



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2026 – 01:26 pm BST

PDB ID : 9SUO / pdb_00009suo
Title : DtxR-like iron-dependent regulator IdeR complexed with cobalt and a mutated consensus DNA-binding sequence
Authors : Griesse, J.J.
Deposited on : 2025-09-29
Resolution : 2.26 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

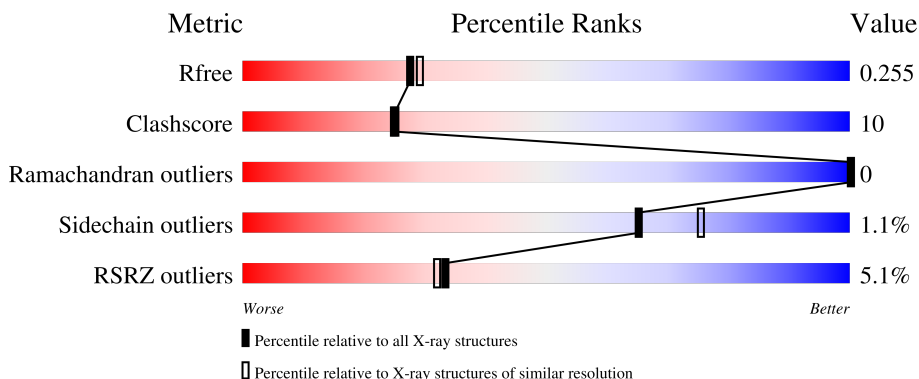
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 $\leq 5\%$. 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	A	233	5% 75% 18% • 6%
1	B	233	5% 78% 16% 5%
2	E	30	7% 30% 53% 13% •
3	F	30	3% 30% 47% 20% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8731 atoms, of which 4102 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
1	A	218	Total	C	H	N	O	S	0	0	0
			3424	1049	1737	312	318	8			
1	B	221	Total	C	H	N	O	S	0	0	0
			3461	1061	1751	315	326	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0ABF7PL34
A	0	HIS	-	expression tag	UNP A0ABF7PL34
B	-1	GLY	-	expression tag	UNP A0ABF7PL34
B	0	HIS	-	expression tag	UNP A0ABF7PL34

- Molecule 2 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	29	Total	C	H	N	O	P	0	29	0
			902	285	309	105	174	29			

- Molecule 3 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	29	Total	C	H	N	O	P	0	29	0
			901	286	305	107	174	29			

- Molecule 4 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Co	0	0
			2	2		
4	B	2	Total	Co	0	0
			2	2		

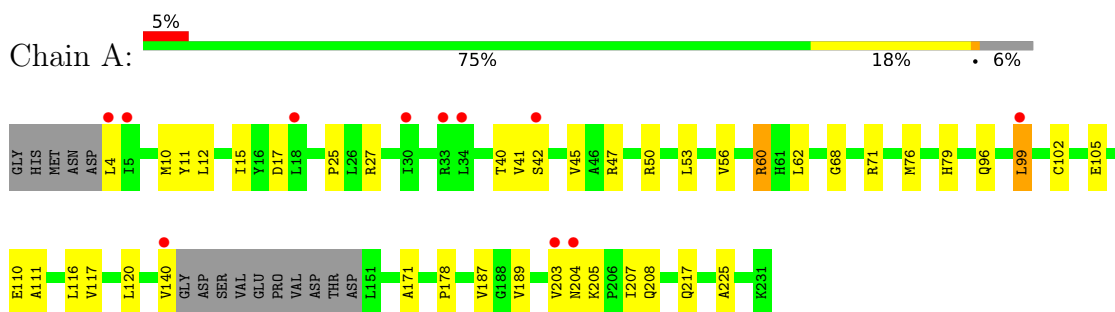
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total 19	O 19	0	0
5	B	17	Total 17	O 17	0	0
5	E	1	Total 1	O 1	0	0
5	F	2	Total 2	O 2	0	0

