

# Full wwPDB X-ray Structure Validation Report (i)

Jun 6, 2024 – 04:13 pm BST

PDB ID : 8QJ4

Title : Receptor Sd-Amt1 (ON-state)

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Deposited on : 2023-09-12

Resolution : 1.70 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 (i) 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 (1)) were used in the production of this report:

MolProbity : FAILED Xtriage (Phenix) : 1.13

EDS : 2.36.2buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

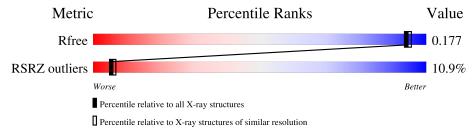
Validation Pipeline (wwPDB-VP) : 2.36.2

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.70 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
$R_{free}$	130704	4298 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6655 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 Ammonium transporter.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	402	Total 3112	C 2043	N 502	O 547	S 20	0	9	0
1	В	402	Total 3112	C 2042	N 502	O 547	S 21	0	9	0

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0
2	В	2	Total Cl 2 2	0	0

• Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 1 1	0	0
3	A	1	Total N 1 1	0	0
3	В	1	Total N 1 1	0	0
3	В	1	Total N 1 1	0	0

#### • Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	204	Total O 204 204	0	0
4	В	219	Total O 219 219	0	0

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## 3 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants	115.10Å 115.10Å 275.72Å	D
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	49.09 - 1.70	Depositor
resolution (A)	49.04 - 1.70	EDS
% Data completeness	90.7 (49.09-1.70)	Depositor
(in resolution range)	90.7 (49.04-1.70)	EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.49 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
D D	0.150 , 0.166	Depositor
$R, R_{free}$	0.164 , $0.177$	DCC
$R_{free}$ test set	6846 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.51, 93.9	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	$\begin{array}{c} 0.000 \; \text{for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k} \\ +1/3*l \\ 0.000 \; \text{for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/} \\ 3*k+1/3*l \\ 0.012 \; \text{for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+} \\ 1/3*l,-4/3*h+4/3*k+1/3*l \\ 0.000 \; \text{for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*} \\ -1/3*l \\ 0.012 \; \text{for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-} \\ 1/3*l,4/3*h-4/3*k-1/3*l \\ 0.000 \; \text{for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3} \\ *k-1/3*l \\ 0.027 \; \text{for h,-h-k,-l} \end{array}$	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 65.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8284e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

### 4 Model quality (i)

#### 4.1 Standard geometry (i)

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#### 4.2 Too-close contacts (i)

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#### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains (i)

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#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 4.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic and 4 are modelled with single atom - 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.

### 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



### 5 Fit of model and data (i)

#### 5.1 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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	402/644 (62%)	0.50	46 (11%) 5 5	3, 15, 42, 91	0
1	В	402/644~(62%)	0.45	42 (10%) 6 7	3, 14, 40, 90	0
All	All	804/1288 (62%)	0.48	88 (10%) 5 6	3, 14, 42, 91	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	192	ASN	15.2
1	A	69	ILE	15.0
1	A	192	ASN	14.2
1	В	194	HIS	13.5
1	В	193	LYS	12.3
1	A	194	HIS	12.1
1	В	69	ILE	10.7
1	A	70	ASP	10.5
1	В	191	ASN	10.4
1	В	195	GLY	10.3
1	A	193	LYS	10.2
1	A	191	ASN	9.9
1	В	70	ASP	9.1
1	A	68	SER	8.1
1	В	196	VAL	7.8
1	В	72	ILE	7.7
1	A	195	GLY	7.7
1	В	404	SER	6.3
1	A	196	VAL	5.4
1	A	4	SER	5.1
1	A	404	SER	5.1
1	В	4	SER	4.7
1	В	257	TRP	4.5
1	A	190	PHE	4.4

