Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:42 AM EDT

PDB ID	:	3GHY
Title	:	Crystal structure of a putative ketopantoate reductase from Ralstonia solanacearum MolK2
Authors	:	Patskovsky, Y.; Ramagopal, U.A.; Toro, R.; Morano, C.; Freeman, J.; Chang, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-03-04
Resolution	:	2.00 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 (1)) were used in the production of this report:

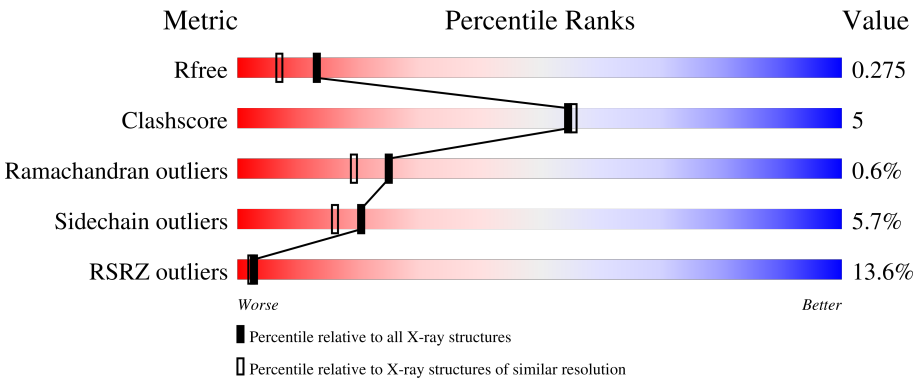
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	335	18% 85% 10% • •
1	B	335	8% 83% 11% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4929 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 Ketopantoate reductase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2364	1490	438	422	14	0	4	0
1	B	321	2354	1479	437	425	13	0	3	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP B5RXG4
A	0	SER	-	expression tag	UNP B5RXG4
A	1	LEU	-	expression tag	UNP B5RXG4
A	21	ALA	VAL	conflict	UNP B5RXG4
A	97	CYS	ARG	conflict	UNP B5RXG4
A	142	CYS	GLY	conflict	UNP B5RXG4
A	326	GLU	-	expression tag	UNP B5RXG4
A	327	GLY	-	expression tag	UNP B5RXG4
A	328	HIS	-	expression tag	UNP B5RXG4
A	329	HIS	-	expression tag	UNP B5RXG4
A	330	HIS	-	expression tag	UNP B5RXG4
A	331	HIS	-	expression tag	UNP B5RXG4
A	332	HIS	-	expression tag	UNP B5RXG4
A	333	HIS	-	expression tag	UNP B5RXG4
B	-1	MET	-	expression tag	UNP B5RXG4
B	0	SER	-	expression tag	UNP B5RXG4
B	1	LEU	-	expression tag	UNP B5RXG4
B	21	ALA	VAL	conflict	UNP B5RXG4
B	97	CYS	ARG	conflict	UNP B5RXG4
B	142	CYS	GLY	conflict	UNP B5RXG4
B	326	GLU	-	expression tag	UNP B5RXG4
B	327	GLY	-	expression tag	UNP B5RXG4
B	328	HIS	-	expression tag	UNP B5RXG4
B	329	HIS	-	expression tag	UNP B5RXG4
B	330	HIS	-	expression tag	UNP B5RXG4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	331	HIS	-	expression tag	UNP B5RXG4
B	332	HIS	-	expression tag	UNP B5RXG4
B	333	HIS	-	expression tag	UNP B5RXG4

- Molecule 2 is water.

