



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:59 PM GMT

PDB ID : 1HQ6
Title : STRUCTURE OF PYRUVOYL-DEPENDENT HISTIDINE DECARBOXY-
LASE AT PH 8
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Deposited on : 2000-12-14
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

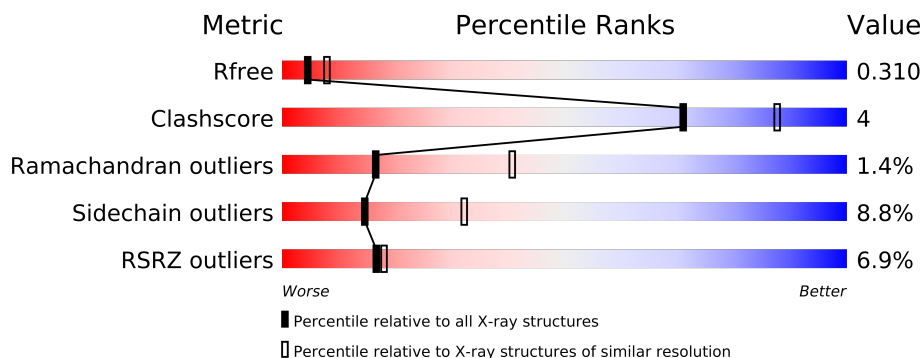
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance





The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	81	
1	C	81	
2	B	229	
2	D	229	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4600 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HISTIDINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	66	Total	C	N	O	S	0	0	0
			506	315	91	98	2			
1	C	66	Total	C	N	O	S	0	0	0
			506	315	91	98	2			

- Molecule 2 is a protein called HISTIDINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1776	1127	286	352	11			
2	D	229	Total	C	N	O	S	0	0	0
			1776	1127	286	352	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	PYR	SER	MODIFIED RESIDUE	UNP P00862
D	82	PYR	SER	MODIFIED RESIDUE	UNP P00862

- Molecule 3 is water.

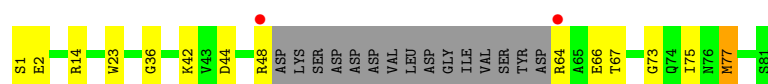
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	3	Total	O	0	0
			3	3		
3	C	10	Total	O	0	0
			10	10		
3	D	12	Total	O	0	0
			12	12		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

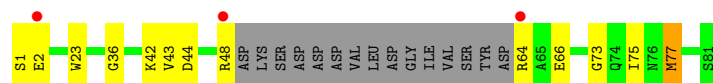
• Molecule 1: HISTIDINE DECARBOXYLASE

Chain A: 



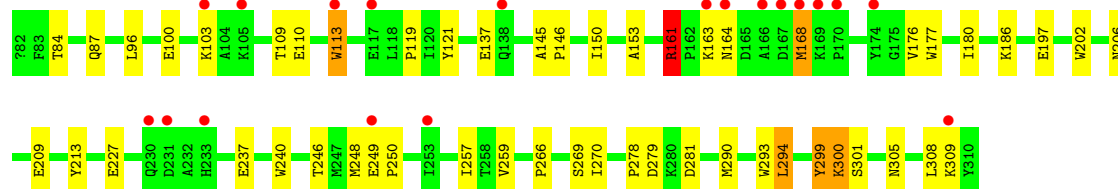
• Molecule 1: HISTIDINE DECARBOXYLASE

Chain C: 



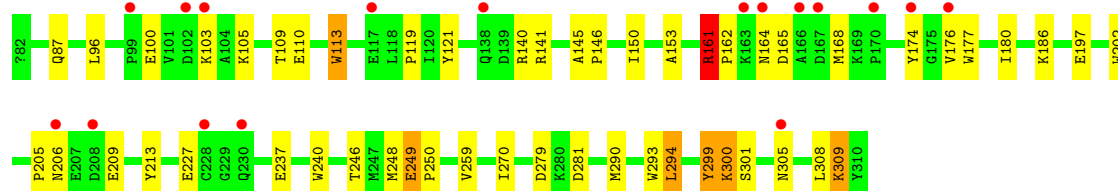
• Molecule 2: HISTIDINE DECARBOXYLASE

Chain B: 



