



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:23 PM UTC

PDB ID : 2SNV / pdb_00002snv
Title : THE REFINED STRUCTURE OF SINDBIS VIRUS CORE PROTEIN IN
COMPARISON WITH OTHER CHYMOTRYPSIN-LIKE SERINE PRO-
TEINASE STRUCTURES
Authors : Tong, L.; Rossmann, M.G.
Deposited on : 1992-07-17
Resolution : 2.80 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 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

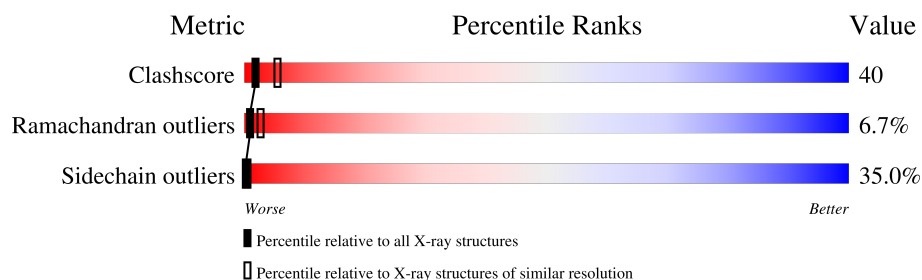
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	151	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1164 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 SINDBIS VIRUS COAT PROTEIN.

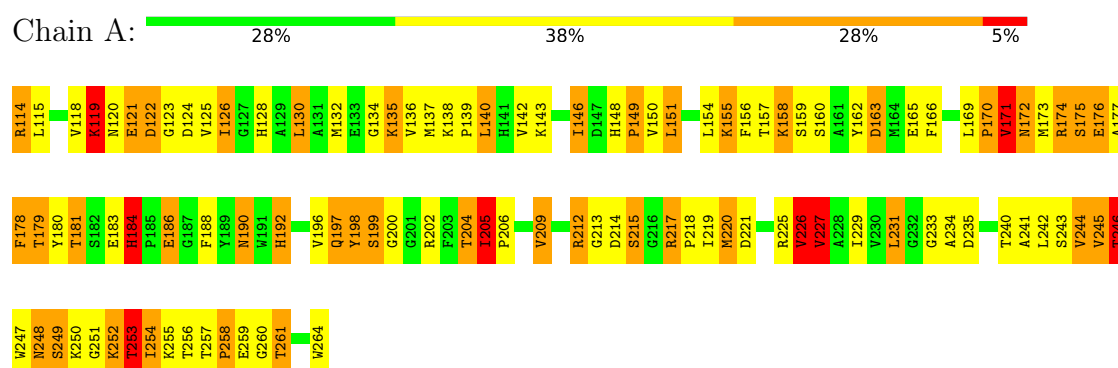
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1164	731	207	221	5			

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 was not executed.

• Molecule 1: SINDBIS VIRUS COAT PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	57.00Å 57.00Å 109.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1164	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

