wwPDB EM Map/Model Validation Report (i)

May 2, 2016 – 10:36 PM EDT

PDB ID	:	3EPC
EMDB ID:	:	EMD-1570
Title	:	CryoEM structure of poliovirus receptor bound to poliovirus type 1
Authors	:	Zhang, P.; Mueller, S.; Morais, M.C.; Bator, C.M.; Bowman, V.D.; Hafenstein, S.; Wimmer, E.; Rossmann, M.G.
Deposited on	:	2008-09-29
Resolution	:	8.00 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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

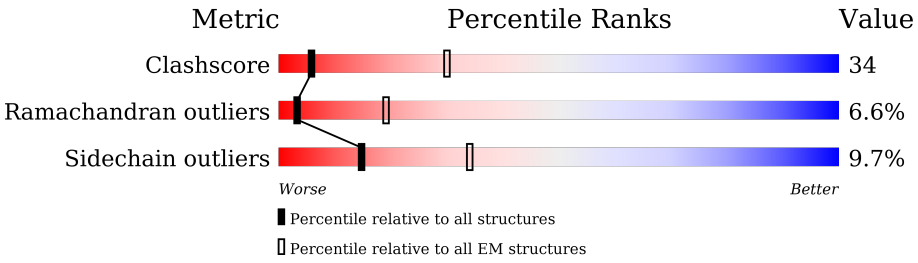
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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
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 <=5%

Mol	Chain	Length	Quality of chain
1	R	213	38% 41% 17% .
2	1	283	55% 35% 9% .
3	2	268	56% 34% 8% .
4	4	68	40% 40% 13% 7%
5	3	235	51% 38% 9% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SPH	1	0	X	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8292 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	213	Total	C	N	O	S	0	0
			1638	1038	281	310	9		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	105	ASP	ASN	ENGINEERED	UNP P15151
R	120	SER	ASN	ENGINEERED	UNP P15151
R	188	GLN	ASN	ENGINEERED	UNP P15151
R	218	GLN	ASN	ENGINEERED	UNP P15151
R	237	SER	ASN	ENGINEERED	UNP P15151

- Molecule 2 is a protein called Protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	283	Total	C	N	O	S	0	0
			2222	1416	378	423	5		

- Molecule 3 is a protein called Protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	268	Total	C	N	O	S	0	0
			2085	1317	358	396	14		

- Molecule 4 is a protein called Protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	63	Total	C	N	O	S	0	1
			477	293	82	101	1		

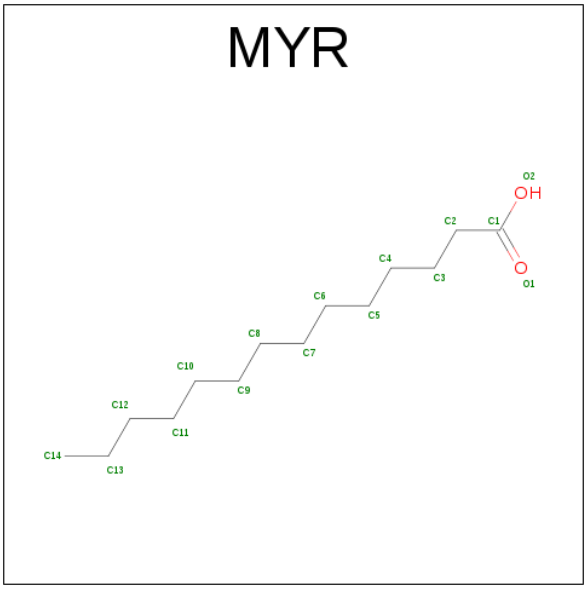
- Molecule 5 is a protein called Protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	235	Total	C	N	O	S	0	0
			1834	1169	299	349	17		

There is a discrepancy between the modelled and reference sequences:

