



wwPDB EM Validation Summary Report ⓘ

Dec 13, 2022 – 12:15 AM EST

PDB ID : 2CSE
Title : Features of Reovirus Outer-Capsid Protein mu1 Revealed by Electron and Image Reconstruction of the virion at 7.0-Å Resolution
Authors : Zhang, X.; Ji, Y.; Zhang, L.; Harrison, S.C.; Marinescu, D.C.; Nibert, M.L.; Baker, T.S.
Deposited on : 2005-05-21
Resolution : 7.00 Å (reported)
Based on initial models : 1EJ6, 1JMU, 1N35

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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
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) : 2.31.2

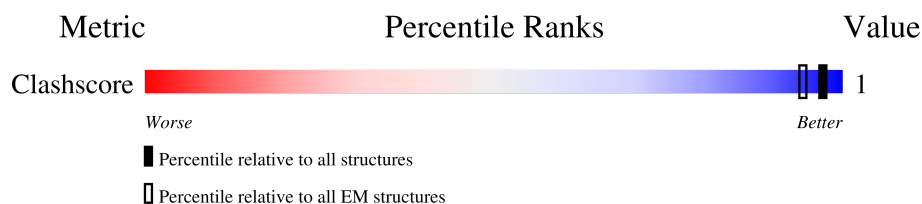
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 7.00 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)	EM structures (#Entries)
Clashscore	158937	4297

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	708	 90% 9%
1	B	708	 91% 9%
1	C	708	 90% 9%
1	J	708	 91% 9%
1	K	708	 90% 9%
1	L	708	 91% 9%
1	P	708	 91% 9%
1	Q	708	 91% 9%
1	R	708	 91% 9%
1	T	708	 91% 9%
2	D	365	 100%

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Mol	Chain	Length	Quality of chain
2	E	365	 100%
2	F	365	 100%
2	G	365	 100%
2	H	365	 100%
2	I	365	 100%
2	M	365	 100%
2	N	365	 100%
2	O	365	 100%
2	S	365	 100%
3	U	1289	 99%
4	V	1275	 81% 19%
4	W	1275	 96% .
5	X	418	 100%
5	Y	418	 100%
5	Z	418	 100%
6	1	1267	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16111 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 major outer-capsid protein mu1.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	641	Total C 641 641	0	641
1	B	641	Total C 641 641	0	641
1	C	641	Total C 641 641	0	641
1	P	641	Total C 641 641	0	641
1	Q	641	Total C 641 641	0	641
1	R	641	Total C 641 641	0	641
1	J	641	Total C 641 641	0	641
1	K	641	Total C 641 641	0	641
1	L	641	Total C 641 641	0	641
1	T	641	Total C 641 641	0	641

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	344	LEU	PRO	conflict	UNP P11077
A	359	PHE	LEU	conflict	UNP P11077
B	344	LEU	PRO	conflict	UNP P11077
B	359	PHE	LEU	conflict	UNP P11077
C	344	LEU	PRO	conflict	UNP P11077
C	359	PHE	LEU	conflict	UNP P11077
J	344	LEU	PRO	conflict	UNP P11077
J	359	PHE	LEU	conflict	UNP P11077
K	344	LEU	PRO	conflict	UNP P11077
K	359	PHE	LEU	conflict	UNP P11077

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Chain	Residue	Modelled	Actual	Comment	Reference
L	344	LEU	PRO	conflict	UNP P11077
L	359	PHE	LEU	conflict	UNP P11077
P	344	LEU	PRO	conflict	UNP P11077
P	359	PHE	LEU	conflict	UNP P11077
Q	344	LEU	PRO	conflict	UNP P11077
Q	359	PHE	LEU	conflict	UNP P11077
R	344	LEU	PRO	conflict	UNP P11077
R	359	PHE	LEU	conflict	UNP P11077
T	344	LEU	PRO	conflict	UNP P11077
T	359	PHE	LEU	conflict	UNP P11077

