



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:31 AM UTC

PDB ID : 7UYN / pdb_00007uyn
Title : Crystal structure of B-form alien DNA 5'-CTTBPPBBSSZZSAAG in a host-guest complex with the N-terminal fragment of Moloney murine leukemia virus reverse transcriptase
Authors : Georgiadis, M.M.
Deposited on : 2022-05-06
Resolution : 1.65 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

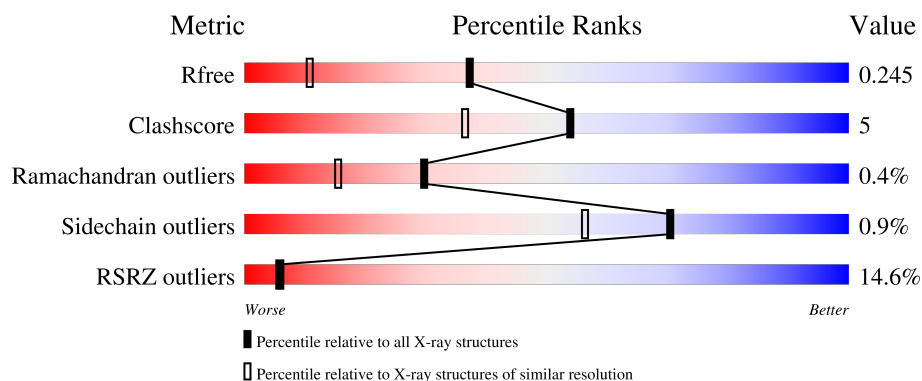
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	266	14% 80% 12% 7%
2	B	8	88% 12%
3	G	8	25% 75%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2476 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 reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1988	1280	346	355	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	expression tag	UNP Q8UN00
A	21	SER	-	expression tag	UNP Q8UN00
A	22	HIS	-	expression tag	UNP Q8UN00
A	23	MET	-	expression tag	UNP Q8UN00
A	249	ASN	ASP	conflict	UNP Q8UN00
A	279	LEU	-	expression tag	UNP Q8UN00
A	280	THR	-	expression tag	UNP Q8UN00
A	281	ARG	-	expression tag	UNP Q8UN00
A	282	GLY	-	expression tag	UNP Q8UN00
A	283	SER	-	expression tag	UNP Q8UN00
A	284	GLY	-	expression tag	UNP Q8UN00
A	285	CYS	-	expression tag	UNP Q8UN00

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*TP*(IGU)P*(1WA)P*(1WA)P*(IGU)P*(IGU))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	P	0	0	0
			166	79	32	48	7			

- Molecule 3 is a DNA chain called DNA (5'-D(P*(JSP)P*(JSP)P*(1W5)P*(1W5)P*(JSP)P*AP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	8	Total	C	N	O	P	0	0	0
			168	80	30	50	8			

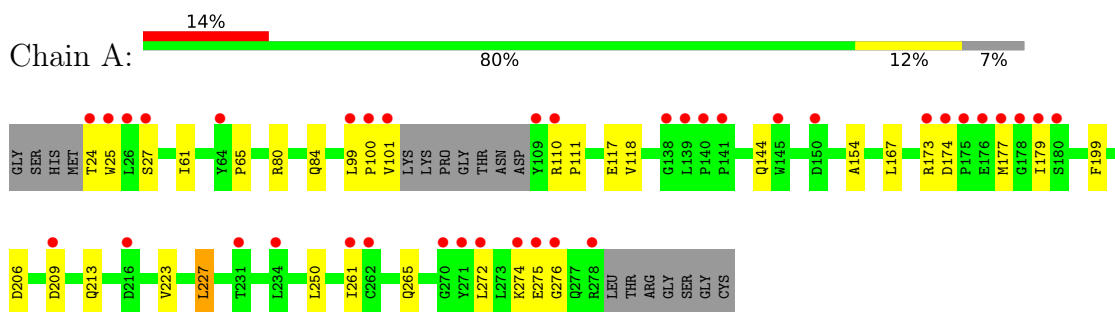
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	152	Total 152	O 152	0	0
4	G	2	Total 2	O 2	0	0

