



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:40 PM GMT

PDB ID : 1C93
Title : Endo-Beta-N-AcetylglucosaminidaseH, D130N/E132Q Double Mutant
Authors : Rao, V.; Cui, T.; Guan, C.; Van Roey, P.
Deposited on : 1999-07-30
Resolution : 2.10 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>

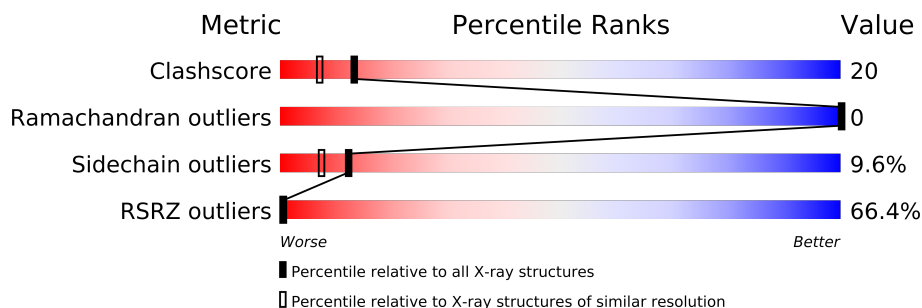
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.10 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	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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 ≥ 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	265	

2 Entry composition

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

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.

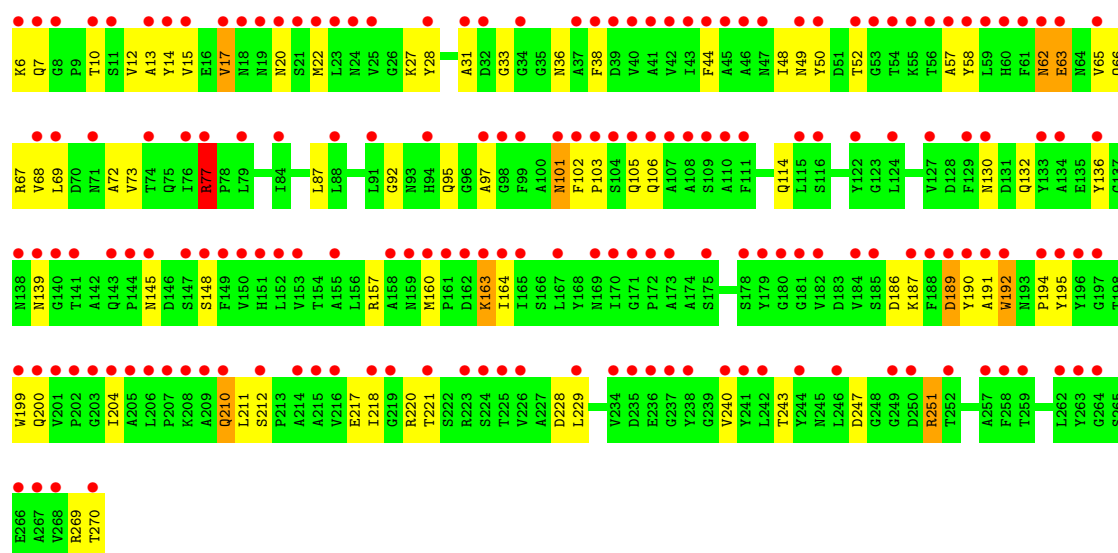
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	124	Total	O	0	0
			124	124		

3 Residue-property plots

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: ENDO-BETA-N-ACETYLGLUCOSAMINIDASEH

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 95.5 (45.21-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.10Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.200 , (Not available) 0.368 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	10.5	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 12430 reflections	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	2140	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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	0.64	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 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	2016	0	1935	81	1
2	A	124	0	0	4	2
All	All	2140	0	1935	81	2

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 20.

All (81) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:72:ALA:HB1	1:A:77:ARG:NH1	2.05	0.71
1:A:17:VAL:HG12	1:A:68:VAL:HG21	1.71	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:HD2	1:A:77:ARG:H	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:73:VAL:O	1:A:77:ARG:HB2	2.09	0.52
1:A:218:ILE:HG12	1:A:243:THR:HG23	1.91	0.52
1:A:28:TYR:CE2	1:A:269:ARG:HB2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:ASP:O	1:A:210:GLN:HB2	2.09	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:17:VAL:CG1	1:A:68:VAL:HG21	2.43	0.43
1:A:102:PHE:N	1:A:148:SER:OG	2.51	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:269:ARG:HG2	1:A:270:THR:N	2.34	0.42
1:A:87:LEU:HD21	1:A:164:ILE:HG22	2.01	0.42
1:A:130:ASN:OD1	1:A:132:GLN:HG3	2.20	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:87:LEU:HD21	1:A:164:ILE:HG21	2.03	0.41
1:A:20:ASN:ND2	1:A:247:ASP:CB	2.84	0.41
1:A:218:ILE:CG1	1:A:243:THR:HG23	2.52	0.40
1:A:192:TRP:HB3	1:A:212:SER:HB3	2.03	0.40
1:A:163:LYS:HA	1:A:163:LYS:HD2	1.87	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	Distance(Å)	Clash(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

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	263/265 (99%)	251 (95%)	12 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	208/208 (100%)	188 (90%)	20 (10%)	12	7

