



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:25 AM GMT

PDB ID : 2AEB
Title : Crystal structure of human arginase I at 1.29 Å resolution and exploration of inhibition in immune response.
Authors : Di Costanzo, L.; Sabio, G.; Mora, A.; Rodriguez, P.C.; Ochoa, A.C.; Centeno, F.; Christianson, D.W.
Deposited on : 2005-07-21
Resolution : 1.29 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

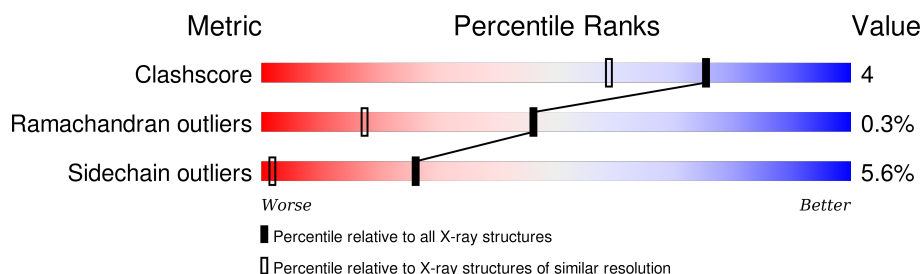
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.29 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	102246	1031 (1.32-1.28)
Ramachandran outliers	100387	1504 (1.34-1.26)
Sidechain outliers	100360	1503 (1.34-1.26)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	322	 81% 14% . .
1	B	322	 79% 15% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10011 atoms, of which 4851 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.

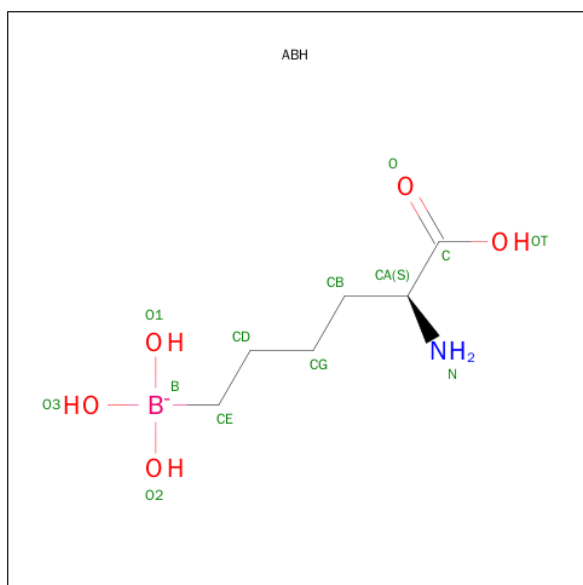
- Molecule 1 is a protein called Arginase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	314	Total	C	H	N	O	S	0	2	0
			4827	1529	2431	408	453	6			
1	B	309	Total	C	H	N	O	S	0	2	0
			4740	1495	2390	401	448	6			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is 2(S)-AMINO-6-BORONOHEXOIC ACID (three-letter code: ABH) (formula: $C_6H_{15}BNO_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 28	B 1	C 6	H 15	N 1	O 5	0	0
3	B	1	Total 28	B 1	C 6	H 15	N 1	O 5	0	0

- Molecule 4 is water.

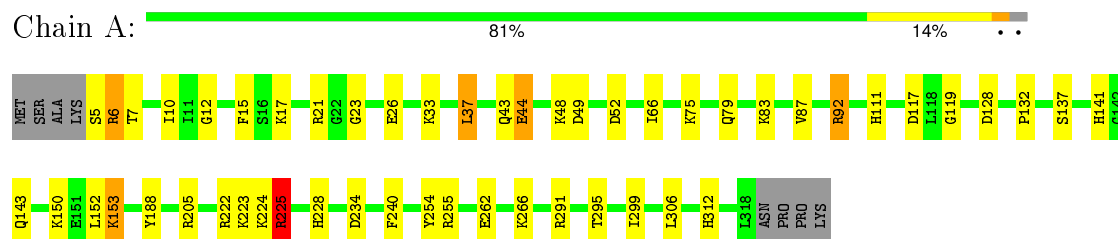
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	218	Total 218	O 218	0	0
4	B	166	Total 166	O 166	0	0

