

Full wwPDB X-ray Structure Validation Report (i)

Jun 10, 2024 – 04:09 PM JST

PDB ID	:	8ZAK
Title	:	Crystal structure of the channel protein CorA from Campylobacter jejuni in
		complex with Ni2 $+$
Authors	:	Ahn, S.Y.; Yoon, S.I.
Deposited on		
Resolution	:	2.40 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:

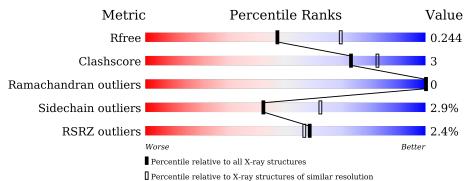
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	: : : : :	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.40 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	$\begin{array}{l} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	А	274	83%	9%	8%
1	В	274	.% 78% 9%	•	12%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4009 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	253	Total	С	Ν	Ο	S	0	0	0
	A	200	1999	1279	323	392	5	0	0	0
1	р	241	Total	С	Ν	0	S	0	0	0
	D	241	1937	1241	317	374	5	0	0	0

• Molecule 1 is a protein called Magnesium transport protein CorA.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-5	GLY	-	expression tag	UNP A0A6C7N0T6
А	-4	SER	-	expression tag	UNP A0A6C7N0T6
A	-3	ALA	-	expression tag	UNP A0A6C7N0T6
A	-2	LYS	-	expression tag	UNP A0A6C7N0T6
А	-1	ASP	-	expression tag	UNP A0A6C7N0T6
A	0	PRO	-	expression tag	UNP A0A6C7N0T6
В	-5	GLY	-	expression tag	UNP A0A6C7N0T6
В	-4	SER	-	expression tag	UNP A0A6C7N0T6
В	-3	ALA	-	expression tag	UNP A0A6C7N0T6
В	-2	LYS	-	expression tag	UNP A0A6C7N0T6
В	-1	ASP	-	expression tag	UNP A0A6C7N0T6
В	0	PRO	-	expression tag	UNP A0A6C7N0T6

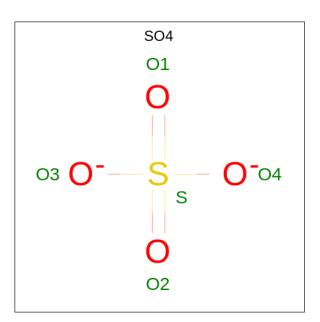
There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

I	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	2	А	1	Total Ni 1 1	0	0
	2	В	1	Total Ni 1 1	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

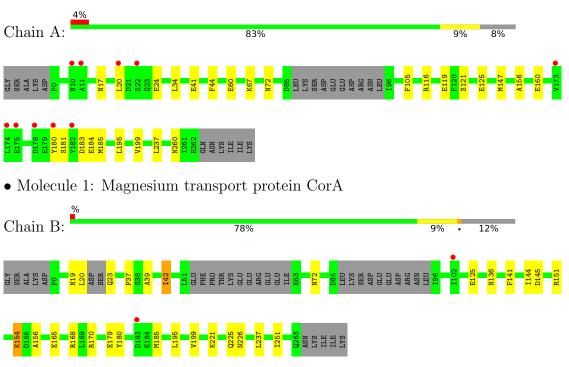
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	24	Total O 24 24	0	0
4	В	17	Total O 17 17	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: Magnesium transport protein CorA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	95.74Å 95.74Å 110.91Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.26 - 2.40	Depositor
Resolution (A)	29.26 - 2.40	EDS
% Data completeness	99.8 (29.26-2.40)	Depositor
(in resolution range)	99.8 (29.26-2.40)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.76 (at 2.39 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
B B.	0.199 , 0.244	Depositor
R, R_{free}	0.199 , 0.244	DCC
R_{free} test set	981 reflections (4.74%)	wwPDB-VP
Wilson B-factor $(Å^2)$	41.2	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 40.2	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4009	wwPDB-VP
Average B, all atoms $(Å^2)$	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NI

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.37	0/2030	0.53	0/2755	
1	В	0.36	0/1964	0.55	0/2658	
All	All	0.37	0/3994	0.54	0/5413	

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	А	1999	0	1907	11	0
1	В	1937	0	1901	16	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	15	0	0	0	0
3	В	15	0	0	0	0
4	А	24	0	0	0	0
4	В	17	0	0	1	0
All	All	4009	0	3808	26	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 3.



