



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2026 – 08:16 AM EDT

PDB ID : 9OBE / pdb\_00009obe  
Title : Crystal structure of human Argonaute2 in complex with a fully modified siRNA with a 5'-phenylpropyl phosphate  
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Deposited on : 2025-04-22  
Resolution : 2.30 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](mailto: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>.

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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

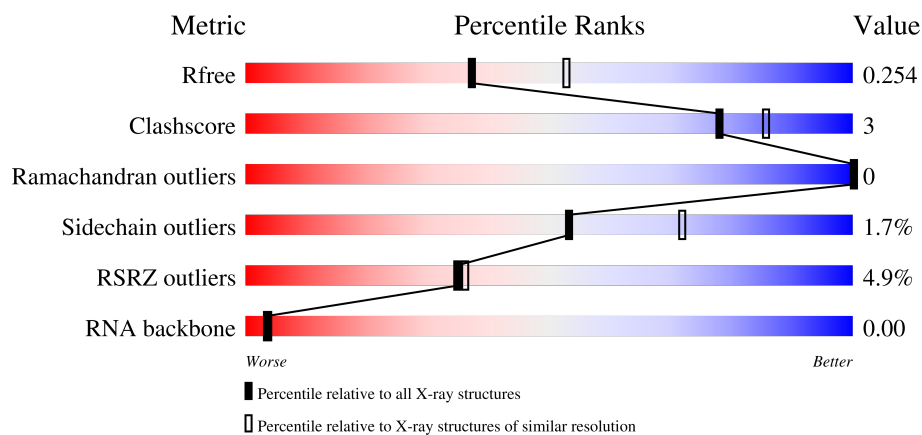
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)
RNA backbone	3983	1090 (2.60-2.00)

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  $\geq 3$ , 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	859	<div> <div>5%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
2	B	21	<div> <div>19%</div> <div>33%</div> <div>48%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6875 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
1	A	803	Total	C	N	O	S	0	0	0
			6447	4105	1159	1143	40			

There are 5 discrepancies between the modelled and reference sequences:

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

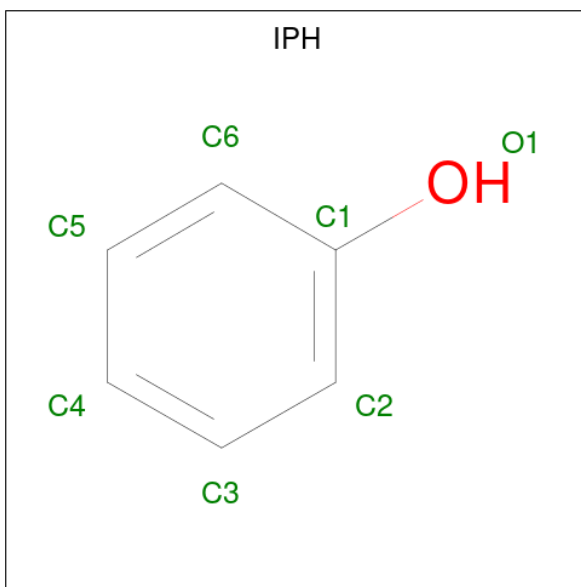
- Molecule 2 is a RNA chain called fully modified siRNA with a 5' phenylpropyl phosphate.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	11	Total	C	F	N	O	P	S	0	0
			252	119	6	40	72	11	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHENOL (CCD ID: IPH) (formula: C<sub>6</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	6	1		
4	A	1	Total	C	O	0	0
			7	6	1		

