



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:01 AM UTC

PDB ID : 3GHY / pdb_00003ghy
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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

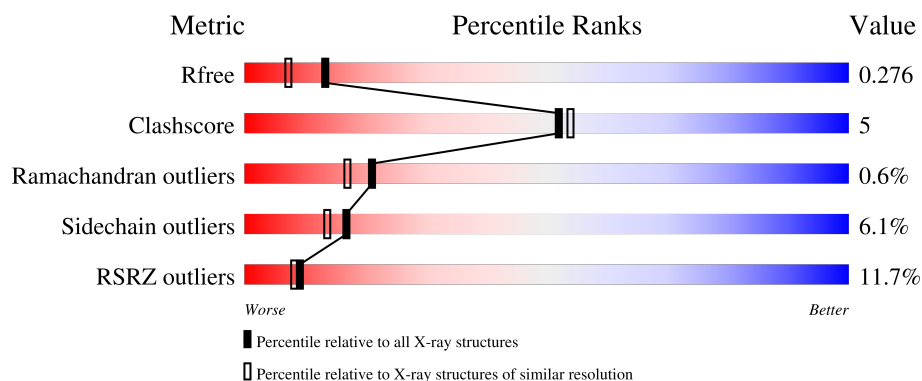
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	335	
1	B	335	

2 Entry composition

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
1	A	321	Total	C	N	O	S	0	4	0
			2364	1490	438	422	14			
1	B	321	Total	C	N	O	S	0	3	0
			2354	1479	437	425	13			

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

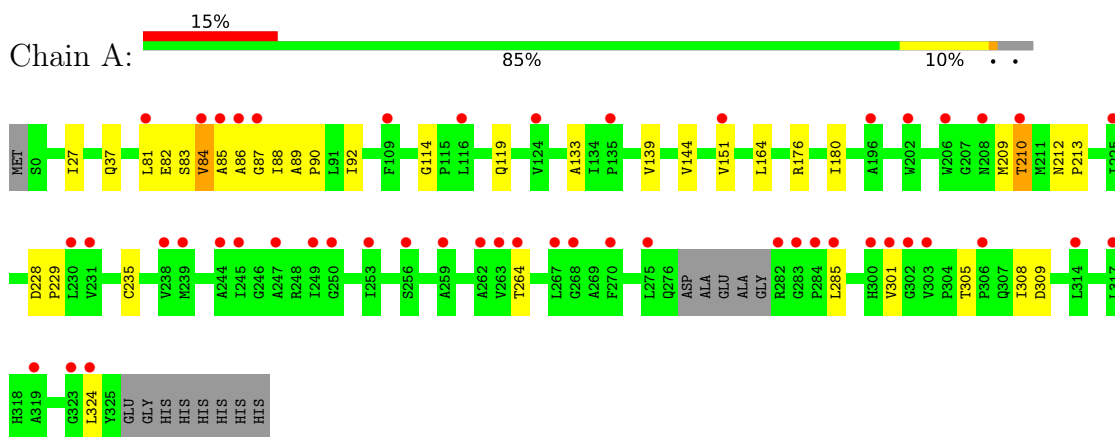
- Molecule 2 is water.

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

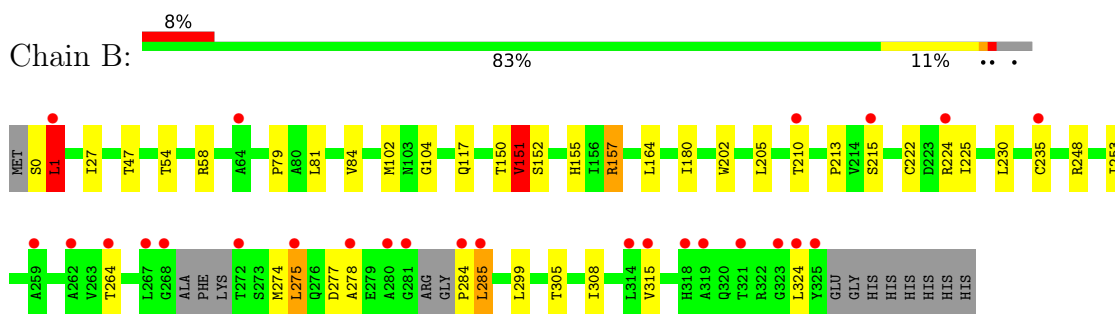
3 Residue-property plots [i](#)

