Full wwPDB X-ray Structure Validation Report (i)

Oct 29, 2026 – 02:08 PM JST

PDB ID	:	25YB / pdb_000025yb
Title	:	Pseudomonas aeruginosa AchC1 (YfdX1) at pH 3.0
Authors	:	Jung, Y.J.; Cha, S.S.
Deposited on	:	2026-04-22
Resolution	:	3.36 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:

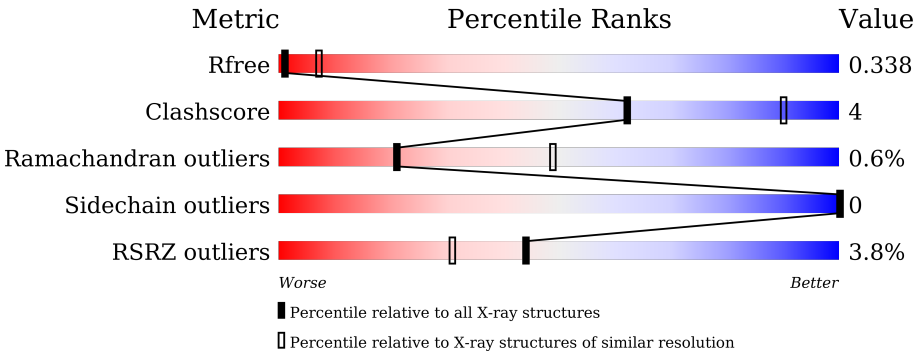
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.36 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}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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% 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	286	4% 80% 10% 10%
1	B	286	4% 81% 7% 12%
1	C	286	3% 72% 10% 18%
1	D	286	3% 76% 11% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7021 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.

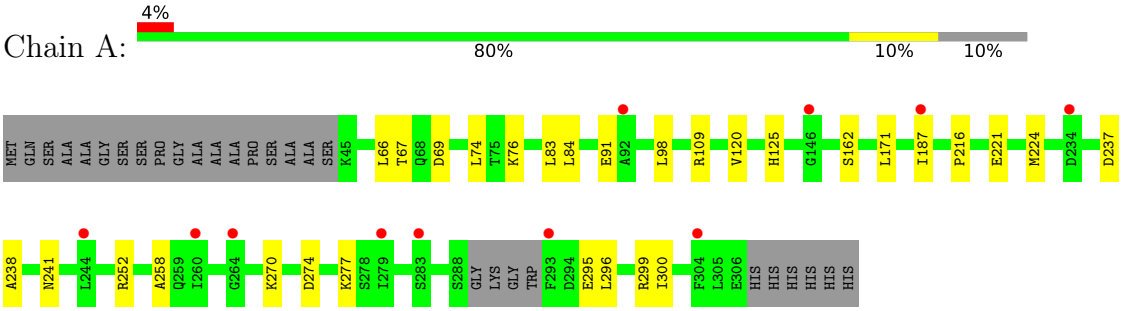
- Molecule 1 is a protein called Heat resistance protein YfdX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1882	1181	329	369	3			
1	B	251	Total	C	N	O	S	0	0	0
			1755	1095	305	352	3			
1	C	234	Total	C	N	O	S	0	0	0
			1666	1051	292	320	3			
1	D	249	Total	C	N	O	S	0	0	0
			1718	1063	307	346	2			

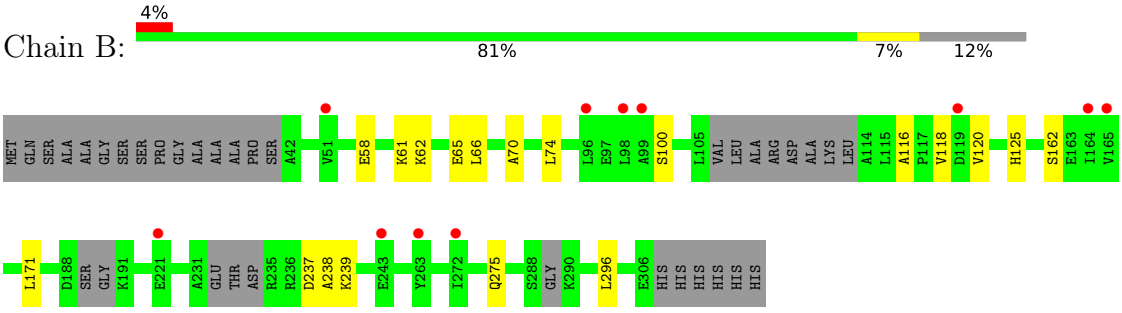
3 Residue-property plots (i)

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 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.

