



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:01 PM UTC

PDB ID : 1N7N / pdb_00001n7n
Title : Streptococcus pneumoniae Hyaluronate Lyase W292A Mutant
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Deposited on : 2002-11-16
Resolution : 1.55 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

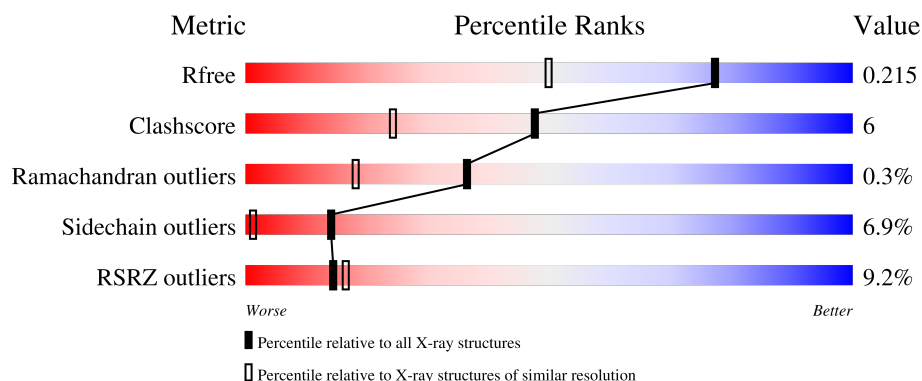
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	721	9% 87% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6507 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 HYALURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	0	0
			5775	3630	967	1156	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	ALA	TRP	engineered mutation	UNP Q54873
A	731	VAL	GLY	SEE REMARK 999	UNP Q54873

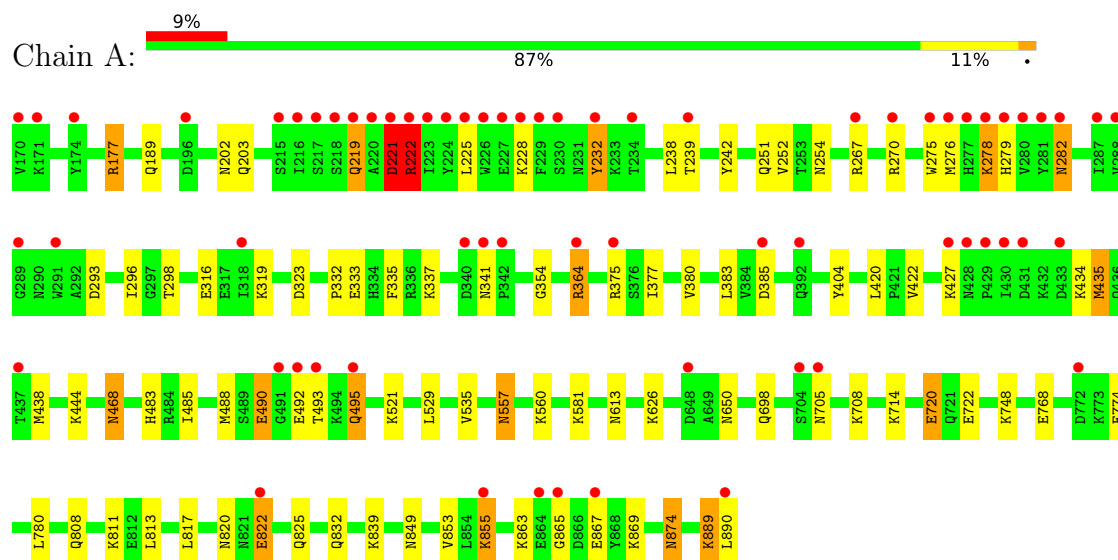
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	732	Total	O	0	0
			732	732		

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 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: HYALURONIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.07Å 103.58Å 101.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55 20.00 – 1.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.55) 97.2 (20.00-1.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.55Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.209 0.198 , 0.215	Depositor DCC
R_{free} test set	1266 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6507	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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	0.73	2/5892 (0.0%)	0.84	0/7957

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	MET	SD-CE	-5.74	1.65	1.79
1	A	438	MET	SD-CE	-5.20	1.66	1.79

There are no bond angle outliers.

