wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:59 PM BST

PDB ID	:	4D1K
EMDB ID:	:	EMD-2638
Title	:	Cryo-electron microscopy of tubular arrays of HIV-1 Gag resolves structures essential for immature virus assembly.
Authors	:	Bharat, T.A.M.; Castillo-Menendez, L.R.; Hagen, W.J.H.; Lux, V.; Igonet, S.; Schorb, M.; Schur, F.K.M.; Krauesslich, H.G.; Briggs, J.A.G.
Deposited on	:	2014-05-02
Resolution	:	9.40 Å(reported)
Based on PDB ID	:	4COP

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

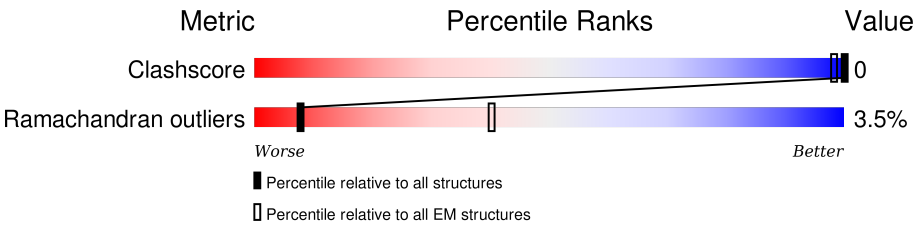
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.40 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

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	A	219	94% 5%
1	B	219	97% .
1	C	219	97% .
1	D	219	95% 5%
1	E	219	95% 5%
1	F	219	95% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3942 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 GAG PROTEIN.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N		
1	A	219	657	438	219	0	0
1	B	219	657	438	219	0	0
1	C	219	657	438	219	0	0
1	D	219	657	438	219	0	0
1	E	219	657	438	219	0	0
1	F	219	657	438	219	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ILE	LEU	VARIANT	UNP Q5D0H3
A	87	HIS	GLN	VARIANT	UNP Q5D0H3
A	120	HIS	SER	VARIANT	UNP Q5D0H3
A	169	SER	TYR	ENGINEERED MUTATION	UNP Q5D0H3
B	15	ILE	LEU	VARIANT	UNP Q5D0H3
B	87	HIS	GLN	VARIANT	UNP Q5D0H3
B	120	HIS	SER	VARIANT	UNP Q5D0H3
B	169	SER	TYR	ENGINEERED MUTATION	UNP Q5D0H3
C	15	ILE	LEU	VARIANT	UNP Q5D0H3
C	87	HIS	GLN	VARIANT	UNP Q5D0H3
C	120	HIS	SER	VARIANT	UNP Q5D0H3
C	169	SER	TYR	ENGINEERED MUTATION	UNP Q5D0H3
D	15	ILE	LEU	VARIANT	UNP Q5D0H3
D	87	HIS	GLN	VARIANT	UNP Q5D0H3
D	120	HIS	SER	VARIANT	UNP Q5D0H3
D	169	SER	TYR	ENGINEERED MUTATION	UNP Q5D0H3
E	15	ILE	LEU	VARIANT	UNP Q5D0H3
E	87	HIS	GLN	VARIANT	UNP Q5D0H3

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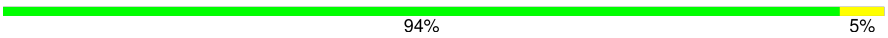
Chain	Residue	Modelled	Actual	Comment	Reference
E	120	HIS	SER	VARIANT	UNP Q5D0H3
E	169	SER	TYR	ENGINEERED MUTATION	UNP Q5D0H3
F	15	ILE	LEU	VARIANT	UNP Q5D0H3
F	87	HIS	GLN	VARIANT	UNP Q5D0H3
F	120	HIS	SER	VARIANT	UNP Q5D0H3
F	169	SER	TYR	ENGINEERED MUTATION	UNP Q5D0H3

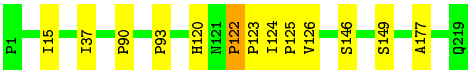
3 Residue-property plots (i)

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: GAG PROTEIN

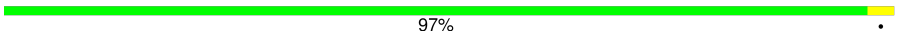
Chain A:





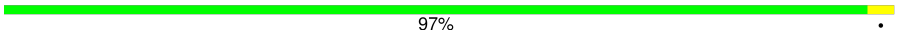
- Molecule 1: GAG PROTEIN

Chain B:



