



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:58 AM UTC

PDB ID : 3B1O / pdb_00003b1o
Title : Structure of Burkholderia thailandensis nucleoside kinase (BthNK) in ligand-free form
Authors : Yasutake, Y.; Ota, H.; Hino, E.; Sakasegawa, S.; Tamura, T.
Deposited on : 2011-07-05
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

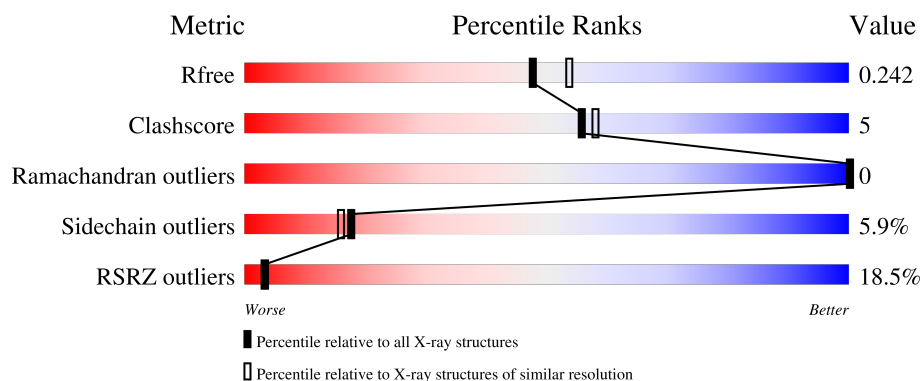
1 Overall quality at a glance

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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of 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	326	83% 11% • •
1	B	326	34% 78% 13% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4900 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 Ribokinase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2391	1502	425	450	14			
1	B	303	Total	C	N	O	S	0	0	0
			2315	1453	411	437	14			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	GLY	-	expression tag	UNP Q2SZE4
A	314	SER	-	expression tag	UNP Q2SZE4
A	315	LYS	-	expression tag	UNP Q2SZE4
A	316	LEU	-	expression tag	UNP Q2SZE4
A	317	ARG	-	expression tag	UNP Q2SZE4
A	318	SER	-	expression tag	UNP Q2SZE4
A	319	LEU	-	expression tag	UNP Q2SZE4
A	320	GLU	-	expression tag	UNP Q2SZE4
A	321	HIS	-	expression tag	UNP Q2SZE4
A	322	HIS	-	expression tag	UNP Q2SZE4
A	323	HIS	-	expression tag	UNP Q2SZE4
A	324	HIS	-	expression tag	UNP Q2SZE4
A	325	HIS	-	expression tag	UNP Q2SZE4
A	326	HIS	-	expression tag	UNP Q2SZE4
B	313	GLY	-	expression tag	UNP Q2SZE4
B	314	SER	-	expression tag	UNP Q2SZE4
B	315	LYS	-	expression tag	UNP Q2SZE4
B	316	LEU	-	expression tag	UNP Q2SZE4
B	317	ARG	-	expression tag	UNP Q2SZE4
B	318	SER	-	expression tag	UNP Q2SZE4
B	319	LEU	-	expression tag	UNP Q2SZE4
B	320	GLU	-	expression tag	UNP Q2SZE4
B	321	HIS	-	expression tag	UNP Q2SZE4
B	322	HIS	-	expression tag	UNP Q2SZE4
B	323	HIS	-	expression tag	UNP Q2SZE4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	324	HIS	-	expression tag	UNP Q2SZE4
B	325	HIS	-	expression tag	UNP Q2SZE4
B	326	HIS	-	expression tag	UNP Q2SZE4

