



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:12 AM UTC

PDB ID : 1ZCD / pdb_00001zcd
Title : Crystal structure of the Na⁺/H⁺ antiporter NhaA
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Deposited on : 2005-04-11
Resolution : 3.45 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) : **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

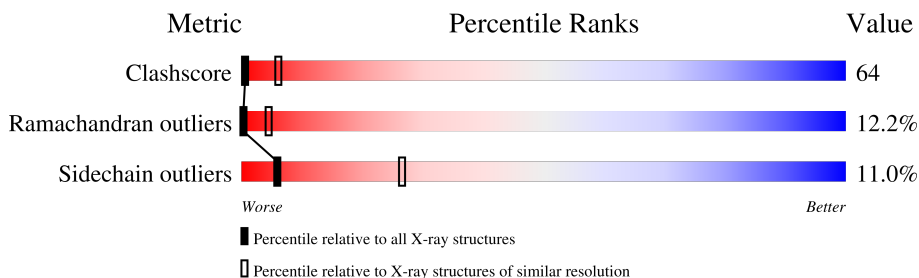
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

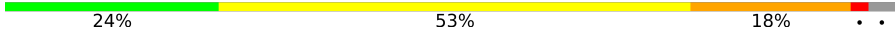
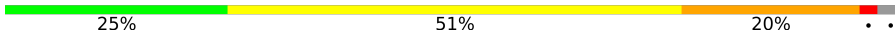
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)

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 ≥ 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	388	 24% 53% 18% . .
1	B	388	 25% 51% 20% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5616 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 Na(+)/H(+) antiporter 1.

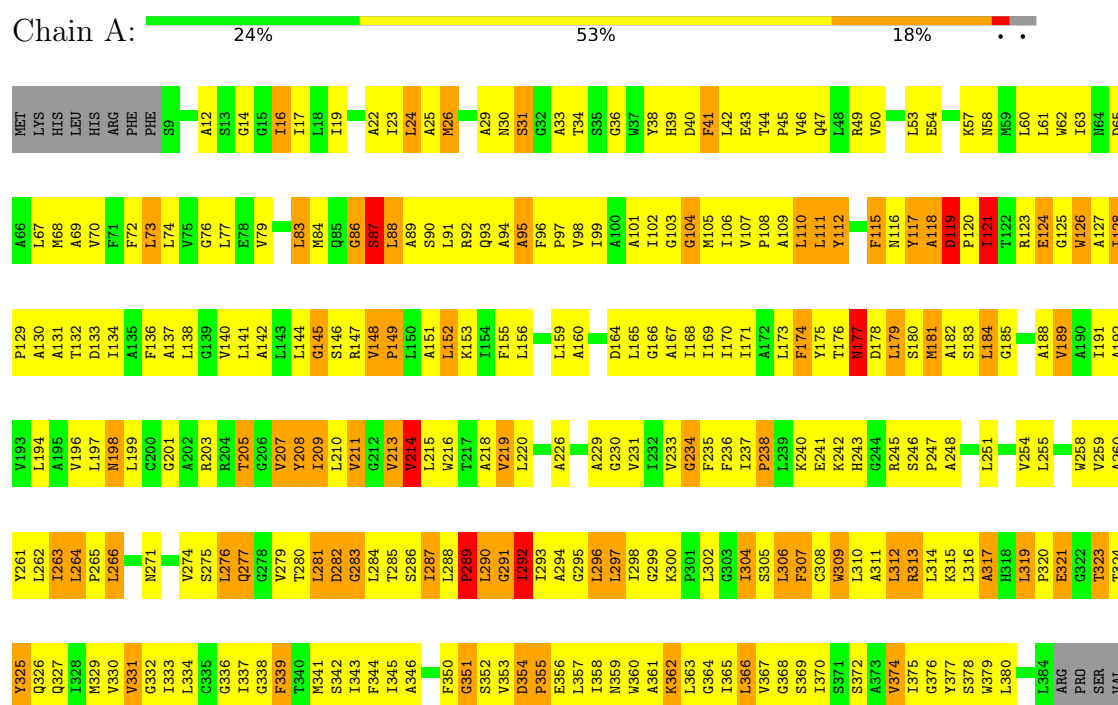
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2808	1865	457	473	13			
1	B	376	Total	C	N	O	S	0	0	0
			2808	1865	457	473	13			

