



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 03:42 AM EDT

PDB ID : 3WZ2
Title : Crystal structure of Pyrococcus furiosus PbaA, an archaeal homolog of proteasome-assembly chaperone
Authors : Sikdar, A.; Satoh, T.; Kawasaki, M.; Kato, K.
Deposited on : 2014-09-18
Resolution : 2.25 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 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

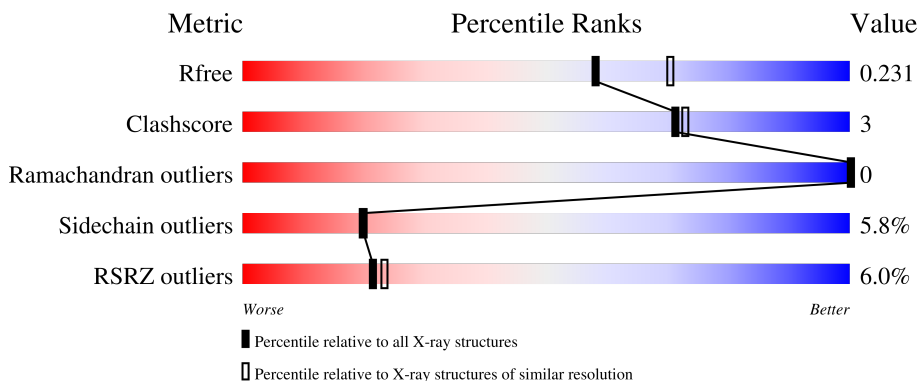
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 $\leq 5\%$. 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	245	 2% 85% 6% • 8%
1	B	245	 2% 84% 8% • 7%
1	C	245	 3% 84% 7% • 7%
1	D	245	 3% 83% 9% • 7%
1	E	245	 17% 80% 9% • 10%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9078 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	Total 1755	C 1135	N 287	O 325	S 8	0	0	0
1	B	228	Total 1772	C 1146	N 290	O 327	S 9	0	0	0
1	C	227	Total 1764	C 1141	N 289	O 326	S 8	0	0	0
1	D	227	Total 1764	C 1141	N 289	O 326	S 8	0	0	0
1	E	221	Total 1715	C 1113	N 276	O 318	S 8	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8U4Q9
A	-1	SER	-	expression tag	UNP Q8U4Q9
A	0	HIS	-	expression tag	UNP Q8U4Q9
B	-2	GLY	-	expression tag	UNP Q8U4Q9
B	-1	SER	-	expression tag	UNP Q8U4Q9
B	0	HIS	-	expression tag	UNP Q8U4Q9
C	-2	GLY	-	expression tag	UNP Q8U4Q9
C	-1	SER	-	expression tag	UNP Q8U4Q9
C	0	HIS	-	expression tag	UNP Q8U4Q9
D	-2	GLY	-	expression tag	UNP Q8U4Q9
D	-1	SER	-	expression tag	UNP Q8U4Q9
D	0	HIS	-	expression tag	UNP Q8U4Q9
E	-2	GLY	-	expression tag	UNP Q8U4Q9
E	-1	SER	-	expression tag	UNP Q8U4Q9
E	0	HIS	-	expression tag	UNP Q8U4Q9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total 86	O 86	0	0
2	B	85	Total 85	O 85	0	0
2	C	60	Total 60	O 60	0	0
2	D	56	Total 56	O 56	0	0
2	E	21	Total 21	O 21	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	111.37Å 155.19Å 172.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.25 37.61 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.25) 99.9 (37.61-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.15 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.196 , 0.220 0.203 , 0.231	Depositor DCC
R_{free} test set	3521 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9078	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.67	0/1788	0.77	2/2417 (0.1%)
1	B	0.65	0/1805	0.77	3/2438 (0.1%)
1	C	0.62	0/1797	0.76	3/2428 (0.1%)
1	D	0.62	0/1797	0.80	4/2429 (0.2%)
1	E	0.55	0/1747	0.78	5/2362 (0.2%)
All	All	0.62	0/8934	0.78	17/12074 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	ARG	CG-CD-NE	9.57	131.90	111.80
1	B	219	LEU	CB-CG-CD2	8.88	126.09	111.00
1	C	57	MET	CA-CB-CG	5.94	123.41	113.30
1	A	166	ARG	CG-CD-NE	5.77	123.91	111.80
1	C	166	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	C	64	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	219	LEU	CA-CB-CG	5.54	128.04	115.30
1	E	182	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	70	ARG	CB-CA-C	-5.38	99.63	110.40
1	D	146	LYS	CA-CB-CG	5.30	125.05	113.40
1	A	230	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	214	MET	CG-SD-CE	5.25	108.60	100.20
1	E	123	ASP	CB-CG-OD1	5.24	123.02	118.30
1	E	123	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	E	109	LYS	CD-CE-NZ	5.19	123.65	111.70
1	E	186	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	D	166	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1755	0	1804	14	0
1	B	1772	0	1826	12	0
1	C	1764	0	1817	9	0
1	D	1764	0	1816	9	0
1	E	1715	0	1762	19	0
2	A	86	0	0	4	0
2	B	85	0	0	3	0
2	C	60	0	0	1	0
2	D	56	0	0	1	0
2	E	21	0	0	0	0
All	All	9078	0	9025	62	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 3.

