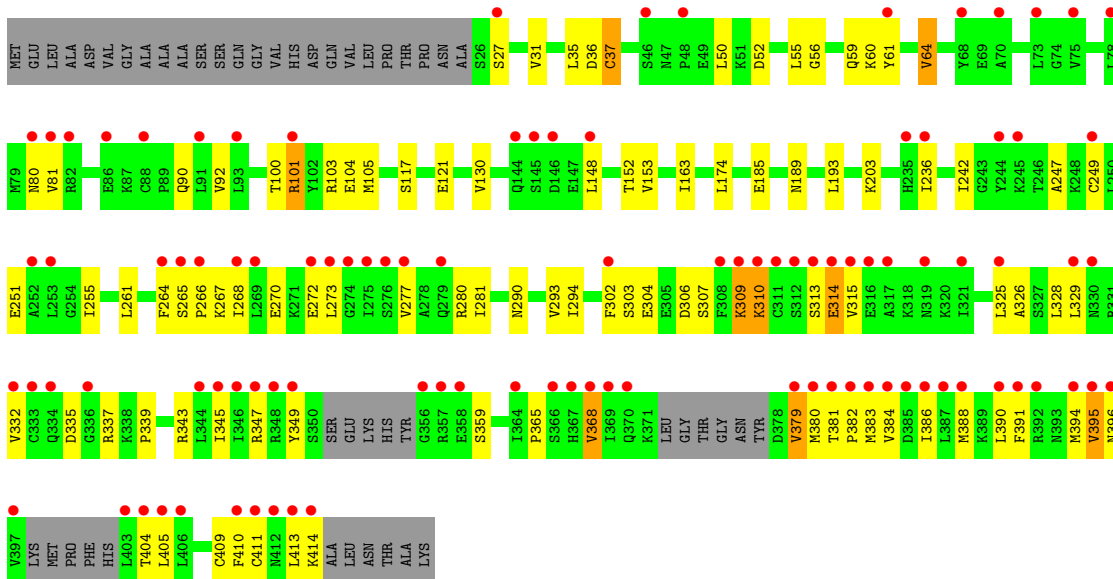
- Molecule 2: DNA (5'-D(P*(MA7)P*GP*GP*GP*TP*CP*CP*T)-3')

Chain T: 



- Molecule 3: DNA polymerase iota

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.92Å 97.92Å 202.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.96 – 1.96 48.96 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.96-1.96) 99.9 (48.96-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.216 , 0.239 0.217 , 0.240	Depositor DCC
R_{free} test set	3153 reflections (7.53%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3442	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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: DOC, MA7, CL

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	P	0.24	0/136	0.35	0/208
2	T	0.29	0/160	0.47	0/245
3	A	0.21	0/2866	0.40	0/3884
All	All	0.21	0/3162	0.40	0/4337

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	P	139	12	79	3	1
2	T	167	14	94	4	1
3	A	2818	0	2794	105	0
4	A	1	0	0	1	0
5	A	257	0	0	17	0
5	P	13	0	0	0	0
5	T	21	0	0	1	0
All	All	3416	26	2967	111	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 18.