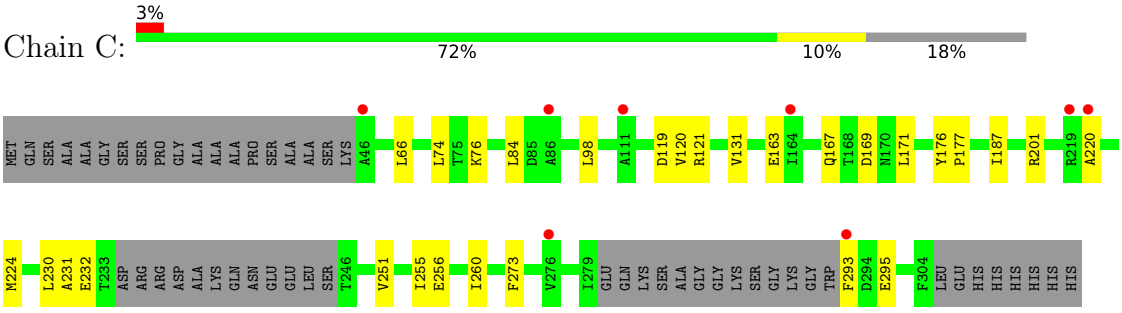
• Molecule 1: Heat resistance protein YfdX1



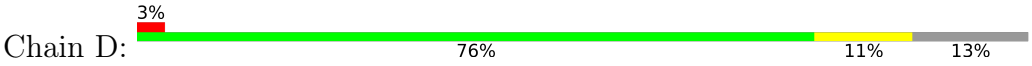
• Molecule 1: Heat resistance protein YfdX1

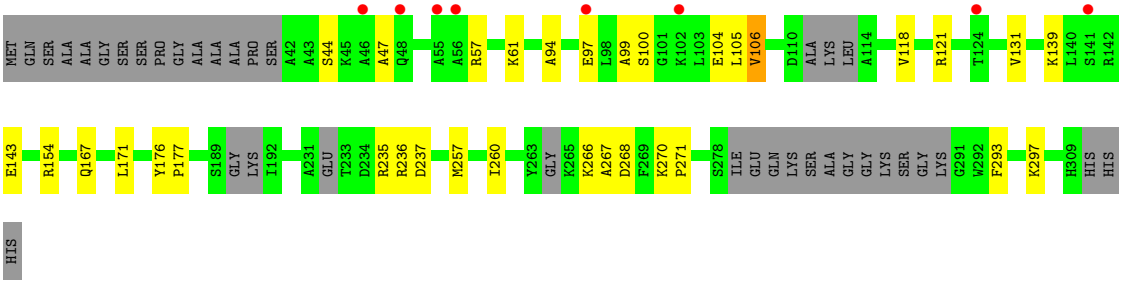


• Molecule 1: Heat resistance protein YfdX1



• Molecule 1: Heat resistance protein YfdX1




MET GLN SER ALA ALA GLY SER SER PRO GLY ALA ALA ALA PRO SER A42 A43 S44 K45 A46 A47 Q48 A55 A56 R57 K61 A94 E97 L98 A99 S100 G101 K102 L103 E104 L105 V106 D110 ALA LYS LEU A114 V118 R121 T124 V131 K139 L140 S141 R142
E143 R154 Q167 L171 Y176 P177 S189 GLY LYS I192 A231 GLU T233 D234 R235 R236 D237 M257 I260 Y263 GLY K265 K266 A267 D268 P269 K270 P271 S278 ILE GLU GLN LYS SER ALA GLY GLY LYS SER GLY LYS G291 W292 F293 K297 H309 HIS HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.57Å 99.79Å 160.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.36 29.75 – 3.36	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.75-3.36) 99.6 (29.75-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.299 , 0.338 0.299 , 0.338	Depositor DCC
R_{free} test set	947 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	88.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7021	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.25 % 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 6.0041e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.09	0/1896	0.21	0/2569
1	B	0.10	0/1767	0.28	1/2405 (0.0%)
1	C	0.09	0/1679	0.22	0/2285
1	D	0.11	0/1728	0.27	0/2353
All	All	0.10	0/7070	0.25	1/9612 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	100	SER	N-CA-C	-5.40	108.46	114.62

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	1882	0	1916	16	0
1	B	1755	0	1673	9	0
1	C	1666	0	1666	16	0
1	D	1718	0	1591	18	0
All	All	7021	0	6846	57	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 4.

