



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:14 am BST

PDB ID : 5KN4
Title : Pavine N-methyltransferase apoenzyme pH 6.0
Authors : Torres, M.A.; Hoffarth, E.; Eugenio, L.; Savtchouk, J.; Chen, X.; Morris, J.;
Facchini, P.J.; Ng, K.K.S.
Deposited on : 2016-06-27
Resolution : 1.99 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

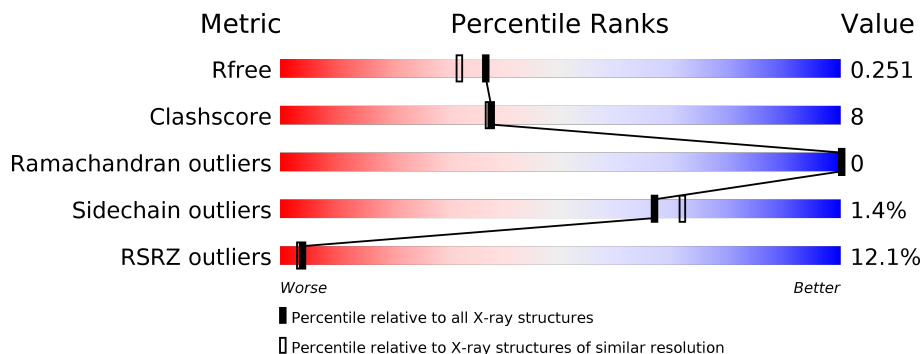
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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 ≥ 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	397	 11% 69% 11% • 20%
1	B	397	 9% 66% 13% • 20%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5420 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 Pavine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2615	1684	426	485	20	0	0	0
1	B	317	2602	1677	424	481	20	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	expression tag	UNP C3SBW0
A	-39	ARG	-	expression tag	UNP C3SBW0
A	-38	GLY	-	expression tag	UNP C3SBW0
A	-37	SER	-	expression tag	UNP C3SBW0
A	-36	HIS	-	expression tag	UNP C3SBW0
A	-35	HIS	-	expression tag	UNP C3SBW0
A	-34	HIS	-	expression tag	UNP C3SBW0
A	-33	HIS	-	expression tag	UNP C3SBW0
A	-32	HIS	-	expression tag	UNP C3SBW0
A	-31	HIS	-	expression tag	UNP C3SBW0
A	-30	GLY	-	expression tag	UNP C3SBW0
A	-29	MET	-	expression tag	UNP C3SBW0
A	-28	ALA	-	expression tag	UNP C3SBW0
A	-27	SER	-	expression tag	UNP C3SBW0
A	-26	MET	-	expression tag	UNP C3SBW0
A	-25	THR	-	expression tag	UNP C3SBW0
A	-24	GLY	-	expression tag	UNP C3SBW0
A	-23	GLY	-	expression tag	UNP C3SBW0
A	-22	GLN	-	expression tag	UNP C3SBW0
A	-21	GLN	-	expression tag	UNP C3SBW0
A	-20	MET	-	expression tag	UNP C3SBW0
A	-19	GLY	-	expression tag	UNP C3SBW0
A	-18	ARG	-	expression tag	UNP C3SBW0
A	-17	ASP	-	expression tag	UNP C3SBW0
A	-16	LEU	-	expression tag	UNP C3SBW0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	TYR	-	expression tag	UNP C3SBW0
A	-14	ASP	-	expression tag	UNP C3SBW0
A	-13	ASP	-	expression tag	UNP C3SBW0
A	-12	ASP	-	expression tag	UNP C3SBW0
A	-11	ASP	-	expression tag	UNP C3SBW0
A	-10	LYS	-	expression tag	UNP C3SBW0
A	-9	ASP	-	expression tag	UNP C3SBW0
A	-8	ARG	-	expression tag	UNP C3SBW0
A	-7	TRP	-	expression tag	UNP C3SBW0
A	-6	ILE	-	expression tag	UNP C3SBW0
A	-5	ARG	-	expression tag	UNP C3SBW0
A	-4	PRO	-	expression tag	UNP C3SBW0
A	-3	ARG	-	expression tag	UNP C3SBW0
A	-2	ASP	-	expression tag	UNP C3SBW0
A	-1	LEU	-	expression tag	UNP C3SBW0