All (111) 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:T:840:MA7:O4'	2:T:840:MA7:C4'	1.69	1.21
1:P:873:DOC:O4'	1:P:873:DOC:C1'	1.65	1.18
3:A:409:CYS:SG	5:A:792:HOH:O	2.18	1.00
3:A:290:ASN:ND2	4:A:501:CL:CL	2.37	0.94
3:A:365:PRO:HB2	3:A:368:VAL:HG23	1.57	0.83
3:A:189[B]:ASN:ND2	5:A:605:HOH:O	2.11	0.83
3:A:90:GLN:OE1	3:A:90:GLN:N	2.12	0.80
3:A:251:GLU:OE2	5:A:603:HOH:O	2.00	0.78
3:A:185:GLU:OE1	5:A:602:HOH:O	2.00	0.78
3:A:304:GLU:HG3	3:A:328:LEU:HG	1.67	0.77
3:A:247:ALA:O	3:A:251:GLU:HG3	1.84	0.76
3:A:314:GLU:HG2	3:A:391:PHE:HZ	1.49	0.76
3:A:380:MET:SD	5:A:807:HOH:O	2.46	0.73
3:A:117:SER:OG	5:A:601:HOH:O	1.88	0.71
3:A:326:ALA:HA	3:A:380:MET:HE1	1.70	0.71
3:A:302:PHE:HE1	3:A:413:LEU:HD21	1.55	0.70
3:A:380:MET:O	3:A:384:VAL:HG23	1.91	0.69
3:A:411:CYS:SG	5:A:792:HOH:O	2.51	0.67
3:A:365:PRO:HB2	3:A:368:VAL:CG2	2.24	0.66
3:A:335:ASP:OD2	3:A:337:ARG:HD3	1.94	0.66
3:A:302:PHE:CE1	3:A:413:LEU:HD21	2.30	0.66
3:A:101:ARG:NH2	5:A:610:HOH:O	2.23	0.65
3:A:27:SER:OG	5:A:606:HOH:O	2.14	0.65
3:A:314:GLU:HG2	3:A:391:PHE:CZ	2.31	0.65
3:A:306:ASP:O	3:A:405:LEU:HD12	1.96	0.65
3:A:391:PHE:CZ	3:A:395:VAL:HG11	2.32	0.64
3:A:413:LEU:O	3:A:414:LYS:HG3	1.98	0.63
3:A:236:ILE:CD1	3:A:261:LEU:HB2	2.30	0.62
3:A:343:ARG:HG2	3:A:345:ILE:HD11	1.82	0.62
3:A:347:ARG:HE	3:A:404:THR:HG23	1.65	0.61
3:A:236:ILE:HD12	3:A:255:ILE:HG22	1.83	0.61
3:A:368:VAL:HG12	3:A:383:MET:HE2	1.83	0.60
3:A:236:ILE:HG22	3:A:242:ILE:HG21	1.84	0.59
3:A:265:SER:HB3	3:A:268:ILE:HD13	1.84	0.59
3:A:396:ASN:O	5:A:607:HOH:O	2.17	0.59
2:T:840:MA7:H8	3:A:59:GLN:OE1	2.04	0.58
3:A:61:TYR:C	3:A:81:VAL:HG23	2.30	0.57
3:A:343:ARG:HD2	3:A:359:SER:HB2	1.87	0.57
3:A:326:ALA:CA	3:A:380:MET:HE1	2.34	0.56
3:A:326:ALA:CB	3:A:380:MET:HE1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:265:SER:CB	3:A:268:ILE:HD13	2.34	0.56
3:A:61:TYR:O	3:A:81:VAL:HG23	2.05	0.56
2:T:846:DC:OP1	5:T:901:HOH:O	2.18	0.55
3:A:35:LEU:HD23	5:A:709:HOH:O	2.07	0.55
3:A:384:VAL:O	3:A:388:MET:HG2	2.07	0.55
3:A:325:LEU:HD21	3:A:383:MET:HB2	1.90	0.54
3:A:339:PRO:HG3	3:A:410:PHE:HB3	1.88	0.54
3:A:236:ILE:HD11	3:A:261:LEU:HB2	1.91	0.53
3:A:105:MET:CG	3:A:193:LEU:HD11	2.39	0.53
3:A:280:ARG:NH2	5:A:609:HOH:O	2.20	0.53
3:A:105:MET:HE1	5:A:748:HOH:O	2.10	0.52
3:A:391:PHE:O	3:A:395:VAL:HG12	2.09	0.52
3:A:55:LEU:HD12	3:A:56:GLY:H	1.76	0.51
3:A:236:ILE:HD13	3:A:261:LEU:HB2	1.93	0.51
3:A:27:SER:N	5:A:606:HOH:O	2.33	0.51
3:A:313:SER:C	3:A:315:VAL:H	2.19	0.51