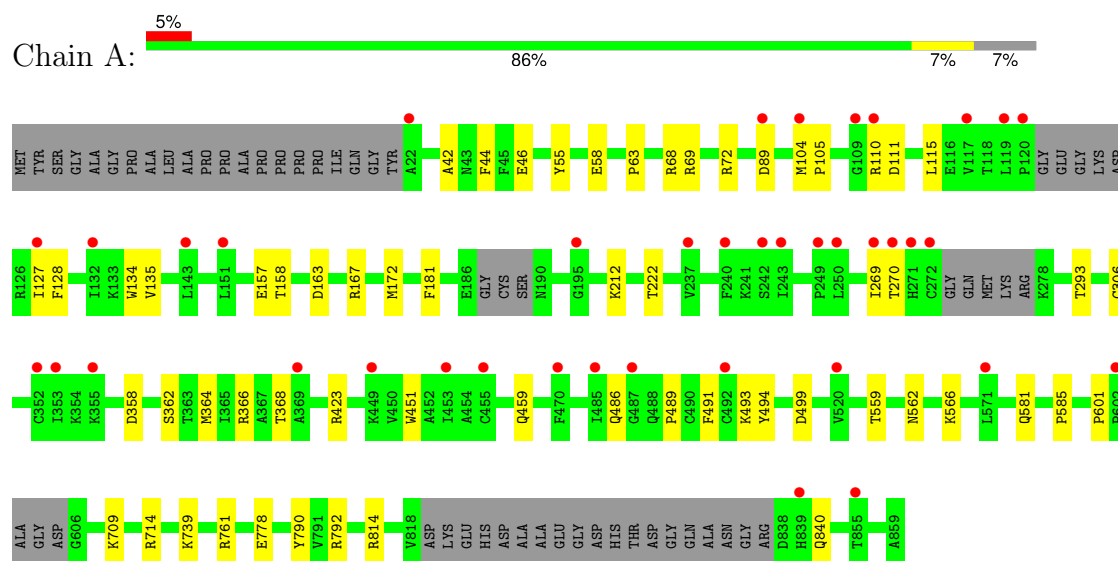
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	157	Total	O	0	0
			157	157		
5	B	4	Total	O	0	0
			4	4		

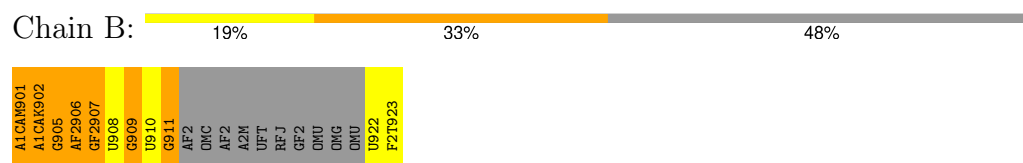
### 3 Residue-property plots

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: Protein argonaute-2



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.12Å 108.24Å 68.53Å 90.00° 107.59° 90.00°	Depositor
Resolution (Å)	60.17 – 2.30 60.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (60.17-2.30) 98.4 (60.17-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.206 , 0.252 0.206 , 0.254	Depositor DCC
$R_{free}$ test set	1916 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.3	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OKT, GF2, A1CAK, UFT, IPH, MG, A1CAM, OMG, RFJ, F2T, AF2

