Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 05:41 PM EDT

PDB ID	:	7LPR
Title	:	STRUCTURAL BASIS FOR BROAD SPECIFICITY IN ALPHA-LYTIC PROTEASE MUTANTS
Authors	:	Fujishige, A.; Bone, R.; Agard, D.A.
Deposited on	:	1991-08-05
Resolution	:	2.05 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 (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:

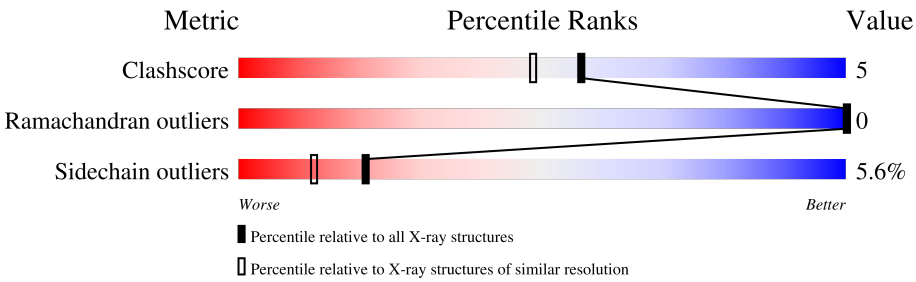
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.05 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	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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	198	75% 20% 5% •
2	P	5	40% 40% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1568 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 ALPHA-LYTIC PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	198	1388	844	262	275	7	0	0	0

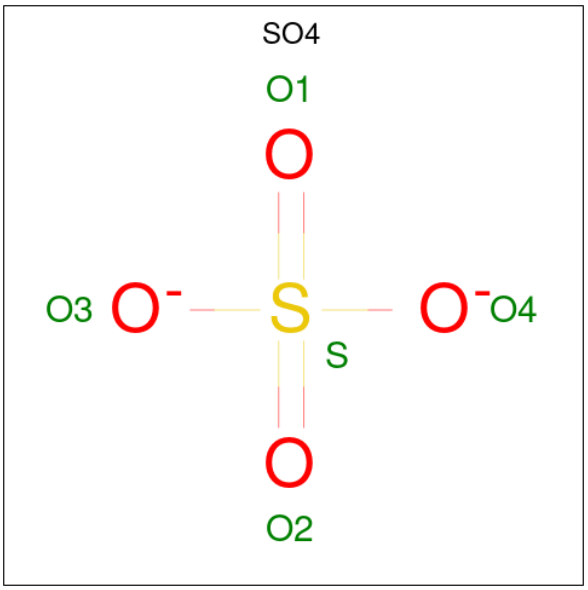
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ALA	MET	conflict	UNP P00778

- Molecule 2 is a protein called METHOXYSUCCINYL-ALA-ALA-PRO-LEUCINE BORONIC ACID INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	B	C	N	O			
2	P	4	26	1	16	4	5	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	146	146	146	0	0
			Total	O		
4	P	3	3	3	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: ALPHA-LYTIC PROTEASE

Chain A: 75% 20% 5%

A15A Y31 R48B T54 H57 C58 N64 R67 F88 R91 N101 D102 S107 S110 T113 R117 S120C S120D R125 E129 V136 C137 R138 S139 G140 R141 Y157 Q158 C159 G160 N166 Y171 A172 E174 R178 G179 N184

M192 G192A R192B G193 D194 S198 W199 I200 A209 V217A I221A P221B Q223 R224 E229 R230 L231 Q232 P233 L239 G244

• Molecule 2: METHOXYSUCCINYL-ALA-ALA-PRO-LEUCINE BORONIC ACID INHIBITOR

Chain P: 40% 40% 20%

MSU A4 A3 P2 L1

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	66.31Å 66.31Å 80.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.05	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.136 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1568	wwPDB-VP
Average B, all atoms ($Å^2$)	11.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BLE, SO4

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	1.19	2/1406 (0.1%)	2.41	59/1906 (3.1%)
2	P	1.10	0/17	2.86	3/23 (13.0%)
All	All	1.19	2/1423 (0.1%)	2.42	62/1929 (3.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120(C)	SER	CA-CB	5.52	1.61	1.52
1	A	174	GLU	CD-OE1	-5.31	1.19	1.25

