Full wwPDB X-ray Structure Validation Report (i)

Sep 27, 2021 – 11:00 am BST

PDB ID	:	7B24
Title	:	DtxR-like iron-dependent regulator IdeR (P39G variant) complexed with cobalt and its consensus DNA-binding sequence
Authors	:	Maurer, D.; Marcos-Torres, F.J.; Griese, J.J.
Deposited on	:	2020-11-26
Resolution	:	2.05 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:

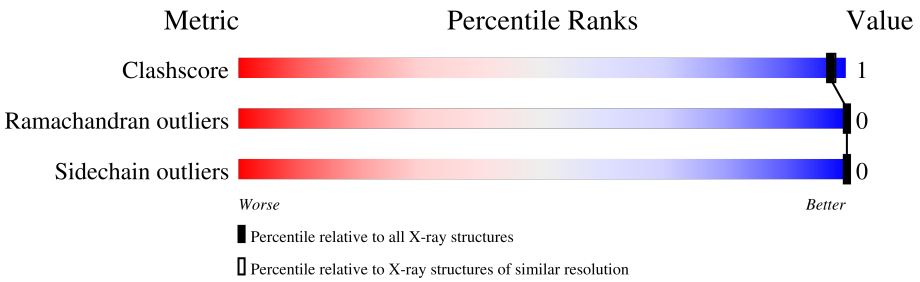
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.05 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))
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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	A	233	60% · 39%
1	B	233	95% · ·
1	C	233	94% · ·
1	D	233	61% 39%
1	aa	233	35% 65%
1	dd	233	36% 64%
2	E	30	83% 13% ·
3	F	30	90% 7% ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8310 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 DtxR family iron (Metal) dependent repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	142	1119	694	204	216	5	0	0	0
			Total	C	N	O	S			
1	B	226	1743	1081	321	333	8	0	0	0
			Total	C	N	O	S			
1	C	224	1727	1071	319	329	8	0	0	0
			Total	C	N	O	S			
1	D	142	1119	694	204	216	5	0	0	0
			Total	C	N	O	S			
1	aa	82	602	371	114	114	3	0	0	0
			Total	C	N	O	S			
1	dd	83	611	377	116	115	3	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A2A9J1W2
A	0	HIS	-	expression tag	UNP A0A2A9J1W2
A	39	GLY	PRO	engineered mutation	UNP A0A2A9J1W2
B	-1	GLY	-	expression tag	UNP A0A2A9J1W2
B	0	HIS	-	expression tag	UNP A0A2A9J1W2
B	39	GLY	PRO	engineered mutation	UNP A0A2A9J1W2
C	-1	GLY	-	expression tag	UNP A0A2A9J1W2
C	0	HIS	-	expression tag	UNP A0A2A9J1W2
C	39	GLY	PRO	engineered mutation	UNP A0A2A9J1W2
D	-1	GLY	-	expression tag	UNP A0A2A9J1W2
D	0	HIS	-	expression tag	UNP A0A2A9J1W2
D	39	GLY	PRO	engineered mutation	UNP A0A2A9J1W2
aa	-1	GLY	-	expression tag	UNP A0A2A9J1W2
aa	0	HIS	-	expression tag	UNP A0A2A9J1W2
aa	39	GLY	PRO	engineered mutation	UNP A0A2A9J1W2
dd	-1	GLY	-	expression tag	UNP A0A2A9J1W2
dd	0	HIS	-	expression tag	UNP A0A2A9J1W2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
dd	39	GLY	PRO	engineered mutation	UNP A0A2A9J1W2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	29	596	284	109	174	29	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	29	593	283	107	174	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
			Total	Co		
4	A	2	2	2	0	0
4	B	2	2	2	0	0
4	C	2	2	2	0	0
4	D	2	2	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	43	43	43	0	0
5	B	26	26	26	0	0
5	C	33	33	33	0	0
5	D	44	44	44	0	0
5	E	12	12	12	0	0
5	F	14	14	14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	aa	7	7	7	0	0
			Total	O		
5	dd	13	13	13	0	0