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: Na(+)/H(+) antiporter 1



V193	L194	A195	V196	L197	M198	L199	G200	G201	A202	R203	R204	T205	G206	V207	Y208	I209	L210	V211	G212	V213	V214	L215	W216	V219	A226	A229	G230	V231	I232	V233	G234	F235	F236	I237	P238	L239	K240	E241	K242	H243	G244	R245	S246	P247	A248	L251	L255	V259	A260	Y261	L262	I263	L264				
P265	L266	N271	V274	S275	L276	Q277	G278	V279	T280	L281	D282	G283	L284	T285	S286	I287	L288	P289	L290	G291	I292	I293	A294	G295	L296	L297	I298	G299	K300	P301	L302	G303	I304	S305	L306	F307	C308	W309	L310	A311	L312	R313	L314	K315	L316	A317	H318	L319	P320	E321	G322	T323	T324	Y325	Q326	Q327	I328
M329	V330	V331	G332	I333	L334	G335	G336	I337	G338	F339	T340	M341	S342	I343	F344	I345	A346	F350	G351	S352	V353	D354	P355	E356	L357	I358	N359	W360	A361	K362	L363	G364	I365	L366	V367	G368	S369	I370	S371	S372	A373	V374	I375	G376	Y377	L380	L384	ARG	PRO	SER	VAL						

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	108.87Å 121.72Å 123.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.45	Depositor
% Data completeness (in resolution range)	91.2 (15.00-3.45)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.316 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5616	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.65	1/2867 (0.0%)	1.11	25/3910 (0.6%)
1	B	0.65	1/2867 (0.0%)	1.10	25/3910 (0.6%)
All	All	0.65	2/5734 (0.0%)	1.10	50/7820 (0.6%)

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
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	ILE	CA-CB	5.42	1.60	1.54
1	B	287	ILE	CA-CB	5.07	1.59	1.54

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	GLU	N-CA-C	-9.86	102.04	114.56
1	B	356	GLU	N-CA-C	-9.55	102.43	114.56
1	B	307	PHE	N-CA-C	-8.26	102.22	111.14
1	A	307	PHE	N-CA-C	-7.75	102.77	111.14
1	B	111	LEU	N-CA-C	-7.37	103.29	112.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	TYR	Sidechain
1	B	112	TYR	Sidechain

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	2808	0	2993	382	0
1	B	2808	0	2993	373	0
All	All	5616	0	5986	748	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 64.

The worst 5 of 748 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:119:ASP:HB3	1:A:120:PRO:HD3	1.19	1.13
1:B:119:ASP:HB3	1:B:120:PRO:HD3	1.20	1.10
1:A:330:VAL:HG11	1:A:380:LEU:HB2	1.32	1.09
1:B:330:VAL:HG11	1:B:380:LEU:HB2	1.32	1.06
1:B:96:PHE:HB3	1:B:97:PRO:HD3	1.47	0.97

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	374/388 (96%)	235 (63%)	94 (25%)	45 (12%)	0	4
1	B	374/388 (96%)	234 (63%)	94 (25%)	46 (12%)	0	4
All	All	748/776 (96%)	469 (63%)	188 (25%)	91 (12%)	0	4

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	GLY
1	A	87	SER
1	A	95	ALA
1	A	119	ASP
1	A	126	TRP

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	291/303 (96%)	259 (89%)	32 (11%)	6	26
1	B	291/303 (96%)	259 (89%)	32 (11%)	6	26
All	All	582/606 (96%)	518 (89%)	64 (11%)	6	26

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	292	ILE
1	B	306	LEU
1	A	289	PRO
1	A	281	LEU
1	B	312	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	198	ASN

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Mol	Chain	Res	Type
1	B	359	ASN
1	B	318	HIS
1	A	318	HIS
1	B	64	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.