

# wwPDB X-ray Structure Validation Summary Report (i)

Sep 27, 2021 - 11:00 am BST

PDB ID	:	7B25
Title	:	DtxR-like iron-dependent regulator IdeR (Q43A variant) complexed with
		cobalt and its consensus DNA-binding sequence
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Deposited on		
Resolution	:	2.34 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 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 2.34 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	2	Percentile Ranks	Value	
Clashscore			2	
Ramachandran outliers			0	
Sidechain outliers			0	
	Worse		Better	
	Percentile relative to all X-ra	y structures		
	Percentile relative to X-ray s	tructures of similar resolution		

Metric	$egin{array}{llllllllllllllllllllllllllllllllllll$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality	of chain
1	А	233	58%	• 41%
1	В	233	94%	•••
1	С	233	93%	5% •
1	D	233	59%	41%
1	aa	233	39%	61%
1	dd	233	39%	61%
2	Е	29	72%	28%
3	F	29	72%	28%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8256 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		At	oms			ZeroOcc	AltConf	Trace
1	А	138	Total	С	Ν	0	S	0	0	0
	A	130	1092	682	198	207	5	0	0	0
1	В	227	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	D	221	1748	1086	320	334	8	0	0	0
1	С	227	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	U	221	1748	1086	320	334	8	0	0	0
1	D	138	Total	С	Ν	0	S	0	0	0
	D	130	1092	682	198	207	5	0	0	0
1	aa	91	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	aa	31	668	410	124	131	3	0	0	0
1	dd	91	Total	С	Ν	Ο	S	0	0	0
	uu	31	668	410	124	131	3		U	U

• Molecule 1 is a protein called DtxR family iron (Metal) dependent repressor.

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	GLY	-	expression tag	UNP A0A2A9J1W2
А	0	HIS	-	expression tag	UNP A0A2A9J1W2
А	43	ALA	GLN	engineered mutation	UNP A0A2A9J1W2
В	-1	GLY	-	expression tag	UNP A0A2A9J1W2
В	0	HIS	-	expression tag	UNP A0A2A9J1W2
В	43	ALA	GLN	engineered mutation	UNP A0A2A9J1W2
С	-1	GLY	-	expression tag	UNP A0A2A9J1W2
С	0	HIS	-	expression tag	UNP A0A2A9J1W2
С	43	ALA	GLN	engineered mutation	UNP A0A2A9J1W2
D	-1	GLY	-	expression tag	UNP A0A2A9J1W2
D	0	HIS	-	expression tag	UNP A0A2A9J1W2
D	43	ALA	GLN	engineered mutation	UNP A0A2A9J1W2
aa	-1	GLY	-	expression tag	UNP A0A2A9J1W2
aa	0	HIS	-	expression tag	UNP A0A2A9J1W2
aa	43	ALA	GLN	engineered mutation	UNP A0A2A9J1W2
dd	-1	GLY	-	expression tag	UNP A0A2A9J1W2
dd	0	HIS	-	expression tag	UNP A0A2A9J1W2

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Chain	Residue	Modelled	Actual	Comment	Reference
dd	43	ALA	GLN	engineered mutation	UNP A0A2A9J1W2

• Molecule 2 is a DNA chain called consensus DNA-binding sequence.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Е	29	Total 593	C 283	N 107	0 174	Р 29	0	0	0

• Molecule 3 is a DNA chain called consensus DNA-binding sequence.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	F	29	Total 596	C 284	N 109	0 174	Р 29	0	0	0

• Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total Co 2 2	0	0
4	В	2	Total Co 2 2	0	0
4	С	2	Total Co 2 2	0	0
4	D	2	$\begin{array}{cc} \text{Total} & \text{Co} \\ 2 & 2 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	7	Total O 7 7	0	0
5	В	5	Total O 5 5	0	0
5	С	7	Total O 7 7	0	0
5	D	10	Total O 10 10	0	0
5	Ε	3	Total O 3 3	0	0
5	aa	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	dd	7	Total O 7 7	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. 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. 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.

Note EDS was not executed.

