



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 05:05 PM UTC

PDB ID : 3BZC / pdb_00003bzc
Title : Crystal Structure of the Tex protein from Pseudomonas aeruginosa, crystal form I
Authors : Johnson, S.J.; Close, D.; Hill, C.P.
Deposited on : 2008-01-17
Resolution : 2.27 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

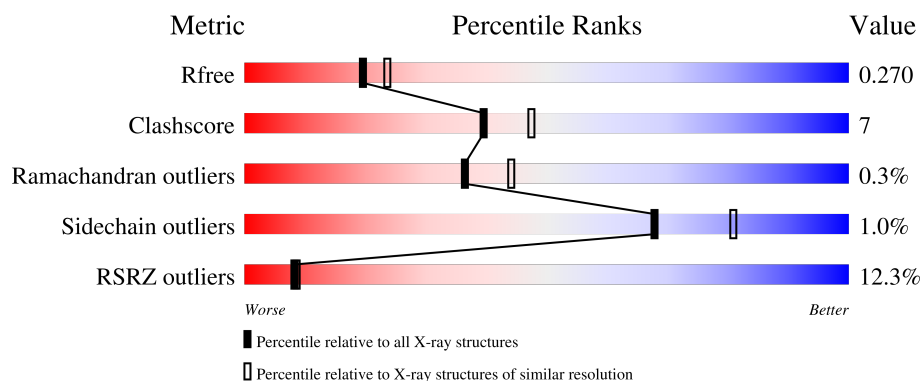
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	785	11% 77% 15% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5691 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 Tex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5618	3537	988	1078	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	780	HIS	-	expression tag	UNP Q9HTY8
A	781	HIS	-	expression tag	UNP Q9HTY8
A	782	HIS	-	expression tag	UNP Q9HTY8
A	783	HIS	-	expression tag	UNP Q9HTY8
A	784	HIS	-	expression tag	UNP Q9HTY8
A	785	HIS	-	expression tag	UNP Q9HTY8

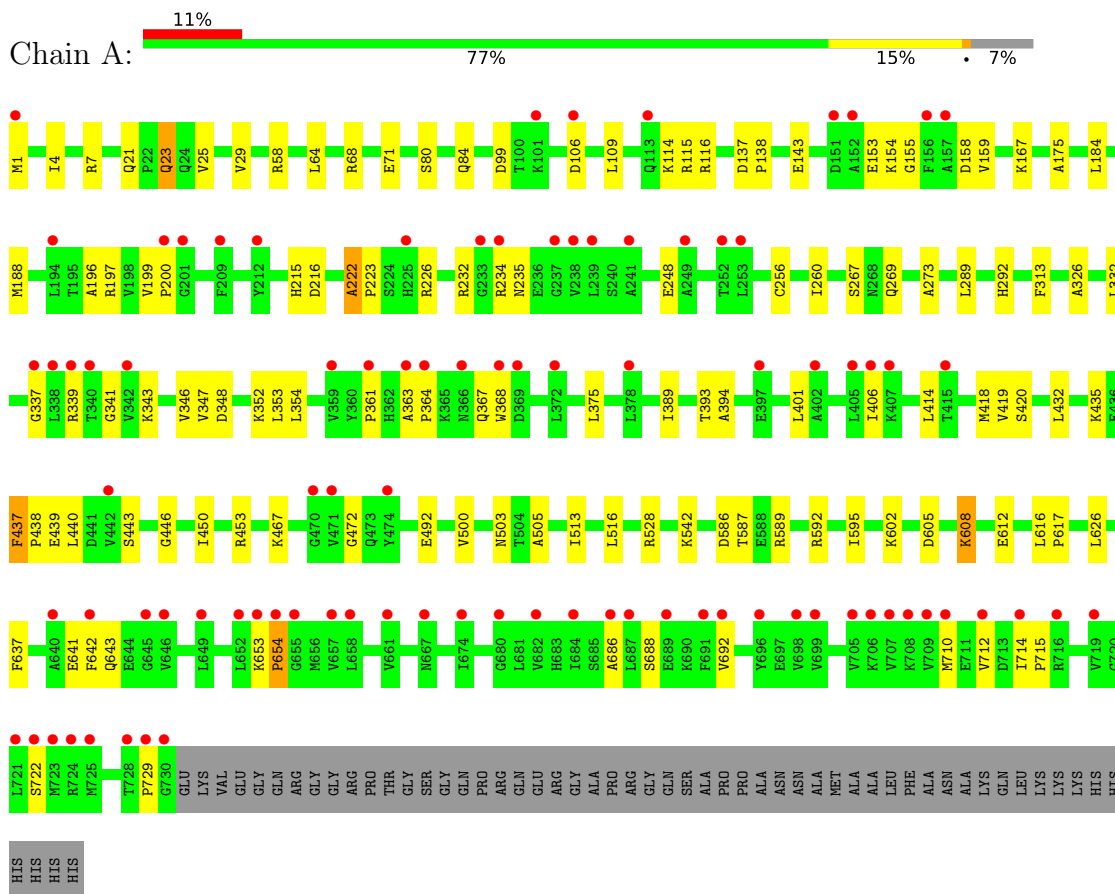
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		

