



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2023 – 12:54 PM EDT

PDB ID : 1BMV
Title : PROTEIN-RNA INTERACTIONS IN AN ICOSAHEDRAL VIRUS AT 3.0
ANGSTROMS RESOLUTION
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Deposited on : 1989-10-09
Resolution : 3.00 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 : 4.02b-467
Xtrriage (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

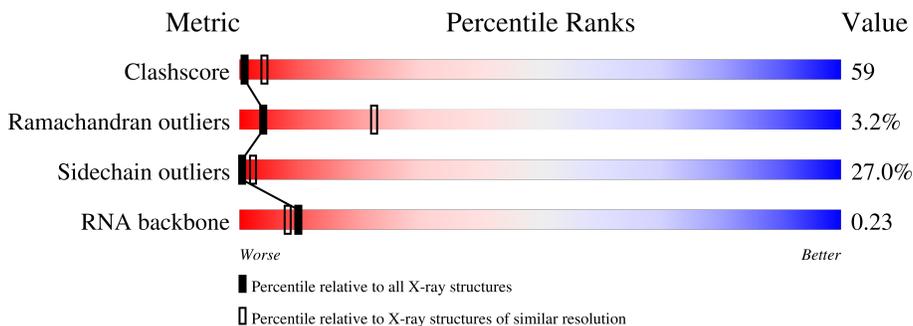
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	M	11	100%
2	1	198	30% 44% 17% 7%
3	2	374	27% 49% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4613 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 (5'-R(*GP*GP*UP*CP*AP*AP*AP*AP*UP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	M	11	238	106	45	76	11	0	0	0

- Molecule 2 is a protein called PROTEIN (ICOSAHEDRAL VIRUS - A DOMAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	1	185	1451	924	244	274	9	0	0	0

- Molecule 3 is a protein called PROTEIN (ICOSAHEDRAL VIRUS - B AND C DOMAIN).

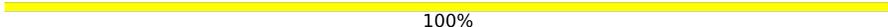
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	2	374	2924	1867	487	542	28	0	6	0

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. 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.

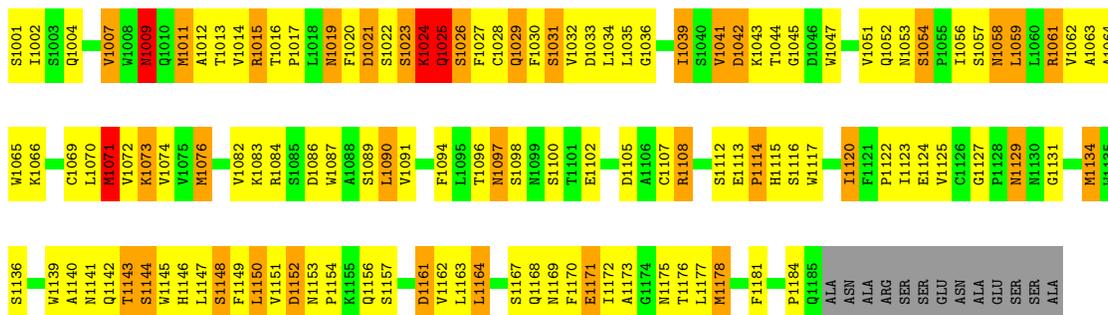
- Molecule 1: RNA (5'-R(*GP*GP*UP*CP*AP*AP*AP*AP*UP*GP*C)-3')

Chain M: 

G1
G2
U3
C4
A5
A6
A7
A8
U9
G10
C11

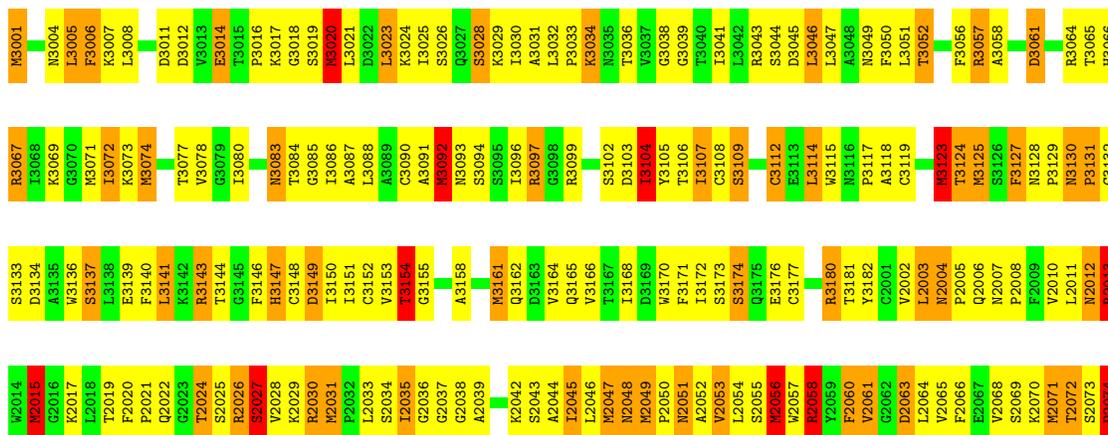
- Molecule 2: PROTEIN (ICOSAHEDRAL VIRUS - A DOMAIN)