• Molecule 1: DtxR family iron (Metal) dependent repressor

Chain A:	58%	41%
GLY HIS MET ASN D3 D3 R60 R60 V117	V140 GLY GLY SER SER SER SER PRD PRD PRD PRD ASP ASP ASP GLY GLY GLY GLY GLY GLY GLY	LEU LEU VAL CYS CYS CYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
VAL PRO GLY GLY ASN GLU TLE ASP TLE VAL	VAL VAL ALA ALA ASN VAL ASN PRO CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	ALA VAL MET VAL VAL LYS LYS
• Molecule 1:	DtxR family iron (Metal) depende	ent repressor
Chain B:	94%	• •
GLY HIS ASN D3 R29 R33 R33	R47 V140 GL14 ASP ASP ASP A171 A171 A171 V167 V167 V128 V228 V228 K231	
• Molecule 1:	DtxR family iron (Metal) depende	ent repressor
Chain C:	93%	5% •
GLY HIS MET ASN D3 R29 R33 R33	V140 GLY ASP ASP ASP 143 144 144 144 144 144 145 145 148 148 148 148 148 148 148 148 171 17 17 17 17 17 17 17 17 17 17 17 17	
• Molecule 1:	DtxR family iron (Metal) depende	ent repressor
Chain D:	59%	41%
GLY HIS ASN ASN D3 B3 R60 V140 C1V	ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	VAL VAL ARG ARG ALL ALE GLU GLU CLEU ASP PRO CLU CLEU CLEU CLEU CLEU CLEU CLEU CLEU
GLY ASN GLU TLE ASP TLE VAL VAL VAL VAL	GLY VAL VAL LYS PRO PRO PRO GLY VAL GLN GLN GLY GLY GLY GLY GLY ALA ALA ALA ALA ALA	MALT ARG VAL LYS
• Molecule 1:	DtvB family iron (Metal) depend	ent repressor

• Molecule 1: DtxR family iron (Metal) dependent repressor

Chain aa:

39%



GLY HIS MET ASN ASP LEU ILEU ASP THR THR	GLU MET TYR TYR ARG ARG THR TYR ASP CLU GLU GLU	VAL VAL PRO PRO ARG ARG ALA ALA ALA ALA CEU CLU CLU CLU CLU CLU CLU CLU CLU	PGLI THR VAL SER ALA ARL ARL ARG GLU GLU GLU CEU	LEU THR VAL ALA GLU
ASP ARG HIS LEU GLU CLEU LEU LVS ALA GLY	ARG ALA ALA ALA ALA TLE SER VAL LYS HIS ARG LYS ALA ALA	GLU LEU LEU VAL LEU VAL ASP VAL ASP VAL CLU CLU CLU CLU CLU CLU CLU VAL	LLU GLU ALA ALA CYS CYS CYS CYS GLU HIS VAL ALA GLU GLU	ANG LYS LEU VAL LYS
LEU LEU GLY ASN PRO THR SER PRO TYR	GLY ASN PRO FRO GLY GLY CLEU GLY GLY GL41 CVAL	1		
• Molecule 1:	DtxR family iron (	Metal) dependent rej	pressor	
Chain dd:	39%		61%	-
GLY HIS MET ASN ASP LEU LEU TLE ASP THR THR	GLU MET TYR LEU LEU TYR TYR TYR TYR GLU GLU GLU GLU	VALL VAL PRO PRO ALA ALA ALA ALA ALA CLU CLU CLU CLU SER SLV CLV	PRO PRO VAL SER ALA ALA ARG GLU GLU ASP GLV CLU	LLEU VAL ALA GLU
ASP ARG HIS LEU CLU CLU LEU THR LYS ALA GLY	ARG ALA ALA ALA ALA SER VAL LYS HIS LYS HIS ARG LYS ALA	AGLO AGLO ASP VAL LEU VAL LEU OLU CLU CLU CLU CLU CLU VAL	LEU LEU GLU ALA ARG CYS ARG TRP OLU HTS NMET NMET NMET SEE ALA ALA ALA	ANG LYS LEU VAL LYS
LEU LEU GLY ASN PRO THR SER SER PRO TYR	GLY ASN PRO PRO PRO PRO PRO CLEU CLEU CLEU VIAL CLEU VIAL	1004		
• Molecule 2:	consensus DNA-bir	nding sequence		
Chain E:	72	%	28%	
C1 A4 A13 G14 A18 A18 A24	628 629 829 829 829			
• Molecule 3:	consensus DNA-bir	nding sequence		
Chain F:	72	%	28%	
<b>C1</b> A4 C5 G10 G10 A13	A18 C28 C28			



# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	192.66Å $110.86$ Å $86.75$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $116.85^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	93.16 - 2.34	Depositor
% Data completeness	53.9 (93.16-2.34)	Depositor
(in resolution range)	00.5 (00.10 2.04)	Depositor
$R_{merge}$	0.13	Depositor
R <sub>sym</sub>	(Not available)	Depositor
Refinement program	REFMAC 5.8.0267	Depositor
$R, R_{free}$	0.267 , $0.283$	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8256	wwPDB-VP
Average B, all atoms $(Å^2)$	67.0	wwPDB-VP



# 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: CO

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	Mol Chain		Bond lengths		angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.64	0/1108	0.73	0/1501
1	В	0.67	0/1770	0.74	0/2396
1	С	0.68	0/1770	0.74	0/2396
1	D	0.64	0/1108	0.73	0/1501
1	aa	0.68	0/674	0.74	0/911
1	dd	0.68	0/674	0.74	0/911
2	Ε	0.34	0/664	0.73	0/1022
3	F	0.32	0/668	0.72	0/1029
All	All	0.62	0/8436	0.74	0/11667

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	1092	0	1110	3	0
1	В	1748	0	1787	5	0
1	С	1748	0	1788	6	0
1	D	1092	0	1110	2	0
1	aa	668	0	684	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	dd	668	0	684	0	0
2	Е	593	0	328	6	0
3	F	596	0	328	6	0
4	А	2	0	0	0	0
4	В	2	0	0	0	0
4	С	2	0	0	0	0
4	D	2	0	0	0	0
5	А	7	0	0	0	0
5	В	5	0	0	0	0
5	С	7	0	0	0	0
5	D	10	0	0	0	0
5	Е	3	0	0	0	0
5	aa	4	0	0	0	0
5	dd	7	0	0	0	0
All	All	8256	0	7819	22	0

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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 2.

The worst 5 of 22 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)
2:E:13:DA:C2	3:F:18:DA:C2	2.98	0.51
3:F:28:DC:H2"	3:F:29:DG:C8	2.45	0.51
1:B:148:ASP:HB2	1:B:151:LEU:HD12	1.95	0.48
1:C:147:VAL:HG23	1:C:147:VAL:O	2.15	0.47
1:A:140:VAL:O	1:A:140:VAL:HG23	2.14	0.46

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	Percen	tiles
1	А	136/233~(58%)	132~(97%)	4(3%)	0	100	100
1	В	223/233~(96%)	218 (98%)	5(2%)	0	100	100
1	С	223/233~(96%)	216 (97%)	7(3%)	0	100	100
1	D	136/233~(58%)	132 (97%)	4 (3%)	0	100	100
1	aa	89/233~(38%)	86~(97%)	3~(3%)	0	100	100
1	dd	89/233~(38%)	84 (94%)	5~(6%)	0	100	100
All	All	896/1398 (64%)	868 (97%)	28 (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	Percer	ntiles
1	А	118/194~(61%)	118 (100%)	0	100	100
1	В	190/194~(98%)	190 (100%)	0	100	100
1	$\mathbf{C}$	190/194~(98%)	190 (100%)	0	100	100
1	D	118/194~(61%)	118 (100%)	0	100	100
1	aa	73/194~(38%)	73~(100%)	0	100	100
1	dd	73/194~(38%)	73~(100%)	0	100	100
All	All	762/1164~(66%)	762 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	aa	208	GLN
1	aa	217	GLN
1	dd	208	GLN
1	dd	217	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, 8 are monoatomic - leaving 0 for Mogul analysis.

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)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