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 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	265/265 (100%)	2.60	176 (66%) 0 0	9, 16, 28, 55	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	97	ALA	7.7
1	A	204	ILE	7.3
1	A	205	ALA	7.1
1	A	179	TYR	6.1
1	A	182	VAL	6.0
1	A	181	GLY	6.0
1	A	7	GLN	5.8
1	A	77	ARG	5.7
1	A	84	ILE	5.4
1	A	206	LEU	5.1
1	A	170	ILE	4.9
1	A	203	GLY	4.8
1	A	103	PRO	4.8
1	A	34	GLY	4.7
1	A	207	PRO	4.7
1	A	229	LEU	4.4
1	A	252	THR	4.3
1	A	200	GLN	4.3
1	A	53	GLY	4.3
1	A	180	GLY	4.3
1	A	216	VAL	4.3
1	A	58	TYR	4.3
1	A	91	LEU	4.2
1	A	190	TYR	4.2
1	A	38	PHE	4.1
1	A	264	GLY	4.1
1	A	106	GLN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	149	PHE	4.0
1	A	241	TYR	4.0
1	A	263	TYR	4.0
1	A	107	ALA	3.9
1	A	257	ALA	3.9
1	A	268	VAL	3.8
1	A	192	TRP	3.8
1	A	25	VAL	3.7
1	A	178	SER	3.7
1	A	238	TYR	3.7
1	A	212	SER	3.7
1	A	6	LYS	3.7
1	A	196	TYR	3.7
1	A	13	ALA	3.6
1	A	57	ALA	3.6
1	A	150	VAL	3.6
1	A	43	ILE	3.6
1	A	59	LEU	3.6
1	A	138	ASN	3.5
1	A	240	VAL	3.5
1	A	209	ALA	3.5
1	A	18	ASN	3.5
1	A	11	SER	3.4
1	A	54	THR	3.4
1	A	270	THR	3.4
1	A	184	VAL	3.3
1	A	63	GLU	3.3
1	A	267	ALA	3.3
1	A	202	PRO	3.3
1	A	74	THR	3.3
1	A	164	ILE	3.3
1	A	195	TYR	3.3
1	A	215	ALA	3.3
1	A	141	THR	3.3
1	A	56	THR	3.2
1	A	133	TYR	3.2
1	A	167	LEU	3.1
1	A	226	VAL	3.1
1	A	102	PHE	3.1
1	A	161	PRO	3.1
1	A	162	ASP	3.1
1	A	14	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	189	ASP	3.0
1	A	79	LEU	3.0
1	A	259	THR	3.0
1	A	127	VAL	3.0
1	A	148	SER	3.0
1	A	44	PHE	3.0
1	A	99	PHE	3.0
1	A	129	PHE	3.0
1	A	124	LEU	3.0
1	A	111	PHE	3.0
1	A	197	GLY	3.0
1	A	28	TYR	3.0
1	A	17	VAL	3.0
1	A	109	SER	3.0
1	A	62	ASN	2.9
1	A	116	SER	2.9
1	A	169	ASN	2.9
1	A	199	TRP	2.9
1	A	101	ASN	2.9
1	A	22	MET	2.9
1	A	223	ARG	2.9
1	A	8	GLY	2.9
1	A	115	LEU	2.9
1	A	225	THR	2.9
1	A	19	ASN	2.8
1	A	31	ALA	2.8
1	A	262	LEU	2.8
1	A	140	GLY	2.8
1	A	173	ALA	2.8
1	A	187	LYS	2.8
1	A	219	GLY	2.8
1	A	76	ILE	2.8
1	A	147	SER	2.8
1	A	249	GLY	2.8
1	A	234	VAL	2.7
1	A	69	LEU	2.7
1	A	246	LEU	2.7
1	A	165	ILE	2.7
1	A	136	TYR	2.7
1	A	104	SER	2.7
1	A	110	ALA	2.7
1	A	221	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	258	PHE	2.7
1	A	49	ASN	2.7
1	A	139	ASN	2.6
1	A	158	ALA	2.6
1	A	175	SER	2.6
1	A	235	ASP	2.6
1	A	134	ALA	2.6
1	A	214	ALA	2.6
1	A	23	LEU	2.6
1	A	88	LEU	2.6
1	A	188	PHE	2.6
1	A	266	GLU	2.6
1	A	130	ASN	2.6
1	A	122	TYR	2.6
1	A	65	VAL	2.6
1	A	68	VAL	2.5
1	A	39	ASP	2.5
1	A	94	HIS	2.5
1	A	185	SER	2.5
1	A	61	PHE	2.5
1	A	45	ALA	2.5
1	A	224	SER	2.5
1	A	50	TYR	2.5
1	A	55	LYS	2.4
1	A	143	GLN	2.4
1	A	171	GLY	2.4
1	A	46	ALA	2.4
1	A	20	ASN	2.4
1	A	24	ASN	2.4
1	A	172	PRO	2.4
1	A	60	HIS	2.4
1	A	244	TYR	2.4
1	A	71	ASN	2.4
1	A	152	LEU	2.4
1	A	210	GLN	2.4
1	A	52	THR	2.3
1	A	32	ASP	2.3
1	A	42	VAL	2.3
1	A	242	LEU	2.3
1	A	10	THR	2.3
1	A	47	ASN	2.3
1	A	98	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	218	ILE	2.2
1	A	21	SER	2.2
1	A	191	ALA	2.2
1	A	155	ALA	2.2
1	A	236	GLU	2.2
1	A	40	VAL	2.2
1	A	151	HIS	2.1
1	A	41	ALA	2.1
1	A	145	ASN	2.1
1	A	144	PRO	2.1
1	A	250	ASP	2.1
1	A	163	LYS	2.1
1	A	201	VAL	2.1
1	A	237	GLY	2.1
1	A	159	ASN	2.1
1	A	37	ALA	2.0
1	A	105	GLN	2.0
1	A	153	VAL	2.0
1	A	108	ALA	2.0
1	A	160	MET	2.0
1	A	15	VAL	2.0
1	A	208	LYS	2.0
1	A	194	PRO	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.