All (62) 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:E:32:ILE:HD11	1:E:219:LEU:CD1	1.86	1.05
1:A:103:LYS:HG2	2:A:345:HOH:O	1.62	1.00
1:D:174:LEU:HD11	1:D:198:MET:HE1	1.58	0.86
1:E:37:LEU:HD21	1:E:195:LEU:HD23	1.57	0.84
1:E:32:ILE:HD11	1:E:219:LEU:HD12	1.60	0.80
1:A:166:ARG:HH11	1:A:166:ARG:HG2	1.52	0.74
1:D:174:LEU:HD11	1:D:198:MET:CE	2.24	0.68
1:D:85:PHE:CZ	1:D:225:GLN:HB3	2.30	0.67
1:E:32:ILE:CD1	1:E:219:LEU:CD1	2.69	0.66
1:C:64:ARG:NH2	2:C:348:HOH:O	2.27	0.66
1:E:66:THR:CG2	1:E:70:ARG:HD3	2.26	0.64
1:A:221:ARG:HG3	1:A:222:MET:H	1.65	0.62
1:B:66:THR:CG2	1:B:70:ARG:HD3	2.30	0.61
1:B:182:ARG:NH1	1:B:216:GLU:OE1	2.34	0.61
1:A:221:ARG:HG3	1:A:222:MET:N	2.16	0.60
1:E:141:GLU:O	1:E:143:LEU:O	2.21	0.59
1:E:66:THR:HG23	1:E:70:ARG:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:LEU:CD2	1:E:195:LEU:HD23	2.33	0.57
1:E:37:LEU:HD11	1:E:192:VAL:HG13	1.87	0.56
1:E:149:LYS:H	1:E:149:LYS:CD	2.19	0.56
1:C:162:TRP:CZ2	1:C:166:ARG:HD3	2.40	0.56
1:E:32:ILE:CD1	1:E:219:LEU:HD11	2.36	0.56
1:B:66:THR:HG23	1:B:70:ARG:HD3	1.87	0.55
1:D:162:TRP:CZ2	1:D:166:ARG:HD3	2.43	0.54
1:E:41:LEU:HD11	1:E:203:VAL:CG2	2.39	0.53
1:A:182:ARG:NH1	1:A:216:GLU:OE2	2.41	0.53
1:B:26:VAL:HG23	2:B:363:HOH:O	2.08	0.52
1:A:16:ASN:N	2:A:323:HOH:O	2.43	0.52
1:B:85:PHE:HB3	2:B:340:HOH:O	2.09	0.52
1:A:84:ILE:HD12	1:A:86:LEU:HD21	1.93	0.51
1:C:182:ARG:NH1	1:C:216:GLU:OE2	2.44	0.51
1:A:166:ARG:NE	1:E:48:TYR:OH	2.44	0.50
1:C:84:ILE:HD12	1:C:86:LEU:HD21	1.93	0.50
1:B:131:GLY:H	1:B:137:ASN:HD21	1.59	0.50
1:B:84:ILE:HD12	1:B:86:LEU:HD21	1.93	0.50
1:D:84:ILE:HD12	1:D:86:LEU:HD21	1.94	0.49
1:B:131:GLY:H	1:B:137:ASN:ND2	2.11	0.48
1:B:166:ARG:NE	1:B:166:ARG:HA	2.28	0.47