- Molecule 2 is a protein called major capsid surface protein sigma-3.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	S	365	Total C 365 365	0	365
2	D	365	Total C 365 365	0	365
2	E	365	Total C 365 365	0	365
2	F	365	Total C 365 365	0	365
2	M	365	Total C 365 365	0	365
2	N	365	Total C 365 365	0	365
2	O	365	Total C 365 365	0	365
2	G	365	Total C 365 365	0	365
2	H	365	Total C 365 365	0	365
2	I	365	Total C 365 365	0	365

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	104	CYS	ALA	conflict	UNP P07939
D	325	ASN	ASP	conflict	UNP P07939
E	104	CYS	ALA	conflict	UNP P07939
E	325	ASN	ASP	conflict	UNP P07939

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Chain	Residue	Modelled	Actual	Comment	Reference
F	104	CYS	ALA	conflict	UNP P07939
F	325	ASN	ASP	conflict	UNP P07939
G	104	CYS	ALA	conflict	UNP P07939
G	325	ASN	ASP	conflict	UNP P07939
H	104	CYS	ALA	conflict	UNP P07939
H	325	ASN	ASP	conflict	UNP P07939
I	104	CYS	ALA	conflict	UNP P07939
I	325	ASN	ASP	conflict	UNP P07939
M	104	CYS	ALA	conflict	UNP P07939
M	325	ASN	ASP	conflict	UNP P07939
N	104	CYS	ALA	conflict	UNP P07939
N	325	ASN	ASP	conflict	UNP P07939
O	104	CYS	ALA	conflict	UNP P07939
O	325	ASN	ASP	conflict	UNP P07939
S	104	CYS	ALA	conflict	UNP P07939
S	325	ASN	ASP	conflict	UNP P07939

- Molecule 3 is a protein called guanylyltransferase.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	U	1284	Total C 1284 1284	0	1284

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	609	GLY	PHE	conflict	UNP P11079

- Molecule 4 is a protein called major core protein lambda 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	V	1031	Total C 1031 1031	0	1031
4	W	1221	Total C 1221 1221	0	1221

- Molecule 5 is a protein called Sigma 2 protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	X	417	Total C 417 417	0	417

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Mol	Chain	Residues	Atoms		AltConf	Trace
5	Y	417	Total 417	C 417	0	417
5	Z	417	Total 417	C 417	0	417


- Molecule 6 is a protein called Minor core protein lambda 3.

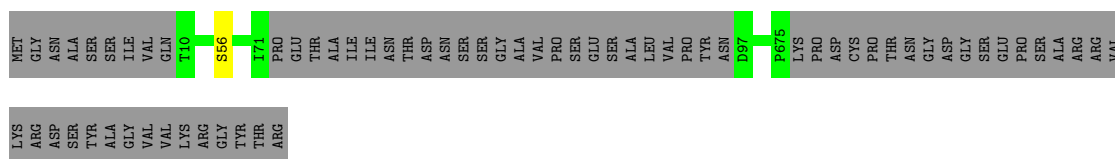
Mol	Chain	Residues	Atoms		AltConf	Trace
6	1	1264	Total 1264	C 1264	0	1264

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.

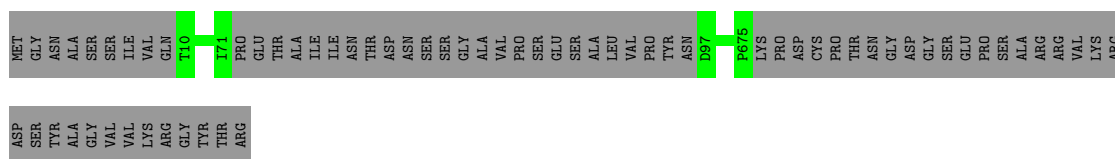
- Molecule 1: major outer-capsid protein mu1

Chain A: 