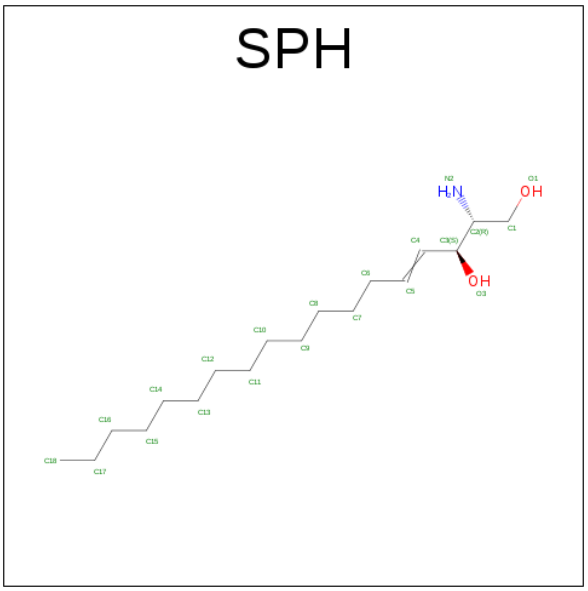
Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	SEE REMARK 999	UNP P03300

- 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	O	0
			15	14	1	

- Molecule 7 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



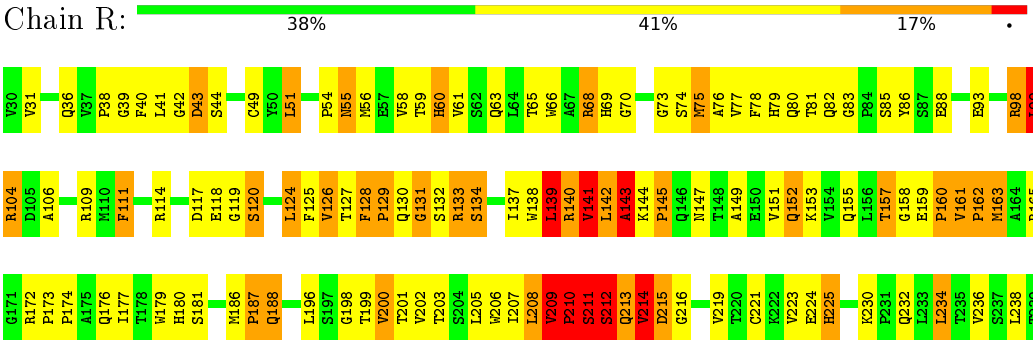
Mol	Chain	Residues	Atoms				AltConf
7	1	1	Total	C	N	O	0
			21	18	1	2	

3 Residue-property plots (i)

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.

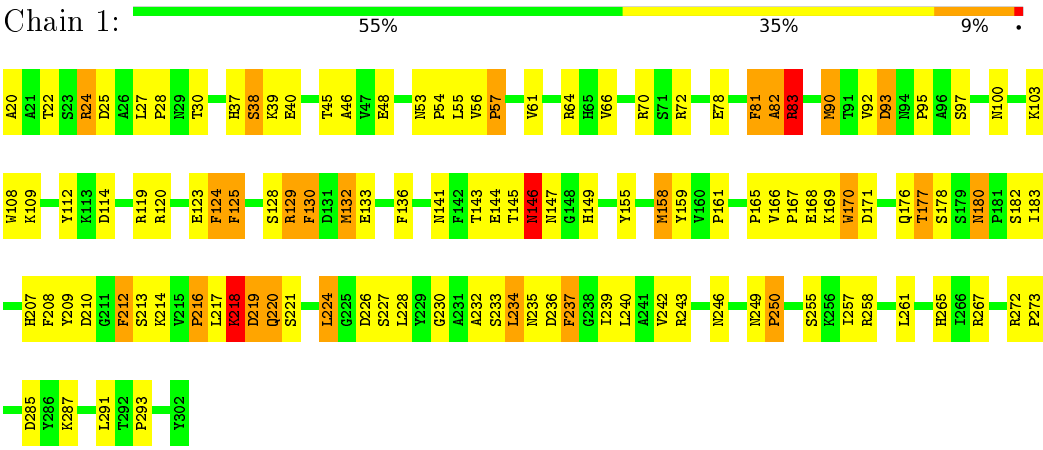
- Molecule 1: Poliovirus receptor

Chain R:



