



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 08:04 am BST

PDB ID : 3M8L
Title : Crystal Structure Analysis of the Feline Calicivirus Capsid Protein
Authors : Zhou, Y.; Prasad, B.V.V.
Deposited on : 2010-03-18
Resolution : 3.40 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

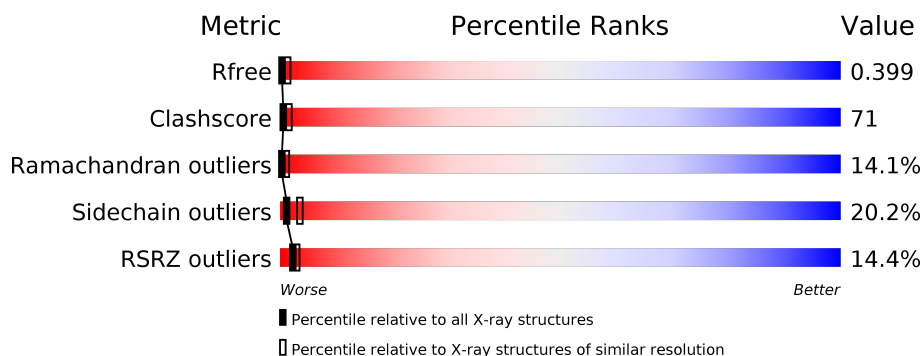
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	534	<div> <div>12%</div> <div>25%</div> <div>52%</div> <div>20%</div> <div>.</div> </div>
1	B	534	<div> <div>16%</div> <div>20%</div> <div>55%</div> <div>21%</div> <div>..</div> </div>
1	C	534	<div> <div>16%</div> <div>23%</div> <div>56%</div> <div>19%</div> <div>.</div> </div>