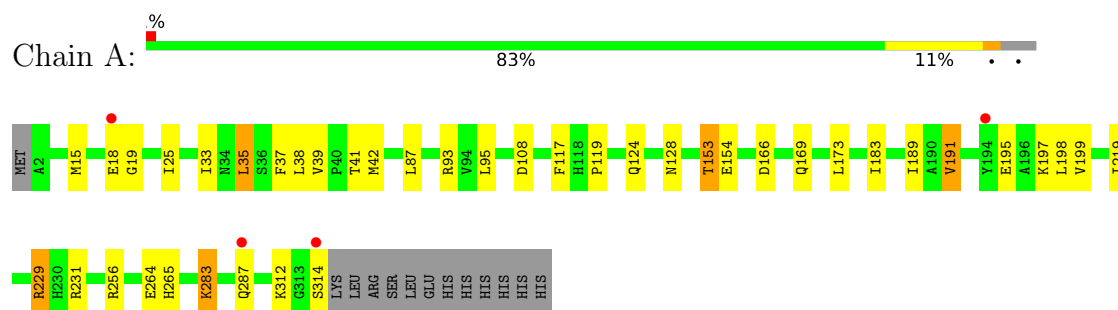
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	145	Total 145	O 145	0	0
2	B	49	Total 49	O 49	0	0

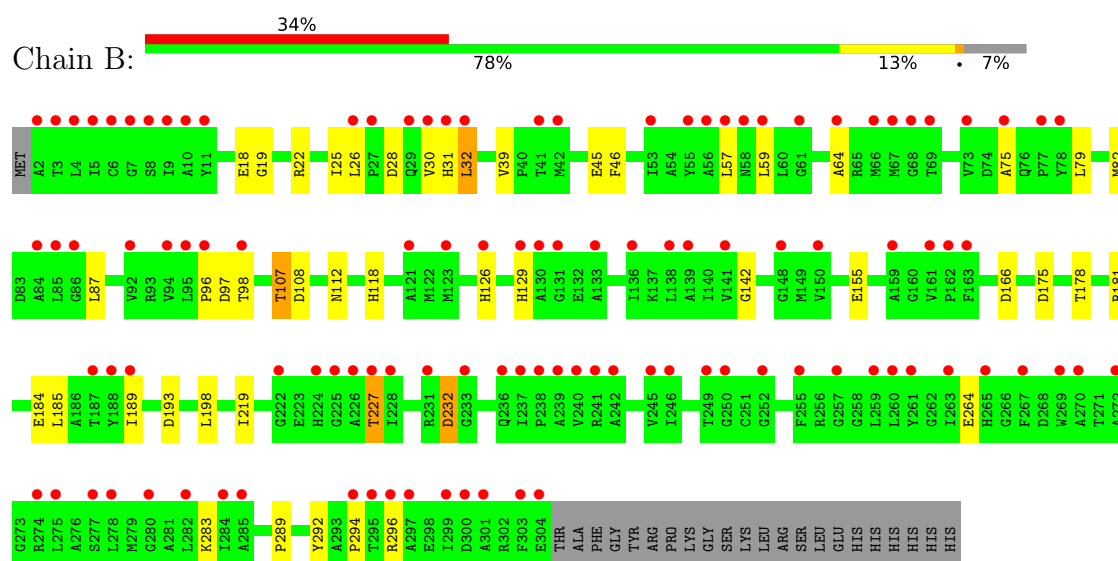
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Ribokinase, putative



- Molecule 1: Ribokinase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.36Å 85.36Å 160.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.68 – 2.10 42.68 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (42.68-2.10) 95.8 (42.68-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.236 , 0.277 0.239 , 0.242	Depositor DCC
R_{free} test set	1683 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4900	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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	0.64	0/2441	0.86	0/3308
1	B	0.56	0/2362	0.87	0/3202
All	All	0.61	0/4803	0.86	0/6510

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	2391	0	2335	22	0
1	B	2315	0	2261	25	0
2	A	145	0	0	2	0
2	B	49	0	0	2	0
All	All	4900	0	4596	44	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 5.

