Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2026 – 12:09 PM EDT

PDB ID	:	36CK / pdb_000036ck
Title	:	Crystal structure of human Argonaute2 in complex with a fully modified siRNA with a 5' methyl phosphate
Authors	:	Gebert, L.F.R.; MacRae, I.J.
Deposited on	:	2026-06-01
Resolution	:	2.21 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:

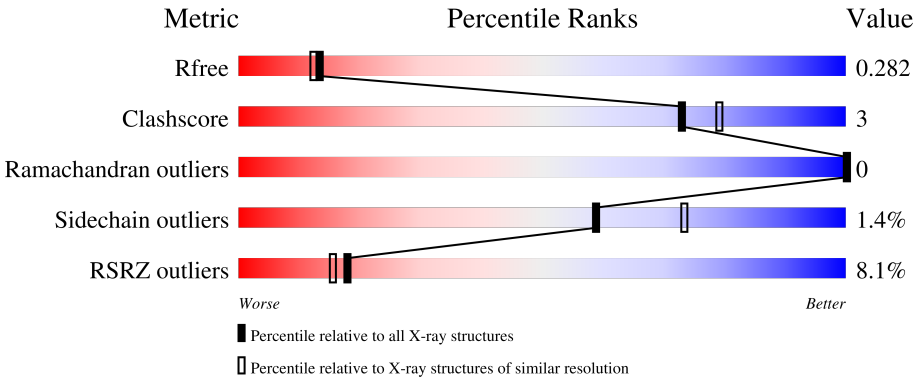
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	859	7% 83% 9% 8%
2	B	21	33% 19% 48%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6638 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 Protein argonaute-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	790	6341	4042	1138	1122	39	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ASP	SER	engineered mutation	UNP Q9UKV8
A	824	ALA	SER	engineered mutation	UNP Q9UKV8
A	828	ASP	SER	engineered mutation	UNP Q9UKV8
A	831	ASP	SER	engineered mutation	UNP Q9UKV8
A	834	ALA	SER	engineered mutation	UNP Q9UKV8

- Molecule 2 is a DNA chain called fully modified siRNA with a 5' methyl phosphate.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	F	N	O	P	S			
2	B	11	244	111	6	40	72	11	4	0	0	0

- Molecule 3 is water.

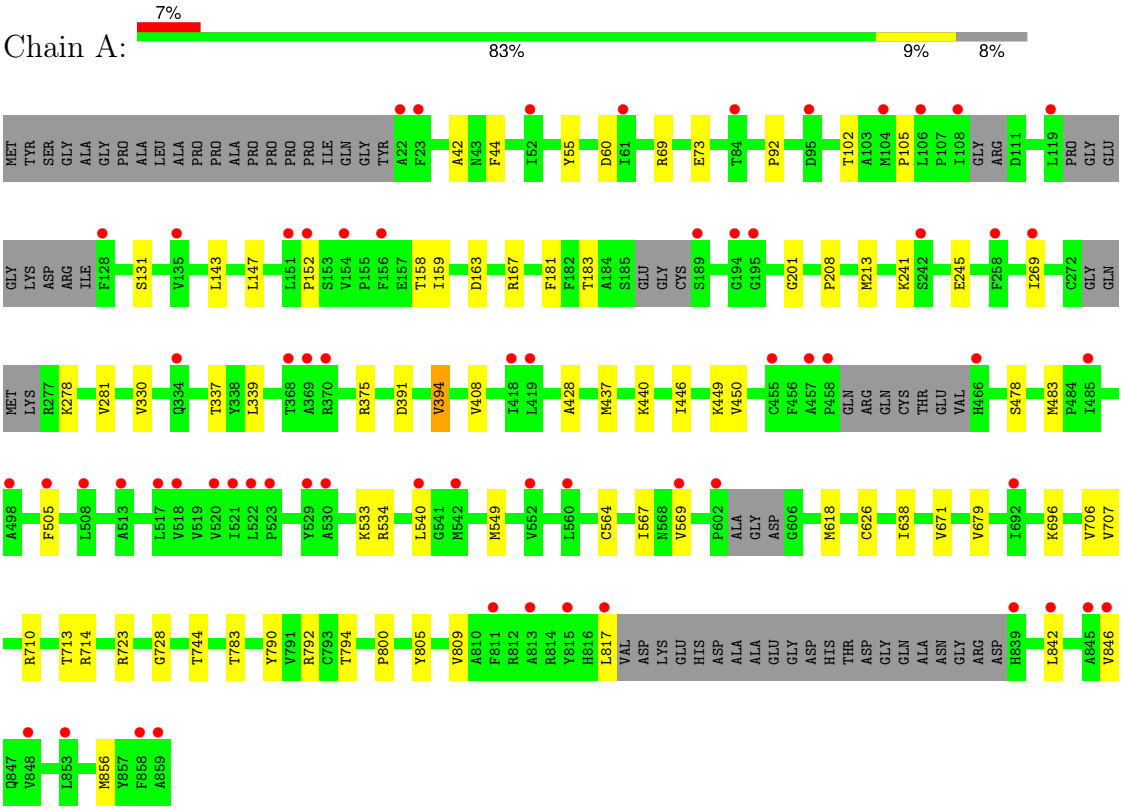
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	47	47	47	0	0
			Total	O		
3	B	6	6	6	0	0

