



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:44 AM UTC

PDB ID : 2SIL / pdb_00002sil
Title : THE STRUCTURES OF SALMONELLA TYPHIMURIUM LT2 NEURAMINIDASE AND ITS COMPLEX WITH A TRANSITION STATE ANALOGUE AT 1.6 ANGSTROMS RESOLUTION
Authors : Taylor, G.L.; Crennell, S.J.; Garman, E.F.; Vimr, E.R.; Laver, W.G.
Deposited on : 1994-07-13
Resolution : 1.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

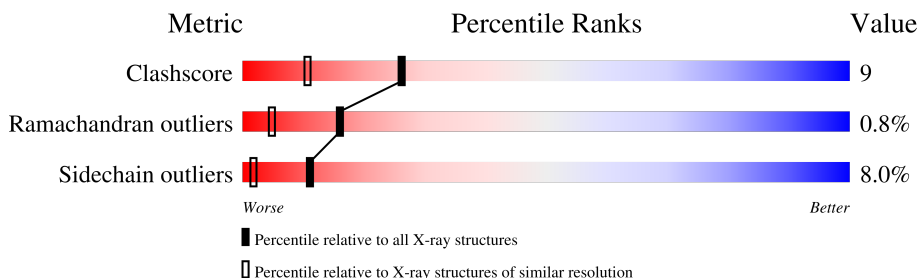
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)

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	381	 73% 20% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3149 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 SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	2954	1847	513	584	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	329	ASP	ALA	conflict	UNP P29768

- Molecule 2 is water.

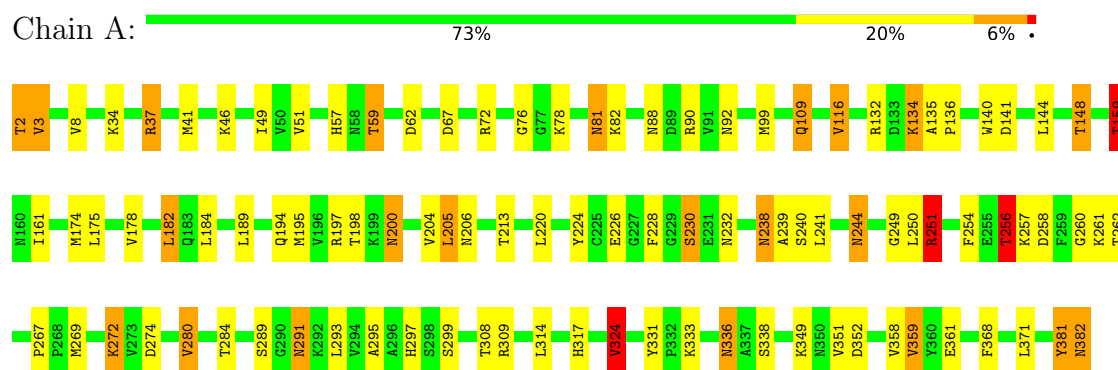
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	195	Total	O	0	0
			195	195		

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: SIALIDASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.50Å 82.50Å 91.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3149	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

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	1.62	1/3012 (0.0%)	1.96	60/4079 (1.5%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	ASN	C-OXT	68.11	2.59	1.23

