



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4AHP / pdb_00004ahp
Title : Crystal Structure of Wild Type N-acetylneuraminic acid lyase from Staphylococcus aureus
Authors : Timms, N.; Polyakova, A.; Windle, C.L.; Trinh, C.H.; Nelson, A.; Trinh, A.R.; Berry, A.
Deposited on : 2012-02-06
Resolution : 2.10 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

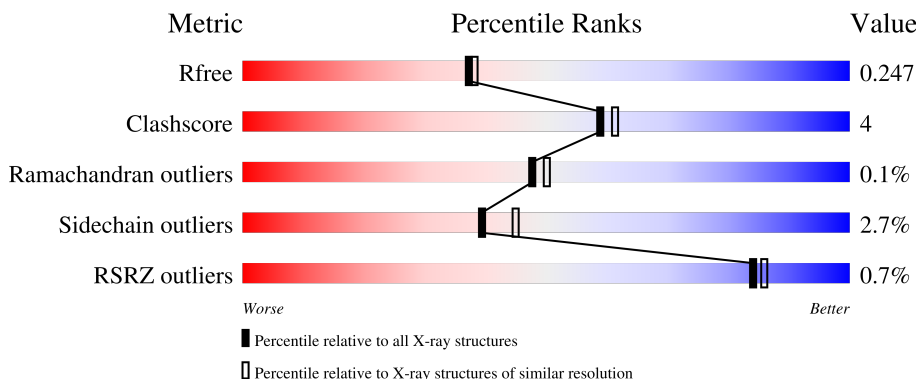
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	298	% 84% 10% 5%
1	B	298	% 89% 6% .
1	C	298	% 84% 13% .
1	D	298	87% 8% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9400 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 N-ACETYLNEURAMINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2246	1440	376	427	3			
1	B	287	Total	C	N	O	S	0	0	0
			2259	1448	379	429	3			
1	C	290	Total	C	N	O	S	0	0	0
			2279	1460	384	432	3			
1	D	283	Total	C	N	O	S	0	0	0
			2231	1432	372	424	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP Q2G160
A	-3	HIS	-	expression tag	UNP Q2G160
A	-2	HIS	-	expression tag	UNP Q2G160
A	-1	HIS	-	expression tag	UNP Q2G160
A	0	HIS	-	expression tag	UNP Q2G160
A	1	HIS	-	expression tag	UNP Q2G160
B	-4	HIS	-	expression tag	UNP Q2G160
B	-3	HIS	-	expression tag	UNP Q2G160
B	-2	HIS	-	expression tag	UNP Q2G160
B	-1	HIS	-	expression tag	UNP Q2G160
B	0	HIS	-	expression tag	UNP Q2G160
B	1	HIS	-	expression tag	UNP Q2G160
C	-4	HIS	-	expression tag	UNP Q2G160
C	-3	HIS	-	expression tag	UNP Q2G160
C	-2	HIS	-	expression tag	UNP Q2G160
C	-1	HIS	-	expression tag	UNP Q2G160
C	0	HIS	-	expression tag	UNP Q2G160
C	1	HIS	-	expression tag	UNP Q2G160
D	-4	HIS	-	expression tag	UNP Q2G160
D	-3	HIS	-	expression tag	UNP Q2G160
D	-2	HIS	-	expression tag	UNP Q2G160

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	HIS	-	expression tag	UNP Q2G160
D	0	HIS	-	expression tag	UNP Q2G160
D	1	HIS	-	expression tag	UNP Q2G160

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	106	Total O 106 106	0	0
3	B	105	Total O 105 105	0	0
3	C	60	Total O 60 60	0	0
3	D	110	Total O 110 110	0	0

- Molecule 1: N-ACETYLNEURAMINATE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.53Å 109.56Å 131.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.52 – 2.10 46.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (46.52-2.10) 97.4 (46.52-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.248 0.195 , 0.247	Depositor DCC
R_{free} test set	3450 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9400	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.72% 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](#)

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	0.85	0/2288	0.93	1/3091 (0.0%)
1	B	0.84	0/2302	0.94	0/3112
1	C	0.88	0/2324	0.93	0/3145
1	D	0.85	0/2272	0.93	0/3071
All	All	0.86	0/9186	0.93	1/12419 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ILE	N-CA-C	5.27	116.00	110.62

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	2246	0	2211	24	0
1	B	2259	0	2214	19	0
1	C	2279	0	2217	29	0
1	D	2231	0	2198	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	106	0	0	1	0
3	B	105	0	0	1	0
3	C	60	0	0	1	0
3	D	110	0	0	1	0
All	All	9400	0	8840	78	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 78 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:LYS:HE2	3:A:2085:HOH:O	1.64	0.96
1:C:33:ASN:HD21	1:C:262:ARG:HH11	1.25	0.82
1:D:33:ASN:HD21	1:D:262:ARG:HH11	1.30	0.79
1:D:277:ASN:ND2	1:D:279:ALA:H	1.85	0.76
1:D:277:ASN:HD22	1:D:277:ASN:C	1.96	0.73

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	280/298 (94%)	274 (98%)	6 (2%)	0	100	100
1	B	283/298 (95%)	277 (98%)	6 (2%)	0	100	100
1	C	286/298 (96%)	279 (98%)	6 (2%)	1 (0%)	36	36
1	D	279/298 (94%)	276 (99%)	3 (1%)	0	100	100
All	All	1128/1192 (95%)	1106 (98%)	21 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	251	ILE

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	234/254 (92%)	229 (98%)	5 (2%)	47	54
1	B	234/254 (92%)	226 (97%)	8 (3%)	32	35
1	C	235/254 (92%)	228 (97%)	7 (3%)	36	41
1	D	232/254 (91%)	227 (98%)	5 (2%)	45	53
All	All	935/1016 (92%)	910 (97%)	25 (3%)	39	45

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	128	GLU
1	C	228	GLN
1	D	277	ASN
1	C	215	ARG
1	C	230	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	52	ASN
1	D	33	ASN
1	C	33	ASN
1	C	277	ASN
1	C	25	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 4 ligands modelled in this entry, 4 are 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, 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	284/298 (95%)	-0.22	3 (1%) 78 80	18, 25, 37, 57	0
1	B	287/298 (96%)	-0.26	2 (0%) 84 86	15, 24, 36, 55	0
1	C	290/298 (97%)	-0.07	3 (1%) 79 81	17, 27, 39, 48	0
1	D	283/298 (94%)	-0.43	0 100 100	15, 21, 34, 55	0
All	All	1144/1192 (95%)	-0.24	8 (0%) 84 86	15, 24, 38, 57	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASN	3.1
1	C	-4	HIS	2.9
1	B	-1	HIS	2.9
1	B	149	ILE	2.8
1	C	169	PRO	2.7

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	CL	C	1294	1/1	0.97	0.05	32,32,32,32	0
2	CL	B	1294	1/1	0.99	0.02	26,26,26,26	0
2	CL	A	1294	1/1	0.99	0.03	28,28,28,28	0
2	CL	D	1294	1/1	0.99	0.03	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.