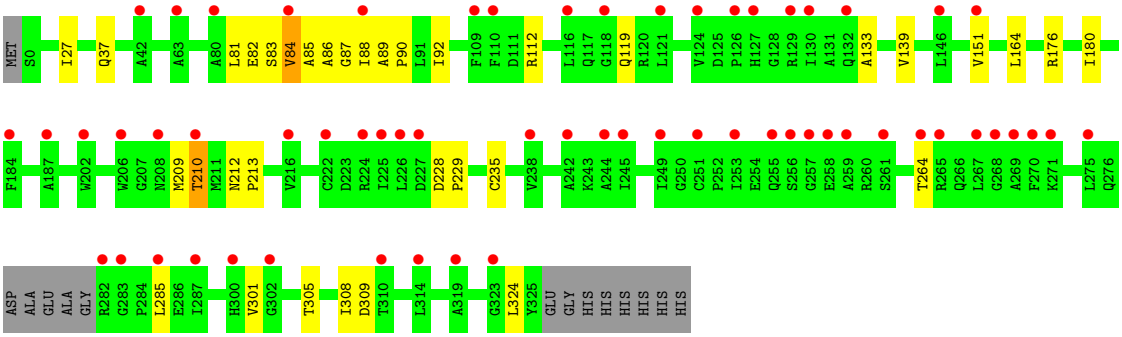
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	78	78	78	0	0
			Total	O		
2	B	133	133	133	0	0

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.

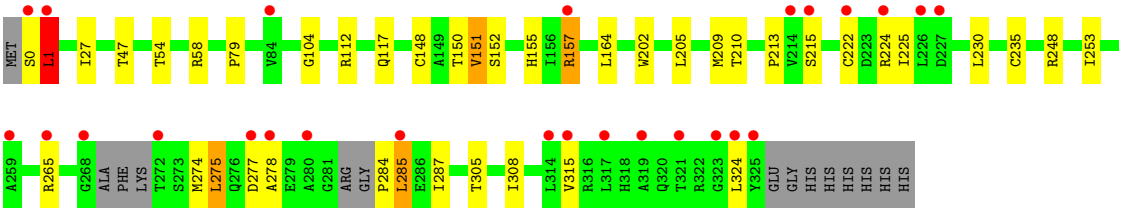
• Molecule 1: Ketopantoate reductase protein

Chain A:



• Molecule 1: Ketopantoate reductase protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	70.65Å 70.65Å 145.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 47.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.00) 99.8 (47.25-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.231 , 0.278 0.231 , 0.275	Depositor DCC
R_{free} test set	1483 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4929	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (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	0.40	0/2417	0.59	0/3290
1	B	0.47	1/2402 (0.0%)	0.64	0/3269
All	All	0.44	1/4819 (0.0%)	0.62	0/6559

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148	CYS	CB-SG	-5.14	1.73	1.81

