



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 10:00 PM EDT

PDB ID : 1C93  
Title : Endo-Beta-N-Acetylglucosaminidase H, D130N/E132Q Double Mutant  
Authors : Rao, V.; Cui, T.; Guan, C.; Van Roey, P.  
Deposited on : unknown  
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

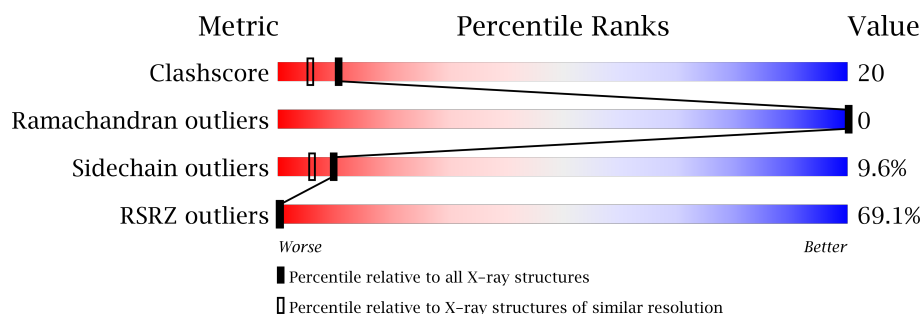
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.10 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))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. 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	265	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2140 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 ENDO-BETA-N-ACETYLGLUCOSAMINIDASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2016	1266	349	399	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	GLN	GLU	ENGINEERED	UNP P04067
A	130	ASN	ASP	ENGINEERED	UNP P04067

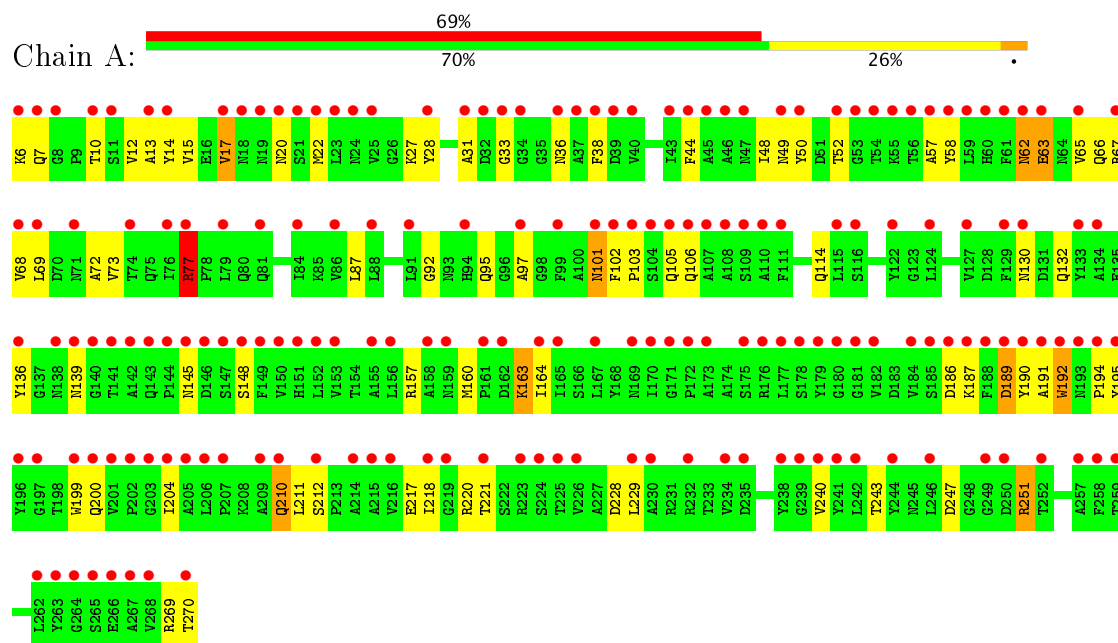
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	124	Total	O	0	0
			124	124		

### 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 ( $\text{RSRZ} > 2$ ). 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: ENDO-BETA-N-ACETYLGLUCOSAMINIDASE H



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.30Å 55.50Å 46.70Å 90.00° 104.50° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 45.21 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.10) 95.6 (45.21-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.05 (at 2.10Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.200 , (Not available) 0.360 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	10.5	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 67.3	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	0.68	EDS
Total number of atoms	2140	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.95% 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	0.64	0/2058	0.85	0/2803

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	77	ARG	Sidechain

### 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	2016	0	1935	81	1
2	A	124	0	0	4	2
All	All	2140	0	1935	81	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 20.