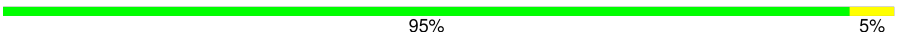
- Molecule 1: GAG PROTEIN

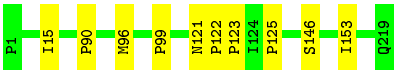
Chain C:



- Molecule 1: GAG PROTEIN

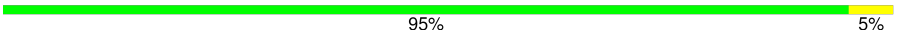
Chain D:





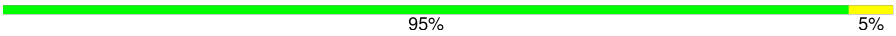
- Molecule 1: GAG PROTEIN

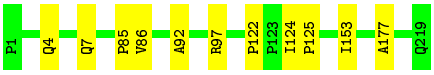
Chain E:



- Molecule 1: GAG PROTEIN

Chain F:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	23	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO-163 FILM	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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	1.51	3/656 (0.5%)	1.46	1/655 (0.2%)
1	B	1.44	0/656	1.44	0/655
1	C	1.46	0/656	1.46	0/655
1	D	1.47	0/656	1.39	0/655
1	E	1.49	0/656	1.43	0/655
1	F	1.46	1/656 (0.2%)	1.45	0/655
All	All	1.47	4/3936 (0.1%)	1.44	1/3930 (0.0%)

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	A	0	1
1	B	0	2
1	D	0	1
1	E	0	2
1	F	0	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	PRO	CA-C	5.87	1.64	1.52
1	F	85	PRO	CA-C	-5.52	1.41	1.52
1	A	37	ILE	C-N	5.52	1.44	1.34
1	A	126	VAL	C-N	5.13	1.42	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	PRO	N-CA-C	-5.15	98.71	112.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ILE	Peptide
1	B	121	ASN	Peptide
1	B	3	VAL	Peptide
1	D	121	ASN	Peptide
1	E	121	ASN	Peptide
1	E	124	ILE	Peptide
1	F	124	ILE	Peptide
1	F	4	GLN	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	657	0	230	0	0
1	B	657	0	230	0	0
1	C	657	0	230	0	0
1	D	657	0	230	0	0
1	E	657	0	230	0	0
1	F	657	0	230	0	0
All	All	3942	0	1380	0	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 0.

There are no clashes within the asymmetric unit.

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	217/219 (99%)	200 (92%)	8 (4%)	9 (4%)	3	35
1	B	217/219 (99%)	205 (94%)	7 (3%)	5 (2%)	8	48
1	C	217/219 (99%)	202 (93%)	8 (4%)	7 (3%)	5	41
1	D	217/219 (99%)	202 (93%)	6 (3%)	9 (4%)	3	35
1	E	217/219 (99%)	205 (94%)	4 (2%)	8 (4%)	4	38
1	F	217/219 (99%)	201 (93%)	8 (4%)	8 (4%)	4	38
All	All	1302/1314 (99%)	1215 (93%)	41 (3%)	46 (4%)	8	39

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	120	HIS
1	A	122	PRO
1	A	123	PRO
1	A	146	SER
1	C	97	ARG
1	C	122	PRO
1	C	123	PRO
1	C	146	SER
1	D	15	ILE
1	D	122	PRO
1	D	123	PRO
1	D	125	PRO
1	E	123	PRO
1	F	97	ARG
1	F	122	PRO
1	A	15	ILE
1	A	177	ALA
1	C	148	THR
1	D	96	MET
1	D	146	SER
1	E	97	ARG
1	E	122	PRO
1	E	178	SER
1	F	125	PRO
1	F	177	ALA
1	A	125	PRO

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Mol	Chain	Res	Type
1	B	122	PRO
1	B	147	PRO
1	E	125	PRO
1	E	149	SER
1	E	177	ALA
1	F	7	GLN
1	A	149	SER
1	B	148	THR
1	C	125	PRO
1	E	85	PRO
1	D	99	PRO
1	F	92	ALA
1	B	123	PRO
1	D	90	PRO
1	C	86	VAL
1	F	86	VAL
1	B	125	PRO
1	F	153	ILE
1	D	153	ILE

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)

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.