



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 4, 2020 – 03:10 pm BST

PDB ID : 1H1K
Title : THE BLUETONGUE VIRUS (BTV) CORE BINDS DSRNA
Authors : Diprose, J.M.; Grimes, J.M.; Sutton, G.C.; Burroughs, J.N.; Meyer, A.; Maan, S.; Mertens, P.P.C.; Stuart, D.I.
Deposited on : 2002-07-17
Resolution : 10.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

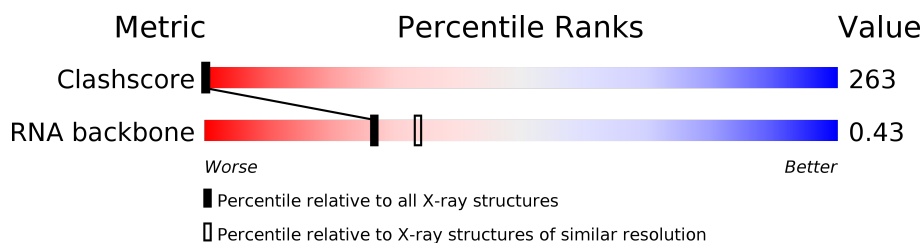
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 10.00 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))
Clashscore	141614	1071 (15.00-3.90)
RNA backbone	3102	1079 (11.50-3.00)

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 on 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	I	412	 78% 21%
2	J	276	 72% 25%
3	K	265	 77% 19%
4	L	412	 79% 21%
5	M	276	 73% 24%
6	N	265	 82% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 40008 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	412	Total	C	N	O	P	0	0	0
			9061	4120	2060	2470	411			

- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	276	Total	C	N	O	P	0	0	0
			6069	2760	1380	1654	275			

- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	265	Total	C	N	O	P	0	0	0
			5827	2650	1325	1588	264			

- Molecule 4 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	412	Total	C	N	O	P	0	0	0
			8237	3708	824	3294	411			

- Molecule 5 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	276	Total	C	N	O	P	0	0	0
			5517	2484	552	2206	275			

- Molecule 6 is a RNA chain called RNA.

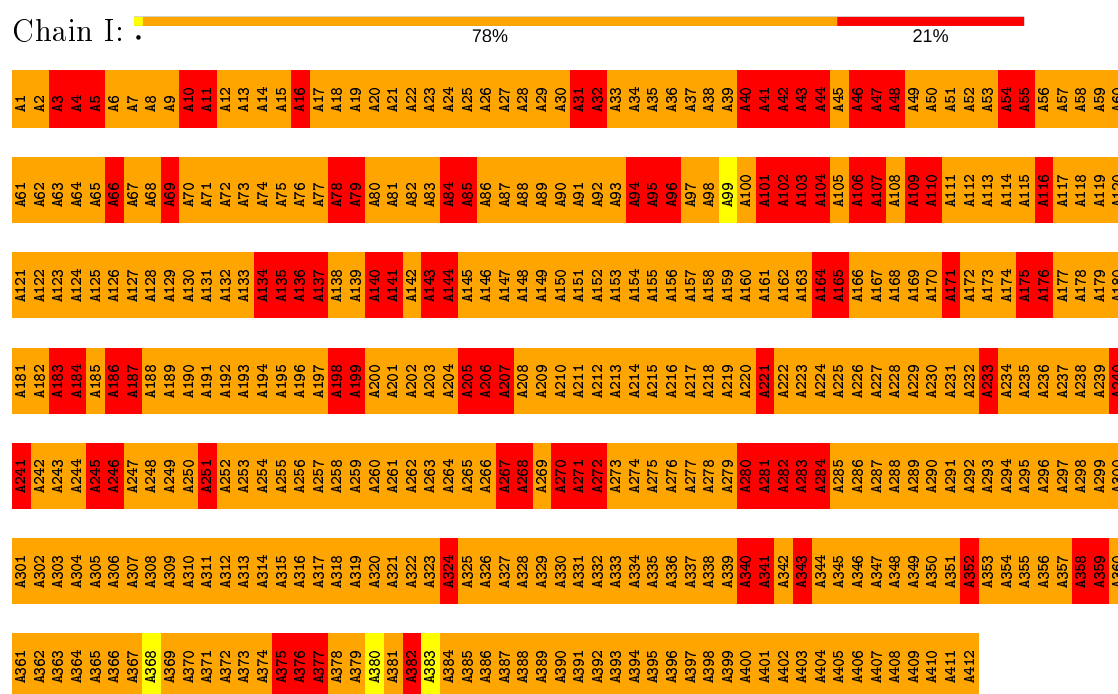
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	265	Total	C	N	O	P	0	0	0
			5297	2385	530	2118	264			