3 Residue-property plots [i](#)

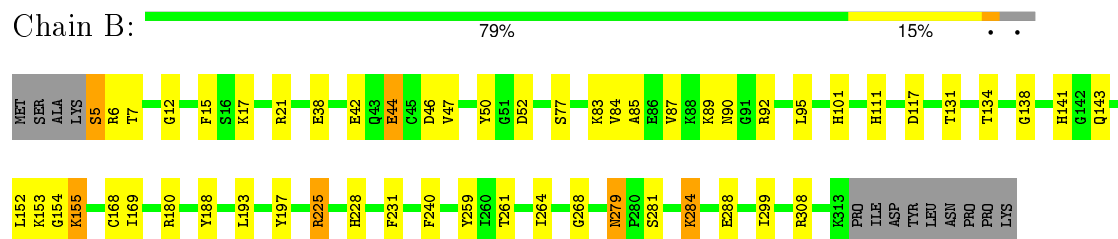
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

• Molecule 1: Arginase 1



• Molecule 1: Arginase 1



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	91.42Å 91.42Å 69.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.29	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.29)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	(Not available) , 0.152	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10011	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: ABH, MN

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	0.69	0/2455	1.46	32/3329 (1.0%)
1	B	0.65	0/2407	1.37	20/3264 (0.6%)
All	All	0.67	0/4862	1.42	52/6593 (0.8%)

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

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	255	ARG	NE-CZ-NH1	13.12	126.86	120.30
1	A	291	ARG	NE-CZ-NH1	10.45	125.52	120.30
1	A	225	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	A	92	ARG	CD-NE-CZ	8.52	135.52	123.60
1	A	228	HIS	CG-ND1-CE1	8.29	119.80	108.20
1	B	92	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	92	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	B	21	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	205	ARG	CD-NE-CZ	7.59	134.23	123.60
1	B	92	ARG	CD-NE-CZ	7.52	134.13	123.60
1	A	111	HIS	CG-ND1-CE1	7.51	118.71	108.20
1	B	188	TYR	CB-CG-CD1	-7.36	116.59	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	TYR	CB-CG-CD1	7.30	125.38	121.00
1	A	6	ARG	CD-NE-CZ	7.22	133.70	123.60
1	A	234	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	225	ARG	CD-NE-CZ	7.10	133.53	123.60
1	B	180	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	312	HIS	CG-ND1-CE1	6.98	117.97	108.20
1	B	50	TYR	CB-CG-CD2	6.94	125.17	121.00
1	B	228	HIS	CG-ND1-CE1	6.76	117.67	108.20
1	A	137	SER	C-N-CA	6.69	136.34	122.30
1	A	240	PHE	CB-CG-CD1	-6.41	116.31	120.80
1	A	222	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	259	TYR	CB-CG-CD1	-6.36	117.18	121.00
1	A	225	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	111	HIS	CG-ND1-CE1	6.06	116.68	108.20
1	B	225	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	128	ASP	CB-CG-OD1	-5.88	113.00	118.30
1	A	132	PRO	C-N-CA	5.88	136.41	121.70
1	A	228	HIS	ND1-CG-CD2	-5.81	97.87	106.00
1	B	180	ARG	CD-NE-CZ	5.72	131.60	123.60
1	A	254	TYR	CB-CG-CD2	5.67	124.40	121.00
1	B	50	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	A	255	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	6	ARG	CG-CD-NE	5.51	123.36	111.80
1	B	47	VAL	CB-CA-C	-5.51	100.94	111.40
1	B	240	PHE	CB-CG-CD2	-5.48	116.96	120.80
1	B	308	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	254	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	132	PRO	O-C-N	-5.42	114.04	122.70
1	A	92	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	188	TYR	CB-CG-CD2	5.41	124.25	121.00
1	B	188	TYR	CB-CG-CD2	5.41	124.25	121.00
1	A	21	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	117	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	291	ARG	NH1-CZ-NH2	-5.16	113.72	119.40
1	A	205	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	B	268	GLY	C-N-CA	5.13	134.53	121.70
1	A	44	GLU	CA-C-N	5.12	128.46	117.20
1	A	255	ARG	C-N-CA	5.06	134.35	121.70
1	B	138	GLY	O-C-N	-5.06	114.61	122.70
1	A	255	ARG	O-C-N	-5.01	114.68	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	GLU	Peptide
1	B	44	GLU	Peptide

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	2396	2431	2450	16	0
1	B	2350	2390	2393	22	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	13	15	12	0	0
3	B	13	15	12	0	0
4	A	218	0	0	1	0
4	B	166	0	0	4	0
All	All	5160	4851	4867	38	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 4.