3 Residue-property plots (i)

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.

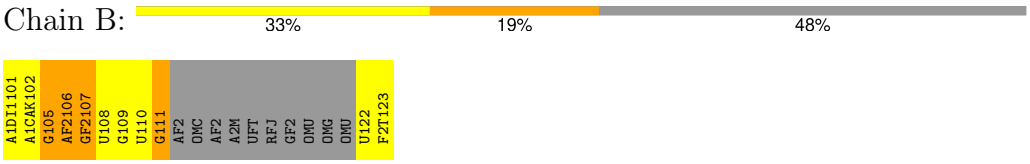
• Molecule 1: Protein argonaute-2

Chain A:



• Molecule 2: fully modified siRNA with a 5' methyl phosphate

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.63Å 108.45Å 68.08Å 90.00° 107.62° 90.00°	Depositor
Resolution (Å)	52.57 – 2.21 52.57 – 2.21	Depositor EDS
% Data completeness (in resolution range)	83.2 (52.57-2.21) 83.1 (52.57-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.241 , 0.283 0.241 , 0.282	Depositor DCC
R_{free} test set	2015 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6638	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: F2T, UFT, A1CAK, GF2, OMG, OKT, A1DI1, AF2, RFJ

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	0.09	0/6490	0.25	0/8781

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	A	6341	0	6400	41	0
2	B	244	0	65	4	0
3	A	47	0	0	0	0
3	B	6	0	0	0	0
All	All	6638	0	6465	42	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 3.

