



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 07:39 am BST

PDB ID : 5J98
Title : Crystal structure of Slow Bee Paralysis Virus at 2.6A resolution
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Deposited on : 2016-04-08
Resolution : 2.60 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 : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

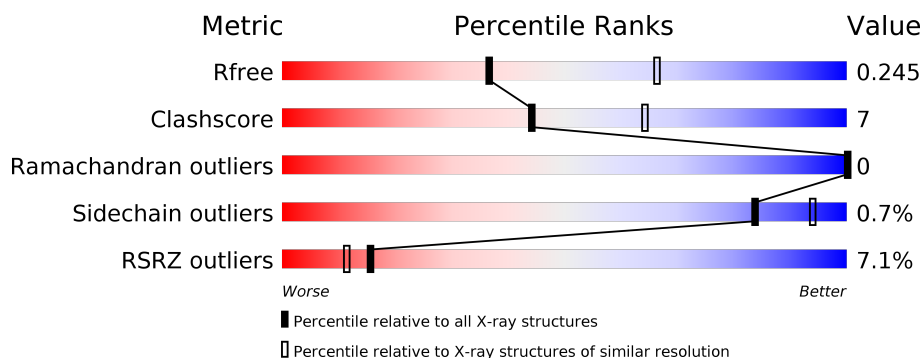
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. 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	A	266	<div> <div>79%</div> <div>15%</div> <div>5%</div> </div>
2	B	261	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
3	C	430	<div> <div>15%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7438 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2023	1293	353	368	9			

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	0	0
			2086	1341	347	384	14			

- Molecule 3 is a protein called VP3.


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	417	Total	C	N	O	S	0	0	0
			3260	2113	538	601	8			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	19	Total	O	0	0
			19	19		
4	C	30	Total	O	0	0
			30	30		

- Molecule 1: VP1

Amino Acid	Frequency (approx.)
P1	10
T6	20
P17	15
T18	15
T19	15
E28	15
A29	15
F30	15
L49	15
E50	15
R54	15
Q64	15
R87	15
I91	15
P92	15
R102	15
G103	15
S116	15
C117	15
Y118	15
W119	15
H123	15
P127	15
R132	15
I139	15
D143	15
F169	15
Y170	15
Q171	15
L174	15
S181	15
D190	15
R191	15
L192	15
G198	15
L201	15
L202	15
G203	15
I210	15
G214	15
I215	15
Y221	15
S222	15
I223	15
F227	15
S228	15
T244	15
Y245	15
D251	15
L252	15
ALA	15
GLN	15
TYR	15
PHE	15
GLU	15
ASP	15
GLU	15
VAL	15
THR	15
ILE	15
ALA	15
GLN	15
PRO	15
GLU	15

Chain B:  82% 17%

The diagram consists of two horizontal rows of colored squares. Each square has a label next to it.

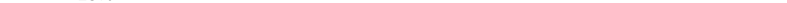
Top Row Labels:

- M1, D2, R3, P4, E5, G6, S7
- T14, S15
- D28, I29
- P36
- D55, R56
- N60, N65
- X30, F31, P32
- N35, V36
- I101, P102, N103, F104, I105, P106
- Q111
- R114, A115, D116, F117
- P125, N126, D127
- N132, F145, K148
- R151, L163, Y178

Bottom Row Labels:

- R182, P183, I190, G193, I197
- E202
- F217
- L229
- L233, F234, V235
- T238, N239, A240
- P260, GLU

A red dot is located above the square labeled G193.

Chain C: 

THR	D832	M223	D1
GLU	K333	E224	F11
TRP	I334	S225	F12
VAL	N335	V226	H18
MET	G336	V230	P29
ALA	W339	I231	R44
GLU	F340	I232	I48
PRO	E343	A245	G63
GLU	G344	V246	L64
	E345	P247	L65
	T346	A251	W70
	W354	S269	H62
	R355	F270	S86
	D356	K271	V93
	G357	S272	T103
	A358	G273	K106
	Y359	I274	P113
	X360	F275	A123
	A361	T276	I124
	K362	V277	T125
	V363	I278	R126
	P364	V279	P139
	F365	G280	R140
	P366	G281	A143
	L367	S281	Y149
	T368	H282	V184
	G371	H283	T188
	I388	S284	D189
	R392	F286	T190
	F393	D287	M191
	T394	S288	G198
	I395	T289	E205
	P396	K290	Y211
	D397	A291	I216
	Y398	I292	L220
	I399	L293	
	V400	K294	
	D401	Y295	
	S402	G296	
	A403	D297	
	A404	V298	
	S405	S299	
	N408	D300	
	I409	H301	
	L410	I302	
	P413	A303	
	R417	Q304	
LEU	ARG	W318	
ALA	GLN	I325	
		K326	
		F327	
		K328	
		I329	

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	340.04Å 396.85Å 431.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.60 49.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.3 (49.50-2.60) 88.6 (49.65-2.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.61Å)	Xtriage
Refinement program	CNS 1.3, PHENIX	Depositor
R, R_{free}	0.279 , (Not available) 0.245 , 0.245	Depositor DCC
R_{free} test set	38971 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.25 , 17.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7438	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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 [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	A	0.24	0/2079	0.46	0/2832
2	B	0.26	0/2139	0.47	0/2907
3	C	0.24	0/3360	0.47	1/4600 (0.0%)
All	All	0.25	0/7578	0.47	1/10339 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	70	TRP	CA-CB-CG	6.00	125.11	113.70

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	A	2023	0	1972	29	0
2	B	2086	0	2072	32	0
3	C	3260	0	3208	45	0
4	A	20	0	0	0	0
4	B	19	0	0	0	0
4	C	30	0	0	0	0
All	All	7438	0	7252	97	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 7.

The worst 5 of 97 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:C:124:TYR:HB2	3:C:245:ALA:HB3	1.61	0.81
3:C:82:HIS:HB3	3:C:216:ILE:HD12	1.63	0.81
2:B:127:ASP:OD2	3:C:140:ARG:NH2	2.15	0.80
1:A:17:PRO:O	3:C:126:ARG:NH2	2.15	0.79
3:C:188:THR:HG22	3:C:190:THR:H	1.47	0.77

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	250/266 (94%)	239 (96%)	11 (4%)	0	100	100
2	B	258/261 (99%)	245 (95%)	13 (5%)	0	100	100
3	C	415/430 (96%)	404 (97%)	11 (3%)	0	100	100
All	All	923/957 (96%)	888 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	218/230 (95%)	215 (99%)	3 (1%)	67	85
2	B	233/234 (100%)	231 (99%)	2 (1%)	78	91
3	C	355/366 (97%)	354 (100%)	1 (0%)	92	98
All	All	806/830 (97%)	800 (99%)	6 (1%)	84	94

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	LEU
3	C	70	TRP
2	B	60	TRP
1	A	221	TYR
2	B	132	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	110	HIS

5.3.3 RNA [i](#)

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 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 ⓘ

There are no chain breaks in this entry.

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	A	252/266 (94%)	-0.30	1 (0%) 92 91	9, 14, 29, 56	0
2	B	260/261 (99%)	-0.33	1 (0%) 92 91	8, 15, 30, 36	0
3	C	417/430 (96%)	0.38	64 (15%) 2 1	9, 18, 56, 66	0
All	All	929/957 (97%)	-0.00	66 (7%) 16 11	8, 15, 52, 66	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	280	GLY	5.6
3	C	302	ILE	5.3
3	C	285	PHE	5.2
3	C	398	TYR	5.2
3	C	286	PHE	4.9

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 carbohydrates 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.