



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:32 PM UTC

PDB ID : 1DLO / pdb_00001dlo
Title : HUMAN IMMUNODEFICIENCY VIRUS TYPE 1
Authors : Hsiou, Y.; Ding, J.; Das, K.; Hughes, S.; Arnold, E.
Deposited on : 1996-04-17
Resolution : 2.70 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 ⓘ 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:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

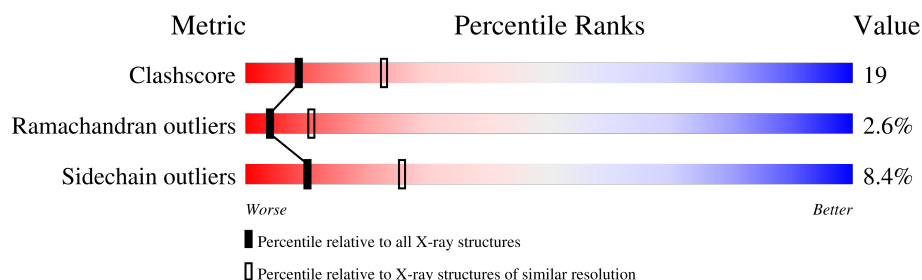
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	556	
2	B	427	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7691 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 HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4370	2835	727	802	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	0	0
			3321	2163	549	604	5			

There is a discrepancy between the modelled and reference sequences:

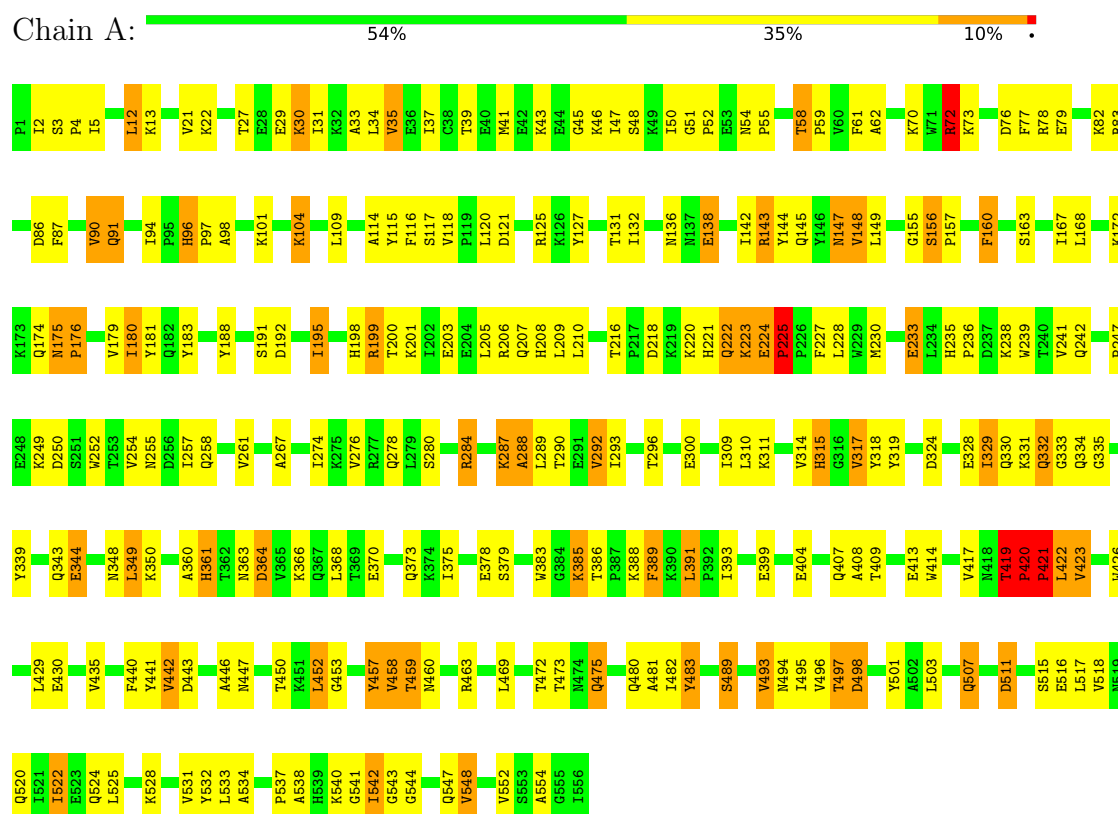
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

3 Residue-property plots

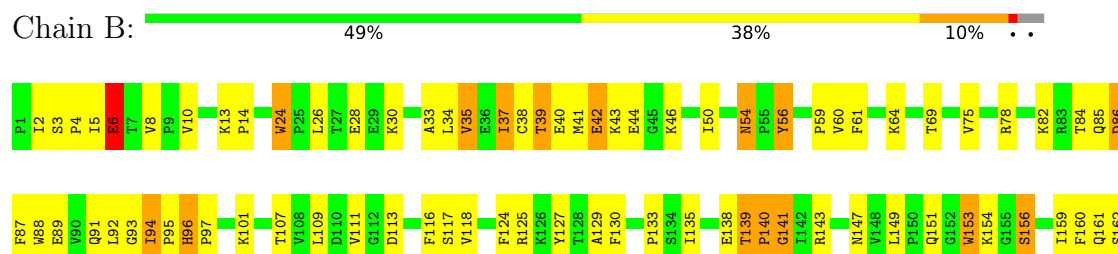
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

- Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE



- Molecule 2: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE



S163	V245	G316	I393	S163
L246	V317	V318	K395	L246
P247	Y319	Y319	E396	P247
E248	D320	D320	T397	E248
K249	P321	P321	W398	K249
D250			E399	D250
	A327	A327	T400	
V254	Q332	Q332	W401	V254
N255			W402	N255
D256	Q336	Q336	T403	D256
I257	K337	K337	W410	I257
	T338	T338		
L260	Y339	Y339	E413	L260
V261	Q340	Q340	W414	V261
	Q343	Q343	E415	
A267	E344	E344	F416	A267
S268	P345	P345	W417	S268
Q269	F346	F346	N418	Q269
L270	K347	K347	T419	L270
Y271	N348	N348	P420	Y271
	L349	L349	P421	
I274	K350	K350	L422	I274
K275	T351	T351	W423	K275
V276	G352	G352		V276
R277	K353	K353		R277
Q278	Y354	Y354		Q278
L279	M357	M357	Y427	L279
S280				S280
K281				K281
L282				L282
L283				L283
G213	T286	T286		G213
L214				L214
T215				T215
T216	L289	L289		T216
P217	T290	T290		P217
D218				D218
LYS	I293	I293		LYS
LYS	P294	P294		LYS
HIS	L295	L295		HIS
GLN	T296	T296		GLN
LYS	E297	E297		LYS
GLU	E298	E298		GLU
PRO	A299	A299		PRO
PRO	E300	E300		PRO
PHE	L301	L301		PHE
LEU	E302	E302		LEU
TRP	L303	L303		TRP
MET	A304	A304		MET
G231	E305	E305		G231
Y232	N306	N306		Y232
E233	R307	R307		E233
L234	E308	E308		L234
H235	I309	I309		H235
P236	L310	L310		P236
D237	K311	K311		D237
K238	E312	E312		K238
W239	F313	F313		W239
	V314	V314		
	H315	H315		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.50Å 70.30Å 93.30Å 90.00° 106.10° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.249 , 0.336	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7691	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.86	3/4486 (0.1%)	1.33	64/6119 (1.0%)
2	B	0.93	3/3415 (0.1%)	1.32	48/4652 (1.0%)
All	All	0.89	6/7901 (0.1%)	1.33	112/10771 (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	A	0	1
2	B	0	2
All	All	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	420	PRO	CA-C	6.70	1.58	1.52
1	A	493	VAL	CA-CB	-6.10	1.49	1.55
2	B	189	VAL	CA-CB	5.67	1.60	1.53
1	A	522	ILE	CA-CB	5.39	1.60	1.54
1	A	386	THR	CA-CB	5.12	1.61	1.52

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	VAL	N-CA-C	15.36	126.48	110.36
1	A	91	GLN	N-CA-C	11.40	125.95	110.55
1	A	360	ALA	N-CA-C	-10.78	100.26	113.41
1	A	225	PRO	N-CA-C	10.36	123.33	110.70
1	A	175	ASN	CA-C-N	9.44	129.67	119.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	501	TYR	Sidechain
2	B	127	TYR	Sidechain
2	B	183	TYR	Sidechain

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	4370	0	4315	165	0
2	B	3321	0	3293	137	0
All	All	7691	0	7608	286	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 19.

The worst 5 of 286 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)
2:B:260:LEU:HD21	2:B:303:LEU:HD21	1.58	0.86
1:A:420:PRO:HB3	1:A:421:PRO:HD2	1.57	0.85
1:A:420:PRO:CB	1:A:421:PRO:HD2	2.06	0.85
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.57	0.83
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.61	0.80

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 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	Percentiles	
1	A	554/556 (100%)	490 (88%)	50 (9%)	14 (2%)	4	11
2	B	411/427 (96%)	353 (86%)	47 (11%)	11 (3%)	4	10
All	All	965/983 (98%)	843 (87%)	97 (10%)	25 (3%)	4	11

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	223	LYS
1	A	225	PRO
1	A	334	GLN
1	A	420	PRO

5.3.2 Protein sidechains ⓘ

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	Percentiles	
1	A	458/496 (92%)	418 (91%)	40 (9%)	9	24
2	B	353/389 (91%)	325 (92%)	28 (8%)	11	28
All	All	811/885 (92%)	743 (92%)	68 (8%)	10	26

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	271	TYR
2	B	275	LYS
2	B	321	PRO
1	A	419	THR
1	A	409	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
2	B	418	ASN
1	A	524	GLN
2	B	278	GLN
1	A	519	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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.