All (42) 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:618:MET:HE3	1:A:626:CYS:HB2	1.71	0.72
1:A:147:LEU:HD21	1:A:213:MET:HE2	1.80	0.64
1:A:147:LEU:HD11	1:A:213:MET:HG2	1.80	0.63
1:A:152:PRO:HA	1:A:744:THR:HG21	1.80	0.62
1:A:428:ALA:HB2	1:A:440:LYS:HE2	1.83	0.60
1:A:449:LYS:HG3	1:A:450:VAL:HG23	1.86	0.58
1:A:375:ARG:HH11	1:A:714:ARG:HD2	1.68	0.57
1:A:710:ARG:NH2	2:B:111:OMG:H2'	2.19	0.57
1:A:143:LEU:HD21	1:A:213:MET:HE3	1.86	0.57
1:A:710:ARG:HH21	2:B:111:OMG:H2'	1.70	0.57
1:A:167:ARG:HB2	1:A:181:PHE:HZ	1.69	0.57
1:A:391:ASP:HB3	1:A:394:VAL:HG22	1.88	0.56
1:A:92:PRO:HB3	1:A:102:THR:HG22	1.90	0.54
1:A:55:TYR:CZ	1:A:105:PRO:HG3	2.44	0.52
2:B:106:AF2:H2'	2:B:107:GF2:C8	2.40	0.52
1:A:281:VAL:HA	1:A:330:VAL:HG12	1.93	0.51
1:A:163:ASP:OD2	1:A:167:ARG:HD2	2.12	0.49
1:A:638:ILE:HD13	1:A:679:VAL:HG12	1.95	0.49
1:A:564:CYS:HA	1:A:567:ILE:HG12	1.95	0.48
1:A:792:ARG:NH2	2:B:105:RFJ:S	2.87	0.48
1:A:790:TYR:CE2	1:A:792:ARG:HB2	2.49	0.48
1:A:437:MET:HG3	1:A:794:THR:HG21	1.96	0.48
1:A:723:ARG:HB3	1:A:728:GLY:HA2	1.95	0.47
1:A:181:PHE:O	1:A:201:GLY:HA3	2.15	0.47
1:A:671:VAL:HG11	1:A:679:VAL:HG21	1.96	0.46
1:A:143:LEU:HB2	1:A:158:THR:HG21	1.98	0.46
1:A:534:ARG:NH2	1:A:817:LEU:HB2	2.31	0.46
1:A:533:LYS:HD3	1:A:533:LYS:HA	1.80	0.45
1:A:375:ARG:NH1	1:A:714:ARG:HH11	2.15	0.44
1:A:783:THR:HG23	1:A:800:PRO:HG3	2.00	0.44
1:A:478:SER:HB3	1:A:483:MET:O	2.17	0.43
1:A:44:PHE:HE1	1:A:713:THR:HG23	1.84	0.43
1:A:159:ILE:HD13	1:A:208:PRO:HG3	2.00	0.43
1:A:69:ARG:O	1:A:73:GLU:HG2	2.18	0.42
1:A:60:ASP:HB2	1:A:131:SER:OG	2.19	0.42
1:A:569:VAL:HB	1:A:856:MET:HE3	2.01	0.42
1:A:241:LYS:HB2	1:A:245:GLU:OE2	2.19	0.42
1:A:269:ILE:HD11	1:A:339:LEU:HD13	2.02	0.42
1:A:42:ALA:C	1:A:44:PHE:H	2.28	0.41
1:A:842:LEU:O	1:A:846:VAL:HG23	2.21	0.41
1:A:505:PHE:HB3	1:A:540:LEU:HG	2.03	0.40
1:A:805:TYR:O	1:A:809:VAL:HG23	2.22	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	774/859 (90%)	738 (95%)	36 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	701/750 (94%)	691 (99%)	10 (1%)	59 73

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	THR
1	A	278	LYS
1	A	337	THR
1	A	394	VAL
1	A	408	VAL
1	A	446	ILE
1	A	549	MET
1	A	696	LYS
1	A	706	VAL
1	A	707	VAL

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

Mol	Chain	Res	Type
1	A	99	ASN
1	A	623	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

11 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	$\#\|Z\| > 2$
2	A1DI1	B	101	2	24,24,24	2.58	7 (29%)	33,35,35	1.06	2 (6%)
2	RFJ	B	105	2	23,26,27	3.33	14 (60%)	32,38,41	2.09	11 (34%)
2	OMG	B	111	2	23,26,27	1.07	2 (8%)	32,38,41	1.07	3 (9%)
2	UFT	B	108	2	18,21,22	4.32	15 (83%)	25,30,33	2.02	7 (28%)
2	A1CAK	B	102	2	22,25,26	3.66	14 (63%)	32,37,40	2.19	10 (31%)
2	UFT	B	110	2	18,21,22	4.29	15 (83%)	25,30,33	1.92	6 (24%)
2	AF2	B	106	2	21,24,25	3.38	9 (42%)	30,35,38	2.60	11 (36%)
2	OMG	B	109	2	23,26,27	1.08	2 (8%)	32,38,41	1.06	3 (9%)
2	F2T	B	123	2	18,21,22	4.82	15 (83%)	25,30,33	2.00	6 (24%)
2	GF2	B	107	2	22,25,26	3.73	14 (63%)	32,37,40	2.24	12 (37%)
2	OKT	B	122	2	19,22,23	4.34	14 (73%)	25,31,34	1.83	5 (20%)

