Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 12:33 PM JST

PDB ID	:	6J25
Title	:	CTX-M-64 beta-lactamase mutant-S130T
Authors	:	Cheng, Q.; Chen, S.
Deposited on	:	2018-12-30
Resolution	:	1.20 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:

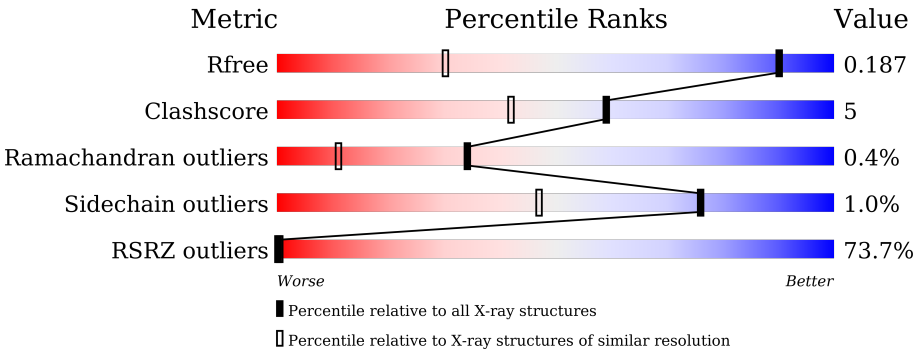
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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 <=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	274	70% 90% 5% 5%
1	B	274	69% 87% 8% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4520 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	1	0
			1953	1216	351	380	6			
1	B	260	Total	C	N	O	S	0	1	0
			1953	1216	351	380	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	expression tag	UNP C8CP57
A	15	SER	-	expression tag	UNP C8CP57
A	16	HIS	-	expression tag	UNP C8CP57
A	17	MET	-	expression tag	UNP C8CP57
A	18	ALA	-	expression tag	UNP C8CP57
A	19	SER	-	expression tag	UNP C8CP57
A	20	GLY	-	expression tag	UNP C8CP57
A	21	GLY	-	expression tag	UNP C8CP57
A	22	THR	-	expression tag	UNP C8CP57
A	23	GLU	-	expression tag	UNP C8CP57
A	24	LEU	-	expression tag	UNP C8CP57
A	130	THR	SER	engineered mutation	UNP C8CP57
B	14	GLY	-	expression tag	UNP C8CP57
B	15	SER	-	expression tag	UNP C8CP57
B	16	HIS	-	expression tag	UNP C8CP57
B	17	MET	-	expression tag	UNP C8CP57
B	18	ALA	-	expression tag	UNP C8CP57
B	19	SER	-	expression tag	UNP C8CP57
B	20	GLY	-	expression tag	UNP C8CP57
B	21	GLY	-	expression tag	UNP C8CP57
B	22	THR	-	expression tag	UNP C8CP57
B	23	GLU	-	expression tag	UNP C8CP57
B	24	LEU	-	expression tag	UNP C8CP57
B	130	THR	SER	engineered mutation	UNP C8CP57

- Molecule 2 is water.

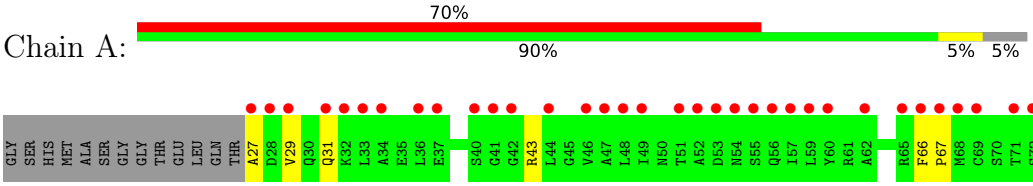
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	295	Total O 295 295	0	0
2	B	319	Total O 319 319	0	0