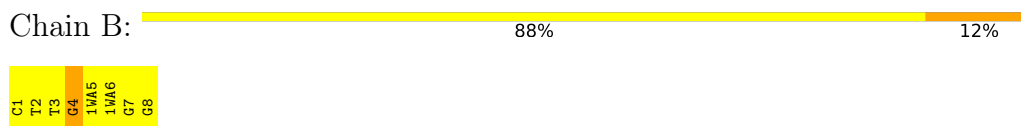
3 Residue-property plots

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: reverse transcriptase



- Molecule 2: DNA (5'-D(*CP*TP*TP*(IGU)P*(1WA)P*(1WA)P*(IGU)P*(IGU))-3')



- Molecule 3: DNA (5'-D(P*(JSP)P*(JSP)P*(1W5)P*(1W5)P*(JSP)P*AP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	54.85Å 146.48Å 46.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.46 – 1.65 30.46 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.46-1.65) 99.8 (30.46-1.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.222 , 0.246 0.223 , 0.245	Depositor DCC
R_{free} test set	2216 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2476	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JSP, IGU, 1WA, 1W5

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	0.32	0/2042	0.54	0/2784
2	B	0.31	0/61	0.56	0/92
3	G	0.30	0/72	0.47	0/109
All	All	0.32	0/2175	0.54	0/2985

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	1988	0	2002	20	0
2	B	166	0	94	2	0
3	G	168	0	56	1	0
4	A	152	0	0	0	0
4	G	2	0	0	0	0
All	All	2476	0	2152	22	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 5.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:HG3	1:A:111:PRO:HD2	1.64	0.78
1:A:24:THR:HG23	1:A:27:SER:H	1.60	0.65
1:A:274:LYS:HG2	1:A:275:GLU:HG3	1.82	0.62
1:A:265:GLN:HG3	1:A:272:LEU:HD11	1.87	0.56
1:A:65:PRO:HA	1:A:173:ARG:HH22	1.72	0.55
1:A:65:PRO:HA	1:A:173:ARG:NH2	2.23	0.54
1:A:118:VAL:HG13	1:A:167:LEU:HD22	1.89	0.54
1:A:206:ASP:HB3	1:A:250:LEU:HD13	1.90	0.52
1:A:209:ASP:O	1:A:213:GLN:HG2	2.10	0.51
1:A:174:ASP:HB3	1:A:177:MET:HB3	1.94	0.50
1:A:110:ARG:HG3	1:A:111:PRO:CD	2.40	0.49
1:A:227:LEU:C	1:A:227:LEU:HD23	2.37	0.49
1:A:144:GLN:HE22	1:A:276:GLY:N	2.11	0.48
1:A:61:ILE:HD11	1:A:117:GLU:HG3	1.98	0.46
1:A:25:TRP:CE2	1:A:261:ILE:HG21	2.52	0.44
1:A:173:ARG:HA	1:A:179:ILE:O	2.16	0.44
1:A:99:LEU:HD11	3:G:16:DG:C6	2.53	0.44
2:B:3:DT:H2''	2:B:4:IGU:C8	2.47	0.44
1:A:80:ARG:O	1:A:84:GLN:HG3	2.19	0.43
1:A:154:ALA:HB1	1:A:199:PHE:CZ	2.55	0.42
2:B:1:DC:H2'	2:B:2:DT:C6	2.56	0.41
1:A:99:LEU:HA	1:A:100:PRO:HD3	1.98	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	244/266 (92%)	242 (99%)	1 (0%)	1 (0%)	30 15

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	VAL

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	218/232 (94%)	216 (99%)	2 (1%)	70 56

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	VAL
1	A	227	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	84	GLN
1	A	144	GLN
1	A	214	HIS
1	A	238	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

10 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
3	1W5	G	11	3	19,23,24	1.70	6 (31%)	18,33,36	3.26	7 (38%)
2	IGU	B	7	2	21,24,25	2.75	10 (47%)	29,35,38	1.74	8 (27%)
3	JSP	G	13	3	17,21,22	1.99	4 (23%)	20,30,33	1.30	3 (15%)
2	IGU	B	8	2,3	21,24,25	2.78	10 (47%)	29,35,38	1.58	4 (13%)
3	1W5	G	12	3	19,23,24	1.66	5 (26%)	18,33,36	2.92	5 (27%)
3	JSP	G	10	3	17,21,22	1.99	4 (23%)	20,30,33	1.18	2 (10%)
3	JSP	G	9	2,3	17,21,22	2.02	4 (23%)	20,30,33	1.22	2 (10%)
2	IGU	B	4	2	21,24,25	2.78	10 (47%)	29,35,38	1.77	9 (31%)
2	1WA	B	6	2	16,24,25	0.98	2 (12%)	16,35,38	1.93	3 (18%)
2	1WA	B	5	2	16,24,25	0.98	1 (6%)	16,35,38	1.84	2 (12%)

