



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2017 – 06:27 AM EST

PDB ID : 5OFP
Title : Structure of the antibacterial peptide ABC transporter McjD in an apo inward occluded conformation
Authors : Beis, K.; Choudhury, H.G.
Deposited on : unknown
Resolution : 4.71 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

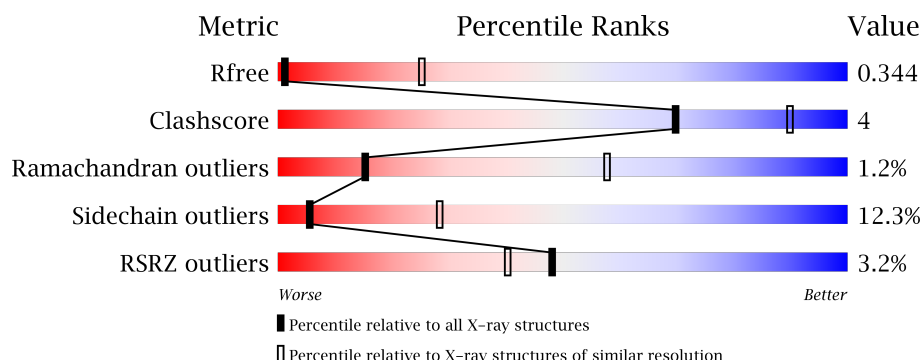
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.71 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	1011 (5.76-3.66)
Clashscore	112137	1059 (5.70-3.70)
Ramachandran outliers	110173	1005 (5.76-3.68)
Sidechain outliers	110143	1027 (5.76-3.66)
RSRZ outliers	101464	1020 (5.76-3.66)

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	580	<div> <div>3%</div> <div>76%</div> <div>22%</div> <div>..</div> </div>

2 Entry composition


There is only 1 type of molecule in this entry. The entry contains 4527 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 Microcin-J25 export ATP-binding/permease protein McjD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	0	0
			4527	2920	739	850	18			

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.

- Chain A: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.85Å 87.85Å 351.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.06 – 4.71 78.58 – 4.71	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.06-4.71) 98.1 (78.58-4.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 4.65Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.313 , 0.334 0.355 , 0.344	Depositor DCC
R_{free} test set	374 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	228.3	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 130.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	4527	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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	0.48	0/4603	0.62	0/6234

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	4527	0	4639	38	0
All	All	4527	0	4639	38	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 4.

All (38) 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:475:ILE:H	1:A:480:ASN:HB2	1.58	0.68
1:A:200:ASP:HA	1:A:203:LEU:HD12	1.80	0.62
1:A:50:THR:HG21	1:A:287:ILE:HG13	1.82	0.62
1:A:334:ILE:N	1:A:335:PRO:HD2	2.16	0.59
1:A:347:ILE:HG12	1:A:402:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLU:HB3	1:A:327:ASN:HA	1.87	0.56
1:A:304:GLY:HA2	1:A:307:LEU:HD12	1.90	0.53
1:A:454:VAL:HG13	1:A:495:PHE:HB2	1.91	0.53
1:A:478:GLY:HA3	1:A:486:LYS:HD3	1.90	0.52
1:A:13:ILE:HG12	1:A:136:ILE:HG12	1.91	0.51
1:A:435:LEU:HD13	1:A:472:THR:HB	1.93	0.50
1:A:409:LEU:HA	1:A:412:ILE:HD12	1.93	0.50
1:A:377:THR:HG21	1:A:542:LEU:HD21	1.93	0.50
1:A:331:SER:N	1:A:332:PRO:HD3	2.27	0.49
1:A:157:THR:HG21	1:A:296:LEU:HD21	1.95	0.49
1:A:36:SER:HB2	1:A:153:GLN:HG3	1.95	0.48
1:A:351:SER:HB2	1:A:399:PHE:HB2	1.96	0.48
1:A:73:MET:HG3	1:A:77:ILE:HD11	1.97	0.47
1:A:127:GLN:HG3	1:A:131:GLN:HE21	1.79	0.47
1:A:341:ARG:HA	1:A:341:ARG:HD3	1.75	0.45
1:A:565:LEU:HB3	1:A:572:ILE:HG13	1.99	0.44
1:A:270:ILE:O	1:A:274:LEU:HG	2.18	0.44
1:A:57:LEU:HA	1:A:61:SER:HB3	2.00	0.44
1:A:354:TYR:HD2	1:A:360:ILE:HG12	1.83	0.44
1:A:162:LEU:HD12	1:A:170:ALA:HB1	2.00	0.43
1:A:217:ILE:HG13	1:A:217:ILE:H	1.65	0.43
1:A:176:TYR:HE1	1:A:260:LEU:HB3	1.84	0.43
1:A:494:LEU:HD21	1:A:523:ILE:HG12	1.99	0.43
1:A:543:GLU:HG2	1:A:563:ARG:HH21	1.83	0.42
1:A:565:LEU:HD22	1:A:572:ILE:HG13	2.01	0.42
1:A:80:LYS:HG2	1:A:84:PHE:HE2	1.85	0.42
1:A:499:PRO:HG2	1:A:502:ILE:HG12	2.02	0.41
1:A:38:ILE:HG13	1:A:38:ILE:H	1.50	0.41
1:A:131:GLN:HE22	1:A:203:LEU:HG	1.85	0.41
1:A:334:ILE:N	1:A:335:PRO:CD	2.83	0.41
1:A:335:PRO:HA	1:A:336:PHE:HA	1.60	0.41
1:A:241:ASN:HA	1:A:244:LYS:HD2	2.03	0.40
1:A:313:SER:O	1:A:317:LEU:HB2	2.21	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	569/580 (98%)	509 (90%)	53 (9%)	7 (1%)	15	58

