



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:07 AM GMT

PDB ID : 1R1O
Title : Amino Acid Sulfonamides as Transition-State Analogue Inhibitors of Arginase
Authors : Cama, E.; Shin, H.; Christianson, D.W.
Deposited on : 2003-09-24
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

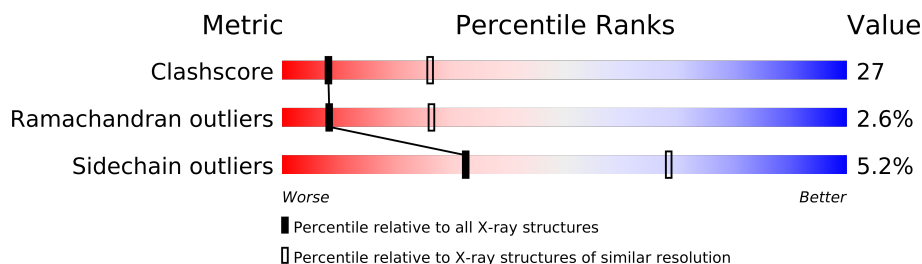
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	
1	B	323	
1	C	323	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7271 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

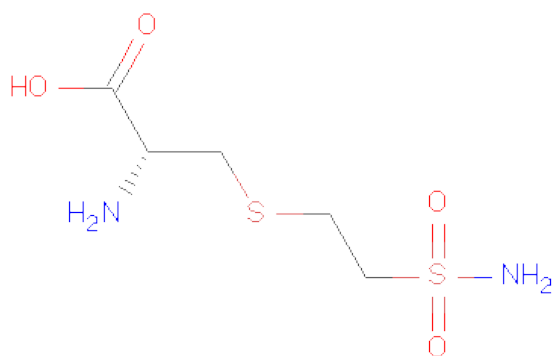
- Molecule 1 is a protein called Arginase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			
1	B	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			
1	C	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			

- 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		
2	C	2	Total	Mn	0	0
			2	2		

- Molecule 3 is S-[2-(AMINOSULFONYL)ETHYL]-D-CYSTEINE (three-letter code: SDC) (formula: C₅H₁₂N₂O₄S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	5	2	4	2		
3	B	1	Total	C	N	O	S	0	0
			13	5	2	4	2		
3	C	1	Total	C	N	O	S	0	0
			13	5	2	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	11	Total	O	0	0
			11	11		
4	C	13	Total	O	0	0
			13	13		

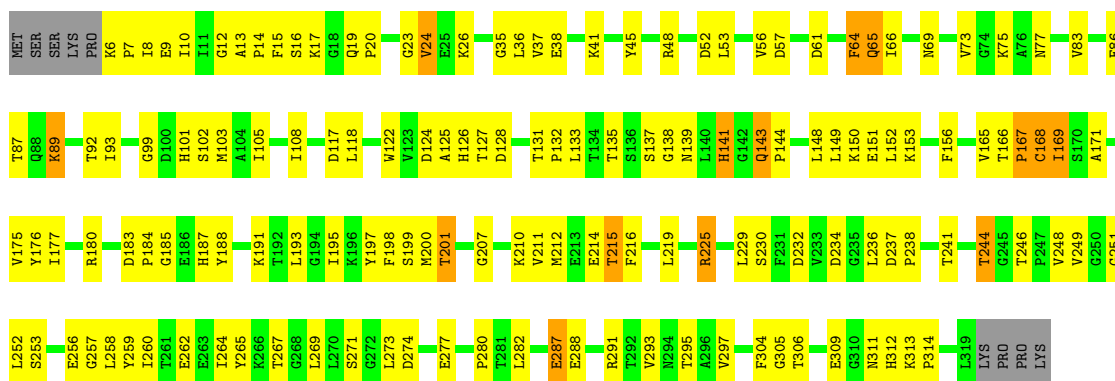
3 Residue-property plots

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 ($RSRZ > 2$). 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.

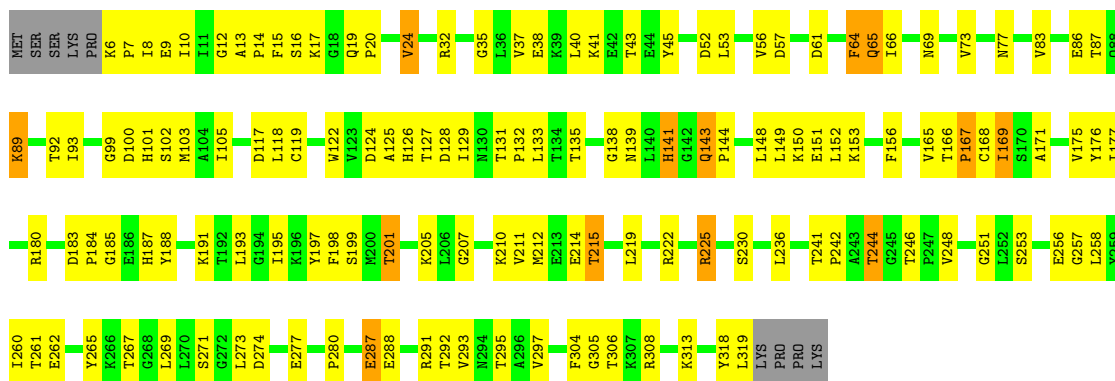
• Molecule 1: Arginase 1

Chain A:



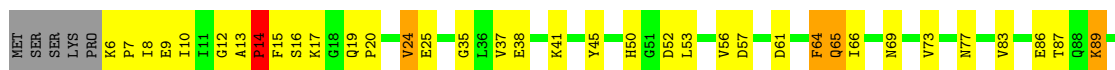
• Molecule 1: Arginase 1

Chain B:



• Molecule 1: Arginase 1

Chain C:



T261	I177	T92
E262	R180	I93
Y265	D183	G99
K266	D100	H101
T267	H187	S102
G268	Y188	M103
L269		A104
L270	K191	I105
S271	T192	D117
G272	L193	L118
L273	F194	C119
D274	K196	W122
E277	Y197	I123
	F198	Y123
P280	S199	D124
E287	R200	A125
E288	T201	H126
	G207	T127
R291		D128
T292	K210	T131
V293	V211	P132
M294	M212	L133
T295	E213	T134
A296	E214	L135
V297	T215	K136
F304	F216	S137
G305		G138
T306	L219	N139
E309	L220	L140
G310	G221	H141
N311	R222	G142
H312		Q143
K313	R225	P144
P314	S230	L148
	L236	L149
L319	T241	K150
LYS	T244	E151
PRO	G245	L152
PRO	T246	K153
PRO	P247	
LYS	V248	F156
	G251	V159
	L252	V165
	S253	T166
	Y254	P167
	R255	C168
	G256	I169
	G257	S170
	L258	A171
	Y259	V175
	T260	Y176

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	88.94Å 88.94Å 112.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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: MN, SDC

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	0.42	0/2448	0.68	0/3325
1	B	0.44	0/2448	0.68	0/3325
1	C	0.44	0/2448	0.69	0/3325
All	All	0.43	0/7344	0.68	0/9975

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2395	0	2420	138	0
1	B	2395	0	2420	129	0
1	C	2395	0	2420	130	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	13	0	9	3	0
3	B	13	0	9	3	0
3	C	13	0	9	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	17	0	0	6	0
4	B	11	0	0	2	0
4	C	13	0	0	1	0
All	All	7271	0	7287	385	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

The worst 5 of 385 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:PRO:HD3	1:A:139:ASN:ND2	1.70	1.05
1:B:20:PRO:HD3	1:B:139:ASN:ND2	1.77	1.00
1:A:175:VAL:HG11	1:A:215:THR:HG22	1.46	0.97
1:C:20:PRO:HD3	1:C:139:ASN:ND2	1.82	0.94
1:C:175:VAL:HG11	1:C:215:THR:HG22	1.53	0.90

There are no symmetry-related clashes.

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	312/323 (97%)	279 (89%)	26 (8%)	7 (2%)	10	32
1	B	312/323 (97%)	280 (90%)	23 (7%)	9 (3%)	7	23
1	C	312/323 (97%)	276 (88%)	28 (9%)	8 (3%)	8	26
All	All	936/969 (97%)	835 (89%)	77 (8%)	24 (3%)	8	26

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	306	THR
1	B	65	GLN

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Mol	Chain	Res	Type
1	C	65	GLN
1	A	64	PHE

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	264/273 (97%)	250 (95%)	14 (5%)	32	67
1	B	264/273 (97%)	251 (95%)	13 (5%)	35	71
1	C	264/273 (97%)	250 (95%)	14 (5%)	32	67
All	All	792/819 (97%)	751 (95%)	41 (5%)	32	68

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	141	HIS
1	B	225	ARG
1	C	244	THR
1	B	169	ILE
1	B	201	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	SDC	A	1000	2	12,12,12	1.77	4 (33%)	16,16,16	2.78	8 (50%)
3	SDC	B	1001	2	12,12,12	1.66	3 (25%)	16,16,16	2.67	7 (43%)
3	SDC	C	1002	2	12,12,12	1.66	3 (25%)	16,16,16	2.78	8 (50%)

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	SDC	A	1000	2	-	0/11/12/12	0/0/0/0
3	SDC	B	1001	2	-	0/11/12/12	0/0/0/0
3	SDC	C	1002	2	-	0/11/12/12	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	SDC	O05-C04	4.01	1.35	1.22
3	A	1000	SDC	O05-C04	3.96	1.35	1.22
3	C	1002	SDC	O05-C04	3.89	1.35	1.22
3	C	1002	SDC	S10-N12	2.79	1.64	1.59
3	A	1000	SDC	O01-C04	-2.66	1.20	1.30

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	SDC	O13-S10-N12	-5.85	97.13	109.08
3	C	1002	SDC	O13-S10-N12	-5.62	97.60	109.08
3	B	1001	SDC	O13-S10-N12	-5.31	98.24	109.08
3	A	1000	SDC	O01-C04-C03	4.94	127.97	116.88
3	C	1002	SDC	O01-C04-C03	4.92	127.93	116.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 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.