• Molecule 2: HISTIDINE DECARBOXYLASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	117.43Å 117.43Å 241.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.00-2.70) 97.5 (19.81-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.15 (at 2.71Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.253 , 0.314 0.254 , 0.310	Depositor DCC
R_{free} test set	1717 reflections (9.84%)	DCC
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 17611 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4600	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PYR

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	0.79	0/512	1.52	7/687 (1.0%)
1	C	0.80	0/512	1.52	8/687 (1.2%)
2	B	0.77	0/1816	1.43	18/2463 (0.7%)
2	D	0.77	0/1816	1.43	21/2463 (0.9%)
All	All	0.77	0/4656	1.45	54/6300 (0.9%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	161	ARG	NE-CZ-NH2	9.11	124.86	120.30
1	C	23	TRP	CD1-CG-CD2	8.49	113.10	106.30
1	A	23	TRP	CD1-CG-CD2	8.37	112.99	106.30
2	D	202	TRP	CD1-CG-CD2	8.30	112.94	106.30
2	B	202	TRP	CD1-CG-CD2	8.22	112.88	106.30
2	B	177	TRP	CD1-CG-CD2	8.20	112.86	106.30
2	D	177	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	C	23	TRP	CE2-CD2-CG	-7.67	101.17	107.30
2	B	113	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	C	48	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	A	23	TRP	CE2-CD2-CG	-7.57	101.24	107.30
2	D	202	TRP	CE2-CD2-CG	-7.57	101.25	107.30
2	B	202	TRP	CE2-CD2-CG	-7.55	101.26	107.30
2	B	177	TRP	CE2-CD2-CG	-7.45	101.34	107.30
2	D	113	TRP	CD1-CG-CD2	7.44	112.25	106.30
2	B	299	TYR	CB-CG-CD2	-7.43	116.54	121.00
2	B	240	TRP	CE2-CD2-CG	-7.40	101.38	107.30
2	D	240	TRP	CE2-CD2-CG	-7.15	101.58	107.30
2	D	113	TRP	CE2-CD2-CG	-7.14	101.59	107.30
2	B	240	TRP	CD1-CG-CD2	7.08	111.97	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	177	TRP	CE2-CD2-CG	-6.90	101.78	107.30
2	D	240	TRP	CD1-CG-CD2	6.88	111.80	106.30
2	B	113	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	A	48	ARG	CA-CB-CG	6.50	127.69	113.40
2	B	293	TRP	CE2-CD2-CG	-6.49	102.11	107.30
2	B	293	TRP	CD1-CG-CD2	6.49	111.49	106.30
2	D	299	TYR	CB-CG-CD2	-6.48	117.11	121.00
2	B	213	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	C	48	ARG	CA-CB-CG	6.44	127.57	113.40
1	C	23	TRP	CG-CD2-CE3	6.19	139.47	133.90
2	D	213	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	A	23	TRP	CG-CD2-CE3	6.13	139.42	133.90
1	A	23	TRP	CG-CD1-NE1	-6.07	104.03	110.10
1	C	64	ARG	NE-CZ-NH1	-6.02	117.29	120.30
2	D	293	TRP	CE2-CD2-CG	-6.00	102.50	107.30
1	C	23	TRP	CG-CD1-NE1	-5.92	104.18	110.10
2	D	293	TRP	CD1-CG-CD2	5.88	111.01	106.30
2	B	161	ARG	NE-CZ-NH2	5.78	123.19	120.30
2	D	141	ARG	NE-CZ-NH1	-5.70	117.45	120.30
2	B	240	TRP	CG-CD2-CE3	5.66	138.99	133.90
2	D	240	TRP	CG-CD2-CE3	5.62	138.96	133.90
2	D	305	ASN	N-CA-C	-5.52	96.09	111.00
2	B	305	ASN	N-CA-C	-5.47	96.22	111.00
