



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 03:28 PM EST

PDB ID : 6N3U
EMDB ID : EMD-0337
Title : MicroED Structure of the CTD-SP1 fragment of HIV-1 Gag with bound maturation inhibitor Bevirimat.
Authors : Purdy, M.D.; Shi, D.; Hattne, J.; Chrustowicz, J.
Deposited on : 2018-11-16
Resolution : 2.90 Å(reported)
Based on initial model : 5I4T

This is a Full wwPDB EM Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
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) : 2.31.2

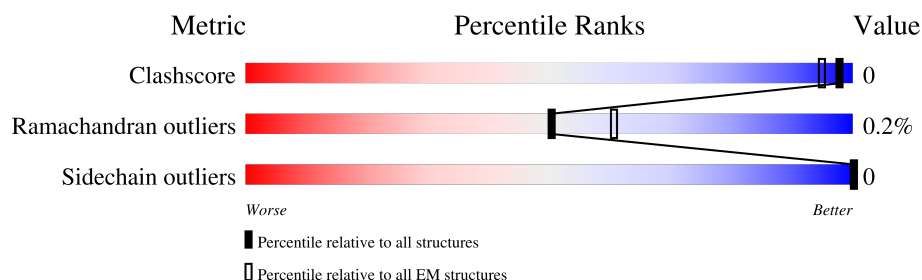
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 2.90 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	110	83% 17%
1	B	110	84% 16%
1	C	110	81% 16%
1	D	110	83% 17%
1	E	110	81% 17%
1	F	110	82% 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7814 atoms, of which 3848 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 CTD-SP1 fragment of HIV-1 Gag.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	91	Total	C	H	N	O	S	0	0
			1272	411	624	117	114	6		
1	B	92	Total	C	H	N	O	S	0	0
			1339	425	664	122	122	6		
1	C	92	Total	C	H	N	O	S	0	0
			1308	419	644	119	120	6		
1	D	91	Total	C	H	N	O	S	0	0
			1304	418	643	120	117	6		
1	E	91	Total	C	H	N	O	S	0	0
			1278	412	627	117	116	6		
1	F	92	Total	C	H	N	O	S	0	0
			1313	422	646	120	119	6		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	HIS	-	expression tag	UNP A0A248SMC7
A	269	MET	-	expression tag	UNP A0A248SMC7
A	270	HIS	-	expression tag	UNP A0A248SMC7
A	271	HIS	-	expression tag	UNP A0A248SMC7
A	272	HIS	-	expression tag	UNP A0A248SMC7
A	273	HIS	-	expression tag	UNP A0A248SMC7
A	274	HIS	-	expression tag	UNP A0A248SMC7
A	275	HIS	-	expression tag	UNP A0A248SMC7
A	276	GLY	-	expression tag	UNP A0A248SMC7
A	277	GLY	-	expression tag	UNP A0A248SMC7
A	373	THR	PRO	engineered mutation	UNP A0A248SMC7
B	268	HIS	-	expression tag	UNP A0A248SMC7
B	269	MET	-	expression tag	UNP A0A248SMC7
B	270	HIS	-	expression tag	UNP A0A248SMC7
B	271	HIS	-	expression tag	UNP A0A248SMC7
B	272	HIS	-	expression tag	UNP A0A248SMC7
B	273	HIS	-	expression tag	UNP A0A248SMC7
B	274	HIS	-	expression tag	UNP A0A248SMC7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	275	HIS	-	expression tag	UNP A0A248SMC7
B	276	GLY	-	expression tag	UNP A0A248SMC7
B	277	GLY	-	expression tag	UNP A0A248SMC7
B	373	THR	PRO	engineered mutation	UNP A0A248SMC7
C	268	HIS	-	expression tag	UNP A0A248SMC7
C	269	MET	-	expression tag	UNP A0A248SMC7
C	270	HIS	-	expression tag	UNP A0A248SMC7
C	271	HIS	-	expression tag	UNP A0A248SMC7
C	272	HIS	-	expression tag	UNP A0A248SMC7
C	273	HIS	-	expression tag	UNP A0A248SMC7
C	274	HIS	-	expression tag	UNP A0A248SMC7
C	275	HIS	-	expression tag	UNP A0A248SMC7
C	276	GLY	-	expression tag	UNP A0A248SMC7
C	277	GLY	-	expression tag	UNP A0A248SMC7
C	373	THR	PRO	engineered mutation	UNP A0A248SMC7
D	268	HIS	-	expression tag	UNP A0A248SMC7
D	269	MET	-	expression tag	UNP A0A248SMC7
D	270	HIS	-	expression tag	UNP A0A248SMC7
D	271	HIS	-	expression tag	UNP A0A248SMC7
D	272	HIS	-	expression tag	UNP A0A248SMC7
D	273	HIS	-	expression tag	UNP A0A248SMC7
D	274	HIS	-	expression tag	UNP A0A248SMC7
D	275	HIS	-	expression tag	UNP A0A248SMC7
D	276	GLY	-	expression tag	UNP A0A248SMC7
D	277	GLY	-	expression tag	UNP A0A248SMC7
D	373	THR	PRO	engineered mutation	UNP A0A248SMC7
E	268	HIS	-	expression tag	UNP A0A248SMC7
E	269	MET	-	expression tag	UNP A0A248SMC7
E	270	HIS	-	expression tag	UNP A0A248SMC7
E	271	HIS	-	expression tag	UNP A0A248SMC7
E	272	HIS	-	expression tag	UNP A0A248SMC7
E	273	HIS	-	expression tag	UNP A0A248SMC7
E	274	HIS	-	expression tag	UNP A0A248SMC7
E	275	HIS	-	expression tag	UNP A0A248SMC7
E	276	GLY	-	expression tag	UNP A0A248SMC7
E	277	GLY	-	expression tag	UNP A0A248SMC7
E	373	THR	PRO	engineered mutation	UNP A0A248SMC7
F	268	HIS	-	expression tag	UNP A0A248SMC7
F	269	MET	-	expression tag	UNP A0A248SMC7
F	270	HIS	-	expression tag	UNP A0A248SMC7
F	271	HIS	-	expression tag	UNP A0A248SMC7
F	272	HIS	-	expression tag	UNP A0A248SMC7