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ARG	CD-NE-CZ	21.44	154.42	124.40
1	A	251	ARG	NE-CZ-NH1	-18.55	102.95	121.50
1	A	90	ARG	NE-CZ-NH2	18.52	135.87	119.20
1	A	251	ARG	NE-CZ-NH2	17.21	134.69	119.20
1	A	90	ARG	NE-CZ-NH1	-16.07	105.43	121.50
1	A	90	ARG	CD-NE-CZ	15.92	146.69	124.40
1	A	159	THR	N-CA-CB	-14.01	90.03	111.05
1	A	37	ARG	NE-CZ-NH1	13.12	134.62	121.50
1	A	37	ARG	NE-CZ-NH2	-12.34	108.10	119.20
1	A	3	VAL	N-CA-C	-10.76	94.49	109.45
1	A	90	ARG	CG-CD-NE	-9.59	90.90	112.00
1	A	238	ASN	CA-C-N	-9.16	109.12	122.40
1	A	238	ASN	C-N-CA	-9.16	109.12	122.40
1	A	148	THR	N-CA-CB	-8.98	96.17	110.98
1	A	59	THR	CB-CA-C	-8.86	94.15	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	THR	CA-CB-OG1	8.58	122.47	109.60
1	A	267	PRO	N-CA-C	8.23	120.74	110.70
1	A	324	VAL	CB-CA-C	-8.07	98.07	110.50
1	A	2	THR	CB-CA-C	7.97	126.64	109.10
1	A	116	VAL	CB-CA-C	-7.88	97.83	110.28
1	A	62	ASP	CA-CB-CG	7.81	120.41	112.60
1	A	256	THR	CB-CA-C	-7.31	96.33	109.71
1	A	159	THR	OG1-CB-CG2	7.10	123.50	109.30
1	A	238	ASN	CB-CA-C	-7.09	101.83	111.89
1	A	148	THR	OG1-CB-CG2	7.04	123.37	109.30
1	A	241	LEU	N-CA-C	-6.98	98.35	109.59
1	A	280	VAL	CB-CA-C	-6.71	101.93	111.40
1	A	291	ASN	CA-CB-CG	6.63	119.23	112.60
1	A	256	THR	N-CA-CB	6.60	121.77	110.68
1	A	280	VAL	CA-CB-CG1	6.43	121.33	110.40
1	A	213	THR	N-CA-C	-6.23	105.81	113.41
1	A	116	VAL	CA-CB-CG2	6.09	120.76	110.40
1	A	220	LEU	CB-CA-C	-5.91	100.67	108.76
1	A	232	ASN	CA-CB-CG	5.87	118.47	112.60
1	A	358	VAL	CA-CB-CG1	5.79	120.25	110.40
1	A	289	SER	N-CA-CB	5.75	120.89	110.95
1	A	116	VAL	N-CA-CB	5.74	120.87	111.58
1	A	257	LYS	N-CA-C	-5.73	105.62	113.30
1	A	230	SER	N-CA-C	5.71	122.96	110.80
1	A	92	ASN	O-C-N	-5.65	116.72	123.27
1	A	99	MET	N-CA-C	5.60	117.31	108.96
1	A	240	SER	N-CA-C	-5.60	100.55	109.23
1	A	72	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	A	3	VAL	O-C-N	-5.54	115.21	122.47
1	A	249	GLY	O-C-N	-5.46	119.53	123.08
1	A	116	VAL	CG1-CB-CG2	5.45	122.79	110.80
1	A	224	TYR	O-C-N	-5.43	116.97	123.27
1	A	72	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	A	34	LYS	N-CA-C	5.36	116.93	111.14
1	A	81	ASN	N-CA-C	-5.35	100.51	109.24
1	A	46	LYS	N-CA-C	-5.32	106.56	113.16
1	A	381	TYR	N-CA-C	5.29	117.81	109.39
1	A	88	ASN	N-CA-C	-5.23	103.98	110.41
1	A	109	GLN	CB-CA-C	-5.19	104.36	111.73
1	A	92	ASN	N-CA-CB	-5.18	102.56	110.65
1	A	109	GLN	CA-C-N	-5.17	113.98	122.20
1	A	109	GLN	C-N-CA	-5.17	113.98	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	PHE	CA-CB-CG	-5.16	108.64	113.80
1	A	59	THR	CA-CB-OG1	5.07	117.20	109.60
1	A	251	ARG	CB-CG-CD	-5.05	99.68	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	ARG	Sidechain

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	2954	0	2883	55	0
2	A	195	0	0	2	0
All	All	3149	0	2883	55	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 9.

