



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 30, 2025 – 02:07 PM EDT

PDB ID : 9Y74 / pdb_00009y74
Title : [22L-7B C|A] 22 bp L-DNA tensegrity triangle that propagates via blunt-end stacking with C stacking on A at the interface
Authors : Horvath, A.; Woloszyn, K.; Vecchioni, S.; Ohayon, Y.P.; Sha, R.
Deposited on : 2025-09-09
Resolution : 8.76 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

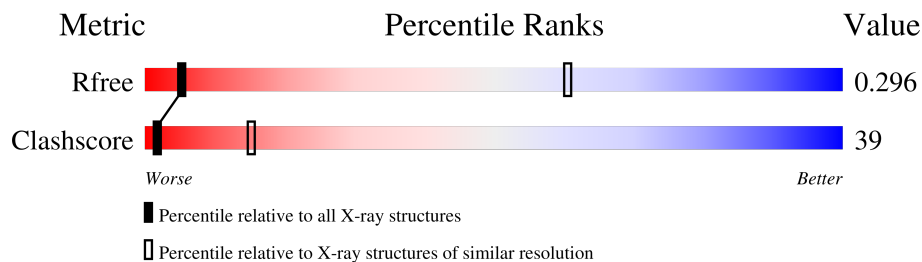
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.76 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}	164625	1107 (10.00-4.00)
Clashscore	180529	1146 (10.00-4.00)

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	22	5%	95%
2	B	7	14%	86%
3	C	7	14%	86%
4	D	8	12%	88%

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
1	ODT	A	111	-	X	-	-
4	ODT	D	102	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ODT	D	105	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 896 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 DNA chain called DNA (5'-D*(0DC)P*(0DG)P*(0DA)P*(0DT)P*(0DG)P*(0DC)P*(0DC)P*(0DT)P*(0DG)P*(0DT)P*(0DA)P*(0DC)P*(0DG)(0DG)P*(0DA)P*(0DC)P*(0DA)P*(0DG)P*(0DA)P*(0DT)P*(0DC)P*(0DA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	22	Total	C	N	O	P	0	0	0
			449	214	86	128	21			

- Molecule 2 is a DNA chain called DNA (5'-D(P*(0DC)P*(0DC)P*(0DG)P*(0DT)P*(0DA)P*(0DC)P*(0DA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	P	0	0	0
			141	67	26	41	7			

- Molecule 3 is a DNA chain called DNA (5'-D(P*(0DG)P*(0DG)P*(0DC)P*(0DA)P*(0DT)P*(0DC)P*(0DG))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	P	0	0	0
			145	68	28	42	7			

- Molecule 4 is a DNA chain called DNA (5'-D*(0DT)P*(0DG)P*(0DA)P*(0DT)P*(0DC)P*(0DT)P*(0DG)P*(0DT))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			161	79	26	49	7			

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*(0DC)P*(0DG)P*(0DA)P*(0DT)P*(0DG)P*(0DC)P*(0DC)P*(0DT)P*(0DG)P*(0DT)P*(0DA)P*(0DC)P*(0DG)(0DG)P*(0DA)P*(0DC)P*(0DA)P*(0DG)P*(0DA)P*(0DT)P*(0DC)P*(0DA))-3')

Chain A: 

G104	G105	A106	T107	G108	G109	C110	T111	G112	T113	A114	C115	G116	G117	A118	C119	A120	G121	A122	T123	C124	A125
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- Molecule 2: DNA (5'-D(P*(0DC)P*(0DC)P*(0DG)P*(0DT)P*(0DA)P*(0DC)P*(0DA))-3')

Chain B: 

G119	C120	G121	T122	A123	C124	A125
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- Molecule 3: DNA (5'-D(P*(0DG)P*(0DG)P*(0DC)P*(0DA)P*(0DT)P*(0DC)P*(0DG))-3')

Chain C: 

G209	G210	C211	A212	T213	C214	G215
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- Molecule 4: DNA (5'-D*(0DT)P*(0DG)P*(0DA)P*(0DT)P*(0DC)P*(0DT)P*(0DG)P*(0DT))-3')

