wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 08:39 AM EDT

PDB ID	:	1PRE
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 (i) 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 (i)) were used in the production of this report:

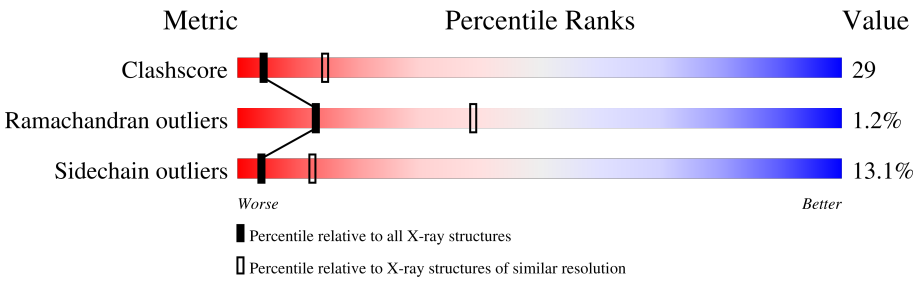
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	470	47% 38% 10% • •
1	B	470	47% 37% 10% • •

2 Entry composition (i)

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	3523	2228	607	679	9	0	0	0
1	B	451	3533	2234	607	683	9	0	0	0

- Molecule 2 is water.

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

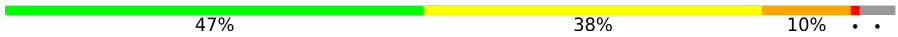
3 Residue-property plots (i)

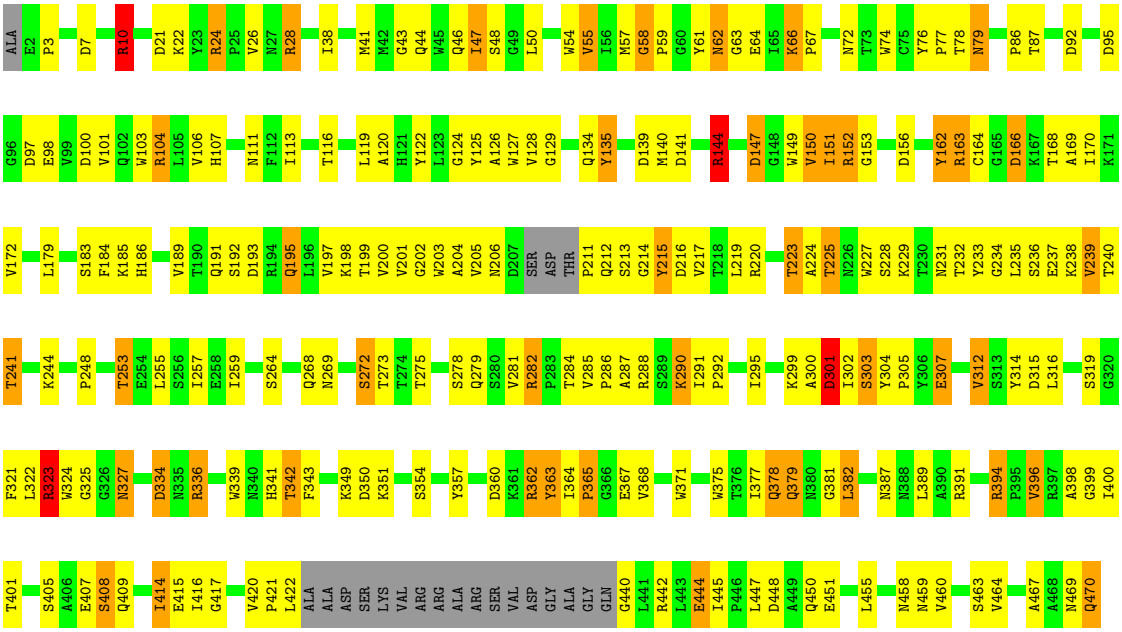
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

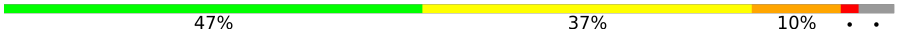
Chain A:

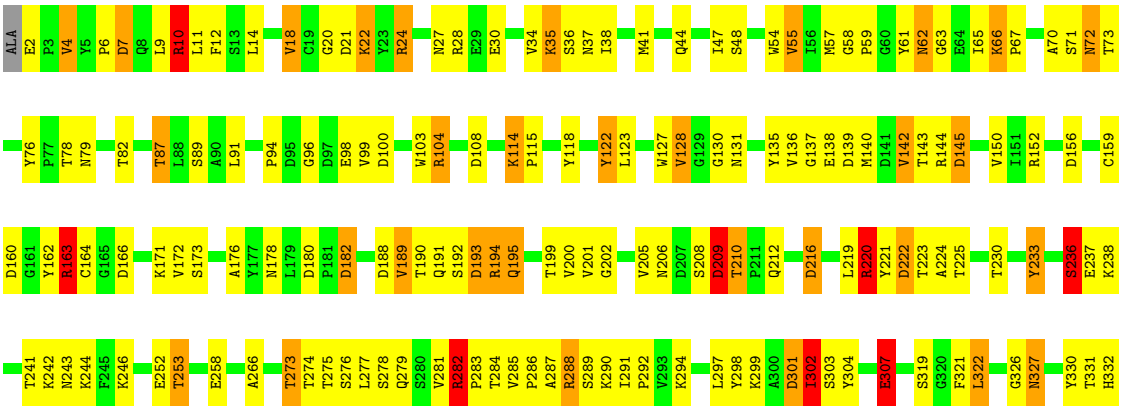


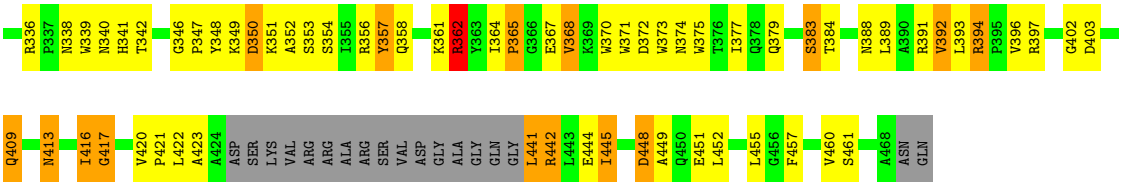


• Molecule 1: PROAEROLYSIN

Chain B:






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
E367
V368
K369
W370
W371
D372
W373
N374
W375
T376
I377
Q378
Q379
S383
T384
N388
L389
A390
R391
V392
L393
R394
P395
V396
R397
G402
D403
Q409
N413
I416
G417
V420
P421
L422
A423
A424
ASP
SER
LYS
VAL
ARG
ARG
ALA
ARG
SER
VAL
ASP
GLY
ALA
GLY
GLN
GLY
L441
R442
L443
E444
I445
D448
A449
Q450
E451
L452
L455
G456
F457
V460
S461
A468
ASN
GLN

4 Data and refinement statistics (i)

Xtriage (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.	Xtriage
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	0.69	0/3620	1.86	72/4938 (1.5%)
1	B	0.68	0/3631	1.82	67/4957 (1.4%)
All	All	0.69	0/7251	1.84	139/9895 (1.4%)

There are no bond length outliers.

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	24	ARG	NE-CZ-NH2	18.22	129.41	120.30
1	A	394	ARG	CD-NE-CZ	16.01	146.01	123.60
1	B	152	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	A	152	ARG	NE-CZ-NH2	-14.48	113.06	120.30
1	B	391	ARG	NE-CZ-NH1	14.31	127.45	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	3523	0	3357	193	0
1	B	3533	0	3366	218	0
2	A	18	0	0	5	0
2	B	15	0	0	2	0
All	All	7089	0	6723	401	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 29.

The worst 5 of 401 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:377:ILE:HD13	1:A:382:LEU:HD13	1.47	0.95

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%)	22 53
1	B	447/470 (95%)	404 (90%)	35 (8%)	8 (2%)	8 28
All	All	890/940 (95%)	805 (90%)	74 (8%)	11 (1%)	13 39

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
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%)	333 (88%)	45 (12%)	5 16
1	B	379/392 (97%)	325 (86%)	54 (14%)	3 10
All	All	757/784 (97%)	658 (87%)	99 (13%)	4 12

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	72	ASN
1	B	199	THR
1	B	87	THR
1	B	143	THR
1	B	222	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	ASN
1	B	388	ASN
1	B	206	ASN
1	B	374	ASN
1	B	195	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 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.