All (38) 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:38:GLU:O	1:B:42:GLU:HG3	1.84	0.78
1:A:66:ILE:HG22	4:A:2495:HOH:O	1.87	0.75
1:A:150:LYS:O	1:A:153[B]:LYS:HG3	1.88	0.73
1:A:79:GLN:O	1:A:83[A]:LYS:HG2	1.88	0.73
1:A:295:THR:O	1:A:299:ILE:HD13	1.91	0.70
1:A:117:ASP:O	1:A:225:ARG:HD3	1.96	0.65
1:B:153:LYS:HA	4:B:1528:HOH:O	2.00	0.62
1:B:84:VAL:O	1:B:87:VAL:HG22	1.99	0.61
1:A:262:GLU:O	1:A:266:LYS:HD3	2.00	0.61
1:A:48:LYS:HG3	1:A:92:ARG:NH2	2.17	0.60
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.40	0.56
1:B:7:THR:HG23	1:B:46:ASP:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:SER:O	1:B:6:ARG:HG2	2.08	0.54
1:A:119:GLY:N	1:A:225:ARG:HD2	2.24	0.53
1:B:155:LYS:N	1:B:155:LYS:HD3	2.24	0.52
1:B:90:ASN:N	1:B:90:ASN:HD22	2.08	0.52
1:A:48:LYS:HG3	1:A:92:ARG:CZ	2.41	0.51
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.45	0.51
1:B:231:PHE:CZ	1:B:299:ILE:HD12	2.46	0.51
1:B:264:ILE:HB	4:B:1427:HOH:O	2.12	0.50
1:B:85:ALA:O	1:B:89:LYS:HG3	2.12	0.49
1:A:37:LEU:HD11	1:A:49:ASP:OD2	2.12	0.49
1:B:168:CYS:HB2	4:B:1429:HOH:O	2.12	0.48
1:B:154:GLY:C	1:B:155:LYS:HD3	2.34	0.48
1:B:6:ARG:HB3	4:B:1455:HOH:O	2.14	0.47
1:B:5:SER:O	1:B:6:ARG:NH1	2.50	0.45
1:B:284:LYS:HE3	1:B:288:GLU:OE2	2.16	0.45
1:B:152:LEU:O	1:B:155:LYS:HB2	2.17	0.45
1:B:12:GLY:HA3	1:B:52:ASP:OD2	2.17	0.44
1:B:131:THR:OG1	1:B:134:THR:HG23	2.19	0.43
1:A:12:GLY:HA3	1:A:52:ASP:OD1	2.19	0.43
1:A:23:GLY:O	1:A:26:GLU:HG2	2.19	0.42
1:A:225:ARG:O	1:A:225:ARG:HG3	2.15	0.42
1:B:261:THR:HG21	1:B:299:ILE:HG23	2.02	0.41
1:B:169:ILE:HG13	1:B:169:ILE:O	2.19	0.41
1:B:279:ASN:HD22	1:B:279:ASN:C	2.25	0.41

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	314/322 (98%)	305 (97%)	8 (2%)	1 (0%)	46 17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	309/322 (96%)	299 (97%)	9 (3%)	1 (0%)	46	17
All	All	623/644 (97%)	604 (97%)	17 (3%)	2 (0%)	46	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	GLN
1	A	143	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	265/270 (98%)	248 (94%)	17 (6%)	22	1
1	B	260/270 (96%)	247 (95%)	13 (5%)	30	2
All	All	525/540 (97%)	495 (94%)	30 (6%)	26	2

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	6	ARG
1	A	7	THR
1	A	10	ILE
1	A	33	LYS
1	A	37	LEU
1	A	43	GLN
1	A	75	LYS
1	A	87	VAL
1	A	141	HIS
1	A	152	LEU
1	A	153[A]	LYS
1	A	153[B]	LYS
1	A	223	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	224	LYS
1	A	225	ARG
1	A	306	LEU
1	B	5	SER
1	B	44	GLU
1	B	77	SER
1	B	83	LYS
1	B	95	LEU
1	B	101	HIS
1	B	141	HIS
1	B	155	LYS
1	B	193	LEU
1	B	225	ARG
1	B	279	ASN
1	B	281	SER
1	B	284	LYS

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

Mol	Chain	Res	Type
1	A	90	ASN
1	B	90	ASN
1	B	279	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	A	551	2	6,12,12	0.34	0	4,16,16	0.95	0
3	ABH	B	552	2	6,12,12	0.39	0	4,16,16	0.86	0

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	A	551	2	-	0/5/12/12	0/0/0/0
3	ABH	B	552	2	-	0/5/12/12	0/0/0/0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.