



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 04:19 am BST

PDB ID : 1Z0V
Title : Crystal Structure of A. fulgidus Lon proteolytic domain
Authors : Dauter, Z.; Botos, I.; LaRonde-LeBlanc, N.; Wlodawer, A.
Deposited on : 2005-03-02
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

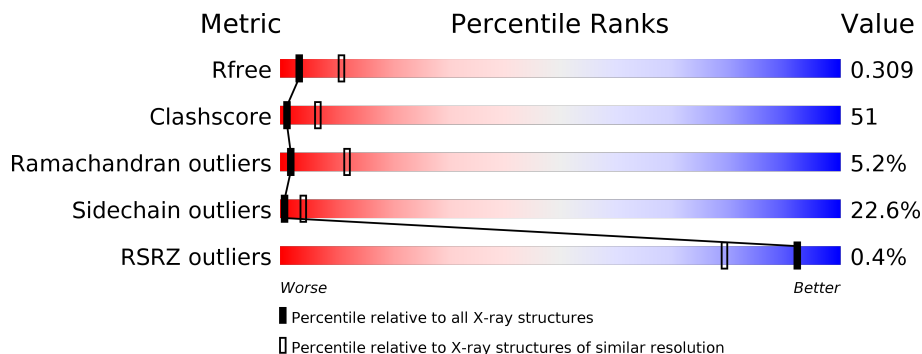
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	205	
1	B	205	
1	C	205	
1	D	205	
1	E	205	
1	F	205	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9236 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 Putative protease La homolog type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	195	1457	921	247	284	5	0	0	0
1	B	195	1457	921	247	284	5	0	0	0
1	C	194	1448	915	245	283	5	0	0	0
1	D	195	1457	921	247	284	5	0	0	0
1	E	195	1457	921	247	284	5	0	0	0
1	F	195	1457	921	247	284	5	0	0	0

- Molecule 2 is water.

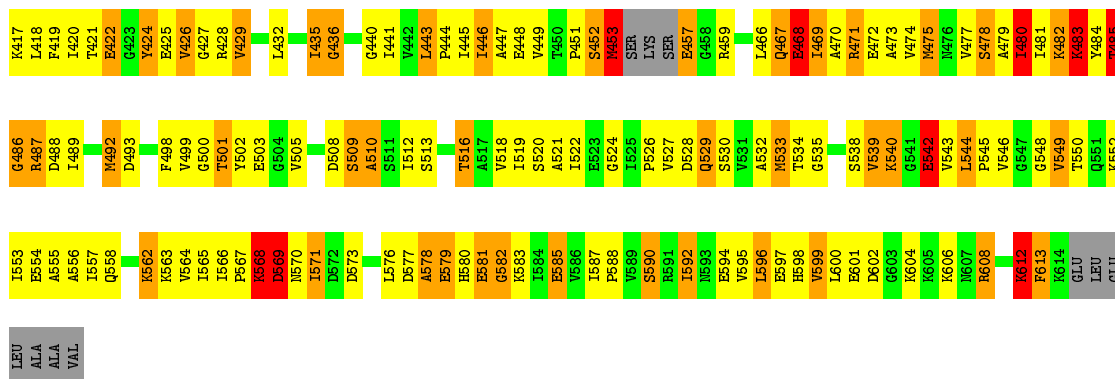
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total 78	O 78	0	0
2	B	74	Total 74	O 74	0	0
2	C	104	Total 104	O 104	0	0
2	D	99	Total 99	O 99	0	0
2	E	69	Total 69	O 69	0	0
2	F	79	Total 79	O 79	0	0

3 Residue-property plots


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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

