



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 07:51 PM EDT

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 : unknown
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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

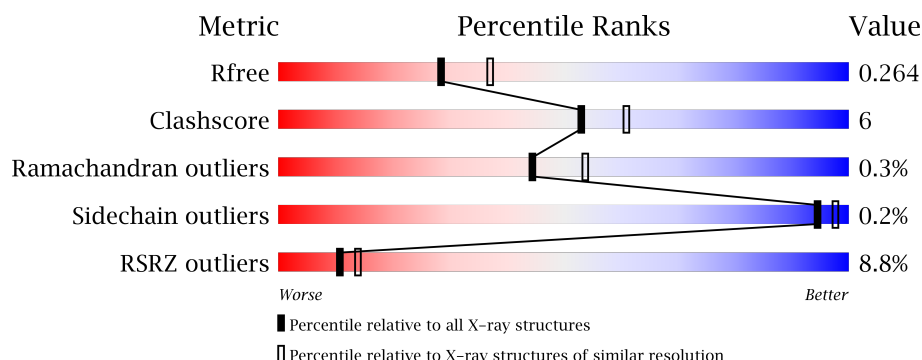
1 Overall quality at a glance

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}	100719	5609 (2.30-2.26)
Clashscore	112137	6364 (2.30-2.26)
Ramachandran outliers	110173	6281 (2.30-2.26)
Sidechain outliers	110143	6281 (2.30-2.26)
RSRZ outliers	101464	5639 (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. 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	<div> <div>8%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>

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 [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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 0.224 , 0.264	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)	0.34 , 44.2	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	0.34	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 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	5618	0	5713	70	0
2	A	73	0	0	2	0
All	All	5691	0	5713	70	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 6.

All (70) 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: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: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: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	Interatomic distance (Å)	Clash overlap (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: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:332:LEU:HD12	1:A:346:VAL:HG22	1.98	0.44
1:A:58:ARG:NH2	1:A:492:GLU:OE2	2.38	0.44
1:A:641:GLU:O	1:A:642:PHE:HB2	2.17	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: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:612:GLU:CD	1:A:612:GLU:H	2.23	0.42
1:A:64:LEU:O	1:A:68:ARG:HG3	2.19	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:500:VAL:HG13	1:A:505:ALA:HB2	2.03	0.41
1:A:7:ARG:NH1	1:A:99:ASP:HB2	2.35	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 [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%)	44 54

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%)	594 (100%)	1 (0%)	94 97

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 [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 ⓘ

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%)	0.77	64 (8%) 11 14	34, 59, 111, 131	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	VAL	10.3
1	A	201	GLY	6.2
1	A	342	VAL	5.7
1	A	338	LEU	5.3
1	A	337	GLY	5.2
1	A	236	GLU	5.2
1	A	202	LYS	4.9
1	A	361	PRO	4.7
1	A	652	LEU	4.6
1	A	209	PHE	4.4
1	A	658	LEU	4.3
1	A	473	GLN	4.3
1	A	728	THR	4.3
1	A	238	VAL	4.0
1	A	714	ILE	4.0
1	A	725	MET	3.9
1	A	204	GLN	3.9
1	A	200	PRO	3.8
1	A	253	LEU	3.8
1	A	687	LEU	3.8
1	A	406	ILE	3.8
1	A	402	ALA	3.7
1	A	407	LYS	3.6
1	A	699	VAL	3.5
1	A	151	ASP	3.4
1	A	474	TYR	3.3
1	A	405	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	235	ASN	3.3
1	A	372	LEU	3.1
1	A	363	ALA	3.1
1	A	472	GLY	3.0
1	A	723	MET	2.9
1	A	366	ASN	2.9
1	A	234	ARG	2.9
1	A	369	ASP	2.8
1	A	689	GLU	2.8
1	A	649	LEU	2.8
1	A	642	PHE	2.7
1	A	116	ARG	2.6
1	A	334	LEU	2.6
1	A	368	TRP	2.6
1	A	710	MET	2.6
1	A	706	LYS	2.6
1	A	707	VAL	2.5
1	A	225	HIS	2.5
1	A	653	LYS	2.5
1	A	692	VAL	2.4
1	A	360	TYR	2.4
1	A	698	VAL	2.3
1	A	716	ARG	2.2
1	A	362	HIS	2.2
1	A	721	LEU	2.2
1	A	93	ARG	2.2
1	A	115	ARG	2.2
1	A	639	THR	2.2
1	A	415	THR	2.1
1	A	730	GLY	2.1
1	A	199	VAL	2.1
1	A	245	VAL	2.1
1	A	682	VAL	2.1
1	A	232	ARG	2.1
1	A	694	ASP	2.1
1	A	640	ALA	2.1
1	A	417	ILE	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 [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.