W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2023 – 12:18 AM EDT

PDB ID	:	3THH
Title	:	Crystal structure of the Co2+2-HAI-ABH complex
Authors	:	D'Antonio, E.L.; Christianson, D.W.
Deposited on	:	2011-08-19
Resolution	:	1.85 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

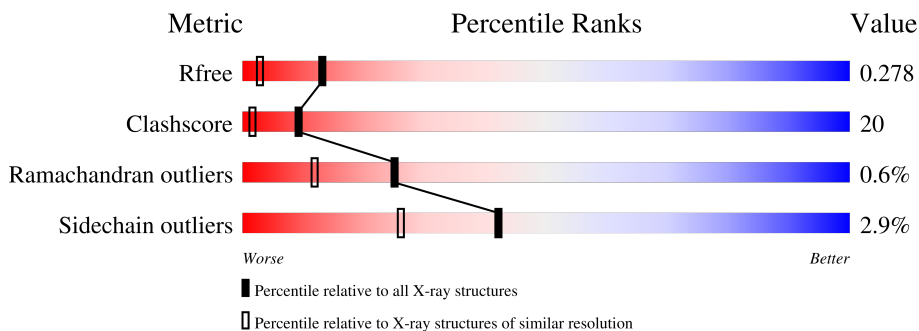|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.85 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
Rfree		0.278
Clashscore		20
Ramachandran outliers		0.6%
Sidechain outliers		2.9%

Worse   *Better*

▐ Percentile relative to all X-ray structures

🯄 Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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%

Mol	Chain	Length	Quality of chain
1	A	322	67% 29% • •
1	B	322	61% 34% • •

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2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5041 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 Arginase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total 2389	C 1523	N 407	O 453	S 6	0	0	0
1	B	314	Total 2389	C 1523	N 407	O 453	S 6	0	0	0

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 3 is 2(S)-AMINO-6-BORONOHEXANOIC ACID (three-letter code: ABH) (formula: $C_6H_{15}BNO_5$).
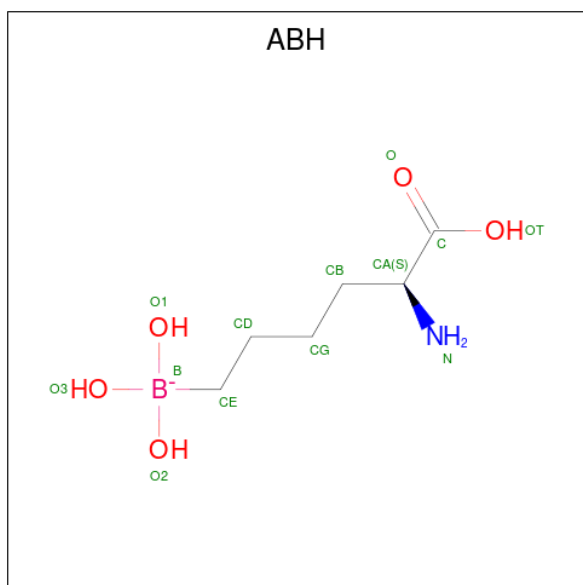
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 13	B 1	C 6	N 1	O 5	0	0
3	B	1	Total 13	B 1	C 6	N 1	O 5	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total 133	O 133	0	0
4	B	100	Total 100	O 100	0	0

3 Residue-property plots ⓘ

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.
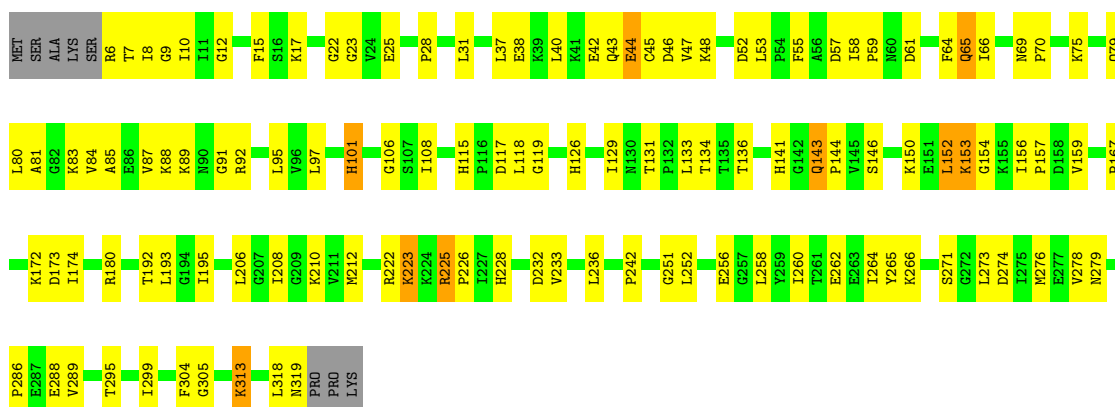
• Molecule 1: Arginase-1

