



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 08:35 AM EDT

PDB ID : 3Q48
Title : Crystal structure of Pseudomonas aeruginosa CupB2 chaperone
Authors : Cai, X.; Wang, R.; Filloux, A.; Waksman, G.; Meng, G.
Deposited on : unknown
Resolution : 2.50 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

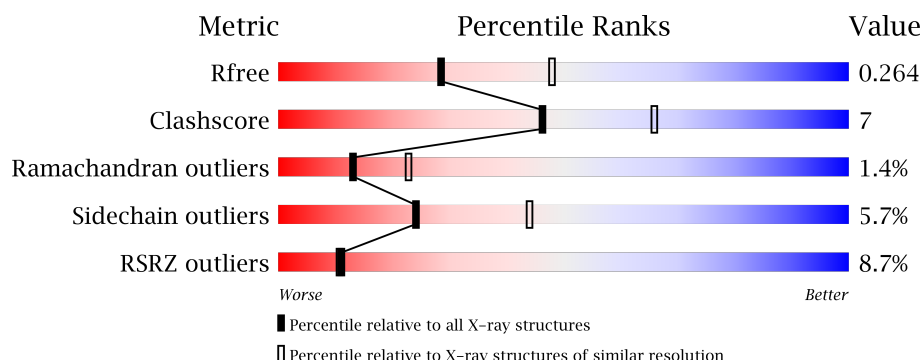
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	257	<div> <div>7%</div> <div>60%</div> <div>12%</div> <div>25%</div> </div>
1	B	257	<div> <div>5%</div> <div>59%</div> <div>12%</div> <div>28%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3136 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 Chaperone CupB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1493	952	262	276	3			
1	B	186	Total	C	N	O	S	0	0	0
			1449	927	253	267	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	ARG	-	EXPRESSION TAG	UNP Q9HWU3
A	250	GLY	-	EXPRESSION TAG	UNP Q9HWU3
A	251	SER	-	EXPRESSION TAG	UNP Q9HWU3
A	252	HIS	-	EXPRESSION TAG	UNP Q9HWU3
A	253	HIS	-	EXPRESSION TAG	UNP Q9HWU3
A	254	HIS	-	EXPRESSION TAG	UNP Q9HWU3
A	255	HIS	-	EXPRESSION TAG	UNP Q9HWU3
A	256	HIS	-	EXPRESSION TAG	UNP Q9HWU3
A	257	HIS	-	EXPRESSION TAG	UNP Q9HWU3
B	249	ARG	-	EXPRESSION TAG	UNP Q9HWU3
B	250	GLY	-	EXPRESSION TAG	UNP Q9HWU3
B	251	SER	-	EXPRESSION TAG	UNP Q9HWU3
B	252	HIS	-	EXPRESSION TAG	UNP Q9HWU3
B	253	HIS	-	EXPRESSION TAG	UNP Q9HWU3
B	254	HIS	-	EXPRESSION TAG	UNP Q9HWU3
B	255	HIS	-	EXPRESSION TAG	UNP Q9HWU3
B	256	HIS	-	EXPRESSION TAG	UNP Q9HWU3
B	257	HIS	-	EXPRESSION TAG	UNP Q9HWU3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	83	Total	O	0	0
			83	83		

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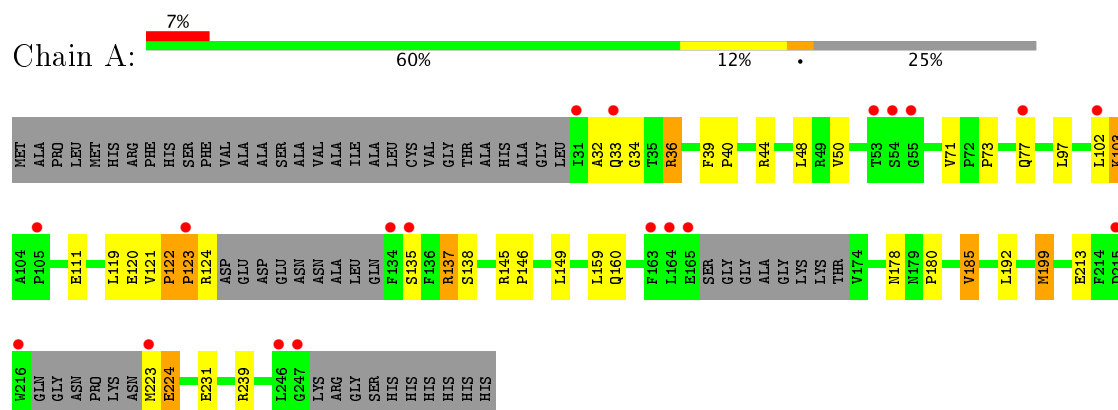
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	111	Total	O	0	0
			111	111		