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Mol	nued fron Chain	$oxed{\mathbf{Res}}$	$\overline{\text{Type}}$	RSRZ
1	В	73	VAL	4.3
1	A	346	GLY	4.1
1	В	190	PHE	4.1
1	A	72	ILE	4.0
1	В	148	THR	3.9
1	A	3	GLU	3.9
1	В	307	LEU	3.7
1	A	20	ILE	3.6
1	A	73	VAL	3.5
1	В	17	LEU	3.4
1	A	75	ALA	3.4
1	A	257	TRP	3.4
1	В	68	SER	3.3
1	A	312	LYS	3.3
1	A	17	LEU	3.3
1	В	20	ILE	3.3
1	В	147	GLU	3.2
1	A	13	LEU	3.2
1	A	147	GLU	3.1
1	В	71	GLY	3.1
1	В	216	LEU	3.0
1	В	16	CYS	3.0
1	В	312	LYS	3.0
1	A	67	ASN	2.9
1	A	216	LEU	2.9
1	В	346	GLY	2.9
1	A	148	THR	2.9
1	A	84	THR	2.8
1	В	403	LYS	2.8
1	В	213	LEU	2.8
1	В	3	GLU	2.8
1	В	399	GLU	2.8
1	A	19	LEU	2.7
1	A	5	PHE	2.7
1	В	343	PHE	2.7
1	В	13	LEU	2.7
1	В	197	ASN	2.7
1	В	345	ALA	2.6
1	A	213	LEU	2.6
1	A	16	CYS	2.6
1	В	145	GLY	2.5
1	A	345	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	В	377	LEU	2.4
1	A	231	ASP	2.4
1	В	18	VAL	2.4
1	A	377	LEU	2.4
1	В	146	SER	2.3
1	В	19	LEU	2.3
1	В	5	PHE	2.3
1	A	341	GLN	2.3
1	A	373[A]	MET	2.3
1	A	403	LYS	2.2
1	В	67	ASN	2.2
1	A	18	VAL	2.2
1	A	310	LYS	2.2
1	В	75	ALA	2.2
1	A	212	PHE	2.1
1	A	146	SER	2.1
1	A	214	LEU	2.1
1	В	84	THR	2.0
1	A	71	GLY	2.0
1	A	49	PHE	2.0
1	A	307[A]	LEU	2.0
1	A	340	GLY	2.0

### 5.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.4 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	$\operatorname{CL}$	A	701	1/1	0.99	0.07	11,11,11,11	0

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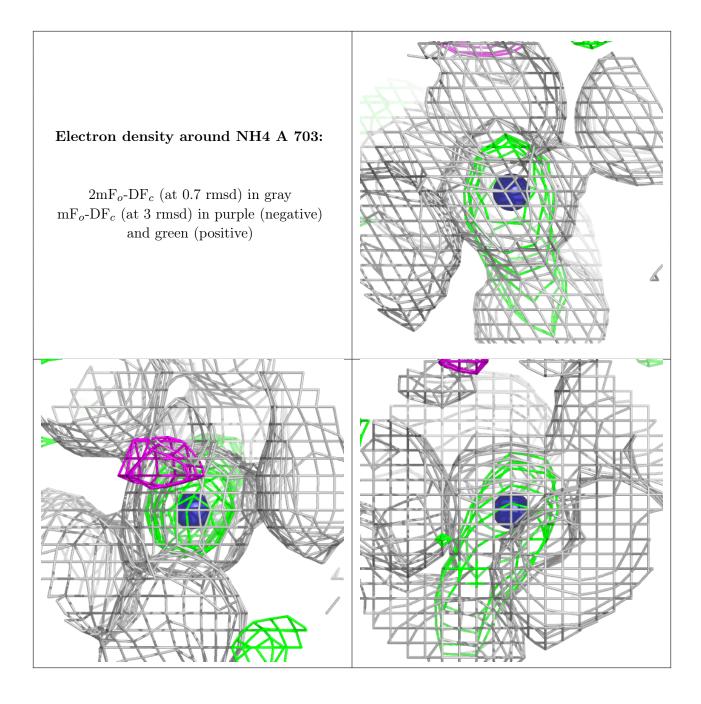


