



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4ZUZ / pdb_00004zuz
Title : SidC 1-871
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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

<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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

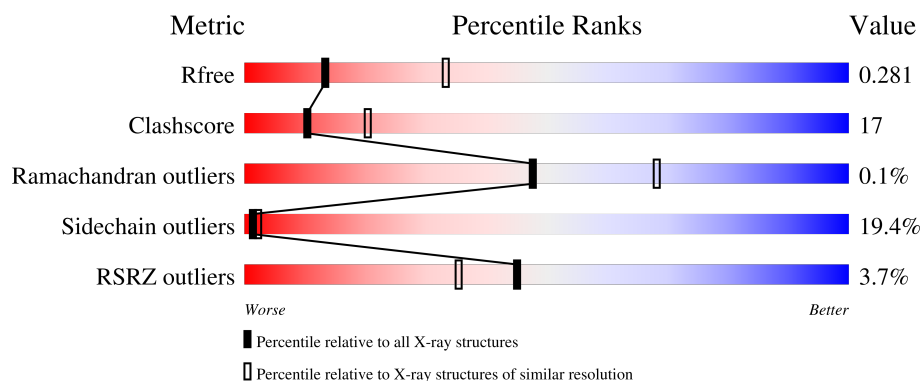
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. 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	
1	B	917	

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

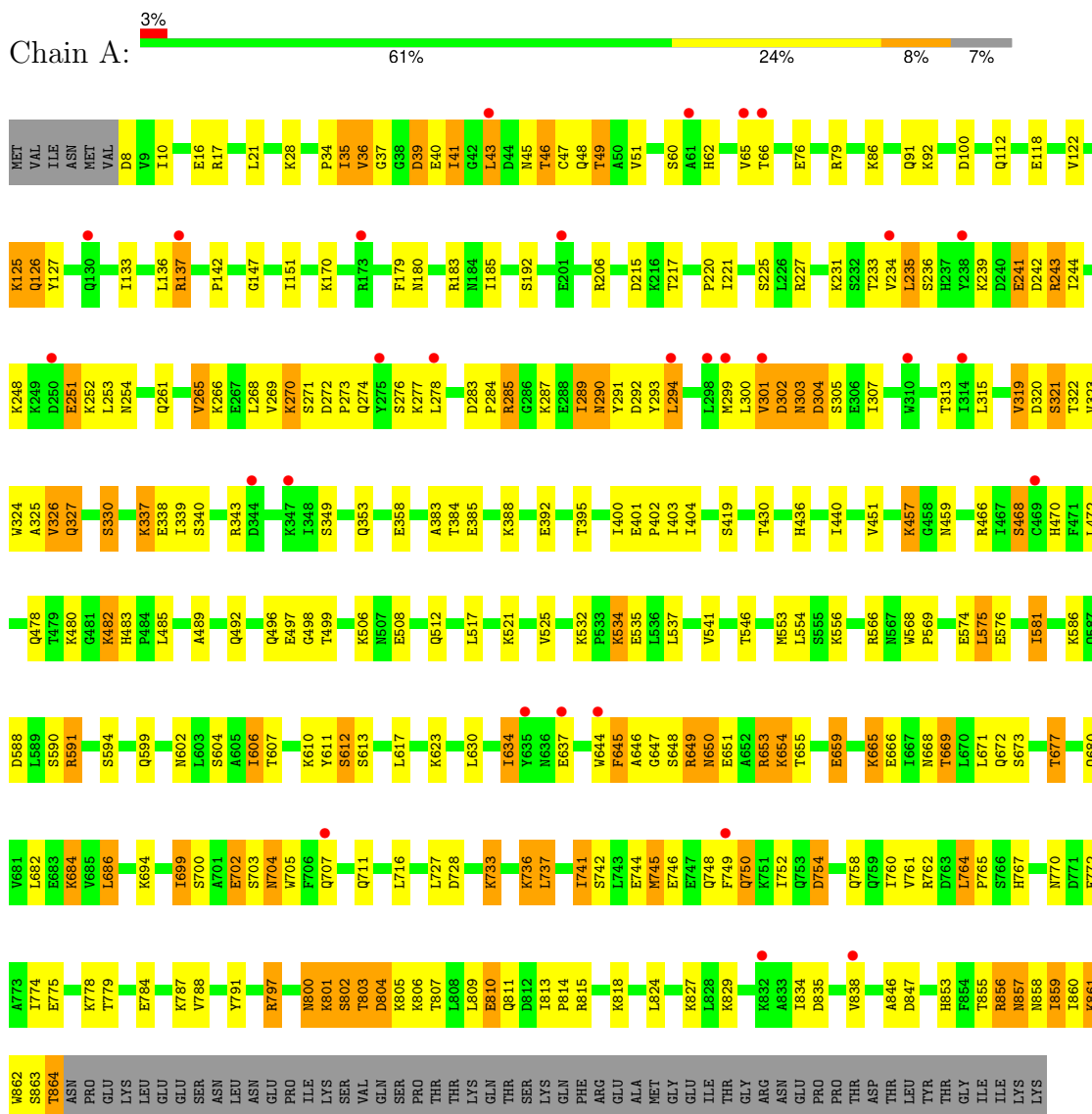
- Molecule 2 is water.

