



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:10 am BST

PDB ID : 6DEU  
Title : Human caspase-6 A109T  
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Deposited on : 2018-05-13  
Resolution : 2.80 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

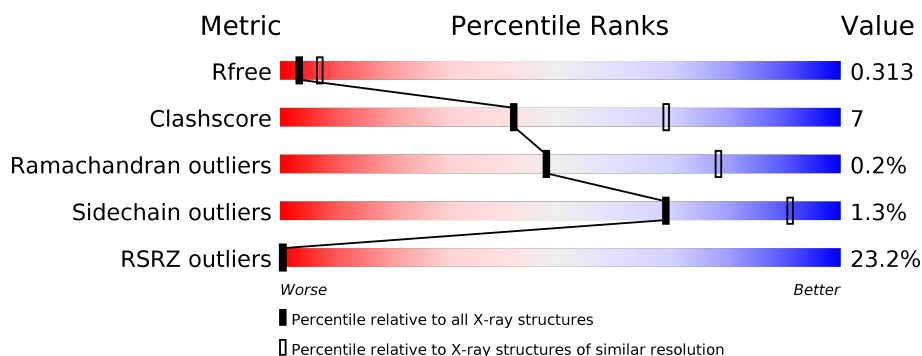
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	302	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>9%</div> <div>25%</div> </div> </div>
1	B	302	<div> <div>28%</div> <div> <div></div> <div>52%</div> <div>20%</div> <div>28%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7155 atoms, of which 3555 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 Caspase-6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	226	Total	C	H	N	O	S	0	0	0
			3632	1171	1806	315	326	14			
1	B	218	Total	C	H	N	O	S	0	0	0
			3511	1128	1749	307	314	13			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P55212
A	1	ALA	-	expression tag	UNP P55212
A	109	THR	ALA	engineered mutation	UNP P55212
A	294	LEU	-	expression tag	UNP P55212
A	295	GLU	-	expression tag	UNP P55212
A	296	HIS	-	expression tag	UNP P55212
A	297	HIS	-	expression tag	UNP P55212
A	298	HIS	-	expression tag	UNP P55212
A	299	HIS	-	expression tag	UNP P55212
A	300	HIS	-	expression tag	UNP P55212
A	301	HIS	-	expression tag	UNP P55212
B	0	MET	-	initiating methionine	UNP P55212
B	1	ALA	-	expression tag	UNP P55212
B	109	THR	ALA	engineered mutation	UNP P55212
B	294	LEU	-	expression tag	UNP P55212
B	295	GLU	-	expression tag	UNP P55212
B	296	HIS	-	expression tag	UNP P55212
B	297	HIS	-	expression tag	UNP P55212
B	298	HIS	-	expression tag	UNP P55212
B	299	HIS	-	expression tag	UNP P55212
B	300	HIS	-	expression tag	UNP P55212
B	301	HIS	-	expression tag	UNP P55212

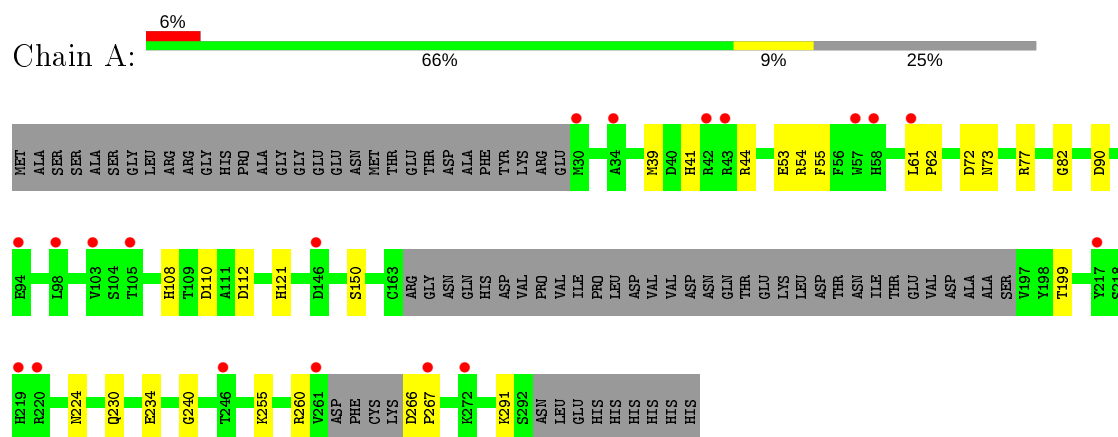
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total 9	O 9	0	0
2	B	3	Total 3	O 3	0	0

