



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:20 AM UTC

PDB ID : 1BY7 / pdb_00001by7
Title : HUMAN PLASMINOGEN ACTIVATOR INHIBITOR-2. LOOP (66-98)
DELETION MUTANT
Authors : Harrop, S.J.; King, G.C.; Mabbutt, B.C.; Curmi, P.M.G.
Deposited on : 1998-10-27
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/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

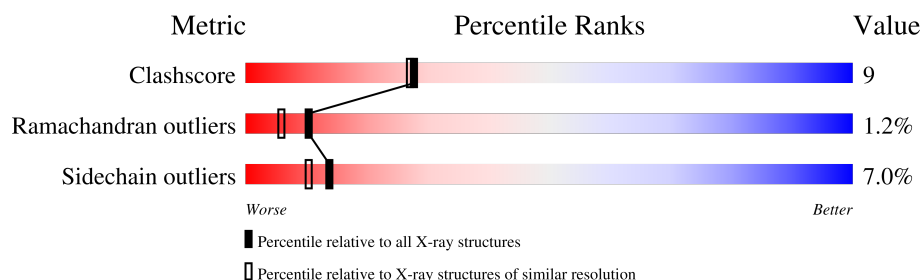
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	382	 60% 26% 6% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3045 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 PROTEIN (PLASMINOGEN ACTIVATOR INHIBITOR-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2836	1816	467	535	18			

- Molecule 2 is water.

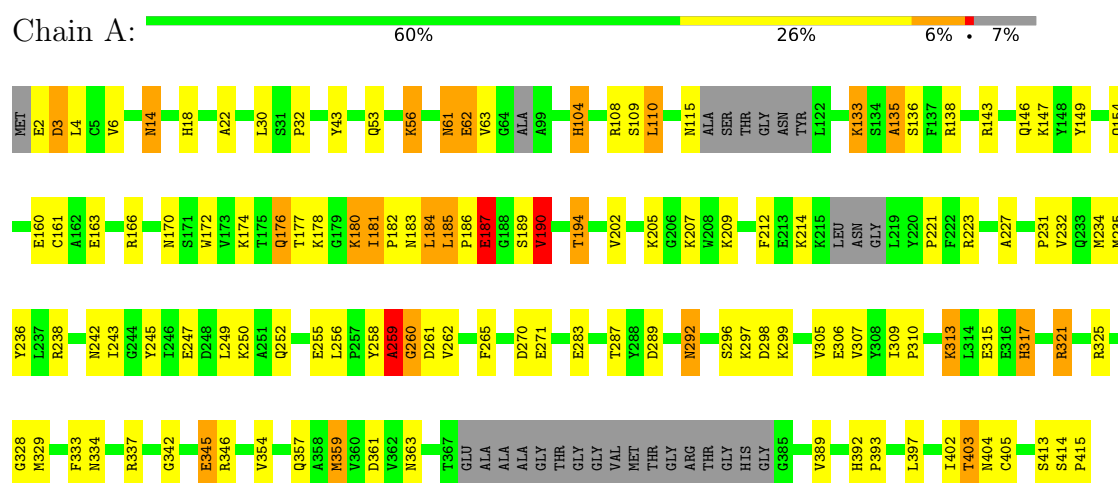
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	209	Total	O	3	0
			209	209		

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: PROTEIN (PLASMINOGEN ACTIVATOR INHIBITOR-2)



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	138.82Å 41.73Å 77.40Å 90.00° 114.88° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.0 (30.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3045	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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	1.11	2/2894 (0.1%)	2.11	83/3894 (2.1%)

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
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	415	PRO	N-CD	6.48	1.56	1.47
1	A	321	ARG	CD-NE	-6.20	1.37	1.46

