



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:35 PM BST

PDB ID : 1NN8  
Title : CryoEM structure of poliovirus receptor bound to poliovirus  
Authors : He, Y.; Mueller, S.; Chipman, P.R.; Bator, C.M.; Peng, X.; Bowman, V.D.;  
Mukhopadhyay, S.; Wimmer, E.; Kuhn, R.J.; Rossmann, M.G.  
Deposited on : 2003-01-13  
Resolution : 15.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

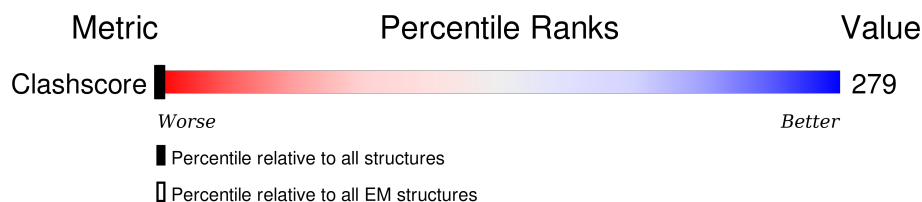
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



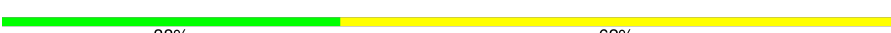




The reported resolution of this entry is 15.00 Å.

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	114402	924

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	R	302	 40% 60%
1	S	302	 33% 67%
1	T	302	 38% 62%
2	1	302	 95% 5%
3	2	272	 98% ..
4	3	235	 100%
5	4	68	 91% 9%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 1757 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 poliovirus receptor.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	R	301	Total 301	C 301	0	301
1	S	301	Total 301	C 301	0	301
1	T	301	Total 301	C 301	0	301

- Molecule 2 is a protein called coat protein VP1.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	1	288	Total 288	C 288	0	288

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	6	GLY	LEU	CONFLICT	UNP P03300
1	7	SER	GLU	CONFLICT	UNP P03300
1	9	SER	MET	CONFLICT	UNP P03300
1	10	THR	ILE	CONFLICT	UNP P03300

- Molecule 3 is a protein called coat protein VP2.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	2	268	Total 268	C 268	0	268

- Molecule 4 is a protein called coat protein VP3.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	3	235	Total 235	C 235	0	235

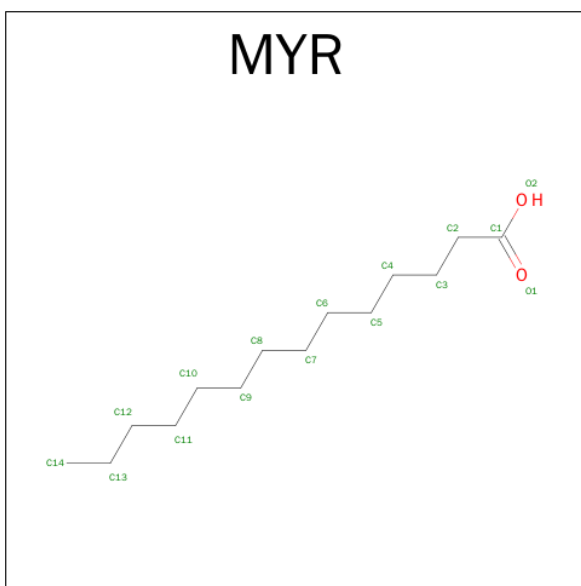
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	CONFLICT	UNP P03300

- Molecule 5 is a protein called coat protein VP4.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	4	62	Total C 62 62	0	62

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).