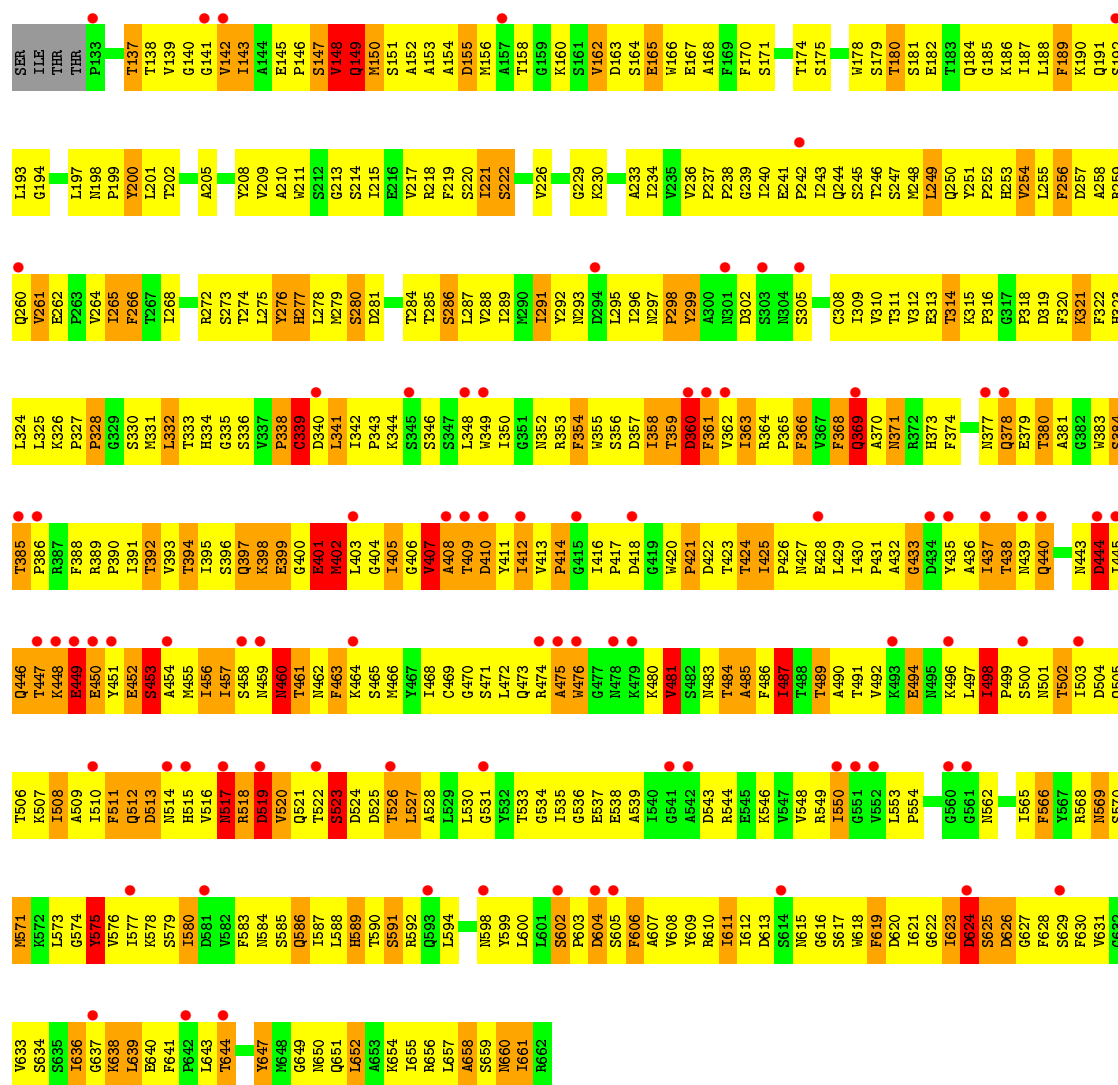
2 Entry composition

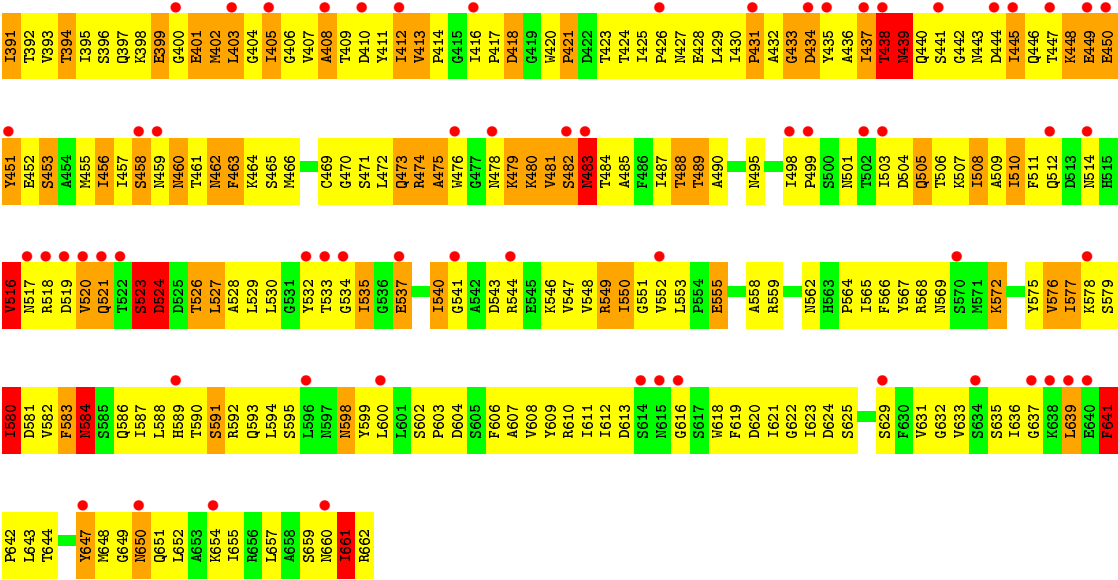
There is only 1 type of molecule in this entry. The entry contains 12360 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4129	2632	687	796	14			
1	B	530	Total	C	N	O	S	0	0	0
			4101	2615	683	789	14			
1	C	534	Total	C	N	O	S	0	0	0
			4130	2632	687	797	14			