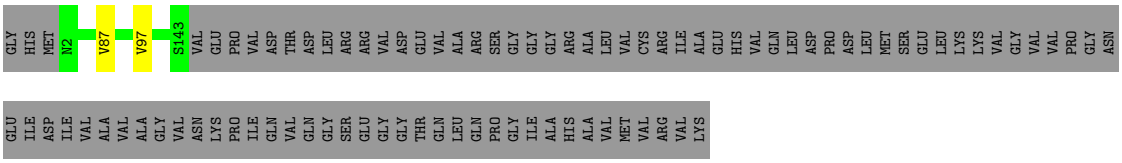
3 Residue-property plots (i)

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.

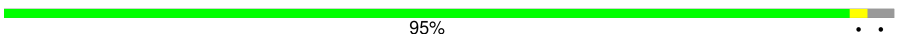
• Molecule 1: DtxR family iron (Metal) dependent repressor

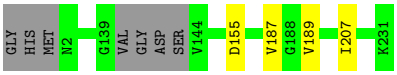
Chain A:



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

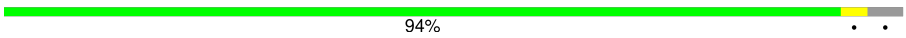
Chain B:

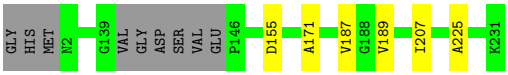




• Molecule 1: DtxR family iron (Metal) dependent repressor

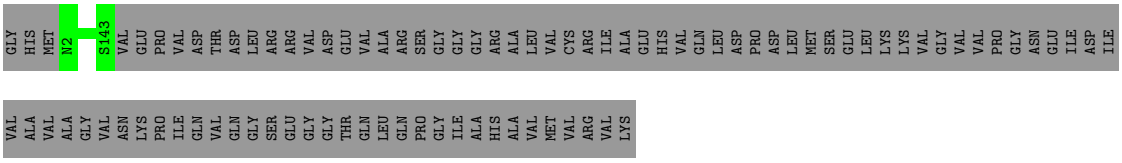
Chain C:





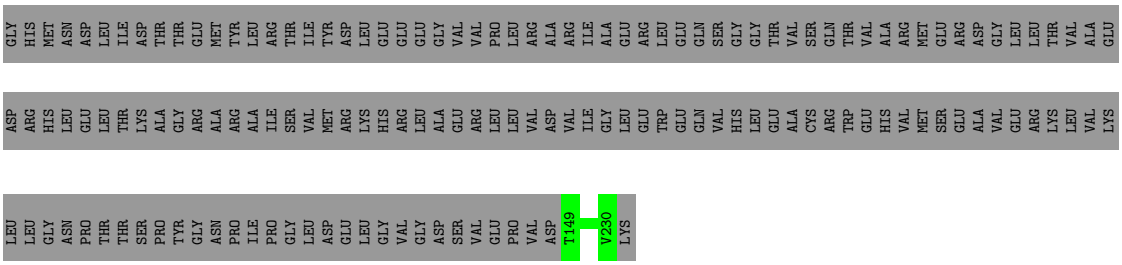
• Molecule 1: DtxR family iron (Metal) dependent repressor

Chain D:



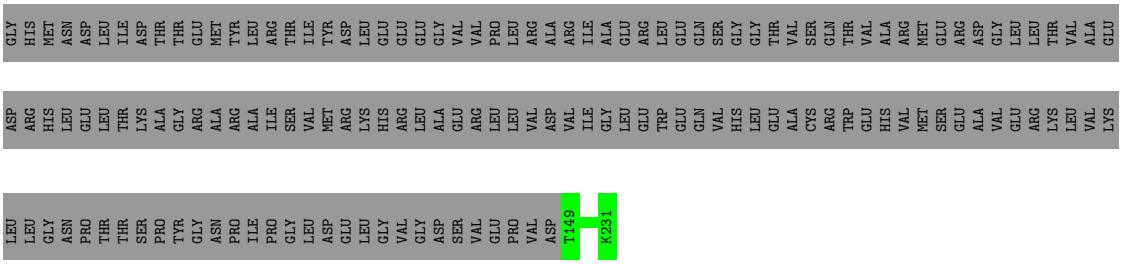
• Molecule 1: DtxR family iron (Metal) dependent repressor