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	0.19	0/6599	0.39	0/8932

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	6447	0	6506	32	0
2	B	252	0	65	9	0
3	A	1	0	0	0	0
4	A	14	0	12	0	0
5	A	157	0	0	0	0
5	B	4	0	0	0	0
All	All	6875	0	6583	37	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 (37) 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:B:901:A1CAM:CB'	2:B:905:RFJ:S	2.86	0.63
1:A:58:GLU:HB2	1:A:135:VAL:HG21	1.81	0.62
1:A:368:THR:HG21	2:B:909:OMG:H5''	1.83	0.61
1:A:222:THR:HA	1:A:364:MET:HE1	1.87	0.56
1:A:167:ARG:HB2	1:A:181:PHE:HZ	1.70	0.56
1:A:709:LYS:O	1:A:761:ARG:HD3	2.06	0.54
1:A:562:ASN:OD1	2:B:902:A1CAK:N2	2.43	0.51
1:A:358:ASP:OD1	1:A:358:ASP:N	2.43	0.50
1:A:790:TYR:CE2	1:A:792:ARG:HB2	2.47	0.49
1:A:585:PRO:HG2	1:A:778:GLU:OE2	2.13	0.48
1:A:491:PHE:CE2	1:A:493:LYS:HD3	2.49	0.48
1:A:840:GLN:H	1:A:840:GLN:CD	2.20	0.48
2:B:906:AF2:H8	2:B:906:AF2:O5'	2.14	0.48
1:A:63:PRO:HD2	1:A:128:PHE:CD2	2.50	0.47
1:A:491:PHE:CZ	1:A:493:LYS:HB2	2.50	0.47
1:A:451:TRP:CZ2	1:A:489:PRO:HD3	2.51	0.46
1:A:459:GLN:HG2	1:A:494:TYR:CD2	2.50	0.46
1:A:42:ALA:C	1:A:44:PHE:H	2.24	0.46
1:A:739:LYS:HA	1:A:739:LYS:HD2	1.85	0.45
1:A:89:ASP:OD1	1:A:89:ASP:N	2.42	0.44
1:A:163:ASP:O	1:A:167:ARG:HG2	2.17	0.44
1:A:790:TYR:OH	1:A:792:ARG:HD2	2.17	0.44
1:A:157:GLU:HG3	1:A:158:THR:N	2.33	0.44
1:A:559:THR:HG23	2:B:902:A1CAK:C4	2.48	0.43
1:A:68:ARG:O	1:A:72:ARG:HG3	2.19	0.43
1:A:46:GLU:OE1	1:A:212:LYS:NZ	2.51	0.42
1:A:55:TYR:CZ	1:A:105:PRO:HG3	2.54	0.42
1:A:362:SER:O	1:A:366:ARG:HG2	2.19	0.42
2:B:909:OMG:H1'	2:B:909:OMG:HM23	1.82	0.42
2:B:907:GF2:O5'	2:B:907:GF2:H8	2.19	0.42
1:A:167:ARG:HB2	1:A:181:PHE:CZ	2.54	0.41
1:A:110:ARG:HH21	1:A:134:TRP:CD1	2.39	0.41
1:A:601:PRO:HG3	1:A:814:ARG:HH22	1.85	0.41
1:A:566:LYS:NZ	2:B:901:A1CAM:OP1	2.39	0.41
1:A:581:GLN:H	1:A:581:GLN:HG3	1.60	0.41
2:B:911:OMG:HM22	2:B:911:OMG:H1'	1.65	0.41
1:A:293:THR:HA	1:A:306:CYS:O	2.22	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	791/859 (92%)	770 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	713/750 (95%)	701 (98%)	12 (2%)	53	72

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	104	MET
1	A	111	ASP
1	A	115	LEU
1	A	127	ILE
1	A	172	MET
1	A	269	ILE
1	A	270	THR
1	A	423	ARG
1	A	486	GLN
1	A	499	ASP
1	A	714	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	GLN
1	A	551	ASN
1	A	640	GLN
1	A	652	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	0/21	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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	OKT	B	922	2	19,22,23	4.40	13 (68%)	25,31,34	1.79	5 (20%)
2	UFT	B	910	2	18,21,22	4.34	15 (83%)	25,30,33	1.90	5 (20%)
2	OMG	B	911	2	23,26,27	1.13	3 (13%)	32,38,41	1.10	1 (3%)
2	F2T	B	923	2	18,21,22	4.65	15 (83%)	25,30,33	2.14	6 (24%)
2	UFT	B	908	2	18,21,22	4.21	13 (72%)	25,30,33	2.16	7 (28%)
2	AF2	B	906	2	21,24,25	3.42	9 (42%)	30,35,38	2.60	11 (36%)
2	GF2	B	907	2	22,25,26	3.67	14 (63%)	32,37,40	2.28	13 (40%)
2	A1CAK	B	902	2	22,25,26	3.62	13 (59%)	32,37,40	2.29	13 (40%)
2	A1CAM	B	901	2	33,33,33	1.49	8 (24%)	44,46,46	1.28	5 (11%)
2	RFJ	B	905	2	23,26,27	3.25	13 (56%)	32,38,41	2.11	11 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMG	B	909	2	23,26,27	1.10	3 (13%)	32,38,41	1.05	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
2	OKT	B	922	2	-	1/9/27/28	0/2/2/2
2	UFT	B	910	2	-	0/7/25/26	0/2/2/2
2	OMG	B	911	2	-	3/9/27/28	0/3/3/3
2	F2T	B	923	2	-	1/7/25/26	0/2/2/2
2	UFT	B	908	2	-	0/7/25/26	0/2/2/2
2	AF2	B	906	2	-	0/7/25/26	0/3/3/3
2	GF2	B	907	2	-	0/7/25/26	0/3/3/3
2	A1CAK	B	902	2	-	1/7/25/26	0/3/3/3
2	A1CAM	B	901	2	-	4/20/36/36	0/3/3/3
2	RFJ	B	905	2	-	1/9/27/28	0/3/3/3
2	OMG	B	909	2	-	2/9/27/28	0/3/3/3

