



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 07:00 PM GMT

PDB ID : 2DPK
Title : The Crystal Structure of the Primary Ca²⁺ Sensor of the Na⁺/Ca²⁺ Exchanger
Authors : Abramson, J.; Sawaya, M.
Deposited on : 2006-05-12
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

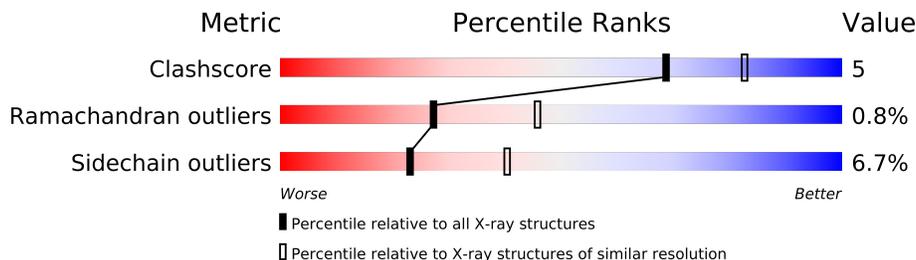
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	152	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 984 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Sodium/calcium exchanger 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	124	944	590	152	199	3	0	0	0

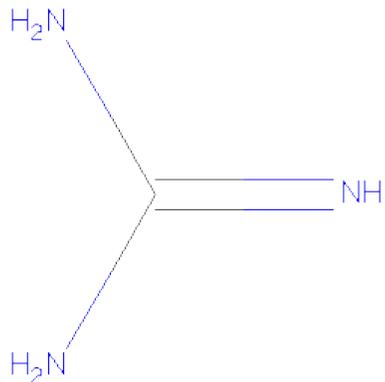
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	358	MET	-	EXPRESSION TAG	UNP P23685
A	359	ARG	-	EXPRESSION TAG	UNP P23685
A	360	GLY	-	EXPRESSION TAG	UNP P23685
A	361	SER	-	EXPRESSION TAG	UNP P23685
A	362	HIS	-	EXPRESSION TAG	UNP P23685
A	363	HIS	-	EXPRESSION TAG	UNP P23685
A	364	HIS	-	EXPRESSION TAG	UNP P23685
A	365	HIS	-	EXPRESSION TAG	UNP P23685
A	366	HIS	-	EXPRESSION TAG	UNP P23685
A	367	HIS	-	EXPRESSION TAG	UNP P23685
A	368	GLY	-	EXPRESSION TAG	UNP P23685
A	369	ILE	-	EXPRESSION TAG	UNP P23685

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

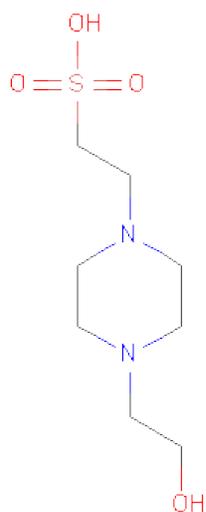
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 is GUANIDINE (three-letter code: GAI) (formula: CH₅N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	4	1	3	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	59.62Å 45.52Å 57.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.26 – 2.50	Depositor
% Data completeness (in resolution range)	98.3 (57.26-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	984	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.39	0/958	0.61	0/1299

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	467	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	944	0	889	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	0	0	0
3	A	4	0	4	0	0
4	A	15	0	17	0	0
5	A	17	0	0	0	0
All	All	984	0	910	9	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (9) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:481:SER:O	1:A:483:LEU:N	2.26	0.68
1:A:501:HIS:O	1:A:502:ALA:HB3	2.03	0.58
1:A:467:SER:HA	1:A:468:GLU:HG2	1.87	0.56
1:A:467:SER:C	1:A:468:GLU:HG2	2.29	0.53
1:A:501:HIS:O	1:A:502:ALA:CB	2.59	0.50
1:A:467:SER:CA	1:A:468:GLU:HG2	2.46	0.45
1:A:369:ILE:HD13	1:A:369:ILE:H	1.83	0.43
1:A:385:GLU:HG2	1:A:446:ASP:HA	2.02	0.42
1:A:380:THR:HG23	1:A:493:THR:HG23	2.02	0.42

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	120/152 (79%)	117 (98%)	2 (2%)	1 (1%)	27 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	ALA

5.3.2 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 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	105/129 (81%)	98 (93%)	7 (7%)	23 40

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	ILE
1	A	383	CYS
1	A	396	ARG
1	A	449	ILE
1	A	455	ASN
1	A	467	SER
1	A	468	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	GLN
1	A	403	ASN
1	A	455	ASN

5.3.3 RNA [i](#)

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAI	A	1008	-	3,3,3	1.97	1 (33%)	3,3,3	1.05	0
4	EPE	A	1009	-	15,15,15	0.70	1 (6%)	20,20,20	1.18	3 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAI	A	1008	-	-	0/0/0/0	0/0/0/0
4	EPE	A	1009	-	-	0/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1009	EPE	C10-S	2.34	1.81	1.77
3	A	1008	GAI	C-N2	-2.23	1.33	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1009	EPE	O2S-S-C10	2.93	109.32	106.81
4	A	1009	EPE	O3S-S-C10	2.87	109.56	105.93
4	A	1009	EPE	O1S-S-C10	2.19	108.68	106.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.