

Full wwPDB X-ray Structure Validation Report (i)

Sep 27, 2021 – 11:01 am BST

PDB ID	:	7B23
Title	:	DtxR-like iron-dependent regulator IdeR complexed with cobalt and the
		SACE_2689 promoter DNA-binding sequence
Authors	:	Maurer, D.; Marcos-Torres, F.J.; Griese, J.J.
Deposited on	:	2020-11-26
Resolution	:	2.15 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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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 2.15 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	Percentile Ranks		Value
Clashscore			1
Ramachandran outliers			0
Sidechain outliers			0
	Worse	Better	
	Percentile relative to all X-ray structures		
	Percentile relative to X-ray structures of similar resolution		

Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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	C	Quality of chain							
1	А	233	58%	·	41%						
1	В	233		93%		• •					
1	С	233		93%		• •					
1	D	233	58%	•	41%						
1	aa	233	39%		61%						
1	dd	233	39%		61%						
2	Е	30		87%		10% •					
3	F	30		93%		• •					



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8203 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
	Л	130	1098	684	199	210	5	0	0	0
1	В	223	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	D	220	1722	1069	316	329	8	0	0	0
1	С	C 223	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	U		1722	1069	316	329	8	0	0	0
1	D	138	Total	С	Ν	0	S	0	0	0
	D	190	1098	684	199	210	5	0	0	0
1	9.9	90	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	1 aa		658	404	122	129	3	0	0	0
1	1 dd	90	Total	С	Ν	Ο	S	0	0	0
		90	658	404	122	129	3		0	U

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	GLY	-	expression tag	UNP A0A2A9J1W2
A	0	HIS	-	expression tag	UNP A0A2A9J1W2
В	-1	GLY	-	expression tag	UNP A0A2A9J1W2
В	0	HIS	-	expression tag	UNP A0A2A9J1W2
С	-1	GLY	-	expression tag	UNP A0A2A9J1W2
С	0	HIS	-	expression tag	UNP A0A2A9J1W2
D	-1	GLY	-	expression tag	UNP A0A2A9J1W2
D	0	HIS	-	expression tag	UNP A0A2A9J1W2
aa	-1	GLY	-	expression tag	UNP A0A2A9J1W2
aa	0	HIS	-	expression tag	UNP A0A2A9J1W2
dd	-1	GLY	-	expression tag	UNP A0A2A9J1W2
dd	0	HIS	-	expression tag	UNP A0A2A9J1W2

• Molecule 2 is a DNA chain called SACE_2689 promoter DNA-binding sequence.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Е	29	Total 597	C 285	N 108	O 175	Р 29	0	0	0

• Molecule 3 is a DNA chain called SACE_2689 promoter DNA-binding sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	29	Total 592	C 283	N 107	0 173	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	Total Co 2 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	10	Total O 10 10	0	0
5	В	9	Total O 9 9	0	0
5	С	5	Total O 5 5	0	0
5	D	11	Total O 11 11	0	0
5	Ε	7	Total O 7 7	0	0
5	F	7	Total O 7 7	0	0
5	aa	1	Total O 1 1	0	0

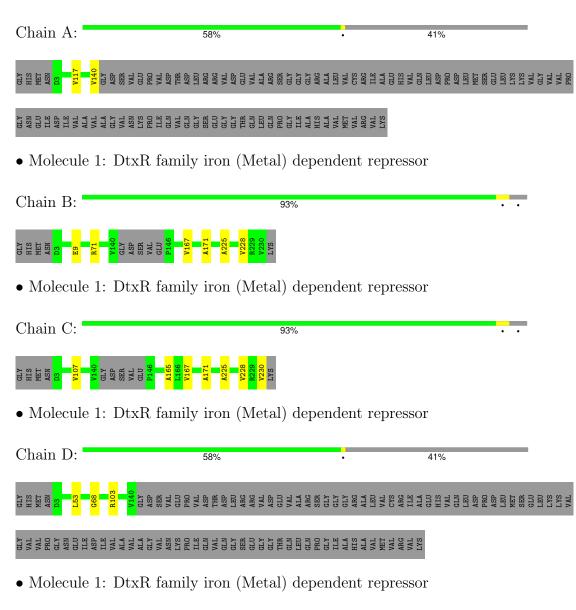


3 Residue-property plots (i)

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 aa:

39%



GLY HIS MET ASN ASP LEU ILEU ASP ASP	THR THR GLU MET TYR LEU THR THR	TYR ASP GLU GLU GLU VAL	VAL PRO LEU ARG ARG ARG ILE	ALA GLU ARG LEU GLU SER	GLY PRO VAL SER GLN	THR VAL ALA ARG MET	ARG ASP GLY LEU	THR VAL ALA GLU
ASP ARG HIS LEU GLU LEU THR TYS	ALA GLY ARG ALA ALA ALA SER SER VAI	MET ARG LYS HIS ARG LEU ALA GLU	ARG LEU VAL ASP VAL TLE	GLY LEU GLU TRP GLU GLU VAL	HIS LEU GLU ALA CSD ARG	TRP GLU HIS VAL MET SFR	GLU GLU VAL GLU	LYS LEU VAL LYS
LEU LEU GLY ASN PRO THR THR SER	PRO TYR GLY ASN PRO FLC GLY I FU	ASP GLU GLU GLY VAL G141 V230	LYS					
• Molecule	1: DtxR fa	mily iron (l	Metal) dej	pendent r	epressor			
Chain dd: '	:	39%			61%			
GLY HIS MET ASN ASP LEU ILE ASP ASP	THR THR GLU MET TYR LEU ARG THR	TYR ASP LEU GLU GLU GLU GLV VAL	VAL PRO LEU ARG ARG ARG ILE	ALA GLU ARG LEU GLU SER	GLY PRO VAL SER GLN	THR VAL ALA ARG MET	ARG ASP GLY LEU	THR VAL ALA GLU
ASP ARG HIS LEU GLU LEU THR TYS	ALA GLY ARG ALA ALA TLE SER VAT	MET ARG LYS LYS HIS ARG LEU ALA GLU	ARG LEU LEU VAL ASP VAL TLE	GLY LEU GLU GLU GLU VAL	HIS LEU GLU ALA CSD	TRP GLU HIS VAL MET SFR	GLU GLU GLU GLU	LFU LEU LYS
LEU LEU GLY ASN THR THR SER	PRO TYR GLY ASN PRO TLE PRO GLY	ALEO GLU GLV GLY VAL G141 V230	LYS					
• Molecule	2: SACE_2	2689 promo	ter DNA-	binding s	equence			
Chain E:			87%			1	0% •	
DG G2 G10 A14 A14	0							
• Molecule	3: SACE_2	2689 promo	ter DNA-	binding s	equence			
Chain F:			93%				• •	
DC C2								



