



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1H1K / pdb_00001h1k
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 ⓘ 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
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

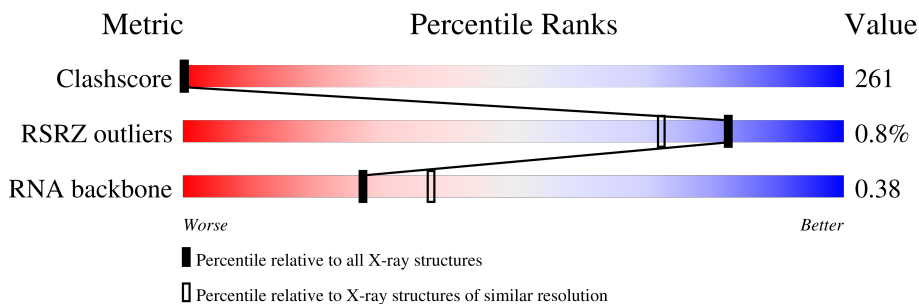
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1002 (15.00-4.06)
RSRZ outliers	180081	1162 (11.50-4.00)
RNA backbone	3983	1057 (11.50-3.10)

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	I	412	2% 78% 21%
2	J	276	2% 72% 25%
3	K	265	% 77% 18%
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			

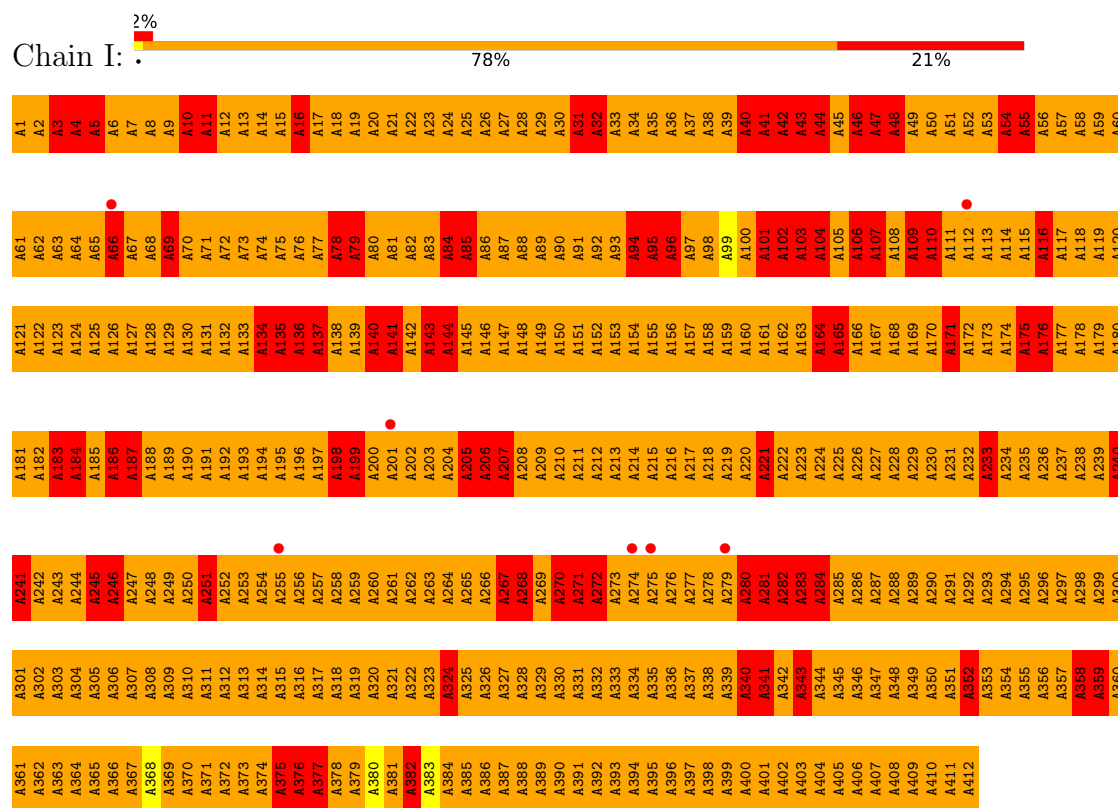
- Molecule 6 is a RNA chain called RNA.

