

Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 06:10 pm BST

PDB ID	:	6F2N
Title	:	Crystal structure of BCII Metallo-beta-lactamase in complex with KDU197
Authors	:	McDonough, M.A.; El-Hussein, A.; Schofield, C.J.; Zhang, D.; Brem, J.
Deposited on	:	2017-11-24
$\operatorname{Resolution}$:	1.15 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.15 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	1492(1.18-1.10)
Clashscore	141614	1537 (1.18-1.10)
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)
RSRZ outliers	127900	1464 (1.18-1.10)

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 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			
			85%			
1	А	227	89%	7%	•	



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2126 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 Metallo-beta-lactamase type 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	219	Total 1756	C 1112	N 299	0 342	${ m S} { m 3}$	0	11	0

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Zn 2 2	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	5	ZeroOcc	AltConf
3	А	1	Total O 5 4	S 1	0	0

• Molecule 4 is ({Z})-3-[2-(naphthalen-2-ylmethyl)phenyl]-2-sulfanyl-prop-2-enoic acid



(three-letter code: CF8) (formula: $\mathrm{C}_{20}\mathrm{H}_{16}\mathrm{O}_2\mathrm{S}).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	А	1	Total 23	C 20	O 2	S 1	0	1

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	336	Total O 340 340	0	14



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: Metallo-beta-lactamase type 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	53.17Å 61.67 Å 69.67 Å	Depositor
a, b, c, α , β , γ	90.00° 93.13° 90.00°	Depositor
$\mathbf{B}_{\mathrm{esolution}}(\mathbf{\hat{A}})$	28.19 - 1.15	Depositor
Resolution (A)	28.19 - 1.15	EDS
$\% { m Data \ completeness}$	97.3 (28.19-1.15)	Depositor
(in resolution range $)$	$97.3\ (28.19-1.15)$	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.14 (at 1.15 Å)	Xtriage
Refinement program	PHENIX	Depositor
D D .	0.134 , 0.151	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.146 , 0.164	DCC
R_{free} test set	2001 reflections (2.57%)	wwPDB-VP
Wilson B-factor $(Å^2)$	11.7	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.34 , 49.3	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2126	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.15% 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: ZN, SO4, CF8 $\,$

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).

Mal	Chain	Bo	nd lengths	Bond angles		
MOI C.	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.88	1/1785~(0.1%)	0.89	1/2418~(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	А	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	130	GLU	CB-CG	-5.35	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	245	ASP	CB-CG-OD1	5.88	123.59	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	117	ALA	Mainchain



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	1756	0	1755	9	0
2	A	2	0	0	0	0
3	А	5	0	0	0	0
4	A	23	0	0	0	0
5	А	340	0	0	3	4
All	All	2126	0	1755	9	4

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.

All (9) 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:82:LEU:HG	1:A:107[A]:LYS:HG3	1.85	0.58
1:A:41:ASN:HB3	1:A:100:MET:HE1	1.88	0.55
1:A:221[B]:THR:HG23	5:A:505:HOH:O	2.09	0.52
1:A:221[B]:THR:HG21	5:A:657[B]:HOH:O	2.13	0.49
1:A:223[B]:ILE:HD11	1:A:252:THR:HG21	2.01	0.43
1:A:59:THR:HA	1:A:71[B]:SER:O	2.19	0.42
1:A:59:THR:HA	1:A:71[A]:SER:O	2.20	0.41
1:A:228:LYS:HG3	5:A:402:HOH:O	2.21	0.41
1:A:218[B]:GLU:O	1:A:221[B]:THR:HG22	2.22	0.40

All (4) 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)
5:A:487:HOH:O	5:A:487:HOH:O[2_556]	1.69	0.51
5:A:734:HOH:O	5:A:734:HOH:O[2_556]	1.79	0.41
5:A:531:HOH:O	5:A:706:HOH:O[2_656]	2.03	0.17
5:A:531:HOH:O	5:A:630:HOH:O[2_656]	2.06	0.14



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	226/227~(100%)	220~(97%)	6 (3%)	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 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	А	191/196~(97%)	189~(99%)	2(1%)	76 42	

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	78	THR
1	А	183	ASN

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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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).