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, 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 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



• Molecule 1: SidC



THR	D804	F766	S612	E508	A328	Q261	I117	MET
SER	R805	Q707	S613	Q512	A336	L264	EL16	VAL
GLN	R806	Q711	L617	L517	K337	V265	Q121	ILE
PHE	L808	L716	K623	K521	E338	K266	V122	ASN
GLU	E810	F717	K634	K522	I339	E267	K126	MET
ALA	Q811	R718	I634	E523	S340	L268	Q126	V7
MET	D812	L727	Y635	E524	I348	V269	Q127	D8
GLY	I813	L733	N636	V525	S349	K270	Y127	Y9
GLU	P814	K733	E637	K634	Q353	S271	D128	I10
ILE	R815	K736	K638	K639	A383	D272	E129	K13
THR	K816	L737	W643	L537	T384	P273	Q130	E16
GLY	L824	F741	W644	D538	T385	Q274	L136	R17
ARG	K827	S742	F645	Y539	E385	S276	R137	L21
ASN	L828	M745	G647	V541	A387	K277	P142	K28
GLU	K829	E746	S648	T546	T395	L278	I151	V29
PRO	L835	F747	R649	L554	I400	D283	K170	P34
THR	K836	Q748	N650	N560	E401	R285	K173	P35
ASP	D835	F749	E651	Y561	P402	G286	S192	V36
LEU	Y838	Q750	R652	R566	I403	E288	E201	G37
TYR	D847	I752	K654	N567	I404	T289	G204	G38
GLY	L855	Q753	E659	W568	Y405	N290	R206	D39
ILE	R856	D754	R662	P569	T430	Y291	G205	E40
LYS	L859	I760	K665	E574	T434	D292	D215	L41
PRO	R860	R761	E666	L575	K435	Y293	K216	L43
GLU	S863	D762	T667	E576	H436	L298	T217	N45
LEU	T864	P765	T669	E576	Y437	L299	P218	O47
ASN	ASN	S766	L670	I581	I440	L300	T219	Q48
PRO	PRO	H767	L671	K586	I440	V301	P220	T49
GLU	GLU	M770	Q672	Q587	K457	D302	I221	A50
SER	GLU	E772	S673	D588	G458	N303	S225	V51
ASN	LEU	A773	T677	R591	N459	D304	K231	S60
ASN	LEU	E775	Q680	S594	I460	S305	S232	H62
LEU	ASN	K778	W681	N597	R466	W310	T233	S63
GLU	ASN	E784	L682	L598	I467	T313	W334	G64
PRO	PRO	E784	K684	Q599	C468	L315	L235	V65
ILE	ILE	V788	W685	H600	H470	D316	S236	T66
LYS	LYS	Y791	L686	D601	F471	A317	E241	R79
SER	VAL	Y791	D693	N602	L472	T318	D242	K86
GLN	GLN	R797	K694	L603	K480	V319	R243	Q91
SER	SER	R797	L699	S604	G481	D320	I244	D100
PRO	THR	R800	E702	I606	K482	S321	E251	Q112
THR	THR	R801	S703	T607	Q492	T322	K252	Y116
LYS	LYS	S802	N704	K610	T499	W324	N254	
GLN	GLN	T803	W705	Y611		V326	Q327	

4 Data and refinement statistics

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 49.16 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.16-2.86) 99.2 (49.16-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.225 , 0.281 0.224 , 0.281	Depositor DCC
R_{free} test set	2708 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	73.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0/7110	0.89	3/9595 (0.0%)
1	B	0.64	0/7117	0.88	1/9605 (0.0%)
All	All	0.67	0/14227	0.89	4/19200 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	SER	N-CA-C	5.98	118.27	109.24
1	A	133	ILE	N-CA-C	-5.19	106.02	110.74
1	A	468	SER	N-CA-C	5.12	116.98	109.24
1	A	846	ALA	N-CA-C	5.12	116.86	111.28

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	6979	0	6935	239	0
1	B	6986	0	6942	239	0
2	A	65	0	0	27	0
2	B	64	0	0	23	0
All	All	14094	0	13877	472	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 472 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:A:703:SER:HB3	1:A:704:ASN:CA	1.48	1.41
1:B:703:SER:CB	1:B:704:ASN:HA	1.41	1.41
1:B:323:VAL:C	1:B:326:VAL:HG21	1.42	1.41
1:B:324:TRP:C	1:B:326:VAL:HB	1.46	1.41

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	855/917 (93%)	829 (97%)	25 (3%)	1 (0%)	48	68
1	B	856/917 (93%)	823 (96%)	33 (4%)	0	100	100
All	All	1711/1834 (93%)	1652 (97%)	58 (3%)	1 (0%)	48	68

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%)	626 (80%)	158 (20%)	1	2
1	B	785/841 (93%)	638 (81%)	147 (19%)	1	2
All	All	1569/1682 (93%)	1264 (81%)	305 (19%)	1	2

5 of 305 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	492	GLN
1	B	800	ASN
1	B	546	THR
1	B	665	LYS
1	B	834	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	720	GLN
1	B	600	HIS
1	B	73	GLN
1	B	572	GLN
1	B	720	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	0.13	29 (3%)	48 38	21, 65, 134, 199	8 (0%)
1	B	858/917 (93%)	0.26	35 (4%)	41 32	27, 76, 140, 181	8 (0%)
All	All	1715/1834 (93%)	0.19	64 (3%)	45 35	21, 71, 139, 199	16 (0%)

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	ARG	7.1
1	B	137	ARG	6.7
1	B	173	ARG	5.9
1	A	130	GLN	4.9
1	B	130	GLN	4.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.