A	0	GLN	-	expression tag	UNP C3SBW0
A	224	ASP	TYR	conflict	UNP C3SBW0
B	-40	MET	-	expression tag	UNP C3SBW0
B	-39	ARG	-	expression tag	UNP C3SBW0
B	-38	GLY	-	expression tag	UNP C3SBW0
B	-37	SER	-	expression tag	UNP C3SBW0
B	-36	HIS	-	expression tag	UNP C3SBW0
B	-35	HIS	-	expression tag	UNP C3SBW0
B	-34	HIS	-	expression tag	UNP C3SBW0
B	-33	HIS	-	expression tag	UNP C3SBW0
B	-32	HIS	-	expression tag	UNP C3SBW0
B	-31	HIS	-	expression tag	UNP C3SBW0
B	-30	GLY	-	expression tag	UNP C3SBW0
B	-29	MET	-	expression tag	UNP C3SBW0
B	-28	ALA	-	expression tag	UNP C3SBW0
B	-27	SER	-	expression tag	UNP C3SBW0
B	-26	MET	-	expression tag	UNP C3SBW0
B	-25	THR	-	expression tag	UNP C3SBW0
B	-24	GLY	-	expression tag	UNP C3SBW0
B	-23	GLY	-	expression tag	UNP C3SBW0
B	-22	GLN	-	expression tag	UNP C3SBW0
B	-21	GLN	-	expression tag	UNP C3SBW0
B	-20	MET	-	expression tag	UNP C3SBW0
B	-19	GLY	-	expression tag	UNP C3SBW0
B	-18	ARG	-	expression tag	UNP C3SBW0
B	-17	ASP	-	expression tag	UNP C3SBW0
B	-16	LEU	-	expression tag	UNP C3SBW0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	TYR	-	expression tag	UNP C3SBW0
B	-14	ASP	-	expression tag	UNP C3SBW0
B	-13	ASP	-	expression tag	UNP C3SBW0
B	-12	ASP	-	expression tag	UNP C3SBW0
B	-11	ASP	-	expression tag	UNP C3SBW0
B	-10	LYS	-	expression tag	UNP C3SBW0
B	-9	ASP	-	expression tag	UNP C3SBW0
B	-8	ARG	-	expression tag	UNP C3SBW0
B	-7	TRP	-	expression tag	UNP C3SBW0
B	-6	ILE	-	expression tag	UNP C3SBW0
B	-5	ARG	-	expression tag	UNP C3SBW0
B	-4	PRO	-	expression tag	UNP C3SBW0
B	-3	ARG	-	expression tag	UNP C3SBW0
B	-2	ASP	-	expression tag	UNP C3SBW0
B	-1	LEU	-	expression tag	UNP C3SBW0
B	0	GLN	-	expression tag	UNP C3SBW0
B	224	ASP	TYR	conflict	UNP C3SBW0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	108	Total O 108 108	0	0
2	B	95	Total O 95 95	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.74Å 72.30Å 97.14Å 90.00° 99.75° 90.00°	Depositor
Resolution (Å)	38.95 – 1.99 38.95 – 1.99	Depositor EDS
% Data completeness (in resolution range)	93.7 (38.95-1.99) 87.2 (38.95-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.196 , 0.253 0.197 , 0.251	Depositor DCC
R_{free} test set	2398 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtrriage
Anisotropy	0.616	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5420	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.52	0/2674	0.57	0/3601
1	B	0.53	0/2660	0.59	0/3580
All	All	0.52	0/5334	0.58	0/7181