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
2	A1DI1	B	101	2	-	3/15/31/31	0/2/2/2
2	RFJ	B	105	2	-	1/9/27/28	0/3/3/3
2	OMG	B	111	2	-	1/9/27/28	0/3/3/3
2	UFT	B	108	2	-	2/7/25/26	0/2/2/2
2	A1CAK	B	102	2	-	0/7/25/26	0/3/3/3
2	UFT	B	110	2	-	0/7/25/26	0/2/2/2
2	AF2	B	106	2	-	2/7/25/26	0/3/3/3
2	OMG	B	109	2	-	3/9/27/28	0/3/3/3
2	F2T	B	123	2	-	2/7/25/26	0/2/2/2
2	GF2	B	107	2	-	0/7/25/26	0/3/3/3
2	OKT	B	122	2	-	2/9/27/28	0/2/2/2

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	107	GF2	C3'-C4'	-9.34	1.29	1.53
2	B	102	A1CAK	C3'-C4'	-9.27	1.29	1.53
2	B	123	F2T	C2-N1	8.79	1.52	1.38
2	B	106	AF2	C3'-C4'	-8.20	1.32	1.53
2	B	123	F2T	C2-N3	8.15	1.52	1.38
2	B	105	RFJ	C2'-C1'	-8.01	1.33	1.53
2	B	122	OKT	O4'-C4'	-8.01	1.27	1.45
2	B	108	UFT	O4'-C4'	-7.89	1.27	1.45
2	B	110	UFT	O4'-C4'	-7.68	1.27	1.45
2	B	108	UFT	C2-N1	7.39	1.50	1.38
2	B	110	UFT	C2-N1	7.26	1.49	1.38
2	B	122	OKT	C2-N3	7.24	1.50	1.38
2	B	106	AF2	C6-N6	7.20	1.52	1.34
2	B	122	OKT	C2-N1	7.14	1.49	1.38
2	B	123	F2T	C6-C5	6.91	1.51	1.35
2	B	106	AF2	O4'-C4'	6.82	1.60	1.45
2	B	105	RFJ	C4-N3	6.79	1.49	1.34
2	B	102	A1CAK	C4-N3	6.79	1.49	1.34
2	B	107	GF2	C4-N3	6.74	1.49	1.34
2	B	108	UFT	C2-N3	6.68	1.49	1.38
2	B	110	UFT	C2-N3	6.64	1.49	1.38
2	B	123	F2T	C2'-C1'	6.35	1.60	1.53
2	B	123	F2T	O4'-C4'	-5.95	1.31	1.45
2	B	108	UFT	C6-C5	5.74	1.48	1.35
2	B	105	RFJ	C2-N3	5.71	1.47	1.33
2	B	110	UFT	C6-C5	5.70	1.48	1.35
2	B	122	OKT	C6-C5	5.69	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	A1CAK	F-C2'	-5.67	1.29	1.40
2	B	107	GF2	F-C2'	-5.66	1.29	1.40
2	B	102	A1CAK	C2-N3	5.58	1.46	1.33
2	B	107	GF2	C2-N3	5.56	1.46	1.33
2	B	101	A1DI1	C2-N1	5.55	1.47	1.38
2	B	122	OKT	C3'-C4'	5.24	1.66	1.53
2	B	110	UFT	F2'-C2'	5.10	1.50	1.40
2	B	108	UFT	F2'-C2'	5.08	1.50	1.40
2	B	106	AF2	O4'-C1'	-4.99	1.30	1.42
2	B	123	F2T	C3'-C4'	4.96	1.65	1.53
2	B	123	F2T	C1'-N1	-4.90	1.33	1.47
2	B	122	OKT	O4'-C1'	4.87	1.53	1.42
2	B	102	A1CAK	C2-N2	4.84	1.45	1.34
2	B	107	GF2	C2-N2	4.84	1.45	1.34
2	B	122	OKT	C1'-N1	-4.80	1.33	1.47
2	B	101	A1DI1	C2-N3	4.77	1.46	1.38
2	B	122	OKT	O01-C2'	4.65	1.54	1.42
2	B	101	A1DI1	P-O5'	4.57	1.77	1.59
2	B	107	GF2	O4'-C1'	-4.56	1.31	1.42
2	B	101	A1DI1	P-OP3	4.54	1.73	1.58
2	B	110	UFT	C1'-N1	-4.53	1.34	1.47
2	B	122	OKT	C4-N3	4.52	1.46	1.38
2	B	123	F2T	C4-N3	4.51	1.46	1.38
2	B	108	UFT	O4'-C1'	4.50	1.52	1.42
2	B	101	A1DI1	O4'-C1'	4.49	1.52	1.42
2	B	108	UFT	C1'-N1	-4.44	1.35	1.47
2	B	110	UFT	O4'-C1'	4.40	1.52	1.42
