



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:53 PM UTC

PDB ID : 4GR4 / pdb\_00004gr4  
Title : Crystal structure of SlgN1deltaAsub  
Authors : Herbst, D.A.; Zocher, G.; Stehle, T.  
Deposited on : 2012-08-24  
Resolution : 2.44 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](mailto: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

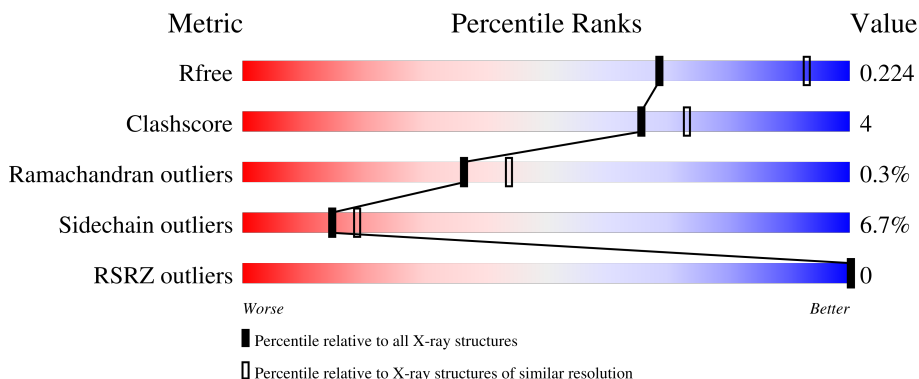
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


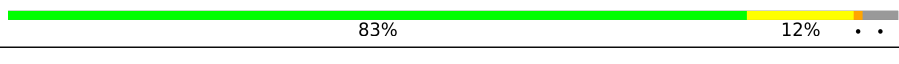
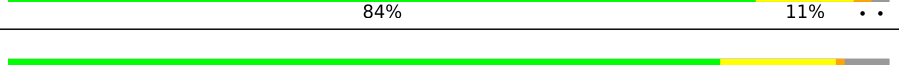

The reported resolution of this entry is 2.44 Å.

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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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  $\geq 3$ , 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	469	 83% 12% . .
1	B	469	 83% 12% . .
1	C	469	 84% 11% . .
1	D	469	 80% 13% . 5%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13783 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 Non-ribosomal peptide synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3357	2122	599	623	13	0	0	0
1	B	451	3339	2109	595	623	12	0	0	0
1	C	458	3353	2121	595	625	12	0	0	0
1	D	444	3291	2080	585	614	12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP D1GLU5
A	-1	SER	-	expression tag	UNP D1GLU5
A	0	HIS	-	expression tag	UNP D1GLU5
B	-2	GLY	-	expression tag	UNP D1GLU5
B	-1	SER	-	expression tag	UNP D1GLU5
B	0	HIS	-	expression tag	UNP D1GLU5
C	-2	GLY	-	expression tag	UNP D1GLU5
C	-1	SER	-	expression tag	UNP D1GLU5
C	0	HIS	-	expression tag	UNP D1GLU5
D	-2	GLY	-	expression tag	UNP D1GLU5
D	-1	SER	-	expression tag	UNP D1GLU5
D	0	HIS	-	expression tag	UNP D1GLU5

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		

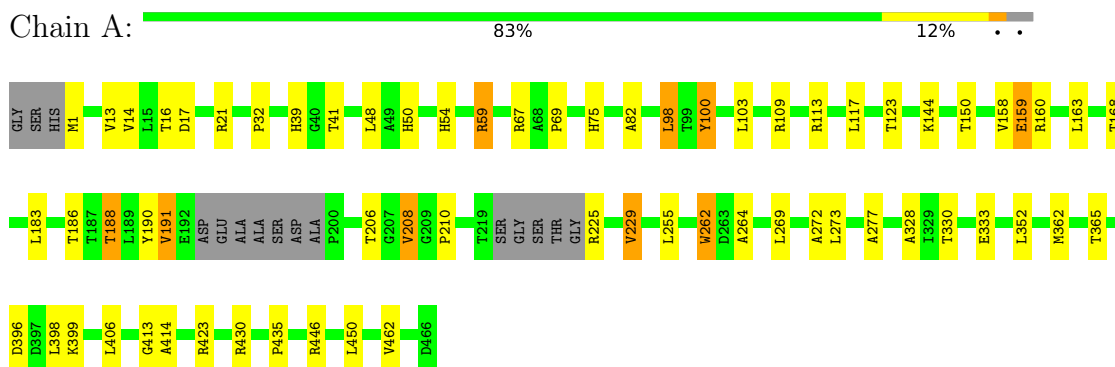
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total 139	O 139	0	0
3	B	108	Total 108	O 108	0	0
3	C	85	Total 85	O 85	0	0
3	D	110	Total 110	O 110	0	0

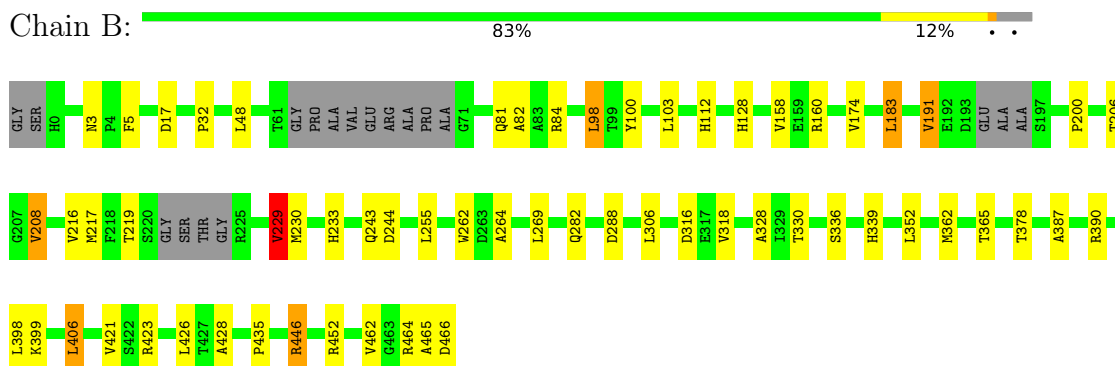
### 3 Residue-property plots [i](#)

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 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.

