



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 10:37 AM UTC

PDB ID : 1PRE / pdb_00001pre
Title : PROAEROLYSIN
Authors : Parker, M.W.; Buckley, J.T.; Postma, J.P.M.; Tucker, A.D.; Tsernoglou, D.
Deposited on : 1995-09-15
Resolution : 2.80 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

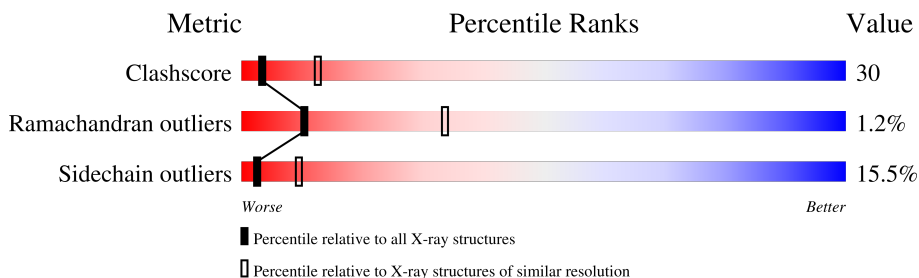
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	470	 37% 39% 18% . .
1	B	470	 37% 38% 18% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7089 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 PROAEROLYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	449	Total 3523	C 2228	N 607	O 679	S 9	0	0	0
1	B	451	Total 3533	C 2234	N 607	O 683	S 9	0	0	0

- Molecule 2 is water.

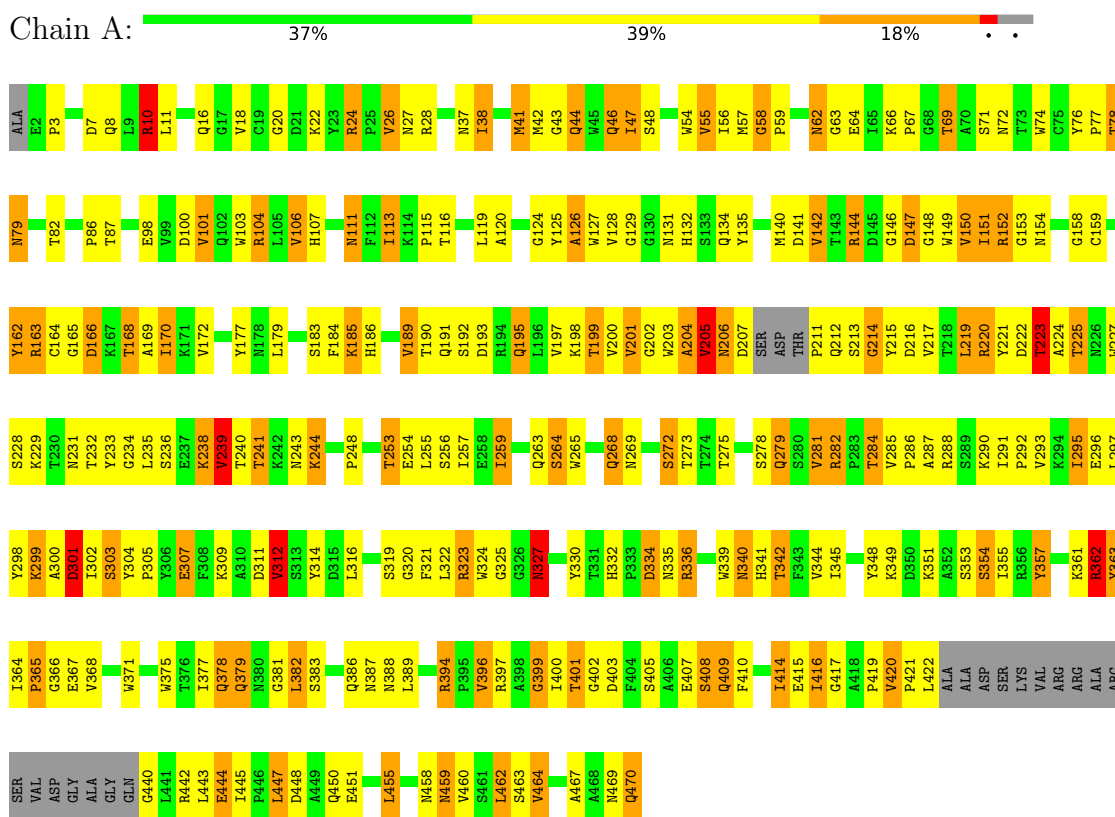
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total 18	O 18	0	0
2	B	15	Total 15	O 15	0	0

