



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:51 pm BST

PDB ID : 4N8K  
Title : E249A mutant, RipA structure  
Authors : Torres, R.; Goulding, C.W.  
Deposited on : 2013-10-17  
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](mailto: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.

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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	:	2.11
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)	:	2.11

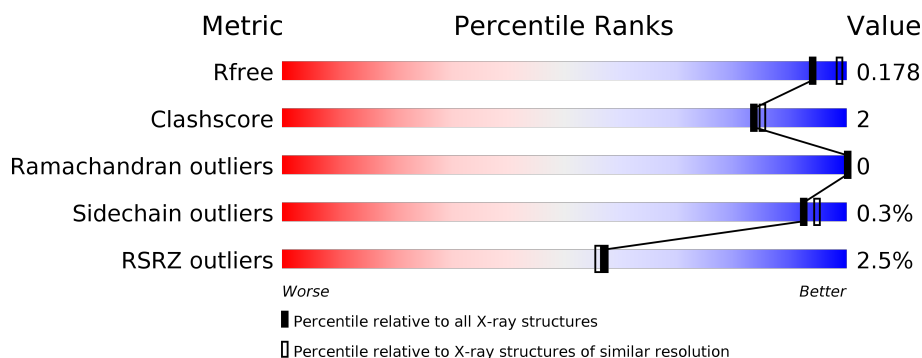
# 1 Overall quality at a glance

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))
$R_{free}$	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	476	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	476	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 14126 atoms, of which 6765 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 Putative 4-hydroxybutyrate coenzyme A transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	440	Total	C	H	N	O	S	0	0	0
			6779	2132	3383	610	637	17			
1	B	440	Total	C	H	N	O	S	0	0	0
			6778	2132	3382	610	637	17			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	INITIATING METHIONINE	UNP Q9ZC36
A	-34	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-33	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-32	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-31	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-30	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-29	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-28	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-27	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-26	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-25	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-24	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-23	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-22	LEU	-	EXPRESSION TAG	UNP Q9ZC36
A	-21	VAL	-	EXPRESSION TAG	UNP Q9ZC36
A	-20	PRO	-	EXPRESSION TAG	UNP Q9ZC36
A	-19	ARG	-	EXPRESSION TAG	UNP Q9ZC36
A	-18	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-17	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-16	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-15	MET	-	EXPRESSION TAG	UNP Q9ZC36
A	-14	ALA	-	EXPRESSION TAG	UNP Q9ZC36
A	-13	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-12	MET	-	EXPRESSION TAG	UNP Q9ZC36
A	-11	THR	-	EXPRESSION TAG	UNP Q9ZC36

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-9	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-8	GLN	-	EXPRESSION TAG	UNP Q9ZC36
A	-7	GLN	-	EXPRESSION TAG	UNP Q9ZC36
A	-6	MET	-	EXPRESSION TAG	UNP Q9ZC36
A	-5	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-4	ARG	-	EXPRESSION TAG	UNP Q9ZC36
A	-3	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-2	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-1	GLU	-	EXPRESSION TAG	UNP Q9ZC36
A	0	PHE	-	EXPRESSION TAG	UNP Q9ZC36
A	249	ALA	GLU	ENGINEERED MUTATION	UNP Q9ZC36
B	-35	MET	-	INITIATING METHIONINE	UNP Q9ZC36
B	-34	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-33	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-32	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-31	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-30	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-29	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-28	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-27	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-26	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-25	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-24	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-23	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-22	LEU	-	EXPRESSION TAG	UNP Q9ZC36
B	-21	VAL	-	EXPRESSION TAG	UNP Q9ZC36
B	-20	PRO	-	EXPRESSION TAG	UNP Q9ZC36
B	-19	ARG	-	EXPRESSION TAG	UNP Q9ZC36
B	-18	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-17	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-16	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-15	MET	-	EXPRESSION TAG	UNP Q9ZC36
B	-14	ALA	-	EXPRESSION TAG	UNP Q9ZC36
B	-13	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-12	MET	-	EXPRESSION TAG	UNP Q9ZC36
B	-11	THR	-	EXPRESSION TAG	UNP Q9ZC36
B	-10	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-9	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-8	GLN	-	EXPRESSION TAG	UNP Q9ZC36
B	-7	GLN	-	EXPRESSION TAG	UNP Q9ZC36
B	-6	MET	-	EXPRESSION TAG	UNP Q9ZC36

