W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 10:28 AM EDT

PDB ID	:	1XUX
Title	:	Structural rationalization of a large difference in RNA affinity despite a small difference in chemistry between two 2'-O-modified nucleic acid analogs
Authors	:	Pattanayek, R.; Sethaphong, L.; Pan, C.; Prhavc, M.; Prakash, T.P.; Manoharan, M.; Egli, M.
Deposited on	:	2004-10-26
Resolution	:	1.30 Å(reported)

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

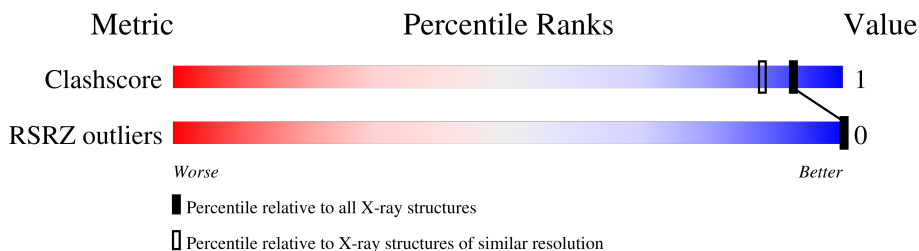|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
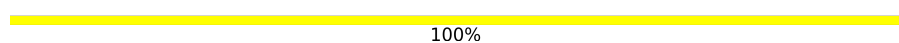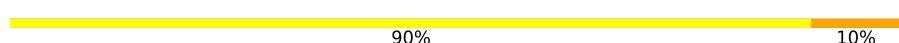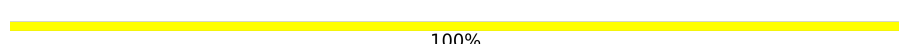*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.30 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	Percentile Ranks	Value
Clashscore		1
RSRZ outliers		0

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1101 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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	10	90% 10%
1	B	10	100%
1	C	10	90% 10%
1	D	10	100%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 1158 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(*GP*CP*GP*TP*AP*(NMS)P*AP*CP*GP *C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	10	Total	C	N	O	P	0	1	0
			214	103	40	62	9			
1	B	10	Total	C	N	O	P	0	4	0
			224	104	40	69	11			
1	C	10	Total	C	N	O	P	0	0	0
			208	100	39	60	9			
1	D	10	Total	C	N	O	P	0	0	0
			208	100	39	60	9			
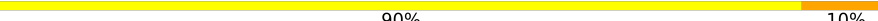
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		
2	B	75	Total	O	0	3
			78	78		
2	C	89	Total	O	0	2
			91	91		
2	D	69	Total	O	0	2
			71	71		

3 Residue-property plots ⓘ
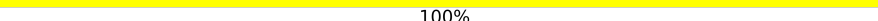
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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(*GP*CP*GP*TP*AP*(NMS)P*AP*CP*GP*C)-3')

Chain A:
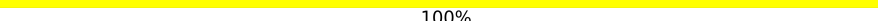
• Molecule 1: DNA (5'-D(*GP*CP*GP*TP*AP*(NMS)P*AP*CP*GP*C)-3')

Chain B:

• Molecule 1: DNA (5'-D(*GP*CP*GP*TP*AP*(NMS)P*AP*CP*GP*C)-3')

Chain C:

• Molecule 1: DNA (5'-D(*GP*CP*GP*TP*AP*(NMS)P*AP*CP*GP*C)-3')

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	27.06Å 44.61Å 44.11Å 90.00° 99.26° 90.00°	Depositor
Resolution (Å)	30.00 – 1.30 9.95 – 1.34	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.30) 92.6 (9.95-1.34)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.27 (at 1.34Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.127 , 0.194 0.125 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.4	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 63.2	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	1158	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: NMS

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	2.86	14/203 (6.9%)	2.79	22/309 (7.1%)
1	B	2.65	18/270 (6.7%)	2.99	34/412 (8.3%)
1	C	2.57	13/203 (6.4%)	2.62	17/309 (5.5%)
1	D	2.74	12/203 (5.9%)	2.84	24/309 (7.8%)
All	All	2.70	57/879 (6.5%)	2.83	97/1339 (7.2%)