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
3	1W5	G	11	3	-	4/8/25/26	0/2/2/2
2	IGU	B	7	2	-	2/7/21/22	0/3/3/3
3	JSP	G	13	3	-	1/6/21/22	0/2/2/2
2	IGU	B	8	2,3	-	2/7/21/22	0/3/3/3
3	1W5	G	12	3	-	6/8/25/26	0/2/2/2
3	JSP	G	10	3	-	4/6/21/22	0/2/2/2
3	JSP	G	9	2,3	-	2/6/21/22	0/2/2/2
2	IGU	B	4	2	-	2/7/21/22	0/3/3/3
2	1WA	B	6	2	-	2/5/21/22	0/2/3/3
2	1WA	B	5	2	-	0/5/21/22	0/2/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	IGU	C5-N7	-6.66	1.25	1.39
2	B	7	IGU	C5-N7	-6.62	1.25	1.39
2	B	8	IGU	C5-N7	-6.50	1.26	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	IGU	C4-N9	-4.92	1.25	1.38
2	B	7	IGU	C4-N9	-4.76	1.25	1.38
2	B	4	IGU	C8-N9	-4.69	1.27	1.37
2	B	8	IGU	C8-N9	-4.62	1.27	1.37
2	B	4	IGU	C4-N9	-4.56	1.26	1.38
2	B	7	IGU	C8-N9	-4.53	1.27	1.37
3	G	13	JSP	C4-N3	-4.47	1.27	1.36
3	G	9	JSP	C4-N3	-4.46	1.27	1.36
3	G	13	JSP	C2-N3	-4.45	1.27	1.34
3	G	9	JSP	C2-N3	-4.42	1.27	1.34
3	G	10	JSP	C2-N3	-4.36	1.27	1.34
3	G	10	JSP	C4-N3	-4.35	1.27	1.36
3	G	9	JSP	C1'-C1	4.32	1.57	1.50
3	G	10	JSP	C1'-C1	4.29	1.57	1.50
3	G	13	JSP	C1'-C1	4.08	1.56	1.50
2	B	4	IGU	C6-N6	-4.07	1.25	1.34
2	B	8	IGU	C6-N6	-3.97	1.25	1.34
2	B	7	IGU	C6-N6	-3.90	1.25	1.34
3	G	11	1W5	C6-C1	-3.74	1.33	1.39
3	G	12	1W5	C6-C1	-3.71	1.33	1.39
2	B	8	IGU	C2-N3	-3.70	1.28	1.36
2	B	7	IGU	C2-N3	-3.59	1.28	1.36
2	B	4	IGU	C2-N3	-3.50	1.28	1.36
2	B	4	IGU	C5-C6	-3.37	1.33	1.40
3	G	11	1W5	C1-C1'	-3.34	1.44	1.52
2	B	7	IGU	C5-C6	-3.33	1.33	1.40
3	G	12	1W5	C1-C1'	-3.27	1.44	1.52
2	B	8	IGU	C5-C6	-3.26	1.33	1.40
2	B	8	IGU	C4-N3	-3.16	1.26	1.33
2	B	4	IGU	C4-N3	-3.14	1.26	1.33
2	B	7	IGU	C4-N3	-3.03	1.27	1.33
2	B	7	IGU	C8-N7	-2.85	1.24	1.32
2	B	8	IGU	C1'-N9	-2.78	1.41	1.48
2	B	4	IGU	C1'-N9	-2.77	1.41	1.48
2	B	4	IGU	C8-N7	-2.74	1.24	1.32
2	B	8	IGU	C8-N7	-2.72	1.24	1.32
2	B	7	IGU	C1'-N9	-2.70	1.41	1.48
2	B	5	1WA	C4-N3	-2.67	1.30	1.35
3	G	9	JSP	C2-N2	-2.63	1.27	1.34
3	G	13	JSP	C2-N2	-2.51	1.27	1.34
3	G	10	JSP	C2-N2	-2.50	1.27	1.34
2	B	6	1WA	C4-N3	-2.48	1.30	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	12	1W5	C6-C5	2.34	1.43	1.39
3	G	11	1W5	ON2-N	-2.27	1.20	1.35
3	G	11	1W5	C6-C5	2.27	1.43	1.39
3	G	12	1W5	ON2-N	-2.24	1.20	1.35
2	B	6	1WA	C8-N9	2.11	1.40	1.38
3	G	11	1W5	O2-C2	-2.10	1.19	1.29
2	B	8	IGU	C5-C4	-2.09	1.33	1.42
3	G	12	1W5	O2-C2	-2.07	1.19	1.29
2	B	7	IGU	C5-C4	-2.06	1.33	1.42
2	B	4	IGU	C5-C4	-2.03	1.34	1.42
3	G	11	1W5	C2-N3	2.01	1.41	1.36