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	A1CAK	C3'-C4'	-9.39	1.29	1.53
2	B	907	GF2	C3'-C4'	-9.23	1.29	1.53
2	B	923	F2T	C2-N1	8.29	1.51	1.38
2	B	908	UFT	O4'-C4'	-8.18	1.26	1.45
2	B	906	AF2	C3'-C4'	-8.16	1.32	1.53
2	B	905	RFJ	C2'-C1'	-8.05	1.33	1.53
2	B	922	OKT	O4'-C4'	-7.82	1.27	1.45
2	B	923	F2T	C2-N3	7.69	1.51	1.38
2	B	910	UFT	O4'-C4'	-7.62	1.28	1.45
2	B	922	OKT	C2-N3	7.60	1.51	1.38
2	B	922	OKT	C2-N1	7.55	1.50	1.38
2	B	910	UFT	C2-N1	7.53	1.50	1.38
2	B	908	UFT	C2-N1	7.08	1.49	1.38
2	B	906	AF2	C6-N6	6.98	1.52	1.34
2	B	910	UFT	C2-N3	6.72	1.49	1.38
2	B	923	F2T	C6-C5	6.65	1.50	1.35
2	B	906	AF2	O4'-C4'	6.56	1.59	1.45
2	B	902	A1CAK	C4-N3	6.51	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	905	RFJ	C4-N3	6.40	1.48	1.34
2	B	907	GF2	C4-N3	6.31	1.48	1.34
2	B	908	UFT	C2-N3	6.30	1.48	1.38
2	B	902	A1CAK	F-C2'	-6.20	1.28	1.40
2	B	923	F2T	O4'-C4'	-6.17	1.31	1.45
2	B	907	GF2	F-C2'	-5.88	1.28	1.40
2	B	922	OKT	C6-C5	5.77	1.48	1.35
2	B	910	UFT	C6-C5	5.75	1.48	1.35
2	B	923	F2T	C2'-C1'	5.74	1.60	1.53
2	B	908	UFT	C6-C5	5.45	1.47	1.35
2	B	905	RFJ	C2-N3	5.44	1.46	1.33
2	B	906	AF2	O4'-C1'	-5.44	1.29	1.42
2	B	902	A1CAK	C2-N3	5.32	1.46	1.33
2	B	907	GF2	O4'-C1'	-5.22	1.29	1.42
2	B	907	GF2	C2-N3	5.21	1.45	1.33
2	B	922	OKT	C3'-C4'	5.20	1.66	1.53
2	B	910	UFT	F2'-C2'	5.18	1.50	1.40
2	B	922	OKT	O4'-C1'	5.16	1.53	1.42
2	B	923	F2T	C1'-N1	-5.13	1.33	1.47
2	B	923	F2T	C3'-C4'	4.89	1.65	1.53
2	B	908	UFT	F2'-C2'	4.78	1.49	1.40
2	B	922	OKT	O01-C2'	4.76	1.54	1.42
2	B	908	UFT	C1'-N1	-4.76	1.34	1.47
2	B	922	OKT	C4-N3	4.74	1.46	1.38
2	B	907	GF2	C2-N2	4.60	1.44	1.34
2	B	922	OKT	C1'-N1	-4.57	1.34	1.47
2	B	910	UFT	C1'-N1	-4.51	1.34	1.47
2	B	902	A1CAK	C2-N2	4.49	1.44	1.34
2	B	910	UFT	O4'-C1'	4.41	1.52	1.42
2	B	910	UFT	C4-N3	4.25	1.45	1.38
2	B	910	UFT	C3'-C4'	4.23	1.63	1.53
2	B	923	F2T	C4-N3	4.15	1.45	1.38
2	B	923	F2T	O2-C2	-4.00	1.16	1.23
2	B	908	UFT	O4'-C1'	3.95	1.51	1.42
2	B	905	RFJ	C2-N2	3.94	1.43	1.34
2	B	908	UFT	C3'-C4'	3.85	1.62	1.53
2	B	908	UFT	C4-N3	3.81	1.45	1.38
2	B	905	RFJ	O3'-C3'	-3.77	1.33	1.43
2	B	923	F2T	O4'-C1'	3.77	1.50	1.42
2	B	901	A1CAM	C2-N1	3.50	1.43	1.38
2	B	923	F2T	F2'-C2'	3.43	1.47	1.40