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-4	ARG	-	EXPRESSION TAG	UNP Q9ZC36
B	-3	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-2	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-1	GLU	-	EXPRESSION TAG	UNP Q9ZC36
B	0	PHE	-	EXPRESSION TAG	UNP Q9ZC36
B	249	ALA	GLU	ENGINEERED MUTATION	UNP Q9ZC36

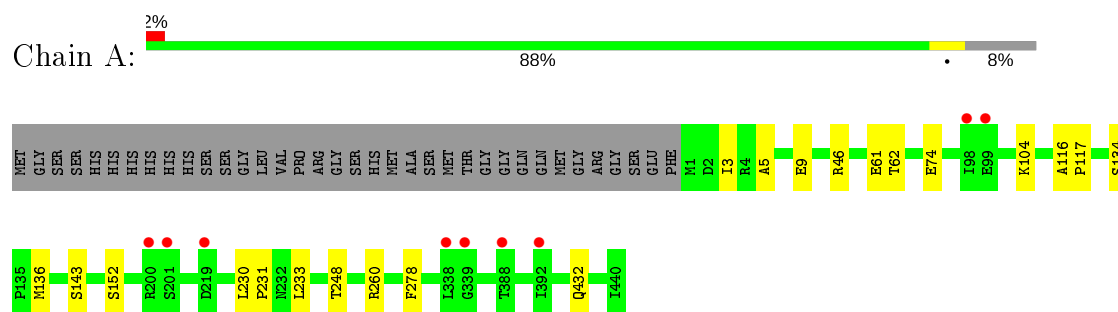
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	304	Total O 304 304	0	0
2	B	265	Total O 265 265	0	0

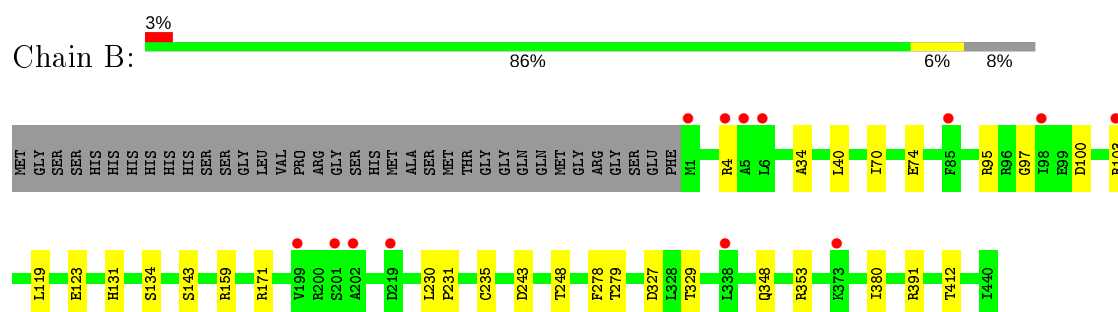
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Putative 4-hydroxybutyrate coenzyme A transferase



- Molecule 1: Putative 4-hydroxybutyrate coenzyme A transferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.18Å 108.18Å 84.99Å 90.00° 120.00° 90.00°	Depositor
Resolution (Å)	43.59 – 2.00 43.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.59-2.00) 99.2 (43.58-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.8.3_1479	Depositor
R, $R_{free}$	0.148 , 0.176 0.150 , 0.178	Depositor DCC
$R_{free}$ test set	2000 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14126	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.58	2/3461 (0.1%)	0.62	1/4696 (0.0%)
1	B	0.61	1/3461 (0.0%)	0.58	0/4696
All	All	0.60	3/6922 (0.0%)	0.60	1/9392 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	235	CYS	CB-SG	-8.45	1.67	1.82
1	A	152	SER	CB-OG	-5.23	1.35	1.42
1	A	61	GLU	CD-OE1	-5.09	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ARG	NE-CZ-NH2	-7.39	116.61	120.30

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	3396	3383	3401	13	0
1	B	3396	3382	3401	20	1
2	A	304	0	0	5	0
2	B	265	0	0	7	0
All	All	7361	6765	6802	32	1



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 2.