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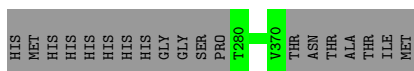
Chain	Residue	Modelled	Actual	Comment	Reference
F	273	HIS	-	expression tag	UNP A0A248SMC7
F	274	HIS	-	expression tag	UNP A0A248SMC7
F	275	HIS	-	expression tag	UNP A0A248SMC7
F	276	GLY	-	expression tag	UNP A0A248SMC7
F	277	GLY	-	expression tag	UNP A0A248SMC7
F	373	THR	PRO	engineered mutation	UNP A0A248SMC7

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.

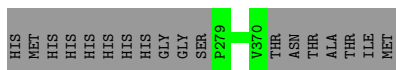
- Molecule 1: CTD-SP1 fragment of HIV-1 Gag

Chain A:  83% 17%




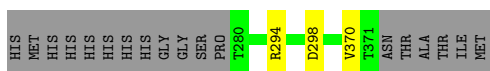
- Molecule 1: CTD-SP1 fragment of HIV-1 Gag

Chain B:  84% 16%




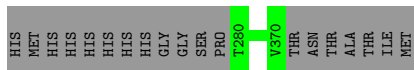
- Molecule 1: CTD-SP1 fragment of HIV-1 Gag

Chain C:  81% 16%




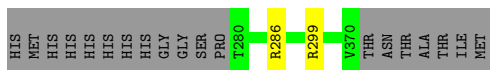
- Molecule 1: CTD-SP1 fragment of HIV-1 Gag

Chain D:  83% 17%




- Molecule 1: CTD-SP1 fragment of HIV-1 Gag

Chain E:  81% 17%



- Molecule 1: CTD-SP1 fragment of HIV-1 Gag

Chain F:  82% 16%

HIS	MET	HIS	HIS	HIS	HIS	HIS	GLY	GLY	SER	PRO	T280		R286		R299		T371	ASN	THR	ALA	THR	ILE	MET
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4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, $a=71.36$ Å, $b=122.98$ Å, $c=81.82$ Å, $\alpha=90^\circ$, $\beta=90^\circ$, $\gamma=95.04^\circ$, space group=C121	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.05	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F416 (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	0.25	0/659	0.40	0/895
1	B	0.25	0/687	0.40	0/931
1	C	0.25	0/675	0.40	0/916
1	D	0.25	0/672	0.42	0/911
1	E	0.25	0/662	0.40	0/899
1	F	0.25	0/678	0.40	0/919
All	All	0.25	0/4033	0.40	0/5471

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 [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	648	624	625	0	0
1	B	675	664	664	0	0
1	C	664	644	645	1	0
1	D	661	643	644	0	0
1	E	651	627	627	1	0
1	F	667	646	647	1	0
All	All	3966	3848	3852	3	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.

All (3) 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:C:294:ARG:NH1	1:C:298:ASP:OD1	2.45	0.48
1:F:286:ARG:O	1:F:299:ARG:NH2	2.46	0.48
1:E:286:ARG:O	1:E:299:ARG:NH2	2.51	0.43

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	89/110 (81%)	87 (98%)	2 (2%)	0	100	100
1	B	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
1	C	90/110 (82%)	88 (98%)	1 (1%)	1 (1%)	14	42
1	D	89/110 (81%)	86 (97%)	3 (3%)	0	100	100
1	E	89/110 (81%)	89 (100%)	0	0	100	100
1	F	90/110 (82%)	88 (98%)	2 (2%)	0	100	100
All	All	537/660 (81%)	527 (98%)	9 (2%)	1 (0%)	50	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	370	VAL

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	59/91 (65%)	59 (100%)	0	100	100
1	B	66/91 (72%)	66 (100%)	0	100	100
1	C	63/91 (69%)	63 (100%)	0	100	100
1	D	62/91 (68%)	62 (100%)	0	100	100
1	E	60/91 (66%)	60 (100%)	0	100	100
1	F	62/91 (68%)	62 (100%)	0	100	100
All	All	372/546 (68%)	372 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0337. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.