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



- Molecule 1: Ketopantoate reductase protein



4 Data and refinement statistics

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 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.00) 99.8 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.231 , 0.278 0.231 , 0.276	Depositor DCC
R_{free} test set	1483 reflections (3.09%)	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 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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	0.56	0/2417	0.94	2/3290 (0.1%)
1	B	0.66	0/2402	0.97	0/3269
All	All	0.61	0/4819	0.95	2/6559 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	GLY	CA-C-N	6.09	126.45	119.93
1	A	114	GLY	C-N-CA	6.09	126.45	119.93

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	22	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	49	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 (49) 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: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:B:0:SER:O	1:B:1:LEU:HB2	2.10	0.50
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:81:LEU:HD22	1:B:102:MET:HE1	1.95	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:A:85:ALA:C	1:A:87:GLY:N	2.73	0.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:228:ASP:HA	1:A:229:PRO:HD3	1.82	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: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%)	21	17
1	B	318/335 (95%)	302 (95%)	14 (4%)	2 (1%)	21	17
All	All	639/670 (95%)	606 (95%)	29 (4%)	4 (1%)	21	17

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%)	20	17
1	B	239/247 (97%)	222 (93%)	17 (7%)	13	10
All	All	480/494 (97%)	450 (94%)	30 (6%)	17	13

All (30) 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	119	GLN
1	A	139	VAL
1	A	144	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	84	VAL
1	B	151	VAL
1	B	157[A]	ARG
1	B	157[B]	ARG
1	B	164	LEU
1	B	180	ILE
1	B	224	ARG
1	B	248	ARG
1	B	264	THR
1	B	275	LEU
1	B	277	ASP
1	B	285	LEU
1	B	299	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	307	GLN
1	A	320	GLN
1	B	190	GLN
1	B	255	GLN
1	B	307	GLN
1	B	320	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 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, 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%)	0.93	49 (15%) 5 4	28, 61, 96, 126	4 (1%)
1	B	321/335 (95%)	0.51	26 (8%) 18 17	25, 46, 85, 111	3 (0%)
All	All	642/670 (95%)	0.72	75 (11%) 9 8	25, 53, 94, 126	7 (1%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	319	ALA	7.9
1	B	215	SER	5.8
1	B	323	GLY	4.4
1	A	267	LEU	4.3
1	A	84	VAL	4.2
1	A	283	GLY	4.2
1	A	86	ALA	4.2
1	A	249	ILE	3.8
1	B	281	GLY	3.7
1	A	259	ALA	3.7
1	A	323	GLY	3.6
1	A	262	ALA	3.5
1	B	278	ALA	3.5
1	A	275	LEU	3.5
1	B	268	GLY	3.4
1	B	285	LEU	3.4
1	B	210	THR	3.4
1	A	270	PHE	3.3
1	B	272	THR	3.3
1	A	301	VAL	3.2
1	A	238	VAL	3.1
1	B	284	PRO	3.0
1	B	259	ALA	2.9
1	A	253	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	64	ALA	2.8
1	A	263	VAL	2.8
1	B	321	THR	2.8
1	B	267	LEU	2.8
1	B	324	LEU	2.8
1	A	85	ALA	2.8
1	A	245	ILE	2.8
1	B	318	HIS	2.7
1	A	247	ALA	2.7
1	A	116	LEU	2.7
1	A	314	LEU	2.7
1	A	151	VAL	2.7
1	A	324	LEU	2.6
1	B	1	LEU	2.6
1	B	235	CYS	2.4
1	B	314	LEU	2.4
1	A	264	THR	2.4
1	A	282	ARG	2.4
1	A	284	PRO	2.4
1	B	325	TYR	2.3
1	A	210	THR	2.3
1	A	196	ALA	2.3
1	A	109	PHE	2.3
1	A	124	VAL	2.3
1	A	306	PRO	2.3
1	A	230	LEU	2.3
1	B	315	VAL	2.3
1	A	208	ASN	2.3
1	A	317	LEU	2.3
1	B	275	LEU	2.3
1	A	268	GLY	2.2
1	B	262	ALA	2.2
1	A	239	MET	2.2
1	A	202	TRP	2.2
1	A	225	ILE	2.2
1	A	319	ALA	2.2
1	B	224	ARG	2.2
1	A	206	TRP	2.2
1	A	135	PRO	2.1
1	A	303	VAL	2.1
1	A	300	HIS	2.1
1	A	81	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	256	SER	2.1
1	A	250	GLY	2.1
1	B	280	ALA	2.1
1	B	264	THR	2.1
1	A	302	GLY	2.1
1	A	285	LEU	2.0
1	A	87	GLY	2.0
1	A	231	VAL	2.0
1	A	244	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 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.