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ARG	CD-NE-CZ	28.52	164.33	124.40
1	A	292	ASN	CA-CB-CG	-11.54	101.06	112.60
1	A	194	THR	CA-CB-OG1	-10.79	93.42	109.60
1	A	256	LEU	CA-C-O	10.08	128.86	119.59
1	A	317	HIS	CA-CB-CG	10.00	123.80	113.80
1	A	342	GLY	O-C-N	-9.12	112.58	122.24
1	A	163	GLU	CA-C-O	8.89	129.98	120.55
1	A	243	ILE	CA-C-O	-8.61	112.32	121.19
1	A	414	SER	CA-C-O	8.57	130.11	120.34
1	A	166	ARG	CD-NE-CZ	8.48	136.28	124.40
1	A	53	GLN	CA-C-O	-8.43	112.02	120.70
1	A	115	ASN	CA-CB-CG	-8.42	104.18	112.60
1	A	154	GLN	CB-CG-CD	8.31	126.74	112.60
1	A	252	GLN	OE1-CD-NE2	-8.22	114.38	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	VAL	N-CA-CB	-8.11	96.75	111.92
1	A	283	GLU	CA-C-O	-7.79	111.01	119.97
1	A	154	GLN	OE1-CD-NE2	-7.66	114.94	122.60
1	A	354	VAL	O-C-N	7.44	130.24	123.03
1	A	262	VAL	CA-C-O	-7.23	112.87	120.39
1	A	231	PRO	CA-C-O	-7.06	112.99	121.03
1	A	403	THR	CA-C-O	6.85	127.29	119.27
1	A	104	HIS	CA-CB-CG	-6.75	107.05	113.80
1	A	334	ASN	CA-C-O	6.74	127.68	120.46
1	A	307	VAL	CA-C-O	-6.60	113.49	120.48
1	A	313	LYS	CA-C-O	-6.41	113.21	120.32
1	A	259	ALA	O-C-N	-6.39	114.09	122.59
1	A	242	ASN	O-C-N	-6.31	115.65	123.04
1	A	305	VAL	CB-CA-C	-6.29	101.13	110.82
1	A	43	TYR	CA-C-O	-6.06	114.12	120.55
1	A	221	PRO	O-C-N	6.06	129.45	123.03
1	A	227	ALA	CA-C-O	-6.03	112.07	119.18
1	A	160	GLU	CA-C-O	-6.01	112.45	119.24
1	A	334	ASN	OD1-CG-ND2	-6.00	116.59	122.60
1	A	328	GLY	CA-C-N	-5.97	113.99	122.41
1	A	328	GLY	C-N-CA	-5.97	113.99	122.41
1	A	289	ASP	CA-C-N	5.94	128.52	120.44
1	A	289	ASP	C-N-CA	5.94	128.52	120.44
1	A	307	VAL	N-CA-C	5.91	116.44	108.17
1	A	143	ARG	CD-NE-CZ	5.90	132.66	124.40
1	A	249	LEU	CA-C-O	5.88	126.23	119.35
1	A	252	GLN	CB-CG-CD	-5.87	102.62	112.60
1	A	255	GLU	CA-C-N	5.76	132.32	122.06
1	A	255	GLU	C-N-CA	5.76	132.32	122.06
1	A	345	GLU	CA-CB-CG	-5.74	102.61	114.10
1	A	307	VAL	O-C-N	5.71	129.18	123.18
1	A	187	GLU	N-CA-C	5.69	122.92	110.80
1	A	170	ASN	CA-C-O	-5.63	113.50	119.97
1	A	258	TYR	CA-CB-CG	5.53	123.85	113.90
1	A	298	ASP	CB-CA-C	-5.53	100.06	110.67
1	A	135	ALA	CA-C-N	5.52	128.94	121.05
1	A	135	ALA	C-N-CA	5.52	128.94	121.05
1	A	62	GLU	N-CA-CB	5.48	118.18	110.12
1	A	310	PRO	CA-C-N	5.47	129.32	121.50
1	A	310	PRO	C-N-CA	5.47	129.32	121.50
1	A	245	TYR	CA-C-O	-5.46	114.26	120.32
1	A	270	ASP	N-CA-C	-5.46	104.26	111.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	LEU	CA-C-O	-5.46	115.06	120.90
1	A	309	ILE	N-CA-C	-5.44	104.73	109.19
1	A	163	GLU	O-C-N	-5.41	116.39	122.12
1	A	287	THR	N-CA-CB	5.36	120.30	111.62
1	A	32	PRO	N-CA-C	-5.34	105.83	113.47
1	A	133	LYS	N-CA-C	5.33	117.84	111.71
1	A	136	SER	CB-CA-C	-5.31	101.88	109.84
1	A	185	LEU	N-CA-CB	5.28	118.81	110.11
1	A	329	MET	CB-CA-C	5.23	120.00	112.05
1	A	205	LYS	CA-C-N	-5.18	116.97	122.30
1	A	205	LYS	C-N-CA	-5.18	116.97	122.30
1	A	176	GLN	N-CA-C	5.16	119.04	112.34
1	A	313	LYS	CA-C-N	-5.15	115.22	122.94
1	A	313	LYS	C-N-CA	-5.15	115.22	122.94
1	A	138	ARG	CA-C-O	5.14	126.84	121.19
1	A	61	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	109	SER	CA-C-N	5.13	127.41	120.38
1	A	109	SER	C-N-CA	5.13	127.41	120.38
1	A	22	ALA	CA-C-O	5.12	125.83	119.79
1	A	14	ASN	CA-C-N	5.10	127.38	120.44
1	A	14	ASN	C-N-CA	5.10	127.38	120.44
1	A	265	PHE	CA-C-O	-5.08	114.90	120.43
1	A	202	VAL	CG1-CB-CG2	-5.06	99.67	110.80
1	A	243	ILE	O-C-N	5.04	128.54	123.00
1	A	287	THR	CA-CB-CG2	5.04	119.07	110.50
1	A	61	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	235	MET	CA-C-O	-5.03	115.27	120.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	PHE	Mainchain

5.2 Too-close contacts ⓘ

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	2836	0	2803	51	0
2	A	209	0	0	9	0
All	All	3045	0	2803	51	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 9.