A. 1	A.L. D.	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:260:ASN:ND2	1:B:37:PRO:O	2.23	0.71
1:B:221:LYS:HE3	1:B:225:GLN:HE21	1.68	0.58
1:B:145:ASP:OD1	1:B:226:ASN:ND2	2.33	0.58
1:B:165:GLU:OE2	1:B:168:ARG:NH1	2.37	0.57
1:A:41:GLU:N	1:A:41:GLU:OE2	2.37	0.54
1:A:181:SER:HB3	1:A:184:GLU:HB2	1.90	0.52
1:B:19:ASN:O	1:B:23:GLN:HB2	2.09	0.52
1:B:125:GLU:HG2	1:B:154:LYS:HE3	1.89	0.52
1:A:20:LEU:HD11	1:A:44:PHE:HB2	1.93	0.49
1:B:151:ARG:NH1	4:B:401:HOH:O	2.32	0.49
1:A:121:SER:O	1:A:125:GLU:HG3	2.13	0.49
1:B:39:ALA:HA	1:B:42:ILE:HB	1.95	0.48
1:B:221:LYS:HE3	1:B:225:GLN:NE2	2.28	0.47
1:A:195:LEU:O	1:A:199:VAL:HG23	2.14	0.47
1:A:34:LEU:HD23	1:A:41:GLU:HB3	1.97	0.47
1:B:179:GLU:HB3	1:B:185:MET:HE2	1.97	0.46
1:A:156:ALA:HB2	1:A:237:LEU:HD11	1.98	0.46
1:A:180:TYR:CZ	1:A:185:MET:HG2	2.50	0.46
1:B:42:ILE:HD13	1:B:42:ILE:HA	1.84	0.45
1:B:156:ALA:HB2	1:B:237:LEU:HD11	1.99	0.44
1:B:180:TYR:CZ	1:B:185:MET:HG2	2.53	0.44
1:B:170:ARG:HB2	1:B:251:ILE:HD11	2.00	0.43
1:A:105:PHE:HE1	1:A:147:MET:SD	2.43	0.41
1:B:141:PHE:O	1:B:144:ILE:HG22	2.21	0.41
1:A:116:ARG:HH12	1:A:119:GLU:CD	2.23	0.41
1:B:195:LEU:O	1:B:199:VAL:HG23	2.21	0.40

All (26) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	А	249/274~(91%)	246 (99%)	3~(1%)	0	100	100
1	В	233/274~(85%)	229~(98%)	4 (2%)	0	100	100
All	All	482/548 (88%)	475 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	210/256~(82%)	203~(97%)	7 (3%)	38 57
1	В	210/256~(82%)	205~(98%)	5(2%)	49 68
All	All	420/512~(82%)	408 (97%)	12 (3%)	42 62

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	17	ASN
1	А	24	GLU
1	А	60	GLU
1	А	67	LYS
1	А	72	ASN
1	А	160	GLU
1	А	183	ASP
1	В	20	LEU
1	В	42	ILE
1	В	72	ASN
1	В	136	ASN
1	В	154	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type		
1	А	258	GLN		
Continued on out on a					

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	В	225	GLN

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)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Trune	Chain Res Link		Tinle	Bond lengths			Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	SO4	В	302	-	4,4,4	0.17	0	$6,\!6,\!6$	0.17	0
3	SO4	А	302	-	4,4,4	0.34	0	$6,\!6,\!6$	0.19	0
3	SO4	В	303	-	4,4,4	0.16	0	$6,\!6,\!6$	0.12	0
3	SO4	В	304	-	4,4,4	0.11	0	$6,\!6,\!6$	0.11	0
3	SO4	А	304	-	4,4,4	0.15	0	$6,\!6,\!6$	0.19	0
3	SO4	А	303	-	4,4,4	0.15	0	$6,\!6,\!6$	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	253/274~(92%)	-0.21	10 (3%) 38 37	28, 44, 88, 113	0
1	В	241/274 (87%)	-0.17	2 (0%) 86 84	27, 43, 78, 92	0
All	All	494/548~(90%)	-0.19	12 (2%) 59 57	27, 44, 86, 113	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	180	TYR	4.7
1	А	173	VAL	2.8
1	А	10	ASN	2.6
1	А	174	LEU	2.5
1	А	178	ASP	2.5
1	А	175	GLU	2.4
1	А	22	SER	2.3
1	А	11	ALA	2.2
1	А	20	LEU	2.2
1	А	182	TYR	2.1
1	В	183	ASP	2.1
1	В	102	ILE	2.1

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.



