



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:26 PM UTC

PDB ID : 5JS2 / pdb_00005js2
Title : Human Argonaute-2 Bound to a Modified siRNA
Authors : Schirle, N.T.; MacRae, I.J.
Deposited on : 2016-05-07
Resolution : 2.95 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)
Xtrriage (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

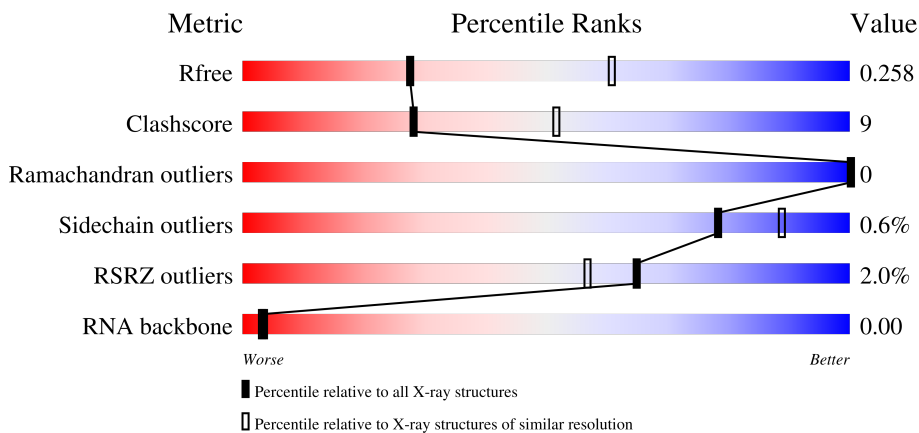
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)
RNA backbone	3983	1046 (3.16-2.76)

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	859	 2% 76% 16% • 7%
2	B	6	 17% 83%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6593 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	800	6432	4095	1156	1142	39	0	0	0

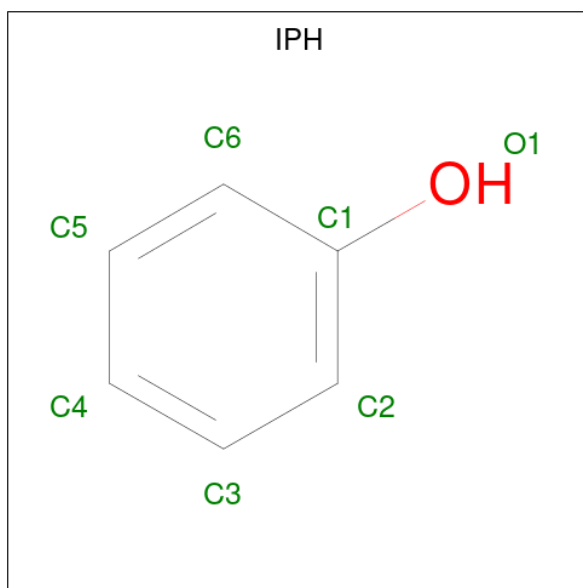
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ASP	SER	engineered mutation	UNP Q9UKV8

- Molecule 2 is a RNA chain called modified siRNA.

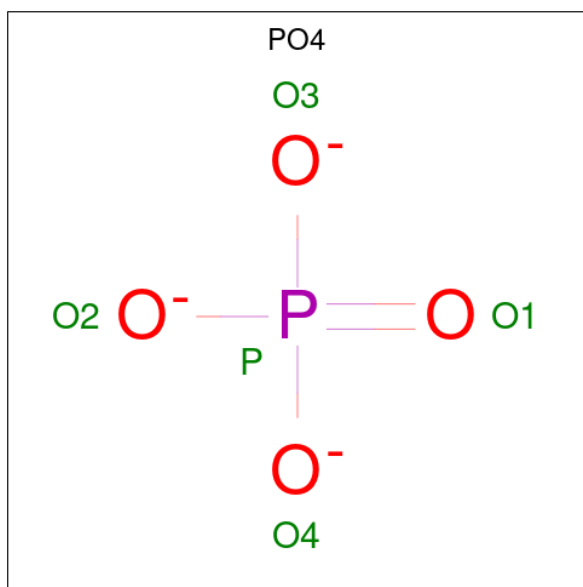
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace	
			Total	C	F	N	O	P				S
2	B	6	130	62	3	16	40	6	3	0	0	0

