wwPDB X-ray Structure Validation Summary Report (i)

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 (i) 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 (i)) were used in the production of this report:

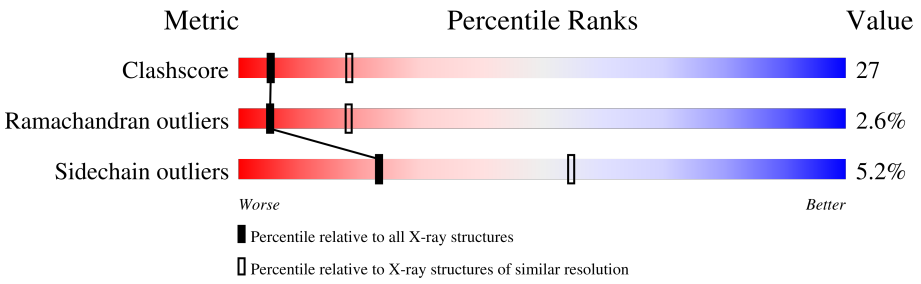
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	51% 42% • •
1	B	323	54% 39% • •
1	C	323	54% 38% • •

2 Entry composition (i)

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.

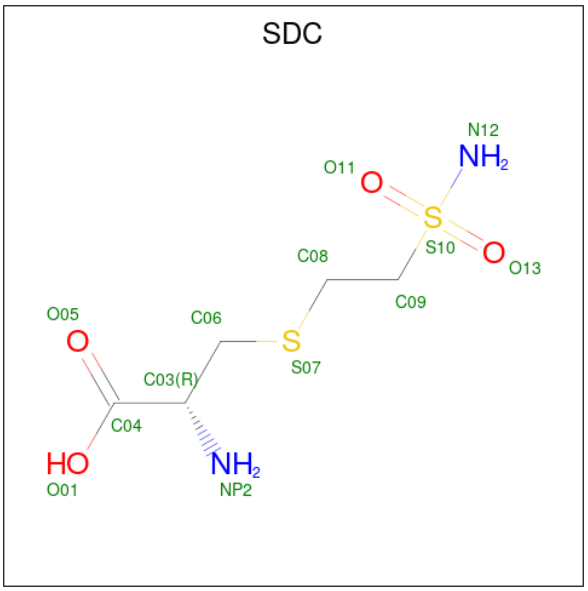
- Molecule 1 is a protein called Arginase 1.

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
			Total	Mn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0

- Molecule 3 is S-[2-(AMINOSULFONYL)ETHYL]-D-CYSTEINE (three-letter code: SDC) (formula: $C_5H_{12}N_2O_4S_2$).



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

- Molecule 4 is water.

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

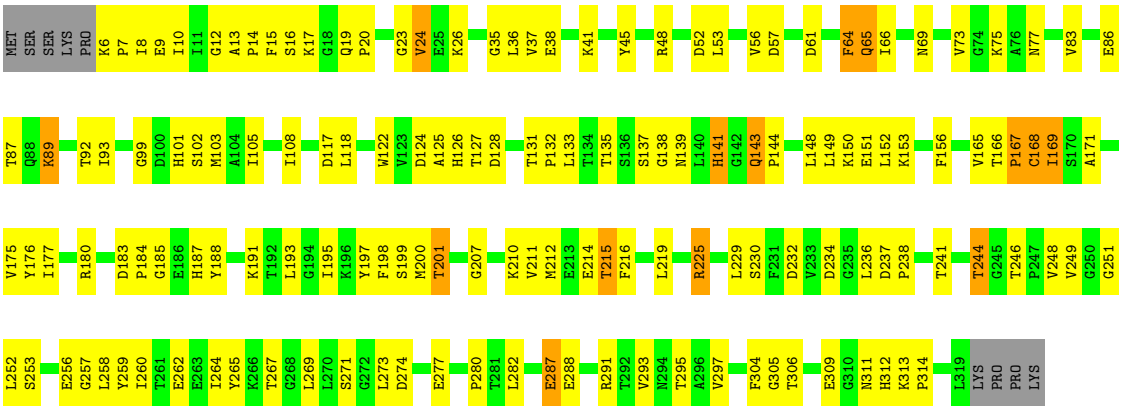
3 Residue-property plots (i)

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.