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	PRO
1	A	506	GLU
1	A	448	GLU
1	A	278	ASN
1	A	279	GLY
1	A	145	GLN
1	A	528	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	520/529 (98%)	456 (88%)	64 (12%)	5	28

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	38	ILE
1	A	46	LEU
1	A	53	LEU

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Mol	Chain	Res	Type
1	A	54	SER
1	A	60	PHE
1	A	85	LEU
1	A	93	LEU
1	A	111	ASN
1	A	139	LEU
1	A	162	LEU
1	A	194	LEU
1	A	197	HIS
1	A	208	LEU
1	A	217	ILE
1	A	248	LEU
1	A	249	LEU
1	A	254	LEU
1	A	255	LEU
1	A	259	LEU
1	A	277	LEU
1	A	292	TYR
1	A	295	LEU
1	A	303	ILE
1	A	310	ILE
1	A	315	SER
1	A	323	ARG
1	A	328	LYS
1	A	330	THR
1	A	338	ASN
1	A	340	GLU
1	A	342	LYS
1	A	345	LEU
1	A	349	GLU
1	A	357	ASP
1	A	373	MET
1	A	376	LEU
1	A	380	SER
1	A	384	LYS
1	A	387	LEU
1	A	395	TYR
1	A	417	LEU
1	A	424	LEU
1	A	425	THR
1	A	426	GLN
1	A	427	ASP

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Mol	Chain	Res	Type
1	A	429	TYR
1	A	433	ASP
1	A	435	LEU
1	A	452	PHE
1	A	455	LEU
1	A	470	LEU
1	A	474	LEU
1	A	491	LEU
1	A	496	LEU
1	A	497	ARG
1	A	511	LEU
1	A	512	ASP
1	A	524	ARG
1	A	540	ASN
1	A	551	LEU
1	A	563	ARG
1	A	564	ASP
1	A	570	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	223	ASN
1	A	278	ASN
1	A	338	ASN
1	A	411	ASN
1	A	480	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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	571/580 (98%)	-0.05	18 (3%) 48 40	24, 94, 127, 165	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	429	TYR	5.9
1	A	430	ILE	5.7
1	A	579	THR	5.4
1	A	481	TYR	3.9
1	A	328	LYS	3.4
1	A	477	ARG	3.4
1	A	329	ALA	3.0
1	A	478	GLY	2.6
1	A	333	SER	2.6
1	A	431	PHE	2.4
1	A	57	LEU	2.4
1	A	428	ASP	2.3
1	A	58	SER	2.3
1	A	394	TYR	2.3
1	A	488	ARG	2.3
1	A	515	ASN	2.1
1	A	427	ASP	2.1
1	A	465	ASN	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.