1:A:223:HIS:NE2	2:A:333:HOH:O	2.22	0.47
1:E:41:LEU:HD11	1:E:203:VAL:HG21	1.97	0.46
1:E:182:ARG:HD2	1:E:216:GLU:OE2	2.15	0.46
1:B:221:ARG:HG2	2:B:336:HOH:O	2.14	0.46
1:C:118:ILE:CD1	1:C:122:LYS:CD	2.93	0.46
1:D:5:LYS:N	1:D:6:PRO:HD2	2.31	0.46
1:D:84:ILE:CD1	1:D:86:LEU:HD21	2.46	0.46
1:C:84:ILE:CD1	1:C:86:LEU:HD21	2.46	0.45
1:D:174:LEU:HD21	1:D:198:MET:HE1	1.97	0.45
1:E:149:LYS:H	1:E:149:LYS:HD3	1.80	0.45
1:B:84:ILE:CD1	1:B:86:LEU:HD21	2.46	0.45
1:C:118:ILE:CD1	1:C:122:LYS:HD3	2.46	0.45
1:A:84:ILE:CD1	1:A:86:LEU:HD21	2.47	0.45
1:B:57:MET:CE	1:B:59:LEU:HD11	2.47	0.45
1:E:41:LEU:CD1	1:E:41:LEU:N	2.79	0.45
1:E:172:TYR:CD1	1:E:172:TYR:N	2.85	0.45
1:D:221:ARG:HG2	2:D:309:HOH:O	2.17	0.44
1:C:118:ILE:HD12	1:C:122:LYS:HD2	2.01	0.42
1:A:221:ARG:CG	1:A:222:MET:H	2.30	0.42
1:A:106:ASN:ND2	2:A:309:HOH:O	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:LEU:N	1:E:41:LEU:HD13	2.36	0.41
1:C:118:ILE:HD11	1:C:122:LYS:HD3	2.03	0.40
1:A:166:ARG:HG2	1:A:166:ARG:NH1	2.29	0.40
1:A:221:ARG:CG	1:A:222:MET:N	2.83	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	224/245 (91%)	218 (97%)	6 (3%)	0	100	100
1	B	226/245 (92%)	219 (97%)	7 (3%)	0	100	100
1	C	225/245 (92%)	221 (98%)	4 (2%)	0	100	100
1	D	225/245 (92%)	220 (98%)	5 (2%)	0	100	100
1	E	217/245 (89%)	212 (98%)	5 (2%)	0	100	100
All	All	1117/1225 (91%)	1090 (98%)	27 (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	189/207 (91%)	181 (96%)	8 (4%)	30	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	191/207 (92%)	182 (95%)	9 (5%)	26	29
1	C	190/207 (92%)	177 (93%)	13 (7%)	16	14
1	D	190/207 (92%)	176 (93%)	14 (7%)	13	12
1	E	185/207 (89%)	174 (94%)	11 (6%)	19	19
All	All	945/1035 (91%)	890 (94%)	55 (6%)	20	20