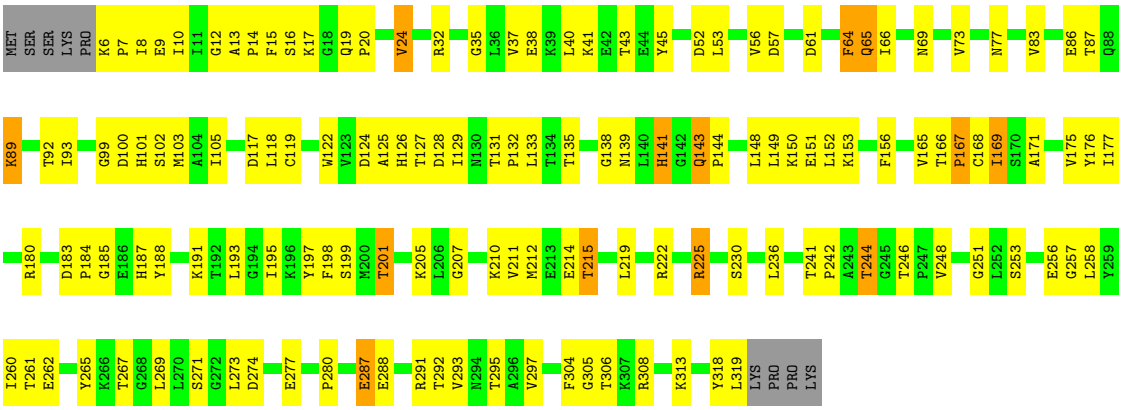
• Molecule 1: Arginase 1

Chain A: 51% 42%



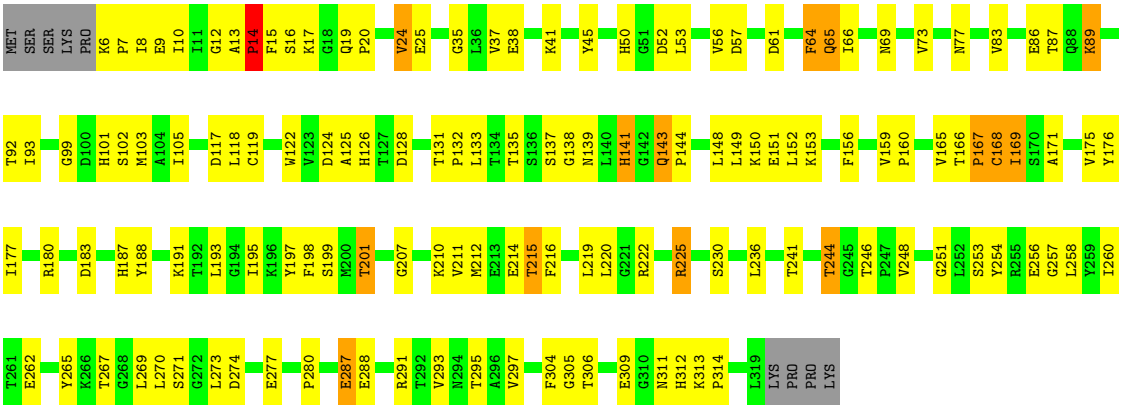
• Molecule 1: Arginase 1

Chain B: 54% 39%



• Molecule 1: Arginase 1

Chain C: 54% 38%


MET SER SER LYS PRO K6 P7 I8 E9 I10 I11 G12 A13 P14 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 T127 D128 T131 P132 L133 T134 T135 S136 S137 G138 N139 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 K196 Y197 F198 S199 M200 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 K266 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 LYS

4 Data and refinement statistics (i)

Xtriage (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.	Xtriage
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(^{o})	Ideal(^{o})
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 (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.