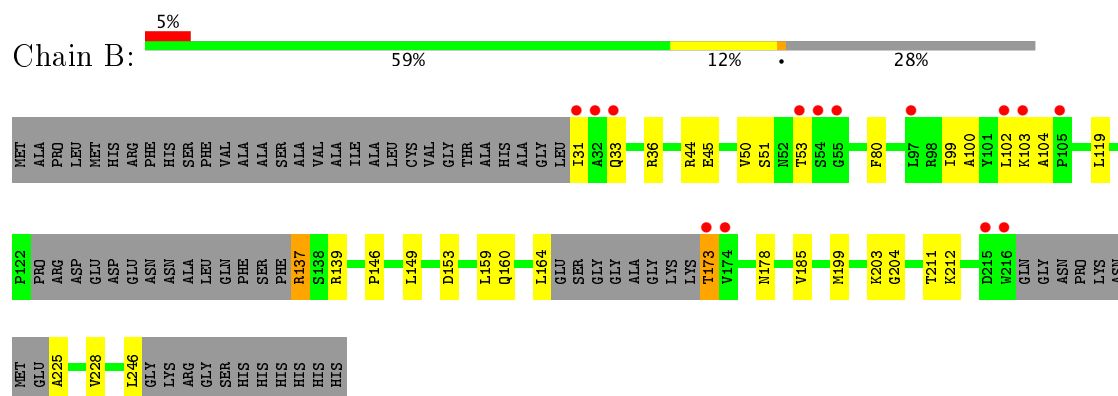
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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: Chaperone CupB2



• Molecule 1: Chaperone CupB2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.52Å 65.78Å 87.51Å 90.00° 105.95° 90.00°	Depositor
Resolution (Å)	28.09 – 2.50 28.09 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.09-2.50) 98.3 (28.09-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.70 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.198 , 0.259 0.202 , 0.264	Depositor DCC
R_{free} test set	892 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3136	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.72% 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