2	B	105	RFJ	C2-N2	4.21	1.44	1.34
2	B	108	UFT	C4-N3	4.18	1.45	1.38
2	B	110	UFT	C3'-C4'	4.16	1.63	1.53
2	B	110	UFT	C4-N3	4.15	1.45	1.38
2	B	123	F2T	O4'-C1'	4.06	1.51	1.42
2	B	105	RFJ	O2'-C2'	3.97	1.52	1.42
2	B	101	A1DI1	C5'-C4'	3.94	1.63	1.51
2	B	123	F2T	F2'-C2'	3.86	1.48	1.40
2	B	108	UFT	C3'-C4'	3.78	1.62	1.53
2	B	105	RFJ	O3'-C3'	-3.78	1.33	1.43
2	B	123	F2T	O2-C2	-3.60	1.16	1.23
2	B	105	RFJ	C2-N1	3.53	1.46	1.37
2	B	102	A1CAK	C2'-C3'	3.43	1.57	1.52
2	B	123	F2T	C5-C4	3.33	1.50	1.43
2	B	107	GF2	C2'-C3'	3.29	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	109	OMG	C2-N2	3.26	1.41	1.34
2	B	122	OKT	C6-N1	3.24	1.45	1.38
2	B	111	OMG	C2-N2	3.22	1.41	1.34
2	B	105	RFJ	C5-C6	3.08	1.55	1.44
2	B	110	UFT	O3'-C3'	3.05	1.50	1.43
2	B	123	F2T	O4-C4	-3.05	1.18	1.24
2	B	123	F2T	C6-N1	3.02	1.45	1.38
2	B	110	UFT	O4-C4	-2.93	1.18	1.24
2	B	108	UFT	O4-C4	-2.91	1.18	1.24
2	B	105	RFJ	C5-N7	-2.82	1.33	1.39
2	B	102	A1CAK	O4'-C4'	2.81	1.51	1.45
2	B	107	GF2	C2-N1	2.80	1.44	1.37
2	B	106	AF2	C5-N7	-2.80	1.34	1.39
2	B	102	A1CAK	C2'-C1'	2.80	1.56	1.53
2	B	107	GF2	C5-N7	-2.79	1.33	1.39
2	B	102	A1CAK	C2-N1	2.79	1.44	1.37
2	B	102	A1CAK	C5-N7	-2.78	1.33	1.39
2	B	122	OKT	O4-C4	-2.77	1.19	1.24
2	B	122	OKT	C5-C4	2.77	1.49	1.43
2	B	108	UFT	O3'-C3'	2.74	1.49	1.43
2	B	108	UFT	C2'-C1'	2.69	1.56	1.53
2	B	107	GF2	C2'-C1'	2.68	1.56	1.53
2	B	106	AF2	C1'-N9	2.64	1.53	1.46
2	B	106	AF2	O3'-C3'	2.63	1.49	1.43
2	B	106	AF2	F-C2'	-2.62	1.35	1.40
2	B	108	UFT	C6-N1	2.59	1.44	1.38
2	B	110	UFT	C6-N1	2.55	1.44	1.38
2	B	102	A1CAK	O3'-C3'	2.54	1.49	1.43
2	B	102	A1CAK	C5-C6	2.53	1.53	1.44
2	B	107	GF2	C5-C6	2.53	1.53	1.44
2	B	101	A1DI1	C4-N3	2.49	1.42	1.38
2	B	107	GF2	O3'-C3'	2.49	1.49	1.43
2	B	110	UFT	O2-C2	-2.46	1.18	1.23
2	B	108	UFT	O2-C2	-2.45	1.18	1.23
2	B	102	A1CAK	O6-C6	-2.45	1.18	1.23
2	B	107	GF2	O6-C6	-2.44	1.18	1.23
2	B	107	GF2	C6-N1	2.43	1.43	1.38
2	B	102	A1CAK	C6-N1	2.39	1.43	1.38
2	B	110	UFT	C2'-C1'	2.35	1.55	1.53
2	B	123	F2T	O3'-C3'	2.32	1.48	1.43
2	B	122	OKT	O2-C2	-2.31	1.19	1.23
2	B	122	OKT	O3'-C3'	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	105	RFJ	O6-C6	-2.19	1.19	1.23
2	B	105	RFJ	O4'-C4'	2.18	1.49	1.45
2	B	106	AF2	C2-N3	2.16	1.37	1.33
2	B	105	RFJ	C1'-N9	-2.16	1.41	1.47
2	B	108	UFT	C5-C4	2.15	1.48	1.43
2	B	110	UFT	C5-C4	2.11	1.48	1.43
2	B	111	OMG	C4-N3	2.05	1.38	1.34
2	B	105	RFJ	C3'-C4'	2.04	1.58	1.53
2	B	109	OMG	C4-N3	2.04	1.38	1.34
2	B	105	RFJ	C5'-C4'	2.02	1.57	1.51