Chain D: 

T102	G103	A104	T105	C106	T107	G108	T109
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4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	130.40Å 130.40Å 61.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.47 – 8.76 56.47 – 8.76	Depositor EDS
% Data completeness (in resolution range)	83.8 (56.47-8.76) 78.8 (56.47-8.76)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 8.36Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.237 , 0.317 0.235 , 0.296	Depositor DCC
R_{free} test set	16 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	-40.3	Xtriage
Anisotropy	1.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	-0.12 , 127.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.07$, $\langle L^2 \rangle = 0.01$	Xtriage
Estimated twinning fraction	0.231 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	896	wwPDB-VP
Average B, all atoms (Å ²)	358.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7941e-03.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0DA, 0DG, 0DT, 0DC

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 [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	449	0	238	29	0
2	B	141	0	75	10	0
3	C	145	0	77	9	0
4	D	161	0	86	14	0
All	All	896	0	476	52	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 39.

The worst 5 of 52 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)
4:D:107:0DT:H73	4:D:107:0DT:H72	1.58	0.85
3:C:209:0DG:H2'	3:C:210:0DG:H8	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:107:0DT:H72	4:D:107:0DT:H71	1.58	0.84
4:D:107:0DT:H73	4:D:107:0DT:H71	1.58	0.83
1:A:125:0DA:H2A	4:D:102:0DT:O2	1.82	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

44 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	ODG	A	108	3,1	18,24,25	4.01	13 (72%)	19,35,38	1.64	4 (21%)
4	ODA	D	104	4	17,23,24	3.74	7 (41%)	17,33,36	3.75	5 (29%)
3	ODC	C	214	3,1	17,20,21	4.40	14 (82%)	23,28,31	1.62	5 (21%)
1	ODT	A	107	1	18,21,22	5.38	15 (83%)	25,30,33	2.56	9 (36%)
1	ODA	A	125	1	17,23,24	3.83	8 (47%)	17,33,36	3.80	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	0DA	A	122	1	17,23,24	3.80	8 (47%)	17,33,36	3.91	3 (17%)
4	0DG	D	103	4,1	18,24,25	3.89	13 (72%)	19,35,38	1.55	4 (21%)
1	0DT	A	111	1	18,21,22	5.30	14 (77%)	25,30,33	2.54	9 (36%)
1	0DT	A	113	1	18,21,22	5.36	15 (83%)	25,30,33	2.58	10 (40%)
3	0DG	C	209	3,1	18,24,25	4.06	13 (72%)	19,35,38	1.73	6 (31%)
1	0DG	A	116	2,1	18,24,25	3.90	13 (72%)	19,35,38	1.92	7 (36%)
3	0DG	C	210	3,1	18,24,25	3.94	12 (66%)	19,35,38	1.91	6 (31%)
3	0DG	C	215	3,1	18,24,25	4.03	13 (72%)	19,35,38	2.47	7 (36%)
1	0DA	A	118	1	17,23,24	3.78	7 (41%)	17,33,36	3.58	4 (23%)
2	0DC	B	124	2,1	17,20,21	4.36	13 (76%)	23,28,31	1.12	2 (8%)
2	0DA	B	123	2	17,23,24	3.82	8 (47%)	17,33,36	3.61	3 (17%)
1	0DC	A	119	1	17,20,21	4.41	14 (82%)	23,28,31	1.60	2 (8%)
1	0DT	A	123	1	18,21,22	5.34	14 (77%)	25,30,33	2.30	9 (36%)
4	0DT	D	102	4	18,18,22	5.26	14 (77%)	26,26,33	2.65	10 (38%)
2	0DG	B	121	2,1	18,24,25	4.03	14 (77%)	19,35,38	2.13	8 (42%)
4	0DC	D	106	4,1	17,20,21	4.54	14 (82%)	23,28,31	1.42	2 (8%)
2	0DC	B	119	2,1	17,20,21	4.38	13 (76%)	23,28,31	1.94	5 (21%)
3	0DT	C	213	3	18,21,22	5.43	14 (77%)	25,30,33	2.55	9 (36%)
4	0DG	D	108	4	18,24,25	4.06	12 (66%)	19,35,38	2.47	8 (42%)
1	0DG	A	105	3,1	18,24,25	3.98	13 (72%)	19,35,38	1.68	5 (26%)
1	0DA	A	114	1	17,23,24	3.72	7 (41%)	17,33,36	3.66	3 (17%)
1	0DC	A	124	4,1	17,20,21	4.29	13 (76%)	23,28,31	1.09	1 (4%)
1	0DA	A	106	1	17,23,24	3.84	9 (52%)	17,33,36	3.48	4 (23%)
3	0DC	C	211	3,1	17,20,21	4.43	14 (82%)	23,28,31	1.33	4 (17%)
4	0DT	D	109	4	18,21,22	5.26	14 (77%)	25,30,33	2.27	8 (32%)
4	0DT	D	107	4	18,21,22	5.40	14 (77%)	25,30,33	2.74	11 (44%)
4	0DT	D	105	4	18,21,22	5.28	14 (77%)	25,30,33	2.59	12 (48%)
1	0DC	A	115	2,1	17,20,21	4.40	14 (82%)	23,28,31	1.56	3 (13%)
1	0DG	A	117	2,1	18,24,25	3.97	13 (72%)	19,35,38	2.07	8 (42%)
1	0DC	A	104	3,1	17,17,21	4.34	13 (76%)	24,24,31	1.35	4 (16%)
2	0DA	B	125	2	17,23,24	3.85	10 (58%)	17,33,36	3.55	5 (29%)
3	0DA	C	212	3	17,23,24	3.78	9 (52%)	17,33,36	3.64	3 (17%)
2	0DT	B	122	2	18,21,22	5.26	14 (77%)	25,30,33	2.50	8 (32%)
2	0DC	B	120	2,1	17,20,21	4.27	13 (76%)	23,28,31	0.86	0
1	0DC	A	110	3,1	17,20,21	4.35	13 (76%)	23,28,31	1.75	6 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	ODG	A	112	2,1	18,24,25	3.87	13 (72%)	19,35,38	1.91	6 (31%)
1	ODC	A	109	3,1	17,20,21	4.33	14 (82%)	23,28,31	1.24	2 (8%)
1	ODG	A	121	4,1	18,24,25	4.00	13 (72%)	19,35,38	1.72	4 (21%)
1	ODA	A	120	1	17,23,24	3.86	9 (52%)	17,33,36	3.78	5 (29%)