All (81) 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:72:ALA:HB1	1:A:77:ARG:CZ	1.90	1.01
1:A:17:VAL:HG21	1:A:65:VAL:HG22	1.47	0.97
1:A:72:ALA:HB1	1:A:77:ARG:NH2	1.83	0.93
1:A:73:VAL:HA	1:A:77:ARG:HD3	1.49	0.93
1:A:62:ASN:HD22	1:A:65:VAL:HG23	1.35	0.89
1:A:62:ASN:ND2	1:A:65:VAL:HG23	1.96	0.80
1:A:72:ALA:CB	1:A:77:ARG:NH1	2.49	0.76
1:A:17:VAL:HG13	1:A:22:MET:HE3	1.72	0.71
1:A:17:VAL:HG12	1:A:68:VAL:HG21	1.71	0.71
1:A:72:ALA:HB1	1:A:77:ARG:NH1	2.05	0.71
1:A:73:VAL:CA	1:A:77:ARG:HD3	2.21	0.70
1:A:72:ALA:CB	1:A:77:ARG:CZ	2.69	0.70
1:A:17:VAL:HG22	1:A:44:PHE:O	1.92	0.70
1:A:101:ASN:ND2	1:A:136:TYR:HD2	1.91	0.69
1:A:77:ARG:N	1:A:77:ARG:HD2	2.09	0.67
1:A:221:THR:HG22	2:A:388:HOH:O	1.94	0.66
1:A:77:ARG:H	1:A:77:ARG:HD2	1.61	0.65
1:A:72:ALA:O	1:A:77:ARG:HD2	1.97	0.64
1:A:101:ASN:ND2	1:A:136:TYR:CD2	2.67	0.62
1:A:12:VAL:O	1:A:243:THR:HB	2.01	0.61
1:A:52:THR:HG22	1:A:139:ASN:HB3	1.82	0.60
1:A:212:SER:HB2	1:A:240:VAL:HB	1.84	0.60
1:A:72:ALA:HB3	1:A:77:ARG:NH1	2.16	0.59
1:A:72:ALA:O	1:A:77:ARG:CD	2.52	0.58
1:A:58:TYR:HA	1:A:114:GLN:HE22	1.68	0.58
1:A:62:ASN:ND2	1:A:65:VAL:H	2.02	0.57
1:A:17:VAL:CG1	1:A:22:MET:HE3	2.34	0.57
1:A:191:ALA:HB3	1:A:211:LEU:CD2	2.35	0.57
1:A:15:VAL:HB	1:A:22:MET:SD	2.45	0.56
1:A:66:GLN:HG3	1:A:67:ARG:HH11	1.71	0.55
1:A:73:VAL:HA	1:A:77:ARG:CD	2.32	0.55
1:A:101:ASN:CG	1:A:136:TYR:HD2	2.10	0.55
1:A:145:ASN:OD1	1:A:148:SER:HB2	2.06	0.54
1:A:17:VAL:HG13	1:A:22:MET:CE	2.36	0.54
1:A:72:ALA:C	1:A:77:ARG:HD3	2.29	0.53
1:A:218:ILE:CG2	1:A:251:ARG:HG2	2.39	0.52
1:A:218:ILE:HG12	1:A:243:THR:HG23	1.91	0.52
1:A:73:VAL:O	1:A:77:ARG:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:O	1:A:210:GLN:HB2	2.09	0.51
1:A:28:TYR:CE2	1:A:269:ARG:HB2	2.45	0.51
1:A:217:GLU:H	1:A:221:THR:CG2	2.24	0.51
1:A:194:PRO:HG2	1:A:195:TYR:CE1	2.46	0.50
1:A:50:TYR:H	1:A:95:GLN:NE2	2.09	0.50
1:A:87:LEU:HD21	1:A:164:ILE:CG2	2.41	0.50
1:A:48:ILE:O	1:A:48:ILE:HG23	2.11	0.50
1:A:157:ARG:NH1	1:A:163:LYS:O	2.39	0.49
1:A:63:GLU:O	1:A:67:ARG:HG2	2.13	0.48
1:A:190:TYR:HA	1:A:210:GLN:O	2.14	0.48
1:A:12:VAL:HG21	1:A:192:TRP:CZ3	2.49	0.48
1:A:73:VAL:HG23	2:A:293:HOH:O	2.13	0.48
1:A:73:VAL:N	1:A:77:ARG:HD3	2.27	0.48
1:A:17:VAL:CG2	1:A:65:VAL:HG22	2.34	0.48
1:A:48:ILE:HG22	1:A:92:GLY:HA2	1.96	0.47
1:A:199:TRP:HB2	1:A:229:LEU:CD2	2.45	0.47
1:A:62:ASN:HD22	1:A:65:VAL:CG2	2.19	0.46
1:A:14:TYR:HD1	1:A:44:PHE:HD1	1.63	0.45
1:A:15:VAL:HB	1:A:22:MET:CE	2.47	0.45
1:A:13:ALA:HB2	1:A:38:PHE:CD1	2.53	0.45
1:A:49:ASN:O	1:A:57:ALA:HA	2.17	0.44
1:A:160:MET:HB2	1:A:163:LYS:HB2	2.00	0.44
1:A:31:ALA:C	1:A:33:GLY:H	2.20	0.44
1:A:27:LYS:O	1:A:269:ARG:HA	2.18	0.43
1:A:102:PHE:N	1:A:148:SER:OG	2.51	0.43
1:A:17:VAL:CG1	1:A:68:VAL:HG21	2.43	0.43
1:A:50:TYR:CD1	1:A:97:ALA:HB2	2.54	0.43
1:A:102:PHE:HA	1:A:103:PRO:HD3	1.86	0.43
1:A:157:ARG:NH2	1:A:187:LYS:O	2.48	0.42
1:A:57:ALA:HB2	1:A:97:ALA:HB1	2.01	0.42
1:A:36:ASN:HB3	2:A:275:HOH:O	2.18	0.42
1:A:221:THR:CG2	2:A:388:HOH:O	2.62	0.42
1:A:130:ASN:OD1	1:A:132:GLN:HG3	2.20	0.42
1:A:87:LEU:HD21	1:A:164:ILE:HG22	2.01	0.42
1:A:269:ARG:HG2	1:A:270:THR:N	2.34	0.42
1:A:191:ALA:HB3	1:A:211:LEU:HD23	2.02	0.41
1:A:217:GLU:H	1:A:221:THR:HG23	1.85	0.41
1:A:101:ASN:CG	1:A:136:TYR:CD2	2.91	0.41
1:A:20:ASN:ND2	1:A:247:ASP:CB	2.84	0.41
1:A:87:LEU:HD21	1:A:164:ILE:HG21	2.03	0.41
1:A:218:ILE:CG1	1:A:243:THR:HG23	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:HA	1:A:163:LYS:HD2	1.87	0.40
1:A:192:TRP:HB3	1:A:212:SER:HB3	2.03	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:228:ASP:OD1	2:A:353:HOH:O[2_748]	2.13	0.07
2:A:334:HOH:O	2:A:370:HOH:O[2_858]	2.16	0.04

