



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:24 PM GMT

PDB ID : 2FP8
Title : Structure of Strictosidine Synthase, the Biosynthetic Entry to the Monoterpenoid Indole Alkaloid Family
Authors : Panjikar, S.
Deposited on : 2006-01-16
Resolution : 2.30 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>

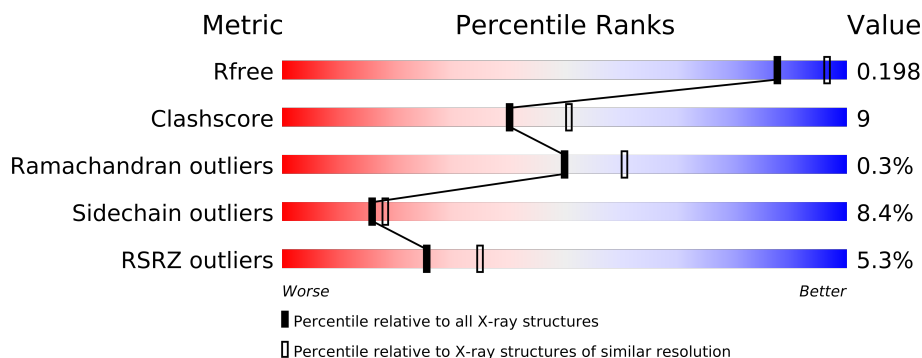
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	322	
1	B	322	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5173 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 Strictosidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2382	1529	388	460	5			
1	B	303	Total	C	N	O	S	0	0	0
			2390	1535	389	461	5			

- Molecule 2 is water.

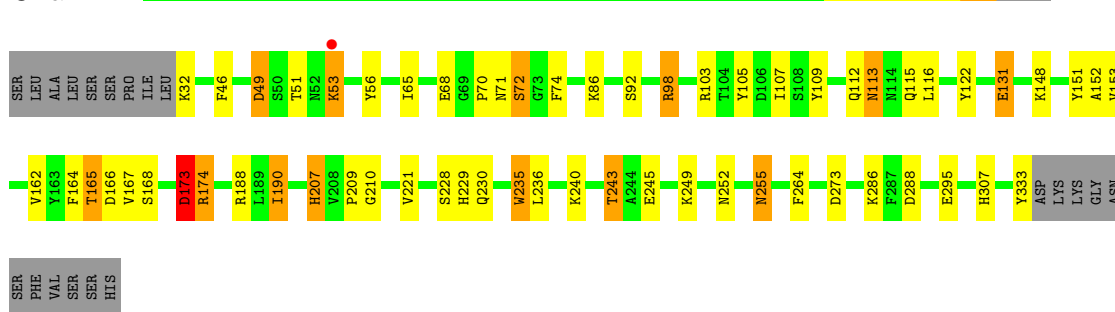
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	279	Total	O	0	0
			279	279		
2	B	122	Total	O	0	0
			122	122		

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.

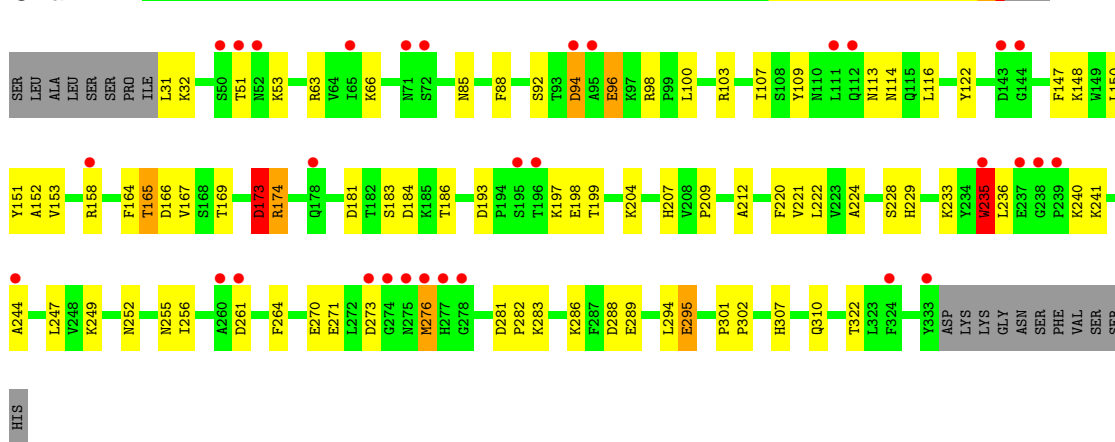
- Molecule 1: Strictosidine synthase

Chain A:



- Molecule 1: Strictosidine synthase

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	147.29Å 147.29Å 122.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.30) 99.7 (19.65-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.217 0.195 , 0.198	Depositor DCC
R_{free} test set	1078 reflections (2.47%)	DCC
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.9	EDS
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43715 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5173	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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	0.80	2/2447 (0.1%)	0.91	6/3329 (0.2%)
1	B	0.73	2/2455 (0.1%)	0.84	6/3340 (0.2%)
All	All	0.76	4/4902 (0.1%)	0.87	12/6669 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	240	LYS	CD-CE	6.70	1.68	1.51
1	A	173	ASP	CB-CG	-6.21	1.38	1.51
1	B	235	TRP	CB-CG	5.58	1.60	1.50
1	A	255	ASN	CG-OD1	5.05	1.35	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	166	ASP	CB-CG-OD2	7.04	124.63	118.30
1	B	94	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	174	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	A	273	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	49	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	288	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	273	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	261	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	193	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	184	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	181	ASP	CB-CG-OD2	5.02	122.81	118.30

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	2382	0	2287	41	0
1	B	2390	0	2298	48	0
2	A	279	0	0	8	0
2	B	122	0	0	8	0
All	All	5173	0	4585	88	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 9.

All (88) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:ASP:OD1	1:A:51:THR:HG22	1.62	0.98
1:A:229:HIS:HD2	1:A:252:ASN:H	1.04	0.95
1:B:229:HIS:HD2	1:B:252:ASN:H	1.04	0.94
1:A:235:TRP:HZ3	1:A:245:GLU:OE2	1.51	0.92
1:A:162:VAL:HG12	2:A:511:HOH:O	1.70	0.89
1:A:122:TYR:OH	1:A:174:ARG:NH1	2.08	0.87
1:B:235:TRP:HE3	2:B:410:HOH:O	1.60	0.83
1:B:229:HIS:CD2	1:B:252:ASN:H	1.95	0.81
1:B:152:ALA:H	1:B:165:THR:HG22	1.45	0.79
1:A:229:HIS:CD2	1:A:252:ASN:H	1.96	0.78
1:A:235:TRP:CZ3	1:A:245:GLU:OE2	2.38	0.76
1:A:153:VAL:HG23	2:A:511:HOH:O	1.85	0.76
1:B:307:HIS:HD2	2:B:465:HOH:O	1.74	0.71
1:A:174:ARG:HH11	1:A:174:ARG:HG3	1.56	0.71
1:B:174:ARG:HG3	1:B:174:ARG:HH11	1.57	0.69
1:A:230:GLN:HE21	1:A:249:LYS:HE2	1.58	0.69
1:B:94:ASP:HB3	1:B:96:GLU:OE1	1.94	0.66
1:B:229:HIS:HD2	1:B:252:ASN:N	1.87	0.65
1:B:98:ARG:HH11	1:B:173:ASP:HB3	1.62	0.65
1:B:233:LYS:HD2	1:B:247:LEU:HD13	1.78	0.65
1:A:229:HIS:HD2	1:A:252:ASN:N	1.88	0.64
1:B:166:ASP:CG	2:B:408:HOH:O	2.35	0.64
1:A:307:HIS:HD2	2:A:406:HOH:O	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:167:VAL:HA	1:B:209:PRO:HD2	1.81	0.63
1:A:164:PHE:HB3	2:A:511:HOH:O	1.98	0.62
