



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 1, 2017 – 11:16 AM EST

PDB ID : 5KU2
EMDB ID: : EMD-8286
Title : expanded poliovirus in complex with VHH 7A
Authors : Strauss, M.; Schotte, L.; Filman, D.J.; Hogle, J.M.
Deposited on : 2016-07-12
Resolution : 4.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : rb-20028442

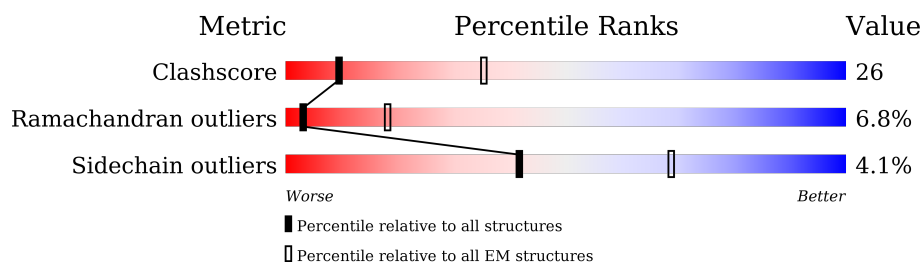
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 ≥ 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	1	209	<div> <div>57%</div> <div>31%</div> <div>• 9%</div> </div>
2	2	268	<div> <div>48%</div> <div>34%</div> <div>5%</div> <div>12%</div> </div>
3	3	230	<div> <div>52%</div> <div>38%</div> <div>5%</div> <div>• •</div> </div>
4	7	125	<div> <div>40%</div> <div>46%</div> <div>10%</div> <div>• •</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5994 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	191	Total	C	N	O	S	0	0
			1543	996	261	281	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	228	ILE	LEU	conflict	UNP P03300

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	235	Total	C	N	O	S	0	0
			1822	1160	310	339	13		

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	221	Total	C	N	O	S	0	0
			1712	1093	279	323	17		

There is a discrepancy between the modelled and reference sequences:

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

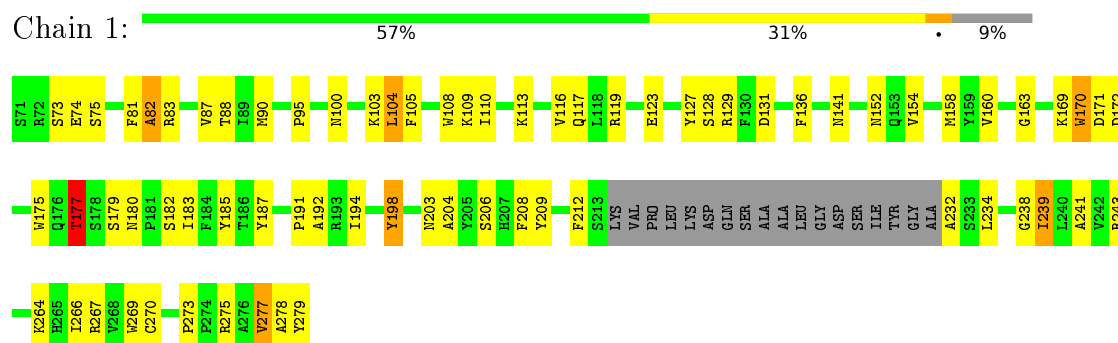
- Molecule 4 is a protein called VHH 7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	124	Total	C	N	O	S	0	0
			917	567	159	186	5		

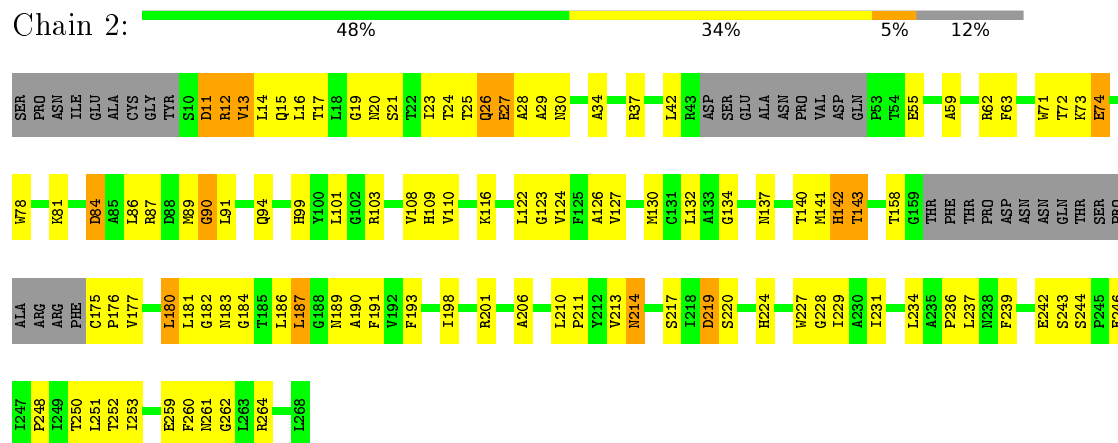
3 Residue-property plots

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.