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	A	1.81	14/1192 (1.2%)	2.04	46/1609 (2.9%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	GLU	C-N	8.05	1.44	1.33
1	A	205	ILE	N-CA	-7.85	1.39	1.46
1	A	122	ASP	N-CA	7.10	1.55	1.46
1	A	246	THR	C-O	-6.93	1.15	1.24
1	A	121	GLU	N-CA	6.92	1.55	1.46
1	A	253	THR	C-N	-6.67	1.25	1.34
1	A	199	SER	N-CA	-6.25	1.38	1.46
1	A	254	ILE	N-CA	-6.07	1.35	1.46
1	A	178	PHE	N-CA	-5.55	1.38	1.45
1	A	122	ASP	CG-OD2	5.25	1.35	1.25
1	A	204	THR	C-N	-5.23	1.28	1.33
1	A	186	GLU	CD-OE1	5.20	1.35	1.25
1	A	176	GLU	CD-OE1	5.12	1.35	1.25
1	A	122	ASP	CA-CB	5.07	1.61	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ASN	CA-C-N	9.52	139.72	121.54
1	A	248	ASN	C-N-CA	9.52	139.72	121.54
1	A	261	THR	N-CA-C	9.06	123.28	110.50
1	A	245	VAL	N-CA-CB	8.83	121.59	110.99
1	A	184	HIS	CA-CB-CG	8.61	122.41	113.80
1	A	221	ASP	CA-CB-CG	8.19	120.79	112.60
1	A	122	ASP	CA-CB-CG	8.16	120.77	112.60
1	A	205	ILE	N-CA-CB	-8.09	102.98	111.87
1	A	205	ILE	CB-CA-C	7.47	117.96	109.89
1	A	209	VAL	CA-C-N	-7.28	115.99	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	VAL	C-N-CA	-7.28	115.99	122.47
1	A	122	ASP	O-C-N	7.15	129.70	122.12
1	A	254	ILE	CB-CA-C	6.84	119.82	111.13
1	A	215	SER	CA-C-N	-6.54	116.36	123.30
1	A	215	SER	C-N-CA	-6.54	116.36	123.30
1	A	248	ASN	N-CA-CB	6.27	120.94	110.59
1	A	227	VAL	CB-CA-C	6.26	116.57	111.06
1	A	226	VAL	CA-C-N	6.23	128.88	121.84
1	A	226	VAL	C-N-CA	6.23	128.88	121.84
1	A	163	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	260	GLY	CA-C-N	6.19	130.66	120.94
1	A	260	GLY	C-N-CA	6.19	130.66	120.94
1	A	123	GLY	N-CA-C	-6.08	98.77	113.18
1	A	246	THR	N-CA-CB	-5.89	101.48	111.31
1	A	244	VAL	N-CA-CB	-5.82	101.26	111.39
1	A	254	ILE	N-CA-CB	-5.70	98.08	111.30
1	A	178	PHE	N-CA-C	-5.62	103.27	110.53
1	A	137	MET	N-CA-CB	5.55	119.45	110.41
1	A	218	PRO	CB-CA-C	-5.54	102.12	110.20
1	A	119	LYS	CA-C-N	5.50	132.88	123.03
1	A	119	LYS	C-N-CA	5.50	132.88	123.03
1	A	251	GLY	N-CA-C	-5.50	104.67	111.70
1	A	218	PRO	N-CA-CB	5.41	109.00	102.72
1	A	257	THR	C-N-CD	-5.39	102.89	125.00
1	A	158	LYS	CB-CA-C	-5.32	100.51	109.50
1	A	253	THR	N-CA-CB	5.32	119.46	110.69
1	A	249	SER	N-CA-C	5.28	122.04	110.80
1	A	136	VAL	CB-CA-C	-5.25	103.89	111.19
1	A	173	MET	N-CA-C	-5.22	105.67	111.36
1	A	253	THR	CA-C-N	5.21	128.37	120.13
1	A	253	THR	C-N-CA	5.21	128.37	120.13
1	A	192	HIS	CA-CB-CG	5.16	118.96	113.80
1	A	261	THR	N-CA-CB	-5.13	102.78	110.17
1	A	170	PRO	N-CA-CB	5.08	107.83	103.31
1	A	122	ASP	N-CA-CB	5.06	117.66	110.06
1	A	248	ASN	O-C-N	5.03	130.23	123.34

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	A	1164	0	1134	91	0
All	All	1164	0	1134	91	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 40.