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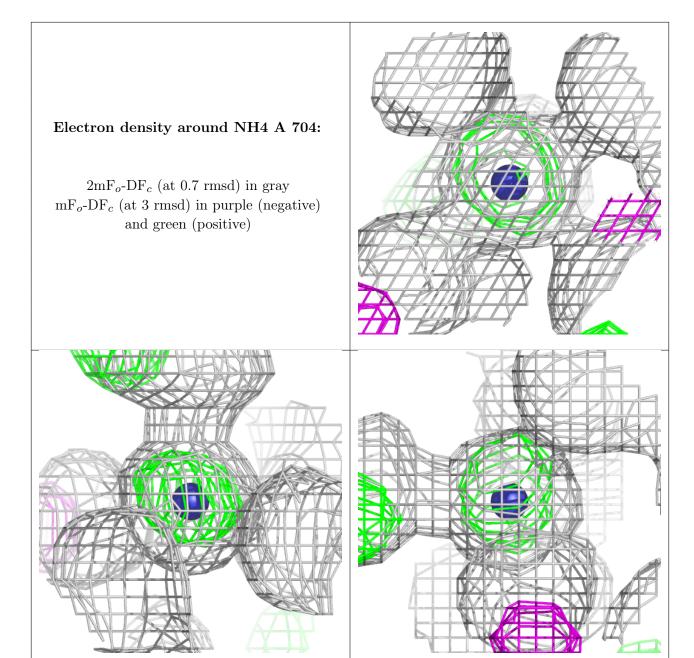
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	CL	A	702	1/1	0.99	0.15	2,2,2,2	0
2	CL	В	701	1/1	0.99	0.15	4,4,4,4	0
2	CL	В	702	1/1	0.99	0.08	10,10,10,10	0
3	NH4	A	703	1/1	0.99	0.24	0,0,0,0	0
3	NH4	A	704	1/1	0.99	0.28	0,0,0,0	0
3	NH4	В	704	1/1	0.99	0.24	0,0,0,0	0
3	NH4	В	703	1/1	1.00	0.25	0,0,0,0	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

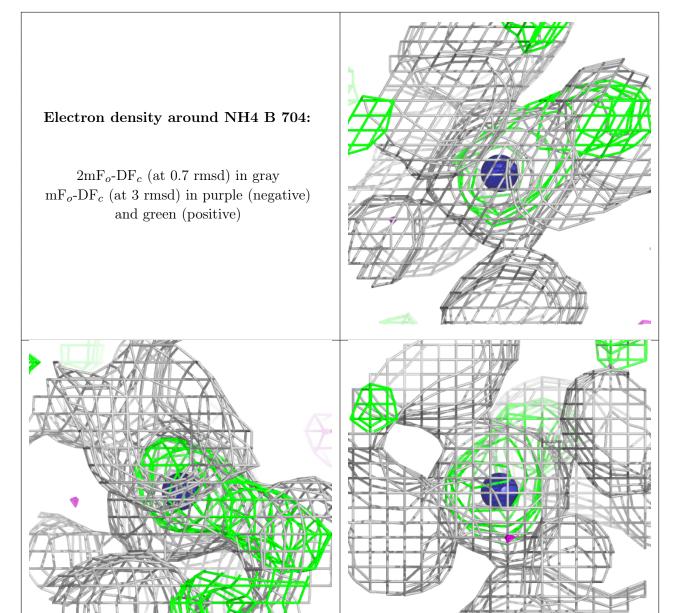




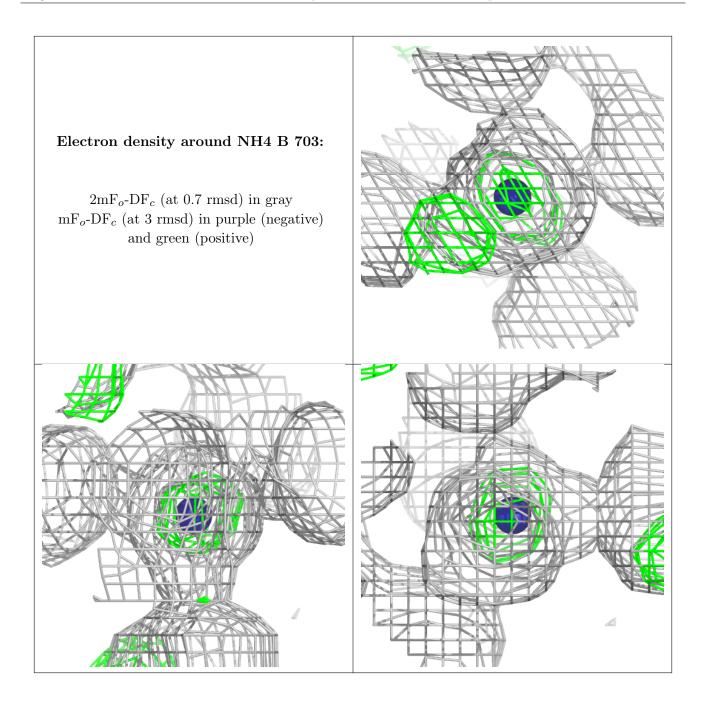












### 5.5 Other polymers (i)

There are no such residues in this entry.