2	B	901	A1CAM	P-O5'	3.35	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	922	OKT	C6-N1	3.34	1.46	1.38
2	B	923	F2T	O4-C4	-3.30	1.18	1.24
2	B	907	GF2	C5-N7	-3.30	1.32	1.39
2	B	911	OMG	C2-N2	3.25	1.41	1.34
2	B	902	A1CAK	C5-N7	-3.22	1.32	1.39
2	B	908	UFT	O4-C4	-3.21	1.18	1.24
2	B	905	RFJ	C5-N7	-3.20	1.32	1.39
2	B	906	AF2	C5-N7	-3.20	1.33	1.39
2	B	905	RFJ	C2-N1	3.19	1.45	1.37
2	B	909	OMG	C2-N2	3.17	1.41	1.34
2	B	923	F2T	C5-C4	3.17	1.50	1.43
2	B	910	UFT	O3'-C3'	3.15	1.50	1.43
2	B	905	RFJ	O2'-C2'	3.08	1.50	1.42
2	B	906	AF2	F-C2'	-3.04	1.34	1.40
2	B	902	A1CAK	C2'-C3'	2.99	1.56	1.52
2	B	910	UFT	O4-C4	-2.89	1.18	1.24
2	B	905	RFJ	C5-C6	2.88	1.55	1.44
2	B	908	UFT	O3'-C3'	2.87	1.50	1.43
2	B	902	A1CAK	O4'-C4'	2.80	1.51	1.45
2	B	923	F2T	C6-N1	2.80	1.44	1.38
2	B	902	A1CAK	O6-C6	-2.79	1.18	1.23
2	B	901	A1CAM	P-OP3	2.79	1.70	1.59
2	B	907	GF2	O6-C6	-2.78	1.18	1.23
2	B	922	OKT	C5-C4	2.75	1.49	1.43
2	B	908	UFT	O2-C2	-2.72	1.18	1.23
2	B	906	AF2	O3'-C3'	2.62	1.49	1.43
2	B	910	UFT	C6-N1	2.60	1.44	1.38
2	B	907	GF2	C2-N1	2.58	1.43	1.37
2	B	905	RFJ	C1'-N9	-2.53	1.40	1.47
2	B	905	RFJ	O6-C6	-2.51	1.18	1.23
2	B	922	OKT	O3'-C3'	2.46	1.49	1.43
2	B	906	AF2	C5-C4	-2.45	1.34	1.39
2	B	902	A1CAK	C2-N1	2.45	1.43	1.37
2	B	907	GF2	C2'-C3'	2.44	1.55	1.52
2	B	910	UFT	C2'-C1'	2.44	1.56	1.53
2	B	902	A1CAK	O3'-C3'	2.42	1.48	1.43
2	B	907	GF2	C4-N9	-2.41	1.31	1.38
2	B	910	UFT	O2-C2	-2.38	1.18	1.23
2	B	922	OKT	O4-C4	-2.38	1.19	1.24
2	B	905	RFJ	C4-N9	-2.38	1.32	1.38
2	B	902	A1CAK	C5-C6	2.35	1.53	1.44
2	B	908	UFT	C6-N1	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	909	OMG	C6-N1	2.30	1.43	1.38
2	B	901	A1CAM	C2-N3	2.29	1.42	1.38
2	B	906	AF2	C1'-N9	2.28	1.52	1.46
2	B	905	RFJ	O5'-C5'	-2.27	1.37	1.44
2	B	901	A1CAM	C1'-N1	2.27	1.54	1.47
2	B	911	OMG	C6-N1	2.24	1.43	1.38
2	B	907	GF2	C5-C6	2.17	1.52	1.44
2	B	907	GF2	C2'-C1'	2.14	1.55	1.53
2	B	910	UFT	C5-C4	2.13	1.48	1.43
2	B	911	OMG	C4-N3	2.10	1.39	1.34
2	B	923	F2T	O3'-C3'	2.10	1.48	1.43
2	B	902	A1CAK	C4-N9	-2.09	1.32	1.38
2	B	907	GF2	O3'-C3'	2.09	1.48	1.43
2	B	901	A1CAM	O4'-C1'	-2.05	1.37	1.42
2	B	909	OMG	C4-N3	2.05	1.38	1.34
2	B	901	A1CAM	C2'-C1'	2.03	1.58	1.53
2	B	901	A1CAM	O5'-C5'	-2.01	1.37	1.44