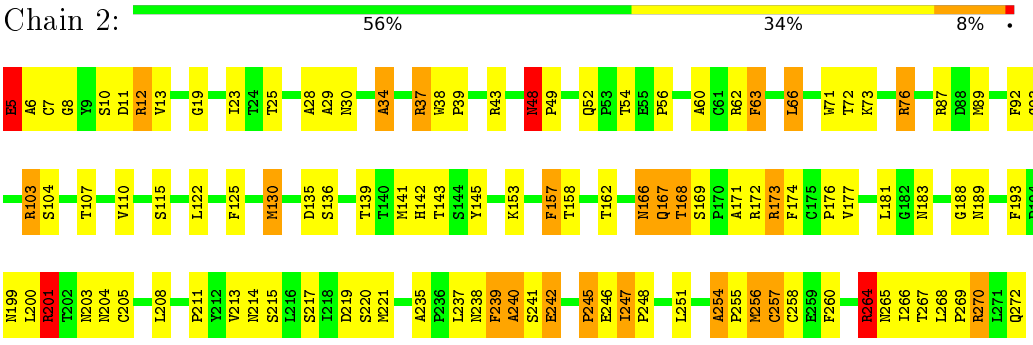
- Molecule 2: Protein VP1

Chain 1:



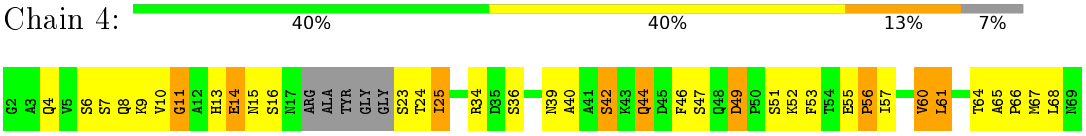
- Molecule 3: Protein VP2

Chain 2:



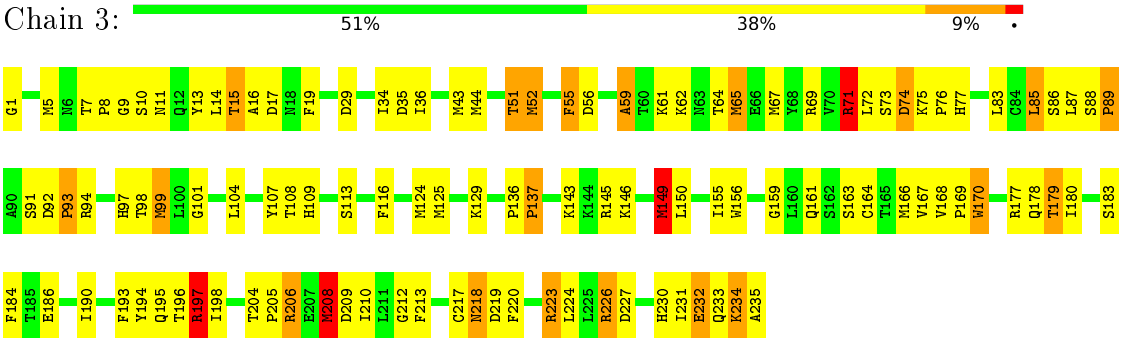
- Molecule 4: Protein VP4

Chain 4:



- Molecule 5: Protein VP3

Chain 3:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/Å^2$)	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

Bond lengths and bond angles in the following residue types are not validated in this section: SPH, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	R	0.41	0/1678	0.77	4/2289 (0.2%)
2	1	1.92	2/2285 (0.1%)	2.09	33/3124 (1.1%)
3	2	1.95	8/2142 (0.4%)	2.10	38/2928 (1.3%)
4	4	1.95	5/484 (1.0%)	2.11	11/653 (1.7%)
5	3	1.92	5/1881 (0.3%)	2.07	33/2562 (1.3%)
All	All	1.74	20/8470 (0.2%)	1.90	119/11556 (1.0%)