3 Residue-property plots

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: Tex



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.16Å 131.85Å 144.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.27 49.28 – 2.27	Depositor EDS
% Data completeness (in resolution range)	75.7 (49.28-2.27) 75.7 (49.28-2.27)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.27Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.240 , 0.274 0.232 , 0.270	Depositor DCC
R_{free} test set	2054 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.789	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.9	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	0.94	EDS
Total number of atoms	5691	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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	0.41	0/5707	0.86	13/7721 (0.2%)

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.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	154	LYS	N-CA-C	-10.01	101.01	113.02
1	A	114	LYS	N-CA-C	-7.70	97.36	108.60
1	A	137	ASP	CA-C-N	6.07	126.19	119.87
1	A	137	ASP	C-N-CA	6.07	126.19	119.87
1	A	437	PHE	CA-C-N	5.57	125.09	119.19
1	A	437	PHE	C-N-CA	5.57	125.09	119.19
1	A	605	ASP	CA-C-N	5.24	125.30	119.32
1	A	605	ASP	C-N-CA	5.24	125.30	119.32
1	A	222	ALA	CA-C-N	5.18	124.94	119.76
1	A	222	ALA	C-N-CA	5.18	124.94	119.76
1	A	116	ARG	N-CA-C	5.09	118.62	111.90
1	A	21	GLN	CA-C-N	5.04	124.70	119.56
1	A	21	GLN	C-N-CA	5.04	124.70	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Peptide

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	5618	0	5713	76	0
2	A	73	0	0	2	0
All	All	5691	0	5713	76	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 7.

