wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	4ZUZ
Title	:	SidC 1-871
Authors	:	Luo, X.; Wasilko, D.J.; Liu, Y.; Sun, J.; Wu, X.; Luo, Z.-Q.; Mao, Y.
Deposited on	:	2015-05-18
Resolution	:	2.86 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

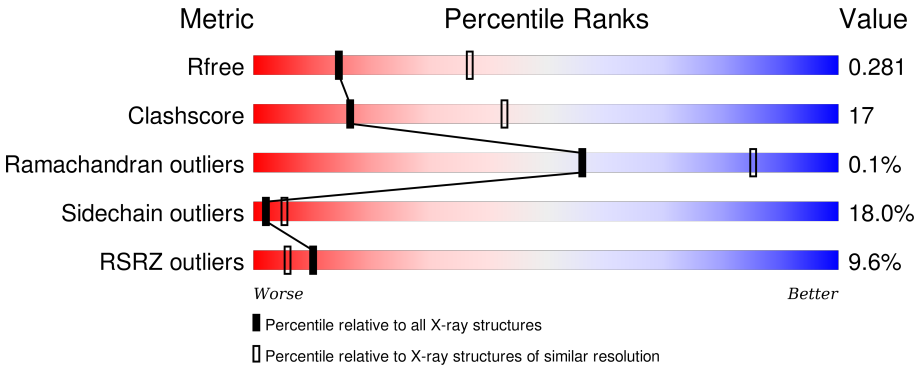
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.86 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))
R_{free}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	917	9% 62% 24% 7% 7%
1	B	917	9% 65% 22% 7% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14094 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 SidC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	857	Total	C	N	O	S	0	0	0
			6979	4405	1190	1374	10			
1	B	858	Total	C	N	O	S	0	0	0
			6986	4410	1191	1375	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	VAL	conflict	UNP Q6RCR4
A	326	VAL	ALA	conflict	UNP Q6RCR4
A	334	GLN	ASP	conflict	UNP Q6RCR4
A	646	ALA	LYS	conflict	UNP Q6RCR4
A	731	TYR	ALA	conflict	UNP Q6RCR4
B	325	ALA	VAL	conflict	UNP Q6RCR4
B	326	VAL	ALA	conflict	UNP Q6RCR4
B	334	GLN	ASP	conflict	UNP Q6RCR4
B	646	ALA	LYS	conflict	UNP Q6RCR4
B	731	TYR	ALA	conflict	UNP Q6RCR4

- Molecule 2 is water.

