



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:13 AM UTC

PDB ID : 3O00 / pdb_00003o00
Title : Crystal Structure of the Salmonella Type III Secretion System Tip Protein SipD-C244S
Authors : Chatterjee, S.; Zhong, D.; Nordhues, B.A.; Battaile, K.P.; Lovell, S.; DeGuzman, R.N.
Deposited on : 2010-07-18
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

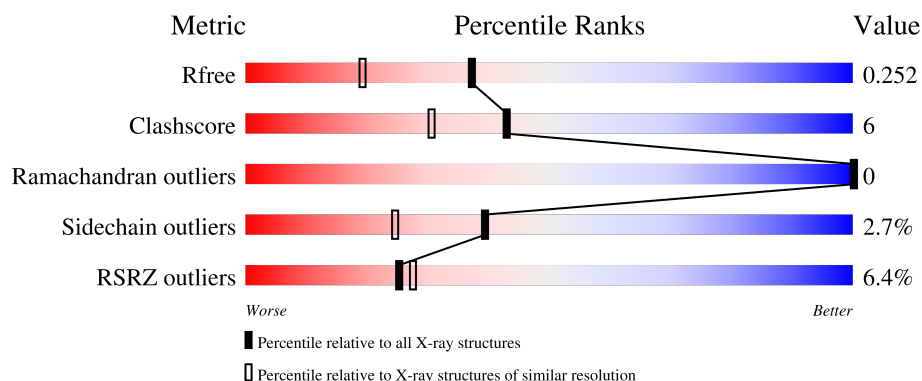
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	308	2% 81% 10% 7%
1	B	308	9% 75% 11% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4598 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 Cell invasion protein sipD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	13	0
			2243	1401	372	463	7			
1	B	266	Total	C	N	O	S	0	3	0
			2056	1286	341	424	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLY	-	expression tag	UNP Q56026
A	37	HIS	-	expression tag	UNP Q56026
A	38	MET	-	expression tag	UNP Q56026
A	244	SER	CYS	engineered mutation	UNP Q56026
B	36	GLY	-	expression tag	UNP Q56026
B	37	HIS	-	expression tag	UNP Q56026
B	38	MET	-	expression tag	UNP Q56026
B	244	SER	CYS	engineered mutation	UNP Q56026

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

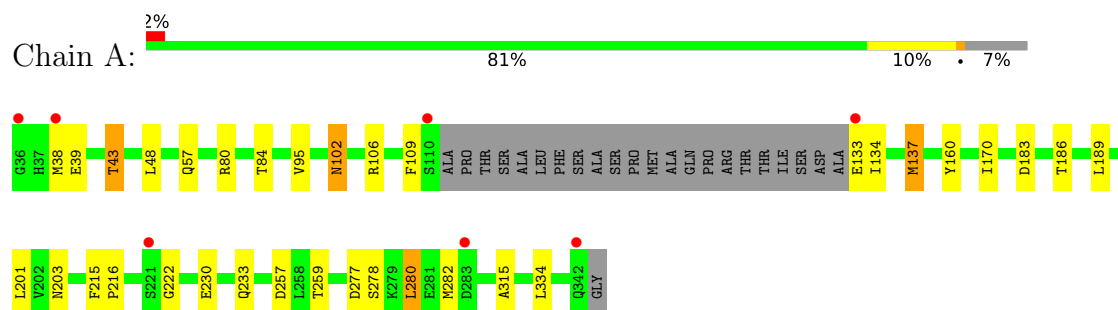
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total	O	0	0
			155	155		
3	B	143	Total	O	0	0
			143	143		

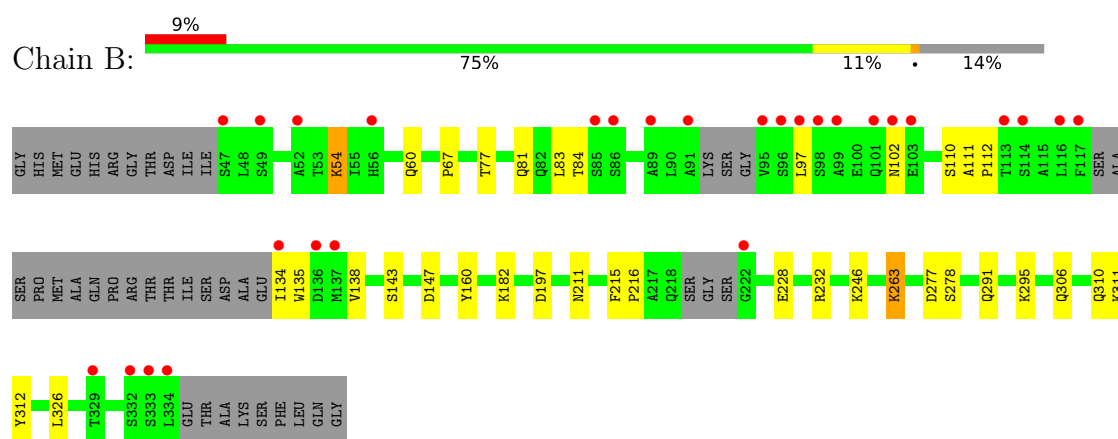
3 Residue-property plots [i](#)