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	427.08 Å 450.73 Å 467.59 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.40 29.98 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.40) 89.1 (29.98-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.39 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.390 , 0.370 0.402 , 0.399	Depositor DCC
R_{free} test set	27284 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	85.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	12360	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	A	0.68	1/4229 (0.0%)	0.84	4/5759 (0.1%)
1	B	1.17	11/4201 (0.3%)	0.89	6/5719 (0.1%)
1	C	0.71	1/4230 (0.0%)	0.89	7/5759 (0.1%)
All	All	0.88	13/12660 (0.1%)	0.87	17/17237 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	624	ASP	CB-CG	33.85	2.22	1.51
1	B	606	PHE	CE1-CZ	24.62	1.84	1.37
1	B	606	PHE	CE2-CZ	22.49	1.80	1.37
1	B	606	PHE	CD2-CE2	20.22	1.79	1.39
1	B	606	PHE	CD1-CE1	20.20	1.79	1.39

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	THR	CB-CA-C	13.09	146.94	111.60
1	A	439	ASN	N-CA-CB	-13.07	87.07	110.60
1	B	624	ASP	CB-CG-OD1	9.58	126.92	118.30
1	C	451	TYR	CB-CA-C	-8.87	92.67	110.40
1	B	360	ASP	N-CA-C	8.51	133.98	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200	TYR	Sidechain

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	4129	0	4062	602	0
1	B	4101	0	4033	615	6
1	C	4130	0	4062	563	7
All	All	12360	0	12157	1731	7

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 71.

The worst 5 of 1731 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:B:606:PHE:CE1	1:B:606:PHE:CZ	1.84	1.62
1:B:606:PHE:CD2	1:B:606:PHE:CE2	1.79	1.62
1:B:606:PHE:CD1	1:B:606:PHE:CE1	1.79	1.62
1:B:606:PHE:CZ	1:B:606:PHE:CE2	1.80	1.61
1:B:606:PHE:CZ	1:B:624:ASP:CB	1.88	1.51

The worst 5 of 7 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:B:299:TYR:CE1	1:C:299:TYR:OH[2_555]	1.77	0.43
1:B:299:TYR:CD1	1:C:299:TYR:CZ[2_555]	1.97	0.23
1:B:229:GLY:N	1:C:222:SER:OG[2_555]	2.06	0.14
1:B:292:TYR:OH	1:C:313:GLU:OE1[2_555]	2.07	0.13
1:B:252:PRO:N	1:C:169:PHE:CE1[2_555]	2.10	0.10

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	532/534 (100%)	310 (58%)	147 (28%)	75 (14%)	0	1
1	B	528/534 (99%)	321 (61%)	132 (25%)	75 (14%)	0	1
1	C	532/534 (100%)	332 (62%)	126 (24%)	74 (14%)	0	1
All	All	1592/1602 (99%)	963 (60%)	405 (25%)	224 (14%)	0	1

5 of 224 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	PRO
1	A	145	GLU
1	A	146	PRO
1	A	151	SER
1	A	279	MET

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	461/461 (100%)	370 (80%)	91 (20%)	1	4
1	B	457/461 (99%)	354 (78%)	103 (22%)	1	2
1	C	461/461 (100%)	377 (82%)	84 (18%)	1	6
All	All	1379/1383 (100%)	1101 (80%)	278 (20%)	1	3

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	369	GLN
1	B	487	ILE
1	C	523	SER
1	B	384	SER
1	B	435	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	277	HIS
1	B	443	ASN
1	C	569	ASN
1	B	369	GLN
1	B	514	ASN

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 [i](#)

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	534/534 (100%)	0.85	62 (11%) 4 5	48, 97, 120, 143	0
1	B	530/534 (99%)	0.99	84 (15%) 2 2	48, 97, 112, 129	0
1	C	534/534 (100%)	1.02	84 (15%) 2 2	49, 95, 113, 123	0
All	All	1598/1602 (99%)	0.95	230 (14%) 2 3	48, 96, 115, 143	0

The worst 5 of 230 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	PRO	7.3
1	A	522	THR	7.1
1	A	447	THR	6.7
1	A	450	GLU	6.4
1	B	412	ILE	6.2

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.