



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2024 – 01:39 PM EST

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 X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

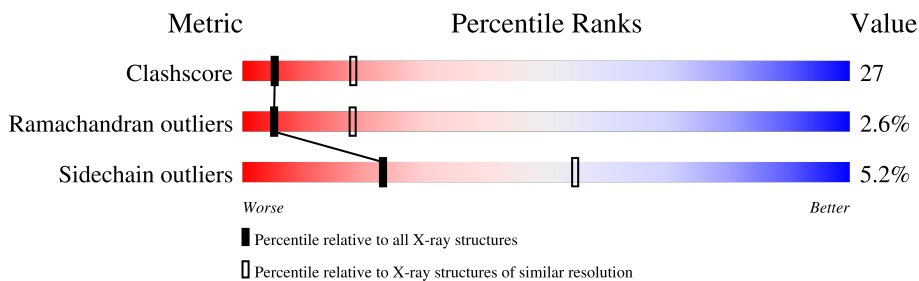
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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	323	51% (green), 42% (yellow), . . (orange, red, grey)
1	B	323	54% (green), 39% (yellow), . . (orange, red, grey)
1	C	323	54% (green), 38% (yellow), . . (orange, red, grey)

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7271 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.

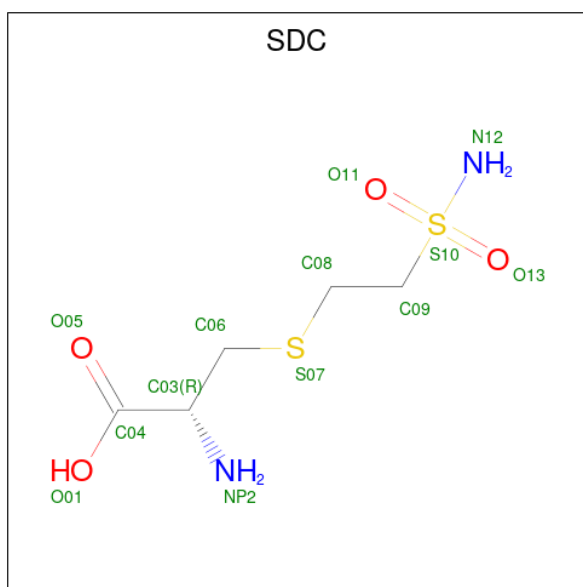
- Molecule 1 is a protein called Arginase 1.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	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
			Total	C	N	O	S		
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.

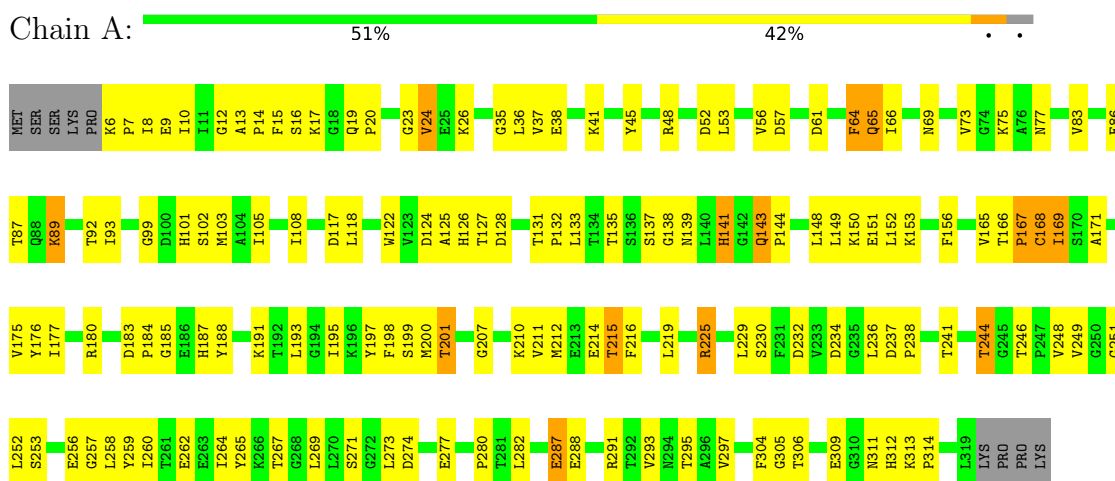
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	11	Total	O	0	0
			11	11		
4	C	13	Total	O	0	0
			13	13		

3 Residue-property plots

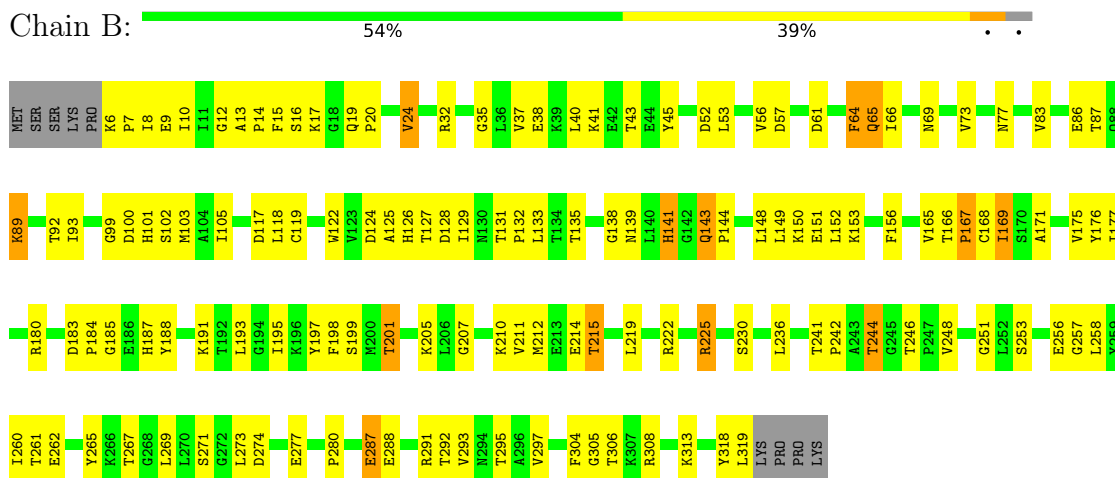
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