- Molecule 3 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

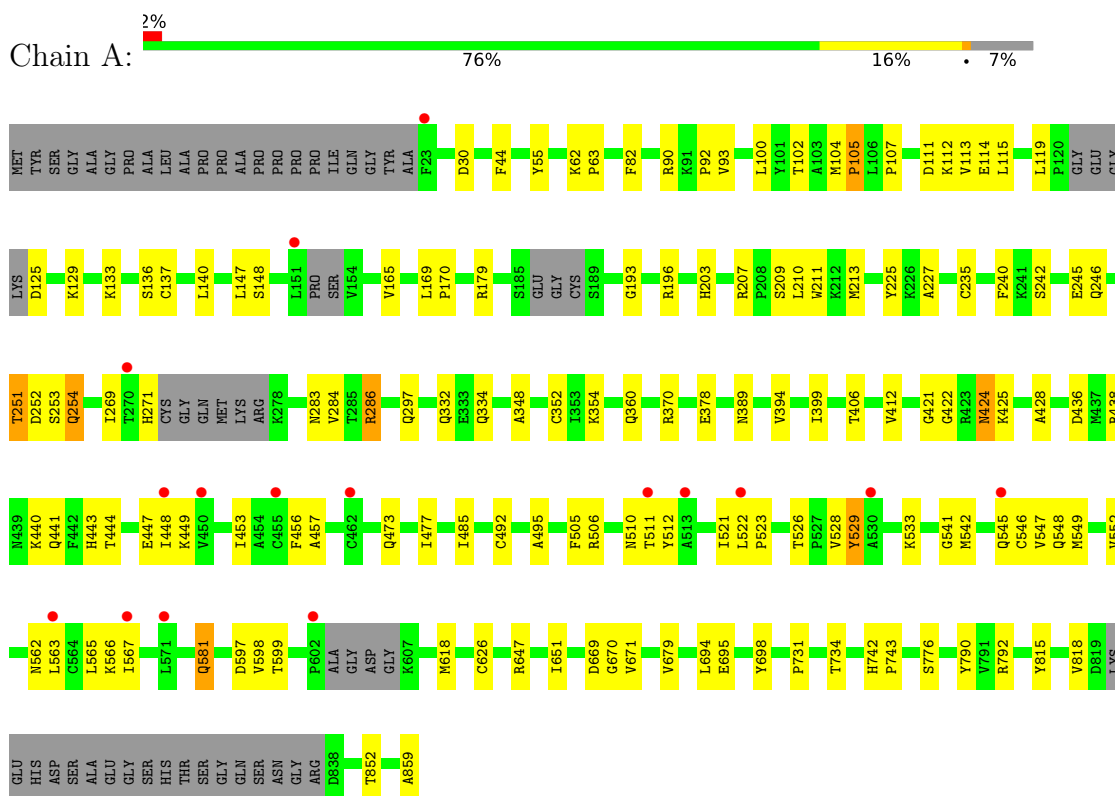
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	11	Total O 11 11	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



- Molecule 2: modified siRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.10Å 107.55Å 68.89Å 90.00° 107.39° 90.00°	Depositor
Resolution (Å)	38.98 – 2.95 38.98 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.98-2.95) 98.1 (38.98-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.95Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.222 , 0.261 0.222 , 0.258	Depositor DCC
R_{free} test set	916 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtrriage
Anisotropy	0.169	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6593	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: UFT, PO4, MG, F2T, 6NW, 6OP, IPH, 6OO