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	2364	0	2449	23	0
1	B	2354	0	2426	28	0
2	A	78	0	0	1	0
2	B	133	0	0	1	0
All	All	4929	0	4875	50	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 (50) 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:B:151:VAL:HG12	1:B:152:SER:N	1.52	1.12
1:A:81:LEU:HD12	1:A:84:VAL:CG1	1.80	1.09
1:B:150:THR:HG23	1:B:150:THR:O	1.63	0.97
1:A:81:LEU:HD12	1:A:84:VAL:HG12	1.46	0.95
1:A:81:LEU:HD12	1:A:84:VAL:HG11	1.51	0.92
1:B:151:VAL:HG12	1:B:152:SER:H	1.35	0.86
1:B:151:VAL:CG1	1:B:152:SER:N	2.29	0.85
1:A:81:LEU:CD1	1:A:84:VAL:HG11	2.10	0.80
1:B:150:THR:O	1:B:150:THR:CG2	2.30	0.80
1:A:81:LEU:CD1	1:A:84:VAL:CG1	2.61	0.79
1:A:85:ALA:HB1	1:A:133:ALA:HB3	1.65	0.78
1:A:89:ALA:HB3	1:A:90:PRO:HD3	1.73	0.70
1:B:151:VAL:CG2	1:B:157[B]:ARG:HH21	2.10	0.65
1:A:85:ALA:HB1	1:A:133:ALA:CB	2.26	0.63
1:A:89:ALA:N	1:A:90:PRO:CD	2.69	0.55
1:B:151:VAL:HG22	1:B:157[B]:ARG:HH21	1.72	0.55
1:A:210:THR:HG21	1:A:235:CYS:HA	1.91	0.52
1:B:0:SER:O	1:B:1:LEU:HB2	2.10	0.51
1:B:151:VAL:HG21	1:B:157[B]:ARG:NH2	2.25	0.51
1:B:151:VAL:CG1	1:B:152:SER:H	2.04	0.51
1:A:89:ALA:O	2:A:402:HOH:O	2.20	0.50
1:A:81:LEU:CD1	1:A:84:VAL:HG12	2.30	0.49
1:B:213:PRO:HB3	1:B:315:VAL:HG21	1.95	0.49
1:B:47:THR:HB	1:B:157[B]:ARG:HG2	1.95	0.49
1:B:305:THR:HB	1:B:308:ILE:HB	1.93	0.49
1:A:88:ILE:O	1:A:88:ILE:HG13	2.13	0.48
1:B:151:VAL:HG21	1:B:157[B]:ARG:HH21	1.79	0.47
1:A:285:LEU:HG	1:A:324:LEU:HB3	1.96	0.47
1:B:202:TRP:HD1	1:B:253:ILE:HD11	1.79	0.47
1:B:151:VAL:HG11	1:B:155:HIS:ND1	2.30	0.47
1:B:222:CYS:HA	1:B:225:ILE:HD12	1.99	0.45
1:A:212:ASN:HB2	1:A:213:PRO:HD3	1.98	0.44
1:B:274:MET:HE1	1:B:287:ILE:HG22	1.99	0.44
1:B:215:SER:HB3	1:B:275:LEU:HB2	2.00	0.43
1:B:117:GLN:NE2	2:B:419:HOH:O	2.51	0.43
1:A:305:THR:HB	1:A:308:ILE:HB	2.01	0.42
1:B:210:THR:HG21	1:B:235:CYS:HA	2.00	0.42
1:B:274:MET:O	1:B:278:ALA:HB3	2.18	0.42
1:B:151:VAL:CG2	1:B:157[B]:ARG:NH2	2.78	0.42
1:A:85:ALA:O	1:A:87:GLY:N	2.53	0.42
1:A:309:ASP:HB3	1:B:230:LEU:HD22	2.01	0.42
1:B:278:ALA:HB1	1:B:285:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ASP:HA	1:A:229:PRO:HD3	1.82	0.41
1:A:85:ALA:C	1:A:87:GLY:N	2.73	0.41
1:A:88:ILE:O	1:A:92:ILE:HG13	2.21	0.41
1:A:176:ARG:O	1:A:180:ILE:HG12	2.21	0.41
1:A:84:VAL:CG1	1:A:85:ALA:N	2.83	0.41
1:B:79:PRO:HG2	1:B:284:PRO:HB3	2.04	0.40
1:B:285:LEU:HD23	1:B:324:LEU:HB3	2.03	0.40
1:B:104:GLY:HA2	1:B:205:LEU:HD13	2.02	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	321/335 (96%)	304 (95%)	15 (5%)	2 (1%)	25	19
1	B	318/335 (95%)	302 (95%)	14 (4%)	2 (1%)	25	19
All	All	639/670 (95%)	606 (95%)	29 (4%)	4 (1%)	25	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	VAL
1	B	1	LEU
1	A	86	ALA
1	A	151	VAL

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	241/247 (98%)	228 (95%)	13 (5%)	22	18
1	B	239/247 (97%)	224 (94%)	15 (6%)	18	13
All	All	480/494 (97%)	452 (94%)	28 (6%)	20	15