All (32) 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:432:GLN:NE2	2:A:728:HOH:O	2.26	0.68
1:B:243:ASP:OD1	2:B:755:HOH:O	2.14	0.65
1:B:353:ARG:NH1	2:B:693:HOH:O	2.32	0.63
1:B:4:ARG:HB3	1:B:4:ARG:CZ	2.29	0.63
1:B:74:GLU:OE2	2:B:699:HOH:O	2.16	0.62
1:A:260:ARG:NH2	2:A:758:HOH:O	2.32	0.62
1:B:4:ARG:HB3	1:B:4:ARG:NH1	2.16	0.61
1:B:329:THR:HB	1:B:391:ARG:HD3	1.89	0.54
1:B:171:ARG:NH1	2:B:633:HOH:O	2.44	0.51
1:B:159:ARG:NH2	2:B:744:HOH:O	2.46	0.49
1:B:348:GLN:NE2	2:B:525:HOH:O	2.43	0.49
1:B:119:LEU:HD12	1:B:123:GLU:HG3	1.95	0.48
1:B:95:ARG:NH1	2:B:678:HOH:O	2.36	0.47
1:B:230:LEU:HB3	1:B:231:PRO:HD3	1.97	0.47
1:B:34:ALA:HB1	1:B:131:HIS:CE1	2.50	0.46
1:B:40:LEU:HD22	1:B:70:ILE:HD13	1.97	0.46
1:A:74:GLU:OE2	2:A:637:HOH:O	2.20	0.46
1:A:5:ALA:O	1:A:9:GLU:HG3	2.15	0.46
1:B:97:GLY:O	1:B:103:ARG:HG2	2.16	0.46
1:A:104:LYS:HE2	1:B:412:THR:OG1	2.16	0.45
1:A:3:ILE:HD11	2:A:802:HOH:O	2.15	0.45
1:A:3:ILE:HG23	1:A:136:MET:HE1	1.98	0.45
1:B:327:ASP:HA	1:B:380:ILE:O	2.17	0.45
1:A:233:LEU:O	2:A:685:HOH:O	2.21	0.44
1:B:248:THR:O	1:B:278:PHE:HA	2.18	0.43
1:A:134:SER:OG	1:A:143:SER:HB3	2.19	0.43
1:A:3:ILE:HG23	1:A:136:MET:CE	2.50	0.42
1:A:116:ALA:N	1:A:117:PRO:CD	2.83	0.41
1:A:230:LEU:HB3	1:A:231:PRO:HD3	2.02	0.41
1:A:248:THR:O	1:A:278:PHE:HA	2.20	0.41
1:B:134:SER:OG	1:B:143:SER:HB3	2.20	0.41
1:B:100:ASP:OD2	1:B:103:ARG:NH1	2.41	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ARG:NE	1:B:4:ARG:NE[2_655]	1.78	0.42

## 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	438/476 (92%)	424 (97%)	14 (3%)	0	100	100
1	B	438/476 (92%)	426 (97%)	12 (3%)	0	100	100
All	All	876/952 (92%)	850 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	365/393 (93%)	364 (100%)	1 (0%)	92	95
1	B	365/393 (93%)	364 (100%)	1 (0%)	92	95
All	All	730/786 (93%)	728 (100%)	2 (0%)	92	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	THR
1	B	279	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	440/476 (92%)	-0.35	9 (2%) 65 63	19, 28, 58, 84	0
1	B	440/476 (92%)	-0.21	13 (2%) 50 49	19, 32, 64, 102	0
All	All	880/952 (92%)	-0.28	22 (2%) 57 56	19, 30, 61, 102	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	LEU	4.6
1	A	201	SER	3.9
1	B	98	ILE	3.6
1	B	1	MET	3.1
1	B	199	VAL	2.8
1	A	338	LEU	2.8
1	A	200	ARG	2.7
1	A	219	ASP	2.7
1	B	373	LYS	2.6
1	A	99	GLU	2.6
1	B	219	ASP	2.6
1	B	5	ALA	2.5
1	A	98	ILE	2.5
1	B	6	LEU	2.4
1	B	202	ALA	2.4
1	B	103	ARG	2.4
1	B	4	ARG	2.3
1	A	339	GLY	2.2
1	B	85	PHE	2.2
1	A	392	ILE	2.1
1	A	388	THR	2.1
1	B	201	SER	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 carbohydrates 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.