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	0.47	1/6582 (0.0%)	0.77	9/8907 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	529	TYR	C-N	-7.35	1.24	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ASP	N-CA-C	7.59	121.23	110.23
1	A	251	THR	N-CA-C	-7.12	100.46	110.50
1	A	252	ASP	N-CA-C	-6.80	103.87	111.28
1	A	818	VAL	N-CA-C	6.40	117.08	110.36
1	A	424	ASN	N-CA-C	6.04	117.94	111.36
1	A	105	PRO	N-CA-C	5.13	119.15	111.14
1	A	107	PRO	CA-C-N	-5.10	116.48	122.14
1	A	107	PRO	C-N-CA	-5.10	116.48	122.14
1	A	209	SER	N-CA-C	-5.06	101.21	108.60

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	6432	0	6487	109	0
2	B	130	0	18	9	0
3	A	14	0	12	0	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
6	A	11	0	0	1	0
All	All	6593	0	6517	116	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 9.

All (116) 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:902:F2T:SP1	2:B:902:F2T:P	1.52	1.49
1:A:251:THR:HB	1:A:254:GLN:HG3	1.21	1.15
1:A:251:THR:HG22	1:A:253:SER:H	1.19	1.04
1:A:389:ASN:ND2	6:A:1001:HOH:O	1.91	1.03
1:A:251:THR:HB	1:A:254:GLN:CG	1.90	1.00
1:A:251:THR:HG22	1:A:253:SER:N	1.77	0.99
1:A:251:THR:CG2	1:A:253:SER:HB3	1.97	0.95
1:A:251:THR:HG21	1:A:253:SER:HB3	1.52	0.89
1:A:114:GLU:O	1:A:115:LEU:HD23	1.78	0.84
2:B:902:F2T:SP1	2:B:902:F2T:OP2	2.37	0.82
1:A:246:GLN:NE2	1:A:254:GLN:HE22	1.78	0.82
1:A:251:THR:CB	1:A:254:GLN:HG3	2.11	0.77
1:A:251:THR:CG2	1:A:253:SER:CB	2.63	0.76
2:B:902:F2T:SP1	2:B:902:F2T:O5'	2.43	0.75
1:A:251:THR:HG22	1:A:253:SER:CB	2.19	0.73
1:A:196:ARG:NH1	1:A:352:CYS:SG	2.63	0.71
1:A:251:THR:HG22	1:A:253:SER:HB3	1.73	0.70
1:A:545:GLN:NE2	1:A:546:CYS:O	2.25	0.69
1:A:669:ASP:OD1	1:A:670:GLY:N	2.27	0.68
1:A:566:LYS:HE3	1:A:859:ALA:OXT	1.94	0.68
1:A:546:CYS:HB2	2:B:901:6OP:C6'	2.25	0.67
1:A:246:GLN:HE21	1:A:254:GLN:HE22	1.42	0.66
1:A:193:GLY:O	1:A:360:GLN:NE2	2.30	0.65
1:A:44:PHE:HE2	1:A:207:ARG:HD2	1.60	0.65
1:A:92:PRO:HB3	1:A:102:THR:HG22	1.77	0.65
1:A:526:THR:HG22	1:A:528:VAL:H	1.62	0.64
1:A:251:THR:HG21	1:A:253:SER:CB	2.24	0.63
1:A:332:GLN:HB3	1:A:334:GLN:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ILE:HD12	1:A:485:ILE:HG12	1.81	0.62