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	11	1W5	C4-N3-C2	8.61	126.93	116.98
3	G	12	1W5	C4-N3-C2	8.60	126.92	116.98
3	G	11	1W5	C3'-C2'-C1'	6.64	108.96	102.73
2	B	6	1WA	O6-C6-N1	6.19	128.12	115.34
2	B	5	1WA	O6-C6-N1	6.00	127.74	115.34
3	G	12	1W5	C3'-C2'-C1'	5.90	108.26	102.73
3	G	11	1W5	C2'-C1'-C1	-4.78	107.87	114.72
3	G	11	1W5	O4'-C1'-C1	4.68	114.29	109.77
2	B	8	IGU	C2'-C1'-N9	4.48	125.00	113.81
2	B	7	IGU	C2'-C1'-N9	4.34	124.66	113.81
2	B	4	IGU	C2'-C1'-N9	4.16	124.22	113.81
2	B	4	IGU	N9-C4-N3	3.48	135.00	127.05
3	G	12	1W5	O4'-C1'-C2'	-3.33	98.17	103.50
2	B	7	IGU	N9-C4-N3	3.26	134.48	127.05
2	B	4	IGU	C5-C4-N3	-3.19	121.05	127.60
3	G	9	JSP	C1-C2-N2	-3.13	116.99	121.39
2	B	7	IGU	C5-C6-N6	-3.07	120.75	124.66
2	B	4	IGU	C5-C6-N6	-3.05	120.78	124.66
3	G	12	1W5	C2'-C1'-C1	-2.99	110.44	114.72
2	B	8	IGU	N9-C4-N3	2.98	133.86	127.05
3	G	11	1W5	C2'-C3'-C4'	-2.97	96.78	102.80
3	G	12	1W5	O4'-C1'-C1	2.89	112.56	109.77
3	G	10	JSP	C1-C2-N2	-2.87	117.35	121.39
2	B	8	IGU	C5-C6-N6	-2.84	121.05	124.66
2	B	4	IGU	C1'-N9-C8	-2.83	121.56	127.91
2	B	7	IGU	C5-C4-N3	-2.81	121.83	127.60
2	B	5	1WA	N3-C2-N1	2.78	128.40	123.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	13	JSP	C1-C2-N2	-2.68	117.62	121.39
3	G	13	JSP	C1'-C1-C2	2.67	124.14	118.73
2	B	6	1WA	N3-C2-N1	2.67	128.21	123.32
2	B	8	IGU	C5-C4-N3	-2.61	122.25	127.60
3	G	10	JSP	C1'-C1-C2	2.52	123.83	118.73
2	B	7	IGU	C3'-C2'-C1'	-2.51	96.46	102.60
3	G	11	1W5	O4'-C1'-C2'	-2.51	99.50	103.50
2	B	4	IGU	C6-C5-N7	-2.50	127.14	130.21
2	B	4	IGU	C6-C5-C4	2.38	121.27	117.72
2	B	7	IGU	C1'-N9-C8	-2.27	122.82	127.91
3	G	11	1W5	C5-C6-C1	2.23	122.77	119.51
2	B	7	IGU	C6-C5-N7	-2.16	127.56	130.21
2	B	4	IGU	C4-N3-C2	2.11	121.42	116.85
2	B	7	IGU	C4-N3-C2	2.11	121.42	116.85
2	B	4	IGU	C1'-N9-C4	2.09	131.14	125.50
3	G	13	JSP	O4-C4-N5	2.09	121.28	118.76
3	G	9	JSP	C1'-C1-C2	2.08	122.93	118.73
2	B	6	1WA	C1'-N9-C8	2.02	126.99	124.37