- Molecule 1: Arginase 1



- Molecule 1: Arginase 1



- Molecule 1: Arginase 1



MET	SER	SER	LYS	PRO	K6	P7	I8	E9	I10	I11	G12	A13	E14	F15	S16	K17	G18	Q19	P20	V24	E25	G35	L36	V37	E38	K41	Y45	H50	G51	D52	L53	V56	D57	D61	F64	Q65	I66	N69	V73	N77	V83	E86	T87	Q88	K89				
T92	I93	G99	D100	H101	S102	M103	A104	I105	D117	L118	C119	W122	V123	D124	A125	H126	I127	D128	T131	V132	L133	T134	T135	S136	G138	M139	L140	H141	G142	Q143	P144	L148	L149	K150	E151	L152	K153	F156	V159	P160	V165	T166	P167	C168	I169	S170	A171	V175	Y176
I177	R180	D183	H187	Y188	K191	T192	L193	G194	I195	R196	Y197	F198	S199	K200	T201	G207	K210	V211	M212	E213	E214	T215	F216	L219	L220	G221	R222	R225	S230	L236	T241	T244	G245	T246	P247	V248	G251	L252	S253	Y254	R255	E256	G257	L258	Y259	I260			
T261	E262	Y265	T267	G268	L269	L270	S271	G272	L273	D274	E277	P280	E287	E288	R291	T292	V293	N294	T295	A296	V297	F304	G305	T306	E309	G310	N311	H312	K313	P314	L319	LYS	PRO	PRO	PRO	LYS													

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore 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	Depositor
R, R_{free}	0.251 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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: SDC, 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	0.42	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 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	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
4	A	17	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	0	0	2	0
4	C	13	0	0	1	0
All	All	7271	0	7287	385	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 27.

The worst 5 of 385 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: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 [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	312/323 (97%)	279 (89%)	26 (8%)	7 (2%)	6	22
1	B	312/323 (97%)	280 (90%)	23 (7%)	9 (3%)	4	15
1	C	312/323 (97%)	276 (88%)	28 (9%)	8 (3%)	5	18
All	All	936/969 (97%)	835 (89%)	77 (8%)	24 (3%)	5	18

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLN

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Mol	Chain	Res	Type
1	A	306	THR
1	B	65	GLN
1	C	65	GLN
1	A	64	PHE

5.3.2 Protein sidechains [i](#)

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%)	22	54
1	B	264/273 (97%)	251 (95%)	13 (5%)	25	57
1	C	264/273 (97%)	250 (95%)	14 (5%)	22	54
All	All	792/819 (97%)	751 (95%)	41 (5%)	23	55

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

Mol	Chain	Res	Type
1	C	24	VAL
1	C	215	THR
1	C	57	ASP
1	C	168	CYS
1	C	244	THR

Sometimes 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 [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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	1002	2	9,12,12	1.87	2 (22%)	10,16,16	2.74	4 (40%)
3	SDC	A	1000	2	9,12,12	1.92	2 (22%)	10,16,16	2.66	4 (40%)
3	SDC	B	1001	2	9,12,12	1.88	2 (22%)	10,16,16	2.61	4 (40%)

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	C	1002	2	-	7/11/12/12	-
3	SDC	A	1000	2	-	7/11/12/12	-
3	SDC	B	1001	2	-	7/11/12/12	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	SDC	O05-C04	4.50	1.35	1.22
3	A	1000	SDC	O05-C04	4.44	1.35	1.22
3	C	1002	SDC	O05-C04	4.36	1.35	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	SDC	O01-C04	-2.98	1.20	1.30
3	C	1002	SDC	O01-C04	-2.81	1.21	1.30

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	SDC	O13-S10-C09	5.19	116.07	107.84
3	B	1001	SDC	O13-S10-C09	4.81	115.46	107.84
3	A	1000	SDC	O13-S10-C09	4.28	114.63	107.84
3	A	1000	SDC	O01-C04-C03	4.28	127.97	113.38
3	C	1002	SDC	O01-C04-C03	4.27	127.93	113.38

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	SDC	C08-C09-S10-O11
3	A	1000	SDC	C08-C09-S10-O13
3	B	1001	SDC	C08-C09-S10-O11
3	B	1001	SDC	C08-C09-S10-O13
3	C	1002	SDC	C08-C09-S10-O11

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	SDC	3	0
3	A	1000	SDC	3	0
3	B	1001	SDC	3	0

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 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.