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	122	OKT	C4-N3-C2	-5.72	119.50	126.61
2	B	106	AF2	C5-C4-N3	-5.70	118.86	126.72
2	B	106	AF2	N3-C2-N1	-5.59	120.11	128.58
2	B	108	UFT	C4-N3-C2	-5.48	119.80	126.61
2	B	123	F2T	C4-N3-C2	-5.41	119.90	126.61
2	B	110	UFT	C4-N3-C2	-5.38	119.93	126.61
2	B	105	RFJ	C5-C4-N3	-5.27	120.00	128.39
2	B	102	A1CAK	C5-C4-N3	-5.25	120.04	128.39
2	B	106	AF2	C1'-N9-C8	5.21	138.65	127.09
2	B	107	GF2	C5-C4-N3	-5.16	120.18	128.39
2	B	105	RFJ	C2-N3-C4	4.70	120.39	112.30
2	B	102	A1CAK	C2-N3-C4	4.49	120.03	112.30
2	B	107	GF2	C2-N3-C4	4.48	120.02	112.30
2	B	107	GF2	C1'-N9-C4	-4.35	113.64	126.49
2	B	102	A1CAK	C1'-N9-C4	-4.07	114.47	126.49
2	B	106	AF2	C4-N9-C1'	-4.05	117.16	126.63
2	B	123	F2T	C2'-C1'-N1	-4.03	108.07	114.27
2	B	106	AF2	N6-C6-N1	-3.94	109.61	118.38
2	B	122	OKT	C5-C4-N3	3.92	120.29	114.80
2	B	108	UFT	N3-C2-N1	3.91	119.98	114.89
2	B	106	AF2	C2-N3-C4	3.86	121.27	111.83
2	B	106	AF2	C5-C4-N9	3.83	109.98	105.81
2	B	110	UFT	N3-C2-N1	3.80	119.83	114.89
2	B	107	GF2	C1'-N9-C8	3.76	137.42	126.73
2	B	123	F2T	N3-C2-N1	3.73	119.75	114.89
2	B	123	F2T	C5-C4-N3	3.67	119.94	114.80
2	B	122	OKT	N3-C2-N1	3.61	119.59	114.89
2	B	108	UFT	C5-C4-N3	3.50	119.70	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	110	UFT	C5-C4-N3	3.48	119.68	114.80
2	B	102	A1CAK	C1'-N9-C8	3.44	136.51	126.73
2	B	102	A1CAK	N9-C4-N3	3.43	132.82	125.95
2	B	106	AF2	C2'-C3'-C4'	3.32	106.80	102.43
2	B	107	GF2	N9-C4-N3	3.26	132.47	125.95
2	B	102	A1CAK	N9-C8-N7	-3.24	107.38	113.40
2	B	110	UFT	C2'-C1'-N1	-3.22	109.32	114.27
2	B	107	GF2	N9-C8-N7	-3.21	107.44	113.40
2	B	105	RFJ	O4'-C1'-C2'	3.15	112.01	106.59