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: PROAEROLYSIN



- Molecule 1: PROAEROLYSIN



GLY	ALA	GLY	GLN	GLY	L441	R442	L443	E444	I445	D448	A449	G450	E451	L452	L455	G456	F457	V460	S461	V464	A468	ASN	GLN	E367	V368	K369	W370	W371	D372	W373	W374	W375	T376	I377	Q378	Q379	N380	S383	T384	M385	N388	L389	A390	R391	V392	L393	R394	P395	V396	R397	A398	G399	I400	T401	G402	G409	G412	M413	I416	G417	A418	F419	V420	P421	L422	A423	A424	ASP	SER	LYS	VAL	ARG	ARG	ALA	ARG	ALA	ARG	ARG	VAL	ASP	K284	L285	Y286	Q287	R288	P283	T284	V285	P286	A287	R288	S289	K290	I291	P292	V293	E294	V295	Y296	L297	Y298	K299	A300	D301	I302	S303	Y304	T230	Y233	G234	L235	S236	E237	K238	V239	T240	T241	K242	N243	K244	F245	K246	W247	P248	E252	T253	E254	E258	Q263	A266	T273	T274	T275	S276	L277	S278	Q279	S280	V281	R282	P283	T284	V285	P286	A287	R288	S289	K290	I291	P292	V293	K294	L295	Y296	L297	Y298	K299	A300	D301	I302	S303	Y304	F308	K309	A310	D311	V312	S313	S319	G320	F321	L322	G326	N327	Y330	T331	H332	R336	P337	N338	W339	N340	H341	T342	G346	P347	Y348	K349	D350	K351	A352	S353	S354	I355	R356	Y357	Q358	K361	R362	Y363	I364	P365	G366	T218	L219	R220	Y221	D222	A224	T225	N226	Y230	Y233	G234	L235	S236	E237	K238	V239	T240	T241	K242	N243	K244	F245	K246	W247	P248	E252	T253	E254	E258	Q263	A266	T273	T274	T275	S276	L277	S278	Q279	S280	V281	R282	P283	T284	V285	P286	A287	R288	S289	K290	I291	P292	V293
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.00Å 104.00Å 222.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.0 (6.00-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7089	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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	0.88	2/3620 (0.1%)	2.27	179/4938 (3.6%)
1	B	0.85	0/3631	2.24	188/4957 (3.8%)
All	All	0.87	2/7251 (0.0%)	2.26	367/9895 (3.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	HIS	C-O	-6.09	1.20	1.23
1	A	397	ARG	NE-CZ	5.16	1.38	1.33

The worst 5 of 367 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CD-NE-CZ	15.43	146.01	124.40
1	A	382	LEU	CA-C-O	-12.40	107.80	120.82
1	A	323	ARG	CD-NE-CZ	12.05	141.27	124.40
1	B	55	VAL	CA-C-O	-11.53	110.22	121.63
1	B	24	ARG	NE-CZ-NH2	11.34	129.41	119.20

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	3523	0	3357	198	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3533	0	3366	227	0
2	A	18	0	0	5	0
2	B	15	0	0	2	0
All	All	7089	0	6723	415	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 30.

The worst 5 of 415 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:B:351:LYS:HD3	1:B:357:TYR:CE2	1.88	1.09
1:B:362:ARG:HG3	1:B:374:ASN:ND2	1.69	1.06
1:B:100:ASP:O	1:B:104:ARG:HG3	1.59	1.03
1:B:292:PRO:HG2	1:B:417:GLY:HA3	1.45	0.97
1:A:47:ILE:HD13	1:A:57:MET:HE3	1.46	0.97

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	443/470 (94%)	401 (90%)	39 (9%)	3 (1%)	18 47
1	B	447/470 (95%)	404 (90%)	35 (8%)	8 (2%)	6 23
All	All	890/940 (95%)	805 (90%)	74 (8%)	11 (1%)	10 34

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO

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Mol	Chain	Res	Type
1	B	190	THR
1	B	362	ARG
1	A	236	SER
1	B	58	GLY

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	Percentiles
1	A	378/392 (96%)	322 (85%)	56 (15%)	3 10
1	B	379/392 (97%)	318 (84%)	61 (16%)	2 8
All	All	757/784 (97%)	640 (84%)	117 (16%)	2 9

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	ARG
1	B	392	VAL
1	B	71	SER
1	B	383	SER
1	B	288	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	ASN
1	B	379	GLN
1	B	178	ASN
1	B	409	GLN
1	B	332	HIS

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.