



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2023 – 01:38 AM JST

PDB ID : 8GY0
Title : Agrocyste pediacides linalool synthase (Ap.LS)
Authors : Rehka, T.; Sharma, D.; Lin, F.; Lim, C.; Choong, Y.K.; Chacko, J.; Zhang, C.
Deposited on : 2022-09-21
Resolution : 1.99 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

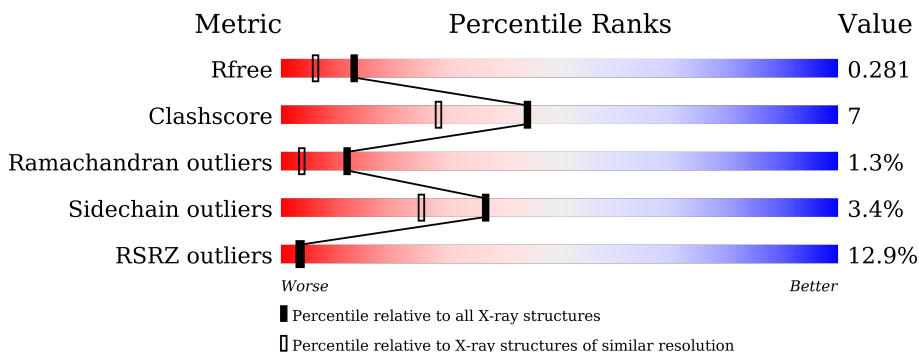
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

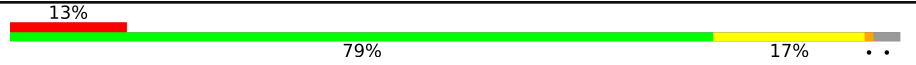

The reported resolution of this entry is 1.99 Å.

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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	325	 13% 79% 17% ..
1	B	325	 12% 81% 14% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5129 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 Terpene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	314	2524	1618	422	473	11	0	0	0
1	A	314	2525	1618	422	474	11	0	0	0

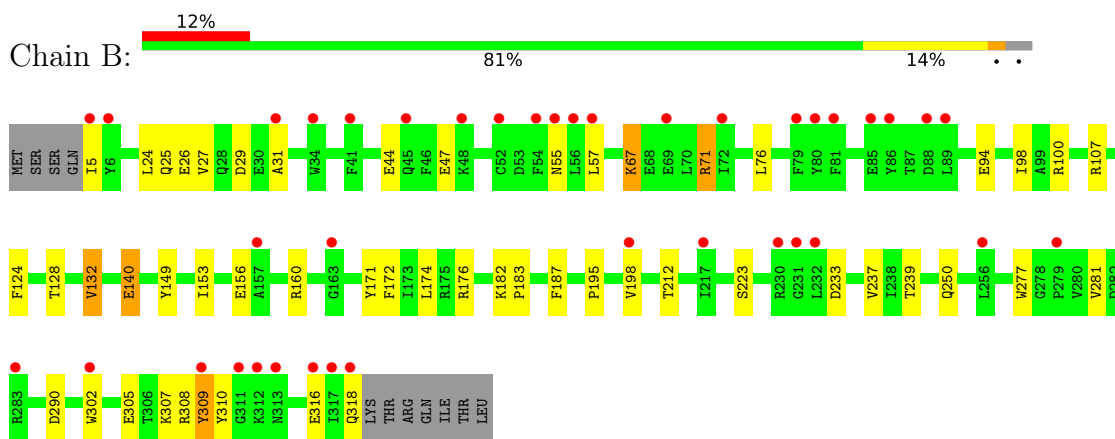
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	39	Total 39	O 39	0	0
2	A	41	Total 41	O 41	0	0