1:A:210:LEU:O	1:A:211:TRP:HB2	2.01	0.60
1:A:246:GLN:NE2	1:A:254:GLN:NE2	2.50	0.59
1:A:251:THR:CG2	1:A:253:SER:H	2.06	0.59
1:A:428:ALA:HB2	1:A:440:LYS:HE2	1.84	0.59
1:A:147:LEU:HD21	1:A:213:MET:HE2	1.86	0.58
1:A:44:PHE:CE2	1:A:207:ARG:HD2	2.41	0.56
1:A:563:LEU:O	1:A:567:ILE:HG13	2.05	0.56
1:A:82:PHE:CZ	1:A:115:LEU:HB3	2.42	0.55
1:A:370:ARG:NH1	1:A:378:GLU:OE2	2.39	0.55
1:A:598:VAL:HG12	1:A:599:THR:N	2.19	0.55
2:B:903:6NW:C8	2:B:903:6NW:C5'	2.85	0.54
1:A:283:ASN:OD1	1:A:284:VAL:N	2.40	0.54
1:A:148:SER:CB	1:A:211:TRP:HZ3	2.22	0.53
1:A:529:TYR:HE1	1:A:815:TYR:CD2	2.27	0.53
1:A:562:ASN:HA	1:A:565:LEU:HD12	1.89	0.52
1:A:436:ASP:OD2	1:A:438:ARG:NE	2.42	0.52
1:A:448:ILE:HB	1:A:485:ILE:HA	1.92	0.52
1:A:92:PRO:HB2	1:A:100:LEU:HD11	1.91	0.52
1:A:505:PHE:HB3	1:A:542:MET:HE1	1.92	0.52
1:A:93:VAL:HG21	1:A:165:VAL:HG22	1.92	0.51
1:A:671:VAL:HG11	1:A:679:VAL:HG11	1.92	0.51
1:A:269:ILE:HG22	1:A:271:HIS:H	1.75	0.51
1:A:251:THR:HB	1:A:254:GLN:HG2	1.89	0.51
1:A:581:GLN:H	1:A:581:GLN:HE21	1.57	0.51
1:A:647:ARG:HG3	1:A:694:LEU:HD11	1.92	0.50
1:A:447:GLU:OE1	1:A:449:LYS:NZ	2.45	0.50
1:A:179:ARG:HE	1:A:203:HIS:HE1	1.60	0.49
1:A:529:TYR:CD1	1:A:529:TYR:C	2.91	0.49
1:A:581:GLN:H	1:A:581:GLN:NE2	2.10	0.49
1:A:412:VAL:HG22	1:A:734:THR:HG22	1.94	0.49
1:A:114:GLU:C	1:A:115:LEU:HG	2.38	0.49
1:A:30:ASP:O	1:A:776:SER:OG	2.28	0.48
1:A:55:TYR:CE2	1:A:105:PRO:HG3	2.49	0.48
1:A:90:ARG:NH2	1:A:104:MET:HG3	2.28	0.48
1:A:119:LEU:O	1:A:125:ASP:N	2.47	0.48
1:A:424:ASN:O	1:A:425:LYS:HB2	2.13	0.48
1:A:235:CYS:HA	1:A:240:PHE:HB2	1.95	0.48
1:A:521:ILE:HD13	1:A:552:VAL:HG21	1.96	0.48
1:A:523:PRO:HB3	1:A:549:MET:HE2	1.96	0.48
1:A:90:ARG:CZ	1:A:104:MET:HB2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:SER:HB3	1:A:211:TRP:HZ3	1.78	0.47
1:A:251:THR:HG22	1:A:253:SER:CA	2.43	0.47
1:A:394:VAL:HG13	1:A:399:ILE:HB	1.97	0.47
1:A:421:GLY:HA3	1:A:443:HIS:HA	1.97	0.47
1:A:456:PHE:HB2	1:A:522:LEU:HD12	1.96	0.47
1:A:112:LYS:HB2	1:A:133:LYS:HD2	1.96	0.47
1:A:114:GLU:O	1:A:115:LEU:CD2	2.57	0.47
1:A:225:TYR:OH	1:A:354:LYS:NZ	2.42	0.47
1:A:456:PHE:HA	1:A:495:ALA:O	2.14	0.47
1:A:790:TYR:CE2	1:A:792:ARG:HB2	2.51	0.46