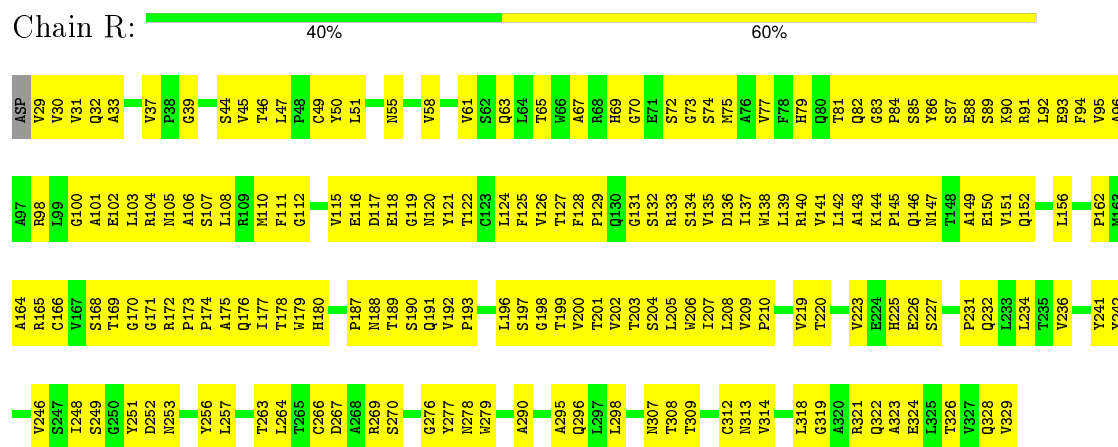


Mol	Chain	Residues	Atoms	AltConf
6	4	1	Total C 1 1	0

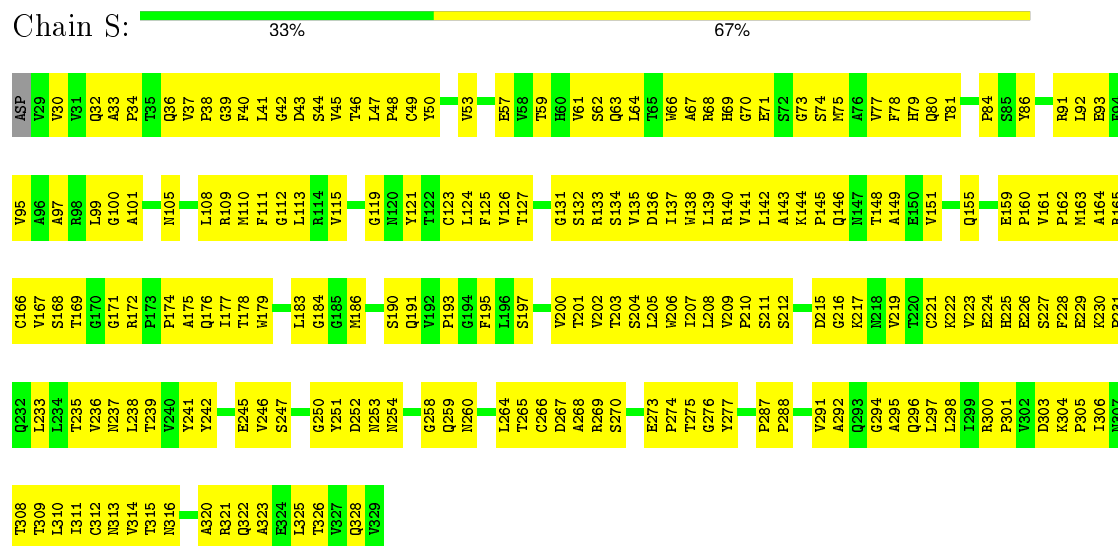
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

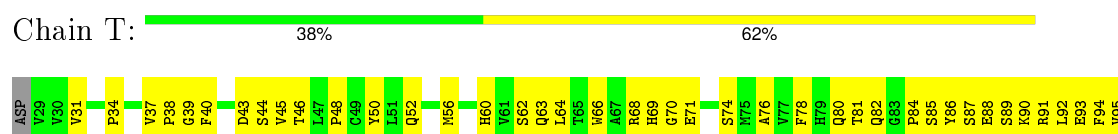
- Molecule 1: poliovirus receptor

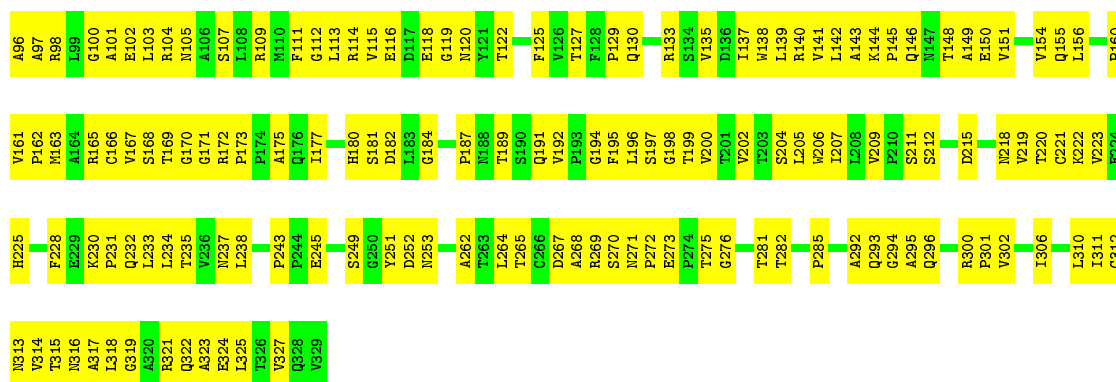


- Molecule 1: poliovirus receptor



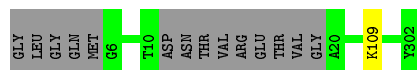
- Molecule 1: poliovirus receptor





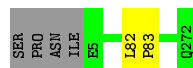
- Molecule 2: coat protein VP1

Chain 1: 95% 5%



- Molecule 3: coat protein VP2

Chain 2: 98% ..



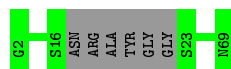
- Molecule 4: coat protein VP3

Chain 3: 100%

There are no outlier residues recorded for this chain.

- Molecule 5: coat protein VP4

Chain 4: 91% 9%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF is corrected for each image	Depositor
Microscope	PHILIPS CM300 FEG	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MYR

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 ⓘ

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	R	301	0	0	312	0
1	S	301	0	0	330	0
1	T	301	0	0	320	0
2	1	288	0	0	1	0
3	2	268	0	0	1	0
4	3	235	0	0	0	0
5	4	62	0	0	0	0
6	4	1	0	0	0	0
All	All	1757	0	0	490	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 279.

The worst 5 of 490 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:R:225:HIS:CA	1:S:223:VAL:CA	1.75	1.63
1:S:79:HIS:CA	1:T:80:GLN:CA	1.77	1.63
1:S:160:PRO:CA	1:T:161:VAL:CA	1.75	1.62
1:R:108:LEU:CA	1:S:109:ARG:CA	1.77	1.62
1:R:328:GLN:CA	1:T:302:VAL:CA	1.78	1.61

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.