wwPDB EM Validation Summary Report (i)

May 13, 2024 – 09:23 pm BST

PDB ID	:	6S2C
EMDB ID	:	EMD-10087
Title	:	Acquired functional capsid structures in metazoan totivirus-like dsRNA virus.
Authors	:	Okamoto, K.; Larsson, S.D.D.; Maia, R.N.C.F.; Murata, K.; Hajdu, J.; Iwasaki, K.; Miyazaki, N.
Deposited on	:	2019-06-20
Resolution	:	3.20 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

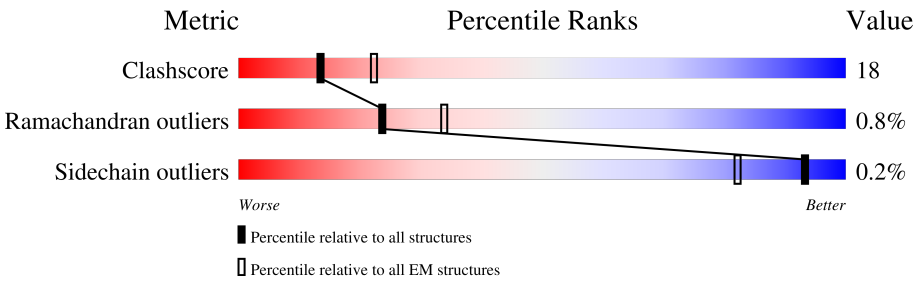
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.20 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
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	840	76% 22% ••
2	B	842	73% 25% ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12716 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	830	6352	4027	1091	1205	29	0	0

- Molecule 2 is a protein called Capsid protein.

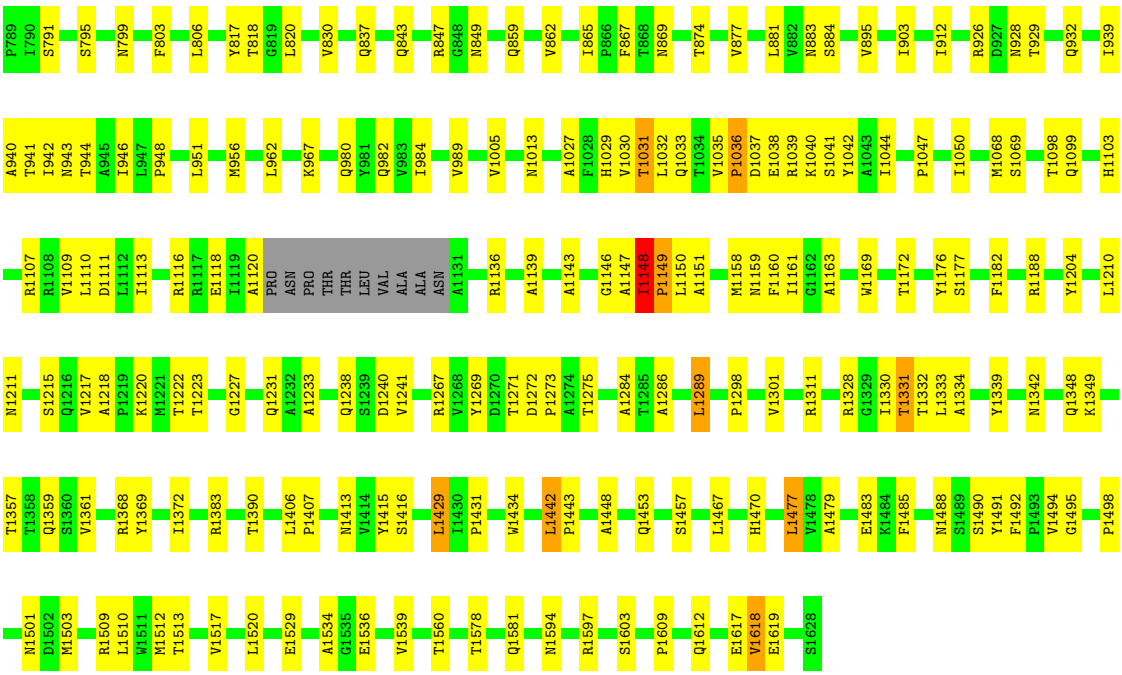
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	831	6364	4037	1093	1208	26	0	0

3 Residue-property plots (i)

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.