1:A:112:LYS:HB2	1:A:133:LYS:HB2	1.97	0.46
1:A:227:ALA:HB2	1:A:348:ALA:HB2	1.98	0.45
1:A:93:VAL:O	1:A:100:LEU:HD12	2.17	0.45
2:B:905:6OO:C3'	2:B:905:6OO:C6	2.95	0.45
1:A:533:LYS:HD3	1:A:533:LYS:HA	1.80	0.44
1:A:506:ARG:O	1:A:510:ASN:ND2	2.50	0.44
1:A:529:TYR:CE1	1:A:815:TYR:CD2	3.05	0.44
1:A:548:GLN:HB2	2:B:902:F2T:SP1	2.58	0.44
1:A:62:LYS:HA	1:A:63:PRO:C	2.44	0.43
1:A:453:ILE:O	1:A:492:CYS:HA	2.18	0.43
1:A:695:GLU:HB2	1:A:698:TYR:HB2	1.99	0.43
1:A:422:GLY:HA3	1:A:441:GLN:HB2	2.01	0.43
1:A:731:PRO:O	1:A:734:THR:HG23	2.19	0.43
1:A:136:SER:OG	1:A:137:CYS:N	2.51	0.43
1:A:286:ARG:H	1:A:286:ARG:HG2	1.63	0.43
1:A:443:HIS:ND1	1:A:444:THR:HG23	2.33	0.43
1:A:62:LYS:HG3	1:A:129:LYS:HB2	2.00	0.43
1:A:742:HIS:CG	1:A:743:PRO:HD2	2.54	0.43
1:A:597:ASP:OD1	1:A:669:ASP:HB3	2.18	0.43
1:A:242:SER:O	1:A:245:GLU:HG2	2.19	0.43
1:A:251:THR:H	1:A:254:GLN:HG3	1.84	0.43
1:A:44:PHE:O	1:A:406:THR:OG1	2.32	0.42
1:A:148:SER:HB3	1:A:211:TRP:CZ3	2.54	0.42
1:A:547:VAL:HG12	1:A:548:GLN:O	2.20	0.42
2:B:905:6OO:C2'	2:B:906:UFT:H5'	2.50	0.42
1:A:511:THR:HG23	1:A:512:TYR:CD2	2.55	0.42
1:A:113:VAL:HG12	1:A:114:GLU:N	2.34	0.42
1:A:618:MET:HE3	1:A:626:CYS:HB3	2.01	0.42
1:A:541:GLY:HA2	1:A:852:THR:OG1	2.20	0.41
1:A:169:LEU:HB3	1:A:170:PRO:HD3	2.02	0.41
1:A:473:GLN:O	1:A:477:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:TRP:CE3	1:A:211:TRP:HA	2.55	0.41
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.90	0.41
2:B:903:6NW:C8	2:B:903:6NW:C3'	2.98	0.41
1:A:457:ALA:HA	1:A:523:PRO:HG3	2.02	0.41
1:A:647:ARG:O	1:A:651:ILE:HG12	2.20	0.41
1:A:581:GLN:HE21	1:A:581:GLN:N	2.18	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	786/859 (92%)	757 (96%)	29 (4%)	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	712/752 (95%)	708 (99%)	4 (1%)	78 89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	286	ARG
1	A	297	GLN
1	A	581	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	246	GLN
1	A	297	GLN
1	A	310	GLN
1	A	324	HIS
1	A	334	GLN
1	A	389	ASN
1	A	507	HIS
1	A	510	ASN
1	A	568	ASN
1	A	576	ASN
1	A	581	GLN
1	A	589	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	0/6	-	-