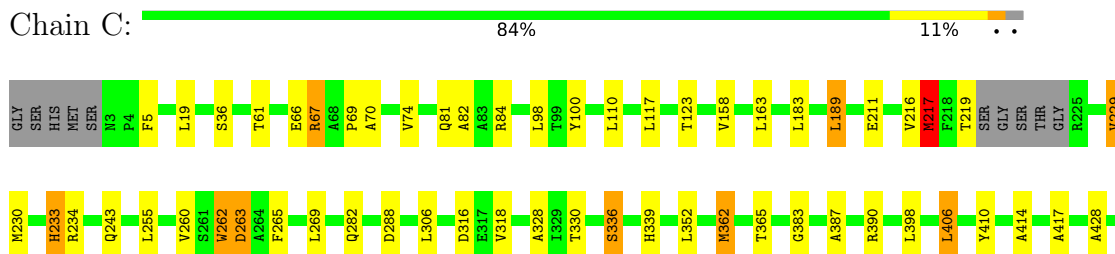
- Molecule 1: Non-ribosomal peptide synthetase



- Molecule 1: Non-ribosomal peptide synthetase



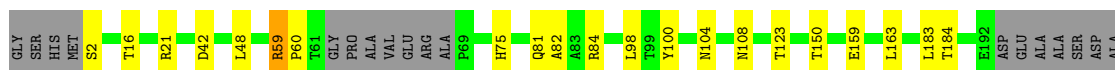
- Molecule 1: Non-ribosomal peptide synthetase





- Molecule 1: Non-ribosomal peptide synthetase

Chain D: 80% 13% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.11Å 148.61Å 109.58Å 90.00° 113.34° 90.00°	Depositor
Resolution (Å)	35.72 – 2.44 35.72 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.72-2.44) 97.7 (35.72-2.44)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.45Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.180 , 0.213 0.192 , 0.224	Depositor DCC
$R_{free}$ test set	4790 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtrriage
Anisotropy	0.195	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 19.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.118 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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

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	0.86	0/3438	1.33	16/4686 (0.3%)
1	B	0.84	0/3419	1.30	12/4659 (0.3%)
1	C	0.85	0/3436	1.32	17/4693 (0.4%)
1	D	0.83	0/3370	1.29	12/4591 (0.3%)
All	All	0.85	0/13663	1.31	57/18629 (0.3%)

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	VAL	N-CA-CB	9.16	120.70	110.72
1	D	283	SER	N-CA-C	8.70	120.76	111.28
1	C	336	SER	CA-C-N	7.59	125.02	120.24
1	C	336	SER	C-N-CA	7.59	125.02	120.24
1	C	263	ASP	N-CA-C	7.17	119.95	111.71

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	3357	0	3277	20	0
1	B	3339	0	3243	27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3353	0	3244	27	0
1	D	3291	0	3195	28	0
2	B	1	0	0	0	0
3	A	139	0	0	1	0
3	B	108	0	0	0	0
3	C	85	0	0	0	0
3	D	110	0	0	0	0
All	All	13783	0	12959	101	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 4.

The worst 5 of 101 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:C:110:LEU:HD11	1:C:189:LEU:HD21	1.57	0.84
1:D:104:ASN:HD21	1:D:203:ASN:HD21	1.33	0.76
1:C:406:LEU:HD11	1:C:462:VAL:HG11	1.72	0.71
1:B:406:LEU:HD11	1:B:462:VAL:HG11	1.74	0.70
1:D:406:LEU:HD11	1:D:462:VAL:HG11	1.75	0.68

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	448/469 (96%)	439 (98%)	8 (2%)	1 (0%)	43 53
1	B	443/469 (94%)	434 (98%)	8 (2%)	1 (0%)	43 53
1	C	454/469 (97%)	441 (97%)	11 (2%)	2 (0%)	30 36
1	D	436/469 (93%)	430 (99%)	5 (1%)	1 (0%)	43 53

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1781/1876 (95%)	1744 (98%)	32 (2%)	5 (0%)	36 44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	MET
1	B	362	MET
1	C	362	MET
1	D	362	MET
1	C	70	ALA

### 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	333/346 (96%)	304 (91%)	29 (9%)	9 11
1	B	332/346 (96%)	313 (94%)	19 (6%)	18 25
1	C	328/346 (95%)	311 (95%)	17 (5%)	21 28
1	D	327/346 (94%)	303 (93%)	24 (7%)	13 15
All	All	1320/1384 (95%)	1231 (93%)	89 (7%)	15 19

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	217	MET
1	D	163	LEU
1	C	255	LEU
1	D	16	THR
1	D	229	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	54	HIS
1	D	282	GLN
1	D	75	HIS
1	D	155	GLN
1	D	312	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](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	454/469 (96%)	-1.65	0 100 100	22, 36, 66, 98	0
1	B	451/469 (96%)	-1.63	0 100 100	23, 38, 68, 96	0
1	C	458/469 (97%)	-1.58	0 100 100	22, 41, 85, 106	0
1	D	444/469 (94%)	-1.61	0 100 100	24, 38, 79, 109	0
All	All	1807/1876 (96%)	-1.62	0 100 100	22, 38, 79, 109	0

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	CL	B	501	1/1	0.99	0.04	58,58,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.