3 Residue-property plots

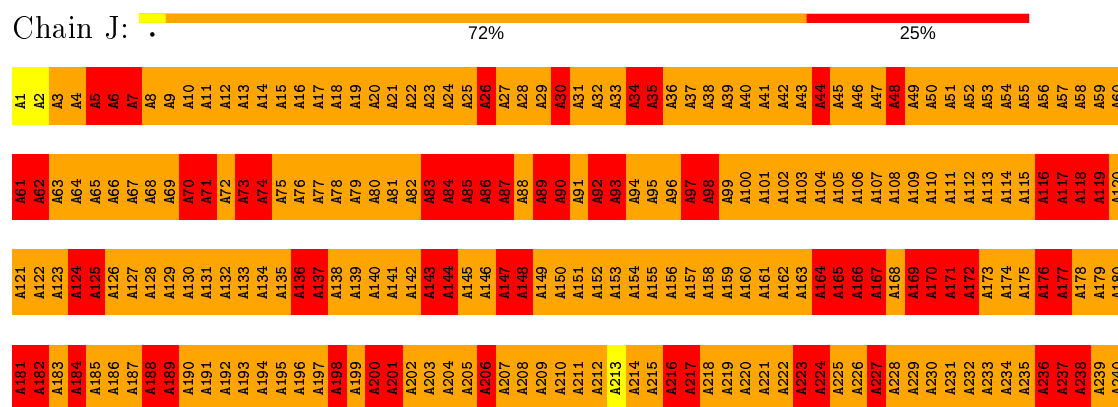
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS failed to run properly.

• Molecule 1: RNA




• Molecule 2: RNA



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• Molecule 3: RNA

Chain K:  77% 19%

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• Molecule 4: RNA

Chain L:  79% 21%

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• Molecule 5: RNA

Chain M:  73% 24%

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4 Data and refinement statistics [i](#)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	795.60 Å 821.80 Å 753.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 10.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-10.00)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 3.49 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.015	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.078 for k,h,-l	Xtriage
Total number of atoms	40008	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.12% 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

5.1 Standard geometry

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	I	3.74	703/10296 (6.8%)	3.73	1049/16060 (6.5%)
2	J	3.72	457/6896 (6.6%)	3.57	672/10756 (6.2%)
3	K	4.26	459/6621 (6.9%)	3.39	627/10327 (6.1%)
4	L	4.08	734/9060 (8.1%)	3.87	1040/14000 (7.4%)
5	M	3.97	464/6068 (7.6%)	3.99	683/9376 (7.3%)
6	N	4.42	459/5824 (7.9%)	3.40	573/8994 (6.4%)
All	All	4.01	3276/44765 (7.3%)	3.68	4644/69513 (6.7%)

The worst 5 of 3276 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	313	U	O3'-P	48.59	2.19	1.61
3	K	12	A	O3'-P	48.05	2.18	1.61
1	I	149	A	O3'-P	47.30	2.17	1.61
3	K	11	A	O3'-P	47.12	2.17	1.61
3	K	75	A	O3'-P	46.95	2.17	1.61

The worst 5 of 4644 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	722	U	OP2-P-O3'	-44.48	7.35	105.20
3	K	120	A	P-O3'-C3'	-44.33	66.50	119.70
1	I	101	A	OP2-P-O3'	-41.80	13.24	105.20
2	J	223	A	P-O3'-C3'	-41.00	70.50	119.70
2	J	92	A	OP2-P-O3'	-40.81	15.42	105.20

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	I	9061	0	4518	4048	715
2	J	6069	0	3032	2589	1135
3	K	5827	0	2926	1867	622
4	L	8237	0	4114	3497	802
5	M	5517	0	2762	2245	1030
6	N	5297	0	2665	1656	473
All	All	40008	0	20017	15802	2447

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 263.

The worst 5 of 15802 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:J:47:A:C2'	2:J:48:A:H5'	1.27	1.65
5:M:319:U:C2'	5:M:320:U:H5'	1.25	1.57
4:L:477:U:C2'	4:L:478:U:H5'	1.35	1.56
3:K:168:A:C2'	3:K:169:A:H5'	1.34	1.54
1:I:65:A:C2'	1:I:66:A:C5'	1.85	1.53

The worst 5 of 2447 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:A:OP2	4:L:465:U:C3'[3_556]	0.12	2.08
4:L:752:U:OP2	5:M:500:U:P[3_556]	0.21	1.99
4:L:758:U:C5'	5:M:510:U:N3[3_556]	0.23	1.97
2:J:48:A:C1'	4:L:754:U:O3'[3_546]	0.25	1.95
2:J:43:A:C1'	4:L:759:U:C2'[3_546]	0.28	1.92

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	411/412 (99%)	57 (13%)	40 (9%)
2	J	275/276 (99%)	46 (16%)	29 (10%)
3	K	264/265 (99%)	32 (12%)	20 (7%)
4	L	411/412 (99%)	55 (13%)	39 (9%)
5	M	275/276 (99%)	47 (17%)	27 (9%)
6	N	262/265 (98%)	25 (9%)	19 (7%)
All	All	1898/1906 (99%)	262 (13%)	174 (9%)

5 of 262 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	4	A
1	I	5	A
1	I	11	A
1	I	16	A
1	I	32	A

5 of 174 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	K	138	A
4	L	551	U
6	N	377	U
3	K	146	A
3	K	243	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	L	134
1	I	113
6	N	112
3	K	104
5	M	68
2	J	64

The worst 5 of 595 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	517:U	O3'	518:U	P	2.23
1	N	456:U	O3'	457:U	P	2.20
1	M	313:U	O3'	314:U	P	2.19
1	K	12:A	O3'	13:A	P	2.18
1	I	149:A	O3'	150:A	P	2.17

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.