



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 05:50 AM EDT

PDB ID : 7OFZ / pdb_00007ofz
Title : Nontypeable Haemophilus influenzae SapA in complex with double stranded RNA
Authors : Lukacik, P.; Owen, C.D.; Nettleship, J.E.; Bird, L.E.; Owens, R.J.; Walsh, M.A.
Deposited on : 2021-05-05
Resolution : 2.62 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

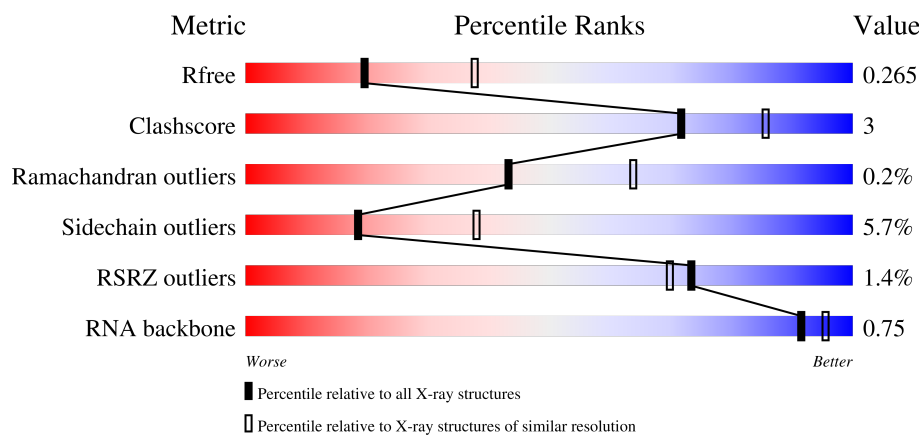
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)
RNA backbone	3983	1035 (2.86-2.38)

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	526	 77% 16% • 6%
2	C	19	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4527 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 ABC-type transport system, periplasmic component, involved in antimicrobial peptide resistance.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	1	0
			4005	2570	675	746	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	LYS	ARG	conflict	UNP Q4QL73

- Molecule 2 is a RNA chain called RNA (5'-R(P*CP*CP*CP*CP*CP*CP*CP*CP*CP*GP*GP*GP*GP*GP*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	19	Total	C	N	O	P	0	0	0
			407	180	75	133	19			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

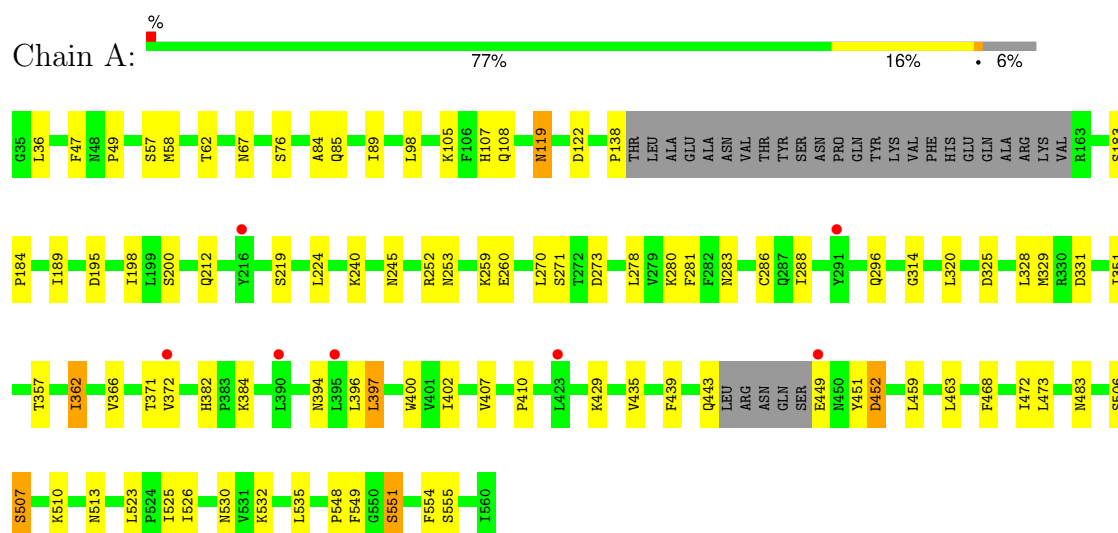
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	C	1	Total	O	0	0
			1	1		

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: ABC-type transport system, periplasmic component, involved in antimicrobial peptide resistance



- Molecule 2: RNA (5'-R(P*CP*CP*CP*CP*CP*CP*CP*CP*CP*GP*GP*GP*GP*GP*GP*GP*GP*GP*G)-3')



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.40Å 144.40Å 62.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.20 – 2.62 72.20 – 2.62	Depositor EDS
% Data completeness (in resolution range)	94.9 (72.20-2.62) 94.9 (72.20-2.62)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.10.3, REFMAC 7.04.09, PHENIX 2.5.6	Depositor
R, R_{free}	0.217 , 0.263 0.224 , 0.265	Depositor DCC
R_{free} test set	940 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4527	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: NA

