



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 04:18 am GMT

PDB ID : 5JS2
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

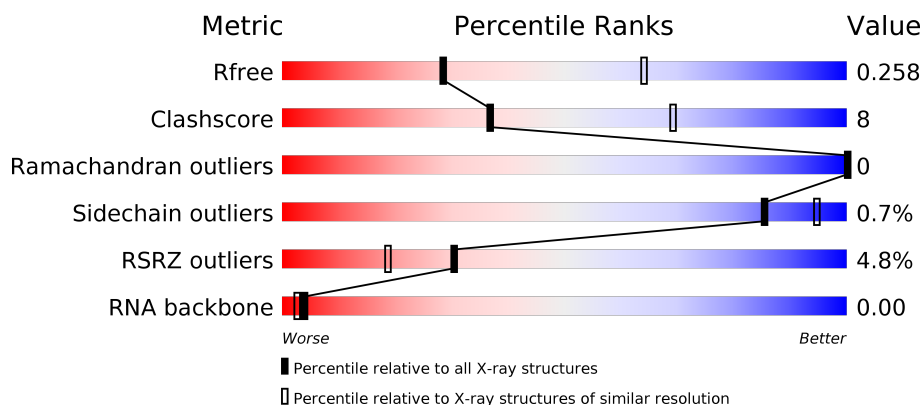
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


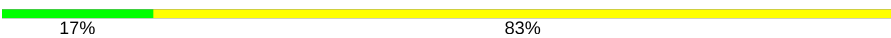
The reported resolution of this entry is 2.95 Å.

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}	111664	2641 (3.00-2.92)
Clashscore	122126	2988 (3.00-2.92)
Ramachandran outliers	120053	2892 (3.00-2.92)
Sidechain outliers	120020	2895 (3.00-2.92)
RSRZ outliers	108989	2527 (3.00-2.92)
RNA backbone	2636	1068 (3.30-2.62)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	B	6	

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

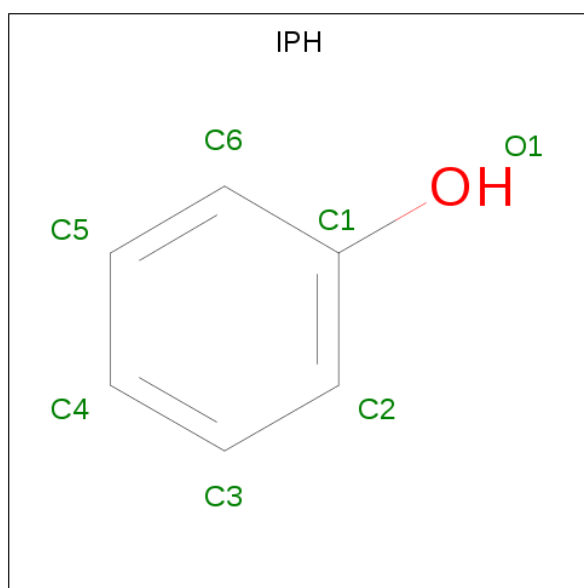
There is a discrepancy between the modelled and reference sequences:

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 (three-letter code: IPH) (formula: C₆H₆O).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.222 , 0.261 0.220 , 0.258	Depositor DCC
R_{free} test set	916 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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: MG, IPH, 6OO, 6NW, 6OP, F2T, UFT, PO4

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	0.34	0/6582	0.46	1/8907 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ASP	CB-CG-OD2	5.22	123.00	118.30

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	104	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	111	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 8.

All (111) 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:OP2	2:B:902:F2T:SP1	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:O5'	2:B:902:F2T:SP1	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
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: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:C5'	2:B:903:6NW:C8	2.85	0.54
1:A:283:ASN:OD1	1:A:284:VAL:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:90:ARG:CZ	1:A:104:MET:HB2	2.44	0.48
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
1:A:505:PHE:HB3	1:A:542:MET:HE1	1.99	0.45
2:B:905:6OO:C3'	2:B:905:6OO:C6	2.95	0.45
1:A:529:TYR:C	1:A:529:TYR:CD1	2.91	0.45
1:A:533:LYS:HA	1:A:533:LYS:HD3	1.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:114:GLU:C	1:A:115:LEU:HG	2.38	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: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: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
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:C3'	2:B:903:6NW:C8	2.98	0.41
1:A:647:ARG:O	1:A:651:ILE:HG12	2.20	0.41
1:A:457:ALA:HA	1:A:523:PRO:HG3	2.02	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 ⓘ

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	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%)	707 (99%)	5 (1%)	85	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	ASP
1	A	254	GLN
1	A	297	GLN
1	A	581	GLN
1	A	804	TYR