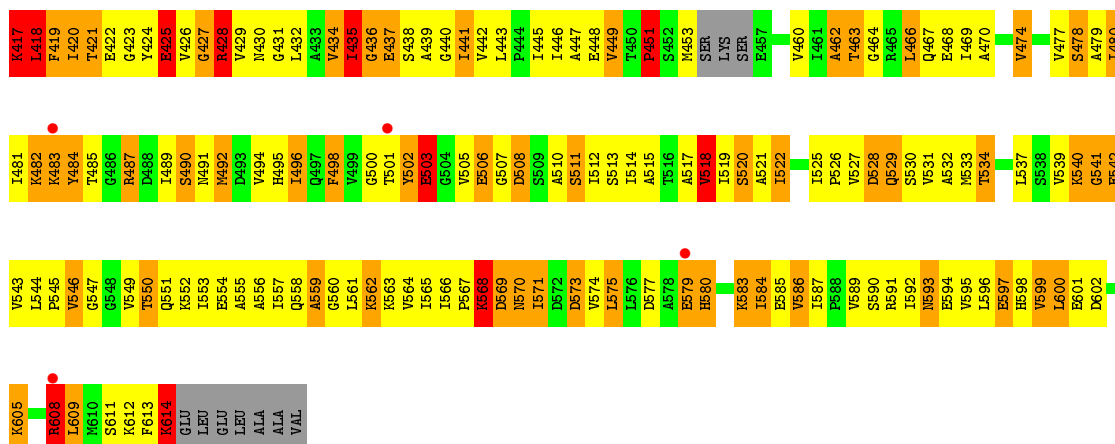
- Molecule 1: Putative protease La homolog type

Chain A: 



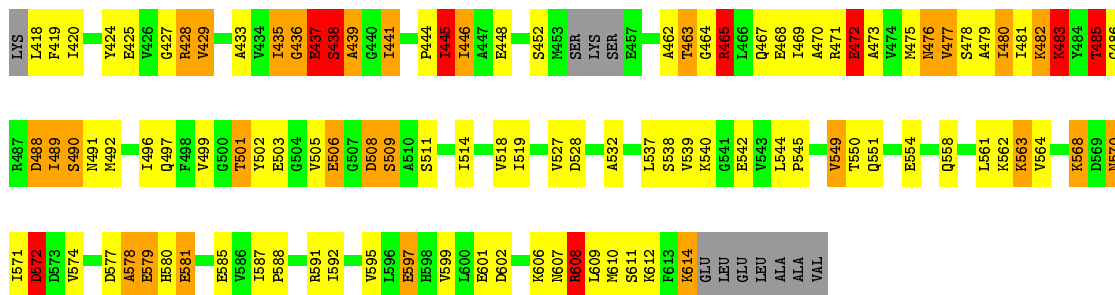
- Molecule 1: Putative protease La homolog type

Chain B: 



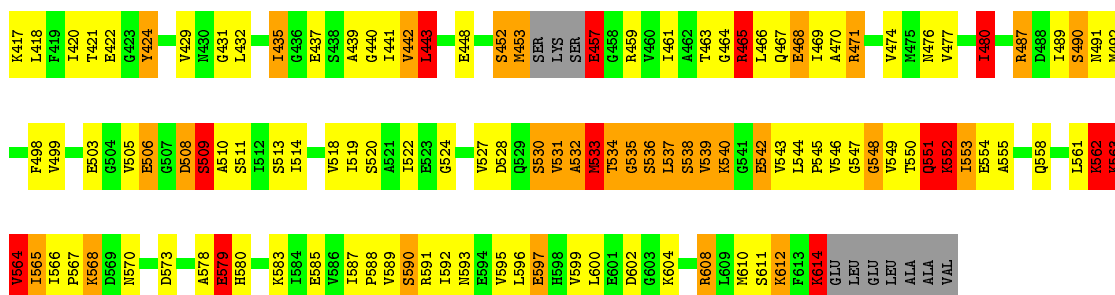
- Molecule 1: Putative protease La homolog type

Chain C: 