All (76) 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:710:MET:HE3	1:A:729:PRO:HA	1.57	0.86
1:A:406:ILE:HG12	1:A:414:LEU:HB2	1.62	0.80
1:A:368:TRP:CH2	1:A:401:LEU:HG	2.25	0.72
1:A:175:ALA:HA	1:A:289:LEU:HD21	1.76	0.68
1:A:437:PHE:HB3	1:A:440:LEU:HD12	1.78	0.66
1:A:313:PHE:CE2	1:A:472:GLY:HA3	2.31	0.65
1:A:363:ALA:HB3	1:A:364:PRO:HD3	1.78	0.63
1:A:587:THR:O	1:A:589:ARG:HG3	2.01	0.61
1:A:223:PRO:HG3	1:A:226:ARG:NH2	2.17	0.60
1:A:313:PHE:CD2	1:A:472:GLY:HA3	2.37	0.59
1:A:25:VAL:O	1:A:29:VAL:HG23	2.04	0.58
1:A:467:LYS:HG3	2:A:797:HOH:O	2.04	0.58
1:A:256:CYS:O	1:A:260:ILE:HG13	2.04	0.57
1:A:1:MET:HE1	1:A:71:GLU:HG3	1.86	0.56
1:A:435:LYS:HG3	2:A:835:HOH:O	2.07	0.55
1:A:513:ILE:HB	1:A:516:LEU:HD12	1.88	0.55
1:A:438:PRO:HD2	1:A:439:GLU:OE2	2.07	0.54
1:A:197:ARG:NH1	1:A:216:ASP:OD2	2.41	0.53
1:A:420:SER:HB3	1:A:453:ARG:NH1	2.24	0.52
1:A:503:ASN:HA	1:A:528:ARG:HD2	1.91	0.52
1:A:710:MET:SD	1:A:722:SER:HB3	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:HA	1:A:352:LYS:O	2.10	0.51
1:A:153:GLU:C	1:A:155:GLY:H	2.18	0.51
1:A:332:LEU:HD21	1:A:375:LEU:HD22	1.92	0.51
1:A:419:VAL:CG1	1:A:453:ARG:HD3	2.41	0.51
1:A:326:ALA:HA	1:A:637:PHE:CG	2.47	0.50
1:A:361:PRO:CB	1:A:401:LEU:HD11	2.40	0.50
1:A:446:GLY:O	1:A:450:ILE:HG13	2.11	0.50
1:A:232:ARG:C	1:A:234:ARG:H	2.21	0.49
1:A:542:LYS:N	1:A:542:LYS:HD2	2.29	0.48
1:A:267:SER:HB3	1:A:269:GLN:OE1	2.14	0.48
1:A:343:LYS:HE2	1:A:443:SER:HB2	1.95	0.48
1:A:654:PRO:HD3	1:A:712:VAL:CG1	2.44	0.48
1:A:184:LEU:O	1:A:188:MET:HG2	2.14	0.47
1:A:688:SER:HB3	1:A:692:VAL:HG23	1.95	0.47
1:A:616:LEU:HB3	1:A:617:PRO:HD3	1.96	0.47
1:A:612:GLU:H	1:A:612:GLU:CD	2.23	0.47
1:A:348:ASP:HB3	1:A:354:LEU:HD11	1.97	0.46
1:A:199:VAL:HB	1:A:200:PRO:HD2	1.97	0.46
1:A:714:ILE:HB	1:A:715:PRO:HD3	1.98	0.46
1:A:654:PRO:HD3	1:A:712:VAL:HG12	1.98	0.46
1:A:686:ALA:HB1	1:A:722:SER:O	2.17	0.45
1:A:80:SER:O	1:A:84:GLN:HG3	2.16	0.45
1:A:595:ILE:HA	1:A:626:LEU:O	2.17	0.45
1:A:326:ALA:HA	1:A:637:PHE:CD2	2.52	0.45
1:A:58:ARG:NH2	1:A:492:GLU:OE2	2.38	0.44
1:A:332:LEU:HD12	1:A:346:VAL:HG22	1.98	0.44
1:A:641:GLU:O	1:A:642:PHE:HB2	2.17	0.44
1:A:393:THR:O	1:A:394:ALA:HB3	2.18	0.44
1:A:710:MET:HE2	1:A:710:MET:HB3	1.90	0.44
1:A:602:LYS:HB3	1:A:602:LYS:HE2	1.64	0.43
1:A:158:ASP:OD1	1:A:159:VAL:N	2.50	0.43
1:A:109:LEU:HA	1:A:109:LEU:HD23	1.83	0.43
1:A:346:VAL:O	1:A:353:LEU:HD12	2.19	0.43
1:A:196:ALA:HB3	1:A:215:HIS:HB3	2.01	0.43
1:A:389:ILE:HB	1:A:418:MET:SD	2.58	0.42
1:A:234:ARG:O	1:A:235:ASN:C	2.63	0.42
1:A:337:GLY:HA3	1:A:341:GLY:O	2.20	0.42
1:A:138:PRO:HA	1:A:273:ALA:HB3	2.02	0.42
1:A:653:LYS:HA	1:A:654:PRO:HD2	1.90	0.42
1:A:64:LEU:O	1:A:68:ARG:HG3	2.19	0.42
1:A:232:ARG:C	1:A:234:ARG:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLN:CD	1:A:23:GLN:C	2.87	0.42
1:A:143:GLU:H	1:A:143:GLU:CD	2.27	0.41
1:A:222:ALA:HA	1:A:223:PRO:HD2	1.86	0.41
1:A:586:ASP:OD2	1:A:608:LYS:HE2	2.20	0.41
1:A:248:GLU:O	1:A:248:GLU:HG3	2.19	0.41
1:A:106:ASP:OD1	1:A:106:ASP:C	2.64	0.41
1:A:292:HIS:ND1	1:A:292:HIS:C	2.78	0.41
1:A:7:ARG:NH1	1:A:99:ASP:HB2	2.35	0.41
1:A:500:VAL:HG13	1:A:505:ALA:HB2	2.03	0.41
1:A:641:GLU:C	1:A:643:GLN:H	2.28	0.41
1:A:1:MET:SD	1:A:4:ILE:HG13	2.61	0.40
1:A:223:PRO:CG	1:A:226:ARG:NH2	2.84	0.40
1:A:184:LEU:HA	1:A:184:LEU:HD23	1.84	0.40
1:A:361:PRO:HB2	1:A:401:LEU:HD11	2.03	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	728/785 (93%)	689 (95%)	37 (5%)	2 (0%)	36	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	ARG
1	A	654	PRO