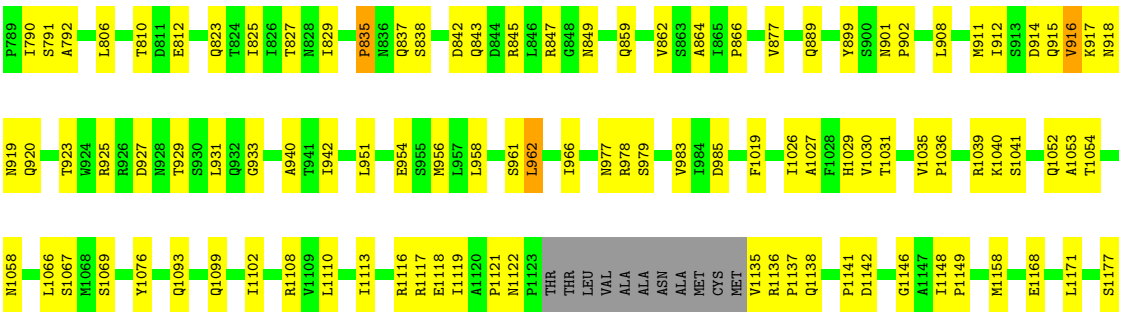
- Molecule 1: Capsid protein

Chain A: 76% 22% ••



- Molecule 2: Capsid protein

Chain B: 73% 25% ••



W1178
F1182
T1185
R1188
Q1189
E1209
L1210
N1211
L1214
S1215
K1220
M1221
T1222
T1223
G1227
A1233
D1240
L1246
R1251
F1256
P1257
Y1269
D1270
N1277
K1278
V1279
L1289
V1301
R1305
F1308
R1311
M1323
R1328
G1329
I1330
T1331
T1332
L1333
A1334
W1335
D1341
Q1348
R1352
T1363
I1364
A1367
V1373
F1381
H1382
R1383
A1386
T1390
I1399
T1400
H1401
F1402
E1403
R1404
N1413
V1414
Y1415
V1421
V1422
N1423
C1424
F1425
S1426
P1427
V1428
L1429
I1430
P1431
D1432
I1433
W1434
C1435
Q1436
Y1437
K1441
L1442
P1443
A1448
Q1453
G1454
Q1455
F1461
H1470
N1476
L1477
Y1478
A1479
E1483
S1489
S1490
Y1491
P1498
N1501
N1507
G1508
R1509
L1510
W1511
M1512
T1513
D1521
P1532
V1539
G1540
K1541
Q1542
I1543
E1549
A1559
Y1566
R1571
L1577
T1578
T1579
A1580
Q1581
N1594
L1601
N1604
V1605
Y1606
L1614
E1617
A1621
F1622
D1623
T1624
L1625
T1626
F1630

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	30363	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	225	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.42	0/6505	0.69	10/8896 (0.1%)
2	B	0.42	0/6520	0.68	6/8920 (0.1%)
All	All	0.42	0/13025	0.69	16/17816 (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
2	B	0	2

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1477	LEU	CA-CB-CG	8.05	133.82	115.30
1	A	1429	LEU	CA-CB-CG	7.37	132.25	115.30
2	B	1432	ASP	N-CA-CB	-7.16	97.71	110.60
2	B	1510	LEU	CA-CB-CG	6.84	131.04	115.30
1	A	1510	LEU	CA-CB-CG	6.68	130.66	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1035	VAL	Peptide
2	B	1256	PHE	Peptide

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	6352	0	6220	270	0
2	B	6364	0	6228	316	0
All	All	12716	0	12448	453	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 18.

The worst 5 of 453 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:944:THR:CG2	2:B:923:THR:HG21	1.18	1.65
1:A:1036:PRO:CG	1:A:1039:ARG:NH2	1.68	1.56
1:A:912:ILE:CD1	1:A:939:ILE:HG12	1.37	1.50
1:A:946:ILE:HD13	2:B:916:VAL:N	1.33	1.41
1:A:944:THR:HG21	2:B:923:THR:CG2	1.50	1.40

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	A	826/840 (98%)	714 (86%)	106 (13%)	6 (1%)	22 61
2	B	827/842 (98%)	689 (83%)	130 (16%)	8 (1%)	15 54
All	All	1653/1682 (98%)	1403 (85%)	236 (14%)	14 (1%)	24 58

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1618	VAL
2	B	916	VAL
2	B	1040	LYS
1	A	1149	PRO
1	A	1331	THR

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	A	675/683 (99%)	673 (100%)	2 (0%)	92 96
2	B	677/685 (99%)	676 (100%)	1 (0%)	93 98
All	All	1352/1368 (99%)	1349 (100%)	3 (0%)	93 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1148	ILE
1	A	1361	VAL
2	B	1429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1507	ASN
2	B	919	ASN
2	B	1501	ASN
2	B	915	GLN
2	B	977	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 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.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10087. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section was not generated.