1	A	77	MET	CA-CB-CG	5.46	122.58	113.30
2	D	140	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	C	77	MET	CA-CB-CG	5.41	122.50	113.30
2	B	163	LYS	CA-C-N	-5.34	105.45	117.20
2	D	202	TRP	CB-CG-CD1	-5.27	120.15	127.00
2	D	202	TRP	CG-CD2-CE3	5.27	138.64	133.90
1	A	14	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	B	84	THR	N-CA-C	-5.11	97.19	111.00
2	D	177	TRP	CG-CD1-NE1	-5.07	105.03	110.10
2	D	153	ALA	N-CA-C	-5.05	97.36	111.00
2	B	153	ALA	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	506	0	511	5	0
1	C	506	0	511	3	0
2	B	1776	0	1706	19	0
2	D	1776	0	1706	20	0
3	A	11	0	0	0	0
3	B	3	0	0	0	0
3	C	10	0	0	0	0
3	D	12	0	0	1	0
All	All	4600	0	4434	40	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (40) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:96:LEU:HB3	2:D:290:MET:HE2	1.69	0.73
2:D:270:ILE:HD13	2:D:281:ASP:HB3	1.72	0.72
2:B:270:ILE:HD13	2:B:281:ASP:HB3	1.72	0.71
2:B:96:LEU:HB3	2:B:290:MET:HE2	1.74	0.70
2:B:161:ARG:HG2	2:B:250:PRO:HA	1.80	0.63
2:D:161:ARG:HG2	2:D:250:PRO:HA	1.81	0.63
2:D:180:ILE:HG13	2:D:197:GLU:HG2	1.82	0.62
2:D:105:LYS:HG3	3:D:18:HOH:O	2.01	0.60
2:B:180:ILE:HG13	2:B:197:GLU:HG2	1.84	0.58
1:C:36:GLY:HA2	2:D:87:GLN:HB3	1.89	0.54
1:A:42:LYS:HB3	2:B:259:VAL:HG13	1.89	0.53
1:C:42:LYS:HB3	2:D:259:VAL:HG13	1.91	0.52
1:A:36:GLY:HA2	2:B:87:GLN:HB3	1.91	0.52
2:B:206:ASN:HB3	2:B:209:GLU:HB2	1.90	0.52
2:D:294:LEU:HD12	2:D:299:TYR:HB2	1.94	0.49
2:D:206:ASN:HB3	2:D:209:GLU:HB2	1.94	0.48
2:D:96:LEU:HB3	2:D:290:MET:CE	2.43	0.48
2:D:100:GLU:HA	2:D:103:LYS:HD2	1.97	0.47
2:B:100:GLU:HA	2:B:103:LYS:HD2	1.99	0.45
2:D:300:LYS:NZ	2:D:300:LYS:H	2.13	0.45
2:B:294:LEU:HD12	2:B:299:TYR:HB2	1.99	0.44
2:B:300:LYS:H	2:B:300:LYS:NZ	2.15	0.44
2:B:109:THR:HG22	2:B:119:PRO:HA	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:278:PRO:O	2:B:281:ASP:HB2	2.17	0.43
1:A:64:ARG:N	1:A:67:THR:HG1	2.16	0.43
2:B:96:LEU:HB3	2:B:290:MET:CE	2.44	0.43
2:D:109:THR:HG22	2:D:119:PRO:HA	2.00	0.43
2:D:119:PRO:HB2	2:D:121:TYR:CE1	2.53	0.43
1:A:42:LYS:HE3	2:B:257:ILE:HD11	2.01	0.43
1:C:77:MET:HA	2:D:150:ILE:O	2.20	0.42
2:B:119:PRO:HB2	2:B:121:TYR:CE1	2.55	0.42
2:D:161:ARG:HH11	2:D:249:GLU:HA	1.84	0.42
1:A:77:MET:HA	2:B:150:ILE:O	2.19	0.42
2:B:266:PRO:O	2:B:269:SER:HB2	2.20	0.42
2:D:162:PRO:HG2	2:D:165:ASP:HB3	2.03	0.41
2:D:174:TYR:CD1	2:D:205:PRO:HB3	2.56	0.41
2:B:168:MET:HG3	2:B:168:MET:H	1.68	0.41
2:D:145:ALA:HA	2:D:146:PRO:HD2	1.95	0.41
2:B:145:ALA:HA	2:B:146:PRO:HD2	1.93	0.40
2:D:309:LYS:O	2:D:309:LYS:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	62/81 (76%)	58 (94%)	3 (5%)	1 (2%)	14	35
1	C	62/81 (76%)	59 (95%)	2 (3%)	1 (2%)	14	35
2	B	226/229 (99%)	205 (91%)	18 (8%)	3 (1%)	18	43
2	D	226/229 (99%)	205 (91%)	18 (8%)	3 (1%)	18	43
All	All	576/620 (93%)	527 (92%)	41 (7%)	8 (1%)	16	41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLY

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Mol	Chain	Res	Type
2	B	113	TRP
1	C	73	GLY
2	D	113	TRP
2	B	164	ASN
2	B	301	SER
2	D	164	ASN
2	D	301	SER

5.3.2 Protein sidechains ⓘ

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	52/66 (79%)	47 (90%)	5 (10%)	12	27
1	C	52/66 (79%)	46 (88%)	6 (12%)	8	19
2	B	188/188 (100%)	172 (92%)	16 (8%)	15	34
2	D	188/188 (100%)	173 (92%)	15 (8%)	17	37
All	All	480/508 (94%)	438 (91%)	42 (9%)	14	32

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	GLU
1	A	44	ASP
1	A	66	GLU
1	A	75	ILE
2	B	110	GLU
2	B	137	GLU
2	B	161	ARG
2	B	168	MET
2	B	176	VAL
2	B	186	LYS
2	B	227	GLU
2	B	237	GLU
2	B	246	THR
2	B	248	MET

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Mol	Chain	Res	Type
2	B	249	GLU
2	B	279	ASP
2	B	294	LEU
2	B	300	LYS
2	B	308	LEU
2	B	309	LYS
1	C	1	SER
1	C	2	GLU
1	C	43	VAL
1	C	44	ASP
1	C	66	GLU
1	C	75	ILE
2	D	110	GLU
2	D	161	ARG
2	D	168	MET
2	D	176	VAL
2	D	186	LYS
2	D	227	GLU
2	D	237	GLU
2	D	246	THR
2	D	248	MET
2	D	249	GLU
2	D	279	ASP
2	D	294	LEU
2	D	300	LYS
2	D	308	LEU
2	D	309	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	255	ASN
2	D	255	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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	66/81 (81%)	-0.08	2 (3%) 48 54	10, 23, 49, 80	0
1	C	66/81 (81%)	-0.10	3 (4%) 32 36	8, 24, 49, 81	0
2	B	229/229 (100%)	0.43	19 (8%) 11 12	13, 37, 61, 73	0
2	D	229/229 (100%)	0.42	17 (7%) 14 15	12, 37, 61, 73	0
All	All	590/620 (95%)	0.31	41 (6%) 17 18	8, 34, 61, 81	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	167	ASP	7.7
2	B	167	ASP	6.9
2	D	166	ALA	6.6
2	B	166	ALA	6.2
2	B	164	ASN	5.3
1	C	48	ARG	4.4
1	A	48	ARG	4.2
1	C	64	ARG	3.6
2	D	230	GLN	3.6
2	D	305	ASN	3.6
2	B	169	LYS	3.5
2	B	309	LYS	3.3
2	D	99	PRO	3.2
2	B	103	LYS	3.1
1	C	2	GLU	3.1
2	B	117	GLU	3.0
2	B	168	MET	3.0
2	D	164	ASN	2.9
2	D	170	PRO	2.9
2	B	230	GLN	2.9
2	B	174	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	170	PRO	2.7
2	D	103	LYS	2.7
2	B	163	LYS	2.6
2	B	249	GLU	2.6
2	D	163	LYS	2.5
2	D	176	VAL	2.5
2	D	174	TYR	2.5
2	B	253	ILE	2.5
2	D	138	GLN	2.5
2	D	208	ASP	2.4
2	D	117	GLU	2.4
1	A	64	ARG	2.4
2	B	231	ASP	2.3
2	B	105	LYS	2.2
2	B	113	TRP	2.2
2	B	138	GLN	2.2
2	D	228	CYS	2.1
2	B	233	HIS	2.0
2	D	102	ASP	2.0
2	D	206	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.