3:A:339:PRO:CG	3:A:410:PHE:HB3	2.41	0.50
3:A:55:LEU:HD12	3:A:56:GLY:N	2.26	0.50
3:A:339:PRO:CB	3:A:410:PHE:HB3	2.42	0.50
3:A:386:ILE:O	3:A:390:LEU:HG	2.12	0.50
3:A:36:ASP:OD1	5:A:608:HOH:O	2.19	0.49
3:A:148:LEU:HD23	3:A:148:LEU:C	2.37	0.49
3:A:36:ASP:O	3:A:37:CYS:C	2.55	0.49
3:A:152:THR:HG22	5:A:656:HOH:O	2.13	0.49
3:A:347:ARG:HB3	3:A:404:THR:HG23	1.95	0.49
1:P:870:DA:H2'	1:P:871:DC:C6	2.48	0.48
3:A:249:CYS:SG	3:A:273:LEU:HD21	2.53	0.48
3:A:329:LEU:HD12	3:A:380:MET:HE2	1.95	0.48
3:A:236:ILE:CG2	3:A:242:ILE:HD13	2.44	0.48
3:A:266:PRO:O	3:A:270:GLU:HG3	2.14	0.47
3:A:103:ARG:HD3	5:A:791:HOH:O	2.13	0.47
3:A:203:LYS:HD3	3:A:293:VAL:HG22	1.96	0.47
3:A:381:THR:OG1	3:A:382:PRO:HD3	2.14	0.47
3:A:329:LEU:O	3:A:332:VAL:HG12	2.15	0.47
3:A:413:LEU:C	3:A:414:LYS:HG3	2.39	0.47
3:A:59:GLN:OE1	3:A:64[B]:VAL:HG11	2.14	0.46
3:A:302:PHE:HE1	3:A:413:LEU:CD2	2.25	0.46
3:A:163:ILE:HG21	3:A:174:LEU:HD11	1.97	0.46
3:A:121:GLU:HB2	3:A:294:ILE:O	2.15	0.46
3:A:310:LYS:HE3	3:A:349:TYR:CB	2.45	0.46
3:A:304:GLU:HG3	3:A:328:LEU:CG	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:345:ILE:N	3:A:345:ILE:HD12	2.30	0.46
3:A:267:LYS:CD	3:A:267:LYS:H	2.27	0.45
3:A:343:ARG:HG2	3:A:345:ILE:CD1	2.46	0.45
3:A:309:LYS:HA	3:A:309:LYS:HD3	1.52	0.45
3:A:105:MET:HG3	3:A:193:LEU:HD11	1.99	0.45
3:A:236:ILE:CD1	3:A:255:ILE:HG22	2.45	0.45
2:T:844:DT:H2''	2:T:845:DC:H5'	1.99	0.45
3:A:60:LYS:HE2	3:A:307:SER:O	2.17	0.44
3:A:255:ILE:HD11	3:A:264:PHE:CG	2.51	0.44
3:A:100:THR:O	3:A:104:GLU:HG3	2.18	0.44
3:A:335:ASP:CG	3:A:337:ARG:HD3	2.42	0.44
3:A:313:SER:O	3:A:315:VAL:N	2.51	0.44
3:A:50:LEU:CD2	3:A:92:VAL:HG11	2.48	0.44
3:A:379:VAL:O	3:A:379:VAL:HG23	2.18	0.44
3:A:268:ILE:HD12	3:A:268:ILE:N	2.33	0.43
3:A:265:SER:OG	3:A:267:LYS:HG2	2.18	0.43
3:A:391:PHE:CE1	3:A:395:VAL:HG11	2.54	0.42
3:A:277:VAL:O	3:A:281:ILE:HG23	2.19	0.42
3:A:325:LEU:O	3:A:329:LEU:HG	2.20	0.42
3:A:329:LEU:HA	3:A:332:VAL:HG12	2.00	0.42
3:A:388:MET:HE3	3:A:388:MET:HA	2.01	0.42
3:A:413:LEU:HD12	3:A:413:LEU:N	2.35	0.42
3:A:339:PRO:HB3	3:A:410:PHE:HB3	2.00	0.41
3:A:379:VAL:O	3:A:383:MET:HG2	2.19	0.41
3:A:31:VAL:CG1	3:A:130:VAL:HB	2.50	0.41
3:A:153:VAL:HB	3:A:174:LEU:HD22	2.03	0.41
3:A:255:ILE:HD11	3:A:264:PHE:CD1	2.56	0.41
3:A:303:SER:O	3:A:304:GLU:HG2	2.21	0.41
1:P:871:DC:H2''	1:P:872:DC:H5'	2.03	0.41
3:A:313:SER:C	3:A:315:VAL:N	2.78	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)
1:P:867:DA:O5'	2:T:847:DT:O3'[10_665]	1.81	0.39