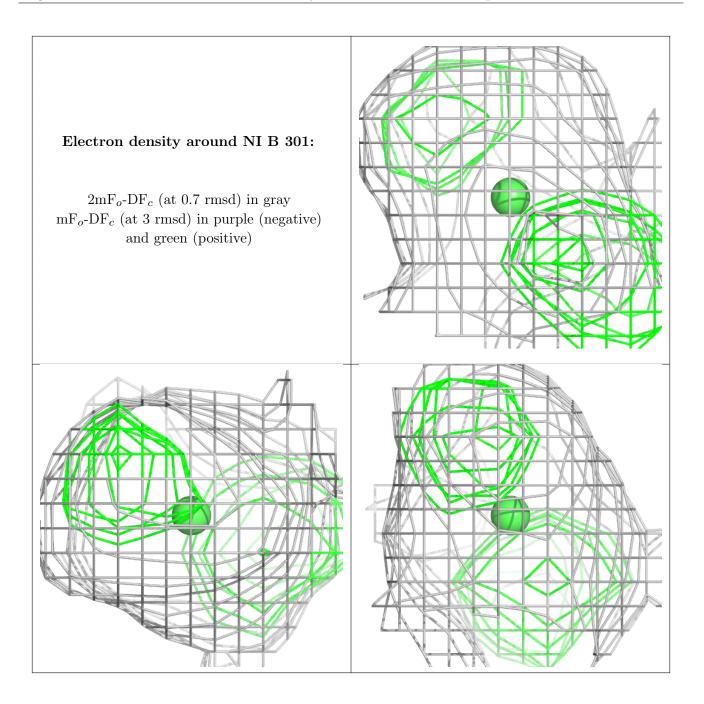
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

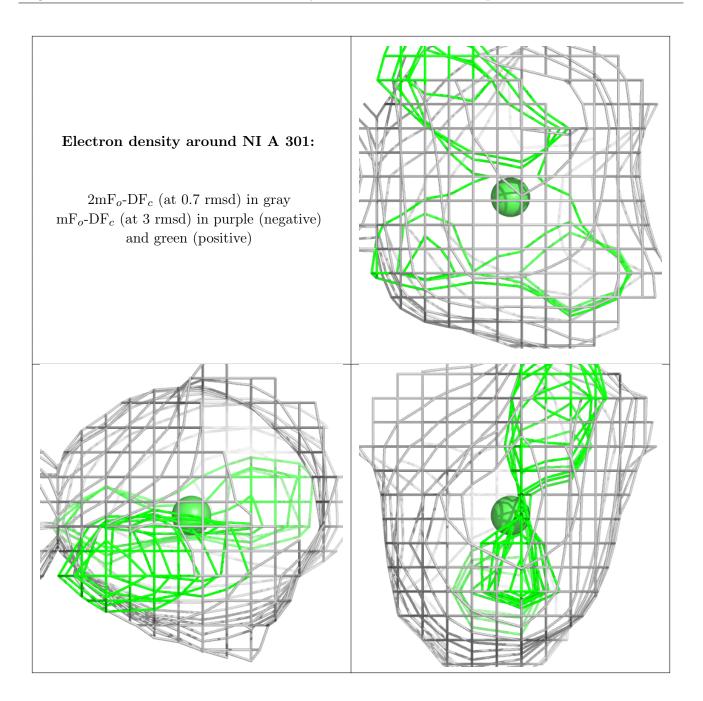
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	NI	В	301	1/1	0.92	0.16	81,81,81,81	0
2	NI	А	301	1/1	0.93	0.17	73,73,73,73	0
3	SO4	В	302	5/5	0.94	0.12	77,78,79,81	0
3	SO4	А	304	5/5	0.96	0.10	$48,\!51,\!53,\!57$	0
3	SO4	А	303	5/5	0.96	0.13	53,57,60,63	0
3	SO4	В	303	5/5	0.97	0.17	78,80,82,86	0
3	SO4	А	302	5/5	0.99	0.16	33,37,39,43	0
3	SO4	В	304	5/5	0.99	0.11	70,70,72,74	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









6.5 Other polymers (i)

There are no such residues in this entry.