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 [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	2615	0	2582	30	0
1	B	2602	0	2566	51	0
2	A	108	0	0	3	0
2	B	95	0	0	0	0
All	All	5420	0	5148	80	0

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 8.

All (80) 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:16:LYS:NZ	1:B:20:HIS:CE1	2.31	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:MET:HG3	1:B:322:LYS:HZ3	1.33	0.93
1:B:16:LYS:HA	1:B:19:GLU:HB2	1.51	0.90
1:B:16:LYS:HZ2	1:B:20:HIS:CE1	1.89	0.84
1:B:83:LEU:HD21	1:B:165:GLU:HG3	1.58	0.83
1:B:83:LEU:CD2	1:B:165:GLU:HG3	2.13	0.78
1:B:16:LYS:NZ	1:B:20:HIS:ND1	2.28	0.74
1:B:16:LYS:HZ1	1:B:20:HIS:CE1	2.07	0.73
1:B:19:GLU:HB3	1:B:322:LYS:NZ	2.03	0.72
1:A:90:CYS:SG	1:A:138:HIS:HD2	2.18	0.66
1:B:147:GLN:HE21	1:B:176:LEU:HD11	1.60	0.66
1:A:160:SER:HB3	1:A:163:GLN:HE21	1.60	0.65
1:B:169:ASP:O	1:B:173:LYS:HD3	1.97	0.65
1:A:139:GLY:HA3	1:A:167:ILE:HG12	1.80	0.63
1:B:190:GLU:HG3	1:B:220:TRP:HE1	1.63	0.62
1:B:89:MET:HA	1:B:298:ARG:HD3	1.81	0.62
1:B:19:GLU:HG2	1:B:325:THR:HG21	1.80	0.62
1:B:173:LYS:HD2	1:B:173:LYS:N	2.16	0.61
1:B:19:GLU:HB3	1:B:322:LYS:HZ2	1.65	0.59
1:B:16:LYS:HG3	1:B:20:HIS:CE1	2.38	0.59
1:A:160:SER:HB3	1:A:163:GLN:NE2	2.17	0.59
1:A:356:LYS:NZ	1:B:356:LYS:O	2.26	0.59
1:B:15:ILE:HG22	1:B:19:GLU:CD	2.25	0.57
1:A:67:MET:HE3	1:A:213:PHE:HD1	1.70	0.57
1:B:240:GLN:HG2	1:B:261:VAL:HG22	1.87	0.56
1:A:15:ILE:O	1:A:19:GLU:HG3	2.09	0.53
1:B:191:THR:HG22	1:B:193:ILE:H	1.74	0.53
1:B:16:LYS:O	1:B:20:HIS:N	2.40	0.52
1:A:20:HIS:HE1	1:A:318:GLU:OE2	1.94	0.51
1:B:166:PHE:O	1:B:170:GLN:HG2	2.10	0.50
1:B:321:MET:HG3	1:B:322:LYS:NZ	2.16	0.50
1:B:185:ASP:OD1	1:B:187:THR:OG1	2.26	0.49
1:B:321:MET:CG	1:B:322:LYS:HZ3	2.16	0.49
1:B:15:ILE:H	1:B:15:ILE:HD12	1.78	0.48
1:A:243:PRO:HA	1:A:248:ASP:OD2	2.13	0.48
1:B:243:PRO:HA	1:B:248:ASP:OD2	2.14	0.48
1:A:165:GLU:HA	1:A:168:MET:HB2	1.96	0.47
1:A:90:CYS:SG	1:A:138:HIS:CD2	3.05	0.47
1:B:283:LEU:O	1:B:347:MET:HB2	2.14	0.47
1:A:17:ARG:O	1:A:22:GLU:HG2	2.15	0.47
1:B:28:ILE:HD13	1:B:329:VAL:HG22	1.97	0.47
1:A:250:TYR:CE1	1:A:254:ILE:HD12	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLN:NE2	2:A:407:HOH:O	2.47	0.46
1:A:26:GLU:OE1	1:A:29:ARG:NH1	2.43	0.46
1:B:16:LYS:NZ	1:B:20:HIS:HE1	2.05	0.46
1:B:139:GLY:HA3	1:B:167:ILE:HG12	1.98	0.46
1:A:160:SER:CB	1:A:163:GLN:HE21	2.28	0.46
1:B:67:MET:HE1	1:B:187:THR:HG22	1.97	0.46
1:B:297:LYS:HD3	1:B:297:LYS:HA	1.63	0.46
1:A:160:SER:O	1:A:183:LEU:HD21	2.15	0.45
1:A:293:LYS:HG3	1:A:335:SER:OG	2.17	0.45
1:A:240:GLN:OE1	1:A:259:THR:OG1	2.35	0.45
1:B:322:LYS:HD3	1:B:322:LYS:HA	1.38	0.45
1:B:355:LYS:O	1:B:356:LYS:HB2	2.17	0.45
1:A:67:MET:HE2	1:A:187:THR:HA	1.99	0.44
1:B:141:LEU:O	1:B:145:VAL:HG23	2.18	0.44
1:B:191:THR:HG21	1:B:193:ILE:HD12	1.99	0.44
1:B:112:GLU:O	1:B:116:MET:HG3	2.18	0.44
1:A:232:HIS:HB3	1:A:338:TYR:OH	2.18	0.43
1:B:172:LYS:HD2	1:B:172:LYS:HA	1.78	0.43
1:B:143:LEU:HB3	1:B:147:GLN:HE22	1.83	0.43
1:B:83:LEU:HD22	1:B:165:GLU:HG3	1.96	0.43
1:A:136:CYS:SG	1:A:158:THR:HG23	2.59	0.42
1:B:16:LYS:CA	1:B:19:GLU:HB2	2.36	0.42
1:B:256:PRO:O	1:B:258:GLY:N	2.52	0.42
1:A:204:ILE:HA	1:A:204:ILE:HD13	1.86	0.42
1:B:311:GLU:HG2	1:B:317:LYS:HA	2.01	0.42
1:A:272:GLN:O	1:A:356:LYS:HE3	2.20	0.42
1:B:18:ILE:HA	1:B:23:VAL:HB	2.01	0.42
1:A:54:GLN:HG2	2:A:418:HOH:O	2.20	0.41
1:B:67:MET:CE	1:B:213:PHE:HD1	2.32	0.41
1:B:153:LYS:HZ1	1:B:180:GLU:N	2.17	0.41
1:A:137:GLY:HA2	1:A:163:GLN:OE1	2.20	0.41
1:A:211:GLU:OE1	2:A:401:HOH:O	2.21	0.41
1:A:300:ASP:O	1:A:303:ILE:HG12	2.20	0.41
1:A:161:VAL:O	1:A:165:GLU:OE2	2.38	0.41
1:B:18:ILE:HG23	1:B:28:ILE:HD11	2.03	0.41
1:B:165:GLU:OE1	1:B:169:ASP:OD2	2.39	0.41
1:B:16:LYS:CE	1:B:20:HIS:HE1	2.34	0.40
1:A:319:LYS:HZ3	1:A:323:PHE:HE2	1.68	0.40