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	DG	C2'-C1'	-12.53	1.39	1.52
1	A	10	DC	C2'-C1'	-11.28	1.41	1.52
1	D	309	DG	C2'-C1'	-11.18	1.41	1.52
1	C	202	DC	C2'-C1'	-10.11	1.42	1.52
1	B	104	DT	C2'-C1'	-10.03	1.42	1.52
1	A	4	DT	C2'-C1'	-9.83	1.42	1.52
1	C	203	DG	C2'-C1'	-9.40	1.42	1.52
1	B	107	DA	C2'-C1'	-9.32	1.43	1.52
1	A	1	DG	C2'-C1'	-9.17	1.43	1.52
1	C	209	DG	C2'-C1'	-9.16	1.43	1.52
1	D	301	DG	C2'-C1'	-9.14	1.43	1.52
1	B	103	DG	C2'-C1'	-8.98	1.43	1.52
1	A	2	DC	C2'-C1'	-8.89	1.43	1.52
1	C	204	DT	C2'-C1'	-8.87	1.43	1.52
1	A	3	DG	C2'-C1'	-8.63	1.43	1.52
1	D	304	DT	C2'-C1'	-8.42	1.43	1.52
1	A	5	DA	C2'-C1'	-8.35	1.43	1.52
1	D	310	DC	C2'-C1'	-8.34	1.44	1.52
1	B	101	DG	O3'-P	-8.27	1.51	1.61
1	D	309	DG	O4'-C1'	8.20	1.52	1.42
1	C	201	DG	C2'-C1'	-8.14	1.44	1.52
1	B	105	DA	C2'-C1'	-7.74	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	DG	C2'-C1'	-7.67	1.44	1.52
1	A	7	DA	C2'-C1'	-7.55	1.44	1.52
1	C	202	DC	O4'-C1'	7.38	1.51	1.42
1	B	108[A]	DC	C2'-C1'	-7.34	1.45	1.52
1	B	108[B]	DC	C2'-C1'	-7.34	1.45	1.52
1	D	305	DA	C2'-C1'	-7.20	1.45	1.52
1	B	109[A]	DG	C2'-C1'	-7.17	1.45	1.52
1	B	109[B]	DG	C2'-C1'	-7.17	1.45	1.52
1	B	103	DG	O4'-C1'	7.14	1.50	1.42
1	A	9	DG	O4'-C1'	7.01	1.50	1.42
1	B	110	DC	C2'-C1'	-6.85	1.45	1.52
1	D	303	DG	C2'-C1'	-6.81	1.45	1.52
1	B	102[A]	DC	C2'-C1'	-6.53	1.45	1.52
1	B	102[B]	DC	C2'-C1'	-6.53	1.45	1.52
1	C	207	DA	C2'-C1'	-6.47	1.45	1.52
1	D	302	DC	C2'-C1'	-6.46	1.45	1.52
1	C	210	DC	C2'-C1'	-6.31	1.46	1.52
1	C	205	DA	C2'-C1'	-6.22	1.46	1.52
1	D	309	DG	C6-O6	-6.16	1.18	1.24
1	C	208	DC	C2'-C1'	-6.09	1.46	1.52
1	A	10	DC	O4'-C1'	5.92	1.49	1.42
1	D	308	DC	C2'-C1'	-5.80	1.46	1.52
1	D	303	DG	O3'-P	-5.79	1.54	1.61
1	D	307	DA	C2'-C1'	-5.78	1.46	1.52
1	A	2	DC	O4'-C1'	5.76	1.49	1.42
1	B	110	DC	C3'-C2'	-5.71	1.45	1.52
1	A	1	DG	O3'-P	-5.71	1.54	1.61
1	B	101	DG	O4'-C1'	5.62	1.49	1.42
1	B	104	DT	O4'-C1'	5.51	1.48	1.42
1	C	203	DG	O4'-C1'	5.47	1.48	1.42
1	A	2	DC	O3'-P	-5.46	1.54	1.61
1	C	204	DT	O4'-C1'	5.34	1.48	1.42
1	C	202	DC	C3'-C2'	-5.26	1.46	1.52
1	B	110	DC	P-O5'	-5.04	1.54	1.59
1	A	4	DT	O4'-C1'	5.04	1.48	1.42