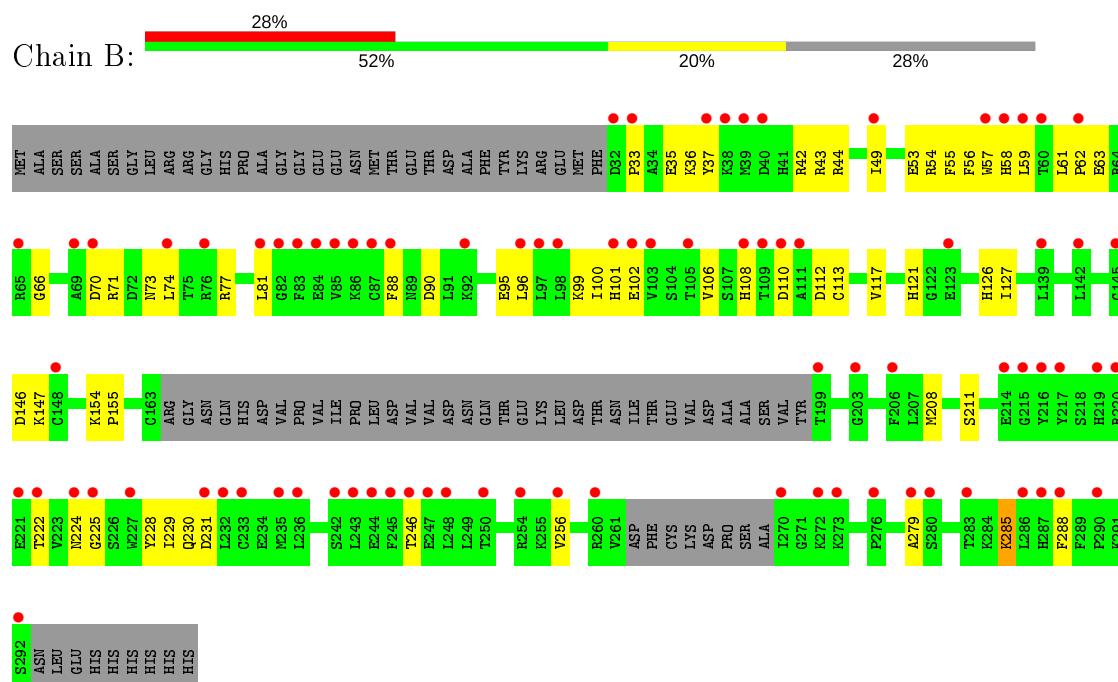
### 3 Residue-property plots [i](#)

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: Caspase-6



#### • Molecule 1: Caspase-6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.11Å 63.93Å 86.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.08 – 2.80 43.27 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.1 (39.08-2.80) 84.3 (43.27-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.85 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.267 , 0.312 0.268 , 0.313	Depositor DCC
$R_{free}$ test set	1158 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 65.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	7155	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.63% 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

### 5.1 Standard geometry

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	0.26	0/1869	0.45	0/2514
1	B	0.28	0/1802	0.47	0/2422
All	All	0.27	0/3671	0.46	0/4936

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

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	1826	1806	1805	15	2
1	B	1762	1749	1748	35	0
2	A	9	0	0	1	0
2	B	3	0	0	1	0
All	All	3600	3555	3553	50	2

