



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:55 PM GMT

PDB ID : 3BZC
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 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>

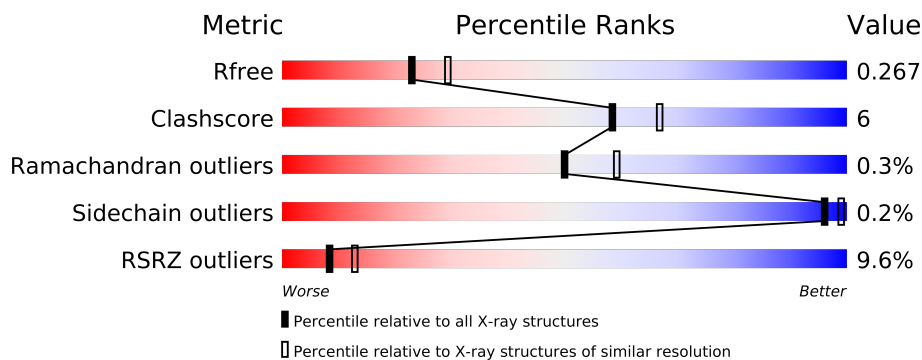
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.27 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}	66092	3861 (2.30-2.26)
Clashscore	79885	4801 (2.30-2.26)
Ramachandran outliers	78287	4729 (2.30-2.26)
Sidechain outliers	78261	4728 (2.30-2.26)
RSRZ outliers	66119	3864 (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 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	785	

2 Entry composition

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

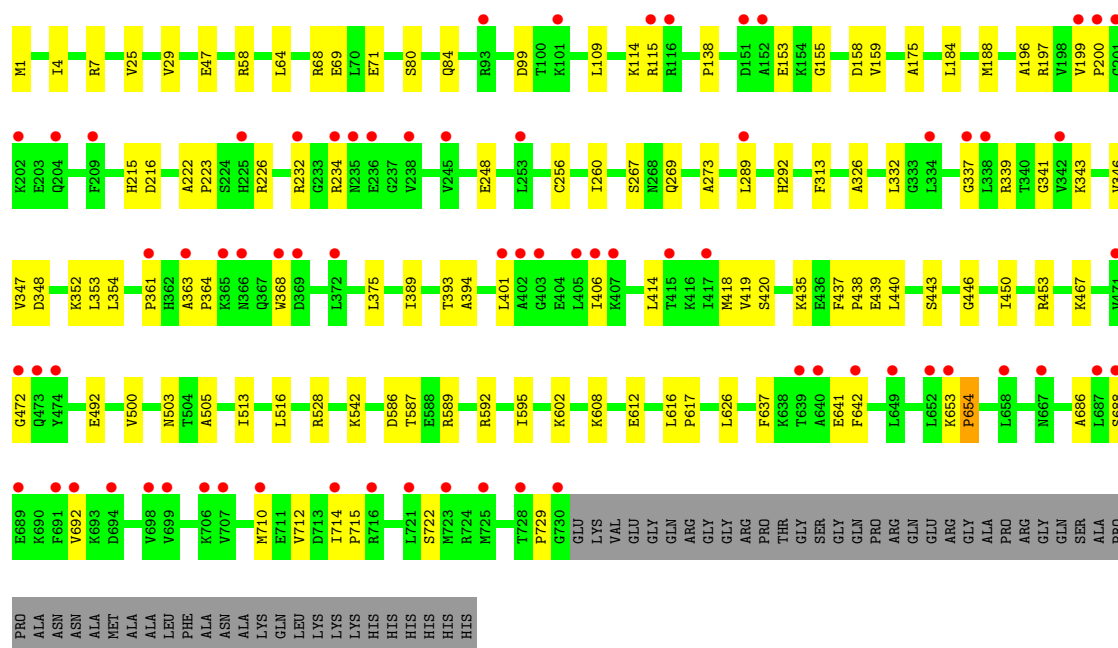
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		

3 Residue-property plots

These plots are drawn for all protein, RNA 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: Tex

Chain A: 



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 0.229 , 0.267	Depositor DCC
R_{free} test set	1934 reflections (4.99%)	DCC
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 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 41052 reflections	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.

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	0.34	2/5707 (0.0%)	0.49	1/7721 (0.0%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	GLU	CD-OE2	7.50	1.33	1.25
1	A	47	GLU	CD-OE2	6.96	1.33	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	LYS	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Peptide

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	5618	0	5713	70	0
2	A	73	0	0	2	0
All	All	5691	0	5713	70	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 6.