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	ODG	A	108	3,1	-	2/3/21/22	0/3/3/3
4	ODA	D	104	4	-	3/3/21/22	0/3/3/3
3	ODC	C	214	3,1	-	3/7/21/22	0/2/2/2
1	ODT	A	107	1	-	2/7/21/22	0/2/2/2
1	ODA	A	125	1	-	2/3/21/22	0/3/3/3
1	ODA	A	122	1	-	0/3/21/22	0/3/3/3
4	ODG	D	103	4,1	-	1/3/21/22	0/3/3/3
1	ODT	A	111	1	-	7/7/21/22	0/2/2/2
1	ODT	A	113	1	-	3/7/21/22	0/2/2/2
3	ODG	C	209	3,1	-	3/3/21/22	0/3/3/3
1	ODG	A	116	2,1	-	2/3/21/22	0/3/3/3
3	ODG	C	210	3,1	-	2/3/21/22	0/3/3/3
3	ODG	C	215	3,1	-	2/3/21/22	0/3/3/3
1	ODA	A	118	1	-	2/3/21/22	0/3/3/3
2	ODC	B	124	2,1	-	0/7/21/22	0/2/2/2
2	ODA	B	123	2	-	0/3/21/22	0/3/3/3
1	ODC	A	119	1	-	7/7/21/22	0/2/2/2
1	ODT	A	123	1	-	2/7/21/22	0/2/2/2
4	ODT	D	102	4	-	6/6/18/22	0/2/2/2
2	ODG	B	121	2,1	-	2/3/21/22	0/3/3/3
4	ODC	D	106	4,1	-	2/7/21/22	0/2/2/2
2	ODC	B	119	2,1	-	4/7/21/22	0/2/2/2
3	ODT	C	213	3	-	2/7/21/22	0/2/2/2
4	ODG	D	108	4	-	2/3/21/22	0/3/3/3
1	ODG	A	105	3,1	-	0/3/21/22	0/3/3/3
1	ODA	A	114	1	-	2/3/21/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	0DC	A	124	4,1	-	6/7/21/22	0/2/2/2
1	0DA	A	106	1	-	2/3/21/22	0/3/3/3
3	0DC	C	211	3,1	-	6/7/21/22	0/2/2/2
4	0DT	D	109	4	-	6/7/21/22	0/2/2/2
4	0DT	D	107	4	-	0/7/21/22	0/2/2/2
4	0DT	D	105	4	-	6/7/21/22	0/2/2/2
1	0DC	A	115	2,1	-	2/7/21/22	0/2/2/2
1	0DG	A	117	2,1	-	3/3/21/22	0/3/3/3
1	0DC	A	104	3,1	-	2/6/18/22	0/2/2/2
2	0DA	B	125	2	-	2/3/21/22	0/3/3/3
3	0DA	C	212	3	-	3/3/21/22	0/3/3/3
2	0DT	B	122	2	-	5/7/21/22	0/2/2/2
2	0DC	B	120	2,1	-	4/7/21/22	0/2/2/2
1	0DC	A	110	3,1	-	2/7/21/22	0/2/2/2
1	0DG	A	112	2,1	-	3/3/21/22	0/3/3/3
1	0DC	A	109	3,1	-	2/7/21/22	0/2/2/2
1	0DG	A	121	4,1	-	2/3/21/22	0/3/3/3
1	0DA	A	120	1	-	0/3/21/22	0/3/3/3