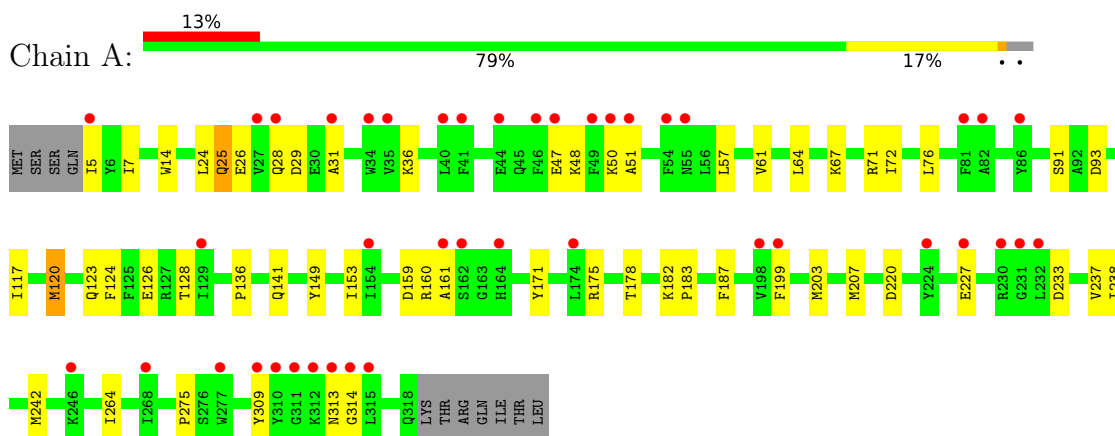
3 Residue-property plots [i](#)

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 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: Terpene synthase



- Molecule 1: Terpene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.92Å 80.67Å 69.91Å 90.00° 96.05° 90.00°	Depositor
Resolution (Å)	46.80 – 1.99 46.76 – 1.99	Depositor EDS
% Data completeness (in resolution range)	82.7 (46.80-1.99) 82.7 (46.76-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.214 , 0.275 0.220 , 0.281	Depositor DCC
R_{free} test set	1831 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtrriage
Anisotropy	0.137	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.457 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5129	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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	0.70	0/2590	0.80	0/3511
1	B	0.70	0/2589	0.80	0/3511
All	All	0.70	0/5179	0.80	0/7022

There are no bond length outliers.

There are no bond angle outliers.

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	2525	0	2416	35	0
1	B	2524	0	2416	30	0
2	A	41	0	0	9	0
2	B	39	0	0	2	0
All	All	5129	0	4832	65	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 7.