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
3	A	368/420 (88%)	357 (97%)	8 (2%)	3 (1%)	16 8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	37	CYS
3	A	310	LYS
3	A	314	GLU

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
3	A	302/376 (80%)	291 (96%)	11 (4%)	31 21

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	52	ASP
3	A	64[A]	VAL
3	A	64[B]	VAL
3	A	80	ASN
3	A	101	ARG
3	A	272	GLU
3	A	309	LYS
3	A	368	VAL

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Mol	Chain	Res	Type
3	A	379	VAL
3	A	394	MET
3	A	395	VAL

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

Mol	Chain	Res	Type
3	A	217	GLN
3	A	361	GLN

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
1	DOC	P	873	1,2	16,19,20	5.14	12 (75%)	20,26,29	1.10	2 (10%)
2	MA7	T	840	2	19,24,25	3.63	7 (36%)	23,35,38	2.38	12 (52%)

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
1	DOC	P	873	1,2	-	0/7/18/19	0/2/2/2
2	MA7	T	840	2	-	4/7/21/22	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	840	MA7	O4'-C4'	10.82	1.69	1.45
1	P	873	DOC	O4'-C1'	10.39	1.65	1.42
1	P	873	DOC	C2'-C1'	-8.39	1.33	1.52
1	P	873	DOC	O4'-C4'	-7.87	1.29	1.44
2	T	840	MA7	C3'-C4'	-7.06	1.34	1.53
1	P	873	DOC	C2-N3	6.54	1.49	1.36
1	P	873	DOC	C6-C5	6.07	1.49	1.35
1	P	873	DOC	C4-N3	5.33	1.45	1.34
2	T	840	MA7	C6-N6	5.25	1.48	1.33
1	P	873	DOC	C4-N4	4.78	1.45	1.33
2	T	840	MA7	O4'-C1'	-4.69	1.31	1.42
1	P	873	DOC	C2-N1	3.77	1.48	1.40
1	P	873	DOC	C6-N1	3.26	1.45	1.38
1	P	873	DOC	C1'-N1	-2.99	1.40	1.48
2	T	840	MA7	C2'-C1'	2.95	1.60	1.52
1	P	873	DOC	O2-C2	-2.49	1.19	1.23
1	P	873	DOC	C5-C4	2.45	1.48	1.42
2	T	840	MA7	C5-C4	-2.14	1.35	1.39
2	T	840	MA7	C2'-C3'	2.12	1.58	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	840	MA7	C5-C4-N3	-4.63	120.34	126.72
2	T	840	MA7	N9-C8-N7	-4.49	107.57	113.94
2	T	840	MA7	N3-C4-N9	3.73	133.52	127.17
2	T	840	MA7	C4-N9-C8	3.69	109.61	105.74
2	T	840	MA7	C5-C6-N6	-3.69	115.44	123.15
1	P	873	DOC	C4'-O4'-C1'	-2.97	107.00	109.81
2	T	840	MA7	C4'-O4'-C1'	-2.90	102.62	109.51
2	T	840	MA7	C5-N7-C8	2.63	107.58	103.45
2	T	840	MA7	O4'-C1'-C2'	-2.41	101.73	106.25
2	T	840	MA7	C2'-C3'-C4'	2.34	107.55	102.80
2	T	840	MA7	O4'-C1'-N9	2.25	112.01	107.96
1	P	873	DOC	C3'-C2'-C1'	2.25	105.47	102.87
2	T	840	MA7	C6-C5-C4	2.24	120.35	118.14
2	T	840	MA7	C2-N3-C4	2.05	119.07	112.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	840	MA7	O4'-C1'-N9-C4
2	T	840	MA7	O4'-C4'-C5'-O5'
2	T	840	MA7	C3'-C4'-C5'-O5'
2	T	840	MA7	O4'-C1'-N9-C8