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	5775	0	5590	64	0
2	A	732	0	0	28	0
All	All	6507	0	5590	64	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 (64) 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:613:ASN:H	1:A:698:GLN:HE22	1.08	0.96
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.35	0.74
1:A:420:LEU:HD22	1:A:435:MET:CE	2.17	0.74
1:A:535:VAL:HG22	2:A:1612:HOH:O	1.89	0.72
1:A:483:HIS:HE1	2:A:1215:HOH:O	1.74	0.70
1:A:557:ASN:HD22	1:A:557:ASN:C	1.99	0.70
1:A:296:ILE:HD11	1:A:335:PHE:CE1	2.29	0.69
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.76	0.67
1:A:705:ASN:HB2	2:A:1335:HOH:O	1.94	0.66
1:A:863:LYS:NZ	1:A:865:GLY:O	2.25	0.66
1:A:874:ASN:C	1:A:874:ASN:HD22	2.04	0.65
1:A:375:ARG:CD	2:A:1579:HOH:O	2.46	0.63
1:A:375:ARG:HD2	2:A:1579:HOH:O	1.98	0.62
1:A:364:ARG:HD3	2:A:1141:HOH:O	1.99	0.61
1:A:296:ILE:HD11	1:A:335:PHE:CZ	2.38	0.59
1:A:267:ARG:HD3	2:A:1177:HOH:O	2.05	0.57
1:A:720:GLU:HG3	2:A:1318:HOH:O	2.05	0.56
1:A:822:GLU:HG3	2:A:1298:HOH:O	2.05	0.55
1:A:354:GLY:CA	1:A:377:ILE:HD11	2.35	0.55
1:A:225:LEU:HD12	1:A:276:MET:HE3	1.89	0.55
1:A:232:TYR:HB3	2:A:1212:HOH:O	2.07	0.55
1:A:708:LYS:HE2	2:A:1386:HOH:O	2.07	0.54
1:A:221:ASP:O	1:A:222:ARG:O	2.26	0.54
1:A:495:GLN:HG2	2:A:1612:HOH:O	2.08	0.54
1:A:177:ARG:HG3	1:A:422:VAL:HG13	1.88	0.53
1:A:557:ASN:ND2	1:A:560:LYS:H	2.07	0.53
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.74	0.52
1:A:254:ASN:C	1:A:254:ASN:HD22	2.18	0.52
1:A:817:LEU:C	1:A:817:LEU:HD13	2.35	0.51
1:A:189:GLN:HG3	2:A:1367:HOH:O	2.10	0.51
1:A:202:ASN:ND2	1:A:251:GLN:HE22	2.09	0.51
1:A:279:HIS:CE1	2:A:1618:HOH:O	2.63	0.50
1:A:267:ARG:CD	2:A:1177:HOH:O	2.59	0.50
1:A:889:LYS:NZ	1:A:889:LYS:H	2.10	0.50
1:A:521:LYS:HD3	2:A:1332:HOH:O	2.12	0.50
1:A:332:PRO:HG2	2:A:1566:HOH:O	2.12	0.49
1:A:839:LYS:HD2	1:A:853:VAL:HG23	1.95	0.49
1:A:420:LEU:HD22	1:A:435:MET:HE1	1.92	0.49
1:A:239:THR:HG21	1:A:293:ASP:OD2	2.13	0.49
1:A:468:ASN:C	1:A:468:ASN:HD22	2.21	0.48
1:A:316:GLU:CD	1:A:316:GLU:N	2.72	0.47
1:A:275:TRP:CZ3	1:A:276:MET:HE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LYS:HG3	1:A:279:HIS:CD2	2.50	0.46
1:A:282:ASN:HB2	2:A:1292:HOH:O	2.15	0.46
1:A:890:LEU:CB	2:A:1455:HOH:O	2.64	0.46
1:A:485:ILE:HD13	1:A:488:MET:HE3	1.97	0.45
1:A:341:ASN:ND2	2:A:1515:HOH:O	2.36	0.45
1:A:341:ASN:HB2	2:A:1459:HOH:O	2.17	0.44
1:A:720:GLU:CG	2:A:1318:HOH:O	2.64	0.44
1:A:581:LYS:HB3	1:A:768:GLU:HB2	2.00	0.44
1:A:855:LYS:HE3	1:A:855:LYS:HB3	1.80	0.44
1:A:316:GLU:CD	1:A:316:GLU:H	2.27	0.43
1:A:323:ASP:HA	2:A:1596:HOH:O	2.18	0.43
1:A:493:THR:HG21	2:A:1344:HOH:O	2.19	0.42
1:A:493:THR:HG22	2:A:1493:HOH:O	2.18	0.42
1:A:296:ILE:CD1	1:A:335:PHE:CE1	3.01	0.42
1:A:375:ARG:NH2	2:A:1611:HOH:O	2.53	0.42
1:A:557:ASN:C	1:A:557:ASN:ND2	2.72	0.41
1:A:242:TYR:CD2	1:A:298:THR:HG23	2.55	0.41
1:A:490:GLU:O	1:A:493:THR:HG22	2.20	0.41
1:A:874:ASN:C	1:A:874:ASN:ND2	2.75	0.41
1:A:238:LEU:HB2	2:A:1621:HOH:O	2.20	0.41
1:A:385:ASP:HB2	2:A:1588:HOH:O	2.20	0.40
1:A:219:GLN:CA	1:A:219:GLN:HE21	2.35	0.40