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	ARG	NE-CZ-NH1	21.33	130.96	120.30
1	A	48(B)	ARG	CD-NE-CZ	18.41	149.37	123.60
1	A	230	ARG	NE-CZ-NH1	17.53	129.06	120.30
1	A	91	ARG	NE-CZ-NH1	16.43	128.52	120.30
1	A	230	ARG	NE-CZ-NH2	-16.00	112.30	120.30
1	A	192(B)	ARG	NE-CZ-NH2	-15.75	112.42	120.30
1	A	48(B)	ARG	NE-CZ-NH1	-14.73	112.93	120.30
1	A	178	ARG	NE-CZ-NH1	12.59	126.59	120.30
1	A	91	ARG	CD-NE-CZ	12.33	140.86	123.60
1	A	117	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	A	125	ARG	NE-CZ-NH1	-10.31	115.14	120.30
1	A	110	SER	CB-CA-C	-10.02	91.06	110.10
1	A	192(B)	ARG	NE-CZ-NH1	9.97	125.28	120.30
1	A	120(D)	SER	N-CA-CB	-9.45	96.33	110.50
1	A	102	ASP	CB-CG-OD2	9.43	126.79	118.30
1	A	138	ARG	NE-CZ-NH2	-9.21	115.70	120.30
1	A	129	GLU	OE1-CD-OE2	8.67	133.70	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48(B)	ARG	NH1-CZ-NH2	8.56	128.82	119.40
1	A	67	ARG	NE-CZ-NH2	-8.52	116.04	120.30
2	P	4	ALA	CB-CA-C	-8.26	97.71	110.10
1	A	110	SER	CA-CB-OG	-7.89	89.91	111.20
1	A	110	SER	O-C-N	7.01	133.91	122.70
1	A	110	SER	N-CA-CB	-6.88	100.19	110.50
1	A	141	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	A	171	TYR	CB-CG-CD2	-6.73	116.96	121.00
1	A	54	THR	CA-CB-CG2	6.65	121.72	112.40
1	A	117	ARG	NH1-CZ-NH2	-6.60	112.14	119.40
1	A	91	ARG	NH1-CZ-NH2	-6.50	112.25	119.40
1	A	217(A)	VAL	CA-CB-CG1	6.39	120.48	110.90
1	A	192(B)	ARG	CG-CD-NE	-6.34	98.48	111.80
1	A	139	SER	N-CA-CB	-6.24	101.14	110.50
1	A	15(A)	ALA	O-C-N	6.21	132.64	122.70
1	A	107	SER	CA-CB-OG	-6.19	94.48	111.20
1	A	88	PHE	CA-C-O	-6.12	107.26	120.10
1	A	129	GLU	CG-CD-OE2	-6.11	106.08	118.30
1	A	67	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
1	A	174	GLU	CG-CD-OE2	-6.05	106.21	118.30
1	A	194	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	160	GLY	N-CA-C	-5.86	98.46	113.10
1	A	57	HIS	CA-C-O	-5.79	107.95	120.10
1	A	171	TYR	CB-CG-CD1	5.77	124.46	121.00
1	A	230	ARG	CD-NE-CZ	-5.72	115.59	123.60
1	A	184	ASN	CB-CG-OD1	5.67	132.94	121.60
1	A	209	ALA	N-CA-CB	-5.60	102.26	110.10
1	A	138	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	217(A)	VAL	N-CA-CB	-5.52	99.36	111.50
2	P	4	ALA	N-CA-C	5.49	125.83	111.00
1	A	57	HIS	CA-C-N	5.44	129.17	117.20
1	A	178	ARG	CD-NE-CZ	-5.39	116.05	123.60
1	A	224	ARG	CA-C-O	-5.39	108.79	120.10
1	A	64	ASN	CA-C-O	-5.38	108.80	120.10
1	A	64	ASN	N-CA-CB	5.37	120.27	110.60
2	P	3	ALA	O-C-N	5.37	131.30	121.10
1	A	58	CYS	CA-CB-SG	-5.37	104.34	114.00
1	A	184	ASN	OD1-CG-ND2	-5.30	109.72	121.90
1	A	113	THR	CA-CB-OG1	-5.29	97.88	109.00
1	A	221(B)	PRO	O-C-N	5.24	131.09	122.70
1	A	200	ILE	O-C-N	5.18	130.99	122.70
1	A	120(C)	SER	CA-CB-OG	-5.14	97.31	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	31	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	157	TYR	N-CA-CB	-5.11	101.40	110.60
1	A	136	VAL	N-CA-CB	-5.09	100.31	111.50

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	1388	0	1356	14	0
2	P	26	0	28	0	0
3	A	5	0	0	0	0
4	A	146	0	0	1	0
4	P	3	0	0	0	0
All	All	1568	0	1384	14	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 5.

All (14) 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:48(B):ARG:HG2	1:A:239:LEU:HD23	1.84	0.60
1:A:137:CYS:HA	1:A:159:CYS:HA	1.88	0.54
1:A:166:ASN:HD22	1:A:179:GLY:HA2	1.72	0.54
1:A:221(A):ILE:HB	1:A:221(B):PRO:HD2	1.92	0.52
1:A:48(B):ARG:CG	1:A:239:LEU:HD23	2.40	0.50
1:A:138:ARG:HD2	1:A:192:MET:HE3	1.95	0.48
1:A:221(B):PRO:HG2	1:A:223:GLN:NE2	2.30	0.46
1:A:138:ARG:HA	1:A:198:SER:O	2.15	0.46
1:A:166:ASN:ND2	1:A:179:GLY:HA2	2.31	0.44
1:A:15(A):ALA:N	4:A:345:HOH:O	2.49	0.44
1:A:232:GLN:N	1:A:233:PRO:HD2	2.33	0.44
1:A:166:ASN:HA	1:A:179:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:HB3	1:A:229:GLU:OE2	2.22	0.40
1:A:138:ARG:HD2	1:A:192:MET:CE	2.51	0.40

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	196/198 (99%)	187 (95%)	9 (5%)	0	100	100
2	P	2/5 (40%)	2 (100%)	0	0	100	100
All	All	198/203 (98%)	189 (96%)	9 (4%)	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	141/141 (100%)	133 (94%)	8 (6%)	20	12
2	P	1/1 (100%)	1 (100%)	0	100	100
All	All	142/142 (100%)	134 (94%)	8 (6%)	21	12

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48(B)	ARG
1	A	91	ARG
1	A	107	SER
1	A	110	SER
1	A	120(D)	SER
1	A	141	ARG
1	A	198	SER
1	A	217(A)	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BLE	P	1	2,1	3,8,8	0.34	0	4,10,10	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BLE	P	1	2,1	-	0/3/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	1	-	4,4,4	0.69	0	6,6,6	1.23	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	SO4	O3-S-O1	-2.27	97.48	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.