There are no symmetry-related clashes.

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	313/397 (79%)	303 (97%)	10 (3%)	0	100	100
1	B	309/397 (78%)	296 (96%)	13 (4%)	0	100	100
All	All	622/794 (78%)	599 (96%)	23 (4%)	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	291/359 (81%)	286 (98%)	5 (2%)	60	65
1	B	288/359 (80%)	285 (99%)	3 (1%)	76	81
All	All	579/718 (81%)	571 (99%)	8 (1%)	67	72

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	THR
1	A	165	GLU
1	A	183	LEU
1	A	284	SER
1	A	317	LYS
1	B	83	LEU
1	B	160	SER
1	B	297	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	20	HIS
1	A	138	HIS
1	B	147	GLN

5.3.3 RNA [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	319/397 (80%)	0.89	42 (13%) 3 2	24, 39, 70, 78	0
1	B	317/397 (79%)	0.68	35 (11%) 5 5	24, 42, 67, 75	0
All	All	636/794 (80%)	0.79	77 (12%) 4 3	24, 41, 69, 78	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	VAL	5.8
1	B	114	TYR	5.8
1	A	105	SER	5.1
1	A	20	HIS	5.1
1	A	16	LYS	4.7
1	A	318	GLU	4.6
1	A	258	GLY	4.6
1	A	246	GLU	4.5
1	A	13	ASN	4.3
1	A	15	ILE	4.3
1	A	14	LEU	4.2
1	B	14	LEU	4.0
1	A	106	THR	4.0
1	A	139	GLY	3.9
1	A	257	SER	3.9
1	B	110	GLU	3.8
1	B	173	LYS	3.7
1	A	323	PHE	3.7
1	A	21	GLY	3.6
1	A	249	TRP	3.5
1	A	17	ARG	3.5
1	B	18	ILE	3.4
1	B	11	VAL	3.4
1	A	138	HIS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	22	GLU	3.3
1	B	174	LEU	3.3
1	B	246	GLU	3.2
1	A	315	GLY	3.1
1	B	147	GLN	3.1
1	A	137	GLY	3.1
1	B	12	ALA	3.1
1	A	136	CYS	3.0
1	A	107	THR	3.0
1	A	321	MET	3.0
1	B	247	ASP	3.0
1	B	204	ILE	2.9
1	A	114	TYR	2.9
1	A	303	ILE	2.9
1	B	175	ASP	2.8
1	B	81	ILE	2.8
1	A	314	TYR	2.8
1	B	269	LEU	2.7
1	A	183	LEU	2.7
1	B	229	VAL	2.6
1	A	159	ASN	2.6
1	B	138	HIS	2.5
1	A	269	LEU	2.5
1	A	204	ILE	2.5
1	A	322	LYS	2.4
1	B	139	GLY	2.4
1	B	159	ASN	2.4
1	B	176	LEU	2.4
1	B	88	ILE	2.4
1	B	201	VAL	2.4
1	A	267	ILE	2.3
1	A	12	ALA	2.3
1	B	15	ILE	2.3
1	A	320	ALA	2.3
1	B	203	LEU	2.3
1	B	20	HIS	2.3
1	A	233	CYS	2.2
1	A	310	PHE	2.2
1	B	168	MET	2.2
1	B	214	LEU	2.2
1	A	23	VAL	2.2
1	A	304	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	233	CYS	2.2
1	A	165	GLU	2.2
1	B	169	ASP	2.2
1	B	109	ASP	2.1
1	B	190	GLU	2.1
1	B	16	LYS	2.1
1	A	264	SER	2.1
1	B	192	GLU	2.0
1	B	27	GLU	2.0
1	A	263	SER	2.0
1	B	90	CYS	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.