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	194.25Å 113.12Å 89.29Å	Depositor
a, b, c, α , β , γ	90.00° 117.25° 90.00°	Depositor
Resolution (Å)	94.63 - 2.15	Depositor
% Data completeness	63.8 (94.63-2.15)	Depositor
(in resolution range)	05.0 (54.05-2.15)	Depositor
R_{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.226 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8203	wwPDB-VP
Average B, all atoms $(Å^2)$	62.0	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, CSD

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	Sond lengths Bon		l angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.64	0/1106	0.70	0/1498	
1	В	0.66	0/1736	0.71	0/2351	
1	С	0.66	0/1736	0.72	0/2351	
1	D	0.64	0/1106	0.70	0/1498	
1	aa	0.69	0/664	0.74	0/900	
1	dd	0.69	0/664	0.74	0/900	
2	Ε	0.30	0/669	0.75	0/1031	
3	F	0.31	0/663	0.76	0/1020	
All	All	0.62	0/8344	0.72	0/11549	

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	1098	0	1114	1	0
1	В	1722	0	1759	3	0
1	С	1722	0	1759	5	0
1	D	1098	0	1114	2	0
1	aa	658	0	671	0	0

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Mol	Chain	Non-H		H(added)	Clashes	Symm-Clashes
1	dd	658	0	671	0	0
2	Е	597	0	329	2	0
3	F	592	0	328	1	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	10	0	0	0	0
5	В	9	0	0	0	0
5	С	5	0	0	0	0
5	D	11	0	0	0	0
5	Е	7	0	0	0	0
5	F	7	0	0	0	0
5	aa	1	0	0	0	0
All	All	8203	0	7745	12	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 1.

All (12) 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:14:DA:C2	3:F:19:DA:C2	3.01	0.48
1:C:107:VAL:HB	1:D:103:ARG:HB3	1.97	0.46
1:D:53:LEU:O	1:D:68:GLY:HA3	2.16	0.45
1:C:165:ALA:HB2	1:C:230:VAL:HG12	1.98	0.45
2:E:10:DG:H2"	2:E:11:DG:O5'	2.20	0.42
1:B:9:GLU:OE2	1:B:71:ARG:NH2	2.52	0.42
1:B:167:VAL:HA	1:B:228:VAL:HG12	2.01	0.42
1:B:171:ALA:HB3	1:B:225:ALA:HB1	2.01	0.41
1:C:165:ALA:HB1	1:C:228:VAL:HB	2.02	0.41
1:A:117:VAL:HG21	1:A:140:VAL:HG21	2.03	0.41
1:C:167:VAL:HA	1:C:228:VAL:HG12	2.02	0.41
1:C:171:ALA:HB3	1:C:225:ALA:HB1	2.03	0.41

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	Percer	ntiles
1	А	135/233~(58%)	131~(97%)	4(3%)	0	100	100
1	В	218/233~(94%)	212~(97%)	6 (3%)	0	100	100
1	С	218/233~(94%)	212~(97%)	6 (3%)	0	100	100
1	D	135/233~(58%)	132 (98%)	3(2%)	0	100	100
1	aa	88/233~(38%)	86~(98%)	2(2%)	0	100	100
1	dd	88/233~(38%)	84 (96%)	4 (4%)	0	100	100
All	All	882/1398~(63%)	857 (97%)	25 (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	118/194~(61%)	118 (100%)	0	100 100
1	В	186/194~(96%)	186 (100%)	0	100 100
1	С	186/194~(96%)	186 (100%)	0	100 100
1	D	118/194 (61%)	118 (100%)	0	100 100
1	aa	72/194~(37%)	72~(100%)	0	100 100
1	dd	72/194~(37%)	72 (100%)	0	100 100
All	All	752/1164~(65%)	752 (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. 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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	Turne	Chain	Dec	Link	B	Bond lengths			Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
1	CSD	В	102	1,4	3,7,8	0.69	0	1,8,10	0.28	0	
1	CSD	А	102	1,4	3,7,8	0.72	0	1,8,10	0.17	0	
1	CSD	D	102	1,4	3,7,8	0.71	0	1,8,10	0.05	0	
1	CSD	С	102	1,4	3,7,8	0.70	0	1,8,10	0.24	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
1	CSD	В	102	1,4	-	1/2/6/8	-
1	CSD	А	102	1,4	-	1/2/6/8	-
1	CSD	D	102	1,4	-	1/2/6/8	-
1	CSD	С	102	1,4	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
1	А	102	CSD	N-CA-CB-SG
1	В	102	CSD	N-CA-CB-SG
1	С	102	CSD	N-CA-CB-SG
1	D	102	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

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.

