

wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2021 – 03:34 AM EDT

PDB ID : 1M9Y

Title : X-ray crystal structure of Cyclophilin A/HIV-1 CA N-terminal domain (1-146)

M-type H87A,G89A Complex.

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Deposited on : 2002-07-30

Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

EDS : 2.23.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

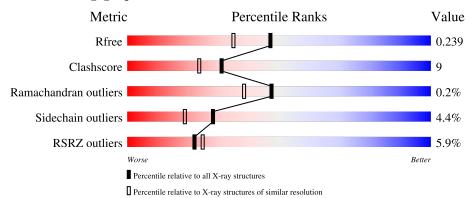
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.90 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain						
1	A	165	91%	9%					
1	В	165	87%	12%					
1	E	165	86%	13%					
1	F		24%		<u> </u>				
1	_	165	.%	12%	•				
2	С	146	68% 279		5%				

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Mol	Chain	Length	Quality of chain						
2	D	146	66%	22%	5% 8%				
2	G	146	7%		15%				
2	Н	146	62%	25%	5% • 8%				



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10531 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Cyclophilin A.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	165	Total	С	N	О	S	0	0	0
1	A		1266	802	218	237	9	U	U	U
1	В	164	Total	С	N	О	S	0	0	0
1	Б	104	1258	797	217	236	8			
1	E	E 165	Total	С	N	О	S	0	0	0
1			1266	802	218	237	9			U
1	F	164	Total	С	N	О	S	0	0	0
		104	1258	797	217	236	8	U	U	U

• Molecule 2 is a protein called HIV-1 Capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	\mathbf{C}	146	Total	С	N	О	S	0	0	0
2		140	1132	716	198	210	8		0	
2	D	135	Total	С	N	О	S	0	0	0
2	ט	133	1048	663	183	195	7			
2	G	146	Total	С	N	О	S	0	0	0
2	G	140	1132	716	198	210	8	U		
2	Н	135	Total	С	N	О	S	0	0	0
	П	133	1048	663	183	195	7	U	U	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	87	ALA	HIS	engineered mutation	UNP Q72497
С	89	ALA	GLY	engineered mutation	UNP Q72497
С	120	HIS	ASN	SEE REMARK 999	UNP Q72497
D	87	ALA	HIS	engineered mutation	UNP Q72497
D	89	ALA	GLY	engineered mutation	UNP Q72497
D	120	HIS	ASN	SEE REMARK 999	UNP Q72497
G	87	ALA	HIS	engineered mutation	UNP Q72497
G	89	ALA	GLY	engineered mutation	UNP Q72497

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Chain	Residue	Modelled	Actual	Comment	Reference
G	120	HIS	ASN	SEE REMARK 999	UNP Q72497
Н	87	ALA	HIS	engineered mutation	UNP Q72497
Н	89	ALA	GLY	engineered mutation	UNP Q72497
Н	120	HIS	ASN	SEE REMARK 999	UNP Q72497

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	171	Total O 171 171	0	0
3	В	177	Total O 177 177	0	0
3	С	178	Total O 178 178	0	0
3	D	61	Total O 61 61	0	0
3	Е	201	Total O 201 201	0	0
3	F	89	Total O 89 89	0	0
3	G	135	Total O 135 135	0	0
3	Н	111	Total O 111 111	0	0

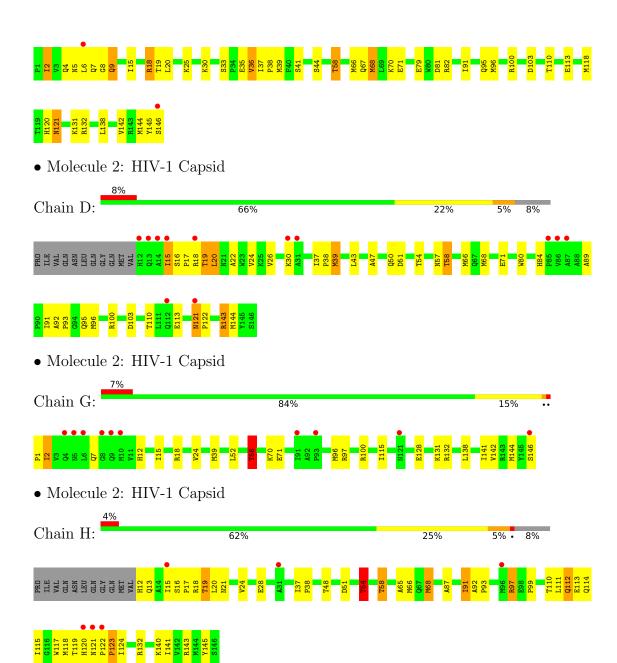


3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Cyclophilin A Chain A: • Molecule 1: Cyclophilin A Chain B: 87% • Molecule 1: Cyclophilin A Chain E: 86% 13% • Molecule 1: Cyclophilin A Chain F: 87% 12% • Molecule 2: HIV-1 Capsid Chain C: 27%