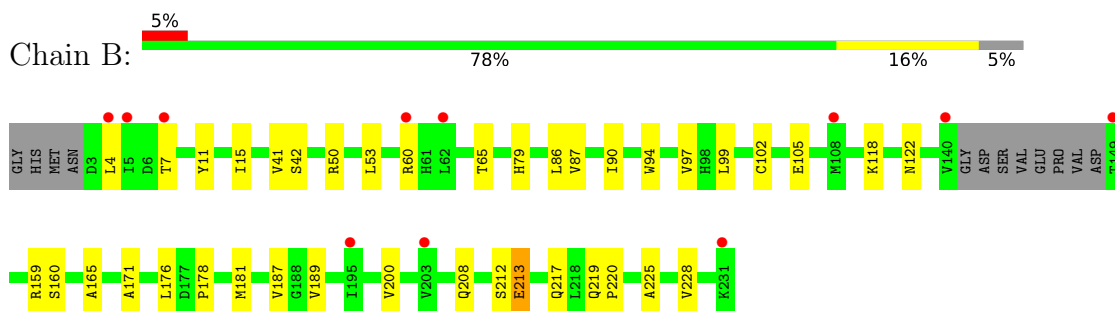
3 Residue-property plots [i](#)

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.

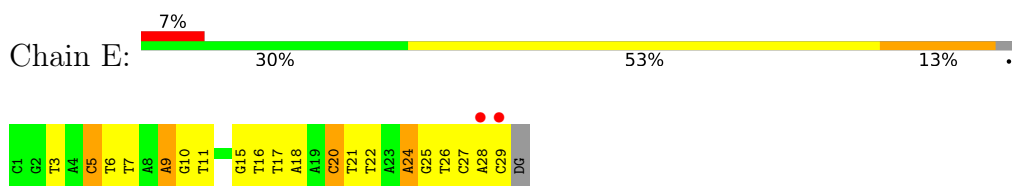
- Molecule 1: DtxR family iron (Metal) dependent repressor



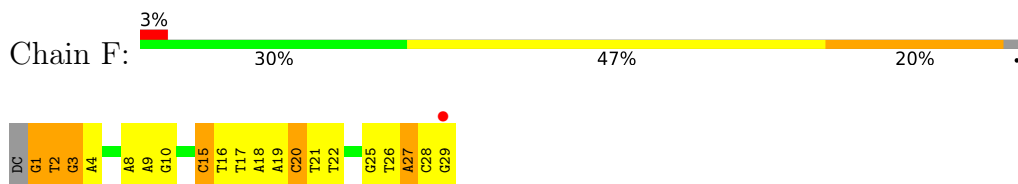
- Molecule 1: DtxR family iron (Metal) dependent repressor



- Molecule 2: DNA (29-MER)



- Molecule 3: DNA (29-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.62Å 39.34Å 96.95Å 90.00° 95.67° 90.00°	Depositor
Resolution (Å)	58.11 – 2.26 58.11 – 2.26	Depositor EDS
% Data completeness (in resolution range)	66.0 (58.11-2.26) 66.3 (58.11-2.26)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.197 , 0.259 0.197 , 0.255	Depositor DCC
R_{free} test set	914 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8731	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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, VI3

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	0.60	0/1699	0.86	1/2295 (0.0%)
1	B	0.69	1/1722 (0.1%)	0.89	0/2327
2	E	1.31	2/664 (0.3%)	1.36	9/1022 (0.9%)
3	F	1.58	9/668 (1.3%)	1.47	9/1029 (0.9%)
All	All	0.95	12/4753 (0.3%)	1.07	19/6673 (0.3%)