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	719/721 (100%)	694 (96%)	23 (3%)	2 (0%)	36 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ARG
1	A	221	ASP

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	637/639 (100%)	593 (93%)	44 (7%)	14 1

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ARG
1	A	203	GLN
1	A	219	GLN
1	A	221	ASP
1	A	222	ARG
1	A	228	LYS
1	A	232	TYR
1	A	252	VAL
1	A	270	ARG
1	A	278	LYS
1	A	282	ASN
1	A	319	LYS
1	A	333	GLU
1	A	337	LYS
1	A	364	ARG
1	A	380	VAL
1	A	383	LEU
1	A	404	TYR
1	A	427	LYS
1	A	434	LYS
1	A	444	LYS
1	A	468	ASN
1	A	490	GLU
1	A	492	GLU
1	A	495	GLN

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Mol	Chain	Res	Type
1	A	529	LEU
1	A	557	ASN
1	A	626	LYS
1	A	714	LYS
1	A	720	GLU
1	A	722	GLU
1	A	748	LYS
1	A	774	GLU
1	A	780	LEU
1	A	808	GLN
1	A	811	LYS
1	A	813	LEU
1	A	822	GLU
1	A	849	ASN
1	A	855	LYS
1	A	867	GLU
1	A	869	LYS
1	A	874	ASN
1	A	889	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	254	ASN
1	A	279	HIS
1	A	282	ASN
1	A	341	ASN
1	A	379	GLN
1	A	386	GLN
1	A	436	GLN
1	A	468	ASN
1	A	483	HIS
1	A	557	ASN
1	A	662	GLN
1	A	667	HIS
1	A	698	GLN
1	A	759	GLN
1	A	789	ASN
1	A	820	ASN
1	A	825	GLN
1	A	832	GLN

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Mol	Chain	Res	Type
1	A	874	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

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	721/721 (100%)	0.41	66 (9%)	14 16	11, 20, 40, 61	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	TYR	7.5
1	A	223	ILE	7.1
1	A	232	TYR	6.4
1	A	225	LEU	5.9
1	A	890	LEU	5.3
1	A	229	PHE	5.1
1	A	219	GLN	4.7
1	A	226	TRP	4.6
1	A	220	ALA	4.4
1	A	216	ILE	4.3
1	A	228	LYS	4.0
1	A	429	PRO	4.0
1	A	170	VAL	4.0
1	A	218	SER	3.9
1	A	433	ASP	3.8
1	A	217	SER	3.8
1	A	280	VAL	3.8
1	A	278	LYS	3.8
1	A	221	ASP	3.7
1	A	174	TYR	3.5
1	A	277	HIS	3.4
1	A	275	TRP	3.4
1	A	493	THR	3.4
1	A	375	ARG	3.3
1	A	230	SER	3.3
1	A	239	THR	3.3
1	A	867	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	222	ARG	3.2
1	A	267	ARG	3.2
1	A	171	LYS	3.1
1	A	340	ASP	3.1
1	A	276	MET	3.1
1	A	341	ASN	3.0
1	A	287	ILE	3.0
1	A	430	ILE	2.8
1	A	215	SER	2.8
1	A	288	VAL	2.8
1	A	227	GLU	2.8
1	A	491	GLY	2.8
1	A	392	GLN	2.7
1	A	427	LYS	2.6
1	A	492	GLU	2.6
1	A	279	HIS	2.6
1	A	281	TYR	2.6
1	A	364	ARG	2.6
1	A	705	ASN	2.5
1	A	318	ILE	2.5
1	A	342	PRO	2.5
1	A	431	ASP	2.4
1	A	385	ASP	2.4
1	A	822	GLU	2.3
1	A	437	THR	2.3
1	A	428	ASN	2.3
1	A	855	LYS	2.2
1	A	234	THR	2.2
1	A	289	GLY	2.2
1	A	865	GLY	2.2
1	A	495	GLN	2.1
1	A	704	SER	2.1
1	A	864	GLU	2.0
1	A	282	ASN	2.0
1	A	772	ASP	2.0
1	A	270	ARG	2.0
1	A	291	TRP	2.0
1	A	196	ASP	2.0
1	A	648	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.