Mal	Turne	Chain	Dec	Timle	Bo	ond leng	sths	B	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CF8	А	304[A]	2	21,25,25	0.40	0	28,34,34	0.46	0
3	SO4	А	303	-	4,4,4	0.29	0	6,6,6	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CF8	А	304[A]	2	-	2/7/12/12	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	304[A]	CF8	C-C2-C3-C4
4	А	304[A]	CF8	C-C2-C3-C8



There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	А	219/227~(96%)	3.64	194 (88%) 0 0	8, 16, 32, 42	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	44	GLY	14.0
1	А	43	THR	13.4
1	А	63	SER	11.6
1	А	45	THR	9.8
1	А	62	GLY	8.7
1	А	89	TRP	8.4
1	А	41	ASN	8.1
1	А	37	THR	7.7
1	А	167	ASN	7.5
1	А	35	GLU	7.3
1	А	36	LYS	7.0
1	А	113	ILE	7.0
1	А	150	TYR	6.4
1	А	211	VAL	6.3
1	А	42	GLU	6.3
1	А	68	ALA	6.1
1	А	184	ILE	6.0
1	А	61	LEU	6.0
1	А	122	ILE	5.9
1	А	133	ILE	5.9
1	А	46	ILE	5.8
1	А	109	VAL	5.8
1	А	249[A]	LEU	5.7
1	А	112	VAL	5.6
1	А	200	VAL	5.6
1	А	85	VAL	5.5
1	А	74	LEU	5.4



Mol	Chain	Res	Type	RSRZ
1	А	166	GLY	5.4
1	А	223[A]	ILE	5.3
1	А	185	VAL	5.3
1	А	84	LEU	5.2
1	А	117	ALA	5.1
1	А	186	VAL	5.1
1	А	217[A]	ASN	5.1
1	А	114	ILE	5.1
1	А	195	VAL	5.0
1	А	83	VAL	4.9
1	А	193	ILE	4.9
1	А	180	THR	4.9
1	А	199	LEU	4.9
1	A	219	TRP	4.8
1	А	51	LEU	4.8
1	А	170	VAL	4.8
1	А	236	VAL	4.7
1	А	48	ILE	4.7
1	А	235	ALA	4.7
1	А	75	VAL	4.7
1	А	187	TRP	4.7
1	А	76	LEU	4.6
1	А	248	LEU	4.6
1	А	101	VAL	4.6
1	А	140	LEU	4.5
1	А	194	LEU	4.5
1	А	237	VAL	4.5
1	А	206	LYS	4.5
1	А	128	LEU	4.5
1	A	230	TYR	4.5
1	A	98	ILE	4.4
1	А	125	ILE	4.4
1	A	198	CYS	4.4
1	А	141	THR	4.3
1	A	70	PRO	4.3
1	A	52	ASN	4.3
1	A	138	THR	4.3
1	A	157	LEU	4.3
1	A	203	THR	4.3
1	A	115	THR	4.2
1	A	244	GLY	4.1
1	A	154	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	А	234	ASN	4.0
1	А	38	VAL	4.0
1	А	82	LEU	4.0
1	А	215	TYR	4.0
1	А	139	ALA	3.9
1	А	240	HIS	3.9
1	А	252	THR	3.9
1	А	256	LEU	3.9
1	А	221[A]	THR	3.8
1	А	174	TYR	3.8
1	А	57	VAL	3.8
1	А	250	LEU	3.8
1	А	253	LEU	3.8
1	А	210	ASN	3.8
1	A	135	ALA	3.8
1	А	183	ASN	3.7
1	А	56	TRP	3.7
1	А	196	GLY	3.7
1	А	239	GLY	3.7
1	А	119	ALA	3.7
1	А	188	LEU	3.7
1	А	146	LYS	3.6
1	А	39	ILE	3.6
1	А	96[A]	GLU	3.6
1	А	216	VAL	3.5
1	А	208	LEU	3.5
1	А	142	ALA	3.5
1	А	227	LEU	3.5
1	A	55	VAL	3.5
1	A	110	THR	3.4
1	A	197	GLY	3.4
1	A	87	SER	3.4
1	A	238	PRO	3.4
1	A	92	LYS	3.4
1	A	144	LEU	3.4
1	A	132	GLY	3.4
1	A	173	PHE	3.3
1	A	97	LEU	3.2
1	A	182	ASP	3.2
1	A	148	ASN	3.2
1	A	58	HIS	3.2
1	A	178	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	А	257	LYS	3.2
1	А	159	THR	3.2
1	А	226	VAL	3.2
1	А	163	LEU	3.1
1	А	175	PRO	3.0
1	А	53	LYS	3.0
1	А	105	PHE	3.0
1	А	93	LEU	3.0
1	А	158	GLN	3.0
1	А	49	SER	3.0
1	А	160	VAL	3.0
1	А	116	HIS	3.0
1	А	191	TYR	3.0
1	A	243	VAL	2.9
1	А	205	ALA	2.9
1	А	214	ALA	2.9
1	А	100	MET	2.9
1	А	78	THR	2.9
1	А	255	LEU	2.9
1	А	162	ASN	2.9
1	А	73	GLY	2.9
1	А	124	GLY	2.9
1	А	137	SER	2.8
1	А	143[A]	GLU	2.8
1	А	242	GLU	2.8
1	А	209	GLY	2.8
1	А	106	GLN	2.8
1	А	177	LYS	2.8
1	А	172	THR	2.7
1	A	147	LYS	2.7
1	А	245	ASP	2.7
1	A	111	ASP	2.7
1	A	232	ASN	2.7
1	А	212	ALA	2.7
1	A	231	ARG	2.7
1	А	246	LYS	2.7
1	А	179	HIS	2.6
1	А	254	ASP	2.6
1	А	161	THR	2.6
1	А	202	SER	2.5
1	А	233	ILE	2.5
1	A	72	ASN	2.5