The worst 5 of 541 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	213	0DT	C2'-C3'	-12.31	1.21	1.52
1	A	111	0DT	C2'-C3'	-12.04	1.22	1.52
4	D	107	0DT	C2'-C3'	-11.94	1.22	1.52
2	B	122	0DT	C2'-C3'	-11.93	1.22	1.52
4	D	109	0DT	C2'-C3'	-11.92	1.22	1.52

The worst 5 of 242 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	0DA	C5A-C6A-N6A	12.28	139.01	120.31
1	A	125	0DA	C5A-C6A-N6A	12.25	138.98	120.31
1	A	120	0DA	C5A-C6A-N6A	11.66	138.07	120.31
1	A	114	0DA	C5A-C6A-N6A	11.52	137.86	120.31
1	A	118	0DA	C5A-C6A-N6A	11.17	137.33	120.31

There are no chirality outliers.

5 of 119 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	108	0DG	O4'-C4'-C5'-O5'
1	A	112	0DG	O4'-C4'-C5'-O5'
1	A	118	0DA	O4'-C4'-C5'-O5'
1	A	121	0DG	O4'-C4'-C5'-O5'
2	B	119	0DC	O4'-C4'-C5'-O5'

There are no ring outliers.

40 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	108	0DG	1	0
4	D	104	0DA	1	0
3	C	214	0DC	1	0
1	A	107	0DT	2	0
1	A	125	0DA	2	0
1	A	122	0DA	2	0
4	D	103	0DG	3	0
1	A	111	0DT	1	0
1	A	113	0DT	1	0
3	C	209	0DG	3	0
1	A	116	0DG	3	0
3	C	210	0DG	5	0
1	A	118	0DA	3	0
2	B	124	0DC	1	0
2	B	123	0DA	1	0
1	A	119	0DC	3	0
1	A	123	0DT	1	0
4	D	102	0DT	4	0
2	B	121	0DG	2	0
2	B	119	0DC	3	0
3	C	213	0DT	2	0
4	D	108	0DG	1	0
1	A	105	0DG	4	0
1	A	114	0DA	4	0
1	A	124	0DC	1	0
1	A	106	0DA	6	0
3	C	211	0DC	3	0
4	D	109	0DT	5	0
4	D	107	0DT	3	0
4	D	105	0DT	1	0
1	A	115	0DC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	117	0DG	4	0
1	A	104	0DC	1	0
3	C	212	0DA	2	0
2	B	122	0DT	4	0
2	B	120	0DC	3	0
1	A	110	0DC	1	0
1	A	112	0DG	1	0
1	A	109	0DC	1	0
1	A	120	0DA	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	0/22	-	-	-	-
2	B	0/7	-	-	-	-
3	C	0/7	-	-	-	-
4	D	0/8	-	-	-	-
All	All	0/44	-	-	-	-