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 [i](#)

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
2	UFT	B	906	2	18,21,22	6.18	12 (66%)	25,30,33	2.36	9 (36%)
2	F2T	B	902	2	18,21,22	6.63	7 (38%)	25,30,33	2.35	8 (32%)
2	6OO	B	905	2	19,22,23	4.17	12 (63%)	25,31,34	1.99	4 (16%)
2	UFT	B	904	2	18,21,22	4.26	12 (66%)	25,30,33	2.22	7 (28%)
2	6OP	B	901	2	25,27,27	3.47	11 (44%)	33,39,39	2.88	10 (30%)
2	6NW	B	903	2	22,25,26	3.93	9 (40%)	30,36,39	2.39	13 (43%)

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	UFT	B	906	2	-	6/7/25/26	0/2/2/2
2	F2T	B	902	2	-	2/7/25/26	0/2/2/2
2	6OO	B	905	2	-	2/9/27/28	0/2/2/2
2	UFT	B	904	2	-	0/7/25/26	0/2/2/2
2	6OP	B	901	2	-	5/12/31/31	0/2/2/2
2	6NW	B	903	2	-	0/9/27/28	0/3/3/3

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	F2T	C2'-C1'	-23.39	1.25	1.53
2	B	906	UFT	C2'-C3'	-18.79	1.27	1.52
2	B	905	6OO	C3'-C2'	-13.83	1.22	1.53
2	B	901	6OP	C2'-C1'	-11.90	1.23	1.53
2	B	906	UFT	O4-C4	11.65	1.47	1.24
2	B	903	6NW	C2'-C1'	-10.94	1.26	1.53
2	B	904	UFT	C3'-C4'	-10.24	1.27	1.53
2	B	906	UFT	C2'-C1'	9.51	1.64	1.53
2	B	902	F2T	O4-C4	8.30	1.40	1.24
2	B	902	F2T	O4'-C1'	8.05	1.60	1.42
2	B	903	6NW	O4'-C4'	-8.03	1.27	1.45
2	B	903	6NW	O4'-C1'	7.89	1.60	1.42
2	B	902	F2T	O4'-C4'	-7.78	1.27	1.45
2	B	904	UFT	O4-C4	7.75	1.39	1.24
2	B	904	UFT	O4'-C4'	6.26	1.58	1.45
2	B	904	UFT	F2'-C2'	-6.16	1.28	1.40
2	B	904	UFT	O4'-C1'	-5.75	1.28	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	905	6OO	O4'-C1'	-5.53	1.29	1.42
2	B	901	6OP	C3'-C2'	5.25	1.64	1.53
2	B	901	6OP	O4'-C4'	5.23	1.53	1.44
2	B	903	6NW	O3'-C3'	-5.15	1.30	1.43
2	B	901	6OP	P-OP1	4.75	1.60	1.54
2	B	906	UFT	O4'-C1'	-4.73	1.31	1.42
2	B	901	6OP	O4'-C1'	4.41	1.52	1.42
2	B	903	6NW	C4-N3	4.11	1.42	1.34
2	B	902	F2T	O3'-C3'	-4.04	1.32	1.43
2	B	905	6OO	C2'-C1'	4.04	1.63	1.53
2	B	906	UFT	C1'-N1	-3.85	1.36	1.47
2	B	906	UFT	C5'-C4'	-3.79	1.40	1.51
2	B	905	6OO	C4-N4	3.74	1.43	1.33
2	B	905	6OO	C2-N1	-3.65	1.32	1.40
2	B	903	6NW	C6-N6	3.63	1.43	1.34
2	B	901	6OP	C4-C5	-3.50	1.39	1.44
2	B	901	6OP	C6-C5	3.37	1.40	1.34
2	B	905	6OO	C6-C5	3.28	1.42	1.35
2	B	906	UFT	C5-C4	-3.22	1.36	1.43
2	B	905	6OO	C5'-C4'	-3.21	1.41	1.51
2	B	904	UFT	C2'-C1'	-3.05	1.49	1.53
2	B	903	6NW	O5'-C5'	-3.02	1.35	1.44
2	B	905	6OO	O3'-C3'	3.00	1.50	1.43
2	B	901	6OP	C4'-C5'	2.99	1.60	1.50
2	B	906	UFT	O4'-C4'	2.97	1.51	1.45
2	B	904	UFT	C4-N3	-2.86	1.33	1.38
2	B	904	UFT	O3'-C3'	2.81	1.49	1.43
2	B	906	UFT	C6-C5	2.81	1.41	1.35
2	B	901	6OP	C2-N1	-2.78	1.34	1.38
2	B	905	6OO	C6-N1	-2.63	1.31	1.38
2	B	906	UFT	C3'-C4'	2.58	1.59	1.53
2	B	906	UFT	O3'-C3'	2.54	1.49	1.43
2	B	902	F2T	C6-C5	2.51	1.40	1.35
2	B	904	UFT	C6-C5	2.47	1.40	1.35
2	B	905	6OO	O2-C2	-2.42	1.19	1.23