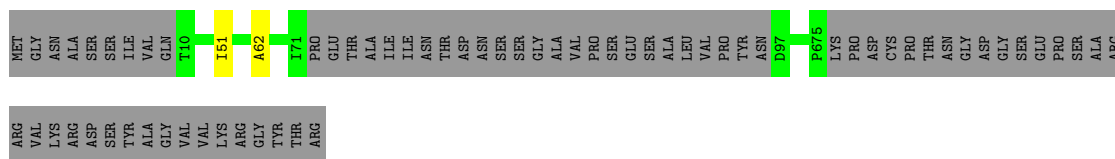
- Molecule 1: major outer-capsid protein mu1

Chain B: 



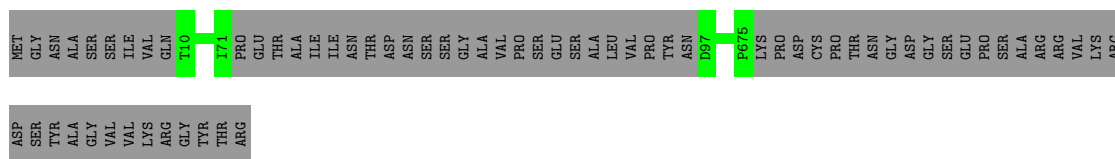
- Molecule 1: major outer-capsid protein mu1

Chain C: 



- Molecule 1: major outer-capsid protein mu1

Chain P: 



- Molecule 1: major outer-capsid protein mu1

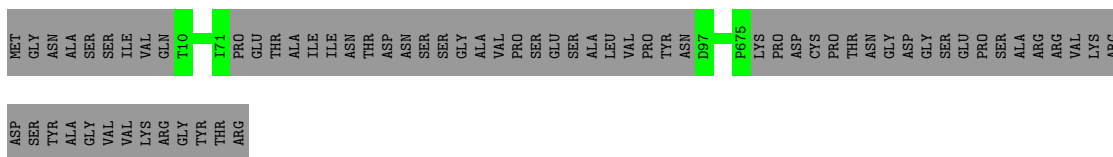
- Molecule 1: major outer-capsid protein mu1

- Molecule 1: major outer-capsid protein mu1

- Molecule 1: major outer-capsid protein mu1

- Molecule 1: major outer-capsid protein mu1

- Molecule 1: major outer-capsid protein mu1



- Molecule 2: major capsid surface protein sigma-3

Chain S: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain F: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain M: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain N: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain 0: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain G:  100%

There are no outlier residues recorded for this chain.

- Chain X: 100%



- Molecule 5: Sigma 2 protein

Chain Y:  100%



- Molecule 5: Sigma 2 protein

Chain Z:  100%



- Molecule 6: Minor core protein lambda 3

Chain 1:  100%



4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 7.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-7.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16111	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	641	0	0	1	0
1	B	641	0	0	0	0
1	C	641	0	0	1	0
1	J	641	0	0	0	0
1	K	641	0	0	1	0
1	L	641	0	0	0	0
1	P	641	0	0	0	0
1	Q	641	0	0	0	0
1	R	641	0	0	0	0
1	T	641	0	0	0	0
2	D	365	0	0	0	0
2	E	365	0	0	0	0
2	F	365	0	0	0	0
2	G	365	0	0	0	0
2	H	365	0	0	0	0
2	I	365	0	0	0	0
2	M	365	0	0	0	0
2	N	365	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	365	0	0	0	0
2	S	365	0	0	0	0
3	U	1284	0	0	2	0
4	V	1031	0	0	2	0
4	W	1221	0	0	1	0
5	X	417	0	0	0	0
5	Y	417	0	0	1	0
5	Z	417	0	0	0	0
6	1	1264	0	0	1	0
All	All	16111	0	0	9	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 1.

The worst 5 of 9 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:56:SER:CA	5:Y:15:GLY:CA	2.13	1.25
1:C:51:ILE:CA	1:C:62:ALA:CA	2.63	0.77
3:U:245:PRO:CA	3:U:246:PRO:CA	2.83	0.56
4:V:1247:LEU:CA	4:V:1248:PRO:CA	2.84	0.56
1:K:51:ILE:CA	1:K:62:ALA:CA	2.85	0.55

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 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](#)

There are no chain breaks in this entry.