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	908	UFT	C4-N3-C2	-5.91	119.28	126.61
2	B	923	F2T	C4-N3-C2	-5.70	119.53	126.61
2	B	906	AF2	N3-C2-N1	-5.69	119.97	128.58
2	B	906	AF2	C5-C4-N3	-5.68	118.90	126.72
2	B	906	AF2	C1'-N9-C8	5.58	139.49	127.09
2	B	910	UFT	C4-N3-C2	-5.39	119.92	126.61
2	B	922	OKT	C4-N3-C2	-5.30	120.03	126.61
2	B	902	A1CAK	C5-C4-N3	-5.29	119.97	128.39
2	B	905	RFJ	C5-C4-N3	-5.04	120.37	128.39
2	B	923	F2T	C2'-C1'-N1	-4.79	106.91	114.27
2	B	907	GF2	C5-C4-N3	-4.78	120.78	128.39
2	B	907	GF2	C1'-N9-C4	-4.76	112.44	126.49
2	B	908	UFT	C2'-C1'-N1	-4.63	107.16	114.27
2	B	906	AF2	C4-N9-C1'	-4.46	116.20	126.63
2	B	905	RFJ	C2-N3-C4	4.44	119.94	112.30
2	B	902	A1CAK	C2-N3-C4	4.31	119.73	112.30
2	B	907	GF2	C2-N3-C4	4.10	119.36	112.30
2	B	906	AF2	N6-C6-N1	-4.03	109.40	118.38
2	B	907	GF2	C1'-N9-C8	4.00	138.10	126.73
2	B	902	A1CAK	C1'-N9-C4	-3.97	114.75	126.49
2	B	906	AF2	C2-N3-C4	3.96	121.51	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	923	F2T	N3-C2-N1	3.96	120.04	114.89
2	B	906	AF2	C5-C4-N9	3.94	110.10	105.81
2	B	908	UFT	N3-C2-N1	3.92	119.99	114.89
2	B	908	UFT	C5-C4-N3	3.91	120.27	114.80
2	B	923	F2T	C5-C4-N3	3.81	120.14	114.80
2	B	910	UFT	N3-C2-N1	3.77	119.79	114.89
2	B	902	A1CAK	N9-C4-N3	3.64	133.23	125.95
2	B	901	A1CAM	N3-C2-N1	3.63	119.61	114.89
2	B	907	GF2	N9-C8-N7	-3.52	106.87	113.40
2	B	922	OKT	C5-C4-N3	3.49	119.69	114.80
2	B	910	UFT	C5-C4-N3	3.47	119.66	114.80
2	B	922	OKT	N3-C2-N1	3.44	119.37	114.89
2	B	922	OKT	O4-C4-C5	-3.43	119.25	125.16
2	B	905	RFJ	C2'-C1'-N9	-3.42	107.75	114.24
2	B	902	A1CAK	O4'-C1'-C2'	-3.40	102.25	105.84
2	B	902	A1CAK	C3'-C2'-C1'	-3.31	99.26	103.10
2	B	902	A1CAK	N9-C8-N7	-3.29	107.29	113.40
2	B	901	A1CAM	C4-N3-C2	-3.28	122.54	126.61
2	B	902	A1CAK	C1'-N9-C8	3.28	136.04	126.73
2	B	905	RFJ	C2-N1-C6	-3.22	119.27	125.11
2	B	901	A1CAM	C6-N1-C2	-3.17	117.14	121.00
2	B	923	F2T	O4-C4-C5	-3.14	119.75	125.16
2	B	907	GF2	N9-C4-N3	3.09	132.13	125.95
2	B	905	RFJ	C3'-C2'-C1'	3.08	108.71	102.81
2	B	905	RFJ	N9-C8-N7	-3.07	107.71	113.40
2	B	907	GF2	C2-N1-C6	-3.04	119.59	125.11
2	B	902	A1CAK	C2-N1-C6	-3.04	119.60	125.11
2	B	910	UFT	O4-C4-C5	-2.94	120.09	125.16
2	B	908	UFT	O4-C4-C5	-2.94	120.09	125.16
2	B	901	A1CAM	O2-C2-N1	-2.85	119.08	122.80
2	B	905	RFJ	N9-C4-N3	2.84	131.64	125.95
2	B	910	UFT	C2'-C1'-N1	-2.83	109.92	114.27
2	B	905	RFJ	C5-C6-N1	2.78	120.34	113.25
2	B	907	GF2	C2'-C1'-N9	-2.74	110.06	114.27
2	B	905	RFJ	O4'-C1'-C2'	2.69	111.21	106.59
2	B	902	A1CAK	C2'-C1'-N9	-2.67	110.16	114.27
2	B	907	GF2	O6-C6-C5	-2.66	119.50	126.53
2	B	907	GF2	C5-C6-N1	2.61	119.90	113.25
2	B	902	A1CAK	C5-C6-N1	2.59	119.84	113.25
2	B	907	GF2	O4'-C4'-C3'	2.50	110.12	105.15
2	B	911	OMG	N1-C2-N3	2.49	127.88	123.32
2	B	909	OMG	N1-C2-N3	2.48	127.86	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	907	GF2	C3'-C2'-C1'	-2.47	100.23	103.10
2	B	902	A1CAK	O6-C6-C5	-2.40	120.21	126.53
2	B	905	RFJ	O6-C6-C5	-2.39	120.23	126.53
2	B	906	AF2	C5-C6-N1	2.38	123.57	117.51
2	B	907	GF2	C8-N7-C5	2.28	108.32	104.26
2	B	901	A1CAM	O2'-C2'-C1'	2.26	113.28	108.99
2	B	906	AF2	N3-C4-N9	2.25	131.00	127.17
2	B	923	F2T	O2-C2-N1	-2.24	119.89	122.80
2	B	902	A1CAK	C8-N7-C5	2.23	108.23	104.26
2	B	922	OKT	O2-C2-N1	-2.18	119.95	122.80
2	B	906	AF2	C4-C5-N7	-2.14	108.13	110.58
2	B	906	AF2	N9-C8-N7	-2.11	110.95	113.94
2	B	908	UFT	O2-C2-N1	-2.10	120.06	122.80
2	B	905	RFJ	C8-N7-C5	2.04	107.89	104.26
2	B	909	OMG	C6-C5-C4	2.01	121.85	118.83
2	B	908	UFT	C2'-C3'-C4'	-2.01	99.79	102.43