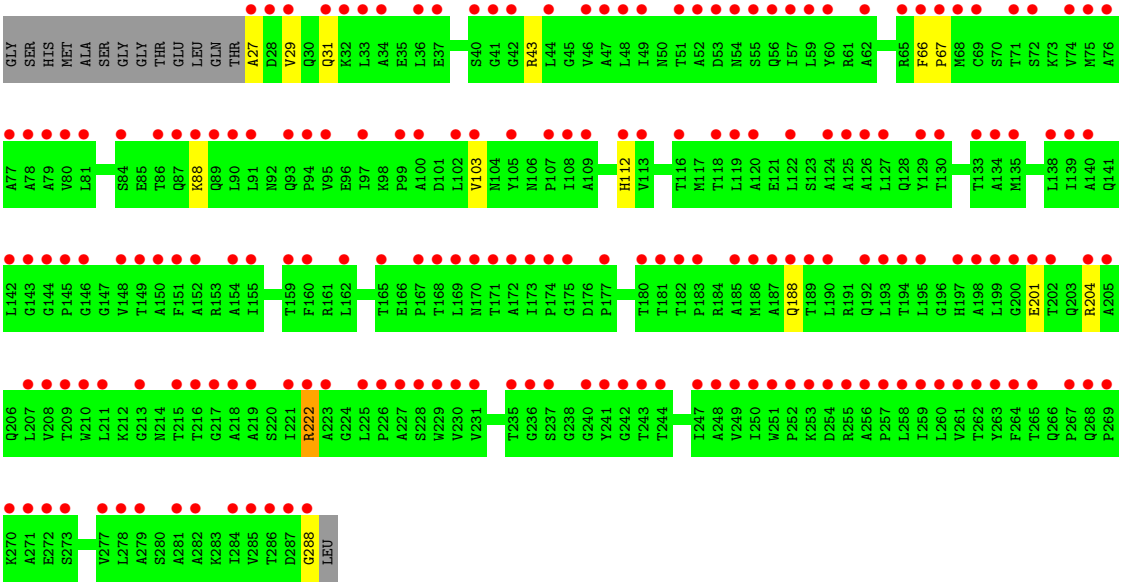
3 Residue-property plots (i)

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: Beta-lactamase

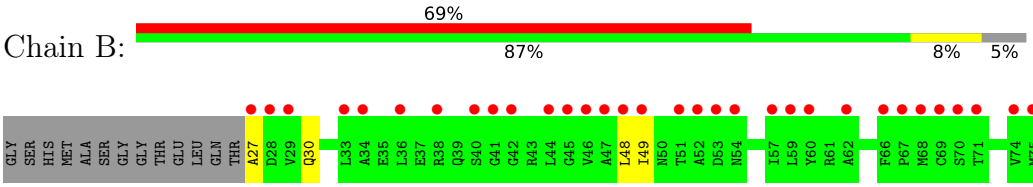
Chain A:

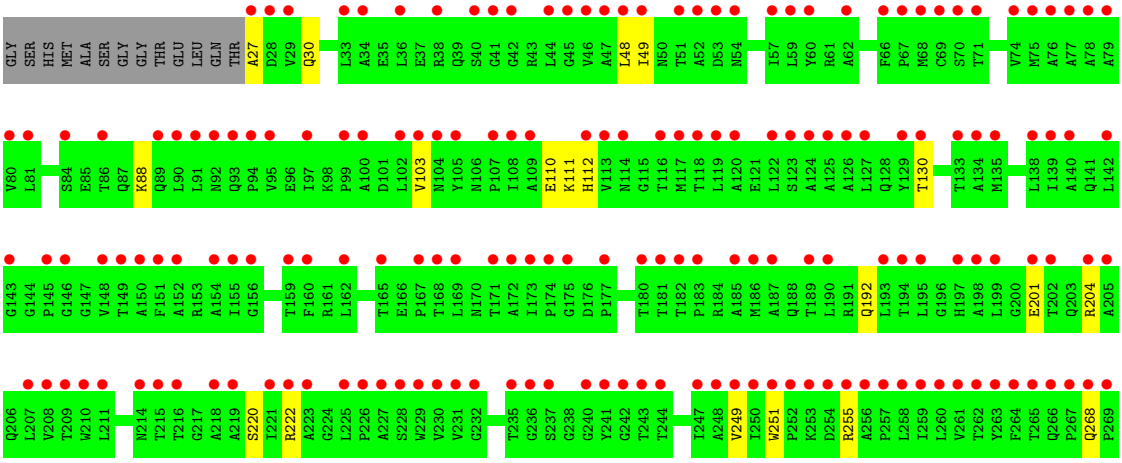


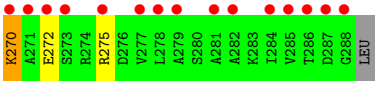


• Molecule 1: Beta-lactamase

Chain B:






K270
A271
E272
S273
R274
R275
D276
V277
L278
A279
S280
A281
A282
K283
I284
V285
T286
D287
G288
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.25Å 105.99Å 47.97Å 90.00° 100.73° 90.00°	Depositor
Resolution (Å)	52.99 – 1.20 47.13 – 1.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (52.99-1.20) 98.3 (47.13-1.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.55 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.182 , 0.194 0.174 , 0.187	Depositor DCC
R_{free} test set	6736 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	10.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4520	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.23	0/1986	1.08	0/2703
1	B	1.26	0/1986	1.13	1/2703 (0.0%)
All	All	1.24	0/3972	1.10	1/5406 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	255	ARG	NE-CZ-NH2	-5.45	117.57	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1953	0	1983	12	0
1	B	1953	0	1983	25	0
2	A	295	0	0	5	1
2	B	319	0	0	10	1
All	All	4520	0	3966	37	1

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 (37) 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:201:GLU:OE1	1:A:204:ARG:NH2	1.91	1.01
1:B:222:ARG:HG3	2:B:400:HOH:O	1.67	0.92
1:B:270:LYS:HE3	1:B:270:LYS:H	1.38	0.88
1:A:288:GLY:O	2:A:301:HOH:O	2.00	0.79
1:B:222:ARG:NH2	2:B:302:HOH:O	2.16	0.77
1:B:270:LYS:HE3	1:B:270:LYS:N	2.05	0.70
1:B:201:GLU:OE2	1:B:204:ARG:NH1	2.24	0.70
1:B:110:GLU:HG3	1:B:111:LYS:HE3	1.78	0.66
1:B:270:LYS:H	1:B:270:LYS:CE	2.09	0.63
1:A:222:ARG:O	1:A:222:ARG:HD3	2.01	0.60
1:A:29:VAL:HG12	2:A:498:HOH:O	2.02	0.59
1:B:110:GLU:HG3	1:B:111:LYS:CE	2.32	0.59
1:B:222:ARG:CZ	2:B:302:HOH:O	2.49	0.58
1:A:43:ARG:NH2	1:A:66:PHE:CZ	2.73	0.56
1:B:192:GLN:HE21	1:B:192:GLN:HA	1.71	0.55
1:B:272:GLU:H	1:B:272:GLU:CD	2.11	0.54
1:A:67:PRO:HD3	2:A:530:HOH:O	2.09	0.52
1:B:27:ALA:HB1	1:B:30:GLN:HB2	1.90	0.52
1:B:88:LYS:HD2	2:B:361:HOH:O	2.12	0.49
1:A:112:HIS:HE1	2:A:517:HOH:O	1.96	0.48
1:B:112:HIS:HE1	2:B:561:HOH:O	1.96	0.48
1:B:222:ARG:NH1	2:B:302:HOH:O	2.45	0.47
1:B:220:SER:OG	1:B:275:ARG:HG2	2.13	0.47
1:A:27:ALA:N	1:A:31:GLN:OE1	2.48	0.46
1:A:222:ARG:HD3	1:A:222:ARG:C	2.36	0.46
1:A:188:GLN:HG3	2:A:437:HOH:O	2.15	0.45
1:A:201:GLU:OE1	1:A:204:ARG:CZ	2.62	0.45
1:B:48:LEU:HD13	1:B:49:ILE:N	2.31	0.45
1:B:88:LYS:HE3	2:B:325:HOH:O	2.15	0.45
1:B:48:LEU:HD13	1:B:48:LEU:C	2.38	0.44
1:B:268:GLN:HB3	1:B:270:LYS:HZ2	1.82	0.43
1:B:110:GLU:CG	1:B:111:LYS:HE3	2.46	0.43
1:B:27:ALA:CA	2:B:530:HOH:O	2.66	0.42
1:A:27:ALA:HB3	1:A:31:GLN:OE1	2.19	0.42
1:B:249:VAL:HG13	1:B:251:TRP:CZ3	2.55	0.42
1:B:27:ALA:HA	2:B:530:HOH:O	2.19	0.42
1:B:27:ALA:HB1	2:B:530:HOH:O	2.19	0.40