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	74	LYS
1	A	166	ARG
1	A	172	TYR
1	A	182	ARG
1	A	224	GLU
1	A	230	ARG
1	A	231	ARG
1	B	9	LEU
1	B	59	LEU
1	B	61	LEU
1	B	74	LYS
1	B	160	LEU
1	B	172	TYR
1	B	182	ARG
1	B	210	LYS
1	B	221	ARG
1	C	59	LEU
1	C	61	LEU
1	C	64	ARG
1	C	74	LYS
1	C	96	LYS
1	C	126	GLU
1	C	142	SER
1	C	166	ARG
1	C	172	TYR
1	C	182	ARG
1	C	208	LEU
1	C	221	ARG
1	C	224	GLU
1	D	64	ARG
1	D	74	LYS

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Mol	Chain	Res	Type
1	D	85	PHE
1	D	96	LYS
1	D	138	LYS
1	D	142	SER
1	D	143	LEU
1	D	166	ARG
1	D	172	TYR
1	D	198	MET
1	D	208	LEU
1	D	214	MET
1	D	228	GLU
1	D	231	ARG
1	E	41	LEU
1	E	143	LEU
1	E	149	LYS
1	E	152	SER
1	E	160	LEU
1	E	165	SER
1	E	166	ARG
1	E	172	TYR
1	E	208	LEU
1	E	221	ARG
1	E	224	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	B	137	ASN
1	E	100	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](#)

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

6.1 Protein, DNA and RNA chains

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	226/245 (92%)	-0.11	6 (2%) 54 57	16, 29, 58, 96	0
1	B	228/245 (93%)	-0.17	6 (2%) 56 59	17, 28, 62, 91	0
1	C	227/245 (92%)	-0.09	7 (3%) 49 52	19, 31, 59, 97	0
1	D	227/245 (92%)	-0.07	8 (3%) 44 46	21, 33, 68, 98	0
1	E	221/245 (90%)	0.98	41 (18%) 1 1	26, 64, 97, 112	0
All	All	1129/1225 (92%)	0.10	68 (6%) 21 23	16, 33, 83, 112	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	202	ASN	5.5
1	E	210	LYS	4.8
1	E	224	GLU	4.5
1	D	224	GLU	4.4
1	E	123	ASP	4.4
1	E	220	ARG	4.4
1	E	42	ASP	4.2
1	A	231	ARG	4.1
1	D	228	GLU	4.1
1	E	200	GLY	4.1
1	E	214	MET	4.1
1	E	138	LYS	4.0
1	E	142	SER	3.9
1	E	122	LYS	3.9
1	C	231	ARG	3.8
1	D	231	ARG	3.8
1	B	231	ARG	3.8
1	E	221	ARG	3.7
1	E	206	GLU	3.6
1	E	211	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	141	GLU	3.3
1	E	40	GLU	3.3
1	E	208	LEU	3.2
1	A	230	ARG	3.0
1	E	207	PRO	2.9
1	C	228	GLU	2.9
1	E	121	PHE	2.9
1	E	120	PHE	2.9
1	A	210	LYS	2.9
1	D	221	ARG	2.9
1	E	16	ASN	2.8
1	C	232	LYS	2.8
1	E	225	GLN	2.8
1	E	12	PRO	2.7
1	E	229	ALA	2.7
1	B	224	GLU	2.7
1	E	217	GLU	2.7
1	A	228	GLU	2.6
1	E	135	GLU	2.6
1	E	134	GLU	2.6
1	B	228	GLU	2.6
1	E	143	LEU	2.6
1	E	124	THR	2.6
1	E	15	GLU	2.6
1	E	105	VAL	2.5
1	E	228	GLU	2.4
1	E	145	VAL	2.4
1	B	214	MET	2.4
1	E	201	LEU	2.4
1	E	106	ASN	2.3
1	C	217	GLU	2.3
1	E	146	LYS	2.3
1	D	85	PHE	2.3
1	C	134	GLU	2.2
1	D	217	GLU	2.2
1	C	141	GLU	2.2
1	E	186	ARG	2.2
1	E	108	GLU	2.2
1	E	113	LEU	2.1
1	B	210	LYS	2.1
1	C	214	MET	2.1
1	E	127	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	221	ARG	2.1
1	A	224	GLU	2.1
1	E	144	GLY	2.1
1	D	220	ARG	2.0
1	D	214	MET	2.0
1	B	230	ARG	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.