1:A:131:GLU:HB3	2:A:492:HOH:O	2.00	0.61
1:A:255:ASN:ND2	2:A:502:HOH:O	2.33	0.60
1:B:152:ALA:N	1:B:165:THR:HG22	2.16	0.59
1:B:235:TRP:CE3	2:B:410:HOH:O	2.42	0.59
1:A:221:VAL:HG23	1:A:236:LEU:HD11	1.85	0.58
1:B:174:ARG:HG3	1:B:174:ARG:NH1	2.19	0.55
1:B:252:ASN:ND2	1:B:271:GLU:H	2.06	0.54
1:A:174:ARG:NH1	1:A:174:ARG:HG3	2.22	0.54
1:B:98:ARG:NH1	1:B:173:ASP:HB3	2.23	0.54
1:B:221:VAL:HG23	1:B:236:LEU:HD11	1.90	0.53
1:B:147:PHE:HB3	2:B:408:HOH:O	2.08	0.53
1:A:98:ARG:HD3	1:A:173:ASP:OD1	2.09	0.52
1:A:71:ASN:ND2	1:A:72:SER:H	2.08	0.52
1:A:113:ASN:ND2	1:A:115:GLN:HG3	2.25	0.52
1:A:207:HIS:HD2	1:A:228:SER:OG	1.93	0.51
1:B:255:ASN:HD22	1:B:310:GLN:HB2	1.76	0.51
1:B:236:LEU:O	1:B:241:LYS:HG3	2.12	0.50
1:B:85:ASN:HD22	1:B:88:PHE:H	1.60	0.50
1:A:51:THR:HG23	1:A:53:LYS:H	1.76	0.49
1:A:221:VAL:CG2	1:A:236:LEU:HD11	2.42	0.48
1:B:151:TYR:HB2	1:B:167:VAL:HG13	1.95	0.48
1:B:224:ALA:HB2	1:B:256:ILE:HD11	1.96	0.48
1:B:264:PHE:O	1:B:286:LYS:HA	2.14	0.47
1:B:158:ARG:CB	1:B:158:ARG:HH11	2.27	0.47
1:A:65:ILE:HD12	1:A:74:PHE:CD2	2.50	0.47
1:B:282:PRO:HD2	2:B:362:HOH:O	2.15	0.47
1:B:252:ASN:HD22	1:B:270:GLU:HA	1.80	0.47
1:B:153:VAL:HG23	1:B:164:PHE:HB3	1.97	0.47
1:A:105:TYR:OH	1:A:173:ASP:OD2	2.21	0.46
1:B:301:PRO:HA	2:B:351:HOH:O	2.15	0.46
1:A:295:GLU:OE2	1:A:333:TYR:OH	2.21	0.46
1:B:122:TYR:OH	1:B:174:ARG:NH1	2.49	0.46
1:B:158:ARG:HB2	1:B:158:ARG:NH1	2.31	0.45
1:B:286:LYS:HB3	1:B:295:GLU:HB2	1.98	0.45
1:A:210:GLY:N	2:A:421:HOH:O	2.49	0.45
1:B:276:MET:HG2	1:B:276:MET:O	2.15	0.45
1:A:107:ILE:HB	1:A:116:LEU:HD11	1.99	0.44
1:A:148:LYS:HD2	1:A:148:LYS:HA	1.69	0.44
1:A:264:PHE:O	1:A:286:LYS:HA	2.17	0.44
1:A:148:LYS:HB2	1:A:168:SER:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210:GLY:CA	2:A:421:HOH:O	2.66	0.44
1:A:240:LYS:O	1:A:243:THR:HB	2.17	0.44
1:A:152:ALA:H	1:A:165:THR:HG22	1.84	0.43
1:A:151:TYR:HB2	1:A:167:VAL:HG13	2.01	0.43
1:B:212:ALA:HA	1:B:222:LEU:O	2.18	0.43
1:B:288:ASP:HB3	1:B:294:LEU:HD11	2.00	0.43
1:B:150:LEU:HD23	1:B:166:ASP:HB2	2.00	0.42
1:B:322:THR:HG22	2:B:352:HOH:O	2.19	0.42
1:A:70:PRO:HG2	1:B:302:PRO:HB3	2.01	0.42
1:B:249:LYS:HB3	1:B:249:LYS:HE3	1.74	0.42
1:A:46:PHE:HA	1:A:56:TYR:O	2.19	0.42
1:B:122:TYR:OH	1:B:173:ASP:HB2	2.18	0.42
1:B:270:GLU:HB3	1:B:281:ASP:HB3	2.02	0.42
1:A:122:TYR:OH	1:A:173:ASP:HB2	2.20	0.41
1:B:220:PHE:HZ	1:B:289:GLU:HB3	1.85	0.41
1:B:233:LYS:O	1:B:244:ALA:HA	2.20	0.41
1:A:165:THR:HG21	1:A:209:PRO:O	2.20	0.41
1:A:188:ARG:HB3	1:A:190:ILE:CD1	2.51	0.40
1:B:148:LYS:HD3	1:B:148:LYS:HA	1.94	0.40
1:B:107:ILE:HB	1:B:116:LEU:HD21	2.04	0.40
1:A:122:TYR:CZ	1:A:174:ARG:NH1	2.88	0.40
1:B:169:THR:HG23	1:B:186:THR:O	2.20	0.40
1:B:221:VAL:CG2	1:B:236:LEU:HD11	2.51	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	300/322 (93%)	288 (96%)	11 (4%)	1 (0%)	50	60
1	B	301/322 (94%)	288 (96%)	12 (4%)	1 (0%)	50	60
All	All	601/644 (93%)	576 (96%)	23 (4%)	2 (0%)	50	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASP
1	B	173	ASP