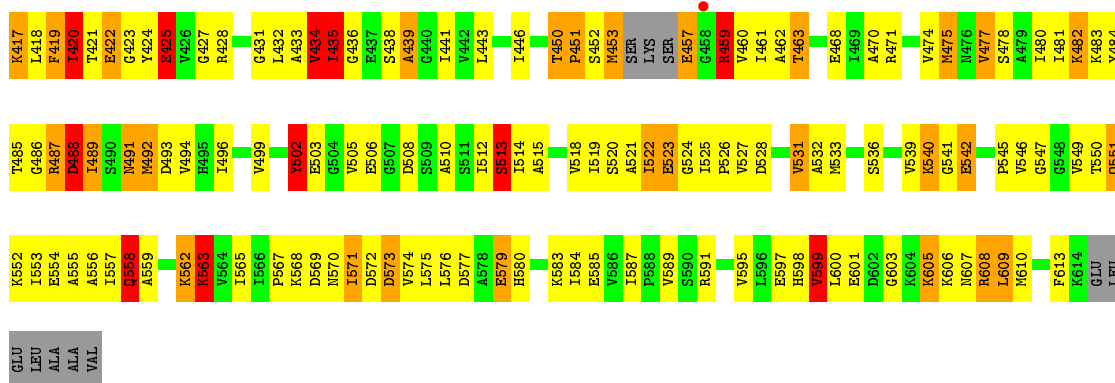
- Molecule 1: Putative protease La homolog type

Chain D: 38% 37% 15% 6% 5%



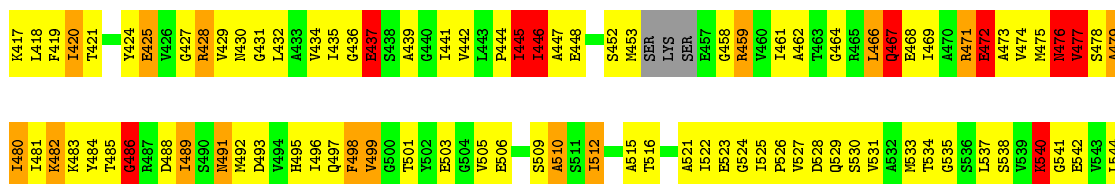
- Molecule 1: Putative protease La homolog type

Chain E: 30% 46% 14% 5% 5%



- Molecule 1: Putative protease La homolog type

Chain F: 28% 48% 13% 5% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.45Å 86.28Å 137.97Å 90.00° 92.30° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 14.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-3.00) 99.1 (14.99-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.310 0.215 , 0.309	Depositor DCC
R_{free} test set	1148 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtrriage
Anisotropy	0.171	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9236	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4102e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.67	19/1470 (1.3%)	1.46	9/1983 (0.5%)
1	B	1.85	23/1470 (1.6%)	1.47	13/1983 (0.7%)
1	C	1.71	17/1461 (1.2%)	1.50	17/1972 (0.9%)
1	D	2.37	58/1470 (3.9%)	2.11	61/1983 (3.1%)
1	E	1.71	16/1470 (1.1%)	1.45	14/1983 (0.7%)
1	F	1.54	16/1470 (1.1%)	1.45	17/1983 (0.9%)
All	All	1.83	149/8811 (1.7%)	1.59	131/11887 (1.1%)

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
1	B	0	5
1	C	0	1
1	D	0	5
1	E	0	3
1	F	0	3
All	All	0	18

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	552	LYS	CE-NZ	23.76	2.08	1.49
1	D	563	LYS	CE-NZ	21.05	2.01	1.49
1	D	534	THR	C-O	19.61	1.60	1.23
1	D	531	VAL	C-N	14.71	1.67	1.34
1	D	508	ASP	CB-CG	-14.54	1.21	1.51

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	536	SER	O-C-N	-19.83	90.98	122.70
1	D	534	THR	CB-CA-C	-16.26	67.69	111.60
1	D	508	ASP	CB-CG-OD1	-16.15	103.77	118.30
1	D	534	THR	CA-CB-CG2	14.87	133.22	112.40
1	D	563	LYS	O-C-N	-14.79	99.03	122.70

