Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 – 12:55 pm GMT

PDB ID	:	6HZQ
Title	:	Apo structure of TP domain from Escherichia coli Penicillin-Binding Protein 3
Authors	:	Bellini, D.; Koekemoer, L.; Newman, H.; Dowson, C.G.
Deposited on	:	2018-10-23
Resolution	:	1.95 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 (i) 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 (1)) were used in the production of this report:

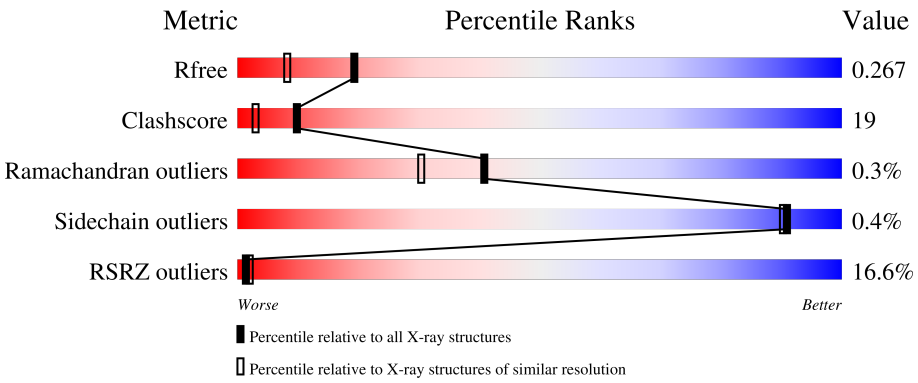
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	348	14% 60% 26% · 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2310 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 Peptidoglycan D,D-transpeptidase FtsI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	2259	1442	388	420	9	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	GLY	-	expression tag	UNP A0A0V7WLC6
A	228	PRO	-	expression tag	UNP A0A0V7WLC6
A	229	GLY	-	expression tag	UNP A0A0V7WLC6
A	230	TYR	-	expression tag	UNP A0A0V7WLC6
A	231	GLN	-	expression tag	UNP A0A0V7WLC6
A	232	ASP	-	expression tag	UNP A0A0V7WLC6
A	233	PRO	-	expression tag	UNP A0A0V7WLC6
A	?	-	SER	deletion	UNP A0A0V7WLC6
A	?	-	TYR	deletion	UNP A0A0V7WLC6
A	?	-	ASN	deletion	UNP A0A0V7WLC6
A	?	-	PRO	deletion	UNP A0A0V7WLC6
A	?	-	ASN	deletion	UNP A0A0V7WLC6
A	?	-	ASN	deletion	UNP A0A0V7WLC6
A	?	-	LEU	deletion	UNP A0A0V7WLC6
A	?	-	SER	deletion	UNP A0A0V7WLC6
A	?	-	GLY	deletion	UNP A0A0V7WLC6
A	?	-	THR	deletion	UNP A0A0V7WLC6
A	?	-	PRO	deletion	UNP A0A0V7WLC6
A	?	-	LYS	deletion	UNP A0A0V7WLC6
A	?	-	GLU	deletion	UNP A0A0V7WLC6
A	?	-	ALA	deletion	UNP A0A0V7WLC6
A	294	GLY	MET	conflict	UNP A0A0V7WLC6

- Molecule 2 is water.

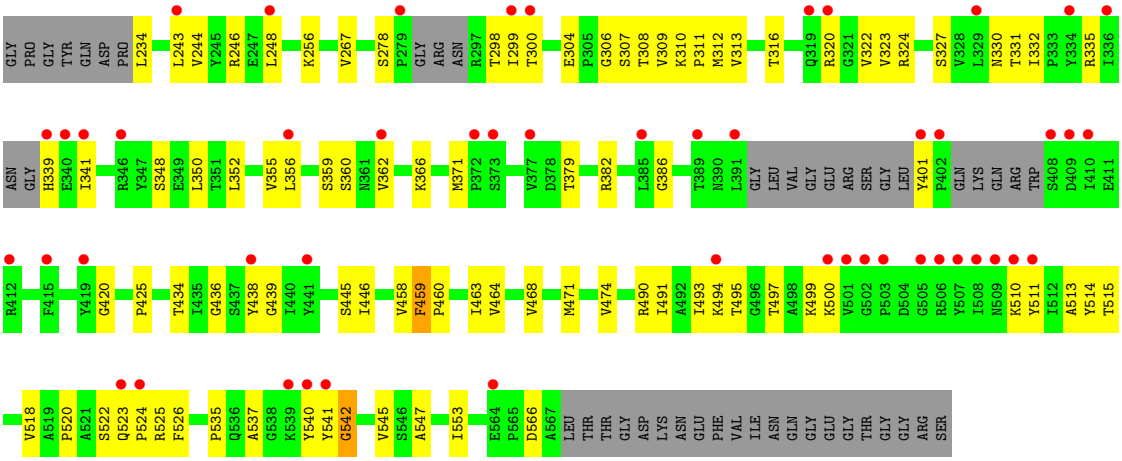
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	51	51	51	0	0

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: Peptidoglycan D,D-transpeptidase FtsI

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	91.87Å 150.03Å 43.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.35 – 1.95 75.01 – 1.95	Depositor EDS
% Data completeness (in resolution range)	53.6 (78.35-1.95) 53.6 (75.01-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.273 , 0.280 0.261 , 0.267	Depositor DCC
R_{free} test set	549 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.001 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	2310	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 6.74% 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 (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	0.60	0/2298	0.73	0/3119

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	2259	0	2323	88	1
2	A	51	0	0	4	0
All	All	2310	0	2323	88	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 19.