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	A1CAM	CB'-CC'-CD'-CE'
2	B	905	RFJ	C1'-C2'-O2'-C
2	B	911	OMG	C1'-C2'-O2'-CM2
2	B	922	OKT	C1'-C2'-O01-C02
2	B	901	A1CAM	C3'-C4'-C5'-O5'
2	B	901	A1CAM	O4'-C4'-C5'-O5'
2	B	909	OMG	O4'-C4'-C5'-O5'
2	B	911	OMG	O4'-C4'-C5'-O5'
2	B	911	OMG	C3'-C4'-C5'-O5'
2	B	923	F2T	O4'-C4'-C5'-O5'
2	B	909	OMG	C3'-C4'-C5'-O5'
2	B	901	A1CAM	OP3-CB'-CC'-CD'
2	B	902	A1CAK	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	911	OMG	1	0
2	B	906	AF2	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	907	GF2	1	0
2	B	902	A1CAK	2	0
2	B	901	A1CAM	2	0
2	B	905	RFJ	1	0
2	B	909	OMG	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
4	IPH	A	904	-	7,7,7	0.64	0	8,8,8	0.33	0
4	IPH	A	903	-	7,7,7	0.60	0	8,8,8	0.32	0

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
4	IPH	A	904	-	-	-	0/1/1/1
4	IPH	A	903	-	-	-	0/1/1/1

