

Full wwPDB NMR Structure Validation Report (i)

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:	2FWS
:	First Ca2+ binding domain of the Na,Ca-exchanger (NCX1)
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:	2006-02-03
	: : :

This is a Full wwPDB NMR 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/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment was not calculated.

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	NMR archive		
	$(\# { m Entries})$	$(\# { m Entries})$		
Clashscore	158937	12864		
Ramachandran outliers	154571	11451		
Sidechain outliers	154315	11428		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain					
1	A	139	55%	12%	•	32%		



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues									
Well-defined core	Well-defined core Residue range (total) Backbone RMSD (Å) Medoid model								
1	A:373-A:397, A:404-A:464,	0.26	4						
	A:491-A:499 (95)								

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 8, 11, 16, 18
2	9, 10, 12, 17
3	2, 3, 6, 20
4	5, 7, 13
5	14, 15
Single-model clusters	19



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2067 atoms, of which 999 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Sodium/calcium exchanger 1.

Mol	Chain	Residues	Atoms					Trace	
1	Λ	120	Total	С	Η	Ν	0	S	0
	A 139	2065	666	999	170	227	3	0	

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms
0	Δ	0	Total Ca
	A	2	2 2



4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Sodium/calcium exchanger 1



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Sodium/calcium exchanger 1



4.2.2 Score per residue for model 2

 \bullet Molecule 1: Sodium/calcium exchanger 1

Chain A: 55% 12% 32%

M482 V371 M482 V371 4485 V390 6485 V390 6485 V390 5488 V390 5489 V390 5480 V390 5481 V390 5483 V390 5484 V390 549 C398 540 C398 1491 T441 1504 C414 1445 D446 1445 D446 1445 D446 1445 C445 1445 C446 1445 C447 1445 C447 1445 C447 1446 C447 1447 C447 1447 C447

4.2.3 Score per residue for model 3

 \bullet Molecule 1: Sodium/calcium exchanger 1



4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Sodium/calcium exchanger 1



4.2.5 Score per residue for model 5

 \bullet Molecule 1: Sodium/calcium exchanger 1



4.2.6 Score per residue for model 6

• Molecule 1: Sodium/calcium exchanger 1





4.2.7 Score per residue for model 7

• Molecule 1: Sodium/calcium exchanger 1



- 4.2.8 Score per residue for model 8
- \bullet Molecule 1: Sodium/calcium exchanger 1



4.2.9 Score per residue for model 9

 \bullet Molecule 1: Sodium/calcium exchanger 1





4.2.10 Score per residue for model 10

• Molecule 1: Sodium/calcium exchanger 1



- 4.2.11 Score per residue for model 11
- \bullet Molecule 1: Sodium/calcium exchanger 1



4.2.12 Score per residue for model 12

• Molecule 1: Sodium/calcium exchanger 1



4.2.13 Score per residue for model 13

• Molecule 1: Sodium/calcium exchanger 1





4.2.14 Score per residue for model 14

• Molecule 1: Sodium/calcium exchanger 1



4.2.15 Score per residue for model 15

• Molecule 1: Sodium/calcium exchanger 1



4.2.16 Score per residue for model 16

 \bullet Molecule 1: Sodium/calcium exchanger 1



4.2.17 Score per residue for model 17

• Molecule 1: Sodium/calcium exchanger 1

Chain A: 53% 14% 32%

4484 1731 6485 1371 6485 1387 6485 1384 8488 638 8488 1384 8488 1384 8488 1384 8488 1384 8488 1384 8498 1398 1496 1398 6401 1401 1402 1401 1403 1445 1446 1446 1446 1446 1445 1446 1445 1447 1445 1447 1445 1447 1445 1447 1445</td

4.2.18 Score per residue for model 18

 \bullet Molecule 1: Sodium/calcium exchanger 1



4.2.19 Score per residue for model 19

 \bullet Molecule 1: Sodium/calcium exchanger 1



4.2.20 Score per residue for model 20

 \bullet Molecule 1: Sodium/calcium exchanger 1





5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: torsion angle dynamics.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	2.0
X-PLOR	refinement	NIH version 2.9.7