All (65) 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:123:GLN:O	2:A:401:HOH:O	1.69	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLN:C	2:A:401:HOH:O	2.06	0.93
1:A:149:TYR:CE1	1:A:153:ILE:HD11	2.19	0.77
1:B:31:ALA:HA	1:B:71:ARG:HH12	1.54	0.72
1:A:275:PRO:O	2:A:402:HOH:O	2.10	0.69
1:B:156:GLU:HG3	1:B:174:LEU:HD21	1.74	0.69
1:B:277:TRP:HB2	1:B:281:VAL:CG2	2.26	0.65
1:A:227:GLU:HB3	1:A:233:ASP:HB3	1.80	0.64
1:B:307:LYS:O	1:B:308:ARG:HD2	1.98	0.64
1:B:149:TYR:CE1	1:B:153:ILE:HD11	2.34	0.62
1:B:233:ASP:O	1:B:239:THR:OG1	2.09	0.62
1:A:24:LEU:HD23	1:A:25:GLN:N	2.14	0.62
1:A:64:LEU:O	2:A:403:HOH:O	2.17	0.57
1:B:55:ASN:HA	2:B:415:HOH:O	2.03	0.57
1:A:175:ARG:NH1	1:A:178:THR:HG21	2.19	0.57
1:A:171:TYR:CZ	1:A:175:ARG:HG3	2.41	0.56
1:B:277:TRP:HB2	1:B:281:VAL:HG21	1.87	0.55
1:B:305:GLU:O	1:B:309:TYR:HA	2.08	0.54
1:A:227:GLU:HB3	1:A:233:ASP:CB	2.37	0.54
1:A:171:TYR:CE2	1:A:175:ARG:HG3	2.43	0.54
1:A:36:LYS:N	2:A:409:HOH:O	2.40	0.53
1:A:76:LEU:HD22	1:A:187:PHE:CD2	2.43	0.53
1:A:171:TYR:CZ	1:A:237:VAL:HB	2.44	0.52
1:B:31:ALA:CA	1:B:71:ARG:HH12	2.23	0.51
1:A:48:LYS:HA	1:A:51:ALA:HB3	1.92	0.51
1:A:171:TYR:OH	1:A:220:ASP:OD2	2.16	0.51
1:A:36:LYS:HB3	2:A:409:HOH:O	2.11	0.50
1:A:117:ILE:HD12	1:A:120:MET:HE3	1.92	0.50
1:B:26:GLU:OE1	1:B:67:LYS:HG2	2.12	0.49
1:B:182:LYS:N	1:B:183:PRO:HD2	2.27	0.49
1:B:24:LEU:C	1:B:26:GLU:H	2.15	0.49
1:A:14:TRP:CE3	1:A:264:ILE:HG12	2.50	0.47
1:A:57:LEU:O	1:A:61:VAL:HB	2.15	0.47
1:B:76:LEU:HD22	1:B:187:PHE:CD2	2.50	0.47
1:B:5:ILE:HG22	1:B:316:GLU:O	2.15	0.47
1:B:171:TYR:CZ	1:B:237:VAL:HB	2.51	0.46
1:A:126:GLU:N	2:A:401:HOH:O	2.48	0.46
1:A:7:ILE:HD12	1:A:314:GLY:O	2.15	0.46
1:A:31:ALA:HA	1:A:71:ARG:CZ	2.46	0.46
1:B:24:LEU:HG	1:B:25:GLN:H	1.80	0.45
1:A:26:GLU:O	1:A:26:GLU:HG2	2.16	0.45
1:B:94:GLU:O	1:B:98:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PRO:HG2	1:B:198:VAL:HG23	1.99	0.45
1:B:223:SER:HB3	1:B:307:LYS:HD2	1.97	0.44
1:B:318:GLN:HA	2:B:426:HOH:O	2.16	0.44
1:A:126:GLU:HB3	2:A:401:HOH:O	2.17	0.44
1:A:160:ARG:HD3	1:A:161:ALA:H	1.83	0.44
1:B:107:ARG:NH1	1:B:140:GLU:OE1	2.50	0.43
1:A:28:GLN:OE1	2:A:404:HOH:O	2.21	0.43
1:A:203:MET:O	1:A:207:MET:HG3	2.17	0.43
1:B:172:PHE:O	1:B:176:ARG:HG3	2.18	0.43
1:A:5:ILE:HD12	1:A:5:ILE:HA	1.92	0.43
1:A:238:ILE:O	1:A:242:MET:HG3	2.19	0.43
1:B:128:THR:O	1:B:132:VAL:HB	2.18	0.42
1:A:24:LEU:O	1:A:25:GLN:CB	2.66	0.42
1:B:5:ILE:HD12	1:B:5:ILE:HA	1.87	0.42
1:A:141:GLN:HG2	1:A:199:PHE:CE1	2.54	0.42
1:B:176:ARG:O	1:B:212:THR:HG21	2.20	0.42
1:B:307:LYS:O	1:B:308:ARG:CD	2.67	0.42
1:A:72:ILE:HG21	1:A:128:THR:HA	2.02	0.42
1:B:24:LEU:HG	1:B:25:GLN:N	2.36	0.41
1:A:182:LYS:N	1:A:183:PRO:HD2	2.35	0.41
1:B:5:ILE:HD12	1:B:250:GLN:OE1	2.20	0.41
1:B:57:LEU:HB2	1:B:302:TRP:CD1	2.56	0.41
1:A:50:LYS:CE	1:A:50:LYS:HA	2.50	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	312/325 (96%)	293 (94%)	16 (5%)	3 (1%)	15 6
1	B	312/325 (96%)	295 (95%)	12 (4%)	5 (2%)	9 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	624/650 (96%)	588 (94%)	28 (4%)	8 (1%)	12 4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	309	TYR
1	B	310	TYR
1	A	309	TYR
1	A	47	GLU
1	A	25	GLN
1	B	44	GLU
1	B	160	ARG
1	B	47	GLU

