



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:51 PM UTC

PDB ID : 1R94 / pdb_00001r94
Title : Crystal Structure of IscA (MERCURY DERIVATIVE)
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Deposited on : 2003-10-28
Resolution : 2.30 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 ⓘ 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 Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

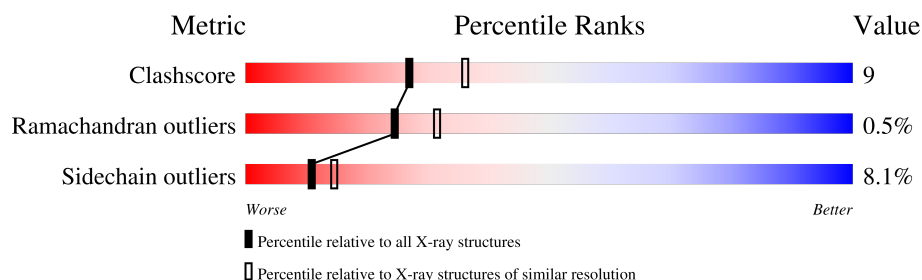
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	118	 64% 17% • 18%
1	B	118	 64% 17% • 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1557 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 Protein yfhF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			735	465	123	145	2			
1	B	97	Total	C	N	O	S	0	0	0
			735	465	123	145	2			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	LYS	-	cloning artifact	UNP P0AAC8
A	107	LEU	-	cloning artifact	UNP P0AAC8
A	108	ALA	-	cloning artifact	UNP P0AAC8
A	109	ALA	-	cloning artifact	UNP P0AAC8
A	110	ALA	-	cloning artifact	UNP P0AAC8
A	111	LEU	-	cloning artifact	UNP P0AAC8
A	112	ASP	-	cloning artifact	UNP P0AAC8
A	113	HIS	-	expression tag	UNP P0AAC8
A	114	HIS	-	expression tag	UNP P0AAC8
A	115	HIS	-	expression tag	UNP P0AAC8
A	116	HIS	-	expression tag	UNP P0AAC8
A	117	HIS	-	expression tag	UNP P0AAC8
A	118	HIS	-	expression tag	UNP P0AAC8
B	106	LYS	-	cloning artifact	UNP P0AAC8
B	107	LEU	-	cloning artifact	UNP P0AAC8
B	108	ALA	-	cloning artifact	UNP P0AAC8
B	109	ALA	-	cloning artifact	UNP P0AAC8
B	110	ALA	-	cloning artifact	UNP P0AAC8
B	111	LEU	-	cloning artifact	UNP P0AAC8
B	112	ASP	-	cloning artifact	UNP P0AAC8
B	113	HIS	-	expression tag	UNP P0AAC8
B	114	HIS	-	expression tag	UNP P0AAC8
B	115	HIS	-	expression tag	UNP P0AAC8
B	116	HIS	-	expression tag	UNP P0AAC8
B	117	HIS	-	expression tag	UNP P0AAC8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	118	HIS	-	expression tag	UNP P0AAC8

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

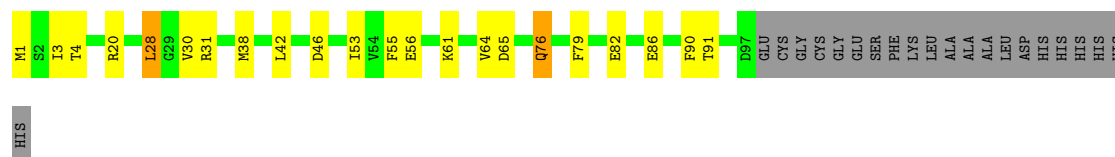
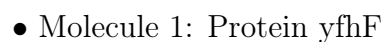
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Hg 1 1	0	0
2	B	1	Total Hg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	43	Total O 43 43	0	0
3	B	42	Total O 42 42	0	0

Note EDS was not executed.