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Mol	Chain	Res	Type	RSRZ		
1	A	207	ASP	2.5		
1	A	54	ASN	2.5		
1	А	145	ALA	2.5		
1	А	79	SER	2.5		
1	А	220[A]	SER	2.5		
1	А	108	ARG	2.5		
1	А	127	THR	2.5		
1	А	176	GLY	2.5		
1	А	121	ARG	2.4		
1	А	168	MET	2.4		
1	А	86	ASP	2.4		
1	А	94	THR	2.4		
1	А	165	PHE	2.3		
1	А	189	PRO	2.3		
1	А	222	SER	2.3		
1	А	247	GLY	2.3		
1	А	218 [A]	GLU	2.3		
1	А	118	HIS	2.3		
1	A	136	HIS	2.2		
1	А	153	PRO	2.2		
1	A	171	GLU	2.2		
1	А	80	LYS	2.2		
1	А	155	GLY	2.2		
1	A	225	ASN	2.2		
1	A	134	LYS	2.2		
1	A	181[A]	GLU	2.2		
1	A	149	GLY	2.2		
1	A	88	SER	2.2		
1	A	99	GLU	2.2		
1	A	69	VAL	2.2		
1	A	229	ARG	2.2		
1	A	241	GLY	2.1		
1	A	126	LYS	2.1		
1	A	91	ASP	2.1		
- 1	A	59	THR	2.1		
- 1	A	169	LYS	2.1		
1	A	47	SER	2.0		
1	A	192	ASN	2.0		
1	A	107[A]	LYS	2.0		
<u> </u>	A	251	HIS	2.0		
1	A	129	LYS	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)

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	\mathbf{Res}	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	А	303	5/5	0.82	0.27	51, 51, 52, 52	0
4	CF8	А	304[A]	23/23	0.85	0.37	$13,\!23,\!28,\!29$	23
2	ZN	А	301	1/1	0.99	0.17	13,13,13,13	1
2	ZN	А	302	1/1	0.99	0.17	12,12,12,12	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.