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 (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:108:HIS:O	1:B:154:LYS:NZ	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:MET:O	1:A:291:LYS:NZ	2.21	0.72
1:A:112:ASP:OD2	1:A:291:LYS:NZ	2.22	0.68
1:A:240:GLY:O	2:A:401:HOH:O	2.13	0.66
1:B:246:THR:OG1	2:B:401:HOH:O	2.16	0.61
1:B:146:ASP:OD1	1:B:147:LYS:NZ	2.34	0.60
1:A:234:GLU:OE1	1:A:255:LYS:NZ	2.36	0.58
1:B:73:ASN:ND2	1:B:230:GLN:OE1	2.37	0.57
1:B:57:TRP:O	1:B:58:HIS:ND1	2.37	0.57
1:B:222:THR:OG1	1:B:224:ASN:OD1	2.25	0.53
1:B:36:LYS:HA	1:B:285:LYS:O	2.10	0.52
1:B:113:CYS:HB2	1:B:155:PRO:HG2	1.91	0.52
1:B:88:PHE:CZ	1:B:99:LYS:HE2	2.46	0.51
1:B:231:ASP:HB2	1:B:256:VAL:HG22	1.94	0.49
1:B:42:ARG:NH2	1:B:110:ASP:OD2	2.41	0.49
1:A:73:ASN:O	1:A:77:ARG:HG2	2.13	0.48
1:B:49:ILE:HG21	1:B:71:ARG:HG3	1.94	0.48
1:B:35:GLU:O	1:B:285:LYS:HG2	2.14	0.48
1:B:54:ARG:HE	1:B:90:ASP:HB2	1.77	0.48
1:A:61:LEU:N	1:A:62:PRO:HD2	2.28	0.47
1:B:61:LEU:N	1:B:62:PRO:HD2	2.29	0.47
1:A:54:ARG:HE	1:A:90:ASP:HB2	1.80	0.47
1:B:37:TYR:CD2	1:B:155:PRO:HD3	2.48	0.47
1:B:74:LEU:HD11	1:B:229:ILE:HG23	1.98	0.46
1:B:113:CYS:CB	1:B:155:PRO:HG2	2.46	0.46
1:B:53:GLU:OE1	1:B:121:HIS:NE2	2.46	0.46
1:B:96:LEU:O	1:B:100:ILE:N	2.35	0.45
1:A:266:ASP:N	1:A:267:PRO:CD	2.80	0.45
1:B:44:ARG:O	1:B:113:CYS:N	2.49	0.44
1:A:53:GLU:OE1	1:A:121:HIS:NE2	2.42	0.44
1:B:54:ARG:HD2	1:B:55:PHE:CE2	2.53	0.43
1:B:59:LEU:HD22	1:B:63:GLU:HB3	1.98	0.43
1:B:126:HIS:CD2	1:B:127:ILE:HG13	2.54	0.43
1:A:44:ARG:HB3	1:A:82:GLY:O	2.19	0.43
1:A:73:ASN:ND2	1:A:230:GLN:OE1	2.52	0.43
1:A:41:HIS:HB3	1:A:110:ASP:O	2.19	0.43
1:B:43:ARG:O	1:B:112:ASP:N	2.52	0.42
1:B:62:PRO:O	1:B:66:GLY:HA3	2.20	0.42
1:B:70:ASP:O	1:B:74:LEU:HD13	2.19	0.42
1:A:108:HIS:H	1:A:150:SER:HB3	1.84	0.42
1:B:95:GLU:O	1:B:99:LYS:HG2	2.19	0.42
1:B:208:MET:O	1:B:279:ALA:N	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLU:O	1:B:106:VAL:HG23	2.21	0.41
1:B:74:LEU:CD2	1:B:117:VAL:HG11	2.51	0.41
1:B:113:CYS:HA	1:B:155:PRO:HD2	2.02	0.41
1:B:81:LEU:HD22	1:B:288:PHE:HB3	2.03	0.41
1:A:54:ARG:HD2	1:A:55:PHE:CE2	2.57	0.40
1:B:211:SER:HA	1:B:228:TYR:CG	2.57	0.40
1:A:199:THR:O	1:A:199:THR:HG22	2.21	0.40
1:B:224:ASN:OD1	1:B:225:GLY:N	2.55	0.40

All (2) 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:A:72:ASP:OD2	1:A:260:ARG:NH1[3_747]	2.12	0.08
1:A:72:ASP:OD2	1:A:260:ARG:HH12[3_747]	1.54	0.06

## 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	220/302 (73%)	212 (96%)	8 (4%)	0	100	100
1	B	212/302 (70%)	202 (95%)	9 (4%)	1 (0%)	29	61
All	All	432/604 (72%)	414 (96%)	17 (4%)	1 (0%)	47	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	PRO

