Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:12 am BST

PDB ID	:	1ARB
Title	:	THE PRIMARY STRUCTURE AND STRUCTURAL CHARACTERISTICS OF ACHROMOBACTER LYTICUS PROTEASE I, A LYSINE-SPECIFIC SERINE PROTEASE
Authors	:	Kitagawa, Y.; Katsube, Y.
Deposited on	:	1993-04-15
Resolution	:	1.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

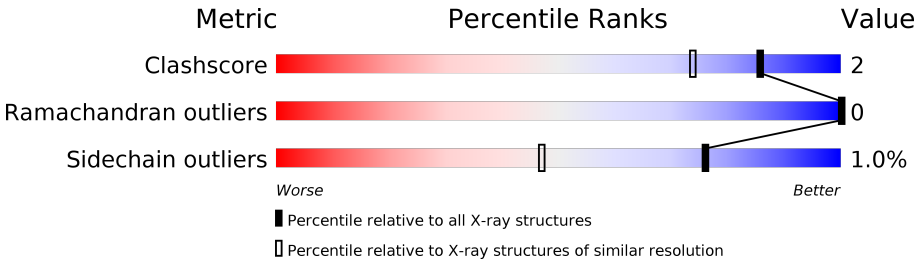
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.20 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	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)

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 on 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	268	81% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2077 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 ACHROMOBACTER PROTEASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	1924	1178	349	388	9	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	153	153	153	0	0

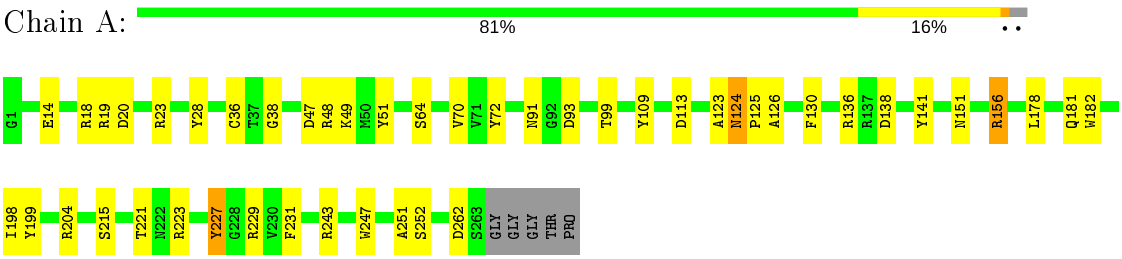
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: ACHROMOBACTER PROTEASE I

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	39.54Å 40.36Å 43.93Å 114.80° 113.73° 74.00°	Depositor
Resolution (Å)	(Not available) – 1.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2077	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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	1.39	4/1971 (0.2%)	1.69	38/2688 (1.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	ARG	NE-CZ	6.75	1.41	1.33
1	A	64	SER	CA-CB	5.68	1.61	1.52
1	A	36	CYS	CB-SG	-5.35	1.73	1.81
1	A	38	GLY	C-O	5.18	1.31	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243	ARG	NE-CZ-NH2	-10.83	114.88	120.30
1	A	136	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	A	20	ASP	CB-CG-OD2	-9.65	109.62	118.30
1	A	48	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	A	262	ASP	CB-CG-OD2	-9.23	110.00	118.30
1	A	109	TYR	CB-CG-CD2	-8.07	116.16	121.00
1	A	182	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	A	138	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	20	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	204	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	156	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	47	ASP	CB-CG-OD2	6.87	124.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	ARG	NH1-CZ-NH2	6.59	126.65	119.40
1	A	18	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	23	ARG	CD-NE-CZ	6.44	132.61	123.60
1	A	91	ASN	CB-CG-OD1	6.33	134.27	121.60
1	A	178	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	227	TYR	CZ-CE2-CD2	-6.14	114.28	119.80
1	A	182	TRP	CD1-CG-CD2	6.07	111.16	106.30
1	A	231	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	A	113	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	28	TYR	CB-CG-CD1	5.95	124.57	121.00
1	A	247	TRP	CG-CD2-CE3	-5.88	128.61	133.90
1	A	70	VAL	O-C-N	5.85	132.05	122.70
1	A	151	ASN	CA-CB-CG	-5.66	100.95	113.40
1	A	141	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	A	123	ALA	O-C-N	5.49	131.48	122.70
1	A	130	PHE	CB-CG-CD1	-5.42	117.00	120.80
1	A	251	ALA	N-CA-CB	-5.41	102.52	110.10
1	A	113	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	199	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	A	19	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	215	SER	N-CA-CB	5.25	118.38	110.50
1	A	247	TRP	CH2-CZ2-CE2	-5.24	112.16	117.40
1	A	14	GLU	CG-CD-OE1	5.15	128.61	118.30
1	A	223	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	93	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	229	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ARG	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	1924	0	1796	8	0
2	A	153	0	0	0	0
All	All	2077	0	1796	8	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 2.

All (8) 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:124:ASN:ND2	1:A:126:ALA:H	1.99	0.60
1:A:124:ASN:HD22	1:A:126:ALA:H	1.50	0.60
1:A:124:ASN:C	1:A:124:ASN:HD22	2.12	0.52
1:A:49:LYS:HD3	1:A:51:TYR:CZ	2.47	0.49
1:A:198:ILE:HB	1:A:227:TYR:CE2	2.50	0.47
1:A:124:ASN:HD22	1:A:125:PRO:N	2.14	0.46
1:A:72:TYR:CD1	1:A:99:THR:HG22	2.50	0.46
1:A:181:GLN:HE22	1:A:221:THR:HA	1.82	0.44

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	261/268 (97%)	256 (98%)	5 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	202/204 (99%)	200 (99%)	2 (1%)	76 47

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	252	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	42	ASN
1	A	74	ASN
1	A	124	ASN
1	A	181	GLN
1	A	183	GLN
1	A	256	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.