All (88) 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:520:PRO:O	1:A:523:GLN:O	1.77	1.02
1:A:300:THR:HG23	1:A:425:PRO:HG2	1.46	0.95
1:A:495:THR:HG21	1:A:547:ALA:HB2	1.61	0.83
1:A:323:VAL:HG13	1:A:327:SER:HB2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:THR:CG2	1:A:425:PRO:HD2	2.11	0.80
1:A:495:THR:HG22	1:A:515:THR:OG1	1.82	0.79
1:A:471:MET:HG2	1:A:494:LYS:HE2	1.64	0.79
1:A:310:LYS:NZ	1:A:359:SER:OG	2.16	0.79
1:A:323:VAL:HG13	1:A:327:SER:CB	2.13	0.78
1:A:323:VAL:HG11	1:A:352:LEU:HD11	1.67	0.77
1:A:323:VAL:CG1	1:A:327:SER:HB2	2.16	0.75
1:A:300:THR:HG22	1:A:425:PRO:HD2	1.69	0.74
1:A:300:THR:HG23	1:A:425:PRO:CG	2.17	0.74
1:A:356:LEU:HB3	1:A:494:LYS:NZ	2.10	0.66
1:A:323:VAL:CG1	1:A:352:LEU:HD11	2.24	0.66
1:A:511:TYR:CE2	1:A:540:TYR:HD2	2.13	0.66
1:A:522:SER:OG	1:A:566:ASP:OD1	2.15	0.65
1:A:330:ASN:O	1:A:366:LYS:HE3	1.98	0.63
1:A:356:LEU:HD22	1:A:494:LYS:NZ	2.13	0.63
1:A:511:TYR:CE2	1:A:540:TYR:CD2	2.87	0.63
1:A:316:THR:HG22	1:A:379:THR:OG1	1.99	0.62
1:A:497:THR:HG21	2:A:601:HOH:O	1.99	0.61
1:A:322:VAL:HG12	1:A:323:VAL:HG23	1.81	0.61
1:A:540:TYR:O	2:A:601:HOH:O	2.16	0.61
1:A:500:LYS:HB3	1:A:510:LYS:HB2	1.82	0.60
1:A:511:TYR:CZ	1:A:541:TYR:HB3	2.37	0.60
1:A:306:GLY:HA3	1:A:514:TYR:OH	2.01	0.59
1:A:459:PHE:CE1	1:A:463:ILE:HG21	2.39	0.58
1:A:511:TYR:CD2	1:A:540:TYR:HD2	2.22	0.57
1:A:499:LYS:HG2	1:A:511:TYR:CE1	2.41	0.56
1:A:300:THR:CG2	1:A:425:PRO:CD	2.84	0.55
1:A:459:PHE:HE1	1:A:463:ILE:HG21	1.72	0.55
1:A:497:THR:HG21	1:A:541:TYR:O	2.08	0.53
1:A:312:MET:O	1:A:316:THR:HG23	2.09	0.53
1:A:520:PRO:O	1:A:523:GLN:C	2.46	0.53
1:A:356:LEU:HD22	1:A:494:LYS:HZ2	1.73	0.53
1:A:355:VAL:HG13	1:A:360:SER:HB3	1.91	0.53
1:A:446:ILE:N	2:A:602:HOH:O	2.25	0.52
1:A:518:VAL:HA	1:A:526:PHE:O	2.09	0.52
1:A:248:LEU:HG	1:A:278:SER:HB2	1.92	0.52
1:A:382:ARG:NH2	1:A:458:VAL:O	2.43	0.51
1:A:313:VAL:O	1:A:316:THR:OG1	2.27	0.51
1:A:316:THR:CG2	1:A:379:THR:OG1	2.60	0.50
1:A:300:THR:CG2	1:A:425:PRO:CG	2.90	0.49
1:A:497:THR:HG22	1:A:513:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:PRO:HD3	1:A:494:LYS:HE3	1.95	0.49
1:A:445:SER:HA	2:A:602:HOH:O	2.14	0.48
1:A:497:THR:HG21	1:A:542:GLY:O	2.14	0.48
1:A:434:THR:O	1:A:439:GLY:N	2.44	0.48
1:A:323:VAL:HG12	1:A:324:ARG:O	2.15	0.47
1:A:332:ILE:HD13	1:A:348:SER:HA	1.96	0.47
1:A:320:ARG:HD3	1:A:371:MET:HG2	1.97	0.47
1:A:267:VAL:CG1	1:A:436:GLY:C	2.84	0.47
1:A:535:PRO:O	1:A:540:TYR:HB3	2.15	0.47
1:A:356:LEU:HB3	1:A:494:LYS:HZ1	1.80	0.46
1:A:438:TYR:OH	1:A:524:PRO:HD2	2.15	0.46
1:A:335:ARG:HA	1:A:339:HIS:O	2.16	0.46
1:A:267:VAL:HG11	1:A:436:GLY:HA3	1.97	0.46
1:A:304:GLU:OE2	1:A:420:GLY:N	2.46	0.45
1:A:307:SER:N	1:A:514:TYR:OH	2.46	0.45
1:A:491:ILE:HD12	1:A:493:ILE:HG21	1.99	0.45
1:A:541:TYR:H	1:A:541:TYR:HD2	1.63	0.45
1:A:535:PRO:O	1:A:540:TYR:CB	2.64	0.45
1:A:234:LEU:CD2	1:A:446:ILE:HG13	2.47	0.45
1:A:300:THR:HG23	1:A:425:PRO:CD	2.47	0.45
1:A:513:ALA:CB	1:A:545:VAL:HB	2.47	0.45
1:A:464:VAL:O	1:A:468:VAL:HG23	2.17	0.45
1:A:331:THR:HG21	1:A:350:LEU:HD12	2.00	0.44
1:A:459:PHE:CD1	1:A:460:PRO:HD2	2.53	0.44
1:A:490:ARG:H	1:A:566:ASP:HB3	1.82	0.44
1:A:511:TYR:HE2	1:A:540:TYR:CD2	2.36	0.43
1:A:306:GLY:O	1:A:309:VAL:HG22	2.18	0.43
1:A:520:PRO:HD2	1:A:523:GLN:O	2.19	0.43
1:A:497:THR:CG2	1:A:542:GLY:O	2.67	0.42
1:A:234:LEU:HD23	1:A:446:ILE:HG13	2.00	0.42
1:A:243:LEU:HB3	1:A:246:ARG:NH2	2.35	0.42
1:A:298:THR:HG22	1:A:299:ILE:N	2.35	0.42
1:A:244:VAL:HG22	1:A:553:ILE:HG23	2.02	0.42
1:A:308:THR:HG23	1:A:514:TYR:CE1	2.55	0.41
1:A:256:LYS:HD2	1:A:537:ALA:HB2	2.02	0.41
1:A:267:VAL:HG11	1:A:436:GLY:C	2.41	0.41
1:A:341:ILE:HG22	1:A:362:VAL:HG22	2.02	0.41
1:A:316:THR:HB	1:A:371:MET:HE1	2.03	0.41
1:A:386:GLY:HA3	1:A:401:TYR:CD2	2.56	0.41
1:A:316:THR:HG23	1:A:379:THR:HG21	2.04	0.40
1:A:474:VAL:HG21	1:A:494:LYS:HZ3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:HH11	1:A:322:VAL:HG22	1.87	0.40
1:A:541:TYR:O	1:A:542:GLY:C	2.60	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)
1:A:324:ARG:NH1	1:A:525:ARG:NH1[6_554]	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	291/348 (84%)	278 (96%)	12 (4%)	1 (0%)	41 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	GLY