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	E	Sond lengths	Bond angles		
1VIOI	RMSZ		$\#Z{>}5$	RMSZ	$\#Z{>}5$	
1	А	$0.99 {\pm} 0.02$	$0{\pm}0/769~(~0.0{\pm}~0.0\%)$	$0.79 {\pm} 0.02$	$1{\pm}1/1043~(~0.1{\pm}~0.1\%)$	
All	All	0.99	2/15380 ($0.0%$)	0.79	29/20860~(~0.1%)	

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	Planarity
1	А	$0.0{\pm}0.0$	0.1 ± 0.3
All	All	0	2

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mal	Chain	Dec	Turne	Atoma	7	Observed (Å)	Ideal(Å)	Moo	dels
	Unain	nes	Type	Atoms		Observed(A)	Ideal(A)	Worst	Total
1	А	385	GLU	CD-OE1	-6.07	1.19	1.25	5	1
1	А	385	GLU	CD-OE2	-5.43	1.19	1.25	10	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mal	Chain	Dec	Turne	Atoma	7	7 $Observed(0)$		Models	
INIOI	Unain	nes	туре	Atoms		Observed()	Ideal()	Worst	Total
1	А	454	GLU	OE1-CD-OE2	-6.77	115.18	123.30	16	12
1	А	447	ASP	CB-CG-OD1	6.49	124.14	118.30	14	14
1	А	385	GLU	OE1-CD-OE2	-5.66	116.50	123.30	5	2
1	А	447	ASP	CB-CG-OD2	5.19	122.97	118.30	13	1

There are no chirality outliers.



All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	А	396	ARG	Sidechain	2

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	А	756	719	719	12 ± 3
2	А	2	0	0	0±1
All	All	15160	14380	14380	231

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 8.

Atom 1	Atom 2	$Clach(\lambda)$	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:416:ALA:HB3	1:A:422:TYR:OH	0.67	1.90	17	3
1:A:384:LEU:HA	1:A:497:PHE:O	0.65	1.91	20	4
1:A:449:ILE:O	1:A:451:GLU:HG3	0.65	1.91	6	17
1:A:422:TYR:CE2	1:A:496:ILE:HD13	0.64	2.28	20	16
1:A:385:GLU:OE2	2:A:600:CA:CA	0.64	1.75	11	1
1:A:451:GLU:OE1	2:A:650:CA:CA	0.64	1.75	12	1
1:A:451:GLU:OE2	2:A:600:CA:CA	0.64	1.75	12	1
1:A:498:ASP:OD2	2:A:600:CA:CA	0.62	1.75	20	3
1:A:411:THR:OG1	1:A:424:PHE:HA	0.61	1.95	1	14
1:A:404:THR:HA	1:A:431:PHE:O	0.59	1.98	9	11
1:A:396:ARG:HB3	1:A:436:THR:O	0.59	1.97	19	1
1:A:442:VAL:HG11	1:A:456:PHE:CZ	0.57	2.34	12	16
1:A:384:LEU:HB2	1:A:387:CYS:SG	0.56	2.40	17	4
1:A:383:CYS:SG	1:A:390:VAL:HB	0.55	2.42	3	7
1:A:385:GLU:HB2	1:A:498:ASP:HA	0.53	1.80	6	2
1:A:421:ASP:O	1:A:445:ILE:HB	0.52	2.04	20	17
1:A:373:LYS:O	1:A:396:ARG:HA	0.51	2.05	18	3
1:A:390:VAL:O	1:A:441:ARG:HA	0.50	2.05	5	17
1:A:406:PHE:CE2	1:A:430:VAL:HG22	0.50	2.42	5	1
1:A:383:CYS:SG	1:A:390:VAL:HG23	0.49	2.47	20	1

All unique clashes are listed below, sorted by their clash magnitude.