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	595/635 (94%)	589 (99%)	6 (1%)	68 81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	167	LYS
1	A	367	GLN
1	A	432	LEU
1	A	592	ARG
1	A	608	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	120	GLN
1	A	367	GLN
1	A	473	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 oligosaccharides 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	730/785 (92%)	0.76	90 (12%) 8 8	34, 59, 111, 131	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	VAL	6.5
1	A	725	MET	4.5
1	A	342	VAL	4.4
1	A	729	PRO	4.3
1	A	200	PRO	4.1
1	A	151	ASP	3.6
1	A	714	ILE	3.6
1	A	709	VAL	3.5
1	A	233	GLY	3.5
1	A	646	VAL	3.4
1	A	640	ALA	3.4
1	A	253	LEU	3.3
1	A	723	MET	3.3
1	A	338	LEU	3.3
1	A	654	PRO	3.3
1	A	722	SER	3.3
1	A	686	ALA	3.3
1	A	209	PHE	3.3
1	A	201	GLY	3.2
1	A	225	HIS	3.2
1	A	406	ILE	3.1
1	A	707	VAL	3.1
1	A	721	LEU	3.1
1	A	728	THR	3.1
1	A	402	ALA	3.1
1	A	407	LYS	3.1
1	A	238	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	652	LEU	2.9
1	A	658	LEU	2.9
1	A	687	LEU	2.9
1	A	364	PRO	2.9
1	A	372	LEU	2.9
1	A	340	THR	2.9
1	A	655	GLY	2.8
1	A	712	VAL	2.8
1	A	642	PHE	2.8
1	A	470	GLY	2.8
1	A	361	PRO	2.7
1	A	106	ASP	2.7
1	A	152	ALA	2.7
1	A	363	ALA	2.7
1	A	710	MET	2.7
1	A	474	TYR	2.7
1	A	337	GLY	2.7
1	A	716	ARG	2.6
1	A	369	ASP	2.6
1	A	405	LEU	2.5
1	A	708	LYS	2.5
1	A	674	ILE	2.5
1	A	696	TYR	2.5
1	A	730	GLY	2.5
1	A	415	THR	2.5
1	A	649	LEU	2.5
1	A	157	ALA	2.5
1	A	661	VAL	2.4
1	A	698	VAL	2.4
1	A	657	VAL	2.4
1	A	699	VAL	2.4
1	A	368	TRP	2.4
1	A	212	TYR	2.4
1	A	366	ASN	2.4
1	A	653	LYS	2.4
1	A	667	ASN	2.4
1	A	359	VAL	2.4
1	A	692	VAL	2.4
1	A	378	LEU	2.3
1	A	645	GLY	2.3
1	A	689	GLU	2.3
1	A	691	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	237	GLY	2.3
1	A	680	GLY	2.3
1	A	682	VAL	2.3
1	A	724	ARG	2.2
1	A	249	ALA	2.2
1	A	706	LYS	2.2
1	A	719	VAL	2.2
1	A	234	ARG	2.2
1	A	239	LEU	2.2
1	A	101	LYS	2.2
1	A	113	GLN	2.2
1	A	156	PHE	2.1
1	A	194	LEU	2.1
1	A	442	VAL	2.1
1	A	397	GLU	2.1
1	A	684	ILE	2.1
1	A	241	ALA	2.1
1	A	705	VAL	2.1
1	A	1	MET	2.0
1	A	339	ARG	2.0
1	A	252	THR	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.