Chain A:
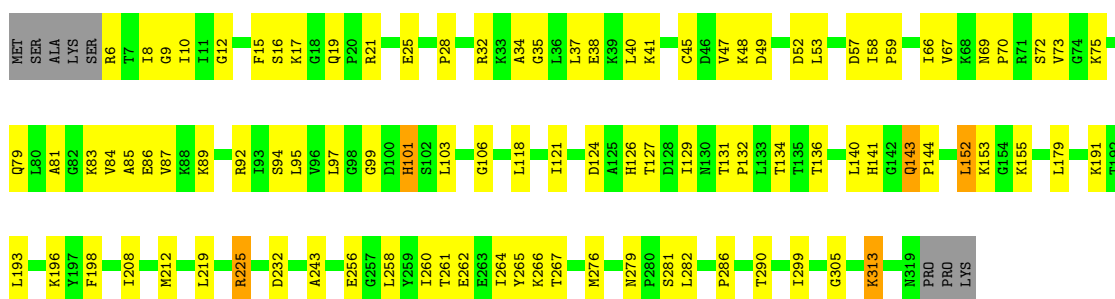
• Molecule 1: Arginase-1

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	90.43Å 90.43Å 69.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.85 34.11 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-1.85) 96.8 (34.11-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 1.85Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.281 0.236 , 0.278	Depositor DCC
R_{free} test set	5272 reflections (9.79%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 30.4	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.41, < L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.234 for -h,-k,l 0.089 for h,-h-k,-l 0.086 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5041	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ABH, 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	0.34	0/2439	0.65	0/3310
1	B	0.33	0/2439	0.63	0/3310
All	All	0.33	0/4878	0.64	0/6620

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	2389	0	2433	87	0
1	B	2389	0	2433	109	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	13	0	12	0	0
3	B	13	0	12	0	0
4	A	133	0	0	6	0
4	B	100	0	0	10	1
All	All	5041	0	4890	193	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 20.

The worst 5 of 193 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:208:ILE:HD11	1:A:260:ILE:HD11	1.31	1.08
1:B:208:ILE:HD11	1:B:260:ILE:HD11	1.40	1.03
1:A:17:LYS:HE2	1:A:17:LYS:HA	1.41	0.99
1:B:6:ARG:CZ	1:B:6:ARG:HA	1.96	0.94
1:A:53:LEU:HD21	1:A:83:LYS:HG3	1.51	0.93

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)
4:B:357:HOH:O	4:B:383:HOH:O[2_455]	2.19	0.01

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	312/322 (97%)	296 (95%)	15 (5%)	1 (0%)	41	26
1	B	312/322 (97%)	288 (92%)	21 (7%)	3 (1%)	15	5
All	All	624/644 (97%)	584 (94%)	36 (6%)	4 (1%)	25	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	153	LYS
1	B	143	GLN
1	A	143	GLN
1	B	65	GLN

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	263/270 (97%)	255 (97%)	8 (3%)	41	24
1	B	263/270 (97%)	256 (97%)	7 (3%)	44	29
All	All	526/540 (97%)	511 (97%)	15 (3%)	42	26

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	313	LYS
1	B	225	ARG
1	B	44	GLU
1	B	313	LYS
1	B	152	LEU

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	79	GLN
1	A	90	ASN
1	B	319	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	#$|Z| > 2$
3	ABH	B	700	2	8,12,12	1.90	2 (25%)	12,16,16	1.08	1 (8%)
3	ABH	A	700	2	8,12,12	1.90	2 (25%)	12,16,16	1.04	2 (16%)

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
3	ABH	B	700	2	-	2/9/12/12	-
3	ABH	A	700	2	-	2/9/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	ABH	O-C	4.25	1.35	1.22
3	A	700	ABH	O-C	4.22	1.35	1.22
3	A	700	ABH	OT-C	-2.51	1.22	1.30
3	B	700	ABH	OT-C	-2.35	1.22	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
3	A	700	ABH	OT-C-CA	2.04	120.33	113.38
3	B	700	ABH	OT-C-CA	2.04	120.32	113.38
3	A	700	ABH	OT-C-O	-2.02	119.50	124.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	ABH	CG-CD-CE-B
3	B	700	ABH	CG-CD-CE-B
3	A	700	ABH	CE-CD-CG-CB
3	B	700	ABH	CE-CD-CG-CB

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3   Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4   Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5   Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.