All (57) 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:D:266:LYS:O	1:D:268:ASP:N	2.23	0.70
1:C:201:ARG:HD2	1:D:47:ALA:HB2	1.74	0.68
1:C:76:LYS:HE3	1:C:98:LEU:HD23	1.77	0.65
1:A:125:HIS:O	1:A:162:SER:HA	1.97	0.65
1:D:121:ARG:NH2	1:D:167:GLN:OE1	2.31	0.64
1:A:69:ASP:OD2	1:A:109:ARG:NH1	2.30	0.64
1:A:83:LEU:HD13	1:A:91:GLU:HB3	1.81	0.62
1:C:163:GLU:OE2	1:D:154:ARG:NH2	2.32	0.60
1:A:252:ARG:HE	1:A:277:LYS:HZ3	1.50	0.60
1:A:270:LYS:NZ	1:A:274:ASP:OD2	2.29	0.58
1:D:235:ARG:HG3	1:D:236:ARG:H	1.73	0.54
1:B:74:LEU:HD11	1:B:118:VAL:HB	1.92	0.52
1:A:76:LYS:HE3	1:A:98:LEU:HD23	1.91	0.51
1:D:118:VAL:HG11	1:D:171:LEU:HG	1.92	0.51
1:B:237:ASP:O	1:B:239:LYS:N	2.45	0.50
1:B:66:LEU:HD21	1:B:120:VAL:HG23	1.93	0.50
1:D:94:ALA:HA	1:D:97:GLU:HB2	1.93	0.50
1:B:116:ALA:HB3	1:B:171:LEU:HB2	1.94	0.49
1:C:293:PHE:O	1:C:295:GLU:N	2.39	0.49
1:B:58:GLU:HA	1:B:61:LYS:HD2	1.94	0.49
1:D:270:LYS:HB3	1:D:271:PRO:HD3	1.94	0.49
1:C:66:LEU:HD21	1:C:120:VAL:HG23	1.94	0.49
1:C:74:LEU:HD13	1:C:171:LEU:HD21	1.95	0.49
1:A:67:THR:HG22	1:A:69:ASP:H	1.77	0.48
1:C:84:LEU:HD11	1:C:187:ILE:HD11	1.95	0.48
1:C:131:VAL:HG13	1:C:260:ILE:HG12	1.96	0.48
1:D:100:SER:O	1:D:104:GLU:N	2.44	0.48
1:D:257:MET:HA	1:D:260:ILE:HG22	1.96	0.47
1:C:220:ALA:HB1	1:C:251:VAL:HG13	1.95	0.47
1:D:131:VAL:HG13	1:D:260:ILE:HG21	1.97	0.47
1:C:256:GLU:HG3	1:C:273:PHE:CZ	2.50	0.46
1:A:295:GLU:OE2	1:A:299:ARG:NE	2.43	0.46
1:A:237:ASP:O	1:A:241:ASN:ND2	2.48	0.46
1:A:296:LEU:O	1:A:300:ILE:HG12	2.15	0.46
1:D:139:LYS:NZ	1:D:143:GLU:OE2	2.45	0.45
1:A:221:GLU:HA	1:A:224:MET:HE2	1.97	0.45
1:A:237:ASP:OD1	1:A:238:ALA:N	2.50	0.45
1:B:275:GLN:HB3	1:B:296:LEU:HD13	1.99	0.45
1:B:62:LYS:O	1:B:65:GLU:HG2	2.17	0.44
1:A:66:LEU:HD21	1:A:120:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:LEU:O	1:C:232:GLU:N	2.51	0.44
1:D:235:ARG:NE	1:D:235:ARG:HA	2.33	0.44
1:C:176:TYR:HB3	1:C:177:PRO:HD3	2.00	0.43
1:D:97:GLU:C	1:D:99:ALA:H	2.26	0.43
1:D:176:TYR:HB3	1:D:177:PRO:HD3	1.99	0.43
1:A:216:PRO:HB2	1:A:258:ALA:HB2	2.00	0.43
1:D:105:LEU:O	1:D:106:VAL:C	2.61	0.43
1:C:224:MET:HE2	1:C:224:MET:HB3	1.77	0.43
1:C:251:VAL:O	1:C:255:ILE:HG12	2.19	0.42
1:A:74:LEU:HD13	1:A:171:LEU:HD21	2.01	0.42
1:B:125:HIS:O	1:B:162:SER:HA	2.20	0.42
1:C:119:ASP:HB3	1:C:169:ASP:HB2	2.02	0.42
1:B:70:ALA:O	1:B:74:LEU:HG	2.19	0.41
1:C:121:ARG:NH1	1:C:167:GLN:OE1	2.47	0.41
1:D:57:ARG:O	1:D:61:LYS:HG3	2.22	0.40
1:D:293:PHE:O	1:D:297:LYS:HG3	2.21	0.40
1:A:84:LEU:HD11	1:A:187:ILE:HD11	2.03	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	254/286 (89%)	239 (94%)	15 (6%)	0	100 100
1	B	241/286 (84%)	226 (94%)	14 (6%)	1 (0%)	30 58
1	C	228/286 (80%)	214 (94%)	13 (6%)	1 (0%)	30 58
1	D	237/286 (83%)	221 (93%)	12 (5%)	4 (2%)	7 27
All	All	960/1144 (84%)	900 (94%)	54 (6%)	6 (1%)	21 49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	106	VAL
1	D	267	ALA
1	C	231	ALA
1	D	237	ASP
1	B	238	ALA
1	D	44	SER