2	B	904	UFT	C2-N3	-2.40	1.33	1.38
2	B	905	6OO	C3'-C4'	2.36	1.59	1.53
2	B	904	UFT	O2-C2	-2.29	1.19	1.23
2	B	906	UFT	C2-N3	-2.20	1.34	1.38
2	B	904	UFT	C6-N1	-2.16	1.32	1.38
2	B	903	6NW	C8-N9	-2.14	1.33	1.37
2	B	902	F2T	C2-N3	-2.14	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	6OP	C7-C5	2.08	1.55	1.50
2	B	905	6OO	C1'-N1	-2.05	1.41	1.47
2	B	901	6OP	C2-N3	-2.03	1.34	1.38
2	B	903	6NW	C4-N9	2.03	1.41	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	6OP	C4'-C5'-C6'	-8.09	109.05	123.89
2	B	905	6OO	C2'-C1'-N1	-6.81	101.33	114.24
2	B	901	6OP	C5-C4-N3	6.60	121.06	115.32
2	B	903	6NW	N3-C2-N1	-6.35	118.97	128.58
2	B	902	F2T	C5-C4-N3	6.07	123.30	114.80
2	B	901	6OP	O4-C4-C5	-6.04	118.01	124.92
2	B	901	6OP	C4-N3-C2	-5.84	119.69	127.34
2	B	901	6OP	N3-C2-N1	5.50	122.05	114.89
2	B	904	UFT	C5-C4-N3	5.24	122.14	114.80
2	B	906	UFT	O4'-C1'-C2'	5.21	111.35	105.84
2	B	906	UFT	N3-C2-N1	4.74	121.07	114.89
2	B	906	UFT	C4-N3-C2	-4.69	120.78	126.61
2	B	902	F2T	C6-C5-C4	-4.44	113.86	119.53
2	B	902	F2T	C4-N3-C2	-4.30	121.28	126.61
2	B	904	UFT	C6-C5-C4	-4.29	114.05	119.53
2	B	903	6NW	C5-C4-N3	-4.05	121.14	126.72
2	B	903	6NW	C2-N3-C4	3.99	121.58	111.83
2	B	904	UFT	O4-C4-C5	-3.86	118.50	125.16
2	B	903	6NW	C2'-C1'-N9	-3.76	107.56	113.75
2	B	902	F2T	O4-C4-C5	-3.74	118.71	125.16
2	B	903	6NW	N3-C4-N9	3.73	133.51	127.17
2	B	906	UFT	F2'-C2'-C3'	3.67	116.39	109.14
2	B	901	6OP	O4'-C1'-C2'	-3.63	100.33	106.59
2	B	902	F2T	F2'-C2'-C3'	-3.61	102.02	109.14
2	B	905	6OO	O2-C2-N3	-3.51	116.80	122.33
2	B	904	UFT	F2'-C2'-C1'	-3.48	101.90	108.88
2	B	901	6OP	C5-C6-N1	-3.48	119.53	123.31
2	B	904	UFT	C4-N3-C2	-3.42	122.37	126.61
2	B	904	UFT	O4'-C1'-N1	3.40	116.06	108.36
2	B	904	UFT	C3'-C2'-C1'	3.06	106.65	103.10
2	B	906	UFT	O4-C4-C5	-2.96	120.05	125.16
2	B	905	6OO	O4'-C1'-N1	2.84	114.79	108.36
2	B	903	6NW	C5'-C4'-C3'	-2.80	105.12	115.21
2	B	903	6NW	N9-C8-N7	-2.75	110.03	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	903	6NW	C4-N9-C8	2.71	108.58	105.74
2	B	906	UFT	C5-C4-N3	2.70	118.58	114.80
2	B	903	6NW	C5-N7-C8	2.69	107.69	103.45
2	B	906	UFT	C4'-O4'-C1'	-2.68	103.55	109.47
2	B	902	F2T	C2'-C1'-N1	-2.66	110.18	114.27
2	B	903	6NW	C2-N1-C6	2.51	122.85	118.73
2	B	903	6NW	O3'-C3'-C4'	-2.50	103.91	111.08
2	B	901	6OP	O2'-C2'-C1'	2.50	113.46	108.97
2	B	906	UFT	O4'-C1'-N1	2.42	113.83	108.36
2	B	905	6OO	C3'-C2'-C1'	2.38	107.36	102.81
2	B	901	6OP	C1'-O4'-C4'	-2.38	105.13	108.91
2	B	901	6OP	O2-C2-N1	-2.31	119.79	122.80
2	B	903	6NW	C6-C5-N7	2.19	136.31	132.09
2	B	902	F2T	C6-N1-C2	2.15	123.62	121.00
2	B	902	F2T	O4'-C4'-C3'	-2.15	100.88	105.15
2	B	906	UFT	C1'-N1-C2	2.07	121.31	117.59
2	B	903	6NW	C5-C6-N6	-2.05	118.21	123.29