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	38.43Å 111.22Å 67.78Å	Depositor
a, b, c, α , β , γ	89.99° 101.45° 89.75°	Depositor
Resolution (Å)	19.69 - 1.90	Depositor
Resolution (A)	19.68 - 1.90	EDS
% Data completeness	97.6 (19.69-1.90)	Depositor
(in resolution range)	96.3 (19.68-1.90)	EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	2.79 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
D D.	0.162 , 0.234	Depositor
R, R_{free}	0.170 , 0.239	DCC
R_{free} test set	8529 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 33.0	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.319 for -h,k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10531	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.86% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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	Bo	nd lengths	Bond angles		
IVIOI	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.80	0/1294	1.36	4/1733~(0.2%)	
1	В	0.85	0/1286	1.41	7/1723 (0.4%)	
1	Е	0.92	0/1294	1.44	14/1733 (0.8%)	
1	F	0.56	0/1286	1.15	3/1723 (0.2%)	
2	С	0.83	0/1159	1.44	$12/1577 \ (0.8\%)$	
2	D	0.62	0/1074	1.28	8/1462 (0.5%)	
2	G	0.72	0/1159	1.30	6/1577 (0.4%)	
2	Н	0.81	1/1074 (0.1%)	1.31	3/1462~(0.2%)	
All	All	0.77	1/9626 (0.0%)	1.34	57/12990 (0.4%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
2	Η	68	MET	SD-CE	-5.79	1.45	1.77

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	G	18	ARG	NE-CZ-NH1	-10.68	114.96	120.30
2	D	143	ARG	NE-CZ-NH1	-9.07	115.76	120.30
2	С	18	ARG	NE-CZ-NH1	-9.03	115.78	120.30
1	В	27	ASP	CB-CG-OD2	8.79	126.21	118.30
1	В	37	ARG	NE-CZ-NH2	-8.63	115.98	120.30

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	1266	0	1237	6	0
1	В	1258	0	1225	8	0
1	Ε	1266	0	1237	8	0
1	F	1258	0	1225	12	0
2	С	1132	0	1135	50	0
2	D	1048	0	1043	29	0
2	G	1132	0	1135	23	0
2	Н	1048	0	1043	46	0
3	A	171	0	0	2	1
3	В	177	0	0	1	0
3	С	178	0	0	8	1
3	D	61	0	0	6	0
3	Ε	201	0	0	2	1
3	F	89	0	0	3	0
3	G	135	0	0	7	1
3	Н	111	0	0	15	0
All	All	10531	0	9280	170	2

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 9.

The worst 5 of 170 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
2:C:30:LYS:NZ	2:C:35:GLU:HG2	1.62	1.13
2:C:6:LEU:HD22	2:C:7:GLN:NE2	1.81	0.95
2:H:115:ILE:O	2:H:119:THR:HG23	1.66	0.94
2:H:91:ILE:HD12	2:H:92:ALA:H	1.39	0.87
2:C:30:LYS:HZ1	2:C:35:GLU:HG2	1.39	0.86

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
3:C:285:HOH:O	3:E:312:HOH:O[1_645]	2.05	0.15
3:A:269:HOH:O	3:G:192:HOH:O[1_655]	2.18	0.02



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 X-ray entries followed by that with respect to entries of similar resolution.

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	Perce	ntiles
1	A	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
1	В	162/165 (98%)	157 (97%)	5 (3%)	0	100	100
1	E	163/165 (99%)	158 (97%)	5 (3%)	0	100	100
1	F	162/165~(98%)	154 (95%)	8 (5%)	0	100	100
2	С	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	D	133/146 (91%)	126 (95%)	5 (4%)	2 (2%)	10	3
2	G	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
2	Н	133/146 (91%)	129 (97%)	4 (3%)	0	100	100
All	All	1204/1244 (97%)	1161 (96%)	41 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	15	ILE
2	D	30	LYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	Percer	ntiles
1	A	133/133 (100%)	128 (96%)	5 (4%)	33	24
1	В	132/133 (99%)	126 (96%)	6 (4%)	27	18
1	E	133/133 (100%)	130 (98%)	3 (2%)	50	45

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	F	132/133 (99%)	130 (98%)	2 (2%)	65	62
2	С	122/122 (100%)	116 (95%)	6 (5%)	25	15
2	D	112/122 (92%)	108 (96%)	4 (4%)	35	26
2	G	122/122 (100%)	115 (94%)	7 (6%)	20	11
2	Н	112/122 (92%)	101 (90%)	11 (10%)	8	3
All	All	998/1020 (98%)	954 (96%)	44 (4%)	28	19

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	15	ILE
2	Н	21	ASN
2	G	58	THR
2	G	146	SER
2	Н	54	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	Н	74	ASN
2	G	74	ASN
2	D	50	GLN
2	G	21	ASN
2	D	21	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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	165/165 (100%)	-0.57	1 (0%) 89 90	15, 23, 38, 63	0
1	В	164/165 (99%)	-0.32	1 (0%) 89 90	13, 21, 36, 53	0
1	E	165/165 (100%)	-0.56	0 100 100	11, 19, 33, 47	0
1	F	164/165~(99%)	1.43	40 (24%) 0 0	27, 41, 59, 70	0
2	С	146/146 (100%)	-0.38	2 (1%) 75 77	14, 23, 44, 51	0
2	D	135/146 (92%)	0.33	12 (8%) 9 11	20, 40, 75, 83	0
2	G	146/146 (100%)	0.17	10 (6%) 17 19	17, 28, 58, 85	0
2	Н	135/146 (92%)	0.02	6 (4%) 34 37	17, 32, 61, 72	0
All	All	1220/1244 (98%)	0.01	72 (5%) 22 25	11, 27, 56, 85	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	8	GLY	8.4
2	D	121	ASN	7.8
1	F	148	ARG	5.9
2	G	10	MET	5.5
1	F	2	VAL	5.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