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

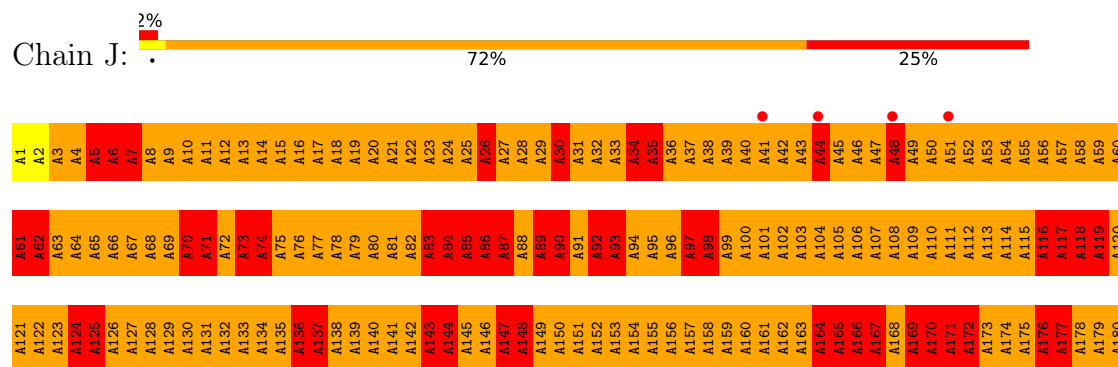
3 Residue-property plots

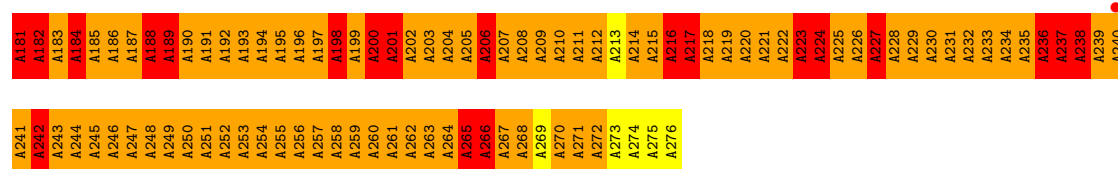
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

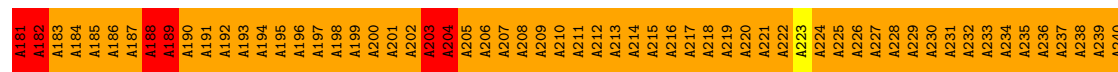
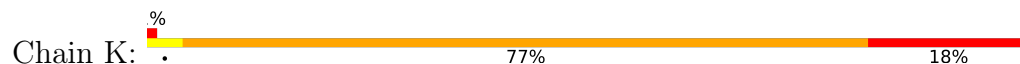


• Molecule 2: RNA

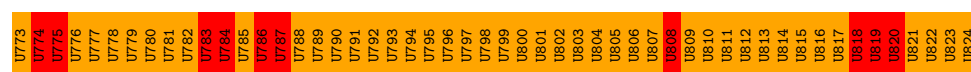
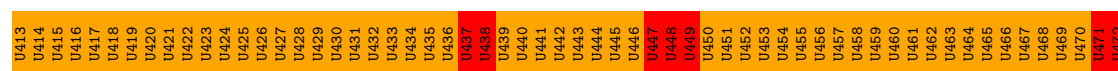
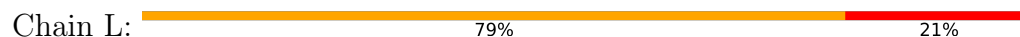