All (70) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:710:MET:HE3	1:A:729:PRO:HA	1.82	0.62
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: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:1:MET:HE1	1:A:71:GLU:HG3	1.92	0.52
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
1:A:347:VAL:HA	1:A:352:LYS:O	2.10	0.51
1:A:419:VAL:CG1	1:A:453:ARG:HD3	2.41	0.51
1:A:332:LEU:HD21	1:A:375:LEU:HD22	1.92	0.51
1:A:361:PRO:CB	1:A:401:LEU:HD11	2.40	0.50
1:A:326:ALA:HA	1:A:637:PHE:CG	2.47	0.50
1:A:446:GLY:O	1:A:450:ILE:HG13	2.11	0.50
1:A:542:LYS:HD2	1:A:542:LYS:N	2.29	0.48
1:A:267:SER:HB3	1:A:269:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:153:GLU:C	1:A:155:GLY:H	2.18	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:348:ASP:HB3	1:A:354:LEU:HD11	1.97	0.46
1:A:292:HIS:HD1	1:A:292:HIS:C	2.19	0.46
1:A:714:ILE:HB	1:A:715:PRO:HD3	1.98	0.46
1:A:199:VAL:HB	1:A:200:PRO:HD2	1.97	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: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:58:ARG:NH2	1:A:492:GLU:OE2	2.38	0.44
1:A:232:ARG:C	1:A:234:ARG:H	2.21	0.44
1:A:393:THR:O	1:A:394:ALA:HB3	2.18	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:337:GLY:HA3	1:A:341:GLY:O	2.20	0.42
1:A:653:LYS:HA	1:A:654:PRO:HD2	1.90	0.42
1:A:138:PRO:HA	1:A:273:ALA:HB3	2.02	0.42
1:A:64:LEU:O	1:A:68:ARG:HG3	2.19	0.42
1:A:612:GLU:CD	1:A:612:GLU:H	2.23	0.42
1:A:710:MET:HE3	1:A:710:MET:HB3	1.89	0.42
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: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:223:PRO:CG	1:A:226:ARG:NH2	2.84	0.40
1:A:1:MET:SD	1:A:4:ILE:HG13	2.61	0.40
1:A:184:LEU:HD23	1:A:184:LEU:HA	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

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	728/785 (93%)	689 (95%)	37 (5%)	2 (0%)	50 59

All (2) Ramachandran outliers are listed below:

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

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	595/635 (94%)	594 (100%)	1 (0%)	96 99

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	592	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	730/785 (92%)	0.87	70 (9%) 8 13	34, 59, 111, 131	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	VAL	9.4
1	A	201	GLY	5.7
1	A	209	PHE	5.0
1	A	361	PRO	5.0
1	A	342	VAL	4.9
1	A	714	ILE	4.8
1	A	338	LEU	4.8
1	A	238	VAL	4.6
1	A	652	LEU	4.5
1	A	725	MET	4.5
1	A	236	GLU	4.5
1	A	337	GLY	4.5
1	A	200	PRO	4.3
1	A	728	THR	4.2
1	A	687	LEU	4.2
1	A	202	LYS	4.1
1	A	253	LEU	4.1
1	A	473	GLN	3.8
1	A	658	LEU	3.8
1	A	204	GLN	3.7
1	A	407	LYS	3.7
1	A	642	PHE	3.7
1	A	235	ASN	3.7
1	A	406	ILE	3.6
1	A	366	ASN	3.5
1	A	699	VAL	3.5
1	A	402	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	151	ASP	3.3
1	A	689	GLU	3.3
1	A	372	LEU	3.3
1	A	405	LEU	3.3
1	A	640	ALA	3.0
1	A	234	ARG	3.0
1	A	692	VAL	3.0
1	A	706	LYS	2.9
1	A	710	MET	2.8
1	A	369	ASP	2.8
1	A	721	LEU	2.7
1	A	730	GLY	2.7
1	A	698	VAL	2.7
1	A	472	GLY	2.7
1	A	723	MET	2.7
1	A	639	THR	2.7
1	A	474	TYR	2.6
1	A	116	ARG	2.6
1	A	363	ALA	2.6
1	A	115	ARG	2.6
1	A	334	LEU	2.5
1	A	707	VAL	2.5
1	A	653	LYS	2.5
1	A	368	TRP	2.5
1	A	417	ILE	2.5
1	A	716	ARG	2.5
1	A	649	LEU	2.4
1	A	245	VAL	2.4
1	A	415	THR	2.4
1	A	365	LYS	2.3
1	A	101	LYS	2.3
1	A	93	ARG	2.3
1	A	232	ARG	2.3
1	A	667	ASN	2.3
1	A	691	PHE	2.3
1	A	152	ALA	2.2
1	A	225	HIS	2.2
1	A	688	SER	2.2
1	A	401	LEU	2.2
1	A	694	ASP	2.2
1	A	403	GLY	2.1
1	A	199	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	289	LEU	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.