All (55) 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:256:THR:HG21	1:A:260:GLY:H	1.15	1.06
1:A:256:THR:HG21	1:A:260:GLY:N	1.89	0.86
1:A:200:ASN:H	1:A:200:ASN:HD22	1.21	0.83
1:A:2:THR:HB	1:A:76:GLY:HA3	1.60	0.83
1:A:159:THR:HG23	1:A:161:ILE:H	1.45	0.80
1:A:200:ASN:H	1:A:200:ASN:ND2	1.74	0.79
1:A:37:ARG:HD2	1:A:361:GLU:OE2	1.84	0.77
1:A:204:VAL:HG12	1:A:205:LEU:HD13	1.68	0.75
1:A:349:LYS:HE2	1:A:352:ASP:HA	1.70	0.74
1:A:41:MET:HE2	1:A:49:ILE:CG2	2.18	0.74
1:A:256:THR:HG23	1:A:262:THR:O	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:THR:CG2	1:A:161:ILE:H	2.02	0.71
1:A:3:VAL:HB	1:A:78:LYS:HG2	1.73	0.70
1:A:3:VAL:HB	1:A:78:LYS:CG	2.26	0.65
1:A:134:LYS:HE2	1:A:135:ALA:H	1.61	0.64
1:A:174:MET:HE2	1:A:195:MET:HE2	1.79	0.64
1:A:8:VAL:O	1:A:82:LYS:HE2	2.00	0.61
1:A:317:HIS:CD2	1:A:324:VAL:HG13	2.36	0.61
1:A:41:MET:HE2	1:A:49:ILE:HG21	1.82	0.61
1:A:132:ARG:NH1	2:A:626:HOH:O	2.35	0.60
1:A:134:LYS:HE2	1:A:135:ALA:N	2.18	0.59
1:A:336:ASN:HD22	1:A:338:SER:H	1.51	0.57
1:A:314:LEU:HD22	1:A:371:LEU:HD13	1.87	0.56
1:A:256:THR:HG22	1:A:258:ASP:H	1.70	0.55
1:A:41:MET:HE1	1:A:368:PHE:CD2	2.42	0.55
1:A:41:MET:HE1	1:A:368:PHE:HD2	1.71	0.54
1:A:159:THR:HG21	2:A:631:HOH:O	2.05	0.54
1:A:57:HIS:HE1	1:A:67:ASP:OD2	1.91	0.53
1:A:41:MET:HE3	1:A:51:VAL:HG22	1.91	0.53
1:A:336:ASN:HD22	1:A:336:ASN:C	2.18	0.52
1:A:244:ASN:C	1:A:244:ASN:HD22	2.20	0.50
1:A:140:TRP:CG	1:A:141:ASP:N	2.80	0.50
1:A:226:GLU:HB2	1:A:228:PHE:CE2	2.47	0.49
1:A:250:LEU:HD23	1:A:274:ASP:HB2	1.93	0.49
1:A:284:THR:OG1	1:A:297:HIS:HD2	1.96	0.47
1:A:204:VAL:HG12	1:A:205:LEU:CD1	2.42	0.46
1:A:336:ASN:ND2	1:A:338:SER:H	2.12	0.46
1:A:269:MET:HA	1:A:272:LYS:HG2	1.98	0.46
1:A:200:ASN:HD22	1:A:200:ASN:N	2.00	0.46
1:A:197:ARG:HH11	1:A:206:ASN:ND2	2.14	0.45
1:A:382:ASN:OXT	1:A:382:ASN:C	2.59	0.45
1:A:182:LEU:HD22	1:A:184:LEU:HD23	1.99	0.45
1:A:297:HIS:HE1	1:A:299:SER:OG	2.00	0.45
1:A:295:ALA:HB3	1:A:317:HIS:HB2	2.00	0.44
1:A:198:THR:CB	1:A:200:ASN:HD21	2.31	0.43
1:A:244:ASN:HD22	1:A:251:ARG:HH21	1.66	0.43
1:A:238:ASN:O	1:A:239:ALA:C	2.61	0.43
1:A:244:ASN:ND2	1:A:251:ARG:HH21	2.16	0.43
1:A:3:VAL:HB	1:A:78:LYS:HG3	1.99	0.42
1:A:382:ASN:C	1:A:382:ASN:ND2	2.78	0.42
1:A:135:ALA:HA	1:A:136:PRO:HA	1.84	0.42
1:A:200:ASN:ND2	1:A:200:ASN:N	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:CE	1:A:359:VAL:HG13	2.50	0.41
1:A:331:TYR:CE1	1:A:333:LYS:HD3	2.55	0.41
1:A:308:THR:O	1:A:309:ARG:C	2.64	0.41

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	379/381 (100%)	366 (97%)	10 (3%)	3 (1%)	16 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	VAL
1	A	230	SER
1	A	351	VAL

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	327/327 (100%)	301 (92%)	26 (8%)	11 2

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	THR
1	A	81	ASN
1	A	109	GLN
1	A	116	VAL
1	A	134	LYS
1	A	144	LEU
1	A	148	THR
1	A	159	THR
1	A	175	LEU
1	A	182	LEU
1	A	189	LEU
1	A	194	GLN
1	A	200	ASN
1	A	205	LEU
1	A	244	ASN
1	A	251	ARG
1	A	256	THR
1	A	261	LYS
1	A	272	LYS
1	A	280	VAL
1	A	291	ASN
1	A	293	LEU
1	A	324	VAL
1	A	336	ASN
1	A	359	VAL
1	A	381	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	107	ASN
1	A	124	ASN
1	A	194	GLN
1	A	200	ASN
1	A	206	ASN
1	A	244	ASN
1	A	247	ASN
1	A	297	HIS
1	A	304	ASN
1	A	317	HIS
1	A	336	ASN
1	A	369	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	374	HIS
1	A	382	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 oligosaccharides 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

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.