Chain aa:



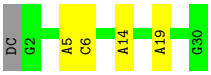
• Molecule 1: DtxR family iron (Metal) dependent repressor

Chain dd: 36% 64%



• Molecule 2: consensus DNA-binding sequence

Chain E: 83% 13% •



• Molecule 3: consensus DNA-binding sequence

Chain F: 90% 7% •

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 a, b, c, α, β, γ	196.40Å 113.84Å 89.80Å 90.00° 117.25° 90.00°	Depositor
Resolution (Å)	54.93 – 2.05	Depositor
% Data completeness (in resolution range)	70.1 (54.93-2.05)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.226 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8310	wwPDB-VP
Average B, all atoms (Å^2)	55.0	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.65	0/1134	0.71	0/1534
1	B	0.67	0/1764	0.71	0/2387
1	C	0.67	0/1748	0.71	0/2364
1	D	0.65	0/1134	0.70	0/1534
1	aa	0.68	0/607	0.72	0/821
1	dd	0.68	0/616	0.73	0/832
2	E	0.26	0/668	0.73	0/1029
3	F	0.25	0/664	0.73	0/1022
All	All	0.62	0/8335	0.72	0/11523

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	1119	0	1128	2	0
1	B	1743	0	1778	2	0
1	C	1727	0	1764	3	0
1	D	1119	0	1128	0	0
1	aa	602	0	624	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	dd	611	0	637	0	0
2	E	596	0	328	3	0
3	F	593	0	328	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	43	0	0	0	0
5	B	26	0	0	0	0
5	C	33	0	0	0	0
5	D	44	0	0	0	0
5	E	12	0	0	0	0
5	F	14	0	0	0	0
5	aa	7	0	0	0	0
5	dd	13	0	0	0	0
All	All	8310	0	7715	10	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 1.

All (10) 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:B:187:VAL:HG23	1:B:189:VAL:HG23	1.93	0.50
1:C:187:VAL:HG23	1:C:189:VAL:HG23	1.96	0.47
2:E:5:DA:H2"	2:E:6:DC:H5"	1.98	0.45
1:B:155:ASP:HA	1:B:207:ILE:HD13	1.97	0.45
1:C:171:ALA:HB3	1:C:225:ALA:HB1	1.99	0.45
2:E:14:DA:C2	3:F:18:DA:C2	3.06	0.44
2:E:19:DA:C2	3:F:13:DA:C2	3.07	0.43
1:A:87:VAL:CG2	1:A:97:VAL:HG21	2.49	0.42
1:C:155:ASP:HA	1:C:207:ILE:HD13	2.02	0.41
1:A:87:VAL:HG22	1:A:97:VAL:HG21	2.03	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	140/233 (60%)	138 (99%)	2 (1%)	0	100	100
1	B	222/233 (95%)	217 (98%)	5 (2%)	0	100	100
1	C	220/233 (94%)	218 (99%)	2 (1%)	0	100	100
1	D	140/233 (60%)	138 (99%)	2 (1%)	0	100	100
1	aa	80/233 (34%)	79 (99%)	1 (1%)	0	100	100
1	dd	81/233 (35%)	80 (99%)	1 (1%)	0	100	100
All	All	883/1398 (63%)	870 (98%)	13 (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 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	121/194 (62%)	121 (100%)	0	100	100
1	B	189/194 (97%)	189 (100%)	0	100	100
1	C	187/194 (96%)	187 (100%)	0	100	100
1	D	121/194 (62%)	121 (100%)	0	100	100
1	aa	65/194 (34%)	65 (100%)	0	100	100
1	dd	66/194 (34%)	66 (100%)	0	100	100
All	All	749/1164 (64%)	749 (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)

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.