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	267/284 (94%)	258 (97%)	9 (3%)	37 25
1	B	267/284 (94%)	258 (97%)	9 (3%)	37 25
All	All	534/568 (94%)	516 (97%)	18 (3%)	37 25

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	VAL
1	B	29	ASP
1	B	67	LYS
1	B	71	ARG
1	B	100	ARG
1	B	124	PHE
1	B	132	VAL
1	B	140	GLU
1	B	290	ASP
1	A	29	ASP

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Mol	Chain	Res	Type
1	A	67	LYS
1	A	91	SER
1	A	93	ASP
1	A	120	MET
1	A	124	PHE
1	A	136	PRO
1	A	159	ASP
1	A	313	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	GLN
1	B	164	HIS
1	A	17	GLN
1	A	28	GLN

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

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	314/325 (96%)	1.06	42 (13%) 3 3	40, 64, 121, 179	0
1	B	314/325 (96%)	1.01	39 (12%) 4 4	40, 65, 118, 160	0
All	All	628/650 (96%)	1.03	81 (12%) 3 3	40, 65, 120, 179	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	GLY	20.0
1	A	315	LEU	10.1
1	A	310	TYR	8.0
1	A	231	GLY	7.8
1	B	41	PHE	7.7
1	B	317	ILE	7.3
1	B	45	GLN	6.7
1	A	314	GLY	6.1
1	B	309	TYR	5.8
1	A	230	ARG	5.6
1	B	318	GLN	5.3
1	B	89	LEU	4.8
1	A	309	TYR	4.8
1	A	232	LEU	4.7
1	A	40	LEU	4.6
1	B	230	ARG	4.4
1	B	48	LYS	4.4
1	B	5	ILE	4.1
1	B	57	LEU	3.8
1	B	163	GLY	3.7
1	A	51	ALA	3.7
1	B	232	LEU	3.7
1	A	162	SER	3.6
1	A	49	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	277	TRP	3.5
1	B	279	PRO	3.5
1	A	44	GLU	3.4
1	B	313	ASN	3.4
1	A	224	TYR	3.4
1	B	316	GLU	3.4
1	A	227	GLU	3.3
1	B	86	TYR	3.3
1	A	27	VAL	3.2
1	B	6	TYR	3.2
1	B	312	LYS	3.2
1	A	31	ALA	3.1
1	B	231	GLY	3.0
1	A	161	ALA	2.9
1	A	313	ASN	2.9
1	A	5	ILE	2.9
1	A	129	ILE	2.9
1	B	54	PHE	2.8
1	B	56	LEU	2.8
1	B	81	PHE	2.7
1	B	256	LEU	2.7
1	A	81	PHE	2.6
1	B	80	TYR	2.6
1	B	198	VAL	2.6
1	A	46	PHE	2.6
1	B	283	ARG	2.6
1	A	154	ILE	2.6
1	A	82	ALA	2.5
1	A	54	PHE	2.5
1	B	88	ASP	2.5
1	A	55	ASN	2.5
1	B	72	ILE	2.5
1	B	217	ILE	2.5
1	A	86	TYR	2.5
1	A	28	GLN	2.4
1	B	311	GLY	2.4
1	A	41	PHE	2.3
1	B	85	GLU	2.3
1	A	312	LYS	2.3
1	A	164	HIS	2.3
1	B	302	TRP	2.2
1	B	52	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	174	LEU	2.2
1	B	55	ASN	2.1
1	A	34	TRP	2.1
1	B	157	ALA	2.1
1	A	35	VAL	2.1
1	A	198	VAL	2.1
1	A	246	LYS	2.1
1	B	34	TRP	2.1
1	B	79	PHE	2.1
1	B	31	ALA	2.1
1	B	69	GLU	2.0
1	A	199	PHE	2.0
1	A	50	LYS	2.0
1	A	268	ILE	2.0
1	A	47	GLU	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.