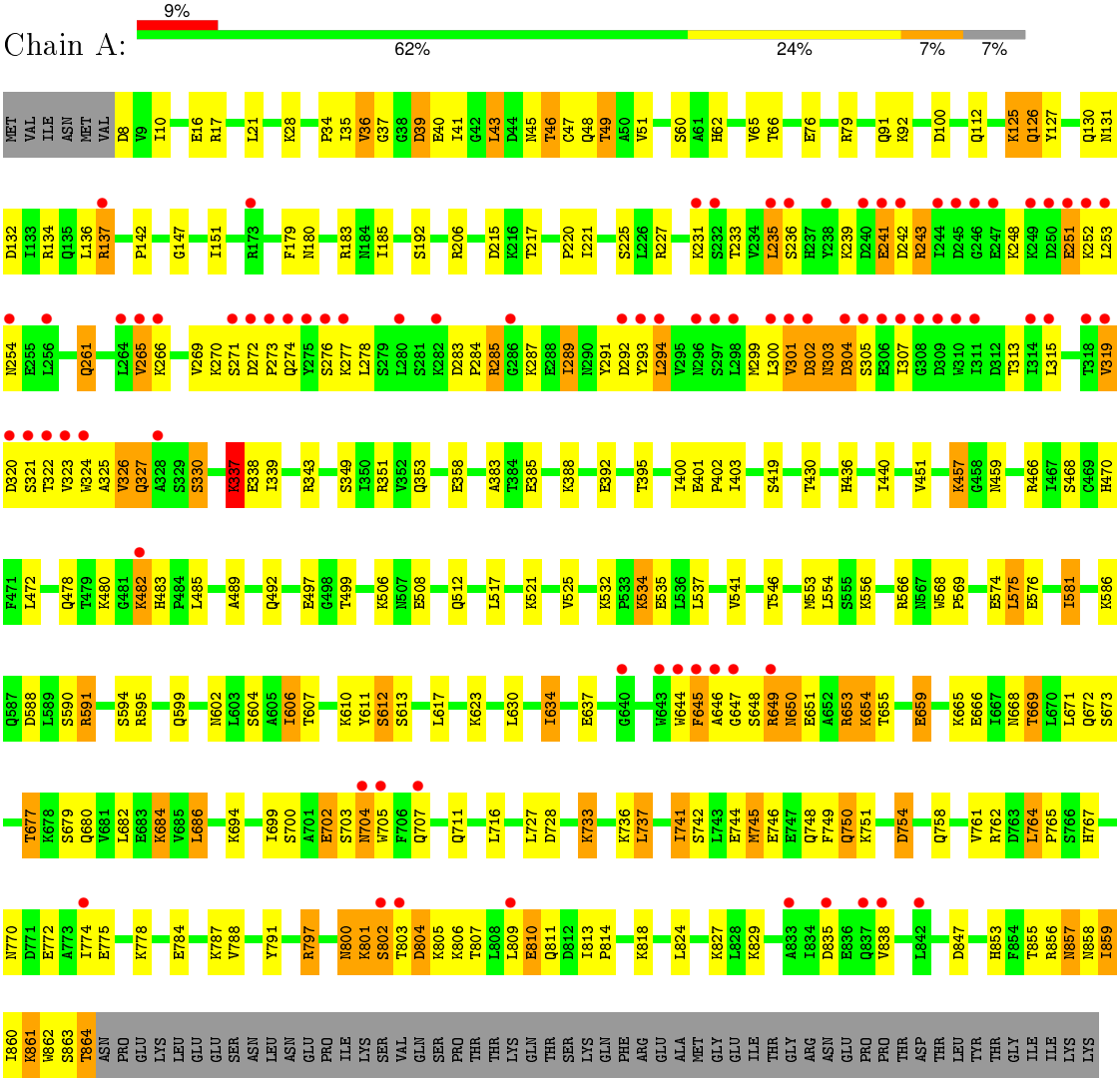
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total	O	0	0
			65	65		
2	B	64	Total	O	0	0
			64	64		

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 (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.