Chain A: 64% 17% 18%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	55.34Å 55.34Å 159.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.22 – 2.30	Depositor
% Data completeness (in resolution range)	95.2 (27.22-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1557	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	0.80	0/746	1.02	0/1005
1	B	0.81	0/746	1.00	0/1005
All	All	0.81	0/1492	1.01	0/2010

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

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	735	0	727	16	0
1	B	735	0	727	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	43	0	0	1	0
3	B	42	0	0	0	1
All	All	1557	0	1454	27	1

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 9.

All (27) 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:53:ILE:HD11	1:B:1:MET:HA	1.55	0.88
1:A:1:MET:HA	1:B:53:ILE:HD11	1.58	0.84
1:A:1:MET:CA	1:B:53:ILE:HD11	2.21	0.70
1:A:53:ILE:HD11	1:B:1:MET:CA	2.19	0.70
1:A:1:MET:C	1:A:3:ILE:H	2.08	0.62
1:B:1:MET:C	1:B:3:ILE:H	2.10	0.59
3:A:160:HOH:O	1:B:55:PHE:HB2	2.07	0.53
1:A:53:ILE:CD1	1:B:1:MET:HA	2.35	0.53
1:B:4:THR:OG1	1:B:76:GLN:HG2	2.08	0.52
1:A:53:ILE:HD11	1:B:1:MET:N	2.25	0.51
1:A:1:MET:N	1:B:53:ILE:HD11	2.26	0.49
1:A:28:LEU:HD12	1:A:42:LEU:CD2	2.42	0.49
1:B:28:LEU:HD12	1:B:42:LEU:CD2	2.43	0.48
1:A:4:THR:OG1	1:A:76:GLN:HG2	2.14	0.46
1:A:79:PHE:CZ	1:A:86:GLU:HG2	2.52	0.45
1:A:90:PHE:CD1	1:A:90:PHE:N	2.85	0.44
1:A:1:MET:C	1:A:3:ILE:N	2.75	0.43
1:B:1:MET:C	1:B:3:ILE:N	2.77	0.43
1:A:3:ILE:HB	1:A:55:PHE:CZ	2.54	0.42
1:A:64:VAL:HG12	1:A:65:ASP:O	2.18	0.42
1:B:79:PHE:CZ	1:B:86:GLU:HG2	2.54	0.42
1:B:64:VAL:HG12	1:B:65:ASP:O	2.19	0.42
1:B:20:ARG:NH2	1:B:46:ASP:OD1	2.52	0.41
1:B:3:ILE:HB	1:B:55:PHE:CZ	2.56	0.41
1:B:56:GLU:OE2	1:B:61:LYS:NZ	2.42	0.41
1:A:56:GLU:OE2	1:A:61:LYS:NZ	2.43	0.41
1:B:90:PHE:CD1	1:B:90:PHE:N	2.88	0.41

All (1) 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)
3:B:129:HOH:O	3:B:151:HOH:O[4_665]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

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	95/118 (80%)	93 (98%)	1 (1%)	1 (1%)	11	13
1	B	95/118 (80%)	93 (98%)	2 (2%)	0	100	100
All	All	190/236 (80%)	186 (98%)	3 (2%)	1 (0%)	24	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER

5.3.2 Protein sidechains

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	80/97 (82%)	74 (92%)	6 (8%)	12	17
1	B	80/97 (82%)	73 (91%)	7 (9%)	9	12
All	All	160/194 (82%)	147 (92%)	13 (8%)	11	14

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	31	ARG
1	A	38	MET
1	A	76	GLN
1	A	82	GLU

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Mol	Chain	Res	Type
1	A	91	THR
1	B	28	LEU
1	B	30	VAL
1	B	31	ARG
1	B	38	MET
1	B	76	GLN
1	B	82	GLU
1	B	91	THR

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

Mol	Chain	Res	Type
1	A	70	GLN
1	A	94	ASN
1	B	70	GLN
1	B	94	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.