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	0.92	1/1526 (0.1%)	0.86	2/2072 (0.1%)
1	B	0.91	0/1481	0.87	2/2015 (0.1%)
All	All	0.92	1/3007 (0.0%)	0.87	4/4087 (0.1%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	VAL	CB-CG1	5.83	1.65	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	36	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	36	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	153	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	GLY	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	1493	0	1463	21	0
1	B	1449	0	1442	21	0
2	A	83	0	0	2	0
2	B	111	0	0	8	0
All	All	3136	0	2905	42	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 (42) 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:123:PRO:HB2	1:A:124:ARG:CA	1.47	1.40
1:A:123:PRO:CB	1:A:124:ARG:CA	2.36	1.03
1:B:160:GLN:CD	2:B:334:HOH:O	2.06	0.94
1:A:122:PRO:N	2:A:290:HOH:O	2.06	0.88
1:A:121:VAL:C	1:A:123:PRO:HD3	1.99	0.82
1:B:160:GLN:NE2	2:B:334:HOH:O	2.13	0.81
1:A:231:GLU:OE1	1:A:239:ARG:NH1	2.16	0.78
1:B:246:LEU:C	2:B:328:HOH:O	2.21	0.78
1:A:223:MET:HA	1:A:224:GLU:CB	2.17	0.74
1:A:122:PRO:N	1:A:123:PRO:HD3	2.03	0.72
1:B:203:LYS:O	2:B:344:HOH:O	2.09	0.70
1:B:173:THR:N	2:B:261:HOH:O	2.27	0.67
1:A:48:LEU:HD23	1:A:97:LEU:HD12	1.76	0.67
1:B:225:ALA:O	2:B:348:HOH:O	2.13	0.66
1:A:120:GLU:O	1:A:135:SER:HB3	1.96	0.66
1:A:192:LEU:HB2	1:A:199:MET:HG3	1.80	0.64
1:B:31:ILE:HD13	1:B:53:THR:HG22	1.81	0.61
1:B:160:GLN:CG	2:B:334:HOH:O	2.49	0.58
1:A:121:VAL:O	1:A:123:PRO:HD3	2.07	0.54
1:A:178:ASN:O	1:A:180:PRO:HD3	2.08	0.53
1:A:159:LEU:HD11	1:A:185:VAL:HG11	1.91	0.51
1:A:146:PRO:HD2	1:A:149:LEU:HD12	1.93	0.51
1:B:119:LEU:HD13	1:B:137:ARG:HB2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PRO:N	1:A:123:PRO:CD	2.75	0.49
1:A:111:GLU:OE2	1:A:145:ARG:NE	2.40	0.49
1:B:45:GLU:HA	1:B:99:ILE:O	2.13	0.48
1:A:50:VAL:O	1:A:50:VAL:HG23	2.12	0.48
1:A:119:LEU:HD13	1:A:137:ARG:HB2	1.96	0.48
1:A:102:LEU:O	1:A:103:LYS:C	2.54	0.46
1:B:50:VAL:O	1:B:50:VAL:HG23	2.16	0.46
1:B:103:LYS:C	1:B:103:LYS:HD2	2.37	0.45
1:B:173:THR:HA	2:B:290:HOH:O	2.17	0.45
1:B:31:ILE:HB	1:B:51:SER:O	2.17	0.44
1:B:103:LYS:HD2	1:B:104:ALA:N	2.33	0.43
1:B:159:LEU:HD11	1:B:185:VAL:HG11	2.01	0.43
1:A:73:PRO:HG2	2:A:285:HOH:O	2.19	0.42
1:B:146:PRO:HD2	1:B:149:LEU:HD12	2.01	0.42
1:B:178:ASN:HD22	1:B:211:THR:HG22	1.86	0.41
1:B:80:PHE:HA	1:B:100:ALA:O	2.21	0.41
1:A:39:PHE:HA	1:A:40:PRO:HD3	1.89	0.40
1:B:204:GLY:HA3	1:B:212:LYS:HE2	2.04	0.40
1:B:228:VAL:O	1:B:228:VAL:HG13	2.20	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	186/257 (72%)	176 (95%)	5 (3%)	5 (3%)	6	9
1	B	178/257 (69%)	170 (96%)	8 (4%)	0	100	100
All	All	364/514 (71%)	346 (95%)	13 (4%)	5 (1%)	13	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	PRO
1	A	123	PRO
1	A	224	GLU
1	A	103	LYS
1	A	32	ALA

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	159/213 (75%)	149 (94%)	10 (6%)	21	38
1	B	157/213 (74%)	149 (95%)	8 (5%)	28	50
All	All	316/426 (74%)	298 (94%)	18 (6%)	24	44

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	36	ARG
1	A	44	ARG
1	A	71	VAL
1	A	77	GLN
1	A	137	ARG
1	A	138	SER
1	A	160	GLN
1	A	199	MET
1	A	213	GLU
1	B	33	GLN
1	B	44	ARG
1	B	102	LEU
1	B	137	ARG
1	B	139	ARG
1	B	164	LEU
1	B	173	THR
1	B	199	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	B	160	GLN
1	B	178	ASN

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	194/257 (75%)	0.33	19 (9%) 8 7	20, 36, 59, 81	0
1	B	186/257 (72%)	0.24	14 (7%) 15 15	15, 31, 52, 65	0
All	All	380/514 (73%)	0.29	33 (8%) 11 11	15, 34, 57, 81	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	GLN	5.4
1	A	134	PHE	5.0
1	A	102	LEU	4.6
1	A	223	MET	4.3
1	B	173	THR	4.2
1	B	102	LEU	4.1
1	A	247	GLY	3.7
1	B	216	TRP	3.4
1	B	54	SER	3.3
1	A	216	TRP	3.1
1	A	54	SER	3.0
1	A	135	SER	2.9
1	A	215	ASP	2.8
1	B	55	GLY	2.8
1	B	32	ALA	2.8
1	B	174	VAL	2.7
1	B	33	GLN	2.7
1	B	53	THR	2.7
1	A	105	PRO	2.7
1	A	165	GLU	2.5
1	B	31	ILE	2.4
1	B	215	ASP	2.3
1	B	103	LYS	2.3
1	A	77	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	105	PRO	2.2
1	A	164	LEU	2.2
1	A	53	THR	2.2
1	A	123	PRO	2.2
1	A	31	ILE	2.0
1	A	246	LEU	2.0
1	B	97	LEU	2.0
1	A	163	PHE	2.0
1	A	55	GLY	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 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.