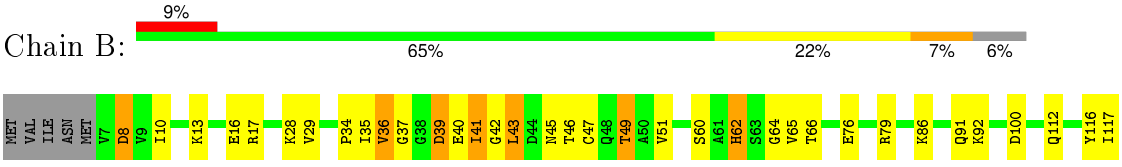
- Molecule 1: SidC

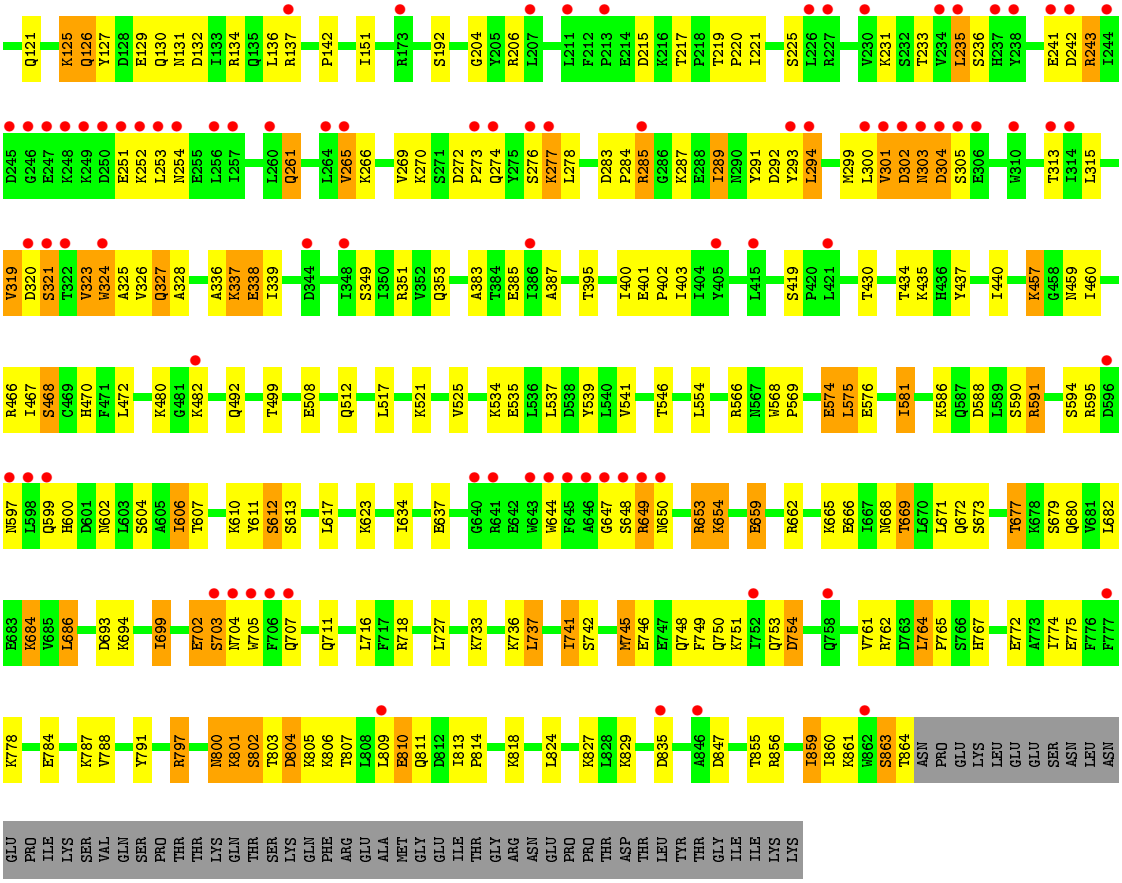
Chain A:



- Molecule 1: SidC

Chain B:




Q121 K125 Q126 Y127 D128 E129 Q130 N131 D132 I133 R134 Q135 L136 R137 P142 I151 R173 S192 G204 Y205 R206 L207 L211 F212 P213 E214 D215 K216 T217 P218 T219 P220 I221 S225 L226 R227 V230 K231 S232 T233 Y234 L235 S236 H237 Y238 E241 D242 R243 I244
D245 G246 E247 K248 K249 D250 E251 K252 L253 N254 E255 L256 I257 L260 Q261 L264 V265 K266 V269 K270 S271 D272 P273 Q274 Y275 S276 K277 L278 D283 P284 R285 G286 K287 E288 I289 N290 Y291 D292 Y293 L294 M299 L300 V301 D302 N303 D304 S305 E306 W310 T313 I314 L315
V319 D320 S321 T322 V323 W324 A325 V326 Q327 A328 A336 K337 E338 I339 D344 I348 S349 I350 R351 V352 Q353 A383 T384 E385 I386 A387 T395 I400 E401 P402 I403 I404 Y405 L415 S419 P420 L421 T430 T434 K435 H436 Y437 I440 K457 G458 N459 I460
R466 I467 S468 C469 H470 F471 L472 K480 G481 K482 Q492 T499 E508 Q512 L517 K521 V525 K534 E535 L536 L537 D538 Y539 L540 V541 T546 L554 R566 N567 W568 P569 E574 L575 E576 I581 K586 Q587 D588 L589 S590 R591 S594 R595 D596
N597 L598 Q599 H600 D601 N602 L603 S604 A605 I606 T607 K610 Y611 S612 S613 L617 K623 I634 E637 G640 R641 E642 W643 W644 F645 A646 G647 S648 R649 N650 R653 K654 E659 R662 K665 E666 I667 N668 T669 L670 L671 Q672 S673 T677 K678 S679 Q680 V681 L682
E683 K684 V685 L686 D693 K694 I699 E702 S703 N704 W705 F706 Q707 Q711 L716 F717 R718 L727 K733 K736 L737 I741 S742 M745 E746 E747 Q748 F749 Q750 K751 I752 Q753 D754 Q758 V761 R762 D763 L764 P765 S766 H767 E772 A773 I774 E775 F776 F777
K778 E784 K787 V788 V791 R797 N800 K801 S802 T803 D804 K805 K806 T807 L808 L809 E810 Q811 D812 I813 P814 K818 L824 K827 I828 K829 D835 A846 D847 T855 R856 I859 I860 K861 W862 S863 T864 ASN PRO GLU LYS LEU GLU GLU SER ASN LEU ASN
GLU PRO ILE LYS SER VAL GLN SER PRO THR THR LYS GLN THR SER LYS GLN PHE ARG GLU ALA MET GLY GLU ILE THR GLY ARG ASN GLU PRO PRO THR ASP THR LEU TYR THR GLY ILE ILE LYS LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	228.16Å 83.93Å 129.41Å 90.00° 108.82° 90.00°	Depositor
Resolution (Å)	49.16 – 2.86 47.14 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.16-2.86) 99.2 (47.14-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.281 0.224 , 0.281	Depositor DCC
R_{free} test set	2708 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	73.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 53343 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14094	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.51	0/7110	0.66	1/9595 (0.0%)
1	B	0.47	0/7117	0.65	1/9605 (0.0%)
All	All	0.49	0/14227	0.66	2/19200 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	337	LYS	CD-CE-NZ	-5.67	98.67	111.70
1	A	337	LYS	CD-CE-NZ	-5.50	99.05	111.70

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	6979	0	6935	236	0
1	B	6986	0	6942	230	0
2	A	65	0	0	27	0
2	B	64	0	0	22	0
All	All	14094	0	13877	461	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 17.

The worst 5 of 461 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:703:SER:HB3	1:B:704:ASN:CA	1.46	1.42
1:B:703:SER:CB	1:B:704:ASN:HA	1.41	1.41
1:A:703:SER:HB3	1:A:704:ASN:CA	1.48	1.41
1:A:703:SER:CB	1:A:704:ASN:HA	1.41	1.40
1:B:323:VAL:C	1:B:326:VAL:HG21	1.42	1.36

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	855/917 (93%)	829 (97%)	25 (3%)	1 (0%)	56 85
1	B	856/917 (93%)	823 (96%)	33 (4%)	0	100 100
All	All	1711/1834 (93%)	1652 (97%)	58 (3%)	1 (0%)	56 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	GLU

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	784/841 (93%)	642 (82%)	142 (18%)	2 5
1	B	785/841 (93%)	645 (82%)	140 (18%)	2 5
All	All	1569/1682 (93%)	1287 (82%)	282 (18%)	2 5

5 of 282 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	802	SER
1	B	131	ASN
1	B	751	LYS
1	A	809	LEU
1	B	36	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	707	GLN
1	B	89	ASN
1	B	661	GLN
1	A	750	GLN
1	A	800	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)

There are no ligands in this entry.

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	857/917 (93%)	0.35	81 (9%)	10	6	31, 65, 134, 199	8 (0%)
1	B	858/917 (93%)	0.44	84 (9%)	10	5	36, 76, 140, 181	8 (0%)
All	All	1715/1834 (93%)	0.40	165 (9%)	10	6	31, 71, 139, 199	16 (0%)

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	707	GLN	9.5
1	A	244	ILE	8.0
1	A	301	VAL	7.1
1	A	294	LEU	7.0
1	A	273	PRO	6.8

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.