

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1H1K
Title	:	THE BLUETONGUE VIRUS (BTV) CORE BINDS DSRNA
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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 (i) 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 (1)) 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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

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



2 Entry composition (i)

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		A	toms			ZeroOcc	AltConf	Trace
1	Ι	412	Total 9061	C 4120	N 2060	O 2470	Р 411	0	0	0

• Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
2	J	276	Total 6069	C 2760	N 1380	0 1654	Р 275	0	0	0

• Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
3	K	265	Total 5827	C 2650	N 1325	O 1588	Р 264	0	0	0

• Molecule 4 is a RNA chain called RNA.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
4	L	412	Total 8237	C 3708	N 824	O 3294	Р 411	0	0	0

• Molecule 5 is a RNA chain called RNA.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
5	М	276	Total 5517	C 2484	N 552	O 2206	Р 275	0	0	0

• Molecule 6 is a RNA chain called RNA.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
6	Ν	265	Total 5297	C 2385	N 530	O 2118	Р 264	0	0	0



Residue-property plots (i) 3

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. 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

Chain I: 78% 21% 124 125 125 126 127 128 128 128 130 33 34 35 35 480 481 482 483 486 487 488 489 491 491 492 493 222 224 225 225 226 227 228 229 229 229 230 231 A 303 A 304 A 304 A 304 A 305 A 305 A 313 A 313





• Molecule 3: RNA



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• Molecule 5: RNA







 \bullet Molecule 6: RNA

Ch	ai	n	Ν	:	•																8	329	6																	1	5%)					
U266 U267	U268 11060	U270	U271	U272 11272	U274	U275	U276	U277	8/20	U280	U281	U282	U283 11004	11705	0.200	U287	U288	U289	U290	1920	U293	U294	U295	U296	U297 11000	0.298	U300	U301	U302	11304	U305	U306	U307 U308	U309	U310	U311	U312 U313	U314	U315	U316	U317 11210	0100	U320	U321	U322	U323 11324	U325
U326 U327	U328 11200	U329 U330	U331	U332 11222	U334	U335	U336	U337	U338 11330	U340	U341	U342	U343	U344 112 AE	0345 11376	U347	U348	U349	U350	U351 11352	U353	U354	U355	U356	U357 112 F 0	1358 11250	U360	U361	U362	U363 11364	U365	U366	U367 11368	U369	U370	U371	U372 11373	U374	U375	U376	U377 11270	11370	U380	U381	U382	U383 11384	U385
U386 U387	U388 110.00	U389 U390	U391	U392 112.02	U394	U395	U396	U397	113 QQ	U400	U401	U402	U403	U404	60400	U407	U408	U409	U410	U411 11412	0412 U413	U414	U415	U416	U417	U418	0413 U420	U421	U422	0423	0425 U425	U426	U427 11428	U429	U430	U431	04.32 114.33	U434	U435	U436	U437	04.30	0439 U440	U441	U442	0443 11444	U445
U446 U447	U448 11440	0449 U450	U451	U452 11/63	U454	U455	U456	U457	U458 11469	U460	U461	U462	U463	U464 11465	0405 11/166	U467	U468	U469	U470	11471 11470	0473 11473	U474	U475	U476	U477 11470	0478 11470	U4/9 U480	U481	U482	U483 11484	U485	U486	U487 11488	U489	U490	U491	U492 11493	U494	U495	U496	U497	0430 11/100	U500	U501	U502	U503 11504	U505
U506 U507	U508	0509 0510	U511	U512 IIE13	U514	U515	U516	U517	U518 11510	U520	U521	U522	U523	U524	11526	U527	U528	U529	U530																												



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	795.60Å 821.80Å 753.30Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) - 10.00	Depositor
% Data completeness	(Not available) ((Not available)-10.00)	Depositor
(in resolution range)		Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.83 (at 3.49 \text{\AA})$	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	$< L > = 0.38, < L^2 > = 0.21$	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

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

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.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

Mal	Chain	B	Bond lengths	Bond angles		
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Ι	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	Κ	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	М	3.97	464/6068~(7.6%)	3.99	683/9376~(7.3%)	
6	Ν	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	М	313	U	O3'-P	48.59	2.19	1.61
3	K	12	А	O3'-P	48.05	2.18	1.61
1	Ι	149	A	O3'-P	47.30	2.17	1.61
3	K	11	А	O3'-P	47.12	2.17	1.61
3	K	75	А	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	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
4	L	722	U	OP2-P-O3'	-44.48	7.35	105.20
3	Κ	120	А	P-O3'-C3'	-44.33	66.50	119.70
1	Ι	101	А	OP2-P-O3'	-41.80	13.24	105.20
2	J	223	А	P-O3'-C3'	-41.00	70.50	119.70
2	J	92	А	OP2-P-O3'	-40.81	15.42	105.20

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	Ι	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	М	5517	0	2762	2245	1030
6	Ν	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	$\begin{array}{c} {\rm Interatomic}\\ {\rm distance}~({\rm \AA}) \end{array}$	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	Ι	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	М	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	\mathbf{Res}	Type
1	Ι	4	А
1	Ι	5	А
1	Ι	11	А
1	Ι	16	А
1	Ι	32	А

5 of 174 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L	736	U
5	М	474	U
4	L	746	U
5	М	338	U
5	М	518	U

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 monosaccharides 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	Ι	113
6	Ν	112
3	Κ	104
5	М	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	Ν	517:U	O3'	518:U	Р	2.23
1	Ν	456:U	O3'	457:U	Р	2.20
1	М	313:U	O3'	314:U	Р	2.19
1	Κ	12:A	O3'	13:A	Р	2.18
1	Ι	149:A	O3'	150:A	Р	2.17



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