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	6OP	C3'-C4'-C5'-C6'
2	B	906	UFT	C2'-C1'-N1-C6
2	B	906	UFT	C2'-C1'-N1-C2
2	B	902	F2T	O4'-C4'-C5'-O5'
2	B	905	6OO	O4'-C4'-C5'-O5'
2	B	906	UFT	O4'-C4'-C5'-O5'
2	B	906	UFT	C3'-C4'-C5'-O5'
2	B	905	6OO	C3'-C4'-C5'-O5'
2	B	901	6OP	O4'-C4'-C5'-C6'
2	B	902	F2T	C3'-C4'-C5'-O5'
2	B	901	6OP	C1'-C2'-O2'-CB'
2	B	906	UFT	O4'-C1'-N1-C6
2	B	901	6OP	CB'-CG'-OD'-CE'
2	B	901	6OP	CG'-CB'-O2'-C2'
2	B	906	UFT	O4'-C1'-N1-C2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	906	UFT	1	0
2	B	902	F2T	4	0
2	B	905	6OO	2	0
2	B	901	6OP	1	0
2	B	903	6NW	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	PO4	A	903	-	4,4,4	0.95	0	6,6,6	0.45	0
3	IPH	A	901	-	7,7,7	0.37	0	8,8,8	0.27	0
3	IPH	A	902	-	7,7,7	0.39	0	8,8,8	0.28	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
3	IPH	A	901	-	-	-	0/1/1/1
3	IPH	A	902	-	-	-	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, 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	800/859 (93%)	0.13	16 (2%) 65 57	30, 58, 97, 140	0
2	B	0/6	-	-	-	-
All	All	800/865 (92%)	0.13	16 (2%) 65 57	30, 58, 97, 140	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	CYS	4.2
1	A	448	ILE	2.8
1	A	522	LEU	2.7
1	A	462	CYS	2.7
1	A	545	GLN	2.5
1	A	151	LEU	2.4
1	A	567	ILE	2.4
1	A	563	LEU	2.3
1	A	270	THR	2.3
1	A	23	PHE	2.2
1	A	450	VAL	2.2
1	A	511	THR	2.1
1	A	513	ALA	2.1
1	A	530	ALA	2.0
1	A	602	PRO	2.0
1	A	571	LEU	2.0

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(\AA^2)	Q<0.9
2	UFT	B	906	20/21	0.73	0.15	74,96,102,103	0
2	F2T	B	902	20/21	0.87	0.09	62,69,85,100	0
2	6OP	B	901	26/26	0.90	0.09	55,75,81,84	0
2	6OO	B	905	21/22	0.91	0.11	48,80,84,87	0
2	6NW	B	903	23/24	0.94	0.08	52,63,69,71	0
2	UFT	B	904	20/21	0.96	0.06	51,66,72,75	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, 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(\AA^2)	Q<0.9
5	MG	A	904	1/1	0.70	0.13	68,68,68,68	0
4	PO4	A	903	5/5	0.87	0.08	70,73,85,95	0
3	IPH	A	901	7/7	0.89	0.11	52,55,59,64	0
3	IPH	A	902	7/7	0.93	0.10	48,52,55,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.