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	DG	P-O3'-C3'	16.36	139.33	119.70
1	B	103	DG	O4'-C1'-N9	-12.61	99.18	108.00
1	B	101	DG	O4'-C1'-N9	-12.53	99.23	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	309	DG	O4'-C1'-N9	-12.52	99.24	108.00
1	C	209	DG	O4'-C1'-N9	-12.17	99.48	108.00
1	C	203	DG	O4'-C1'-N9	-11.91	99.66	108.00
1	D	310	DC	O4'-C1'-N1	-11.18	100.17	108.00
1	B	107	DA	O4'-C1'-N9	-10.81	100.43	108.00
1	A	9	DG	O4'-C1'-N9	-10.74	100.48	108.00
1	B	102[A]	DC	N3-C4-C5	-10.65	117.64	121.90
1	B	102[B]	DC	N3-C4-C5	-10.65	117.64	121.90
1	A	10	DC	O4'-C1'-N1	-10.61	100.57	108.00
1	D	301	DG	O4'-C1'-N9	-10.49	100.65	108.00
1	C	204	DT	O4'-C1'-N1	-9.59	101.29	108.00
1	A	5	DA	O4'-C1'-N9	-9.57	101.30	108.00
1	C	202	DC	O4'-C1'-N1	-9.46	101.38	108.00
1	A	3	DG	O4'-C1'-N9	-9.29	101.50	108.00
1	D	303	DG	O4'-C4'-C3'	-9.12	100.53	106.00
1	D	308	DC	C6-N1-C2	9.11	123.94	120.30
1	A	2	DC	O4'-C1'-N1	-8.84	101.81	108.00
1	B	102[A]	DC	C2-N3-C4	8.54	124.17	119.90
1	B	102[B]	DC	C2-N3-C4	8.54	124.17	119.90
1	C	201	DG	O4'-C1'-N9	-8.45	102.09	108.00
1	B	107	DA	O4'-C4'-C3'	-8.40	100.96	106.00
1	A	1	DG	O4'-C1'-N9	-8.19	102.27	108.00
1	D	303	DG	O4'-C1'-N9	-8.16	102.29	108.00
1	D	304	DT	O4'-C4'-C3'	-8.01	101.19	106.00
1	A	10	DC	C6-N1-C2	7.97	123.49	120.30
1	C	208	DC	O4'-C4'-C3'	-7.89	101.27	106.00
1	A	8	DC	O4'-C4'-C3'	-7.87	101.28	106.00
1	B	108[A]	DC	C2-N3-C4	7.51	123.66	119.90
1	B	108[B]	DC	C2-N3-C4	7.51	123.66	119.90
1	D	309	DG	C4-C5-N7	-7.36	107.86	110.80
1	D	310	DC	N1-C2-O2	7.30	123.28	118.90
1	B	104	DT	O4'-C4'-C3'	-7.24	101.60	104.50
1	C	202	DC	N3-C4-C5	-7.18	119.03	121.90
1	A	7	DA	O4'-C4'-C3'	-7.11	101.66	104.50
1	A	1	DG	O4'-C4'-C3'	-7.05	101.68	104.50
1	C	205	DA	N1-C2-N3	-7.04	125.78	129.30
1	C	202	DC	C2-N3-C4	6.76	123.28	119.90
1	D	309	DG	C6-C5-N7	6.75	134.45	130.40
1	A	4	DT	O4'-C4'-C3'	-6.63	101.85	104.50
1	B	104	DT	O4'-C1'-N1	-6.57	103.40	108.00
1	B	103	DG	C4-N9-C1'	-6.55	117.98	126.50
1	B	109[A]	DG	O4'-C1'-N9	-6.53	103.43	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	109[B]	DG	O4'-C1'-N9	-6.53	103.43	108.00
1	D	308	DC	C5-C4-N4	6.52	124.76	120.20
