

Full wwPDB X-ray Structure Validation Report (i)

May 28, 2020 – 07:38 pm BST

PDB ID	:	1IAE
Title	:	CRYSTAL STRUCTURES, SPECTROSCOPIC FEATURES, AND CAT-
		ALYTIC PROPERTIES OF COBALT(II), COPPER(II), NICKEL(II),
		AND MERCURY(II) DERIVATIVES OF THE ZINC ENDOPEPTIDASE
		ASTACIN. A CORRELATION OF STRUCTURE AND PROTEOLYTIC AC-
		TIVITY
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Deposited on		
Resolution	:	1.83 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 (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 25 th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.83 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	Percent	tile Ranks	Value	
Cl	ashscore 📕			3	
	Wa	orse		Better	
	∎ P	Percentile relative to all X-ray stru	ictures		
	0 P	Percentile relative to X-ray structu	ires of similar resolutior	1	
	Metric	Whole archive	Simi	lar resolution	
	viernc		/ ··· ·		. 0

Matria	Whole archive	Similar resolution		
Metric	$(\# {\it Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
Clashscore	141614	4233 (1.86-1.82)		

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 on 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	200	93%	8%



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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1776 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 ASTACIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	200	Total 1591	C 1004	N 259	O 318	S 10	5	0	0

• Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Ni 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	184	Total O 184 184	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 colorcoded 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: ASTACIN

Chain A: 93% 8%



4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 31 2 1	Depositor	
Cell constants	61.89Å 61.89 Å 98.55 Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	10.00 - 1.83	Depositor	
% Data completeness	(Not available) (10.00-1.83)	Depositor	
(in resolution range)	(100 available) (10.00-1.05)	-	
R_{merge}	(Not available)	Depositor	
R _{sym}	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
R, R_{free}	0.143 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1776	wwPDB-VP	
Average B, all atoms $(Å^2)$	16.0	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: NI

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	Chain	Bond	lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.45	0/1631	0.56	0/2218	

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	А	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	8	TYR	Sidechain

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	1591	0	1475	10	0
2	А	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	184	0	0	1	0
All	All	1776	0	1475	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 3.

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:A:124:MET:HG2	1:A:127:ASN:ND2	2.08	0.68
1:A:200:LEU:HD22	3:A:425:HOH:O	2.05	0.55
1:A:124:MET:HG2	1:A:127:ASN:HD21	1.71	0.54
1:A:16:PRO:HA	1:A:46:VAL:O	2.08	0.53
1:A:198:CYS:HB2	1:A:200:LEU:HD13	1.91	0.51
1:A:102:HIS:HB3	1:A:104:HIS:CE1	2.51	0.46
1:A:198:CYS:CB	1:A:200:LEU:HD13	2.47	0.45
1:A:34:MET:O	1:A:38:GLU:HG3	2.17	0.45
1:A:149:TYR:HB3	1:A:153:SER:OG	2.17	0.45
1:A:121:ASP:HA	1:A:122:PRO:HD3	1.87	0.42

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

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

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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.