All (1) 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)
2:A:571:HOH:O	2:B:428:HOH:O[1_556]	2.09	0.11

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	259/274 (94%)	254 (98%)	4 (2%)	1 (0%)	34 11
1	B	259/274 (94%)	253 (98%)	5 (2%)	1 (0%)	34 11
All	All	518/548 (94%)	507 (98%)	9 (2%)	2 (0%)	34 11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	B	103	VAL

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	205/214 (96%)	203 (99%)	2 (1%)	76 47
1	B	205/214 (96%)	203 (99%)	2 (1%)	76 47
All	All	410/428 (96%)	406 (99%)	4 (1%)	76 47

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
1	A	222	ARG
1	B	130	THR
1	B	270	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	112	HIS
1	A	188	GLN
1	A	192	GLN
1	B	92	ASN
1	B	112	HIS
1	B	192	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 monosaccharides 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^{th} 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	260/274 (94%)	2.91	193 (74%)	0	0	6, 9, 18, 30	0
1	B	260/274 (94%)	2.85	190 (73%)	0	0	6, 9, 19, 42	0
All	All	520/548 (94%)	2.88	383 (73%)	0	0	6, 9, 19, 42	0

All (383) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ALA	15.0
1	A	288	GLY	10.2
1	A	66	PHE	9.9
1	B	27	ALA	8.3
1	B	229	TRP	7.4
1	B	227	ALA	6.0
1	B	288	GLY	5.9
1	B	231	VAL	5.7
1	B	94	PRO	5.6
1	A	250	ILE	5.5
1	B	263	TYR	5.3
1	B	251	TRP	5.3
1	A	29	VAL	5.2
1	B	230	VAL	5.2
1	A	41	GLY	5.2
1	A	284	ILE	5.1
1	B	261	VAL	5.0
1	B	252	PRO	5.0
1	B	90	LEU	4.9
1	A	251	TRP	4.9
1	A	230	VAL	4.9
1	B	139	ILE	4.9
1	A	263	TYR	4.8
1	A	88	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	231	VAL	4.7
1	B	259	ILE	4.7
1	B	210	TRP	4.6
1	A	229	TRP	4.6
1	B	284	ILE	4.6
1	B	155	ILE	4.5
1	B	221	ILE	4.5
1	A	210	TRP	4.5
1	A	28	ASP	4.5
1	A	46	VAL	4.4
1	B	148	VAL	4.4
1	B	226	PRO	4.4
1	A	33	LEU	4.3
1	B	47	ALA	4.3
1	A	138	LEU	4.3
1	B	277	VAL	4.3
1	A	105	TYR	4.3
1	A	221	ILE	4.3
1	A	259	ILE	4.3
1	B	250	ILE	4.3
1	A	207	LEU	4.2
1	A	261	VAL	4.2