1	C	210	DC	O4'-C1'-N1	-6.51	103.44	108.00
1	D	309	DG	C1'-O4'-C4'	-6.48	103.62	110.10
1	B	101	DG	O4'-C4'-C3'	-6.47	101.91	104.50
1	A	9	DG	C8-N9-C4	6.35	108.94	106.40
1	A	9	DG	O4'-C4'-C3'	-6.32	101.97	104.50
1	A	10	DC	C2-N1-C1'	-6.28	111.89	118.80
1	B	102[A]	DC	C6-N1-C1'	6.24	128.28	120.80
1	B	102[B]	DC	C6-N1-C1'	6.24	128.28	120.80
1	D	305	DA	C5-C6-N6	6.17	128.63	123.70
1	B	103	DG	C8-N9-C1'	6.15	134.99	127.00
1	D	309	DG	C8-N9-C1'	6.08	134.91	127.00
1	A	9	DG	C4-N9-C1'	-6.05	118.63	126.50
1	B	109[A]	DG	C4-N9-C1'	-5.98	118.73	126.50
1	B	109[B]	DG	C4-N9-C1'	-5.98	118.73	126.50
1	D	309	DG	C4-N9-C1'	-5.98	118.73	126.50
1	C	203	DG	C1'-O4'-C4'	-5.96	104.14	110.10
1	A	4	DT	O4'-C1'-N1	-5.83	103.92	108.00
1	D	301	DG	C8-N9-C4	5.80	108.72	106.40
1	C	203	DG	C2-N3-C4	-5.79	109.00	111.90
1	B	102[A]	DC	C2-N1-C1'	-5.78	112.44	118.80
1	B	102[B]	DC	C2-N1-C1'	-5.78	112.44	118.80
1	D	305	DA	O4'-C1'-N9	-5.75	103.97	108.00
1	A	7	DA	C4'-C3'-C2'	-5.75	97.92	103.10
1	D	307	DA	O4'-C4'-C3'	-5.73	102.21	104.50
1	C	209	DG	C4-N9-C1'	-5.71	119.08	126.50
1	D	309	DG	C5-N7-C8	5.70	107.15	104.30
1	A	9	DG	N7-C8-N9	-5.68	110.26	113.10
1	C	202	DC	C5-C4-N4	5.67	124.17	120.20
1	B	103	DG	C1'-O4'-C4'	-5.66	104.44	110.10
1	A	5	DA	C1'-O4'-C4'	-5.49	104.61	110.10
1	D	310	DC	C2-N1-C1'	-5.46	112.80	118.80
1	A	7	DA	O4'-C1'-N9	-5.37	104.24	108.00
1	D	309	DG	C5-C6-N1	5.36	114.18	111.50
1	B	108[A]	DC	C4'-C3'-O3'	-5.34	96.34	109.70
1	B	108[B]	DC	C4'-C3'-O3'	-5.34	96.34	109.70
1	D	303	DG	C2-N3-C4	5.34	114.57	111.90
1	A	3	DG	C8-N9-C1'	5.33	133.93	127.00
1	D	308	DC	N3-C4-N4	-5.31	114.28	118.00
1	B	108[A]	DC	C4'-C3'-C2'	-5.28	98.34	103.10
1	B	108[B]	DC	C4'-C3'-C2'	-5.28	98.34	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	302	DC	O4'-C4'-C3'	-5.28	102.39	104.50
1	C	209	DG	C1'-O4'-C4'	-5.25	104.85	110.10
1	C	210	DC	C2-N3-C4	-5.19	117.31	119.90
1	B	109[A]	DG	C8-N9-C1'	5.16	133.71	127.00
1	B	109[B]	DG	C8-N9-C1'	5.16	133.71	127.00
1	A	3	DG	C4-N9-C1'	-5.10	119.87	126.50
1	B	103	DG	C5-C6-O6	5.09	131.65	128.60
1	B	108[A]	DC	N1-C2-N3	-5.08	115.64	119.20
1	B	108[B]	DC	N1-C2-N3	-5.08	115.64	119.20
1	C	202	DC	C2-N1-C1'	-5.04	113.26	118.80