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	to us page		\mathbf{D}	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:422:TYR:CE1	1:A:456:PHE:HD2	0.49	2.26	6	12
1:A:406:PHE:CE1	1:A:430:VAL:HG13	0.49	2.42	7	1
1:A:413:ASP:OD1	1:A:417:ASN:HA	0.49	2.08	16	1
1:A:456:PHE:CE2	1:A:496:ILE:HD11	0.48	2.43	12	9
1:A:384:LEU:HD13	1:A:497:PHE:O	0.48	2.09	11	7
1:A:390:VAL:HG11	1:A:494:VAL:HG11	0.48	1.86	20	7
1:A:455:ASN:HB3	1:A:495:THR:HA	0.47	1.84	5	2
1:A:409:PHE:O	1:A:426:GLU:HA	0.47	2.09	18	1
1:A:415:THR:HG22	1:A:455:ASN:O	0.47	2.09	19	1
1:A:412:GLU:O	1:A:456:PHE:HB2	0.46	2.10	1	5
1:A:422:TYR:OH	1:A:454:GLU:HG2	0.46	2.11	10	5
1:A:422:TYR:CZ	1:A:456:PHE:HD2	0.45	2.28	17	1
1:A:413:ASP:HB2	1:A:416:ALA:O	0.45	2.11	12	1
1:A:406:PHE:HB2	1:A:464:LYS:HB3	0.45	1.87	18	1
1:A:425:THR:HG21	1:A:442:VAL:HG22	0.45	1.88	18	8
1:A:378:GLN:HB2	1:A:381:TYR:CZ	0.45	2.47	3	3
1:A:378:GLN:HB2	1:A:381:TYR:CE1	0.44	2.47	7	3
1:A:384:LEU:HD12	1:A:386:ASN:OD1	0.44	2.13	16	2
1:A:384:LEU:CD1	1:A:499:ASP:HB2	0.44	2.42	17	1
1:A:422:TYR:CZ	1:A:496:ILE:HD13	0.44	2.47	8	2
1:A:406:PHE:HA	1:A:429:VAL:O	0.43	2.14	15	1
1:A:458:VAL:O	1:A:491:THR:HA	0.43	2.13	9	2
1:A:381:TYR:CE2	1:A:392:LEU:HA	0.43	2.48	7	2
1:A:377:GLU:HB3	1:A:381:TYR:OH	0.42	2.13	5	1
1:A:397:ARG:NE	1:A:397:ARG:HA	0.42	2.30	19	1
1:A:389:THR:HG22	1:A:443:GLY:HA2	0.42	1.91	8	1
1:A:418:ALA:HB1	1:A:424:PHE:HB3	0.41	1.92	18	1
1:A:385:GLU:HB2	1:A:498:ASP:CB	0.41	2.45	11	1
1:A:380:THR:HA	1:A:493:THR:O	0.41	2.15	20	1
1:A:413:ASP:HA	1:A:416:ALA:O	0.41	2.16	20	1
1:A:375:PHE:CZ	1:A:397:ARG:HG2	0.40	2.52	16	1
1:A:389:THR:HA	1:A:442:VAL:O	0.40	2.17	18	1
1:A:451:GLU:HB2	1:A:498:ASP:HB2	0.40	1.92	7	1
1:A:382:GLN:HA	1:A:495:THR:O	0.40	2.16	9	1
1:A:422:TYR:CD2	1:A:496:ILE:HD13	0.40	2.52	17	2

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6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	А	95/139~(68%)	88±1 (93±1%)	$5\pm1~(6\pm1\%)$	1±1 (1±1%)	16 63
All	All	1900/2780~(68%)	1767~(93%)	108 (6%)	25~(1%)	16 63

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	462	ASN	14
1	А	414	GLY	10
1	А	413	ASP	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	А	84/118 (71%)	80 ± 1 (96 $\pm2\%$)	$4\pm1~(4\pm2\%)$	31 80
All	All	1680/2360~(71%)	1605 (96%)	75 (4%)	31 80

All 18 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	422	TYR	20
1	А	447	ASP	15
1	А	432	LYS	6
1	А	455	ASN	5
1	А	423	GLU	4
1	А	384	LEU	3
1	А	453	ASP	3

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		1	1 0	
Mol	Chain	Res	Type	Models (Total)
1	А	498	ASP	3
1	А	377	GLU	3
1	А	386	ASN	2
1	А	382	GLN	2
1	А	424	PHE	2
1	А	426	GLU	2
1	А	397	ARG	1
1	А	410	ARG	1
1	А	462	ASN	1
1	А	499	ASP	1
1	А	404	THR	1

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6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