1	B	247	ILE	4.2
1	A	69	CYS	4.2
1	A	36	LEU	4.2
1	A	195	LEU	4.2
1	B	91	LEU	4.2
1	B	95	VAL	4.2
1	B	97	ILE	4.2
1	B	249	VAL	4.2
1	A	108	ILE	4.2
1	A	247	ILE	4.2
1	B	49	ILE	4.2
1	A	127	LEU	4.1
1	A	227	ALA	4.1
1	B	256	ALA	4.1
1	A	148	VAL	4.1
1	B	66	PHE	4.1
1	A	90	LEU	4.1
1	A	139	ILE	4.1
1	A	249	VAL	4.1
1	A	252	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	162	LEU	4.0
1	B	173	ILE	4.0
1	B	80	VAL	4.0
1	B	218	ALA	4.0
1	B	109	ALA	4.0
1	A	48	LEU	4.0
1	B	36	LEU	4.0
1	A	122	LEU	3.9
1	A	99	PRO	3.9
1	B	271	ALA	3.9
1	A	258	LEU	3.9
1	B	199	LEU	3.9
1	A	95	VAL	3.9
1	A	113[A]	VAL	3.9
1	B	113[A]	VAL	3.9
1	B	103	VAL	3.8
1	B	69	CYS	3.8
1	B	48	LEU	3.8
1	B	241	TYR	3.8
1	A	225	LEU	3.8
1	B	44	LEU	3.8
1	B	211	LEU	3.8
1	A	77	ALA	3.8
1	A	87	GLN	3.8
1	B	193	LEU	3.8
1	B	207	LEU	3.8
1	B	57	ILE	3.7
1	A	91	LEU	3.7
1	A	169	LEU	3.7
1	A	257	PRO	3.7
1	A	277	VAL	3.7
1	B	208	VAL	3.7
1	B	152	ALA	3.7
1	A	102	LEU	3.7
1	B	285	VAL	3.7
1	B	100	ALA	3.7
1	B	38	ARG	3.7
1	A	264	PHE	3.7
1	B	160	PHE	3.7
1	B	264	PHE	3.7
1	A	81	LEU	3.7
1	A	190	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	94	PRO	3.6
1	A	149	THR	3.6
1	A	44	LEU	3.6
1	A	49	ILE	3.6
1	A	285	VAL	3.6
1	A	279	ALA	3.6
1	A	71	THR	3.6
1	A	260	LEU	3.6
1	B	119	LEU	3.6
1	B	127	LEU	3.6
1	A	47	ALA	3.6
1	B	108	ILE	3.6
1	B	150	ALA	3.6
1	B	138	LEU	3.6
1	B	278	LEU	3.6
1	A	185	ALA	3.5
1	A	256	ALA	3.5
1	B	52	ALA	3.5
1	A	199	LEU	3.5
1	B	81	LEU	3.5
1	B	260	LEU	3.5
1	A	173	ILE	3.5
1	A	89	GLN	3.5
1	A	78	ALA	3.5
1	A	152	ALA	3.5
1	B	28	ASP	3.5
1	A	160	PHE	3.5
1	B	29	VAL	3.5
1	B	74	VAL	3.5
1	B	219	ALA	3.5
1	A	241	TYR	3.5
1	A	177	PRO	3.5
1	B	272	GLU	3.5
1	B	151	PHE	3.5
1	B	189	THR	3.4
1	A	278	LEU	3.4
1	B	46	VAL	3.4
1	A	107	PRO	3.4
1	A	168	THR	3.4
1	A	286	THR	3.4
1	B	51	THR	3.4
1	B	105	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	287	ASP	3.4
1	A	211	LEU	3.4
1	B	122	LEU	3.4
1	B	190	LEU	3.4
1	B	225	LEU	3.4
1	A	182	THR	3.4
1	A	151	PHE	3.3
1	A	126	ALA	3.3
1	B	145	PRO	3.3
1	B	222	ARG	3.3