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: Cell invasion protein sipD



• Molecule 1: Cell invasion protein sipD



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.35Å 52.15Å 57.55Å 90.00° 90.45° 90.00°	Depositor
Resolution (Å)	41.30 – 1.85 41.30 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.1 (41.30-1.85) 97.0 (41.30-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.249 (Not available) , 0.252	Depositor DCC
R_{free} test set	2550 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4598	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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	1.03	0/2314	1.00	1/3135 (0.0%)
1	B	1.01	0/2094	1.03	0/2841
All	All	1.02	0/4408	1.02	1/5976 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	315	ALA	N-CA-C	-5.19	105.71	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	GLY	Peptide

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	2243	0	2241	27	0
1	B	2056	0	2031	30	0
2	A	1	0	0	0	0
3	A	155	0	0	5	0
3	B	143	0	0	4	0
All	All	4598	0	4272	53	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 6.

All (53) 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:228:GLU:CD	1:B:232:ARG:HH12	1.60	1.08
1:A:109:PHE:O	1:A:137:MET:HE1	1.64	0.97
1:B:246:LYS:HE3	3:B:405:HOH:O	1.68	0.91
1:B:228:GLU:HG2	1:B:232:ARG:NH1	1.96	0.81
1:B:138:VAL:HG11	1:B:326:LEU:HD21	1.64	0.80
1:A:109:PHE:O	1:A:137:MET:CE	2.30	0.79
1:B:84:THR:HG21	1:B:143[A]:SER:OG	1.87	0.75
1:B:147:ASP:OD1	3:B:444:HOH:O	2.05	0.74
1:A:39:GLU:OE1	3:A:346:HOH:O	2.07	0.72
1:B:228:GLU:CG	1:B:232:ARG:HH12	2.02	0.72
1:B:228:GLU:CD	1:B:232:ARG:NH1	2.43	0.70
1:B:228:GLU:CG	1:B:232:ARG:NH1	2.55	0.70
1:A:57:GLN:HE22	1:B:311:LYS:NZ	1.91	0.68
1:A:257:ASP:OD1	1:A:259:THR:HG23	1.95	0.67
1:A:80:ARG:O	1:A:84[B]:THR:HG22	1.94	0.66
1:A:109:PHE:HB3	1:A:137:MET:HE1	1.80	0.64
1:B:291:GLN:HG2	1:B:295:LYS:HE2	1.79	0.63
1:A:277:ASP:O	1:A:278:SER:HB2	1.99	0.62
1:A:84[B]:THR:HG21	3:A:404:HOH:O	2.00	0.61
1:A:38[A]:MET:HE2	3:A:384:HOH:O	2.02	0.60
1:B:84:THR:CG2	1:B:143[A]:SER:OG	2.50	0.58
1:B:211:ASN:HB3	3:B:407:HOH:O	2.04	0.57
1:A:189:LEU:CD2	1:A:282:MET:HE1	2.35	0.57
1:A:57:GLN:HE22	1:B:311:LYS:HZ1	1.52	0.56
1:A:203:ASN:HB2	3:A:442:HOH:O	2.07	0.54
1:B:215:PHE:CD1	1:B:216:PRO:HA	2.42	0.54
1:A:230:GLU:O	1:A:233:GLN:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD23	1:A:282:MET:HE1	1.89	0.54
1:A:48:LEU:HD21	1:A:95:VAL:HG11	1.89	0.54
1:B:54:LYS:N	1:B:54:LYS:HD3	2.23	0.53
1:A:43[A]:THR:OG1	1:B:110:SER:HB2	2.09	0.53
1:A:137:MET:O	1:A:137:MET:HE2	2.10	0.52
1:B:228:GLU:OE1	1:B:232:ARG:NH1	2.37	0.52
1:B:67:PRO:HG3	1:B:312:TYR:CZ	2.45	0.51
1:B:97:LEU:HB2	1:B:102:ASN:OD1	2.10	0.51
1:A:109:PHE:CB	1:A:137:MET:HE1	2.41	0.50
1:B:97:LEU:HD21	1:B:135:TRP:CZ2	2.47	0.50
1:B:277:ASP:O	1:B:278:SER:OG	2.23	0.49
1:A:183:ASP:OD2	1:A:186[A]:THR:HG22	2.12	0.49
1:B:112:PRO:HB2	3:B:426:HOH:O	2.13	0.48
1:A:84[B]:THR:CG2	3:A:404:HOH:O	2.59	0.47
1:A:133:GLU:HG2	1:A:134:ILE:N	2.29	0.47
1:B:97:LEU:HD21	1:B:135:TRP:HZ2	1.79	0.47
1:B:83:LEU:HD23	1:B:83:LEU:C	2.39	0.47
1:A:102:ASN:HD22	1:A:106:ARG:NH1	2.13	0.47
1:A:43[A]:THR:HG23	1:B:111:ALA:C	2.40	0.46
1:B:67:PRO:HG3	1:B:312:TYR:CE1	2.52	0.45
1:B:306:GLN:O	1:B:310:GLN:HG3	2.17	0.45
1:B:263:LYS:HA	1:B:263:LYS:HD3	1.84	0.44
1:A:215:PHE:CD1	1:A:216:PRO:HA	2.53	0.43
1:B:77:THR:O	1:B:81:GLN:HG3	2.19	0.42
1:A:280:LEU:HD13	1:A:282:MET:CG	2.49	0.42
1:A:170:ILE:HD12	1:A:201:LEU:HD22	2.01	0.41