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	260/278 (94%)	243 (94%)	17 (6%)	24	30
1	B	261/278 (94%)	234 (90%)	27 (10%)	10	11
All	All	521/556 (94%)	477 (92%)	44 (8%)	16	18

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	53	LYS
1	A	68	GLU
1	A	72	SER
1	A	86	LYS
1	A	92	SER
1	A	103	ARG
1	A	109	TYR
1	A	112	GLN
1	A	113	ASN
1	A	131	GLU
1	A	165	THR
1	A	173	ASP
1	A	190	ILE
1	A	207	HIS
1	A	235	TRP
1	A	243	THR
1	B	31	LEU
1	B	32	LYS
1	B	51	THR
1	B	53	LYS
1	B	63	ARG
1	B	66	LYS
1	B	92	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	96	GLU
1	B	100	LEU
1	B	103	ARG
1	B	109	TYR
1	B	113	ASN
1	B	114	ASN
1	B	165	THR
1	B	173	ASP
1	B	174	ARG
1	B	183	SER
1	B	197	LYS
1	B	198	GLU
1	B	199	THR
1	B	204	LYS
1	B	207	HIS
1	B	228	SER
1	B	235	TRP
1	B	276	MET
1	B	283	LYS
1	B	295	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	91	ASN
1	A	112	GLN
1	A	113	ASN
1	A	207	HIS
1	A	229	HIS
1	A	230	GLN
1	A	252	ASN
1	A	255	ASN
1	A	310	GLN
1	A	312	GLN
1	B	85	ASN
1	B	91	ASN
1	B	113	ASN
1	B	229	HIS
1	B	230	GLN
1	B	252	ASN
1	B	255	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	275	ASN
1	B	310	GLN
1	B	312	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	302/322 (93%)	-0.30	1 (0%) 91 96	16, 21, 28, 33	0
1	B	303/322 (94%)	0.52	31 (10%) 7 12	16, 22, 29, 50	0
All	All	605/644 (93%)	0.11	32 (5%) 25 35	16, 22, 29, 50	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	GLY	10.1
1	B	276	MET	4.9
1	B	196	THR	4.8
1	B	275	ASN	4.8
1	B	195	SER	4.2
1	B	333	TYR	3.9
1	B	158	ARG	3.9
1	B	277	HIS	3.9
1	B	112	GLN	3.6
1	B	278	GLY	3.6
1	B	144	GLY	3.4
1	B	51	THR	3.4
1	B	143	ASP	3.4
1	B	50	SER	3.3
1	B	178	GLN	3.1
1	B	239	PRO	3.1
1	B	94	ASP	3.1
1	B	72	SER	3.1
1	B	260	ALA	2.9
1	B	261	ASP	2.9
1	B	235	TRP	2.8
1	B	244	ALA	2.8
1	B	238	GLY	2.8
1	B	52	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	95	ALA	2.6
1	B	71	ASN	2.4
1	A	53	LYS	2.3
1	B	111	LEU	2.3
1	B	273	ASP	2.2
1	B	237	GLU	2.1
1	B	65	ILE	2.0
1	B	324	PHE	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.