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	R	1	6

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	1	GLY	N-CA	9.08	1.59	1.46
2	1	20	ALA	N-CA	7.91	1.62	1.46
4	4	23	SER	N-CA	7.73	1.61	1.46
4	4	14	GLU	CD-OE2	6.59	1.32	1.25
3	2	5	GLU	N-CA	5.85	1.58	1.46

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	211	SER	O-C-N	-8.58	108.97	122.70
5	3	197	ARG	NE-CZ-NH2	7.74	124.17	120.30
5	3	69	ARG	NE-CZ-NH2	7.63	124.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	3	223	ARG	NE-CZ-NH2	7.63	124.11	120.30
3	2	264	ARG	NE-CZ-NH2	7.62	124.11	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	R	141	VAL	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	140	ARG	Peptide
1	R	143	ALA	Peptide
1	R	210	PRO	Peptide
1	R	211	SER	Peptide
1	R	212	SER	Mainchain

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	R	1638	0	1617	246	0
2	1	2222	0	2173	190	0
3	2	2085	0	2000	97	0
4	4	477	0	457	33	0
5	3	1834	0	1815	131	0
6	4	15	0	27	1	0
7	1	21	0	36	23	0
All	All	8292	0	8125	564	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 34.

The worst 5 of 564 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:130:GLN:NE2	2:1:105:PHE:CE1	1.75	1.52
1:R:128:PHE:HE2	2:1:108:TRP:NE1	1.18	1.40
1:R:130:GLN:CG	2:1:105:PHE:O	1.70	1.37
1:R:130:GLN:NE2	2:1:105:PHE:CZ	1.97	1.32
3:2:5:GLU:CG	3:2:7:CYS:HB3	1.58	1.32

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	R	211/213 (99%)	136 (64%)	50 (24%)	25 (12%)	0 9
2	1	281/283 (99%)	222 (79%)	43 (15%)	16 (6%)	2 28
3	2	266/268 (99%)	222 (84%)	36 (14%)	8 (3%)	5 42
4	4	59/68 (87%)	47 (80%)	7 (12%)	5 (8%)	1 18
5	3	233/235 (99%)	180 (77%)	38 (16%)	15 (6%)	2 25
All	All	1050/1067 (98%)	807 (77%)	174 (17%)	69 (7%)	3 24

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	55	ASN
1	R	99	LEU
1	R	143	ALA
1	R	188	GLN
1	R	210	PRO

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 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	R	185/185 (100%)	150 (81%)	35 (19%)	2 13
2	1	245/245 (100%)	230 (94%)	15 (6%)	23 60
3	2	228/228 (100%)	208 (91%)	20 (9%)	12 45
4	4	54/57 (95%)	46 (85%)	8 (15%)	4 24
5	3	210/210 (100%)	199 (95%)	11 (5%)	29 65
All	All	922/925 (100%)	833 (90%)	89 (10%)	15 40

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	143	THR
2	1	287	LYS
5	3	143	LYS
2	1	146	ASN
2	1	220	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	232	GLN
2	1	37	HIS
4	4	13	HIS
1	R	152	GLN
1	R	155	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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	SPH	1	0	-	19,20,20	1.27	1 (5%)	16,21,21	1.17	1 (6%)
6	MYR	4	1	4	14,14,15	0.96	1 (7%)	13,13,15	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SPH	1	0	-	2/2/2/4	0/21/21/21	0/0/0/0
6	MYR	4	1	4	-	0/12/12/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	4	1	MYR	O2-C1	-3.20	1.24	1.42
7	1	0	SPH	C4-C5	4.69	1.53	1.31

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1	0	SPH	C6-C5-C4	-3.85	113.38	125.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	1	0	SPH	C2
7	1	0	SPH	C3

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	1	0	SPH	23	0
6	4	1	MYR	1	0

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.