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	873	DOC	1	0
2	T	840	MA7	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	P	6/7 (85%)	0.70	0	100 100	33, 47, 50, 56	0
2	T	8/11 (72%)	0.11	0	100 100	31, 37, 46, 63	0
3	A	373/420 (88%)	1.15	101 (27%)	1 1	18, 44, 83, 105	3 (0%)
All	All	387/438 (88%)	1.12	101 (26%)	1 1	18, 44, 82, 105	3 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	349	TYR	6.8
3	A	403	LEU	5.6
3	A	391	PHE	5.2
3	A	395	VAL	5.0
3	A	348	ARG	4.9
3	A	311	CYS	4.6
3	A	315	VAL	4.6
3	A	252	ALA	4.5
3	A	333	CYS	4.4
3	A	302	PHE	4.1
3	A	411	CYS	4.1
3	A	379	VAL	4.0
3	A	397	VAL	4.0
3	A	334	GLN	4.0
3	A	73	LEU	3.8
3	A	235[A]	HIS	3.8
3	A	381	THR	3.8
3	A	244	TYR	3.6
3	A	269	LEU	3.6
3	A	413	LEU	3.6
3	A	396	ASN	3.5
3	A	276	SER	3.5
3	A	385	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
3	A	146	ASP	3.3
3	A	347	ARG	3.3
3	A	386	ILE	3.3
3	A	144	GLN	3.3
3	A	368	VAL	3.2
3	A	313	SER	3.2
3	A	384	VAL	3.2
3	A	273	LEU	3.2
3	A	329	LEU	3.2
3	A	346	ILE	3.1
3	A	356	GLY	3.1
3	A	367	HIS	3.1
3	A	253	LEU	3.1
3	A	332	VAL	3.1
3	A	317	ALA	3.1
3	A	390	LEU	3.1
3	A	309	LYS	3.1
3	A	310	LYS	3.1
3	A	406	LEU	3.0
3	A	75	VAL	2.9
3	A	404	THR	2.9
3	A	405	LEU	2.9
3	A	61	TYR	2.8
3	A	382	PRO	2.8
3	A	88	CYS	2.8
3	A	394	MET	2.8
3	A	412	ASN	2.8
3	A	325	LEU	2.8
3	A	364	ILE	2.8
3	A	268	ILE	2.7
3	A	46	SER	2.7
3	A	81	VAL	2.7
3	A	275	ILE	2.6
3	A	277	VAL	2.6
3	A	380	MET	2.6
3	A	148	LEU	2.5
3	A	321	ILE	2.5
3	A	145	SER	2.5
3	A	383	MET	2.5
3	A	357	ARG	2.5
3	A	314	GLU	2.5
3	A	279	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	358	GLU	2.5
3	A	369	ILE	2.4
3	A	70	ALA	2.4
3	A	245	LYS	2.4
3	A	336	GLY	2.4
3	A	78	LEU	2.4
3	A	387	LEU	2.4
3	A	80	ASN	2.4
3	A	388	MET	2.4
3	A	366	SER	2.4
3	A	68	TYR	2.3
3	A	236	ILE	2.3
3	A	266	PRO	2.3
3	A	414	LYS	2.3
3	A	319	ASN	2.3
3	A	265	SER	2.3
3	A	312	SER	2.3
3	A	86	GLU	2.3
3	A	316	GLU	2.3
3	A	82	ARG	2.2
3	A	410	PHE	2.2
3	A	392	ARG	2.2
3	A	93	LEU	2.2
3	A	27	SER	2.2
3	A	249	CYS	2.2
3	A	330	ASN	2.1
3	A	274	GLY	2.1
3	A	344	LEU	2.1
3	A	264	PHE	2.1
3	A	345	ILE	2.1
3	A	370	GLN	2.1
3	A	308	PHE	2.0
3	A	91	LEU	2.0
3	A	101	ARG	2.0
3	A	272	GLU	2.0
3	A	48	PRO	2.0

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

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
2	MA7	T	840	22/23	0.90	0.15	41,58,72,79	0
1	DOC	P	873	18/19	0.97	0.07	27,34,44,44	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
4	CL	A	501	1/1	0.86	0.12	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.