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	187/224 (84%)	187 (100%)	0	100	100
1	B	161/224 (72%)	161 (100%)	0	100	100
1	C	158/224 (70%)	158 (100%)	0	100	100
1	D	151/224 (67%)	151 (100%)	0	100	100
All	All	657/896 (73%)	657 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	125	HIS
1	A	170	ASN
1	A	194	ASN
1	B	241	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 oligosaccharides 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, 95^{th} 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	258/286 (90%)	0.35	11 (4%)	40	28	33, 69, 103, 113	0
1	B	251/286 (87%)	0.50	11 (4%)	39	28	38, 81, 117, 127	0
1	C	234/286 (81%)	0.43	8 (3%)	48	34	38, 71, 104, 115	0
1	D	249/286 (87%)	0.53	8 (3%)	50	36	39, 85, 115, 138	0
All	All	992/1144 (86%)	0.45	38 (3%)	44	31	33, 76, 111, 138	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	GLY	4.6
1	A	92	ALA	4.3
1	B	51	VAL	3.5
1	B	272	ILE	3.0
1	A	234	ASP	2.9
1	A	244	LEU	2.9
1	C	111	ALA	2.8
1	C	293	PHE	2.8
1	A	283	SER	2.8
1	B	99	ALA	2.7
1	D	141	SER	2.7
1	B	96	LEU	2.7
1	B	243	GLU	2.6
1	C	86	ALA	2.5
1	D	56	ALA	2.5
1	C	220	ALA	2.5
1	C	276	VAL	2.5
1	A	304	PHE	2.4
1	B	119	ASP	2.4
1	D	46	ALA	2.3
1	D	48	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	55	ALA	2.3
1	A	293	PHE	2.3
1	B	165	VAL	2.3
1	C	164	ILE	2.2
1	C	219	ARG	2.2
1	D	124	THR	2.2
1	B	221	GLU	2.2
1	C	46	ALA	2.2
1	B	164	ILE	2.2
1	A	260	ILE	2.1
1	A	279	ILE	2.1
1	D	102	LYS	2.1
1	D	97	GLU	2.1
1	A	146	GLY	2.1
1	A	187	ILE	2.0
1	B	263	TYR	2.0
1	B	98	LEU	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 oligosaccharides 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.