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	242/277 (87%)	241 (100%)	1 (0%)	91 90

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

Mol	Chain	Res	Type
1	A	459	PHE

Sometimes 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 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	301/348 (86%)	1.15	50 (16%) 1 2	2, 32, 79, 107	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	TYR	9.7
1	A	402	PRO	9.5
1	A	409	ASP	9.5
1	A	501	VAL	8.7
1	A	507	TYR	7.6
1	A	502	GLY	7.2
1	A	503	PRO	6.3
1	A	508	ILE	6.1
1	A	408	SER	5.9
1	A	506	ARG	5.7
1	A	505	GLY	5.6
1	A	509	ASN	5.6
1	A	540	TYR	5.0
1	A	339	HIS	4.8
1	A	539	LYS	4.2
1	A	541	TYR	4.1
1	A	300	THR	3.9
1	A	299	ILE	3.7
1	A	341	ILE	3.4
1	A	523	GLN	3.4
1	A	336	ILE	3.3
1	A	340	GLU	3.2
1	A	389	THR	3.1
1	A	410	ILE	3.1
1	A	441	TYR	3.0
1	A	494	LYS	3.0
1	A	372	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	373	SER	2.9
1	A	346	ARG	2.9
1	A	412	ARG	2.8
1	A	510	LYS	2.8
1	A	391	LEU	2.7
1	A	500	LYS	2.5
1	A	279	PRO	2.5
1	A	438	TYR	2.4
1	A	320	ARG	2.4
1	A	362	VAL	2.4
1	A	243	LEU	2.3
1	A	415	PHE	2.3
1	A	334	TYR	2.3
1	A	356	LEU	2.3
1	A	319	GLN	2.2
1	A	385	LEU	2.1
1	A	419	TYR	2.1
1	A	329	LEU	2.1
1	A	248	LEU	2.1
1	A	511	TYR	2.1
1	A	377	VAL	2.1
1	A	524	PRO	2.1
1	A	564	GLU	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.