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	7	IGU	O4'-C4'-C5'-O5'
3	G	12	1W5	C2-C1-C1'-C2'
3	G	12	1W5	C2-C1-C1'-O4'
3	G	12	1W5	C6-C1-C1'-C2'
3	G	12	1W5	C6-C1-C1'-O4'
2	B	7	IGU	C3'-C4'-C5'-O5'
2	B	8	IGU	C3'-C4'-C5'-O5'
3	G	11	1W5	C3'-C4'-C5'-O5'
3	G	11	1W5	O4'-C4'-C5'-O5'
2	B	8	IGU	O4'-C4'-C5'-O5'
3	G	10	JSP	O4'-C4'-C5'-O5'
3	G	12	1W5	O4'-C4'-C5'-O5'
3	G	12	1W5	C3'-C4'-C5'-O5'
2	B	6	1WA	O4'-C4'-C5'-O5'
3	G	10	JSP	C3'-C4'-C5'-O5'
2	B	4	IGU	O4'-C4'-C5'-O5'
2	B	6	1WA	C3'-C4'-C5'-O5'
2	B	4	IGU	C3'-C4'-C5'-O5'
3	G	9	JSP	C2-C1-C1'-O4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	10	JSP	C2-C1-C1'-O4'
3	G	9	JSP	C6-C1-C1'-O4'
3	G	10	JSP	C6-C1-C1'-O4'
3	G	13	JSP	O4'-C4'-C5'-O5'
3	G	11	1W5	C2-C1-C1'-O4'
3	G	11	1W5	C2-C1-C1'-C2'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	IGU	1	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

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	248/266 (93%)	0.81	37 (14%) 5 6	15, 26, 49, 76	0
2	B	3/8 (37%)	0.69	0 100 100	38, 38, 41, 47	0
3	G	3/8 (37%)	0.70	0 100 100	30, 30, 42, 51	0
All	All	254/282 (90%)	0.81	37 (14%) 6 6	15, 27, 49, 76	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	ILE	9.6
1	A	101	VAL	7.9
1	A	173	ARG	4.5
1	A	174	ASP	4.4
1	A	177	MET	4.0
1	A	175	PRO	3.9
1	A	109	TYR	3.8
1	A	176	GLU	3.5
1	A	64	TYR	3.4
1	A	100	PRO	3.2
1	A	216	ASP	3.2
1	A	278	ARG	3.1
1	A	276	GLY	3.1
1	A	262	CYS	3.0
1	A	180	SER	2.9
1	A	140	PRO	2.9
1	A	99	LEU	2.9
1	A	27	SER	2.8
1	A	178	GLY	2.8
1	A	24	THR	2.8
1	A	139	LEU	2.7
1	A	270	GLY	2.6
1	A	26	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	141	PRO	2.6
1	A	275	GLU	2.5
1	A	272	LEU	2.5
1	A	234	LEU	2.5
1	A	274	LYS	2.4
1	A	150	ASP	2.4
1	A	138	GLY	2.4
1	A	110	ARG	2.3
1	A	231	THR	2.3
1	A	261	ILE	2.3
1	A	209	ASP	2.3
1	A	25	TRP	2.2
1	A	145	TRP	2.2
1	A	271	TYR	2.1

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
3	JSP	G	10	20/21	0.58	0.21	69,78,93,94	0
3	1W5	G	12	22/23	0.60	0.20	59,65,76,82	0
3	1W5	G	11	22/23	0.62	0.18	65,72,85,90	0
2	1WA	B	6	22/23	0.68	0.20	62,68,77,78	0
2	IGU	B	8	22/23	0.69	0.21	66,70,79,81	0
2	IGU	B	7	22/23	0.70	0.17	63,69,77,80	0
3	JSP	G	13	20/21	0.71	0.18	53,58,72,74	0
3	JSP	G	9	20/21	0.73	0.19	68,81,86,90	0
2	1WA	B	5	22/23	0.76	0.16	57,64,71,73	0
2	IGU	B	4	22/23	0.83	0.13	52,55,59,67	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.