1	A	86	THR	3.3
1	A	142	LEU	3.3
1	A	103	VAL	3.3
1	B	99	PRO	3.3
1	B	174	PRO	3.3
1	A	100	ALA	3.3
1	B	124	ALA	3.3
1	B	270	LYS	3.3
1	B	171	THR	3.3
1	A	60	TYR	3.3
1	A	187	ALA	3.3
1	B	182	THR	3.3
1	B	235	THR	3.3
1	A	62	ALA	3.3
1	A	125	ALA	3.3
1	B	223	ALA	3.3
1	A	59	LEU	3.3
1	A	222	ARG	3.3
1	B	33	LEU	3.3
1	A	74	VAL	3.3
1	B	253	LYS	3.2
1	A	120	ALA	3.2
1	A	124	ALA	3.2
1	B	102	LEU	3.2
1	B	118	THR	3.2
1	B	254	ASP	3.2
1	A	218	ALA	3.2
1	B	134	ALA	3.2
1	A	67	PRO	3.2
1	A	267	PRO	3.2
1	A	262	THR	3.2
1	A	97	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	281	ALA	3.2
1	B	140	ALA	3.2
1	A	265	THR	3.2
1	B	71	THR	3.2
1	B	202	THR	3.2
1	A	193	LEU	3.2
1	B	60	TYR	3.2
1	B	287	ASP	3.2
1	B	267	PRO	3.1
1	A	57	ILE	3.1
1	A	165	THR	3.1
1	B	130	THR	3.1
1	A	76	ALA	3.1
1	B	125	ALA	3.1
1	B	187	ALA	3.1
1	A	118	THR	3.1
1	B	149	THR	3.1
1	B	269	PRO	3.1
1	A	134	ALA	3.1
1	A	271	ALA	3.1
1	A	129	TYR	3.1
1	A	51	THR	3.1
1	A	171	THR	3.1
1	B	255	ARG	3.1
1	B	67	PRO	3.1
1	A	155	ILE	3.1
1	B	78	ALA	3.1
1	B	228	SER	3.1
1	A	145	PRO	3.1
1	A	208	VAL	3.1
1	B	248	ALA	3.0
1	B	282	ALA	3.0
1	A	180	THR	3.0
1	B	181	THR	3.0
1	A	269	PRO	3.0
1	B	195	LEU	3.0
1	A	282	ALA	3.0
1	B	185	ALA	3.0
1	A	226	PRO	3.0
1	B	273	SER	3.0
1	B	59	LEU	3.0
1	A	219	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	146	GLY	3.0
1	A	181	THR	3.0
1	A	209	THR	3.0
1	A	31	GLN	3.0
1	B	142	LEU	3.0
1	B	258	LEU	3.0
1	A	80	VAL	3.0
1	A	215	THR	3.0
1	A	244	THR	3.0
1	B	209	THR	3.0
1	B	244	THR	3.0
1	B	154	ALA	2.9
1	A	174	PRO	2.9
1	A	119	LEU	2.9
1	B	169	LEU	2.9
1	A	130	THR	2.9
1	B	262	THR	2.9
1	B	126	ALA	2.9
1	A	202	THR	2.9
1	B	194	THR	2.9
1	B	183	PRO	2.9
1	A	197	HIS	2.9
1	B	62	ALA	2.9
1	B	120	ALA	2.9
1	B	205	ALA	2.9
1	A	253	LYS	2.9
1	A	188	GLN	2.9
1	A	75	MET	2.9
1	B	135	MET	2.9
1	A	143	GLY	2.9
1	B	257	PRO	2.9
1	A	194	THR	2.8
1	B	129	TYR	2.8
1	B	159	THR	2.8
1	B	265	THR	2.8
1	A	53	ASP	2.8
1	A	183	PRO	2.8
1	A	228	SER	2.8
1	A	52	ALA	2.8
1	A	243	THR	2.8
1	B	243	THR	2.8