All (44) 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:25:ILE:HG22	1:B:25:ILE:HD11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:HH11	1:A:229:ARG:HB3	1.60	0.65
1:A:153:THR:HG21	2:A:361:HOH:O	1.96	0.65
1:A:283:LYS:C	1:A:283:LYS:HE3	2.24	0.62
1:B:107:THR:HG23	2:B:338:HOH:O	2.00	0.62
1:B:26:LEU:HD12	1:B:32:LEU:HB3	1.82	0.61
1:B:219:ILE:HB	1:B:227:THR:HG22	1.81	0.61
1:B:175:ASP:OD2	1:B:178:THR:HG23	2.02	0.60
1:B:59:LEU:HD13	1:B:294:PRO:HD2	1.85	0.56
1:A:18:GLU:HG2	1:A:18:GLU:O	2.06	0.55
1:B:129:HIS:HB3	1:B:155:GLU:OE1	2.10	0.52
1:A:183:ILE:HG23	1:A:189:ILE:HD11	1.91	0.52
1:B:283:LYS:HG3	1:B:292:TYR:CE1	2.45	0.51
1:B:22:ARG:O	1:B:25:ILE:HD12	2.10	0.51
1:B:232:ASP:OD2	1:B:232:ASP:N	2.46	0.49
1:A:15:MET:HG2	1:A:42:MET:HG2	1.95	0.48
1:A:93:ARG:HD2	1:A:128:ASN:ND2	2.27	0.48
1:B:28:ASP:OD2	1:B:32:LEU:HD12	2.13	0.48
1:A:128:ASN:ND2	2:A:382:HOH:O	2.46	0.48
1:B:96:PRO:O	1:B:98:THR:HG23	2.14	0.48
1:A:15:MET:HB3	1:A:39:VAL:HG11	1.97	0.46
1:A:153:THR:HG22	1:A:154:GLU:N	2.30	0.46
1:B:30:VAL:O	1:B:31:HIS:C	2.59	0.45
1:B:46:PHE:O	1:B:289:PRO:HG2	2.15	0.45
1:A:19:GLY:O	1:A:108:ASP:HB2	2.17	0.45
1:A:35:LEU:HD22	1:A:37:PHE:HD1	1.81	0.45
1:A:191:VAL:O	1:A:219:ILE:HA	2.17	0.45
1:B:19:GLY:O	1:B:108:ASP:HB2	2.17	0.44
1:A:264:GLU:HG3	1:A:265:HIS:CD2	2.53	0.44
1:A:42:MET:HG3	1:B:118:HIS:CG	2.54	0.42
1:B:181:ARG:CZ	1:B:185:LEU:HD21	2.48	0.42
1:A:169:GLN:HA	1:A:169:GLN:OE1	2.19	0.42
1:A:33:ILE:HB	1:B:112:ASN:HB3	2.02	0.42
1:B:142:GLY:HA2	1:B:166:ASP:O	2.19	0.42
1:B:39:VAL:HG23	1:B:39:VAL:O	2.20	0.41
1:B:75:ALA:O	1:B:79:LEU:HG	2.20	0.41
1:A:117:PHE:O	1:A:119:PRO:HD3	2.21	0.41
1:B:57:LEU:HD23	1:B:64:ALA:HB2	2.03	0.41
1:A:166:ASP:CG	1:A:256:ARG:HE	2.29	0.40
1:A:195:GLU:O	1:A:199:VAL:HG23	2.21	0.40
1:A:95:LEU:HD22	1:A:124:GLN:CD	2.46	0.40
1:B:45:GLU:HG2	1:B:289:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:HIS:HD2	2:B:333:HOH:O	2.04	0.40
1:B:79:LEU:HA	1:B:82:MET:HE3	2.04	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	311/326 (95%)	307 (99%)	4 (1%)	0	100	100
1	B	301/326 (92%)	293 (97%)	8 (3%)	0	100	100
All	All	612/652 (94%)	600 (98%)	12 (2%)	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	242/255 (95%)	227 (94%)	15 (6%)	16	14
1	B	235/255 (92%)	222 (94%)	13 (6%)	19	18
All	All	477/510 (94%)	449 (94%)	28 (6%)	18	16

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	LEU
1	A	41	THR
1	A	87	LEU
1	A	153	THR
1	A	173	LEU
1	A	191	VAL
1	A	197	LYS
1	A	198	LEU
1	A	229	ARG
1	A	231	ARG
1	A	283	LYS
1	A	287	GLN
1	A	312	LYS
1	A	314	SER
1	B	18	GLU
1	B	32	LEU
1	B	87	LEU
1	B	97	ASP
1	B	107	THR
1	B	184	GLU
1	B	189	ILE
1	B	193	ASP
1	B	198	LEU
1	B	227	THR
1	B	232	ASP
1	B	264	GLU
1	B	296	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	76	GLN
1	A	128	ASN
1	A	236	GLN
1	B	126	HIS
1	B	129	HIS
1	B	224	HIS
1	B	286	HIS