2	B	123	F2T	O4-C4-C5	-3.05	119.89	125.16
2	B	105	RFJ	C2-N1-C6	-3.05	119.58	125.11
2	B	105	RFJ	N9-C8-N7	-3.05	107.74	113.40
2	B	122	OKT	O4-C4-C5	-3.02	119.95	125.16
2	B	105	RFJ	N9-C4-N3	3.01	131.98	125.95
2	B	102	A1CAK	C2-N1-C6	-3.00	119.67	125.11
2	B	107	GF2	C2-N1-C6	-3.00	119.67	125.11
2	B	108	UFT	C2'-C1'-N1	-2.98	109.70	114.27
2	B	110	UFT	O4-C4-C5	-2.90	120.15	125.16
2	B	108	UFT	O4-C4-C5	-2.90	120.16	125.16
2	B	105	RFJ	C5-C6-N1	2.72	120.19	113.25
2	B	107	GF2	C3'-C2'-C1'	-2.70	99.96	103.10
2	B	101	A1DI1	C2'-C1'-N1	-2.68	109.16	114.24
2	B	102	A1CAK	C5-C6-N1	2.65	120.01	113.25
2	B	107	GF2	C5-C6-N1	2.65	120.00	113.25
2	B	111	OMG	N1-C2-N3	2.56	128.01	123.32
2	B	105	RFJ	C3'-C2'-C1'	2.55	107.69	102.81
2	B	109	OMG	N1-C2-N3	2.52	127.93	123.32
2	B	102	A1CAK	O6-C6-C5	-2.49	119.95	126.53
2	B	107	GF2	O6-C6-C5	-2.49	119.96	126.53
2	B	105	RFJ	O4'-C4'-C3'	-2.44	100.31	105.15
2	B	105	RFJ	O6-C6-C5	-2.43	120.12	126.53
2	B	106	AF2	N3-C4-N9	2.35	131.16	127.17
2	B	107	GF2	O4'-C4'-C3'	2.32	109.76	105.15
2	B	106	AF2	C5-C6-N1	2.26	123.25	117.51
2	B	102	A1CAK	C8-N7-C5	2.24	108.25	104.26
2	B	107	GF2	C8-N7-C5	2.21	108.20	104.26
2	B	105	RFJ	C8-N7-C5	2.21	108.19	104.26
2	B	122	OKT	O2-C2-N1	-2.20	119.93	122.80
2	B	106	AF2	C4-C5-N7	-2.15	108.12	110.58
2	B	101	A1DI1	C2'-C3'-C4'	2.15	106.61	101.99
2	B	111	OMG	C6-C5-C4	2.14	122.05	118.83
2	B	108	UFT	C5'-C4'-C3'	-2.11	107.60	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	110	UFT	O2-C2-N1	-2.11	120.05	122.80
2	B	108	UFT	O2-C2-N1	-2.08	120.09	122.80
2	B	109	OMG	C6-C5-C4	2.04	121.90	118.83
2	B	109	OMG	O6-C6-C5	2.03	131.88	126.53
2	B	111	OMG	O6-C6-C5	2.02	131.87	126.53
2	B	123	F2T	O2-C2-N1	-2.00	120.19	122.80