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	294/308 (96%)	291 (99%)	3 (1%)	0	100	100
1	B	261/308 (85%)	258 (99%)	3 (1%)	0	100	100
All	All	555/616 (90%)	549 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	260/264 (98%)	253 (97%)	7 (3%)	39	24
1	B	234/264 (89%)	227 (97%)	7 (3%)	36	21
All	All	494/528 (94%)	480 (97%)	14 (3%)	39	23

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43[A]	THR
1	A	43[B]	THR
1	A	102	ASN
1	A	137	MET
1	A	160	TYR
1	A	280	LEU
1	A	334	LEU
1	B	54	LYS
1	B	60	GLN
1	B	134	ILE
1	B	160	TYR
1	B	182	LYS
1	B	197	ASP
1	B	263	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	57	GLN
1	A	88	ASN
1	A	102	ASN
1	A	185	ASN
1	A	203	ASN
1	A	284	ASN
1	B	57	GLN
1	B	60	GLN
1	B	82	GLN
1	B	207	GLN
1	B	291	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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

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	285/308 (92%)	0.20	7 (2%) 58 62	9, 24, 40, 50	13 (4%)
1	B	266/308 (86%)	0.44	28 (10%) 11 11	12, 24, 49, 56	3 (1%)
All	All	551/616 (89%)	0.31	35 (6%) 25 27	9, 24, 45, 56	16 (2%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	LEU	5.1
1	B	91	ALA	5.1
1	B	99	ALA	4.3
1	B	117	PHE	3.9
1	A	283	ASP	3.7
1	A	133	GLU	3.7
1	B	136	ASP	3.4
1	B	47	SER	3.4
1	B	95	VAL	3.3
1	B	56	HIS	3.3
1	B	113	THR	3.2
1	B	116	LEU	3.1
1	B	89	ALA	3.1
1	A	36	GLY	3.1
1	B	333	SER	3.1
1	A	342	GLN	3.1
1	B	97	LEU	3.0
1	B	114	SER	3.0
1	B	134	ILE	3.0
1	B	98	SER	2.9
1	B	102	ASN	2.8
1	B	101	GLN	2.7
1	B	49	SER	2.7
1	A	38[A]	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	222	GLY	2.4
1	B	52	ALA	2.4
1	B	137	MET	2.4
1	A	221	SER	2.4
1	B	85	SER	2.3
1	B	332	SER	2.2
1	B	86	SER	2.2
1	A	110	SER	2.1
1	B	103	GLU	2.1
1	B	96	SER	2.1
1	B	329	THR	2.0

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	A	1	1/1	0.99	0.02	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.