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 oligosaccharides 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, 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	313/326 (96%)	0.02	4 (1%) 75 77	15, 24, 39, 49	0
1	B	303/326 (92%)	1.71	110 (36%) 1 1	26, 47, 70, 157	0
All	All	616/652 (94%)	0.85	114 (18%) 3 3	15, 34, 65, 157	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	9.5
1	B	4	LEU	7.0
1	B	5	ILE	6.9
1	B	3	THR	5.9
1	B	130	ALA	4.9
1	B	267	PHE	4.7
1	B	57	LEU	4.7
1	B	7	GLY	4.4
1	B	237	ILE	4.3
1	B	263	ILE	4.3
1	B	9	ILE	3.9
1	B	32	LEU	3.9
1	B	138	LEU	3.9
1	B	133	ALA	3.9
1	B	226	ALA	3.9
1	A	18	GLU	3.8
1	B	77	PRO	3.8
1	B	297	ALA	3.8
1	B	259	LEU	3.5
1	B	275	LEU	3.5
1	B	163	PHE	3.4
1	B	240	VAL	3.4
1	B	238	PRO	3.4
1	B	6	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	84	ALA	3.3
1	B	242	ALA	3.3
1	B	188	TYR	3.3
1	B	239	ALA	3.3
1	B	92	VAL	3.2
1	B	245	VAL	3.2
1	B	301	ALA	3.2
1	B	94	VAL	3.1
1	B	161	VAL	3.1
1	B	269	TRP	3.1
1	B	303	PHE	3.1
1	B	285	ALA	3.1
1	B	278	LEU	3.1
1	B	68	GLY	3.0
1	B	75	ALA	3.0
1	B	55	TYR	3.0
1	B	270	ALA	2.9
1	B	225	GLY	2.9
1	B	224	HIS	2.9
1	B	227	THR	2.8
1	B	272	ALA	2.8
1	B	299	ILE	2.8
1	B	8	SER	2.8
1	B	159	ALA	2.8
1	B	73	VAL	2.8
1	B	59	LEU	2.7
1	B	136	ILE	2.7
1	B	255	PHE	2.7
1	B	228	ILE	2.7
1	B	265	HIS	2.6
1	B	53	ILE	2.6
1	B	98	THR	2.6
1	B	295	THR	2.6
1	B	150	VAL	2.6
1	B	260	LEU	2.6
1	A	194	TYR	2.5
1	B	61	GLY	2.5
1	B	27	PRO	2.5
1	B	284	ILE	2.5
1	B	95	LEU	2.5
1	B	121	ALA	2.5
1	B	233	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	66	MET	2.4
1	B	123	MET	2.4
1	B	139	ALA	2.4
1	B	236	GLN	2.4
1	B	300	ASP	2.4
1	B	131	GLY	2.4
1	B	29	GLN	2.4
1	B	96	PRO	2.4
1	B	282	LEU	2.4
1	B	58	ASN	2.4
1	B	252	GLY	2.4
1	B	69	THR	2.3
1	B	280	GLY	2.3
1	A	287	GLN	2.3
1	B	261	TYR	2.3
1	B	26	LEU	2.3
1	B	42	MET	2.3
1	B	304	GLU	2.2
1	B	30	VAL	2.2
1	B	141	VAL	2.2
1	B	56	ALA	2.2
1	B	129	HIS	2.2
1	B	222	GLY	2.2
1	B	10	ALA	2.2
1	B	85	LEU	2.2
1	B	274	ARG	2.2
1	B	249	THR	2.2
1	B	246	ILE	2.1
1	B	67	MET	2.1
1	B	78	TYR	2.1
1	B	187	THR	2.1
1	B	31	HIS	2.1
1	B	126	HIS	2.1
1	B	250	GLY	2.1
1	B	277	SER	2.1
1	B	294	PRO	2.1
1	B	241	ARG	2.1
1	B	296	ARG	2.1
1	B	64	ALA	2.1
1	B	41	THR	2.1
1	B	231	ARG	2.1
1	B	86	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	314	SER	2.1
1	B	11	TYR	2.0
1	B	148	GLY	2.0
1	B	189	ILE	2.0
1	B	162	PRO	2.0
1	B	257	GLY	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 oligosaccharides 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.