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	37	GLN
1	A	82	GLU
1	A	83	SER
1	A	84	VAL
1	A	112	ARG
1	A	119	GLN
1	A	139	VAL
1	A	164	LEU
1	A	209	MET
1	A	210	THR
1	A	264	THR
1	A	301	VAL
1	B	1	LEU
1	B	27	ILE
1	B	54	THR
1	B	58	ARG
1	B	112	ARG
1	B	157[A]	ARG
1	B	157[B]	ARG
1	B	164	LEU
1	B	209	MET
1	B	224	ARG
1	B	248	ARG
1	B	265	ARG
1	B	275	LEU
1	B	277	ASP
1	B	285	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	119	GLN
1	A	276	GLN
1	A	320	GLN
1	B	117	GLN
1	B	190	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 (i)

There are no chain breaks in this entry.

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	321/335 (95%)	1.13	61 (19%) 1 1	33, 61, 96, 126	0
1	B	321/335 (95%)	0.57	26 (8%) 12 11	30, 46, 85, 111	0
All	All	642/670 (95%)	0.85	87 (13%) 3 2	30, 53, 94, 126	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	LEU	8.4
1	A	84	VAL	7.5
1	A	249	ILE	7.3
1	A	264	THR	7.2
1	B	278	ALA	6.7
1	A	253	ILE	6.5
1	B	319	ALA	6.0
1	A	323	GLY	5.9
1	B	323	GLY	5.6
1	A	270	PHE	5.2
1	A	226	LEU	5.1
1	B	268	GLY	5.0
1	B	1	LEU	4.9
1	A	283	GLY	4.9
1	A	265	ARG	4.8
1	A	116	LEU	4.8
1	A	151	VAL	4.6
1	A	238	VAL	4.6
1	A	282	ARG	4.6
1	A	245	ILE	4.4
1	B	0	SER	4.2
1	A	261	SER	4.1
1	A	130	ILE	4.0
1	A	242	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	268	GLY	3.9
1	A	256	SER	3.9
1	A	129	ARG	3.8
1	A	314	LEU	3.8
1	A	132	GLN	3.8
1	B	215	SER	3.8
1	A	224	ARG	3.8
1	B	277	ASP	3.8
1	A	126	PRO	3.7
1	A	302	GLY	3.7
1	A	269	ALA	3.6
1	A	210	THR	3.6
1	A	110	PHE	3.5
1	B	224	ARG	3.5
1	A	258	GLU	3.5
1	B	324	LEU	3.4
1	A	285	LEU	3.3
1	A	225	ILE	3.2
1	A	275	LEU	3.2
1	B	321	THR	3.1
1	A	300	HIS	3.1
1	A	310	THR	3.1
1	A	222	CYS	3.1
1	B	325	TYR	3.0
1	A	244	ALA	3.0
1	A	118	GLY	3.0
1	A	42	ALA	3.0
1	B	265	ARG	2.9
1	A	257	GLY	2.9
1	B	314	LEU	2.9
1	B	285	LEU	2.8
1	A	127	HIS	2.8
1	B	280	ALA	2.8
1	A	255	GLN	2.8
1	A	208	ASN	2.7
1	A	206	TRP	2.7
1	B	272	THR	2.7
1	B	317	LEU	2.7
1	A	121	LEU	2.6
1	A	319	ALA	2.6
1	A	202	TRP	2.6
1	B	222	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	109	PHE	2.5
1	B	259	ALA	2.4
1	B	157[A]	ARG	2.4
1	A	216	VAL	2.4
1	A	80	ALA	2.3
1	B	226	LEU	2.3
1	B	214	VAL	2.3
1	A	251	CYS	2.3
1	A	88	ILE	2.2
1	A	187	ALA	2.2
1	A	124	VAL	2.2
1	A	287	ILE	2.1
1	B	227	ASP	2.1
1	B	315	VAL	2.1
1	A	271	LYS	2.1
1	A	146	LEU	2.1
1	B	84	VAL	2.1
1	A	184	PHE	2.1
1	A	227	ASP	2.0
1	A	259	ALA	2.0
1	A	63	ALA	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.