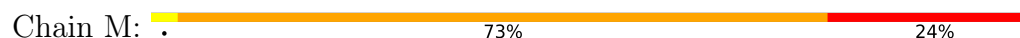
• Molecule 3: RNA

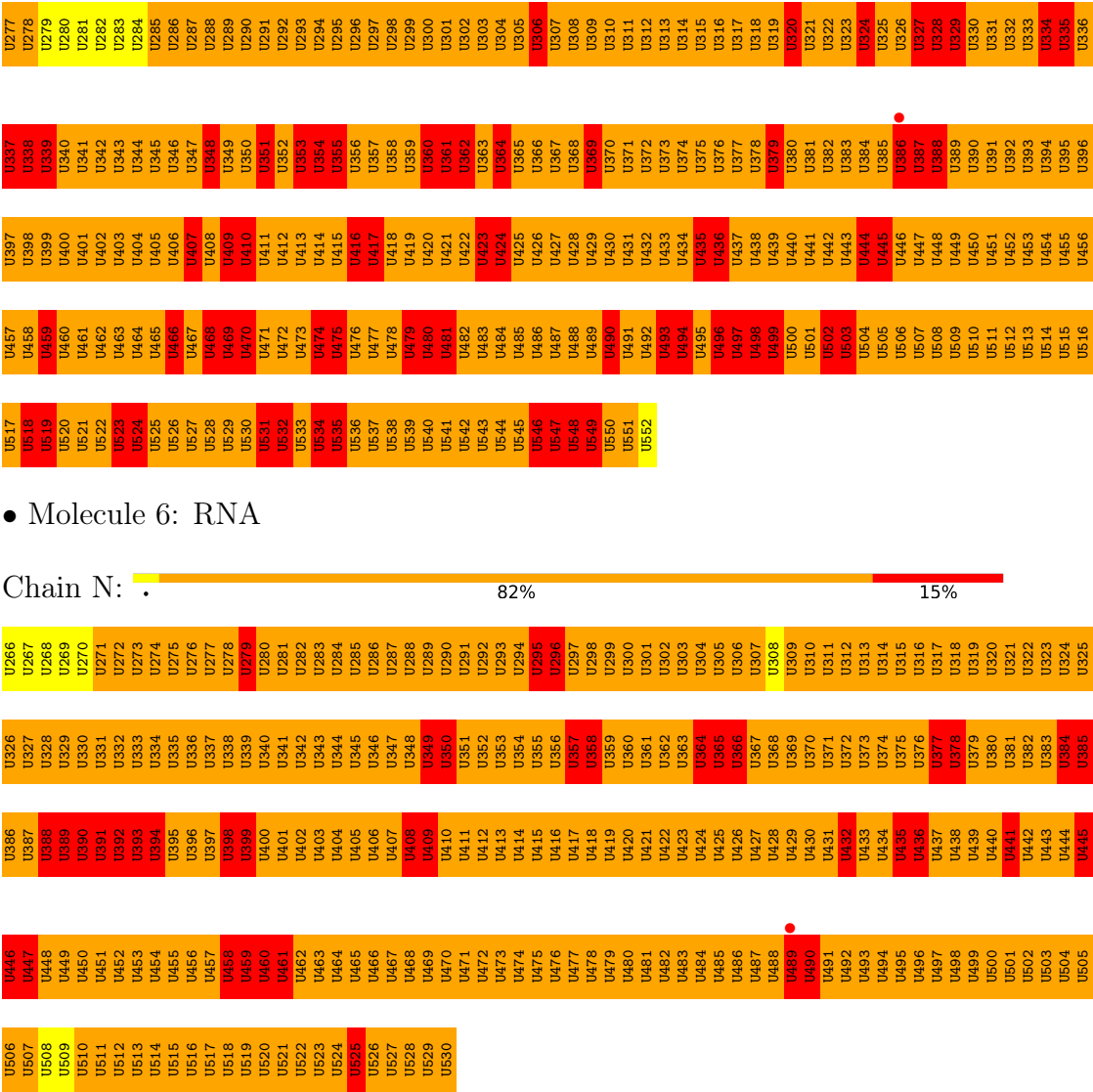


• Molecule 4: RNA



• Molecule 5: RNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	795.60Å 821.80Å 753.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 10.00 200.00 – 10.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-10.00) 73.2 (200.00-10.00)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 35.6	EDS
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
F_o, F_c correlation	0.19	EDS
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	3.18	666/10296 (6.5%)	3.41	942/16060 (5.9%)
2	J	3.17	438/6896 (6.4%)	3.27	631/10756 (5.9%)
3	K	3.58	445/6621 (6.7%)	3.12	553/10327 (5.4%)
4	L	3.50	706/9060 (7.8%)	3.53	935/14000 (6.7%)
5	M	3.42	434/6068 (7.2%)	3.63	631/9376 (6.7%)
6	N	3.76	442/5824 (7.6%)	3.18	494/8994 (5.5%)
All	All	3.42	3131/44765 (7.0%)	3.37	4186/69513 (6.0%)

The worst 5 of 3131 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	313	U	O3'-P	38.87	2.19	1.61
3	K	12	A	O3'-P	38.44	2.18	1.61
1	I	149	A	O3'-P	37.84	2.17	1.61
3	K	11	A	O3'-P	37.70	2.17	1.61
3	K	75	A	O3'-P	37.56	2.17	1.61

The worst 5 of 4186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	425	U	O3'-P-O5'	-42.82	39.77	104.00
4	L	712	U	O3'-P-O5'	-41.72	41.42	104.00
5	M	453	U	O3'-P-O5'	-37.78	47.33	104.00
4	L	811	U	O3'-P-O5'	-36.55	49.18	104.00
4	L	766	U	O3'-P-O5'	-36.06	49.91	104.00

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	4003	715
2	J	6069	0	3032	2565	1135
3	K	5827	0	2926	1851	622
4	L	8237	0	4114	3463	802
5	M	5517	0	2762	2209	1030
6	N	5297	0	2665	1647	473
All	All	40008	0	20017	15638	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 261.

The worst 5 of 15638 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%)	19 (7%)
4	L	411/412 (99%)	55 (13%)	39 (9%)
5	M	275/276 (99%)	47 (17%)	27 (9%)
6	N	264/265 (99%)	25 (9%)	19 (7%)
All	All	1900/1906 (99%)	262 (13%)	173 (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 173 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L	737	U
5	M	479	U
4	L	750	U
5	M	354	U
5	M	523	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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	I	412/412 (100%)	0.01	7 (1%) 69 59	50, 50, 50, 50	0
2	J	276/276 (100%)	-0.10	5 (1%) 67 58	50, 50, 50, 50	0
3	K	265/265 (100%)	-0.11	2 (0%) 82 72	50, 50, 50, 50	0
4	L	412/412 (100%)	-0.13	0 100 100	50, 50, 50, 50	0
5	M	276/276 (100%)	-0.20	1 (0%) 88 79	50, 50, 50, 50	0
6	N	265/265 (100%)	-0.13	1 (0%) 88 79	50, 50, 50, 50	0
All	All	1906/1906 (100%)	-0.10	16 (0%) 82 72	50, 50, 50, 50	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	275	A	3.5
2	J	240	A	2.8
2	J	48	A	2.7
2	J	44	A	2.6
1	I	66	A	2.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.