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

Mol	Chain	Res	Type
1	A	246	GLN
1	A	297	GLN
1	A	334	GLN
1	A	581	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	6OP	B	901	2	20,27,27	4.76	7 (35%)	23,39,39	2.32	6 (26%)
2	F2T	B	902	2	14,21,22	7.43	6 (42%)	17,30,33	2.56	4 (23%)
2	6NW	B	903	2	19,25,26	4.42	7 (36%)	20,36,39	2.90	4 (20%)
2	UFT	B	904	2	14,21,22	4.77	10 (71%)	17,30,33	2.86	4 (23%)
2	6OO	B	905	2	15,22,23	4.64	9 (60%)	19,31,34	1.64	3 (15%)
2	UFT	B	906	2	14,21,22	6.47	11 (78%)	17,30,33	3.07	5 (29%)

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	6OP	B	901	2	-	0/7/31/31	0/2/2/2
2	F2T	B	902	2	-	0/2/25/26	0/2/2/2
2	6NW	B	903	2	-	0/4/27/28	0/3/3/3
2	UFT	B	904	2	-	0/3/25/26	0/2/2/2
2	6OO	B	905	2	-	0/4/27/28	0/2/2/2
2	UFT	B	906	2	-	0/3/25/26	0/2/2/2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	F2T	C2'-C1'	-20.75	1.25	1.52
2	B	906	UFT	C2'-C3'	-17.55	1.27	1.52
2	B	901	6OP	C3'-C4'	-17.18	1.23	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	905	6OO	C3'-C2'	-13.84	1.22	1.53
2	B	904	UFT	C3'-C4'	-10.08	1.27	1.53
2	B	904	UFT	O4'-C1'	-8.96	1.28	1.41
2	B	905	6OO	O4'-C1'	-8.60	1.29	1.41
2	B	903	6NW	O4'-C4'	-7.98	1.27	1.45
2	B	902	F2T	O4'-C4'	-7.73	1.27	1.45
2	B	906	UFT	O4'-C1'	-7.27	1.31	1.41
2	B	903	6NW	O5'-C5'	-6.81	1.35	1.44
2	B	903	6NW	O3'-C3'	-5.19	1.30	1.43
2	B	904	UFT	F2'-C2'	-4.97	1.28	1.40
2	B	902	F2T	O5'-C5'	-4.15	1.39	1.44
2	B	902	F2T	O3'-C3'	-4.08	1.32	1.43
2	B	906	UFT	O5'-C5'	-4.06	1.39	1.44
2	B	906	UFT	C5'-C4'	-3.56	1.40	1.51
2	B	904	UFT	O5'-C5'	-3.39	1.40	1.44
2	B	905	6OO	C5'-C4'	-3.03	1.41	1.51
2	B	905	6OO	C6-N1	-2.97	1.31	1.35
2	B	904	UFT	C2'-C1'	-2.63	1.49	1.52
2	B	903	6NW	C8-N9	-2.51	1.33	1.36
2	B	904	UFT	C2-N3	-2.21	1.33	1.38
2	B	904	UFT	C6-N1	-2.13	1.32	1.35
2	B	906	UFT	C2-N3	-2.03	1.34	1.38
2	B	905	6OO	C2-N3	-2.03	1.34	1.38
2	B	905	6OO	C6-C5	2.09	1.42	1.38
2	B	903	6NW	C6-N6	2.32	1.43	1.34
2	B	905	6OO	C3'-C4'	2.32	1.59	1.53
2	B	905	6OO	C4-N4	2.50	1.43	1.35
2	B	906	UFT	C3'-C4'	2.53	1.59	1.53
2	B	906	UFT	O3'-C3'	2.55	1.49	1.43
2	B	901	6OP	C7-C5	2.59	1.55	1.51
2	B	901	6OP	C4'-C5'	2.69	1.60	1.50
2	B	904	UFT	O3'-C3'	2.82	1.49	1.43
2	B	906	UFT	O4'-C4'	2.95	1.51	1.45
2	B	905	6OO	O3'-C3'	3.02	1.50	1.43
2	B	906	UFT	C4-N3	3.23	1.38	1.33
2	B	903	6NW	C4-N3	4.54	1.42	1.35
2	B	901	6OP	P-OP1	4.58	1.60	1.54
2	B	901	6OP	O4'-C4'	4.83	1.53	1.44
2	B	901	6OP	C3'-C2'	5.24	1.64	1.53
2	B	904	UFT	O4-C4	5.99	1.39	1.24
2	B	904	UFT	O4'-C4'	6.22	1.58	1.45
2	B	902	F2T	O4-C4	6.42	1.40	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	6OP	O4'-C1'	7.84	1.52	1.41
2	B	906	UFT	C2'-C1'	8.56	1.64	1.52
2	B	906	UFT	O4-C4	9.02	1.47	1.24
2	B	903	6NW	O4'-C1'	13.59	1.60	1.41
2	B	902	F2T	O4'-C1'	13.87	1.60	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	903	6NW	N3-C2-N1	-11.56	118.97	128.86
2	B	901	6OP	C4'-C5'-C6'	-7.40	109.05	124.08
2	B	906	UFT	C4'-O4'-C1'	-6.02	103.55	109.83
2	B	902	F2T	C4'-O4'-C1'	-3.87	105.80	109.83
2	B	901	6OP	O4'-C1'-C2'	-3.60	100.33	106.60
2	B	904	UFT	F2'-C2'-C1'	-3.60	101.90	109.28
2	B	902	F2T	F2'-C2'-C3'	-3.42	102.02	109.13
2	B	903	6NW	C5'-C4'-C3'	-2.70	105.12	115.29
2	B	903	6NW	O3'-C3'-C4'	-2.47	103.91	111.06
2	B	901	6OP	C5-C6-N1	-2.42	119.53	122.15
2	B	901	6OP	C1'-O4'-C4'	-2.41	105.13	109.11
2	B	902	F2T	O4'-C4'-C3'	-2.16	100.88	105.15
2	B	905	6OO	C3'-C2'-C1'	2.35	107.36	102.89
2	B	903	6NW	C2-N1-C6	2.41	122.85	118.75
2	B	901	6OP	O2'-C2'-C1'	2.45	113.46	108.76
2	B	904	UFT	C3'-C2'-C1'	2.75	106.65	103.08
2	B	906	UFT	O4'-C1'-N1	2.91	113.83	108.05
2	B	905	6OO	O4'-C1'-N1	3.39	114.79	108.05
2	B	905	6OO	O2'-C2'-C3'	3.45	120.56	111.33
2	B	906	UFT	F2'-C2'-C3'	3.49	116.39	109.13
2	B	904	UFT	O4'-C1'-N1	4.03	116.06	108.05
2	B	906	UFT	O4'-C1'-C2'	5.29	111.35	105.74
2	B	901	6OP	C4-N3-C2	5.34	119.69	115.14
2	B	906	UFT	C4-N3-C2	7.72	120.78	114.14
2	B	902	F2T	C4-N3-C2	8.29	121.28	114.14
2	B	904	UFT	C4-N3-C2	9.57	122.37	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
3	IPH	A	901	-	7,7,7	0.38	0	8,8,8	0.22	0
3	IPH	A	902	-	7,7,7	0.39	0	8,8,8	0.23	0
4	PO4	A	903	-	4,4,4	0.75	0	6,6,6	0.37	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	-	-	0/0/0/0	0/1/1/1
3	IPH	A	902	-	-	0/0/0/0	0/1/1/1
4	PO4	A	903	-	-	0/0/0/0	0/0/0/0