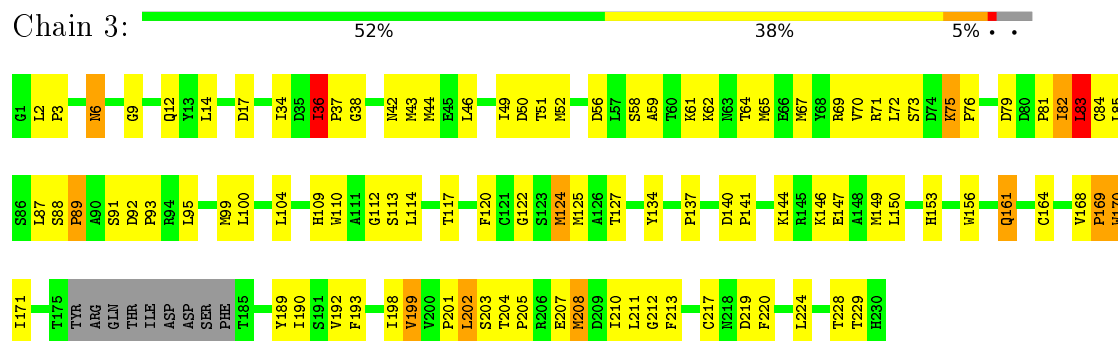
• Molecule 1: VP1



• Molecule 2: VP2



• Molecule 3: VP3



● Molecule 4: VHH 7A

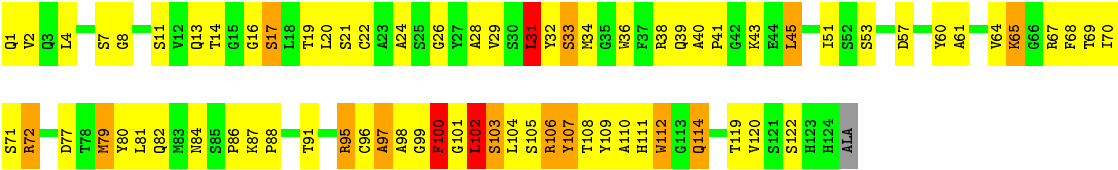
Chain 7:

40%

46%

10%

..



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	17654	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

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 >2	RMSZ	# Z >2
1	1	0.60	0/1590	0.96	1/2169 (0.0%)
2	2	0.64	0/1870	1.01	3/2553 (0.1%)
3	3	0.65	0/1756	1.07	4/2392 (0.2%)
4	7	0.82	0/935	1.29	5/1265 (0.4%)
All	All	0.67	0/6151	1.06	13/8379 (0.2%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7	31	LEU	CA-CB-CG	8.08	133.89	115.30
4	7	102	LEU	CA-CB-CG	7.81	133.27	115.30
4	7	104	LEU	CA-CB-CG	6.60	130.49	115.30
3	3	202	LEU	CA-CB-CG	6.01	129.12	115.30
4	7	31	LEU	CB-CG-CD2	5.93	121.08	111.00

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	1	1543	0	1503	57	0
2	2	1822	0	1762	100	0
3	3	1712	0	1697	96	0
4	7	917	0	872	94	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5994	0	5834	309	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 26.

The worst 5 of 309 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)
2:2:140:THR:O	2:2:141:MET:CG	1.84	1.25
2:2:140:THR:O	2:2:141:MET:HG2	1.34	1.23
1:1:209:TYR:CE1	2:2:224:HIS:HD2	1.66	1.13
3:3:56:ASP:OD2	4:7:106:ARG:HD3	1.50	1.09
1:1:209:TYR:HE1	2:2:224:HIS:CD2	1.78	1.01

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 PDB entries followed by that with respect to all EM entries.

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	1	187/209 (90%)	154 (82%)	19 (10%)	14 (8%)	1	21
2	2	229/268 (85%)	180 (79%)	29 (13%)	20 (9%)	1	17
3	3	217/230 (94%)	182 (84%)	30 (14%)	5 (2%)	8	50
4	7	122/125 (98%)	90 (74%)	20 (16%)	12 (10%)	1	14
All	All	755/832 (91%)	606 (80%)	98 (13%)	51 (7%)	3	24

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	104	LEU
1	1	172	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	177	THR
1	1	198	TYR
1	1	234	LEU

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 PDB entries followed by that with respect to all EM entries.

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	1	170/183 (93%)	169 (99%)	1 (1%)	90	95
2	2	198/228 (87%)	194 (98%)	4 (2%)	63	86
3	3	196/206 (95%)	186 (95%)	10 (5%)	29	67
4	7	96/97 (99%)	84 (88%)	12 (12%)	6	31
All	All	660/714 (92%)	633 (96%)	27 (4%)	42	72

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	161	GLN
4	7	13	GLN
4	7	102	LEU
3	3	199	VAL
2	2	264	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	224	HIS
3	3	6	ASN
4	7	13	GLN
2	2	137	ASN
3	3	161	GLN

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.