## 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	263/265 (99%)	251 (95%)	12 (5%)	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	208/208 (100%)	188 (90%)	20 (10%)	10	6

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	7	GLN
1	A	10	THR
1	A	17	VAL
1	A	62	ASN
1	A	63	GLU
1	A	69	LEU
1	A	77	ARG
1	A	101	ASN
1	A	105	GLN
1	A	106	GLN
1	A	163	LYS
1	A	186	ASP
1	A	189	ASP
1	A	192	TRP
1	A	200	GLN
1	A	204	ILE
1	A	210	GLN
1	A	220	ARG
1	A	251	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	20	ASN
1	A	36	ASN
1	A	62	ASN
1	A	82	GLN
1	A	93	ASN
1	A	95	GLN
1	A	101	ASN
1	A	105	GLN
1	A	114	GLN
1	A	139	ASN
1	A	159	ASN
1	A	200	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates 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, 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	265/265 (100%)	2.61	183 (69%) <b>0</b> <b>0</b>	9, 16, 28, 55	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ILE	7.9
1	A	181	GLY	7.5
1	A	182	VAL	6.9
1	A	97	ALA	6.9
1	A	179	TYR	6.0
1	A	77	ARG	6.0
1	A	203	GLY	5.7
1	A	205	ALA	5.6
1	A	34	GLY	5.3
1	A	170	ILE	5.2
1	A	207	PRO	5.1
1	A	7	GLN	5.0
1	A	252	THR	4.8
1	A	84	ILE	4.8
1	A	53	GLY	4.6
1	A	206	LEU	4.6
1	A	103	PRO	4.6
1	A	190	TYR	4.6
1	A	229	LEU	4.6
1	A	38	PHE	4.5
1	A	149	PHE	4.5
1	A	216	VAL	4.4
1	A	58	TYR	4.4
1	A	264	GLY	4.3
1	A	192	TRP	4.2
1	A	200	GLN	4.2
1	A	241	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	91	LEU	4.1
1	A	180	GLY	4.1
1	A	18	ASN	4.0
1	A	257	ALA	4.0
1	A	178	SER	3.9
1	A	106	GLN	3.9
1	A	238	TYR	3.9
1	A	107	ALA	3.8
1	A	196	TYR	3.8
1	A	31	ALA	3.8
1	A	209	ALA	3.7
1	A	184	VAL	3.7
1	A	6	LYS	3.7
1	A	74	THR	3.7
1	A	202	PRO	3.6
1	A	59	LEU	3.6
1	A	270	THR	3.6
1	A	268	VAL	3.6
1	A	249	GLY	3.5
1	A	263	TYR	3.5
1	A	195	TYR	3.5
1	A	259	THR	3.4
1	A	116	SER	3.4
1	A	133	TYR	3.4
1	A	79	LEU	3.4
1	A	76	ILE	3.3
1	A	199	TRP	3.3
1	A	240	VAL	3.3
1	A	124	LEU	3.3
1	A	13	ALA	3.3
1	A	11	SER	3.2
1	A	56	THR	3.2
1	A	150	VAL	3.2
1	A	62	ASN	3.2
1	A	134	ALA	3.2
1	A	57	ALA	3.2
1	A	212	SER	3.2
1	A	111	PHE	3.2
1	A	167	LEU	3.2
1	A	136	TYR	3.2
1	A	99	PHE	3.1