All (91) 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)
1:A:248:ASN:HB3	1:A:255:LYS:HZ2	1.22	1.04
1:A:212:ARG:HH11	1:A:212:ARG:HG2	1.26	1.00
1:A:231:LEU:HD11	1:A:245:VAL:HG23	1.50	0.93
1:A:169:LEU:HD13	1:A:174:ARG:HA	1.51	0.92
1:A:248:ASN:HB3	1:A:255:LYS:NZ	1.84	0.92
1:A:120:ASN:ND2	1:A:124:ASP:HB2	1.85	0.91
1:A:202:ARG:HE	1:A:241:ALA:HB2	1.48	0.79
1:A:206:PRO:HG2	1:A:209:VAL:HG21	1.65	0.78
1:A:202:ARG:NE	1:A:241:ALA:HB2	2.02	0.75
1:A:254:ILE:O	1:A:255:LYS:HG3	1.88	0.73
1:A:132:MET:SD	1:A:226:VAL:HG11	2.32	0.69
1:A:247:TRP:HA	1:A:253:THR:O	1.93	0.67
1:A:245:VAL:HA	1:A:255:LYS:O	1.97	0.65
1:A:135:LYS:HB3	1:A:135:LYS:NZ	2.12	0.65
1:A:119:LYS:HA	1:A:124:ASP:O	1.95	0.64
1:A:114:ARG:HG2	1:A:178:PHE:CD2	2.33	0.63
1:A:134:GLY:HA2	1:A:174:ARG:HD3	1.81	0.62
1:A:248:ASN:CB	1:A:255:LYS:HZ2	2.08	0.61
1:A:184:HIS:HD2	1:A:227:VAL:HG22	1.66	0.60
1:A:130:LEU:O	1:A:130:LEU:HD13	2.02	0.60
1:A:240:THR:HG21	1:A:264:TRP:HH2	1.65	0.59
1:A:169:LEU:CD1	1:A:174:ARG:HA	2.27	0.59
1:A:212:ARG:HG2	1:A:212:ARG:NH1	2.01	0.59
1:A:202:ARG:HE	1:A:241:ALA:CB	2.16	0.58
1:A:139:PRO:HB3	1:A:231:LEU:HD23	1.85	0.58
1:A:162:TYR:HA	1:A:256:THR:OG1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:CD2	1:A:165:GLU:HB2	2.35	0.56
1:A:120:ASN:HD21	1:A:124:ASP:HB2	1.66	0.56
1:A:146:ILE:HD11	1:A:151:LEU:HB3	1.87	0.56
1:A:148:HIS:CD2	1:A:149:PRO:HD2	2.40	0.56
1:A:214:ASP:O	1:A:217:ARG:HG3	2.05	0.56
1:A:135:LYS:HB3	1:A:135:LYS:HZ2	1.70	0.56
1:A:148:HIS:HB3	1:A:151:LEU:HB2	1.87	0.55
1:A:186:GLU:HA	1:A:198:TYR:HB3	1.90	0.54
1:A:235:ASP:HA	1:A:240:THR:HA	1.90	0.54
1:A:171:VAL:HG13	1:A:171:VAL:O	2.08	0.54
1:A:114:ARG:HG2	1:A:178:PHE:CE2	2.44	0.53
1:A:205:ILE:HD12	1:A:242:LEU:HD11	1.90	0.53
1:A:159:SER:HG	1:A:162:TYR:HD2	1.55	0.53
1:A:126:ILE:HG13	1:A:142:VAL:HG13	1.91	0.52
1:A:205:ILE:CD1	1:A:242:LEU:HD11	2.40	0.52
1:A:140:LEU:HD22	1:A:165:GLU:HB2	1.91	0.51
1:A:246:THR:CG2	1:A:247:TRP:N	2.74	0.51
1:A:146:ILE:HD11	1:A:151:LEU:CB	2.40	0.51
1:A:252:LYS:O	1:A:252:LYS:HG3	2.12	0.50
1:A:233:GLY:HA3	1:A:264:TRP:CH2	2.47	0.50
1:A:234:ALA:HB3	1:A:259:GLU:HB2	1.94	0.49
1:A:132:MET:HB2	1:A:178:PHE:HB2	1.93	0.49
1:A:119:LYS:HD3	1:A:125:VAL:HG22	1.94	0.49
1:A:157:THR:HB	1:A:166:PHE:CZ	2.48	0.49
1:A:120:ASN:CG	1:A:124:ASP:HB2	2.36	0.49
1:A:188:PHE:HA	1:A:196:VAL:O	2.13	0.49
1:A:214:ASP:HA	1:A:217:ARG:HG3	1.94	0.49
1:A:155:LYS:HA	1:A:155:LYS:NZ	2.28	0.49
1:A:114:ARG:HB3	1:A:178:PHE:CE2	2.47	0.49
1:A:170:PRO:O	1:A:172:ASN:N	2.43	0.48
1:A:198:TYR:HD1	1:A:198:TYR:HA	1.58	0.48
1:A:214:ASP:OD1	1:A:217:ARG:NH1	2.44	0.48
1:A:197:GLN:HG3	1:A:198:TYR:N	2.29	0.47
1:A:155:LYS:HA	1:A:155:LYS:HZ2	1.78	0.47
1:A:132:MET:SD	1:A:226:VAL:CG1	3.02	0.47
1:A:256:THR:C	1:A:258:PRO:HD3	2.40	0.47
1:A:247:TRP:CD1	1:A:252:LYS:HB2	2.50	0.47
1:A:162:TYR:CE1	1:A:254:ILE:HG23	2.50	0.46
1:A:243:SER:OG	1:A:261:THR:HG21	2.16	0.46
1:A:159:SER:OG	1:A:162:TYR:HD2	1.98	0.46
1:A:196:VAL:HG11	1:A:219:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:THR:O	1:A:258:PRO:HD3	2.17	0.45
1:A:254:ILE:C	1:A:255:LYS:HG3	2.42	0.45
1:A:134:GLY:O	1:A:169:LEU:HB2	2.17	0.45
1:A:120:ASN:HD22	1:A:126:ILE:HG23	1.82	0.44
1:A:139:PRO:HB3	1:A:231:LEU:CD2	2.46	0.44
1:A:179:THR:O	1:A:226:VAL:HG12	2.16	0.44
1:A:118:VAL:HG11	1:A:142:VAL:HG12	1.99	0.44
1:A:126:ILE:H	1:A:126:ILE:HG12	1.68	0.44
1:A:180:TYR:CG	1:A:181:THR:N	2.86	0.44
1:A:248:ASN:CB	1:A:255:LYS:NZ	2.70	0.44
1:A:132:MET:HE2	1:A:132:MET:HB3	1.93	0.43
1:A:174:ARG:O	1:A:177:ALA:HB2	2.18	0.43
1:A:190:ASN:OD1	1:A:190:ASN:N	2.52	0.42
1:A:202:ARG:NE	1:A:241:ALA:CB	2.77	0.42
1:A:160:SER:C	1:A:162:TYR:H	2.27	0.42
1:A:162:TYR:O	1:A:163:ASP:HB3	2.20	0.41
1:A:202:ARG:CZ	1:A:241:ALA:HB2	2.50	0.41
1:A:220:MET:H	1:A:220:MET:HG2	1.69	0.41
1:A:156:PHE:HB3	1:A:165:GLU:CG	2.50	0.41
1:A:134:GLY:HA2	1:A:169:LEU:HD12	2.01	0.41
1:A:206:PRO:CG	1:A:209:VAL:HG21	2.44	0.41
1:A:135:LYS:NZ	1:A:135:LYS:CB	2.81	0.40
1:A:240:THR:HG21	1:A:264:TRP:CH2	2.52	0.40
1:A:128:HIS:ND1	1:A:213:GLY:O	2.54	0.40