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	0.88	1/4106 (0.0%)	1.38	28/5579 (0.5%)
2	C	0.83	0/453	0.67	0/705
All	All	0.87	1/4559 (0.0%)	1.32	28/6284 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	MET	SD-CE	-6.29	1.63	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	PHE	CA-CB-CG	7.94	121.74	113.80
1	A	270	LEU	CA-C-N	6.76	129.65	120.38
1	A	270	LEU	C-N-CA	6.76	129.65	120.38
1	A	506	SER	CA-C-N	6.48	128.86	120.44
1	A	506	SER	C-N-CA	6.48	128.86	120.44
1	A	325	ASP	N-CA-C	-5.90	106.12	113.38
1	A	362	ILE	N-CA-C	-5.86	107.20	112.12
1	A	259	LYS	CA-C-N	5.76	129.45	120.75
1	A	259	LYS	C-N-CA	5.76	129.45	120.75
1	A	273	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	84	ALA	CA-C-N	5.60	127.78	120.28
1	A	84	ALA	C-N-CA	5.60	127.78	120.28
1	A	331	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	47	PHE	N-CA-C	-5.31	106.38	112.92
1	A	119	ASN	CA-C-N	5.26	128.06	120.38
1	A	119	ASN	C-N-CA	5.26	128.06	120.38
1	A	472	ILE	N-CA-C	5.26	115.47	110.53
1	A	507	SER	CA-C-N	5.19	127.18	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	SER	C-N-CA	5.19	127.18	120.44
1	A	452	ASP	N-CA-C	-5.13	106.70	113.12
1	A	57	SER	N-CA-C	5.13	116.61	108.96
1	A	67	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	483	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	271	SER	N-CA-C	5.07	117.46	111.33
1	A	283	ASN	CA-C-N	5.06	129.30	122.07
1	A	283	ASN	C-N-CA	5.06	129.30	122.07
1	A	245	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	468	PHE	CA-CB-CG	5.05	118.85	113.80

There are no chirality outliers.

There are no planarity outliers.

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	4005	0	3938	28	0
2	C	407	0	210	0	0
3	A	1	0	0	0	0
4	A	113	0	0	1	0
4	C	1	0	0	0	0
All	All	4527	0	4148	28	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 3.

All (28) 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:357:THR:HB	1:A:530:ASN:HB2	1.73	0.70
1:A:314:GLY:HA2	1:A:366:VAL:HG21	1.80	0.64
1:A:371:THR:HG22	1:A:513:ASN:ND2	2.17	0.60
1:A:36:LEU:HD21	1:A:288:ILE:HD12	1.86	0.58
1:A:252:ARG:HD2	1:A:260:GLU:HG2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:HG13	1:A:439:PHE:HD2	1.72	0.55
1:A:195:ASP:HB3	1:A:198:ILE:HG12	1.90	0.54
1:A:382:HIS:CE1	1:A:384:LYS:HB2	2.44	0.53
1:A:98:LEU:HD11	1:A:189:ILE:HD11	1.91	0.53
1:A:200:SER:HB3	4:A:779:HOH:O	2.10	0.52
1:A:351:ILE:HG22	1:A:410:PRO:HD2	1.92	0.51
1:A:362:ILE:HD12	1:A:525:ILE:HD11	1.95	0.49
1:A:119:ASN:HB2	1:A:184:PRO:O	2.13	0.48
1:A:329:MET:HE2	1:A:397:LEU:HD22	1.97	0.47
1:A:400:TRP:CD2	1:A:451:TYR:HB3	2.49	0.47
1:A:396:LEU:HD13	1:A:429:LYS:HD3	1.97	0.45
1:A:281:PHE:HA	1:A:286:CYS:HB3	1.97	0.45
1:A:122:ASP:HA	1:A:212:GLN:HB2	2.00	0.44
1:A:548:PRO:HD2	1:A:549:PHE:CE2	2.53	0.43
1:A:138:PRO:HD2	1:A:219:SER:HB3	2.01	0.43
1:A:320:LEU:HD23	1:A:526:ILE:HD12	2.00	0.43
1:A:400:TRP:CG	1:A:451:TYR:HB3	2.54	0.43
1:A:382:HIS:HE1	1:A:384:LYS:HB2	1.84	0.43
1:A:329:MET:HE2	1:A:452:ASP:HB3	2.01	0.42
1:A:107:HIS:CE1	1:A:253:ASN:HD22	2.38	0.41
1:A:407:VAL:HG11	1:A:459:LEU:HD22	2.01	0.41
1:A:49:PRO:HD3	1:A:62:THR:HG21	2.03	0.41
1:A:278:LEU:HD12	1:A:296:GLN:HB3	2.03	0.40

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	492/526 (94%)	474 (96%)	17 (4%)	1 (0%)	43 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	SER

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	440/466 (94%)	415 (94%)	25 (6%)	18 38

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	SER
1	A	85	GLN
1	A	89	ILE
1	A	105	LYS
1	A	108	GLN
1	A	183	SER
1	A	224	LEU
1	A	240	LYS
1	A	280	LYS
1	A	328	LEU
1	A	372	VAL
1	A	394	ASN
1	A	397	LEU
1	A	402	ILE
1	A	443	GLN
1	A	449	GLU
1	A	463	LEU
1	A	473	LEU
1	A	507	SER
1	A	510	LYS
1	A	523	LEU
1	A	532	LYS
1	A	535	LEU
1	A	551	SER
1	A	555	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	99	ASN
1	A	246	GLN
1	A	253	ASN
1	A	340	GLN
1	A	343	ASN
1	A	398	ASN
1	A	403	ASN
1	A	406	GLN
1	A	450	ASN
1	A	479	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	18/19 (94%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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 [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	497/526 (94%)	0.17	7 (1%) 73 70	32, 62, 93, 121	1 (0%)
2	C	19/19 (100%)	0.68	0 100 100	60, 112, 172, 176	0
All	All	516/545 (94%)	0.19	7 (1%) 73 70	32, 63, 96, 176	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291[A]	TYR	3.4
1	A	372	VAL	2.8
1	A	423	LEU	2.6
1	A	395	LEU	2.5
1	A	390	LEU	2.5
1	A	216	TYR	2.2
1	A	449	GLU	2.1

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
3	NA	A	601	1/1	0.90	0.07	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.