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	485	THR	Peptide
1	B	417	LYS	Peptide
1	B	441	ILE	Peptide
1	B	451	PRO	Peptide
1	B	462	ALA	Peptide

5.2 Too-close contacts

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	1457	0	1523	160	0
1	B	1457	0	1523	229	0
1	C	1448	0	1510	136	0
1	D	1457	0	1523	129	0
1	E	1457	0	1523	147	0
1	F	1457	0	1523	154	1
2	A	78	0	0	12	0
2	B	74	0	0	13	0
2	C	104	0	0	5	0
2	D	99	0	0	10	0
2	E	69	0	0	13	0
2	F	79	0	0	11	0
All	All	9236	0	9125	906	1

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 51.

The worst 5 of 906 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:C:445:ILE:CG1	1:C:445:ILE:CD1	1.78	1.56
1:A:483:LYS:NZ	1:A:483:LYS:CE	1.70	1.55
1:D:531:VAL:CA	1:D:531:VAL:N	1.68	1.55
1:A:568:LYS:NZ	1:A:568:LYS:CE	1.68	1.55
1:C:483:LYS:CG	1:C:483:LYS:CB	1.74	1.55

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:GLY:O	1:F:578:ALA:CB[1_455]	1.65	0.55

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	191/205 (93%)	164 (86%)	16 (8%)	11 (6%)	1	10
1	B	191/205 (93%)	140 (73%)	35 (18%)	16 (8%)	1	4
1	C	190/205 (93%)	162 (85%)	18 (10%)	10 (5%)	2	11
1	D	191/205 (93%)	169 (88%)	16 (8%)	6 (3%)	4	23
1	E	191/205 (93%)	151 (79%)	35 (18%)	5 (3%)	5	27
1	F	191/205 (93%)	155 (81%)	25 (13%)	11 (6%)	1	10
All	All	1145/1230 (93%)	941 (82%)	145 (13%)	59 (5%)	2	12

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	GLY
1	A	549	VAL
1	A	578	ALA
1	A	581	GLU

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Mol	Chain	Res	Type
1	A	582	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	160/168 (95%)	116 (72%)	44 (28%)	0	2
1	B	160/168 (95%)	115 (72%)	45 (28%)	0	2
1	C	159/168 (95%)	125 (79%)	34 (21%)	1	5
1	D	160/168 (95%)	133 (83%)	27 (17%)	2	11
1	E	160/168 (95%)	122 (76%)	38 (24%)	0	3
1	F	160/168 (95%)	131 (82%)	29 (18%)	1	9
All	All	959/1008 (95%)	742 (77%)	217 (23%)	1	4

5 of 217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	465	ARG
1	C	608	ARG
1	F	489	ILE
1	C	477	VAL
1	C	508	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	580	HIS
1	F	558	GLN
1	E	558	GLN
1	B	551	GLN
1	D	598	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 carbohydrates 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	531:VAL	C	532:ALA	N	1.67
1	D	532:ALA	C	533:MET	N	1.66

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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	195/205 (95%)	-0.42	0 100 100	5, 17, 35, 47	0
1	B	195/205 (95%)	-0.02	4 (2%) 63 34	11, 25, 43, 61	0
1	C	194/205 (94%)	-0.69	0 100 100	2, 10, 27, 35	0
1	D	195/205 (95%)	-0.71	0 100 100	2, 8, 24, 34	0
1	E	195/205 (95%)	-0.35	1 (0%) 91 75	5, 17, 42, 57	0
1	F	195/205 (95%)	-0.50	0 100 100	2, 17, 36, 50	0
All	All	1169/1230 (95%)	-0.45	5 (0%) 92 79	2, 16, 37, 61	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	THR	2.7
1	B	608	ARG	2.2
1	E	458	GLY	2.2
1	B	483	LYS	2.2
1	B	579	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.