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%)	0.23	38 (4%) 30 19	30, 58, 97, 140	0
2	B	0/6	-	-	-	-
All	All	800/865 (92%)	0.23	38 (4%) 30 19	30, 58, 97, 140	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	LYS	4.5
1	A	448	ILE	3.9
1	A	513	ALA	3.9
1	A	455	CYS	3.8
1	A	485	ILE	3.7
1	A	271	HIS	3.7
1	A	85	GLN	3.5
1	A	819	ASP	3.4
1	A	439	ASN	3.3
1	A	110	ARG	3.0
1	A	447	GLU	3.0
1	A	607	LYS	2.9
1	A	125	ASP	2.9
1	A	317	LYS	2.8
1	A	334	GLN	2.7
1	A	512	TYR	2.7
1	A	844	LYS	2.7
1	A	602	PRO	2.7
1	A	486	GLN	2.6
1	A	451	TRP	2.6
1	A	151	LEU	2.5
1	A	154	VAL	2.4
1	A	81	HIS	2.4
1	A	488	GLN	2.3
1	A	522	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	321	ARG	2.3
1	A	353	ILE	2.2
1	A	332	GLN	2.2
1	A	127	ILE	2.2
1	A	80	GLN	2.2
1	A	484	PRO	2.1
1	A	270	THR	2.1
1	A	507	HIS	2.1
1	A	423	ARG	2.1
1	A	462	CYS	2.1
1	A	65	LYS	2.1
1	A	461	GLN	2.0
1	A	247	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UFT	B	906	20/21	0.83	0.23	74,96,102,103	0
2	6OO	B	905	21/22	0.92	0.17	48,80,84,87	0
2	6OP	B	901	26/26	0.94	0.15	55,75,81,84	0
2	F2T	B	902	20/21	0.94	0.15	62,69,85,100	0
2	UFT	B	904	20/21	0.96	0.20	51,66,72,75	0
2	6NW	B	903	23/24	0.97	0.18	52,63,69,71	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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	0.78	0.18	68,68,68,68	0
4	PO4	A	903	5/5	0.93	0.18	70,73,85,95	0
3	IPH	A	901	7/7	0.94	0.28	52,55,59,64	0
3	IPH	A	902	7/7	0.97	0.14	48,52,55,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.