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	A	0	1
1	B	0	1
All	All	0	2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	ASN	C-O	-8.50	1.20	1.23
2	E	20[A]	DC	C3'-C2'	7.12	1.57	1.52
3	F	29[B]	DG	C2-N3	-6.74	1.27	1.32
3	F	29[B]	DG	C2'-C1'	6.54	1.58	1.52
3	F	1[B]	DG	C2'-C1'	6.33	1.58	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	29[B]	DG	O4'-C1'-N9	9.76	114.83	108.00
3	F	2[B]	DT	O4'-C1'-N1	9.43	114.60	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	20[A]	DC	O4'-C4'-C3'	-8.43	100.94	106.00
3	F	1[B]	DG	O4'-C1'-N9	7.37	113.16	108.00
2	E	20[A]	DC	O4'-C1'-N1	6.88	112.82	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ARG	Sidechain
1	B	50	ARG	Sidechain

5.2 Too-close contacts

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	1687	1737	1731	28	0
1	B	1710	1751	1746	29	0
2	E	593	309	306	17	0
3	F	596	305	303	17	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	19	0	0	2	0
5	B	17	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
All	All	4629	4102	4086	84	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 10.

The worst 5 of 84 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:41:VAL:O	1:A:45:VAL:HG23	1.69	0.93
1:B:208:GLN:NE2	1:B:217:GLN:OE1	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:C	1:B:65:THR:HG23	2.11	0.76
1:A:204:ASN:O	1:A:204:ASN:OD1	2.04	0.74
1:B:212:SER:C	1:B:213:GLU:OE2	2.30	0.74

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	213/233 (91%)	209 (98%)	4 (2%)	0	100	100
1	B	216/233 (93%)	211 (98%)	5 (2%)	0	100	100
All	All	429/466 (92%)	420 (98%)	9 (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	181/194 (93%)	179 (99%)	2 (1%)	65	75
1	B	184/194 (95%)	182 (99%)	2 (1%)	65	75
All	All	365/388 (94%)	361 (99%)	4 (1%)	65	75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	207	ILE
1	B	160	SER
1	B	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	HIS
1	B	130	ASN
1	B	173	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	VI3	A	102	4,1	2,7,8	1.15	0	2,8,10	11.09	2 (100%)
1	VI3	B	102	4,1	2,7,8	1.14	0	2,8,10	9.34	2 (100%)

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	VI3	A	102	4,1	-	2/3/6/8	-
1	VI3	B	102	4,1	-	2/3/6/8	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	VI3	O2-SG-CB	13.81	125.40	105.35
1	B	102	VI3	O1-SG-CB	9.77	119.54	105.35
1	B	102	VI3	O2-SG-CB	8.90	118.27	105.35
1	A	102	VI3	O1-SG-CB	7.44	116.15	105.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	102	VI3	N-CA-CB-SG
1	A	102	VI3	CA-CB-SG-O2
1	B	102	VI3	N-CA-CB-SG
1	B	102	VI3	CA-CB-SG-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 ⓘ

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	A	217/233 (93%)	0.23	11 (5%) 33 32	33, 52, 85, 128	0
1	B	220/233 (94%)	0.30	11 (5%) 34 33	32, 54, 83, 123	0
2	E	29/30 (96%)	0.48	2 (6%) 23 21	22, 28, 62, 68	29 (100%)
3	F	29/30 (96%)	0.34	1 (3%) 48 48	27, 36, 78, 86	29 (100%)
All	All	495/526 (94%)	0.28	25 (5%) 33 32	22, 52, 84, 128	58 (11%)

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	ILE	4.5
1	A	140	VAL	4.2
1	A	203	VAL	3.9
1	A	4	LEU	3.9
3	F	29[B]	DG	3.4

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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	B-factors(Å ²)	Q<0.9
1	VI3	A	102	8/9	0.93	0.10	36,46,54,58	0
1	VI3	B	102	8/9	0.98	0.05	31,49,59,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	B-factors(Å ²)	Q<0.9
4	CO	A	301	1/1	0.97	0.05	66,66,66,66	0
4	CO	B	301	1/1	0.99	0.04	58,58,58,58	0
4	CO	B	302	1/1	1.00	0.03	36,36,36,36	0
4	CO	A	302	1/1	1.00	0.04	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.