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	ODT	A	113	20/21	0.88	0.18	180,193,215,221	0
4	ODG	D	108	22/23	0.93	0.08	214,229,255,261	0
1	ODC	A	124	19/20	0.94	0.07	493,517,534,541	0
4	ODT	D	105	20/21	0.95	0.08	409,426,463,468	0
1	ODT	A	111	20/21	0.95	0.19	230,253,264,269	0
1	ODA	A	118	21/22	0.96	0.12	251,279,294,296	0
1	ODG	A	112	22/23	0.96	0.21	201,222,237,242	0
2	ODA	B	123	21/22	0.96	0.13	221,242,253,264	0
1	ODC	A	109	19/20	0.96	0.09	349,356,401,408	0
1	ODA	A	114	21/22	0.96	0.28	167,182,197,202	0
1	ODG	A	121	22/23	0.97	0.08	314,326,339,344	0
1	ODT	A	123	20/21	0.97	0.12	376,422,433,434	0
1	ODC	A	104	16/20	0.97	0.09	366,403,413,414	0
1	ODC	A	115	19/20	0.97	0.22	180,198,212,213	0
3	ODG	C	210	22/23	0.97	0.09	323,334,340,349	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	0DA	C	212	21/22	0.97	0.13	533,551,567,578	0
4	0DG	D	103	22/23	0.97	0.07	505,531,578,592	0
1	0DG	A	116	22/23	0.97	0.12	192,218,228,236	0
4	0DT	D	107	20/21	0.97	0.05	243,265,285,294	0
1	0DA	A	106	21/22	0.97	0.13	459,469,487,487	0
4	0DT	D	109	20/21	0.97	0.06	182,194,211,211	0
2	0DG	B	121	22/23	0.98	0.07	194,220,238,247	0
2	0DT	B	122	20/21	0.98	0.07	209,231,246,255	0
1	0DG	A	108	22/23	0.98	0.07	507,521,547,567	0
2	0DC	B	124	19/20	0.98	0.13	229,242,250,260	0
2	0DA	B	125	21/22	0.98	0.10	252,261,270,280	0
3	0DG	C	209	22/23	0.98	0.09	304,318,351,360	0
1	0DA	A	120	21/22	0.98	0.07	275,293,327,340	0
3	0DC	C	211	19/20	0.98	0.14	405,447,451,452	0
1	0DG	A	105	22/23	0.98	0.11	446,474,485,493	0
1	0DA	A	122	21/22	0.98	0.11	339,355,371,378	0
4	0DA	D	104	21/22	0.98	0.06	477,498,546,569	0
1	0DC	A	110	19/20	0.98	0.09	281,299,310,311	0
4	0DC	D	106	19/20	0.98	0.05	420,435,465,477	0
1	0DG	A	117	22/23	0.98	0.07	198,226,250,253	0
2	0DC	B	119	19/20	0.98	0.13	180,186,199,202	0
2	0DC	B	120	19/20	0.98	0.06	186,209,219,221	0
1	0DC	A	119	19/20	0.99	0.20	249,268,285,291	0
1	0DT	A	107	20/21	0.99	0.17	466,483,514,527	0
3	0DT	C	213	20/21	0.99	0.09	551,574,596,598	0
3	0DG	C	215	22/23	0.99	0.07	592,613,637,656	0
4	0DT	D	102	17/21	0.99	0.05	527,548,598,607	0
1	0DA	A	125	21/22	0.99	0.10	561,604,623,626	0
3	0DC	C	214	19/20	1.00	0.07	567,580,600,607	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.