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	105	RFJ	C1'-C2'-O2'-C
2	B	106	AF2	O4'-C4'-C5'-O5'
2	B	109	OMG	C1'-C2'-O2'-CM2
2	B	122	OKT	C1'-C2'-O01-C02
2	B	106	AF2	C3'-C4'-C5'-O5'
2	B	108	UFT	C3'-C4'-C5'-O5'
2	B	109	OMG	O4'-C4'-C5'-O5'
2	B	109	OMG	C3'-C4'-C5'-O5'
2	B	123	F2T	O4'-C4'-C5'-O5'
2	B	123	F2T	C3'-C4'-C5'-O5'
2	B	108	UFT	O4'-C4'-C5'-O5'
2	B	101	A1DI1	C4'-C5'-O5'-P
2	B	101	A1DI1	C3'-C2'-O2'-CO2'
2	B	122	OKT	O4'-C4'-C5'-O5'
2	B	111	OMG	O4'-C1'-N9-C4
2	B	101	A1DI1	C1'-C2'-O2'-CO2'

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	105	RFJ	1	0
2	B	111	OMG	2	0
2	B	106	AF2	1	0
2	B	107	GF2	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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

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, 95^{th} 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	790/859 (91%)	0.73	64 (8%) 18 15	34, 63, 96, 106	0
2	B	0/21	-	-	-	-
All	All	790/880 (89%)	0.73	64 (8%) 18 15	34, 63, 96, 106	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	PRO	4.3
1	A	151	LEU	4.3
1	A	369	ALA	4.0
1	A	458	PRO	3.7
1	A	455	CYS	3.3
1	A	542	MET	3.1
1	A	22	ALA	3.1
1	A	498	ALA	3.1
1	A	530	ALA	3.1
1	A	128	PHE	3.0
1	A	858	PHE	3.0
1	A	853	LEU	3.0
1	A	846	VAL	3.0
1	A	195	GLY	3.0
1	A	194	GLY	2.9
1	A	108	ILE	2.9
1	A	119	LEU	2.7
1	A	817	LEU	2.7
1	A	813	ALA	2.7
1	A	334	GLN	2.7
1	A	95	ASP	2.6
1	A	154	VAL	2.6
1	A	839	HIS	2.6
1	A	518	VAL	2.6
1	A	540	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	23	PHE	2.5
1	A	859	ALA	2.5
1	A	692	ILE	2.4
1	A	508	LEU	2.4
1	A	52	ILE	2.4
1	A	842	LEU	2.4
1	A	848	VAL	2.4
1	A	156	PHE	2.3
1	A	845	ALA	2.3
1	A	269	ILE	2.3
1	A	520	VAL	2.3
1	A	815	TYR	2.3
1	A	505	PHE	2.2
1	A	522	LEU	2.2
1	A	370	ARG	2.2
1	A	61	ILE	2.2
1	A	569	VAL	2.2
1	A	466	HIS	2.2
1	A	513	ALA	2.2
1	A	529	TYR	2.2
1	A	106	LEU	2.2
1	A	419	LEU	2.2
1	A	84	THR	2.1
1	A	189	SER	2.1
1	A	418	ILE	2.1
1	A	521	ILE	2.1
1	A	457	ALA	2.1
1	A	104	MET	2.1
1	A	135	VAL	2.1
1	A	368	THR	2.1
1	A	517	LEU	2.1
1	A	523	PRO	2.1
1	A	602	PRO	2.1
1	A	242	SER	2.0
1	A	552	VAL	2.0
1	A	258	PHE	2.0
1	A	811	PHE	2.0
1	A	560	LEU	2.0
1	A	485	ILE	2.0

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, 95^{th} 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
2	OKT	B	122	21/22	0.73	0.17	71,78,86,102	0
2	OMG	B	111	24/25	0.74	0.17	48,73,84,87	0
2	A1DI1	B	101	23/23	0.90	0.14	66,72,75,79	0
2	UFT	B	110	20/21	0.90	0.11	54,66,74,75	0
2	OMG	B	109	24/25	0.91	0.11	55,67,71,73	0
2	A1CAK	B	102	23/24	0.91	0.10	55,63,70,85	0
2	RFJ	B	105	24/25	0.93	0.10	49,54,64,65	0
2	AF2	B	106	22/23	0.93	0.10	42,53,58,59	0
2	GF2	B	107	23/24	0.93	0.09	44,53,61,68	0
2	UFT	B	108	20/21	0.93	0.12	41,61,75,80	0
2	F2T	B	123	20/21	0.93	0.11	50,59,69,73	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.