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	A	214	0	116	1	0
1	B	224	0	95	0	0
1	C	208	0	119	1	0
1	D	208	0	119	0	0
2	A	64	0	0	0	0
2	B	78	0	0	0	0
2	C	91	0	0	0	0
2	D	71	0	0	0	0
All	All	1158	0	449	2	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 1.

All (2) 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:C:206:NMS:O5'	1:C:206:NMS:H6	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	NMS	A	6[B]	-	24,27,28	1.07	1 (4%)	32,38,41	1.08	3 (9%)
1	NMS	B	106[A]	-	24,27,28	1.19	4 (16%)	32,38,41	1.24	3 (9%)
1	NMS	B	106[B]	-	24,27,28	1.11	3 (12%)	32,38,41	1.17	2 (6%)
1	NMS	C	206	1	24,27,28	1.07	1 (4%)	32,38,41	1.38	5 (15%)
1	NMS	A	6[A]	-	24,27,28	1.13	1 (4%)	32,38,41	1.50	4 (12%)
1	NMS	D	306	1	24,27,28	1.28	3 (12%)	32,38,41	1.01	2 (6%)

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	NMS	A	6[B]	-	-	2/14/32/33	0/2/2/2
1	NMS	B	106[A]	-	-	2/14/32/33	0/2/2/2
1	NMS	B	106[B]	-	-	2/14/32/33	0/2/2/2
1	NMS	C	206	1	-	0/14/32/33	0/2/2/2
1	NMS	A	6[A]	-	-	0/14/32/33	0/2/2/2
1	NMS	D	306	1	-	4/14/32/33	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	306	NMS	C2'-C1'	-3.43	1.44	1.53
1	A	6[A]	NMS	C2'-C1'	-3.16	1.44	1.53
1	A	6[B]	NMS	C2'-C1'	-3.16	1.44	1.53
1	C	206	NMS	C2'-C1'	-3.13	1.45	1.53
1	B	106[A]	NMS	C2'-C1'	-3.02	1.45	1.53
1	B	106[B]	NMS	C2'-C1'	-3.02	1.45	1.53
1	D	306	NMS	O2-C2	-2.55	1.18	1.23
1	B	106[A]	NMS	O6'-C2'	-2.46	1.38	1.43
1	D	306	NMS	O4'-C1'	2.36	1.47	1.42
1	B	106[A]	NMS	C3'-C2'	-2.26	1.47	1.52
1	B	106[B]	NMS	C3'-C2'	-2.26	1.47	1.52
1	B	106[A]	NMS	O4'-C1'	2.14	1.47	1.42
1	B	106[B]	NMS	O4'-C1'	2.14	1.47	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6[A]	NMS	C7'-O6'-C2'	-5.36	106.17	114.32
1	C	206	NMS	C6-N1-C2	3.60	124.94	121.30
1	B	106[A]	NMS	C7'-O6'-C2'	3.11	119.05	114.32
1	C	206	NMS	C1'-N1-C2	-2.99	112.16	117.57
1	A	6[A]	NMS	O6'-C2'-C3'	2.69	117.63	110.94
1	C	206	NMS	N3-C2-N1	-2.53	111.53	114.89
1	B	106[A]	NMS	C1'-N1-C6	2.48	125.25	121.12
1	B	106[B]	NMS	C1'-N1-C6	2.48	125.25	121.12
1	A	6[A]	NMS	C1'-N1-C2	-2.35	113.32	117.57
1	A	6[B]	NMS	C1'-N1-C2	-2.35	113.32	117.57
1	B	106[A]	NMS	C1'-N1-C2	-2.34	113.33	117.57
1	B	106[B]	NMS	C1'-N1-C2	-2.34	113.33	117.57
1	D	306	NMS	C7'-O6'-C2'	-2.16	111.03	114.32
1	A	6[B]	NMS	O8'-C8'-C7'	2.13	125.60	119.61
1	C	206	NMS	O2-C2-N1	2.13	125.62	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6[A]	NMS	C1'-N1-C6	2.11	124.64	121.12
1	A	6[B]	NMS	C1'-N1-C6	2.11	124.64	121.12
1	C	206	NMS	C5-C6-N1	-2.09	121.19	123.34
1	D	306	NMS	C1'-N1-C2	-2.02	113.91	117.57

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	306	NMS	C7'-C8'-N9'-C10
1	D	306	NMS	O8'-C8'-N9'-C10
1	A	6[B]	NMS	O6'-C7'-C8'-N9'
1	B	106[A]	NMS	O6'-C7'-C8'-N9'
1	B	106[B]	NMS	O6'-C7'-C8'-N9'
1	D	306	NMS	O6'-C7'-C8'-N9'
1	B	106[B]	NMS	O6'-C7'-C8'-O8'
1	D	306	NMS	O6'-C7'-C8'-O8'
1	A	6[B]	NMS	O6'-C7'-C8'-O8'
1	B	106[A]	NMS	O6'-C7'-C8'-O8'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	206	NMS	1	0
1	A	6[A]	NMS	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	9/10 (90%)	-0.50	0	100	100	17, 17, 21, 21	0
1	B	9/10 (90%)	-0.53	0	100	100	16, 19, 22, 22	0
1	C	9/10 (90%)	-0.65	0	100	100	15, 16, 18, 20	0
1	D	9/10 (90%)	-0.51	0	100	100	15, 16, 19, 23	0
All	All	36/40 (90%)	-0.55	0	100	100	15, 17, 22, 23	0

There are no RSRZ outliers to report.

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(Å²)	Q<0.9
1	NMS	A	6[A]	26/27	0.96	0.09	16,21,30,35	6
1	NMS	A	6[B]	26/27	0.96	0.09	16,21,28,42	6
1	NMS	B	106[A]	26/27	0.96	0.09	16,22,28,40	6
1	NMS	B	106[B]	26/27	0.96	0.09	16,22,31,36	6
1	NMS	C	206	26/27	0.98	0.06	13,16,31,34	0
1	NMS	D	306	26/27	0.98	0.06	13,16,28,55	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

There are no ligands in this entry.

6.5   Other polymers ⓘ

There are no such residues in this entry.