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
1	A	149/151 (99%)	123 (83%)	16 (11%)	10 (7%)	1 3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	GLU
1	A	172	ASN
1	A	249	SER
1	A	258	PRO
1	A	171	VAL
1	A	192	HIS
1	A	175	SER
1	A	200	GLY
1	A	149	PRO
1	A	174	ARG

5.3.2 Protein sidechains ⓘ

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	123/123 (100%)	80 (65%)	43 (35%)	0 0

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ARG
1	A	115	LEU
1	A	119	LYS
1	A	122	ASP
1	A	126	ILE
1	A	130	LEU
1	A	135	LYS
1	A	138	LYS
1	A	140	LEU
1	A	143	LYS
1	A	146	ILE
1	A	150	VAL
1	A	151	LEU
1	A	154	LEU
1	A	155	LYS

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Mol	Chain	Res	Type
1	A	158	LYS
1	A	171	VAL
1	A	175	SER
1	A	176	GLU
1	A	179	THR
1	A	181	THR
1	A	183	GLU
1	A	184	HIS
1	A	190	ASN
1	A	197	GLN
1	A	198	TYR
1	A	199	SER
1	A	204	THR
1	A	205	ILE
1	A	212	ARG
1	A	215	SER
1	A	217	ARG
1	A	220	MET
1	A	225	ARG
1	A	226	VAL
1	A	227	VAL
1	A	229	ILE
1	A	231	LEU
1	A	244	VAL
1	A	246	THR
1	A	250	LYS
1	A	252	LYS
1	A	253	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	184	HIS
1	A	222	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.