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	803/859 (93%)	0.51	39 (4%) 35 36	26, 55, 87, 105	0
2	B	0/21	-	-	-	-
All	All	803/880 (91%)	0.51	39 (4%) 35 36	26, 55, 87, 105	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	ALA	4.3
1	A	602	PRO	3.7
1	A	243	ILE	3.5
1	A	271	HIS	3.1
1	A	272	CYS	3.1
1	A	151	LEU	2.9
1	A	270	THR	2.8
1	A	127	ILE	2.7
1	A	355	LYS	2.7
1	A	269	ILE	2.6
1	A	104	MET	2.6
1	A	485	ILE	2.6
1	A	353	ILE	2.5
1	A	117	VAL	2.5
1	A	132	ILE	2.5
1	A	839	HIS	2.5
1	A	89	ASP	2.4
1	A	855	THR	2.4
1	A	520	VAL	2.4
1	A	249	PRO	2.4
1	A	109	GLY	2.4
1	A	453	ILE	2.4
1	A	120	PRO	2.3
1	A	195	GLY	2.3
1	A	571	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	110	ARG	2.3
1	A	237	VAL	2.3
1	A	352	CYS	2.3
1	A	240	PHE	2.2
1	A	492	CYS	2.2
1	A	242	SER	2.2
1	A	487	GLY	2.2
1	A	369	ALA	2.2
1	A	449	LYS	2.1
1	A	455	CYS	2.1
1	A	143	LEU	2.0
1	A	470	PHE	2.0
1	A	119	LEU	2.0
1	A	250	LEU	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	OMG	B	911	24/25	0.58	0.18	64,83,98,99	0
2	OKT	B	922	21/22	0.68	0.16	67,75,90,96	0
2	OMG	B	909	24/25	0.82	0.13	67,74,81,83	0
2	UFT	B	910	20/21	0.87	0.10	66,74,81,82	0
2	A1CAM	B	901	31/31	0.93	0.09	52,61,70,70	0
2	UFT	B	908	20/21	0.93	0.10	35,59,68,68	0
2	RFJ	B	905	24/25	0.94	0.08	42,49,57,60	0
2	A1CAK	B	902	23/24	0.94	0.07	46,52,55,62	0
2	F2T	B	923	20/21	0.94	0.09	45,56,65,68	0
2	AF2	B	906	22/23	0.96	0.08	36,43,56,58	0
2	GF2	B	907	23/24	0.96	0.08	34,48,59,62	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	IPH	A	904	7/7	0.82	0.19	40,43,51,54	0
4	IPH	A	903	7/7	0.86	0.14	40,42,46,60	0
3	MG	A	902	1/1	0.95	0.04	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.