



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:30 PM UTC

PDB ID : 1BML / pdb_00001bml
Title : COMPLEX OF THE CATALYTIC DOMAIN OF HUMAN PLASMIN AND STREPTOKINASE
Authors : Wang, X.; Zhang, X.C.
Deposited on : 1999-05-25
Resolution : 2.90 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 ⓘ 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
Xtrriage (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

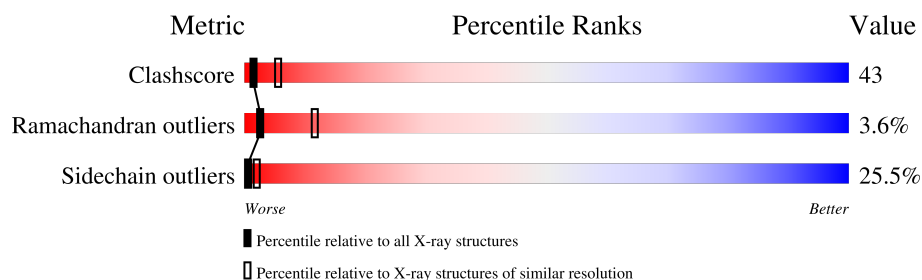
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8940 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 PLASMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1917	1217	339	347	14	0	0	0
1	B	250	1917	1217	339	347	14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	ALA	SER	engineered mutation	UNP P00747
B	741	ALA	SER	engineered mutation	UNP P00747

- Molecule 2 is a protein called STREPTOKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	318	2553	1610	426	514	3	0	0	0
2	D	318	2553	1610	426	514	3	0	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.03Å 125.05Å 86.79Å 90.00° 105.41° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	91.3 (20.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.201 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8940	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

4 Model quality [i](#)

4.1 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	0.63	0/1967	1.19	19/2673 (0.7%)
1	B	0.61	0/1967	1.17	20/2673 (0.7%)
2	C	0.51	0/2597	0.96	11/3522 (0.3%)
2	D	0.50	0/2597	1.05	22/3522 (0.6%)
All	All	0.56	0/9128	1.08	72/12390 (0.6%)

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
2	C	0	1

There are no bond length outliers.

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	HIS	N-CA-C	-11.21	95.60	109.83
2	D	130	GLN	N-CA-C	9.87	125.59	112.17
1	A	745	LEU	N-CA-C	-9.47	93.09	108.52
2	D	22	VAL	N-CA-C	9.34	120.22	108.82
2	D	335	LEU	N-CA-C	8.59	120.41	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	327	TYR	Sidechain

4.2 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	1917	0	1892	126	0
1	B	1917	0	1892	149	0
2	C	2553	0	2485	252	0
2	D	2553	0	2485	251	0
All	All	8940	0	8754	767	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 43.

The worst 5 of 767 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:C:170:ASN:HB2	2:C:171:PRO:HD2	1.24	1.13
2:D:170:ASN:HB2	2:D:171:PRO:HD2	1.14	1.10
1:B:749:GLU:HG2	1:B:754:ILE:HD13	1.33	1.05
2:D:186:LYS:HB3	2:D:188:LEU:HD21	1.40	1.03
2:C:302:VAL:HG22	2:C:368:TYR:HB3	1.45	0.96

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	246/250 (98%)	212 (86%)	28 (11%)	6 (2%)	4 18
1	B	128/250 (51%)	105 (82%)	18 (14%)	5 (4%)	2 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	58/186 (31%)	45 (78%)	11 (19%)	2 (3%)	3	12
2	D	62/186 (33%)	44 (71%)	13 (21%)	5 (8%)	1	1
All	All	494/872 (57%)	406 (82%)	70 (14%)	18 (4%)	2	11

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	629	HIS
2	D	188	LEU
1	B	628	PRO
1	B	644	ARG
2	D	185	LEU

4.3.2 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	Percentiles	
1	A	209/209 (100%)	157 (75%)	52 (25%)	0	2
1	B	209/209 (100%)	168 (80%)	41 (20%)	1	5
2	C	288/162 (178%)	204 (71%)	84 (29%)	0	1
2	D	288/162 (178%)	212 (74%)	76 (26%)	0	2
All	All	994/742 (134%)	741 (74%)	253 (26%)	0	2

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	157	SER
2	D	211	HIS
2	C	232	ARG
2	D	209	LYS
2	D	267	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	208	ASN
2	D	358	HIS
2	C	320	ASN
2	D	357	ASN
2	D	250	GLN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	561:ARG	C	562:VAL	N	19.28
1	B	561:ARG	C	562:VAL	N	18.27

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

5.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

5.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.