### 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	199/264 (75%)	198 (100%)	1 (0%)	88	96
1	B	192/264 (73%)	188 (98%)	4 (2%)	53	84
All	All	391/528 (74%)	386 (99%)	5 (1%)	69	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	B	56	PHE
1	B	77	ARG
1	B	101	HIS
1	B	285	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	B	73	ASN
1	B	230	GLN

### 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	226/302 (74%)	0.65	19 (8%) 11 5	8, 42, 82, 98	0
1	B	218/302 (72%)	1.85	84 (38%) 0 0	41, 77, 107, 119	0
All	All	444/604 (73%)	1.24	103 (23%) 0 0	8, 62, 101, 119	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	LEU	8.9
1	B	59	LEU	8.2
1	B	65	ARG	5.7
1	B	97	LEU	5.6
1	B	74	LEU	5.2
1	B	214	GLU	4.9
1	B	32	ASP	4.6
1	B	40	ASP	4.6
1	B	270	ILE	4.6
1	B	33	PRO	4.5
1	B	111	ALA	4.3
1	B	105	THR	4.2
1	B	217	TYR	4.1
1	B	76	ARG	4.1
1	B	215	GLY	4.1
1	B	224	ASN	4.1
1	A	146	ASP	4.1
1	B	216	TYR	3.9
1	A	217	TYR	3.9
1	B	231	ASP	3.9
1	B	101	HIS	3.8
1	B	39	MET	3.8
1	B	199	THR	3.7
1	B	232	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	108	HIS	3.5
1	B	109	THR	3.5
1	B	123	GLU	3.4
1	B	288	PHE	3.4
1	B	292	SER	3.4
1	B	96	LEU	3.4
1	B	37	TYR	3.3
1	A	98	LEU	3.3
1	B	49	ILE	3.3
1	B	221	GLU	3.3
1	B	60	THR	3.1
1	B	235	MET	3.1
1	B	85	VAL	3.1
1	B	84	GLU	3.0
1	B	219	HIS	2.9
1	B	81	LEU	2.9
1	A	267	PRO	2.9
1	B	148	CYS	2.9
1	A	220	ARG	2.8
1	B	86	LYS	2.8
1	B	83	PHE	2.8
1	B	103	VAL	2.8
1	B	88	PHE	2.8
1	B	220	ARG	2.8
1	A	58	HIS	2.7
1	B	247	GLU	2.7
1	B	248	LEU	2.7
1	A	272	LYS	2.7
1	A	42	ARG	2.7
1	B	38	LYS	2.7
1	B	82	GLY	2.7
1	B	87	CYS	2.7
1	B	62	PRO	2.6
1	B	58	HIS	2.6
1	B	290	PRO	2.6
1	B	286	LEU	2.6
1	B	280	SER	2.6
1	B	276	PRO	2.6
1	B	227	TRP	2.5
1	B	279	ALA	2.5
1	A	261	VAL	2.5
1	B	222	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	203	GLY	2.5
1	B	70	ASP	2.5
1	B	256	VAL	2.5
1	B	69	ALA	2.5
1	B	102	GLU	2.5
1	A	219	HIS	2.4
1	B	245	PHE	2.4
1	A	105	THR	2.4
1	B	225	GLY	2.4
1	B	236	LEU	2.4
1	B	283	THR	2.4
1	B	250	THR	2.4
1	B	272	LYS	2.4
1	B	254	ARG	2.4
1	B	233	CYS	2.3
1	B	142	LEU	2.3
1	B	246	THR	2.3
1	B	242	SER	2.3
1	A	43	ARG	2.3
1	A	103	VAL	2.3
1	B	287	HIS	2.2
1	A	94	GLU	2.2
1	B	244	GLU	2.2
1	B	92	LYS	2.2
1	B	273	LYS	2.2
1	B	243	LEU	2.2
1	B	260	ARG	2.2
1	B	139	LEU	2.2
1	A	30	MET	2.1
1	A	61	LEU	2.1
1	B	110	ASP	2.1
1	B	206	PHE	2.1
1	A	34	ALA	2.1
1	B	57	TRP	2.0
1	B	145	GLY	2.0
1	A	246	THR	2.0
1	A	57	TRP	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 [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.