1	A	129	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	188	PHE	3.1
1	A	101	ASN	3.1
1	A	246	LEU	3.1
1	A	25	VAL	3.1
1	A	234	VAL	3.1
1	A	141	THR	3.1
1	A	14	TYR	3.1
1	A	165	ILE	3.1
1	A	169	ASN	3.0
1	A	43	ILE	3.0
1	A	226	VAL	3.0
1	A	161	PRO	3.0
1	A	109	SER	3.0
1	A	127	VAL	3.0
1	A	162	ASP	3.0
1	A	187	LYS	3.0
1	A	258	PHE	3.0
1	A	244	TYR	3.0
1	A	138	ASN	3.0
1	A	267	ALA	3.0
1	A	19	ASN	3.0
1	A	54	THR	2.9
1	A	102	PHE	2.9
1	A	148	SER	2.9
1	A	215	ALA	2.9
1	A	33	GLY	2.9
1	A	22	MET	2.9
1	A	214	ALA	2.9
1	A	185	SER	2.8
1	A	55	LYS	2.8
1	A	164	ILE	2.8
1	A	63	GLU	2.8
1	A	197	GLY	2.8
1	A	44	PHE	2.8
1	A	8	GLY	2.8
1	A	139	ASN	2.8
1	A	152	LEU	2.8
1	A	17	VAL	2.8
1	A	50	TYR	2.8
1	A	52	THR	2.7
1	A	110	ALA	2.7
1	A	218	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	28	TYR	2.7
1	A	225	THR	2.7
1	A	86	VAL	2.7
1	A	140	GLY	2.6
1	A	20	ASN	2.6
1	A	239	GLY	2.6
1	A	24	ASN	2.6
1	A	115	LEU	2.6
1	A	104	SER	2.6
1	A	262	LEU	2.6
1	A	147	SER	2.6
1	A	194	PRO	2.6
1	A	39	ASP	2.5
1	A	242	LEU	2.6
1	A	94	HIS	2.5
1	A	69	LEU	2.5
1	A	45	ALA	2.5
1	A	10	THR	2.5
1	A	32	ASP	2.5
1	A	173	ALA	2.5
1	A	201	VAL	2.5
1	A	221	THR	2.5
1	A	189	ASP	2.5
1	A	235	ASP	2.5
1	A	158	ALA	2.5
1	A	71	ASN	2.4
1	A	175	SER	2.4
1	A	177	LEU	2.4
1	A	146	ASP	2.4
1	A	145	ASN	2.4
1	A	186	ASP	2.4
1	A	155	ALA	2.4
1	A	223	ARG	2.4
1	A	159	ASN	2.3
1	A	105	GLN	2.3
1	A	265	SER	2.3
1	A	23	LEU	2.3
1	A	153	VAL	2.3
1	A	224	SER	2.3
1	A	122	TYR	2.2
1	A	65	VAL	2.2
1	A	21	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	108	ALA	2.2
1	A	156	LEU	2.2
1	A	60	HIS	2.2
1	A	266	GLU	2.2
1	A	68	VAL	2.2
1	A	172	PRO	2.2
1	A	219	GLY	2.2
1	A	88	LEU	2.2
1	A	47	ASN	2.2
1	A	230	ALA	2.2
1	A	232	ARG	2.2
1	A	61	PHE	2.1
1	A	144	PRO	2.1
1	A	130	ASN	2.1
1	A	36	ASN	2.1
1	A	250	ASP	2.1
1	A	143	GLN	2.1
1	A	81	GLN	2.1
1	A	40	VAL	2.1
1	A	193	ASN	2.1
1	A	37	ALA	2.1
1	A	210	GLN	2.0
1	A	49	ASN	2.0
1	A	151	HIS	2.0
1	A	191	ALA	2.0
1	A	176	ARG	2.0
1	A	46	ALA	2.0
1	A	142	ALA	2.0
1	A	67	ARG	2.0
1	A	171	GLY	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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.