All (51) 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:181:ILE:HD12	1:A:357:GLN:NE2	2.06	0.70
1:A:161:CYS:SG	2:A:583:HOH:O	2.51	0.68
1:A:186:PRO:HD2	1:A:189:SER:OG	1.94	0.67
1:A:104:HIS:HD2	1:A:149:TYR:OH	1.77	0.67
1:A:110:LEU:HD11	2:A:567:HOH:O	1.98	0.62
1:A:315:GLU:OE2	1:A:357:GLN:NE2	2.33	0.62
1:A:104:HIS:HE1	2:A:429:HOH:O	1.82	0.61
1:A:321:ARG:HG3	1:A:333:PHE:CD1	2.37	0.59
1:A:56:LYS:HD2	1:A:61:ASN:OD1	2.03	0.59
1:A:313:LYS:HG2	1:A:361:ASP:OD1	2.03	0.58
1:A:2:GLU:O	1:A:3:ASP:HB2	2.01	0.58
1:A:321:ARG:HD3	1:A:325:ARG:NH1	2.18	0.58
1:A:4:LEU:HD12	1:A:110:LEU:HD12	1.86	0.57
1:A:402:ILE:HG12	2:A:447:HOH:O	2.06	0.55
1:A:180:LYS:HB3	1:A:359:MET:HE1	1.88	0.54
1:A:238:ARG:HG3	1:A:306:GLU:HG2	1.88	0.54
1:A:180:LYS:HD2	1:A:359:MET:HE1	1.89	0.54
1:A:321:ARG:HD3	1:A:325:ARG:CZ	2.39	0.52
1:A:397:LEU:C	1:A:397:LEU:HD12	2.35	0.52
1:A:186:PRO:HD2	1:A:189:SER:CB	2.40	0.51
1:A:337:ARG:NH1	2:A:608:HOH:O	2.43	0.51
1:A:135:ALA:HA	1:A:346:ARG:HD2	1.93	0.51
1:A:413:SER:HB2	2:A:549:HOH:O	2.10	0.51
1:A:180:LYS:HD2	1:A:359:MET:CE	2.41	0.50
1:A:14:ASN:HD21	1:A:18:HIS:CE1	2.29	0.50
1:A:247:GLU:HG2	2:A:616:HOH:O	2.10	0.49
1:A:108:ARG:HD2	1:A:147:LYS:O	2.11	0.49
1:A:260:GLY:O	1:A:261:ASP:HB2	2.12	0.49
1:A:223:ARG:O	1:A:393:PRO:HD3	2.12	0.48
1:A:190:VAL:HG22	1:A:194:THR:HG21	1.96	0.48
1:A:296:SER:OG	1:A:299:LYS:HG2	2.13	0.48
1:A:4:LEU:HB2	1:A:110:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TYR:OH	1:A:306:GLU:OE1	2.32	0.46
1:A:181:ILE:HD12	1:A:357:GLN:HE22	1.79	0.46
1:A:232:VAL:CG2	1:A:234:MET:HE2	2.46	0.46
1:A:259:ALA:O	1:A:261:ASP:N	2.47	0.45
1:A:177:THR:O	1:A:178:LYS:C	2.59	0.44
1:A:174:LYS:CG	1:A:182:PRO:HA	2.48	0.44
1:A:135:ALA:CA	1:A:346:ARG:HD2	2.48	0.43
1:A:363:ASN:OD1	1:A:363:ASN:C	2.62	0.42
1:A:183:ASN:O	1:A:184:LEU:C	2.61	0.42
1:A:3:ASP:OD2	1:A:6:VAL:HG23	2.20	0.42
1:A:345:GLU:HG2	2:A:443:HOH:O	2.20	0.42
1:A:392:HIS:HD2	2:A:418:HOH:O	2.02	0.42
1:A:172:TRP:CZ2	1:A:176:GLN:HG3	2.55	0.41
1:A:174:LYS:HG3	1:A:182:PRO:HA	2.03	0.41
1:A:133:LYS:HB2	1:A:133:LYS:HE3	1.82	0.41
1:A:135:ALA:CB	1:A:346:ARG:HD2	2.51	0.41
1:A:403:THR:O	1:A:404:ASN:CB	2.69	0.41
1:A:135:ALA:HB2	1:A:346:ARG:HD2	2.02	0.41
1:A:232:VAL:HG21	1:A:234:MET:HE2	2.03	0.41

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	344/382 (90%)	326 (95%)	14 (4%)	4 (1%)	10 6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLU
1	A	259	ALA

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Mol	Chain	Res	Type
1	A	3	ASP
1	A	260	GLY

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	313/329 (95%)	291 (93%)	22 (7%)	14	10

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	56	LYS
1	A	62	GLU
1	A	63	VAL
1	A	110	LEU
1	A	146	GLN
1	A	180	LYS
1	A	181	ILE
1	A	185	LEU
1	A	187	GLU
1	A	190	VAL
1	A	207	LYS
1	A	209	LYS
1	A	214	LYS
1	A	250	LYS
1	A	271	GLU
1	A	292	ASN
1	A	297	LYS
1	A	317	HIS
1	A	359	MET
1	A	389	VAL
1	A	405	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	26	GLN
1	A	104	HIS
1	A	183	ASN
1	A	200	ASN
1	A	242	ASN
1	A	252	GLN

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.