Chain 1: 



- Molecule 3: PROTEIN (ICOSAHEDRAL VIRUS - B AND C DOMAIN)

Chain 2: 



Y2075	Y2076	K2077	C2078	T2079	V2080	S2081	F2082	F2083	I2084	A2085	F2086	G2087	N2088	D2091	D2092	T2093	T2094	N2095	F2096	E2097	A2098	F2099	P2100	H2101	K2102	L2103	V2104	Q2105	F2106	G2107	E2108	T2109	Q2110	E2111	K2112	V2113	V2114	L2115	K2116	Q2119	F2120	E2121	F2122	L2123	T2124	A2125	Q2126	S2127	T2128	Q2129	V2130	R2131	P2132	A2133	T2134	T2135	L2136
L2137	A2138	D2139	P2142	Y2143	L2144	Y2145	A2146	M2147	V2148	H2149	D2150	S2151	S2152	V2153	S2154	G2158	D2159	F2160	V2161	I2162	G2163	V2164	K2165	L2166	T2167	I2168	I2169	E2170	N2171	M2172	G2176	L2177	N2178	P2179	G2180	I2181	S2182	R2185	L2186	L2187	G2188	T2189	I2190	P2191	Q2192												

4 Data and refinement statistics i

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

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	311.20Å 284.20Å 350.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	NONE	Depositor
R, R_{free}	0.330 , (Not available)	Depositor
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4613	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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](#)

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	M	1.11	0/266	1.44	0/411
2	1	1.13	0/1490	1.57	21/2031 (1.0%)
3	2	1.11	6/2988 (0.2%)	1.58	54/4056 (1.3%)
All	All	1.12	6/4744 (0.1%)	1.57	75/6498 (1.2%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	2070	LYS	N-CA	7.13	1.60	1.46
3	2	2074	PRO	C-N	6.91	1.50	1.34
3	2	3052	THR	C-N	6.03	1.48	1.34
3	2	2071	MET	C-N	-5.98	1.20	1.34
3	2	2077	LYS	CA-C	-5.62	1.38	1.52

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	2072	THR	N-CA-CB	-15.01	81.78	110.30
3	2	2070	LYS	CB-CA-C	10.13	130.65	110.40
3	2	2077	LYS	CB-CA-C	9.81	130.01	110.40
3	2	2079	THR	N-CA-CB	-8.48	94.19	110.30
3	2	2070	LYS	N-CA-C	-7.92	89.63	111.00

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	M	238	0	120	16	0
2	1	1451	0	1402	146	0
3	2	2924	0	2938	401	0
All	All	4613	0	4460	537	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 59.

The worst 5 of 537 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)
3:2:2190[A]:ILE:HG12	3:2:2191[A]:PRO:CD	1.51	1.39
3:2:2066:PHE:CE2	3:2:2166:LEU:HD12	1.63	1.32
3:2:2186:LEU:C	3:2:2187[B]:LEU:HA	1.56	1.24
3:2:2033:LEU:HB2	3:2:2142:PRO:O	1.40	1.18
3:2:2190[A]:ILE:CG1	3:2:2191[A]:PRO:HD2	1.72	1.17

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
2	1	183/198 (92%)	158 (86%)	20 (11%)	5 (3%)	5 26
3	2	377/374 (101%)	316 (84%)	46 (12%)	15 (4%)	3 17
All	All	560/572 (98%)	474 (85%)	66 (12%)	20 (4%)	4 19

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	1022	SER
2	1	1024	LYS

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Mol	Chain	Res	Type
2	1	1025	GLN
2	1	1136	SER
3	2	3057	ARG

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	
2	1	165/174 (95%)	124 (75%)	41 (25%)	0	3
3	2	329/324 (102%)	236 (72%)	93 (28%)	0	2
All	All	494/498 (99%)	360 (73%)	134 (27%)	0	2

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	2121	GLU
3	2	2139	ASP
3	2	2187[A]	LEU
3	2	3023	LEU
3	2	3021	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	2	3083	ASN
3	2	2004	ASN
3	2	2119	GLN
3	2	2048	ASN
3	2	2101	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	M	10/11 (90%)	5 (50%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	M	7	A
1	M	8	A
1	M	9	U
1	M	10	G
1	M	11	C

There are no RNA pucker outliers to report.

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
3	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	2186:LEU	C	2187[B]:LEU	N	2.97
1	2	2071:MET	C	2072:THR	N	1.20

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.