1	A	237	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	34	ALA	2.8
1	A	236	GLY	2.8
1	A	167	PRO	2.8
1	B	133	THR	2.8
1	B	198	ALA	2.8
1	B	281	ALA	2.8
1	A	116	THR	2.8
1	B	116	THR	2.8
1	B	168	THR	2.8
1	B	162	LEU	2.8
1	A	201	GLU	2.8
1	B	275	ARG	2.8
1	A	235	THR	2.7
1	B	180	THR	2.7
1	B	286	THR	2.7
1	A	172	ALA	2.7
1	A	34	ALA	2.7
1	B	279	ALA	2.7
1	B	86	THR	2.7
1	A	254	ASP	2.7
1	B	104	ASN	2.7
1	A	109	ALA	2.7
1	A	223	ALA	2.7
1	B	77	ALA	2.7
1	A	140	ALA	2.6
1	A	65	ARG	2.6
1	A	216	THR	2.6
1	B	215	THR	2.6
1	B	172	ALA	2.6
1	A	84	SER	2.6
1	B	75	MET	2.6
1	B	165	THR	2.6
1	B	268	GLN	2.6
1	A	248	ALA	2.6
1	A	144	GLY	2.6
1	B	232	GLY	2.6
1	A	198	ALA	2.6
1	B	76	ALA	2.6
1	B	167	PRO	2.6
1	B	177	PRO	2.6
1	B	156	GLY	2.5
1	B	216	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	93	GLN	2.5
1	B	40	SER	2.5
1	A	205	ALA	2.5
1	B	143	GLY	2.5
1	B	112	HIS	2.5
1	A	159	THR	2.5
1	A	68	MET	2.5
1	A	135	MET	2.5
1	A	200	GLY	2.5
1	B	242	GLY	2.5
1	A	54	ASN	2.5
1	B	107	PRO	2.5
1	B	175	GLY	2.5
1	B	92	ASN	2.4
1	A	189	THR	2.4
1	B	42	GLY	2.4
1	B	45	GLY	2.4
1	B	79	ALA	2.4
1	A	270	LYS	2.4
1	A	40	SER	2.4
1	A	192	GLN	2.4
1	A	217	GLY	2.4
1	B	41	GLY	2.4
1	A	133	THR	2.4
1	A	186	MET	2.4
1	B	186	MET	2.4
1	B	53	ASP	2.4
1	B	237	SER	2.4
1	A	37	GLU	2.4
1	A	272	GLU	2.4
1	B	68	MET	2.4
1	A	150	ALA	2.3
1	A	154	ALA	2.3
1	A	213	GLY	2.3
1	A	273	SER	2.3
1	B	214	ASN	2.3
1	B	240	GLY	2.3
1	A	56	GLN	2.3
1	A	32	LYS	2.3
1	A	42	GLY	2.3
1	A	93	GLN	2.3
1	B	204	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	54	ASN	2.2
1	A	268	GLN	2.2
1	A	79	ALA	2.2
1	B	201	GLU	2.2
1	A	55	SER	2.2
1	B	84	SER	2.2
1	A	255	ARG	2.2
1	B	123	SER	2.2
1	A	170	ASN	2.1
1	B	70	SER	2.1
1	A	146	GLY	2.1
1	B	89	GLN	2.1
1	A	72	SER	2.1
1	B	117	MET	2.1
1	B	266	GLN	2.1
1	B	236	GLY	2.0
1	A	175	GLY	2.0
1	A	240	GLY	2.0
1	A	204	ARG	2.0
1	A	112	HIS	2.0
1	B	197	HIS	2.0
1	A	242	GLY	2.0
1	B	114	ASN	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 monosaccharides 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.